Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 06:10 PM JST

PDB ID	:	8IB5 / pdb_00008ib5
EMDB ID	:	EMD-35332
Title	:	Respiratory complex Peripheral Arm of CI, focus-refined map of type IA, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-09
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

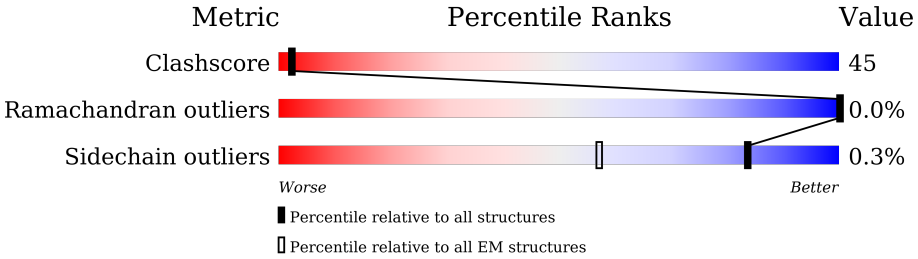
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

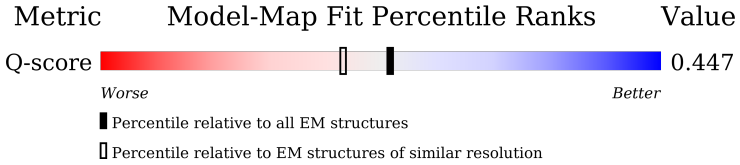
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	14% 22% 53% 5% 20%
2	B	224	• 29% 34% 7% 30%
3	C	263	• 36% 37% • 25%
4	D	463	5% 34% 46% • 17%

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Mol	Chain	Length	Quality of chain
5	E	248	46% 25% 54% 5% 15%
6	F	464	33% 32% 53% 7% 8%
7	G	727	5% 38% 49% 7% 6%
8	H	318	7% 29% 58% 12%
9	I	212	39% 38% 5% 18%
10	P	377	31% 32% 52% 6% 10%
11	Q	175	10% 37% 27% 33%
12	R	116	47% 26% 40% 6% 28%
13	S	99	11% 30% 44% 9% 16%
14	T	156	25% 12% 30% 6% 52%
15	V	116	50% 41% 6%
16	W	131	11% 36% 46% 5% 13%
17	X	172	11% 33% 44% 5% 17%
18	Z	144	10% 41% 53%
19	a	70	30% 61%
20	b	84	15% 29% 65% 5%
21	q	145	56% 37% 39% 7% 17%
22	r	113	27% 21% 18% 6% 55%
23	s	104	13% 11% 87%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	SF4	B	301	-	-	X	-
25	SF4	F	502	-	-	X	-
25	SF4	G	802	-	-	X	-
25	SF4	I	303	-	-	X	-
25	SF4	I	304	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	UQ1	B	302	-	-	X	-
28	FES	E	301	-	-	X	-
28	FES	G	803	-	-	X	-
34	CDL	a	101	-	-	X	-

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 33943 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	92	754	523	107	119	5	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	157	1258	802	227	215	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	198	1641	1060	279	299	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	386	3095	1974	534	564	23	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1635	1039	275	310	11	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	426	3288	2073	588	605	22	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	687	5287	3316	918	1012	41	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	314	2510	1687	380	421	22	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	174	1398	880	240	266	12	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	P	340	2730	1765	479	479	7	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Q	118	957	608	165	180	4	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	R	83	660	411	120	126	3	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	S	83	667	419	126	119	3	0	0

- Molecule 14 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	T	75	604	388	89	122	5	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	V	112	915	596	152	164	3	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	W	114	970	619	180	165	6	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	X	142	1164	736	209	209	10	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Z	139	1152	741	204	199	8	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	a	67	548	356	97	91	4	0	0

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	b	80	628	414	99	111	4	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	q	120	1004	645	178	177	4	0	0

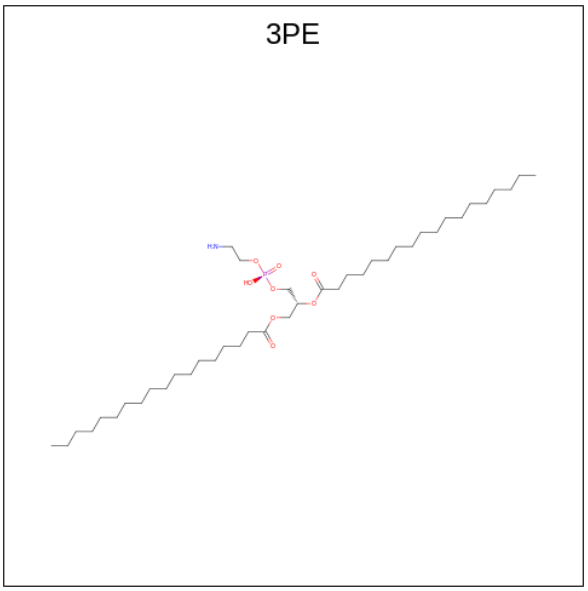
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	r	51	418	266	78	73	1	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

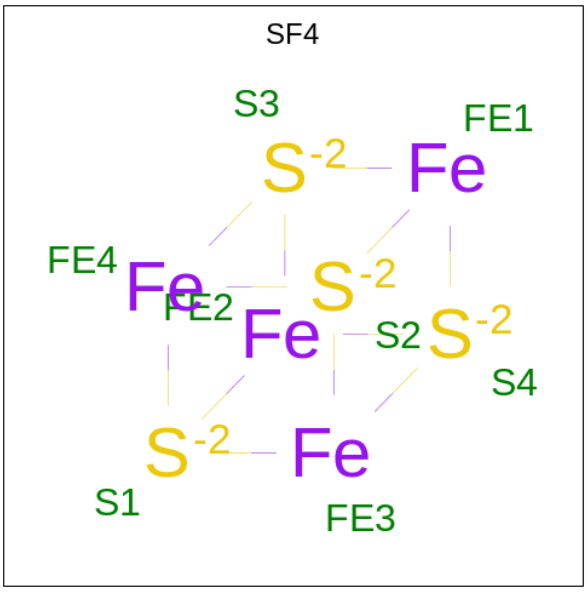
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	s	14	115	75	17	23	0	0

- Molecule 24 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



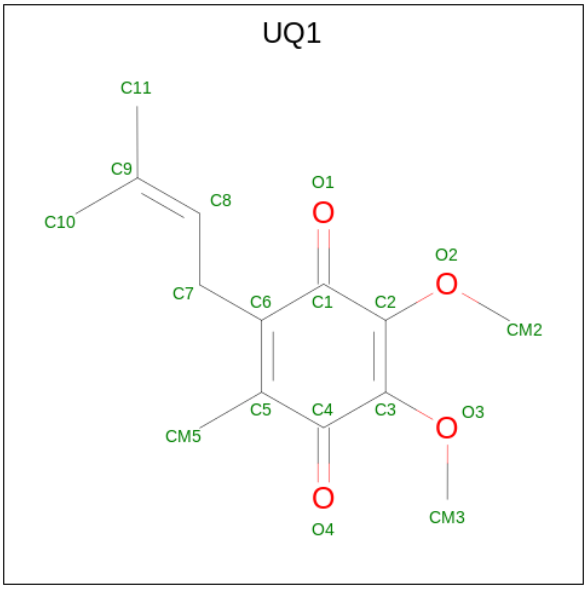
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	A	1	46	36	1	8	1	0
			Total	C	N	O	P	
24	I	1	51	41	1	8	1	0
			Total	C	N	O	P	
24	b	1	46	36	1	8	1	0

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



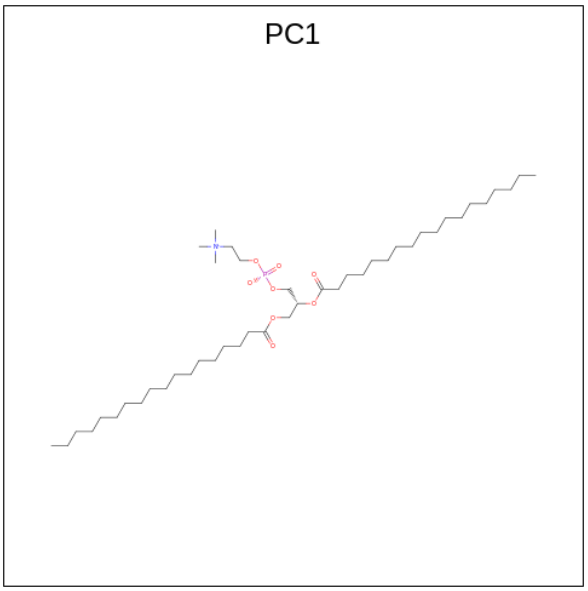
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
25	B	1	8	4	4	0
25	F	1	8	4	4	0
25	G	1	8	4	4	0
25	G	1	8	4	4	0
25	I	1	8	4	4	0
25	I	1	8	4	4	0

- Molecule 26 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



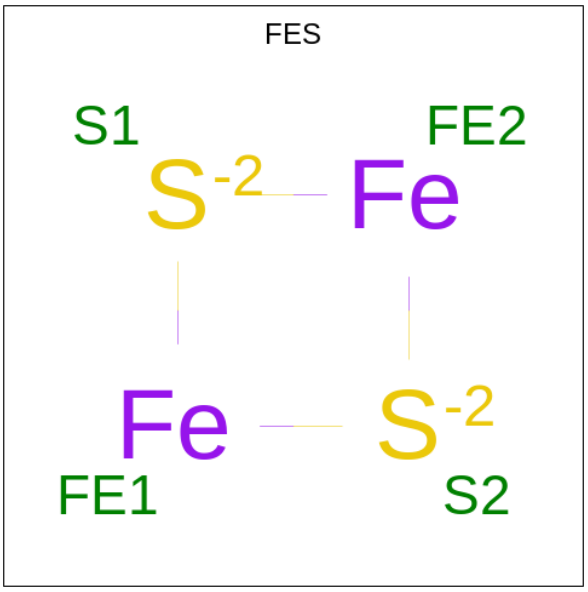
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	B	1	18	14	4	0

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



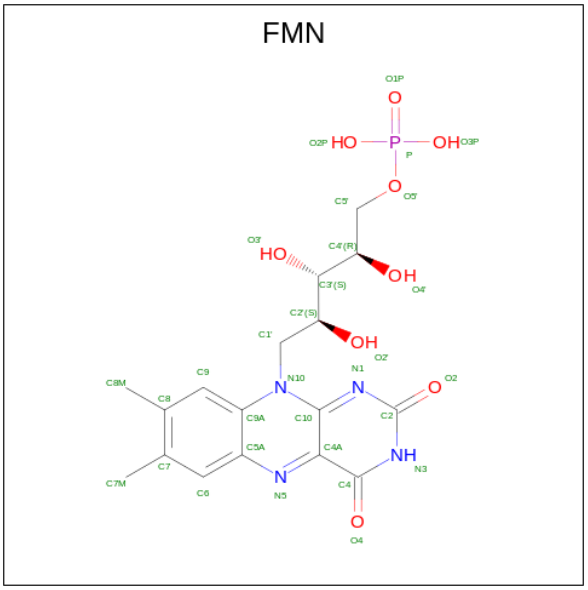
Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
27	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
27	I	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 28 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



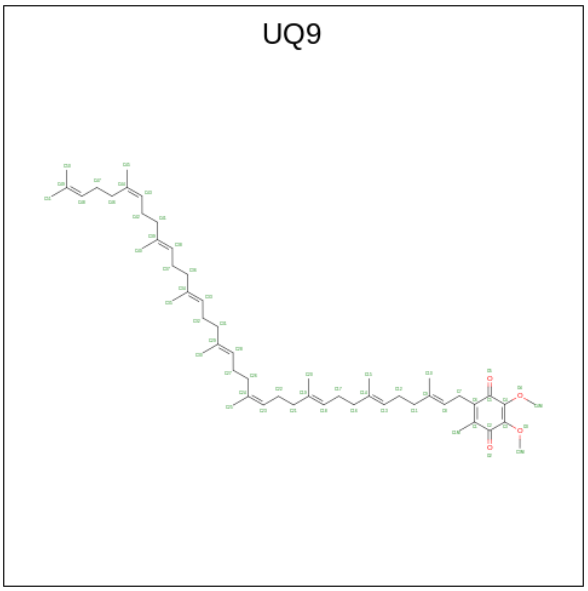
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
28	E	1	4	2	2	0
			Total	Fe	S	
28	G	1	4	2	2	0

- Molecule 29 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



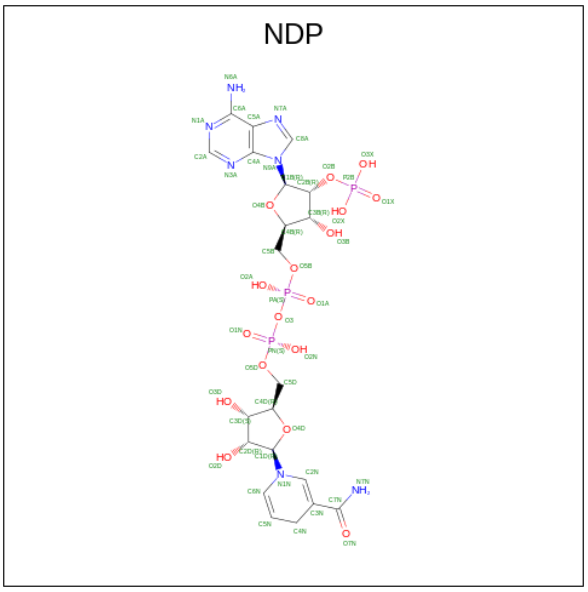
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
29	F	1	31	17	4	9	1	0

- Molecule 30 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	H	1	35	31	4	0

- Molecule 31 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



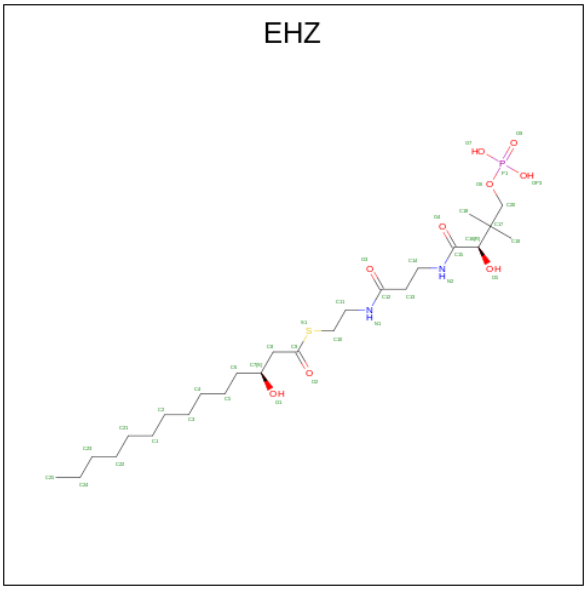
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
31	P	1	48	21	7	17	3	0

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

depositor).

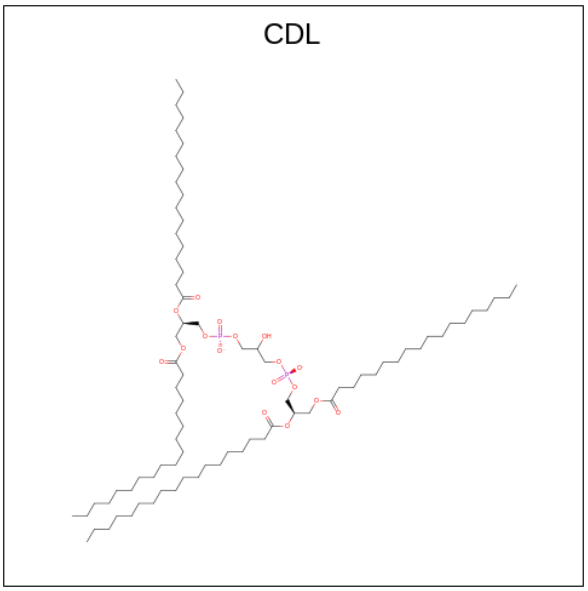
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
32	R	1	1	1	0

- Molecule 33 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
33	W	1	32	19	2	9	1	1	0

- Molecule 34 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



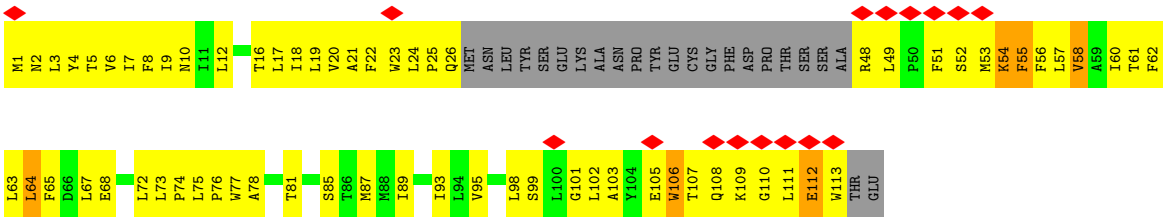
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
34	a	1	57	38	17	2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

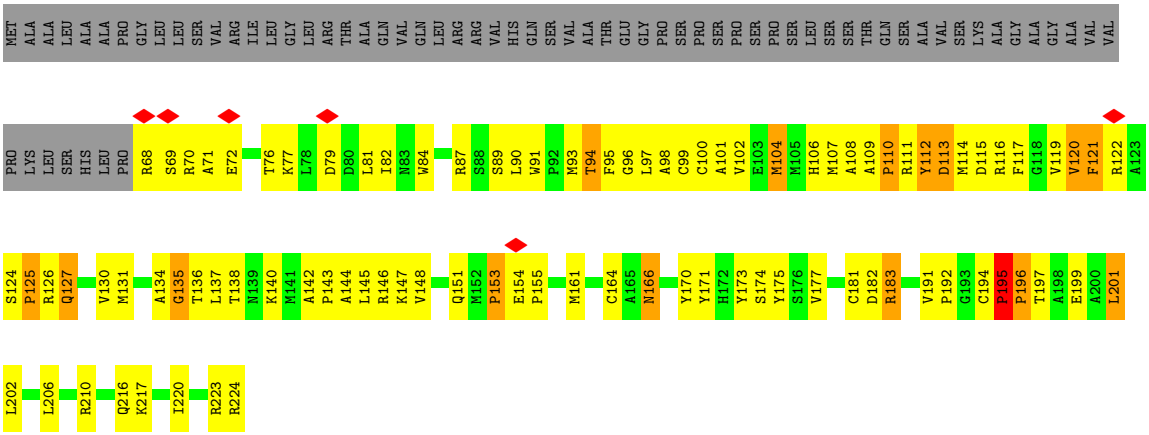
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 14% 22% 53% 5% 20%



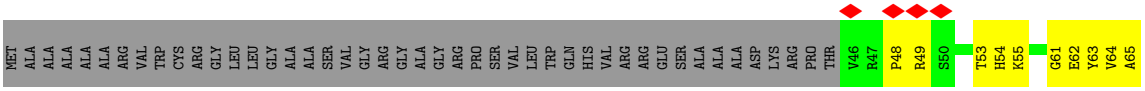
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

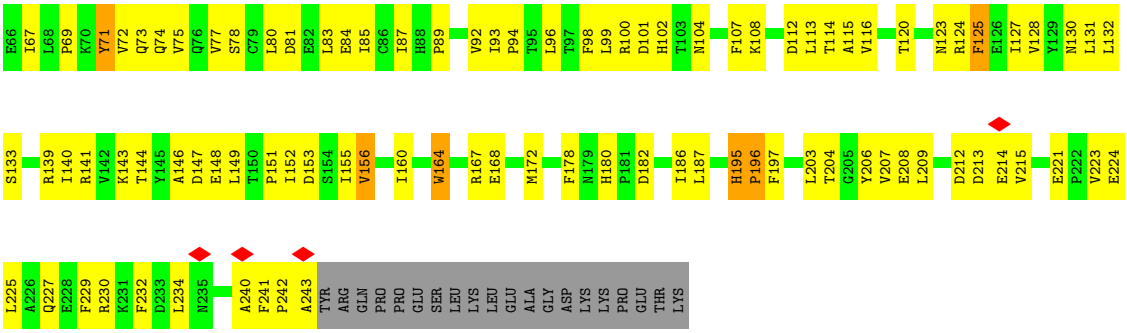
Chain B: 29% 34% 7% 30%



• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

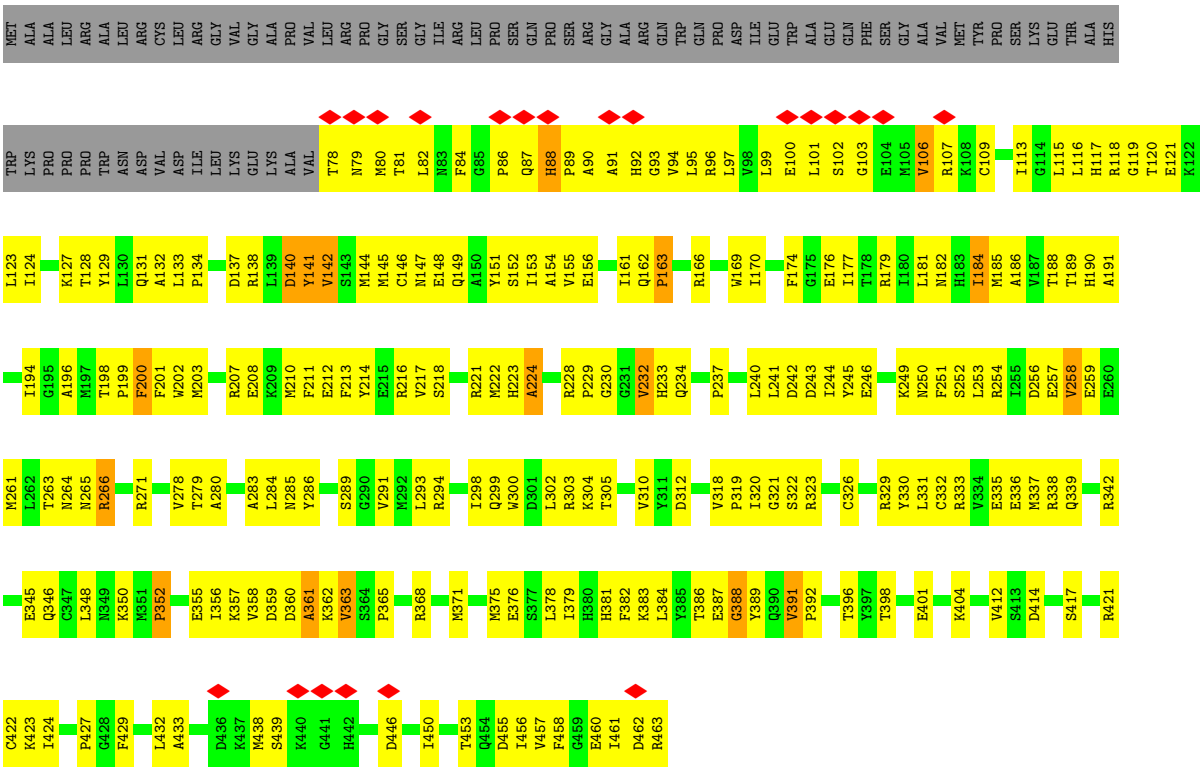
Chain C: 36% 37% • 25%





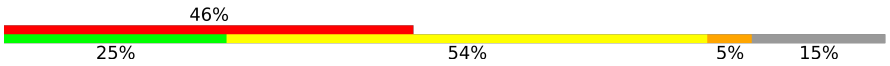
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

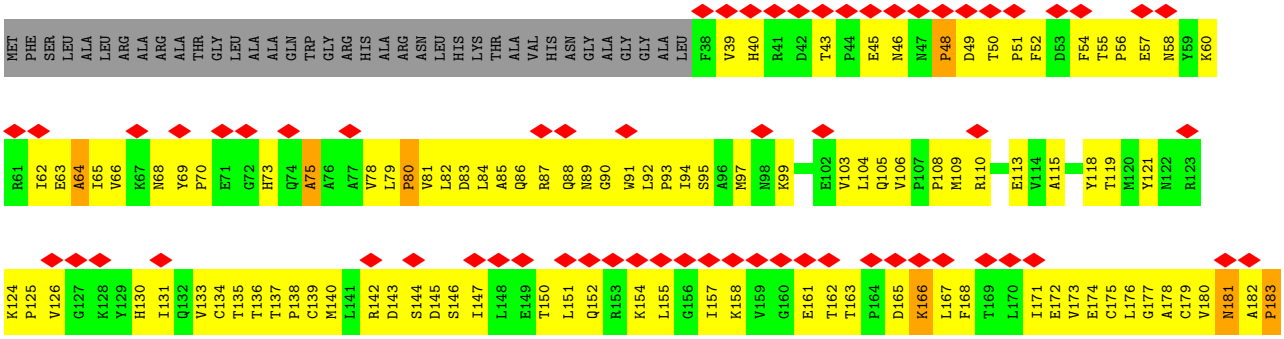
Chain D:



• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

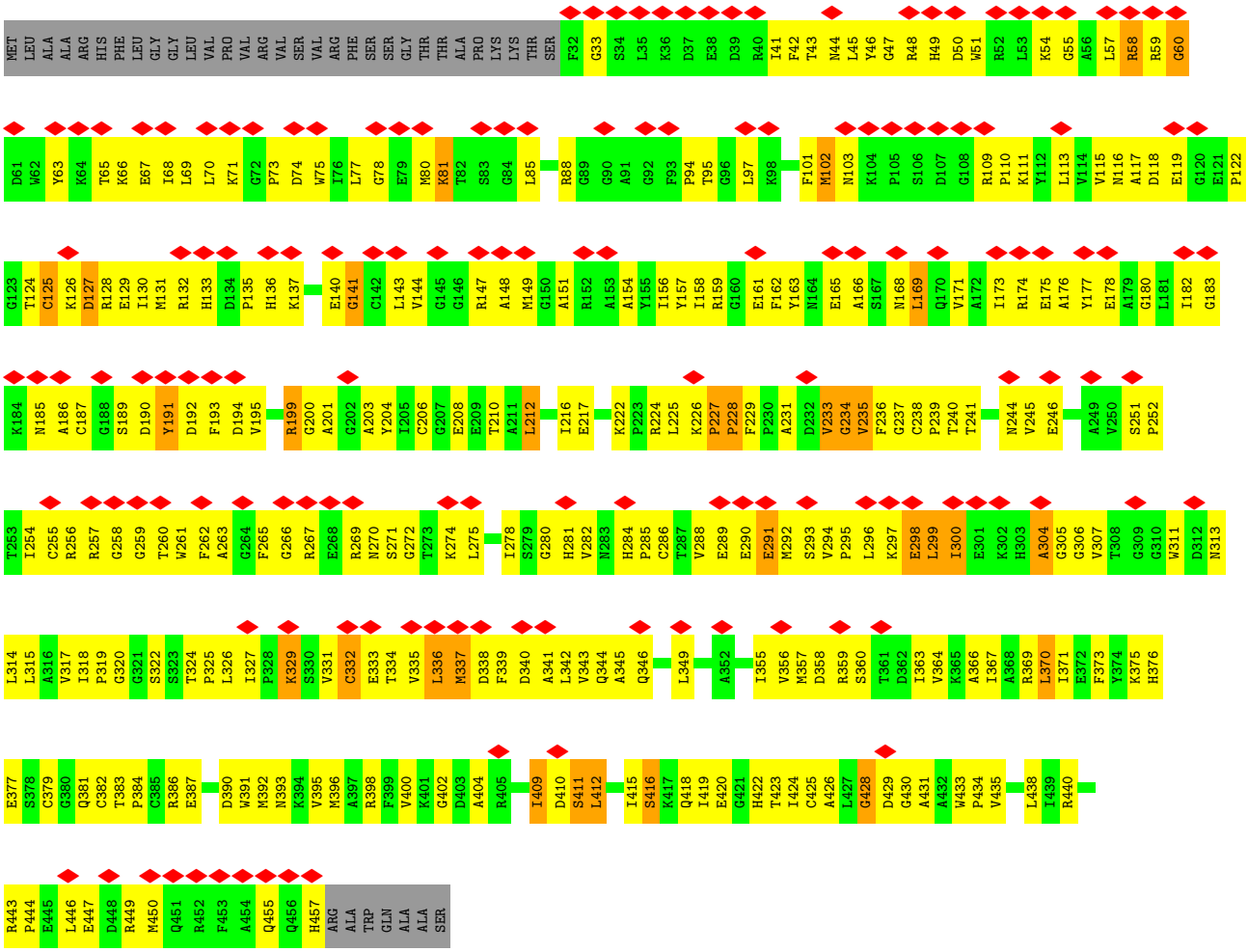
Chain E:





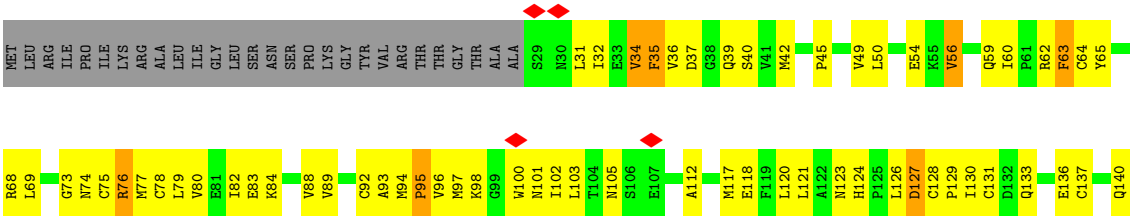
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

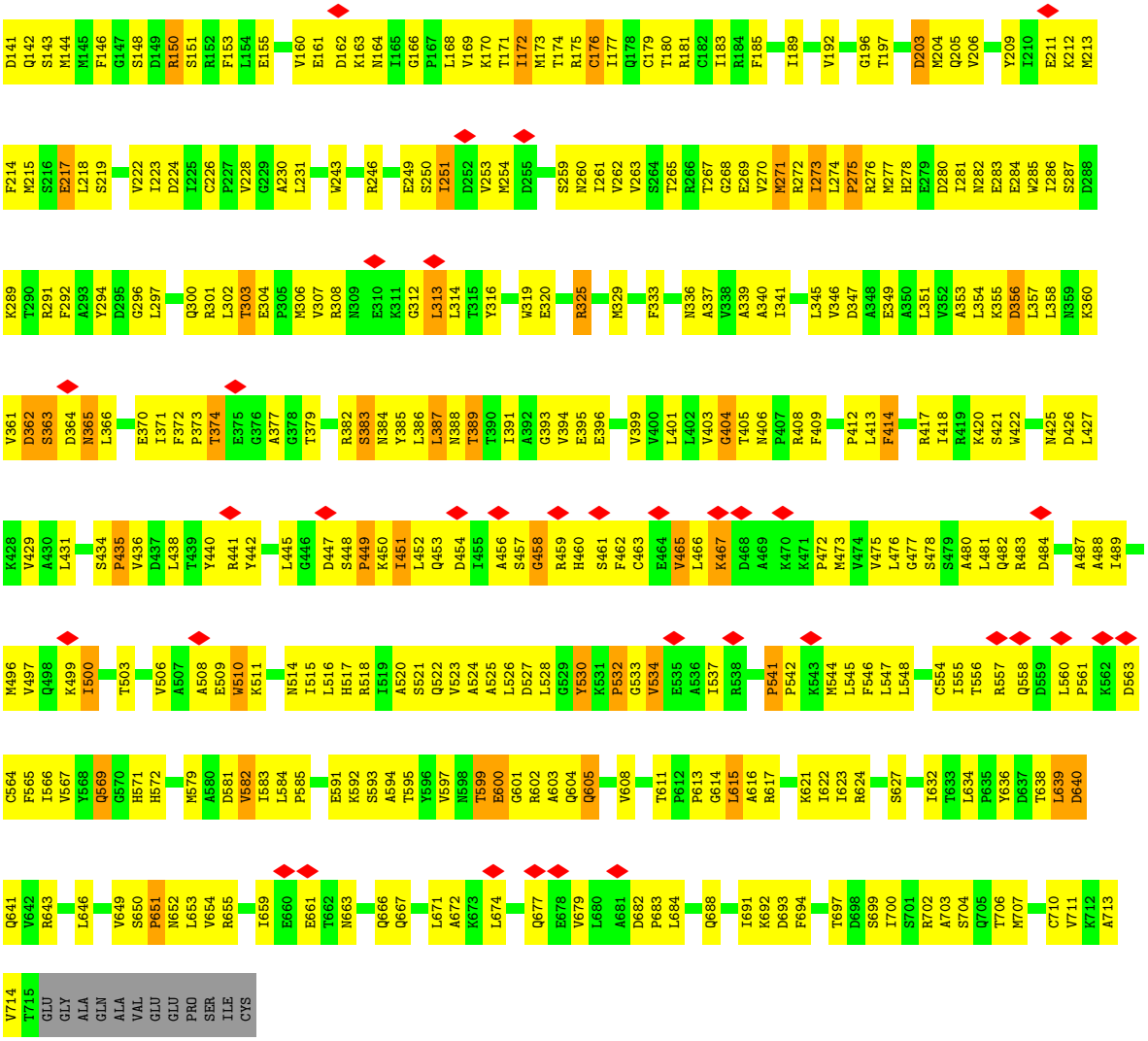
Chain F:



• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

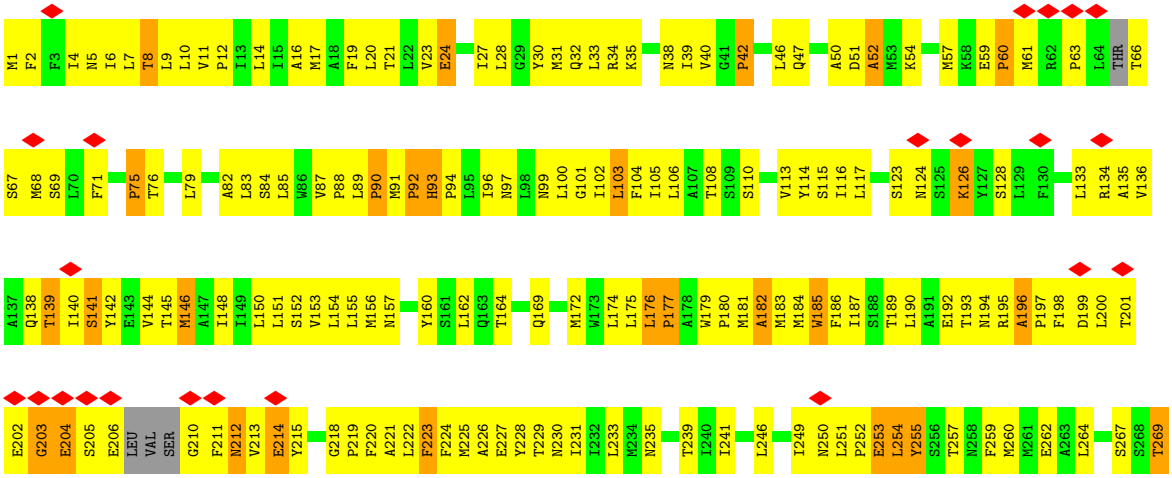
Chain G:





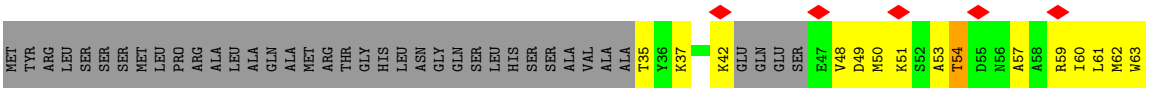
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

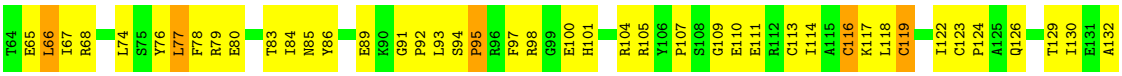
Chain H:



• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

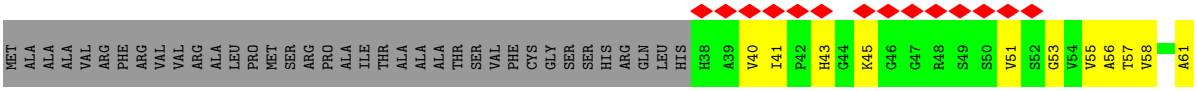
Chain I:

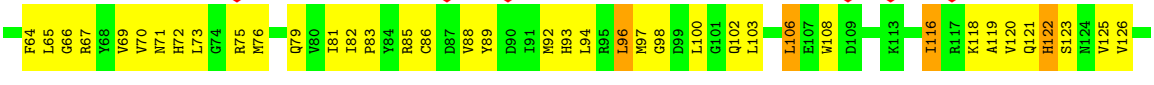


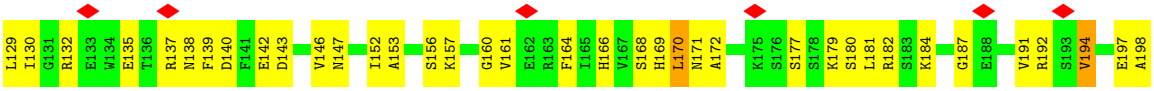


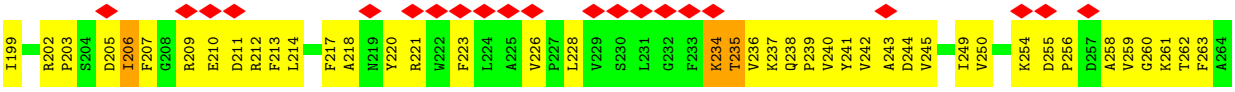
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

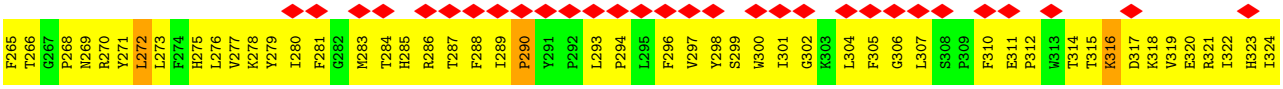
Chain P:

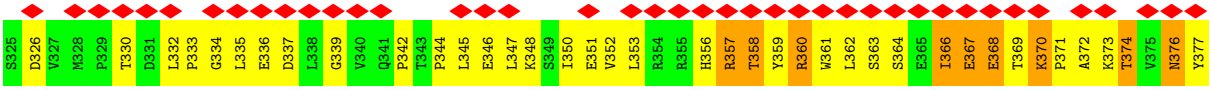






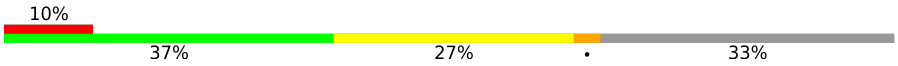


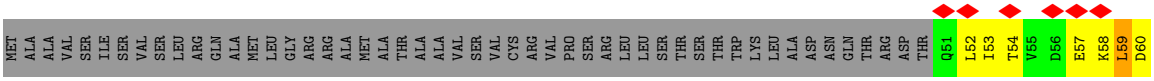


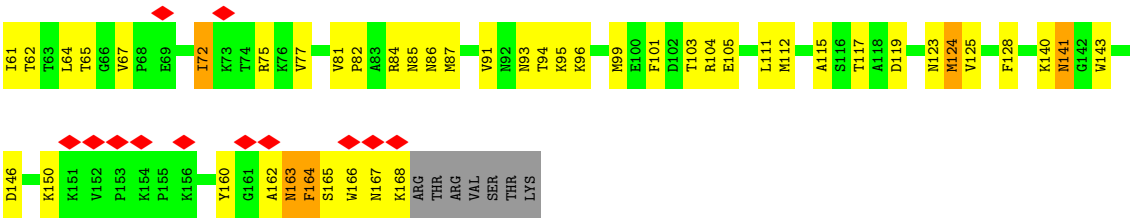


• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:

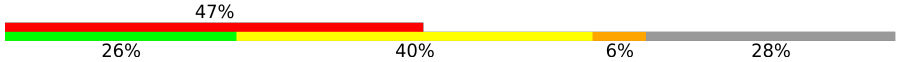


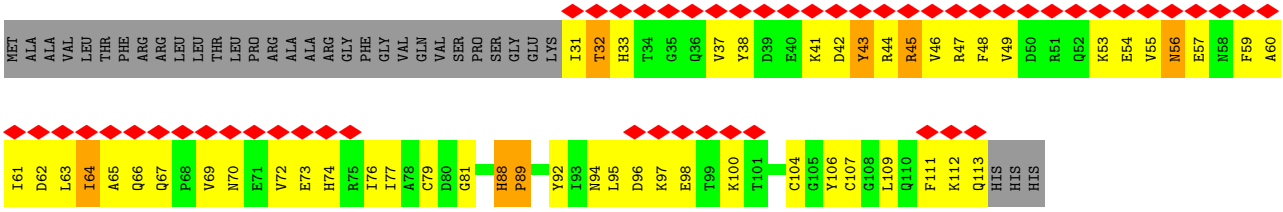




• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

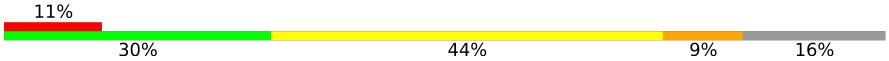
Chain R:

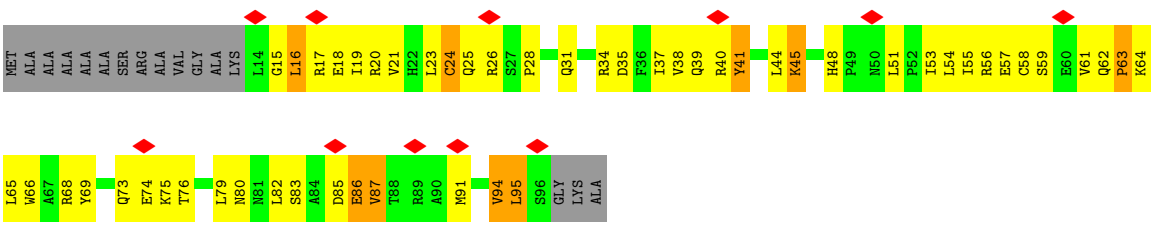




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

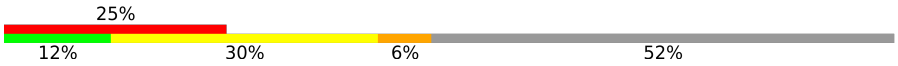
Chain S:

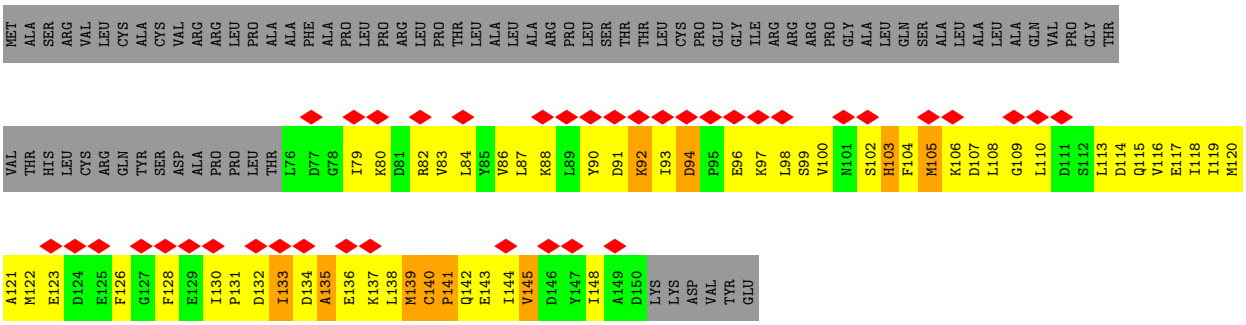




• Molecule 14: Acyl carrier protein, mitochondrial

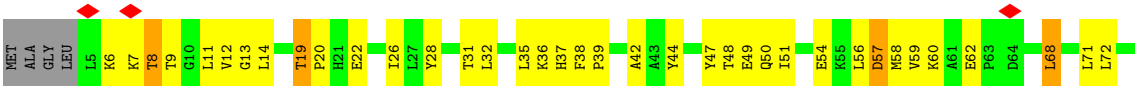
Chain T:

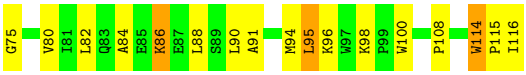




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

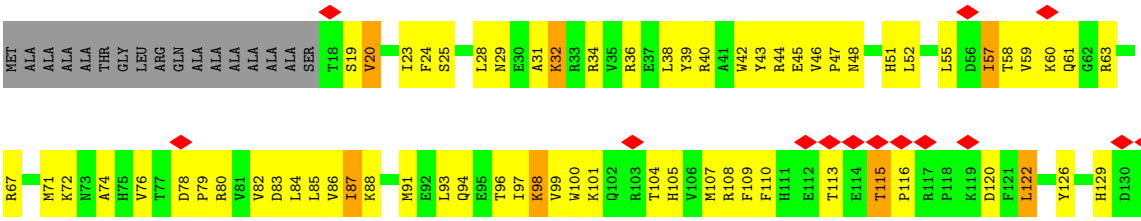
Chain V:





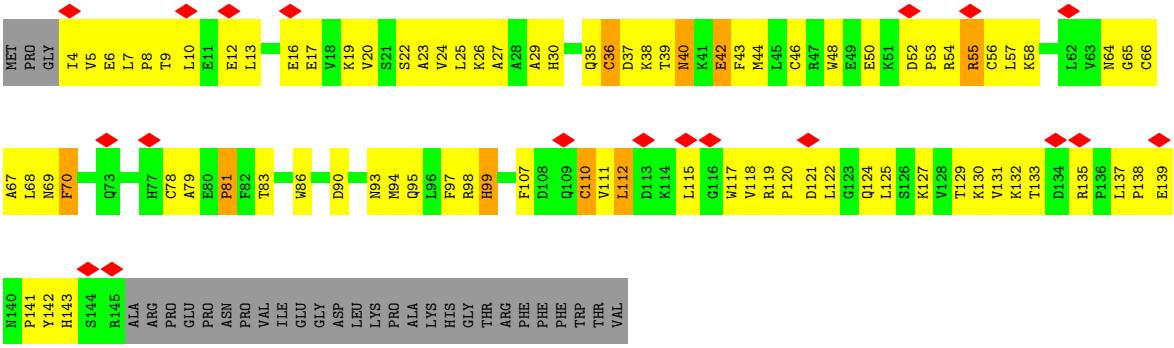
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



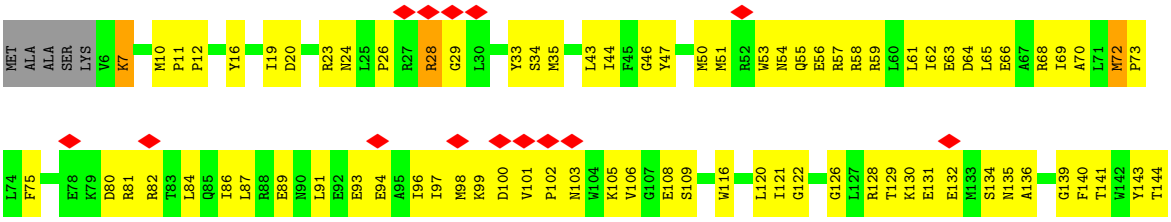
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



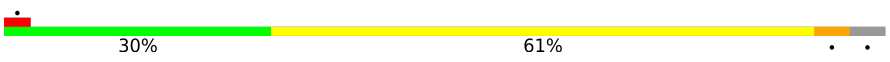
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



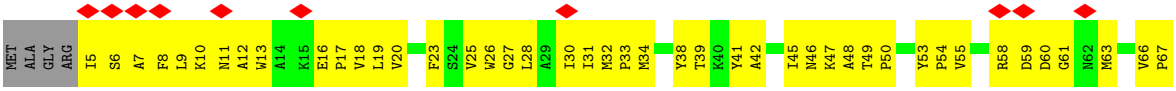
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:



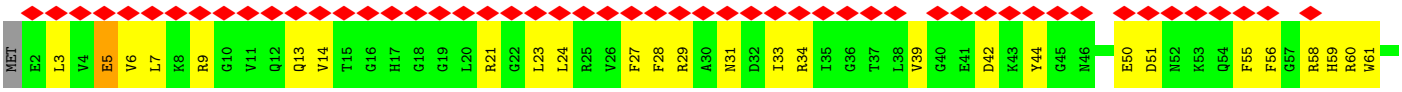
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

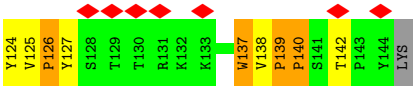
Chain b:



• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

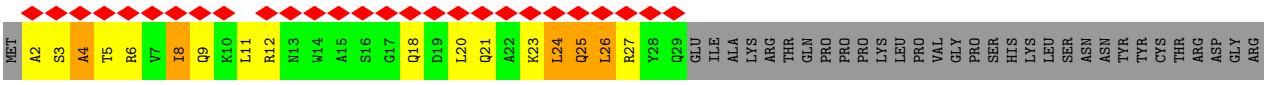
Chain q:

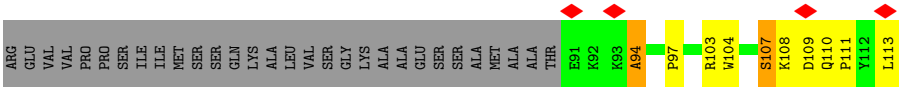




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

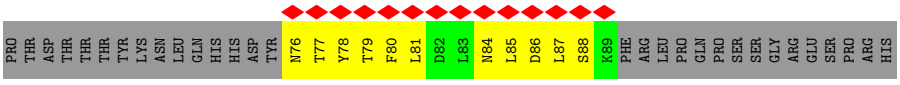
Chain r:





• Molecule 23: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.168	Depositor
Minimum map value	-1.846	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, ZN, NDP, UQ1, PC1, CDL, SF4, EHZ, UQ9, FMN, 3PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.83	0/774	1.33	11/1056 (1.0%)
2	B	0.97	1/1289 (0.1%)	1.45	18/1744 (1.0%)
3	C	0.87	1/1687 (0.1%)	1.31	14/2297 (0.6%)
4	D	0.98	8/3169 (0.3%)	1.40	30/4286 (0.7%)
5	E	0.86	3/1675 (0.2%)	1.35	24/2282 (1.1%)
6	F	0.96	6/3363 (0.2%)	1.54	64/4543 (1.4%)
7	G	0.92	10/5374 (0.2%)	1.60	109/7281 (1.5%)
8	H	0.98	5/2585 (0.2%)	1.52	59/3529 (1.7%)
9	I	0.93	1/1427 (0.1%)	1.54	18/1927 (0.9%)
10	P	0.88	4/2804 (0.1%)	1.35	43/3802 (1.1%)
11	Q	0.87	1/980 (0.1%)	1.29	12/1324 (0.9%)
12	R	0.87	1/671 (0.1%)	1.22	10/903 (1.1%)
13	S	1.09	3/678 (0.4%)	1.74	20/915 (2.2%)
14	T	1.03	1/613 (0.2%)	1.56	13/826 (1.6%)
15	V	0.86	0/937	1.47	14/1270 (1.1%)
16	W	0.80	0/993	1.32	15/1335 (1.1%)
17	X	0.84	1/1191 (0.1%)	1.44	22/1605 (1.4%)
18	Z	0.76	0/1183	1.10	7/1597 (0.4%)
19	a	0.83	0/561	1.47	7/755 (0.9%)
20	b	0.70	0/651	0.91	1/895 (0.1%)
21	q	1.07	2/1037 (0.2%)	1.52	17/1408 (1.2%)
22	r	1.04	2/426 (0.5%)	1.57	11/573 (1.9%)
23	s	0.98	0/116	1.78	3/157 (1.9%)
All	All	0.92	50/34184 (0.1%)	1.45	542/46310 (1.2%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	89	PRO	N-CD	-15.05	1.26	1.47
21	q	139	PRO	N-CD	-13.44	1.28	1.47
10	P	371	PRO	N-CD	12.93	1.65	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	532	PRO	N-CD	-12.51	1.30	1.47
13	S	28	PRO	N-CD	-11.91	1.31	1.47
14	T	141	PRO	N-CD	11.75	1.64	1.47
8	H	42	PRO	N-CD	10.87	1.62	1.47
6	F	234	GLY	CA-C	-10.22	1.41	1.52
6	F	227	PRO	N-CD	10.05	1.61	1.47
6	F	235	VAL	N-CA	-9.64	1.34	1.46
10	P	290	PRO	N-CD	9.62	1.61	1.47
7	G	275	PRO	N-CD	-9.48	1.34	1.47
8	H	75	PRO	N-CD	9.27	1.60	1.47
6	F	319	PRO	N-CD	9.11	1.60	1.47
9	I	107	PRO	N-CD	8.56	1.59	1.47
4	D	163	PRO	N-CD	-8.44	1.35	1.47
5	E	218	ARG	CA-C	7.96	1.62	1.53
4	D	352	PRO	N-CD	-7.90	1.36	1.47
13	S	63	PRO	N-CD	-7.89	1.36	1.47
11	Q	53	ILE	C-O	7.78	1.33	1.24
22	r	111	PRO	N-CD	-7.44	1.37	1.47
10	P	138	ASN	CA-C	7.23	1.62	1.53
7	G	449	PRO	N-CD	6.82	1.57	1.47
7	G	541	PRO	N-CD	-6.74	1.38	1.47
6	F	233	VAL	CA-C	-6.72	1.44	1.52
7	G	203	ASP	CA-C	6.71	1.62	1.52
4	D	106	VAL	C-N	-6.55	1.24	1.33
7	G	600	GLU	CA-C	6.45	1.61	1.52
2	B	110	PRO	C-O	-6.28	1.16	1.24
4	D	266	ARG	C-O	-6.25	1.16	1.24
7	G	127	ASP	CA-C	6.25	1.62	1.52
7	G	76	ARG	CA-C	6.14	1.61	1.53
6	F	384	PRO	N-CD	-6.12	1.39	1.47
5	E	93	PRO	N-CD	-5.92	1.39	1.47
7	G	361	VAL	CA-C	5.88	1.60	1.52
17	X	54	ARG	CA-C	5.83	1.60	1.52
22	r	25	GLN	CA-C	5.82	1.60	1.52
4	D	88	HIS	CA-C	-5.79	1.45	1.52
8	H	60	PRO	N-CD	5.77	1.55	1.47
5	E	80	PRO	N-CD	5.70	1.55	1.47
4	D	107	ARG	C-N	5.51	1.40	1.33
4	D	392	PRO	C-O	-5.50	1.20	1.24
13	S	95	LEU	CA-C	5.49	1.59	1.52
7	G	683	PRO	N-CD	-5.42	1.40	1.47
21	q	126	PRO	N-CD	5.39	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	235	THR	CA-C	5.38	1.59	1.53
8	H	211	PHE	CA-C	5.33	1.59	1.52
4	D	266	ARG	CA-C	-5.23	1.45	1.52
3	C	61	GLY	C-N	-5.08	1.27	1.33
8	H	310	PHE	CA-C	5.00	1.59	1.52

All (542) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	142	VAL	N-CA-CB	19.24	132.39	110.65
4	D	142	VAL	N-CA-C	-19.04	92.53	110.42
7	G	174	THR	N-CA-C	-16.81	89.08	114.64
6	F	125	CYS	N-CA-C	-15.64	93.46	113.17
6	F	332	CYS	N-CA-C	15.63	130.09	111.02
21	q	139	PRO	N-CA-CB	-13.60	95.57	103.19
7	G	251	ILE	N-CA-C	13.33	126.83	108.17
7	G	77	MET	N-CA-C	-13.07	97.31	113.38
9	I	164	VAL	N-CA-C	-12.85	100.11	112.83
7	G	500	ILE	N-CA-C	-12.52	98.77	110.53
19	a	3	PHE	CB-CA-C	-12.42	89.56	110.68
10	P	106	LEU	N-CA-C	12.25	128.79	109.07
6	F	171	VAL	N-CA-C	-11.82	99.42	110.53
7	G	204	MET	N-CA-C	-11.65	91.43	109.25
6	F	449	ARG	N-CA-C	-11.61	98.70	111.36
6	F	334	THR	N-CA-CB	11.47	127.25	109.82
11	Q	60	ASP	N-CA-C	-11.34	90.30	109.24
7	G	599	THR	N-CA-C	11.32	126.19	112.38
13	S	39	GLN	N-CA-C	11.19	125.45	111.69
16	W	87	ILE	N-CA-C	-11.13	99.73	110.42
15	V	57	ASP	N-CA-C	-11.04	99.26	111.07
1	A	54	LYS	N-CA-C	-10.98	98.18	111.69
8	H	259	PHE	N-CA-C	-10.96	99.41	111.36
23	s	86	ASP	N-CA-C	-10.95	99.32	111.14
17	X	70	PHE	N-CA-C	-10.60	99.73	111.07
9	I	77	LEU	N-CA-C	-10.46	99.68	111.71
5	E	68	ASN	N-CA-C	-10.41	99.93	111.07
14	T	139	MET	N-CA-C	-10.40	97.46	113.89
2	B	195	PRO	N-CA-C	-10.33	98.10	110.70
8	H	284	GLN	N-CA-C	-10.32	100.02	111.07
16	W	59	VAL	N-CA-C	-10.30	100.53	110.42
4	D	337	MET	N-CA-C	-10.30	100.05	111.07
7	G	280	ASP	N-CA-C	10.26	122.47	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	140	ASP	CB-CA-C	-10.20	98.06	111.42
10	P	366	ILE	N-CA-C	10.19	121.02	110.62
7	G	414	PHE	N-CA-C	-10.06	101.51	113.88
19	a	4	GLU	N-CA-C	10.05	124.81	112.54
9	I	161	ALA	N-CA-C	10.05	122.24	111.28
14	T	135	ALA	N-CA-C	-10.05	100.32	111.28
7	G	325	ARG	N-CA-C	-9.87	100.21	110.97
6	F	178	GLU	N-CA-C	-9.87	99.26	111.11
9	I	166	ALA	N-CA-C	-9.87	100.79	113.12
6	F	103	ASN	N-CA-C	-9.81	101.00	113.16
6	F	144	VAL	N-CA-C	-9.77	101.35	110.53
6	F	141	GLY	N-CA-C	-9.76	101.18	112.50
7	G	654	VAL	N-CA-C	9.76	123.28	111.09
7	G	35	PHE	N-CA-C	9.68	124.35	108.96
5	E	64	ALA	N-CA-C	-9.65	99.53	111.11
10	P	371	PRO	N-CA-CB	9.63	111.84	103.36
6	F	418	GLN	N-CA-C	-9.62	100.75	111.14
7	G	337	ALA	N-CA-C	-9.59	100.79	114.12
19	a	2	TRP	N-CA-C	-9.53	101.65	113.28
8	H	52	ALA	N-CA-C	-9.50	100.90	111.07
4	D	427	PRO	N-CA-C	-9.48	95.62	110.50
10	P	358	THR	N-CA-C	9.44	121.89	110.19
21	q	139	PRO	CA-N-CD	9.37	125.12	112.00
14	T	133	ILE	N-CA-C	9.35	119.89	110.82
7	G	694	PHE	N-CA-C	9.35	121.47	111.28
7	G	692	LYS	N-CA-C	-9.30	100.52	112.23
10	P	367	GLU	N-CA-C	9.26	122.56	111.82
10	P	369	THR	N-CA-CB	9.26	123.50	110.17
7	G	640	ASP	N-CA-C	-9.22	101.31	111.36
10	P	157	LYS	N-CA-C	-9.14	101.39	111.36
7	G	389	THR	N-CA-C	-9.13	96.26	109.96
5	E	85	ALA	N-CA-C	-9.12	101.42	111.36
17	X	55	ARG	N-CA-C	9.04	130.06	110.80
2	B	121	PHE	CB-CA-C	8.91	124.69	110.96
6	F	411	SER	N-CA-C	-8.89	101.56	111.07
7	G	133	GLN	N-CA-CB	8.76	121.48	110.45
7	G	212	LYS	N-CA-C	-8.76	94.63	108.90
7	G	365	ASN	N-CA-C	-8.74	102.17	112.92
8	H	60	PRO	N-CA-CB	8.69	108.56	102.65
9	I	154	TYR	N-CA-CB	-8.69	99.19	111.62
16	W	20	VAL	N-CA-C	8.68	120.78	108.36
10	P	96	LEU	N-CA-C	8.65	121.66	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	212	ASN	N-CA-C	-8.63	101.88	114.39
19	a	3	PHE	CA-CB-CG	8.55	122.35	113.80
13	S	86	GLU	N-CA-C	-8.53	102.07	111.36
12	R	57	GLU	N-CA-C	-8.51	98.25	110.59
13	S	18	GLU	N-CA-C	8.49	123.23	109.40
10	P	373	LYS	N-CA-C	8.45	121.84	110.35
10	P	360	ARG	N-CA-C	8.44	121.67	110.53
16	W	100	TRP	N-CA-C	-8.43	99.90	112.04
17	X	99	HIS	N-CA-C	-8.40	102.20	111.36
7	G	452	LEU	N-CA-C	-8.36	102.17	111.28
3	C	108	LYS	N-CA-C	8.35	120.00	111.07
16	W	57	ILE	N-CA-C	8.34	122.02	109.17
8	H	141	SER	N-CA-C	-8.34	102.15	111.07
11	Q	54	THR	N-CA-C	8.34	123.30	109.46
7	G	532	PRO	CA-N-CD	8.32	123.64	112.00
7	G	558	GLN	N-CA-C	-8.27	102.23	111.07
1	A	55	PHE	N-CA-C	-8.26	102.23	111.07
8	H	311	THR	N-CA-C	-8.23	102.55	112.59
5	E	218	ARG	CB-CA-C	-8.22	99.78	112.12
8	H	196	ALA	N-CA-C	8.22	127.99	109.81
3	C	196	PRO	N-CA-C	8.18	124.90	113.53
7	G	691	ILE	N-CA-C	8.14	123.62	111.89
6	F	411	SER	N-CA-CB	8.14	121.81	110.01
7	G	484	ASP	N-CA-C	8.14	121.07	111.71
1	A	64	LEU	N-CA-C	-8.14	102.36	111.07
6	F	298	GLU	N-CA-C	8.13	120.14	111.28
16	W	96	THR	N-CA-C	-8.13	102.36	111.14
6	F	191	TYR	N-CA-C	8.12	121.69	110.24
23	s	86	ASP	N-CA-CB	8.12	121.84	110.07
15	V	86	LYS	N-CA-C	-8.10	102.39	111.14
7	G	500	ILE	N-CA-CB	8.09	120.92	110.57
2	B	110	PRO	N-CA-C	8.07	124.55	113.65
5	E	219	SER	N-CA-CB	8.07	124.07	111.56
13	S	76	THR	N-CA-C	8.00	121.95	108.90
8	H	271	LEU	N-CA-C	-8.00	102.50	111.14
7	G	534	VAL	N-CA-C	-7.99	104.80	111.91
17	X	43	PHE	N-CA-C	-7.99	102.51	111.14
17	X	112	LEU	N-CA-C	-7.98	102.52	111.14
16	W	98	LYS	N-CA-C	-7.97	101.60	113.72
9	I	201	ILE	N-CA-C	-7.97	102.67	110.72
1	A	9	ILE	N-CA-C	-7.97	102.49	110.62
21	q	67	GLU	CB-CA-C	-7.94	99.60	112.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	360	ARG	N-CA-CB	-7.93	99.02	110.36
7	G	651	PRO	CB-CA-C	-7.93	98.48	111.56
10	P	206	ILE	N-CA-C	7.93	120.92	108.87
2	B	121	PHE	CA-CB-CG	-7.92	105.88	113.80
17	X	46	CYS	N-CA-C	-7.90	102.75	111.36
13	S	28	PRO	CA-N-CD	7.90	123.06	112.00
8	H	311	THR	N-CA-CB	7.86	123.50	110.92
15	V	6	LYS	N-CA-C	-7.86	100.15	110.53
7	G	270	VAL	N-CA-CB	-7.85	100.66	110.31
17	X	55	ARG	N-CA-CB	-7.84	97.24	110.49
9	I	160	GLU	N-CA-C	7.82	124.19	111.37
10	P	235	THR	CB-CA-C	-7.82	100.03	112.07
7	G	389	THR	N-CA-CB	7.79	121.46	109.85
17	X	58	LYS	N-CA-C	-7.76	102.77	111.07
1	A	53	MET	N-CA-C	-7.76	103.96	113.19
9	I	74	LEU	N-CA-C	-7.75	102.83	111.28
4	D	141	TYR	CA-C-N	7.73	130.16	120.72
4	D	141	TYR	C-N-CA	7.73	130.16	120.72
6	F	334	THR	N-CA-C	-7.70	101.62	111.02
21	q	44	TYR	N-CA-C	-7.68	98.91	110.28
21	q	89	TRP	N-CA-C	-7.67	102.86	111.14
8	H	253	GLU	N-CA-C	7.67	121.90	112.54
6	F	58	ARG	N-CA-C	-7.65	103.02	111.36
7	G	56	VAL	N-CA-C	-7.63	103.02	110.72
6	F	171	VAL	N-CA-CB	7.62	120.33	110.57
2	B	153	PRO	CB-CA-C	-7.62	98.98	111.56
4	D	361	ALA	N-CA-C	-7.62	103.08	112.38
7	G	569	GLN	N-CA-C	7.60	122.00	108.24
5	E	68	ASN	N-CA-CB	7.59	121.02	110.01
13	S	35	ASP	N-CA-C	-7.59	103.09	111.36
12	R	32	THR	N-CA-C	7.58	119.60	110.19
5	E	166	LYS	N-CA-C	-7.57	102.22	113.72
12	R	74	HIS	N-CA-C	7.55	121.15	110.50
14	T	141	PRO	N-CA-C	-7.55	103.04	113.53
8	H	223	PHE	CB-CA-C	-7.54	99.05	110.88
9	I	119	CYS	N-CA-C	-7.50	103.18	111.36
7	G	277	MET	N-CA-C	7.49	120.60	109.59
7	G	467	LYS	N-CA-C	-7.49	102.27	111.33
9	I	158	CYS	N-CA-C	-7.47	103.13	111.28
7	G	510	TRP	N-CA-CB	7.43	120.93	109.85
7	G	303	THR	N-CA-C	7.43	123.06	113.18
2	B	183	ARG	N-CA-C	-7.41	104.48	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	430	GLY	N-CA-C	7.41	121.62	112.73
15	V	57	ASP	N-CA-CB	7.37	120.70	110.01
4	D	350	LYS	CB-CA-C	-7.36	101.03	111.85
21	q	24	LEU	N-CA-C	-7.34	103.28	111.28
13	S	94	VAL	N-CA-C	7.32	117.45	110.42
8	H	309	ILE	N-CA-C	7.32	117.40	110.30
14	T	105	MET	N-CA-C	7.28	119.29	111.36
3	C	195	HIS	CB-CA-C	7.25	117.35	110.17
7	G	374	THR	CB-CA-C	-7.24	99.85	111.28
7	G	384	ASN	N-CA-C	-7.23	103.43	111.82
7	G	497	VAL	N-CA-C	-7.23	103.25	110.62
8	H	212	ASN	N-CA-CB	7.22	120.50	110.98
8	H	50	ALA	N-CA-C	7.21	118.78	111.07
7	G	661	GLU	N-CA-C	7.19	118.81	110.97
8	H	139	THR	N-CA-CB	7.19	120.44	110.01
6	F	73	PRO	N-CA-C	-7.17	103.79	113.40
15	V	68	LEU	N-CA-C	-7.17	103.47	111.28
6	F	81	LYS	N-CA-C	-7.16	103.55	111.36
7	G	465	VAL	N-CA-CB	7.15	118.45	110.51
7	G	217	GLU	N-CA-C	-7.13	101.63	110.41
8	H	254	LEU	N-CA-C	-7.13	103.55	111.82
8	H	214	GLU	N-CA-CB	-7.12	98.89	110.42
6	F	78	GLY	N-CA-C	-7.09	104.22	112.73
15	V	95	LEU	N-CA-C	-7.09	103.55	111.28
11	Q	162	ALA	N-CA-C	7.06	118.97	111.28
7	G	461	SER	N-CA-C	7.05	119.86	111.33
7	G	148	SER	N-CA-C	7.03	120.86	109.40
8	H	176	LEU	CA-C-N	-7.03	113.56	120.52
8	H	176	LEU	C-N-CA	-7.03	113.56	120.52
6	F	169	LEU	N-CA-C	7.00	118.91	111.28
21	q	77	VAL	N-CA-C	-7.00	99.69	109.21
23	s	84	ASN	N-CA-C	7.00	118.55	111.07
6	F	455	GLN	N-CA-C	6.99	118.55	111.07
7	G	150	ARG	N-CA-C	6.99	119.55	109.14
2	B	166	ASN	N-CA-C	-6.98	103.36	110.97
6	F	418	GLN	N-CA-CB	6.97	120.18	110.07
6	F	428	GLY	N-CA-C	-6.97	103.85	112.77
7	G	294	TYR	N-CA-C	-6.96	104.59	113.23
8	H	292	ASN	N-CA-C	6.96	118.94	111.36
6	F	103	ASN	N-CA-CB	6.95	121.08	110.44
6	F	246	GLU	N-CA-C	-6.95	103.70	111.28
7	G	582	VAL	N-CA-C	6.94	118.48	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	W	87	ILE	N-CA-CB	6.94	118.67	110.55
3	C	69	PRO	N-CA-C	-6.93	104.29	113.65
14	T	145	VAL	N-CA-C	-6.92	103.72	110.72
10	P	235	THR	CA-C-O	6.92	128.11	121.67
8	H	204	GLU	N-CA-C	-6.92	104.96	113.19
5	E	152	GLN	N-CA-C	-6.90	103.69	111.07
7	G	300	GLN	N-CA-CB	6.90	122.50	112.08
6	F	148	ALA	N-CA-C	-6.89	103.85	111.36
18	Z	34	SER	N-CA-C	-6.87	103.71	111.07
7	G	362	ASP	N-CA-C	6.87	125.44	110.80
6	F	233	VAL	O-C-N	6.85	131.12	123.10
18	Z	28	ARG	N-CA-C	6.85	119.68	108.52
6	F	329	LYS	N-CA-C	6.83	119.59	111.33
8	H	300	LEU	N-CA-C	-6.82	104.22	112.54
1	A	112	GLU	N-CA-C	-6.82	102.25	111.87
8	H	305	ILE	N-CA-C	-6.82	103.37	113.39
7	G	133	GLN	N-CA-C	-6.81	101.21	110.68
12	R	56	ASN	N-CA-C	6.80	119.99	108.90
7	G	268	GLY	N-CA-C	6.80	124.75	115.30
6	F	244	ASN	N-CA-C	-6.79	100.93	110.50
6	F	233	VAL	CA-C-O	-6.76	113.29	120.53
22	r	11	LEU	N-CA-C	-6.74	104.01	111.36
7	G	434	SER	N-CA-C	-6.74	100.99	110.29
8	H	8	THR	N-CA-C	-6.71	101.23	110.35
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
5	E	199	ASP	N-CA-C	-6.69	103.68	110.97
10	P	371	PRO	CA-N-CD	-6.68	102.64	112.00
15	V	8	THR	N-CA-C	6.68	119.01	108.79
16	W	105	HIS	N-CA-C	-6.68	104.95	113.23
14	T	141	PRO	N-CA-CB	6.66	110.66	103.33
15	V	114	TRP	N-CA-CB	6.66	120.22	110.30
7	G	601	GLY	N-CA-C	6.66	124.89	115.30
17	X	129	THR	N-CA-C	6.64	120.86	110.17
3	C	125	PHE	N-CA-CB	-6.64	100.61	110.17
7	G	640	ASP	N-CA-CB	6.64	119.98	110.16
10	P	116	ILE	N-CA-C	-6.64	104.02	110.72
8	H	93	HIS	CB-CA-C	6.62	117.83	108.76
17	X	97	PHE	N-CA-C	6.62	118.58	111.36
6	F	344	GLN	N-CA-C	-6.62	103.99	111.07
15	V	86	LYS	N-CA-CB	6.62	119.66	110.07
6	F	228	PRO	N-CA-C	-6.60	98.88	112.47
7	G	287	SER	N-CA-C	6.60	119.24	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	184	ILE	N-CA-C	-6.59	103.90	110.62
13	S	40	ARG	N-CA-C	6.59	122.83	113.02
5	E	166	LYS	CB-CA-C	6.58	123.47	110.65
8	H	182	ALA	N-CA-C	-6.57	104.04	111.07
6	F	336	LEU	N-CA-CB	-6.57	100.99	111.43
7	G	435	PRO	N-CA-C	-6.56	100.20	110.50
6	F	234	GLY	CA-C-N	-6.55	111.72	120.50
6	F	234	GLY	C-N-CA	-6.55	111.72	120.50
11	Q	141	ASN	N-CA-CB	6.55	120.74	110.46
7	G	605	GLN	N-CA-C	6.52	119.15	108.52
8	H	223	PHE	N-CA-C	-6.51	104.10	111.07
13	S	16	LEU	N-CA-C	-6.50	98.31	108.90
8	H	267	SER	N-CA-C	-6.49	104.28	111.36
7	G	275	PRO	CB-CA-C	-6.49	102.48	110.98
17	X	81	PRO	N-CA-C	-6.49	104.19	113.47
14	T	141	PRO	CA-N-CD	-6.48	102.92	112.00
17	X	98	ARG	N-CA-C	6.47	120.44	112.54
4	D	388	GLY	N-CA-C	6.47	119.57	110.38
10	P	137	ARG	N-CA-C	6.46	122.04	111.37
21	q	75	TRP	N-CA-C	6.46	121.43	112.45
12	R	81	GLY	N-CA-C	-6.46	106.82	115.21
15	V	49	GLU	N-CA-C	-6.45	104.25	111.28
7	G	250	SER	N-CA-C	6.45	116.78	108.34
8	H	255	TYR	N-CA-CB	6.44	119.35	110.01
3	C	125	PHE	N-CA-C	6.43	119.57	110.50
8	H	177	PRO	N-CA-C	-6.43	101.56	111.13
22	r	24	LEU	N-CA-C	6.42	119.55	110.50
6	F	178	GLU	N-CA-CB	6.41	119.49	109.94
4	D	140	ASP	N-CA-C	-6.40	96.54	107.23
7	G	273	ILE	N-CA-C	-6.40	98.29	107.77
7	G	275	PRO	CA-N-CD	6.40	120.97	112.00
12	R	43	TYR	N-CA-C	-6.40	99.80	109.79
9	I	66	LEU	N-CA-C	-6.40	104.39	111.36
6	F	370	LEU	N-CA-C	-6.39	104.39	111.36
8	H	271	LEU	N-CA-CB	6.38	119.32	110.07
9	I	205	ILE	N-CA-C	-6.37	104.29	110.72
7	G	95	PRO	N-CA-C	-6.37	101.19	110.80
11	Q	59	LEU	N-CA-C	-6.35	100.77	110.30
6	F	144	VAL	N-CA-CB	6.33	118.68	110.57
7	G	176	CYS	N-CA-C	6.32	119.64	110.42
22	r	8	ILE	N-CA-C	-6.29	104.36	110.72
15	V	71	LEU	N-CA-C	6.29	118.13	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	26	ILE	N-CA-C	-6.29	104.52	113.07
21	q	28	PHE	N-CA-C	6.28	117.79	111.07
17	X	99	HIS	N-CA-CB	6.28	119.46	110.16
5	E	64	ALA	N-CA-CB	6.28	119.29	109.94
1	A	101	GLY	N-CA-C	-6.27	105.23	112.50
7	G	356	ASP	N-CA-CB	6.27	119.34	110.12
6	F	415	ILE	N-CA-C	-6.27	104.39	110.72
15	V	91	ALA	N-CA-C	-6.26	104.46	111.28
4	D	141	TYR	N-CA-C	6.25	120.91	113.16
2	B	113	ASP	N-CA-CB	6.25	119.52	109.28
6	F	255	CYS	N-CA-C	-6.24	104.55	111.36
21	q	69	ASN	N-CA-CB	6.24	121.39	111.66
6	F	101	PHE	N-CA-C	6.23	118.87	111.33
5	E	50	THR	N-CA-CB	6.22	121.45	110.37
7	G	383	SER	N-CA-C	-6.22	106.91	114.75
8	H	269	THR	N-CA-C	6.22	118.06	111.28
10	P	139	PHE	N-CA-CB	6.22	121.72	110.95
8	H	52	ALA	N-CA-CB	6.22	119.03	110.01
11	Q	141	ASN	N-CA-C	-6.21	105.71	113.28
6	F	192	ASP	N-CA-C	6.20	119.05	109.07
17	X	36	CYS	CB-CA-C	-6.20	97.25	110.76
8	H	76	THR	N-CA-C	-6.20	104.53	111.28
7	G	451	ILE	N-CA-C	-6.18	104.96	113.00
13	S	28	PRO	N-CA-CB	-6.18	96.71	103.39
22	r	26	LEU	N-CA-CB	-6.18	101.15	110.35
10	P	368	GLU	N-CA-CB	6.17	119.81	110.30
6	F	409	ILE	N-CA-C	6.17	116.34	110.42
10	P	118	LYS	N-CA-C	6.17	118.98	111.82
6	F	212	LEU	N-CA-C	-6.17	104.56	111.28
7	G	418	ILE	N-CA-C	-6.16	103.42	112.04
18	Z	44	ILE	N-CA-C	-6.13	104.77	110.53
13	S	40	ARG	N-CA-CB	-6.13	101.09	111.27
4	D	291	VAL	N-CA-C	-6.13	103.43	111.09
7	G	325	ARG	N-CA-CB	6.12	118.85	109.91
7	G	420	LYS	N-CA-C	6.12	118.73	111.33
7	G	508	ALA	N-CA-C	6.09	117.92	111.28
8	H	276	SER	N-CA-C	6.09	118.89	111.82
13	S	87	VAL	N-CA-C	-6.06	104.44	110.62
8	H	103	LEU	N-CA-C	-6.04	104.78	111.36
10	P	370	LYS	N-CA-C	6.03	119.26	108.47
8	H	185	TRP	N-CA-C	-6.03	104.07	112.45
21	q	137	TRP	N-CA-C	-6.02	100.93	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	7	LEU	N-CA-C	-6.01	104.35	111.03
8	H	24	GLU	N-CA-C	-6.01	104.09	112.45
22	r	108	LYS	N-CA-C	6.01	117.91	111.36
13	S	61	VAL	N-CA-C	-6.00	99.60	107.88
7	G	353	ALA	N-CA-C	-6.00	104.67	112.23
7	G	532	PRO	N-CA-CB	-6.00	97.08	103.38
8	H	203	GLY	N-CA-C	-5.99	103.92	112.55
2	B	196	PRO	N-CA-C	-5.98	101.82	111.03
7	G	638	THR	N-CA-C	-5.96	100.24	109.24
5	E	66	VAL	N-CA-C	5.96	116.62	110.36
6	F	291	GLU	N-CA-C	5.95	118.23	110.43
9	I	116	CYS	N-CA-C	-5.94	105.52	112.89
7	G	387	LEU	CB-CA-C	-5.93	101.72	111.68
17	X	40	ASN	N-CA-C	-5.93	104.73	111.07
21	q	5	GLU	N-CA-C	-5.91	104.92	111.36
4	D	352	PRO	N-CA-CB	-5.89	97.36	103.08
1	A	58	VAL	CB-CA-C	-5.87	104.19	111.70
14	T	94	ASP	N-CA-CB	-5.87	105.14	111.66
3	C	71	TYR	N-CA-C	5.86	120.23	113.38
6	F	127	ASP	N-CA-C	5.84	118.43	111.71
7	G	480	ALA	N-CA-C	-5.84	104.99	111.36
3	C	209	LEU	N-CA-CB	-5.84	100.66	110.83
13	S	86	GLU	N-CA-CB	5.84	118.80	110.16
4	D	258	VAL	N-CA-C	-5.83	103.98	110.62
7	G	639	LEU	N-CA-C	5.83	118.58	111.82
7	G	289	LYS	N-CA-C	5.82	117.62	111.28
8	H	116	ILE	N-CA-C	-5.82	104.83	110.42
15	V	19	THR	N-CA-CB	5.82	120.72	110.37
21	q	65	THR	N-CA-C	5.82	119.15	110.14
8	H	315	PRO	O-C-N	5.81	123.88	121.15
10	P	367	GLU	CB-CA-C	-5.81	99.51	110.67
7	G	672	ALA	N-CA-C	-5.81	104.95	111.28
8	H	211	PHE	CA-C-O	5.80	126.97	119.95
10	P	157	LYS	N-CA-CB	5.80	118.75	110.16
7	G	34	VAL	N-CA-C	5.79	116.22	108.11
10	P	122	HIS	N-CA-C	5.79	120.03	112.92
11	Q	164	PHE	N-CA-CB	5.78	119.78	110.42
19	a	3	PHE	N-CA-CB	5.77	118.72	110.06
12	R	45	ARG	N-CA-C	-5.77	104.96	113.61
6	F	102	MET	CB-CA-C	-5.77	101.43	110.94
4	D	414	ASP	N-CA-C	-5.76	101.42	110.36
6	F	299	LEU	N-CA-C	5.76	118.51	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Z	72	MET	CA-C-N	-5.76	113.25	119.24
18	Z	72	MET	C-N-CA	-5.76	113.25	119.24
10	P	234	LYS	CB-CA-C	-5.76	103.39	111.80
7	G	275	PRO	N-CA-CB	-5.73	98.00	103.33
6	F	393	ASN	N-CA-C	-5.73	104.94	111.07
13	S	73	GLN	N-CA-C	-5.72	100.38	109.59
8	H	126	LYS	N-CA-C	5.72	117.51	111.28
2	B	135	GLY	CA-C-O	-5.71	118.01	122.52
17	X	79	ALA	N-CA-C	5.71	117.18	111.07
5	E	119	THR	N-CA-C	-5.71	105.81	112.89
21	q	140	PRO	N-CA-C	-5.70	102.19	110.80
8	H	252	PRO	N-CA-CB	-5.70	98.04	103.51
1	A	55	PHE	N-CA-CB	5.69	118.26	110.01
10	P	272	LEU	N-CA-C	-5.68	101.87	110.28
6	F	41	ILE	N-CA-C	5.68	115.76	110.42
7	G	59	GLN	N-CA-C	5.65	117.98	107.99
17	X	65	GLY	N-CA-C	-5.65	105.95	112.50
10	P	119	ALA	N-CA-C	-5.64	105.04	111.14
6	F	457	HIS	N-CA-CB	-5.64	100.91	110.50
7	G	599	THR	CA-C-N	-5.63	114.16	122.83
7	G	599	THR	C-N-CA	-5.63	114.16	122.83
6	F	416	SER	N-CA-C	5.62	117.86	111.11
6	F	304	ALA	CB-CA-C	-5.62	110.08	116.54
11	Q	124	MET	CA-C-N	-5.61	115.01	122.98
11	Q	124	MET	C-N-CA	-5.61	115.01	122.98
2	B	112	TYR	N-CA-C	5.61	122.74	110.80
6	F	176	ALA	N-CA-C	5.60	118.11	111.33
5	E	222	PHE	CB-CA-C	-5.60	100.62	109.80
17	X	56	CYS	N-CA-C	5.60	119.80	112.92
4	D	352	PRO	N-CA-C	5.59	117.52	110.70
9	I	191	LEU	N-CA-C	-5.59	105.27	111.36
13	S	63	PRO	CA-N-CD	5.59	119.82	112.00
7	G	530	TYR	N-CA-C	-5.58	102.02	110.28
7	G	615	LEU	N-CA-C	-5.58	106.25	113.16
12	R	89	PRO	N-CA-CB	-5.57	98.25	103.27
21	q	142	THR	N-CA-CB	5.57	119.87	109.68
2	B	71	ALA	N-CA-CB	-5.57	101.34	110.14
5	E	183	PRO	N-CA-C	-5.56	102.20	111.26
4	D	163	PRO	N-CA-CB	-5.55	97.69	103.08
17	X	54	ARG	CB-CA-C	5.55	119.50	110.96
2	B	201	LEU	N-CA-C	-5.54	105.14	111.07
7	G	127	ASP	CA-C-O	5.53	129.02	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	130	ILE	N-CA-C	5.53	115.22	107.37
2	B	120	VAL	CA-C-N	-5.53	113.36	120.65
2	B	120	VAL	C-N-CA	-5.53	113.36	120.65
6	F	294	VAL	CA-C-N	-5.53	114.07	119.76
6	F	294	VAL	C-N-CA	-5.53	114.07	119.76
21	q	68	MET	N-CA-C	5.52	119.28	112.54
21	q	71	LYS	N-CA-C	5.51	120.00	113.16
14	T	135	ALA	N-CA-CB	5.50	118.21	110.12
6	F	118	ASP	N-CA-C	-5.50	102.14	110.28
3	C	71	TYR	CB-CA-C	-5.50	102.27	111.23
7	G	313	LEU	N-CA-C	5.49	118.51	109.72
7	G	363	SER	N-CA-C	-5.49	100.23	109.07
19	a	25	TYR	N-CA-C	-5.49	107.84	114.75
8	H	141	SER	N-CA-CB	5.47	117.94	110.01
22	r	94	ALA	N-CA-C	-5.47	101.75	109.96
4	D	200	PHE	CA-CB-CG	5.46	119.26	113.80
7	G	404	GLY	N-CA-C	5.46	121.45	113.48
10	P	86	CYS	N-CA-C	-5.46	103.18	110.55
4	D	132	ALA	N-CA-C	-5.45	106.63	113.72
7	G	682	ASP	CA-C-N	-5.45	114.15	119.76
7	G	682	ASP	C-N-CA	-5.45	114.15	119.76
22	r	111	PRO	N-CA-C	-5.45	106.44	113.57
7	G	150	ARG	N-CA-CB	-5.44	102.81	111.62
10	P	357	ARG	N-CA-C	5.42	117.53	110.43
7	G	420	LYS	N-CA-CB	-5.42	101.94	110.06
17	X	27	ALA	N-CA-C	-5.41	105.04	111.69
10	P	374	THR	N-CA-C	5.40	117.53	108.73
3	C	81	ASP	N-CA-C	-5.40	104.45	111.74
12	R	88	HIS	CB-CA-C	5.39	117.33	109.08
14	T	92	LYS	N-CA-C	-5.39	106.29	112.92
5	E	48	PRO	N-CA-C	5.38	120.84	113.84
13	S	24	CYS	N-CA-C	-5.37	103.30	110.55
13	S	41	TYR	N-CA-C	-5.37	105.51	111.36
18	Z	50	MET	N-CA-C	-5.37	105.43	111.28
6	F	199	ARG	N-CA-C	5.36	117.47	109.59
11	Q	163	ASN	CB-CA-C	-5.35	99.30	109.95
7	G	510	TRP	N-CA-C	-5.35	101.94	109.96
4	D	201	PHE	N-CA-C	-5.34	105.54	111.36
5	E	219	SER	N-CA-C	-5.34	100.61	108.79
18	Z	55	GLN	N-CA-C	-5.34	105.46	111.28
4	D	391	VAL	CA-C-N	-5.33	115.82	119.66
4	D	391	VAL	C-N-CA	-5.33	115.82	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Q	164	PHE	N-CA-C	-5.33	106.75	113.20
7	G	356	ASP	N-CA-C	-5.33	105.47	111.28
8	H	94	PRO	N-CA-C	5.33	118.68	111.22
4	D	93	GLY	N-CA-C	5.33	121.84	114.92
4	D	141	TYR	N-CA-CB	-5.31	102.32	110.44
8	H	252	PRO	CA-N-CD	5.30	119.43	112.00
10	P	339	GLY	N-CA-C	5.30	122.64	115.00
16	W	32	LYS	N-CA-C	-5.30	104.92	111.33
11	Q	72	ILE	N-CA-C	-5.28	108.36	113.53
9	I	54	THR	N-CA-C	-5.27	104.95	111.33
10	P	330	THR	N-CA-C	-5.27	106.75	114.39
9	I	160	GLU	N-CA-CB	-5.27	100.77	109.72
4	D	363	VAL	N-CA-C	5.26	116.34	111.81
16	W	122	LEU	N-CA-C	-5.26	105.54	111.28
7	G	435	PRO	CB-CA-C	-5.26	105.83	111.56
5	E	48	PRO	CB-CA-C	-5.26	104.39	111.85
8	H	46	LEU	N-CA-C	-5.25	106.65	113.16
16	W	120	ASP	N-CA-C	-5.25	102.51	110.28
6	F	300	ILE	N-CA-CB	5.25	119.32	110.56
6	F	412	LEU	N-CA-C	-5.24	105.74	111.82
8	H	146	MET	N-CA-C	-5.24	105.46	111.07
7	G	362	ASP	CA-CB-CG	5.24	117.84	112.60
10	P	260	GLY	N-CA-C	-5.24	108.39	115.36
5	E	221	ARG	N-CA-C	5.23	117.81	110.23
7	G	449	PRO	N-CA-CB	5.22	109.03	103.39
8	H	310	PHE	N-CA-C	5.22	119.28	113.01
7	G	277	MET	N-CA-CB	-5.22	101.67	109.71
10	P	192	ARG	N-CA-C	-5.21	105.60	111.28
22	r	111	PRO	CA-N-CD	5.21	119.29	112.00
22	r	107	SER	N-CA-C	-5.20	102.16	109.96
7	G	713	ALA	N-CA-C	-5.20	105.51	111.07
22	r	25	GLN	N-CA-C	5.20	118.88	112.54
10	P	194	VAL	N-CA-CB	5.20	118.38	110.58
7	G	556	THR	N-CA-C	-5.19	101.52	109.41
10	P	137	ARG	CA-C-N	-5.19	114.93	122.86
10	P	137	ARG	C-N-CA	-5.19	114.93	122.86
3	C	164	TRP	N-CA-C	5.18	117.01	111.36
7	G	600	GLU	CB-CA-C	-5.18	103.03	111.06
13	S	85	ASP	N-CA-C	5.17	117.82	111.82
7	G	172	ILE	N-CA-C	-5.16	98.62	109.34
8	H	277	TYR	N-CA-C	5.16	117.99	110.10
2	B	125	PRO	CB-CA-C	-5.15	104.82	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	196	ALA	CA-C-N	-5.15	113.49	119.47
8	H	196	ALA	C-N-CA	-5.15	113.49	119.47
1	A	106	TRP	CB-CA-C	-5.15	102.44	110.94
6	F	337	MET	CB-CA-C	-5.15	103.03	111.68
7	G	63	PHE	CA-C-O	-5.15	115.09	121.06
7	G	569	GLN	CB-CA-C	-5.15	104.23	112.05
15	V	84	ALA	N-CA-C	5.15	116.58	111.07
7	G	387	LEU	N-CA-C	-5.14	98.32	107.98
10	P	198	ALA	N-CA-C	-5.14	100.14	108.52
8	H	101	GLY	N-CA-C	5.13	118.45	112.50
10	P	360	ARG	CA-C-O	-5.13	115.92	121.87
8	H	90	PRO	CA-C-O	-5.13	117.43	121.38
20	b	82	LYS	N-CA-C	-5.13	103.76	110.53
7	G	458	GLY	N-CA-C	-5.13	108.25	115.32
4	D	391	VAL	N-CA-C	5.12	113.79	109.02
16	W	115	THR	CA-C-N	-5.12	113.44	119.84
16	W	115	THR	C-N-CA	-5.12	113.44	119.84
2	B	94	THR	N-CA-CB	-5.11	102.25	110.69
6	F	60	GLY	N-CA-C	-5.10	106.01	114.48
3	C	156	VAL	N-CA-C	-5.10	104.13	111.17
8	H	214	GLU	N-CA-C	5.09	119.36	113.20
16	W	91	MET	N-CA-C	-5.09	105.91	111.82
10	P	356	HIS	N-CA-C	-5.09	105.86	111.71
7	G	203	ASP	CA-C-O	5.08	127.22	121.32
5	E	181	ASN	N-CA-C	-5.08	99.51	108.20
5	E	222	PHE	N-CA-C	5.08	117.89	109.46
9	I	95	PRO	N-CA-C	5.08	121.17	113.81
10	P	376	ASN	CB-CA-C	-5.07	102.23	110.85
14	T	140	CYS	CB-CA-C	-5.06	104.08	109.85
10	P	170	LEU	N-CA-C	5.05	117.05	110.43
8	H	254	LEU	N-CA-CB	5.05	118.11	110.28
7	G	280	ASP	N-CA-CB	-5.05	102.70	110.12
7	G	393	GLY	N-CA-C	-5.05	107.79	115.66
17	X	42	GLU	N-CA-C	-5.05	105.86	111.36
2	B	127	GLN	N-CA-CB	-5.04	103.16	110.47
22	r	4	ALA	N-CA-C	-5.04	105.88	112.23
1	A	54	LYS	N-CA-CB	5.04	117.70	110.20
3	C	208	GLU	CA-C-O	-5.04	115.71	121.40
13	S	45	LYS	N-CA-C	-5.03	105.87	111.36
4	D	224	ALA	CA-C-O	-5.03	115.52	120.90
3	C	221	GLU	N-CA-C	-5.03	102.42	108.25
5	E	213	PRO	CB-CA-C	-5.03	106.31	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	X	110	CYS	CB-CA-C	-5.03	103.22	110.96
5	E	75	ALA	N-CA-C	5.01	117.39	111.33
12	R	65	ALA	N-CA-C	-5.01	105.95	111.71
14	T	140	CYS	N-CA-C	5.00	116.65	109.04
4	D	106	VAL	O-C-N	-5.00	116.84	122.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	754	0	814	112	0
2	B	1258	0	1270	160	0
3	C	1641	0	1596	134	0
4	D	3095	0	3066	300	0
5	E	1635	0	1626	185	0
6	F	3288	0	3243	357	0
7	G	5287	0	5323	551	0
8	H	2510	0	2593	386	0
9	I	1398	0	1359	151	0
10	P	2730	0	2747	233	0
11	Q	957	0	949	74	0
12	R	660	0	639	78	0
13	S	667	0	685	72	0
14	T	604	0	596	92	0
15	V	915	0	954	81	0
16	W	970	0	991	78	0
17	X	1164	0	1150	84	0
18	Z	1152	0	1148	95	0
19	a	548	0	562	78	0
20	b	628	0	628	93	0
21	q	1004	0	962	83	0
22	r	418	0	434	44	0
23	s	115	0	113	14	0
24	A	46	0	69	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	I	51	0	82	14	0
24	b	46	0	69	16	0
25	B	8	0	0	6	0
25	F	8	0	0	10	0
25	G	16	0	0	5	0
25	I	16	0	0	16	0
26	B	18	0	18	13	0
27	B	35	0	44	7	0
27	H	42	0	58	6	0
27	I	47	0	71	9	0
28	E	4	0	0	5	0
28	G	4	0	0	4	0
29	F	31	0	19	1	0
30	H	35	0	43	4	0
31	P	48	0	26	7	0
32	R	1	0	0	0	0
33	W	32	0	0	7	0
34	a	57	0	58	22	0
All	All	33943	0	34005	3028	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (3028) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
10:P:93:HIS:CD2	10:P:94:LEU:HD12	1.75	1.22
8:H:251:LEU:HD12	8:H:251:LEU:O	1.42	1.20
7:G:126:LEU:HD12	7:G:126:LEU:O	1.37	1.19
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.38	1.19
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
15:V:44:TYR:CE1	15:V:48:THR:HG21	1.77	1.18
10:P:156:SER:HB2	10:P:161:VAL:CG2	1.75	1.16
6:F:392:MET:CE	6:F:419:ILE:HD12	1.76	1.15
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.64	1.13
13:S:51:LEU:HD13	13:S:95:LEU:HD21	1.23	1.12
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.38	1.12
9:I:123:CYS:SG	25:I:303:SF4:FE1	1.40	1.12
6:F:392:MET:HE3	6:F:419:ILE:CD1	1.78	1.12
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:40:VAL:HG22	12:R:43:TYR:CE2	1.86	1.10
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.10
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.09
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.43	1.09
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.09
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
7:G:399:VAL:HG21	7:G:462:PHE:CZ	1.88	1.08
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.10	1.07
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.37	1.06
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.06
9:I:152:CYS:SG	25:I:303:SF4:FE2	1.46	1.06
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.33	1.06
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.06
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.06
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.37	1.06
2:B:100:CYS:SG	25:B:301:SF4:FE4	1.48	1.05
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.37	1.05
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	1.05
3:C:102:HIS:HE1	15:V:48:THR:HG22	1.20	1.05
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.05
22:r:2:ALA:N	22:r:26:LEU:HD12	1.69	1.05
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.92	1.04
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.04
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.04
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.36	1.03
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.23	1.03
10:P:156:SER:HB2	10:P:161:VAL:HG22	1.34	1.03
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
2:B:82:ILE:HG23	8:H:57:MET:SD	1.99	1.03
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.41	1.02
6:F:199:ARG:HD3	23:s:80:PHE:CE2	1.95	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.42	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.02
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.95	1.01
6:F:300:ILE:HG23	6:F:305:GLY:O	1.58	1.01
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.01
10:P:358:THR:HG22	10:P:359:TYR:N	1.72	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:179:CYS:SG	28:E:301:FES:FE2	1.50	1.01
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.86	1.00
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	1.00
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	1.00
9:I:155:CYS:SG	25:I:303:SF4:FE4	1.51	1.00
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	1.00
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.00
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.99
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.98
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.98
3:C:168:GLU:CB	3:C:186:ILE:HD11	1.92	0.98
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
2:B:82:ILE:HG12	8:H:57:MET:CE	1.94	0.97
7:G:399:VAL:HG21	7:G:462:PHE:HZ	1.30	0.97
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.97
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.43	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.96
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.96
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.96
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.74	0.95
7:G:92:CYS:SG	28:G:803:FES:S1	2.63	0.95
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.95
10:P:40:VAL:HG22	12:R:43:TYR:CD2	1.99	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.95
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.95
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.95
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.94
13:S:19:ILE:HG13	13:S:95:LEU:HD11	1.49	0.94
6:F:300:ILE:HG22	6:F:306:GLY:HA2	1.47	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
9:I:152:CYS:HG	25:I:303:SF4:FE2	0.70	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.45	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.94
9:I:113:CYS:SG	25:I:304:SF4:FE3	1.59	0.93
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.49	0.93
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.51	0.93
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.32	0.92
10:P:93:HIS:CD2	10:P:94:LEU:CD1	2.52	0.92
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.92
34:a:101:CDL:HB4	21:q:3:LEU:HD13	1.49	0.92
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.92
5:E:179:CYS:HG	28:E:301:FES:FE2	0.66	0.92
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.92
7:G:399:VAL:CG2	7:G:462:PHE:HZ	1.82	0.92
21:q:85:GLU:HG2	21:q:98:PRO:HB3	1.53	0.91
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.63	0.91
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.91
6:F:382:CYS:HG	25:F:502:SF4:FE3	0.72	0.91
2:B:120:VAL:HG21	30:H:401:UQ9:H1MA	1.52	0.90
8:H:200:LEU:HD12	8:H:201:THR:N	1.86	0.90
4:D:232:VAL:HG12	4:D:356:ILE:HD13	1.53	0.90
10:P:93:HIS:NE2	10:P:94:LEU:CD1	2.35	0.90
2:B:81:LEU:HG	27:B:303:PC1:H261	1.52	0.90
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.55	0.90
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.52	0.90
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.89
21:q:76:ASP:OD1	21:q:76:ASP:O	1.90	0.89
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.53	0.89
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.36	0.89
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.89
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.62	0.89
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.54	0.89
2:B:95:PHE:HZ	2:B:148:VAL:HB	1.35	0.89
7:G:226:CYS:HG	25:G:802:SF4:FE1	0.71	0.89
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:96:LEU:HD12	10:P:97:MET:N	1.88	0.88
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.88
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.88
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.88
9:I:61:LEU:HD21	20:b:17:PRO:O	1.74	0.88
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.56	0.88
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.87
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.87
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.87
20:b:60:ASP:OD1	20:b:61:GLY:N	2.07	0.87
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.55	0.87
22:r:2:ALA:N	22:r:26:LEU:CD1	2.37	0.87
8:H:93:HIS:CE1	19:a:24:ALA:HA	2.10	0.87
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.57	0.87
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.87
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.86
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.86
10:P:358:THR:CG2	10:P:359:TYR:N	2.37	0.86
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.86
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.86
8:H:199:ASP:O	8:H:279:ARG:HD2	1.74	0.86
3:C:168:GLU:HB2	3:C:186:ILE:CD1	2.04	0.86
7:G:78:CYS:SG	28:G:803:FES:FE2	1.68	0.86
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.76	0.86
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.85
9:I:162:CYS:SG	25:I:304:SF4:FE4	1.68	0.85
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.85
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.55	0.85
2:B:122:ARG:HH11	4:D:89:PRO:HB3	1.40	0.85
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.90	0.85
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.85
1:A:49:LEU:HD23	4:D:80:MET:HB2	1.57	0.85
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.58	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.85
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.77	0.85
10:P:132:ARG:HG2	31:P:401:NDP:H8A	1.56	0.85
3:C:80:LEU:CD1	4:D:396:THR:HG22	2.07	0.85
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.85
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.85
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.84
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.84
4:D:89:PRO:HB2	8:H:204:GLU:HG3	1.58	0.84
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.95	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.08	0.84
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.42	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
2:B:93:MET:HE1	2:B:148:VAL:HG11	1.59	0.84
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.84
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
4:D:271:ARG:HD2	8:H:279:ARG:O	1.78	0.84
5:E:178:ALA:HA	6:F:125:CYS:SG	2.18	0.84
7:G:78:CYS:HG	28:G:803:FES:FE2	0.53	0.83
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.83
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.83
4:D:86:PRO:HG3	4:D:96:ARG:HG2	1.58	0.83
20:b:23:PHE:HB3	24:b:201:3PE:H2D2	1.58	0.83
1:A:108:GLN:HG2	1:A:109:LYS:H	1.43	0.83
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.83
10:P:358:THR:HG22	10:P:359:TYR:H	1.43	0.83
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.82
3:C:186:ILE:CD1	4:D:429:PHE:HZ	1.93	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
8:H:1:MET:HG3	19:a:30:THR:HG22	1.58	0.82
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.59	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.81
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.94	0.81
9:I:162:CYS:HG	25:I:304:SF4:FE4	0.52	0.81
10:P:358:THR:CG2	10:P:359:TYR:H	1.92	0.81
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.81
8:H:1:MET:HE3	19:a:29:PHE:CE2	2.15	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
8:H:1:MET:HG3	19:a:30:THR:CG2	2.08	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.81
22:r:4:ALA:HB1	22:r:9:GLN:HB2	1.60	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
3:C:102:HIS:CE1	15:V:48:THR:HG22	2.11	0.81
27:H:402:PC1:H342	27:H:402:PC1:H382	1.61	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
4:D:84:PHE:HZ	4:D:90:ALA:HB3	1.46	0.80
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.80
6:F:234:GLY:HA3	6:F:238:CYS:O	1.81	0.80
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.80
7:G:73:GLY:HA2	28:G:803:FES:S1	2.21	0.80
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
9:I:80:GLU:HG3	19:a:1:MET:SD	2.22	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.12	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.80
9:I:123:CYS:HG	25:I:303:SF4:FE1	0.51	0.80
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.80
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.61	0.80
34:a:101:CDL:HB4	21:q:3:LEU:CD1	2.11	0.80
2:B:122:ARG:HH12	26:B:302:UQ1:H71	1.45	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
2:B:89:SER:O	8:H:54:LYS:HD3	1.82	0.79
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.79
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.79
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79
17:X:4:ILE:HG22	17:X:5:VAL:H	1.48	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.79
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.79
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.79
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.62	0.79
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.24	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.78
13:S:51:LEU:HD13	13:S:95:LEU:CD2	2.11	0.78
6:F:109:ARG:HD2	6:F:237:GLY:O	1.83	0.78
13:S:20:ARG:HG3	13:S:54:LEU:HB2	1.65	0.78
7:G:617:ARG:NH1	16:W:129:HIS:HA	1.97	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
8:H:30:TYR:OH	19:a:4:GLU:HB2	1.82	0.78
10:P:40:VAL:CG2	12:R:43:TYR:CE2	2.66	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.78
9:I:113:CYS:HG	25:I:304:SF4:FE3	0.49	0.78
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.78
2:B:89:SER:O	8:H:54:LYS:CD	2.32	0.78
3:C:186:ILE:HD12	4:D:429:PHE:CZ	2.19	0.78
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.78
10:P:142:GLU:O	10:P:146:VAL:HG12	1.83	0.78
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.78
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.78
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.78
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.99	0.77
16:W:47:PRO:HG3	16:W:63:ARG:HH21	1.48	0.77
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.77
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.66	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.66	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.77
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
1:A:61:THR:CG2	8:H:290:TRP:CH2	2.67	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
20:b:66:VAL:HG13	20:b:72:ASP:HB2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.77
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.77
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.77
3:C:80:LEU:CD1	4:D:396:THR:CG2	2.63	0.76
8:H:183:MET:HE2	27:I:302:PC1:H2A1	1.67	0.76
1:A:112:GLU:O	1:A:112:GLU:CD	2.28	0.76
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.76
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.76
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.66	0.76
1:A:61:THR:HG21	8:H:290:TRP:CZ3	2.20	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	0.76
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.24	0.76
21:q:96:ASP:OD1	21:q:97:PRO:HD2	1.85	0.76
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.32	0.76
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.76
5:E:183:PRO:HB2	5:E:195:LEU:H	1.50	0.76
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.76
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.76
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.75
2:B:68:ARG:HD3	2:B:70:ARG:HG2	1.69	0.75
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.75
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.75
4:D:84:PHE:CZ	4:D:90:ALA:HB3	2.22	0.75
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.16	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
2:B:112:TYR:OH	9:I:91:GLY:CA	2.27	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.75
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.87	0.74
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.74
21:q:55:PHE:CD1	22:r:26:LEU:HD22	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:SER:O	8:H:54:LYS:HE2	1.87	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.74
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.74
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.67	0.74
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.74
9:I:57:ALA:HB2	20:b:13:TRP:O	1.87	0.74
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.74
5:E:139:CYS:SG	28:E:301:FES:FE1	1.78	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.74
14:T:117:GLU:HA	14:T:120:MET:HE3	1.68	0.74
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.69	0.74
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.48	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.74
3:C:99:LEU:HD13	3:C:140:ILE:HD11	1.70	0.74
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.78	0.74
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.74
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.52	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.74
8:H:195:ARG:O	8:H:199:ASP:HB2	1.87	0.74
8:H:272:TRP:HH2	27:I:302:PC1:H381	1.52	0.74
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.74
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.70	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
6:F:293:SER:HA	6:F:336:LEU:HD13	1.68	0.74
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.74
1:A:61:THR:HG21	8:H:290:TRP:CH2	2.23	0.73
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.68	0.73
5:E:192:TYR:CE1	5:E:215:PRO:HA	2.23	0.73
9:I:110:GLU:OE2	12:R:64:ILE:HB	1.88	0.73
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.73
2:B:122:ARG:NH1	26:B:302:UQ1:H71	2.02	0.73
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.22	0.73
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.73
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.69	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
4:D:280:ALA:CB	15:V:11:LEU:HG	2.19	0.73
21:q:68:MET:SD	21:q:81:MET:HB3	2.28	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:40:VAL:CG2	12:R:43:TYR:CD2	2.71	0.73
20:b:69:HIS:HD2	20:b:70:PRO:HD2	1.54	0.73
10:P:203:PRO:HG2	31:P:401:NDP:H6N	1.69	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.73
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.73
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.73
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.71	0.73
16:W:110:PHE:HZ	33:W:201:EHZ:C2	2.00	0.73
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	2.04	0.72
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
8:H:292:ASN:O	20:b:18:VAL:HG11	1.88	0.72
27:I:302:PC1:H112	18:Z:29:GLY:HA3	1.71	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
2:B:95:PHE:HE1	2:B:131:MET:HE2	1.54	0.72
17:X:90:ASP:OD2	19:a:62:VAL:HG11	1.90	0.72
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.71	0.72
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.72
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.72
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.68	0.72
10:P:262:THR:H	10:P:332:LEU:HD12	1.54	0.72
13:S:51:LEU:CD1	13:S:95:LEU:HD21	2.12	0.72
18:Z:98:MET:HE3	18:Z:101:VAL:HG21	1.70	0.72
34:a:101:CDL:HA32	21:q:13:GLN:HE22	1.54	0.72
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.72
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.70	0.72
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.72
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.72
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.19	0.72
4:D:81:THR:HA	4:D:100:GLU:HA	1.71	0.72
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.52	0.72
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.72
1:A:4:TYR:CE2	24:A:401:3PE:H231	2.25	0.72
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.72
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.71
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.72	0.71
3:C:102:HIS:HE1	15:V:48:THR:CG2	2.01	0.71
5:E:232:SER:HB3	6:F:288:VAL:HG23	1.71	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
6:F:236:PHE:HA	11:Q:166:TRP:CD1	2.25	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
27:I:302:PC1:H2D1	27:I:302:PC1:H291	1.73	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
8:H:30:TYR:HE2	19:a:5:ILE:HG22	1.54	0.71
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.72	0.71
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.71
13:S:48:HIS:ND1	13:S:95:LEU:HD23	2.05	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.73	0.71
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
8:H:312:ALA:HB2	20:b:38:TYR:HB3	1.73	0.71
2:B:93:MET:HE1	2:B:148:VAL:CG1	2.21	0.70
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.72	0.70
8:H:187:ILE:HD12	24:I:301:3PE:H242	1.71	0.70
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.70
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.70
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
8:H:318:MET:HG2	19:a:40:ARG:NH2	2.06	0.70
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.72	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.70
8:H:134:ARG:NH2	8:H:200:LEU:HD13	2.06	0.70
16:W:42:TRP:CD2	16:W:93:LEU:HD12	2.26	0.70
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.26	0.70
2:B:101:ALA:HB1	26:B:302:UQ1:HM53	1.73	0.70
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.70
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.70
8:H:30:TYR:CE2	19:a:5:ILE:CG2	2.75	0.70
8:H:67:SER:HA	27:H:402:PC1:H121	1.72	0.70
9:I:155:CYS:HG	25:I:303:SF4:FE4	1.08	0.70
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.70
16:W:110:PHE:CZ	33:W:201:EHZ:C2	2.75	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.73	0.70
16:W:58:THR:HB	16:W:61:GLN:CB	2.22	0.70
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.70
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.70
19:a:37:ARG:CB	19:a:48:MET:HE2	2.22	0.70
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.70
2:B:122:ARG:NH1	4:D:89:PRO:HB3	2.05	0.69
7:G:127:ASP:HA	12:R:106:TYR:OH	1.90	0.69
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.69
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.69
9:I:93:LEU:O	21:q:93:MET:HG2	1.93	0.69
3:C:84:GLU:HG2	3:C:141:ARG:HH11	1.56	0.69
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.69
13:S:23:LEU:HD12	13:S:23:LEU:O	1.93	0.69
13:S:34:ARG:O	13:S:38:VAL:HG23	1.92	0.69
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.69
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.23	0.69
6:F:300:ILE:HG22	6:F:306:GLY:CA	2.22	0.69
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.69
9:I:200:GLU:OE2	21:q:93:MET:SD	2.51	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.69
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.69
13:S:19:ILE:HG13	13:S:95:LEU:CD1	2.22	0.69
5:E:190:ASN:HB3	5:E:192:TYR:CE2	2.28	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.68
3:C:186:ILE:HB	4:D:113:ILE:HD11	1.76	0.68
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.73	0.68
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.68
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.76	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.23	0.68
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.74	0.68
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.68
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.68
8:H:283:ASP:OD1	8:H:284:GLN:N	2.26	0.68
34:a:101:CDL:H341	34:a:101:CDL:H171	1.74	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.58	0.68
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.68
6:F:227:PRO:HG3	7:G:94:MET:SD	2.34	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.68
16:W:84:LEU:HD21	16:W:88:LYS:HE3	1.74	0.68
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.68
2:B:89:SER:O	8:H:54:LYS:CE	2.42	0.68
5:E:78:VAL:HG12	5:E:104:LEU:HD13	1.76	0.68
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.68
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.68
17:X:64:ASN:O	17:X:68:LEU:HG	1.94	0.68
1:A:61:THR:HG22	8:H:290:TRP:CH2	2.29	0.67
7:G:126:LEU:CD1	12:R:89:PRO:HB3	2.25	0.67
17:X:78:CYS:SG	17:X:111:VAL:HG13	2.34	0.67
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.67
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.67
1:A:61:THR:HG22	8:H:290:TRP:HH2	1.59	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
2:B:93:MET:HE3	4:D:87:GLN:NE2	2.09	0.67
2:B:95:PHE:HZ	2:B:148:VAL:CB	2.05	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.67
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.67
19:a:60:TYR:O	19:a:62:VAL:HG13	1.95	0.67
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
18:Z:121:ILE:HD11	18:Z:136:ALA:CB	2.24	0.67
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.60	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
10:P:180:SER:O	10:P:184:LYS:HG3	1.95	0.67
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.67
18:Z:121:ILE:HD11	18:Z:136:ALA:HB1	1.77	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
8:H:1:MET:HE3	19:a:29:PHE:HE2	1.58	0.67
9:I:188:GLU:CD	12:R:56:ASN:HB2	2.19	0.67
9:I:188:GLU:OE2	12:R:56:ASN:HB2	1.94	0.67
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.25	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
13:S:26:ARG:H	13:S:34:ARG:NH1	1.92	0.67
1:A:112:GLU:O	1:A:112:GLU:OE1	2.12	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
8:H:1:MET:CE	19:a:29:PHE:HE2	2.08	0.67
4:D:92:HIS:HB2	4:D:458:PHE:CD2	2.30	0.67
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.67
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.67
10:P:320:GLU:O	10:P:324:ILE:HG12	1.95	0.67
21:q:138:VAL:CG2	21:q:139:PRO:HD2	2.25	0.67
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.21	0.66
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.66
23:s:78:TYR:HA	23:s:81:LEU:HD12	1.76	0.66
2:B:82:ILE:HA	8:H:57:MET:HE1	1.78	0.66
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.76	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.77	0.66
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.77	0.66
9:I:67:ILE:HG13	27:I:302:PC1:H251	1.77	0.66
10:P:94:LEU:HA	10:P:97:MET:HE3	1.77	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
5:E:240:PRO:HG3	6:F:57:LEU:O	1.94	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.26	0.66
6:F:300:ILE:HD11	6:F:356:VAL:HG21	1.77	0.66
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.30	0.66
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.49	0.66
9:I:35:THR:CG2	22:r:107:SER:HA	2.26	0.66
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.10	0.66
6:F:300:ILE:CG2	6:F:307:VAL:N	2.59	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
9:I:92:PRO:HA	21:q:91:HIS:O	1.96	0.66
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.76	0.66
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.06	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.66
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.24	0.66
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.66
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.66
1:A:54:LYS:O	1:A:58:VAL:HG23	1.95	0.66
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.57	0.66
9:I:80:GLU:OE2	22:r:26:LEU:CD1	2.44	0.66
10:P:156:SER:CB	10:P:161:VAL:HG22	2.20	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.66
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.66
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.77	0.66
6:F:110:PRO:O	6:F:238:CYS:HB3	1.96	0.66
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.31	0.66
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.66
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.66
10:P:263:PHE:HD2	10:P:333:PRO:O	1.79	0.65
18:Z:97:ILE:HG13	18:Z:98:MET:H	1.61	0.65
8:H:93:HIS:HE1	19:a:24:ALA:HA	1.61	0.65
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.73	0.65
8:H:311:THR:HB	18:Z:51:MET:SD	2.36	0.65
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.77	0.65
13:S:24:CYS:HA	13:S:58:CYS:O	1.97	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65
16:W:24:PHE:HB2	16:W:83:ASP:CG	2.20	0.65
18:Z:98:MET:CE	18:Z:101:VAL:HG21	2.27	0.65
2:B:122:ARG:HH11	4:D:89:PRO:CB	2.08	0.65
6:F:300:ILE:HG21	6:F:307:VAL:N	2.11	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65
4:D:84:PHE:HZ	4:D:90:ALA:CB	2.09	0.65
4:D:101:LEU:CD1	4:D:106:VAL:HA	2.25	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
8:H:30:TYR:CE2	19:a:5:ILE:HG22	2.31	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.65
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.27	0.65
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.65
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.65
18:Z:75:PHE:CD1	19:a:46:TYR:HE2	2.15	0.65
7:G:651:PRO:HG3	13:S:57:GLU:H	1.61	0.65
8:H:180:PRO:HD3	18:Z:43:LEU:HD21	1.79	0.65
10:P:156:SER:CB	10:P:161:VAL:CG2	2.66	0.65
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.62	0.65
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.78	0.65
10:P:363:SER:HB3	16:W:51:HIS:CD2	2.32	0.65
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.65
10:P:169:HIS:H	10:P:184:LYS:HE3	1.61	0.65
3:C:99:LEU:HD13	3:C:140:ILE:CD1	2.27	0.64
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.64
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.33	0.64
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64
12:R:38:TYR:HB2	12:R:45:ARG:HD3	1.79	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
18:Z:69:ILE:HD12	20:b:53:TYR:HA	1.78	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.79	0.64
16:W:115:THR:O	16:W:116:PRO:C	2.39	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.13	0.64
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.77	0.64
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.62	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.64
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.26	0.64
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.28	0.64
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.62	0.64
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.32	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
10:P:299:SER:CB	10:P:316:LYS:HE3	2.23	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.64
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.64
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.79	0.64
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.64
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.64
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.28	0.64
5:E:81:VAL:HB	5:E:104:LEU:HD11	1.79	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.80	0.64
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.64
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.63
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.80	0.63
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.63
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.63
18:Z:62:ILE:HG12	20:b:49:THR:HG22	1.79	0.63
1:A:54:LYS:HD2	1:A:113:TRP:HB2	1.79	0.63
2:B:122:ARG:HG2	26:B:302:UQ1:H102	1.81	0.63
4:D:90:ALA:O	4:D:91:ALA:HB3	1.96	0.63
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.78	0.63
4:D:348:LEU:O	18:Z:11:PRO:HB3	1.98	0.63
5:E:87:ARG:HD2	23:s:77:THR:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:449:PRO:HG3	7:G:483:ARG:HH22	1.62	0.63
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.34	0.63
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.63
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.63
1:A:99:SER:HB3	24:b:201:3PE:H392	1.81	0.63
4:D:88:HIS:NE2	8:H:205:SER:HA	2.14	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
10:P:93:HIS:NE2	10:P:94:LEU:HD11	2.14	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
4:D:375:MET:HE1	7:G:126:LEU:HA	1.80	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
13:S:19:ILE:CG1	13:S:95:LEU:HD11	2.26	0.63
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.63
4:D:142:VAL:HG13	4:D:207:ARG:NH1	2.14	0.63
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.63
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.81	0.63
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.60	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.63
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.63	0.63
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
10:P:132:ARG:HG2	31:P:401:NDP:C8A	2.29	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.63
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.63
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.63
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.28	0.63
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.64	0.62
8:H:1:MET:HE3	19:a:29:PHE:CD2	2.33	0.62
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.80	0.62
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.62
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.28	0.62
6:F:33:GLY:HA2	6:F:291:GLU:CB	2.16	0.62
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.62
16:W:83:ASP:O	16:W:86:VAL:HG22	1.99	0.62
17:X:53:PRO:O	17:X:57:LEU:HG	1.99	0.62
18:Z:65:LEU:HB3	20:b:50:PRO:O	1.99	0.62
6:F:48:ARG:HH11	6:F:48:ARG:HA	1.64	0.62
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.62
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.62
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.62
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.62
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62
34:a:101:CDL:H1	22:r:3:SER:HB2	1.81	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.62
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.81	0.62
7:G:176:CYS:SG	25:G:802:SF4:FE4	1.78	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	0.62
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.62
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.30	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.62
1:A:3:LEU:HD23	24:A:401:3PE:H251	1.80	0.62
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.35	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
6:F:299:LEU:CD1	6:F:300:ILE:HG13	2.30	0.62
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.62
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.82	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.62
9:I:78:PHE:HD1	19:a:2:TRP:CD1	2.17	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.81	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.61
10:P:169:HIS:H	10:P:184:LYS:CE	2.13	0.61
10:P:179:LYS:HA	10:P:182:ARG:HG2	1.82	0.61
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.61
4:D:89:PRO:HB2	8:H:204:GLU:CG	2.29	0.61
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.82	0.61
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.61
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.82	0.61
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.35	0.61
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.15	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
16:W:32:LYS:NZ	33:W:201:EHZ:C19	2.63	0.61
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.30	0.61
1:A:113:TRP:CE2	8:H:283:ASP:HB2	2.35	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.61
34:a:101:CDL:H311	21:q:7:LEU:HD23	1.82	0.61
20:b:8:PHE:C	20:b:9:LEU:HD12	2.25	0.61
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.61
1:A:51:PHE:CD1	4:D:102:SER:HB2	2.36	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.83	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	0.61
8:H:306:SER:HG	8:H:310:PHE:HE2	1.31	0.61
16:W:24:PHE:HB2	16:W:83:ASP:HB3	1.82	0.61
16:W:25:SER:HB2	16:W:31:ALA:HB2	1.83	0.61
18:Z:58:ARG:NH2	20:b:49:THR:HG21	2.15	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
6:F:426:ALA:HB3	29:F:501:FMN:HM81	1.81	0.61
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.61
11:Q:167:ASN:O	11:Q:168:LYS:CG	2.49	0.61
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.61
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.61
21:q:74:PHE:CD2	21:q:75:TRP:CD1	2.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:ARG:HH12	15:V:86:LYS:NZ	1.99	0.61
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.66	0.61
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.83	0.61
5:E:233:LEU:HD22	6:F:43:THR:HA	1.83	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.61
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.33	0.61
8:H:183:MET:HE2	27:I:302:PC1:H271	1.83	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.01	0.61
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.61
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.61
4:D:86:PRO:HG3	4:D:96:ARG:CG	2.30	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
16:W:97:ILE:HG23	16:W:98:LYS:HG3	1.82	0.61
19:a:3:PHE:CE2	34:a:101:CDL:HA4	2.36	0.61
3:C:186:ILE:HG13	3:C:187:LEU:HG	1.83	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.01	0.60
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.49	0.60
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
7:G:126:LEU:CD1	12:R:89:PRO:HB2	2.31	0.60
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.60
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.31	0.60
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.35	0.60
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.60
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.60
10:P:146:VAL:HG23	10:P:187:GLY:HA2	1.83	0.60
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.60
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.60
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.60
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.83	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
8:H:93:HIS:CD2	19:a:27:HIS:ND1	2.70	0.60
17:X:53:PRO:HD3	18:Z:116:TRP:CD1	2.36	0.60
1:A:54:LYS:HE3	1:A:55:PHE:CE1	2.37	0.60
1:A:113:TRP:O	1:A:113:TRP:CD1	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:CYS:SG	25:B:301:SF4:S2	2.99	0.60
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.15	0.60
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.60
16:W:58:THR:HB	16:W:61:GLN:HB2	1.83	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.32	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.60
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.37	0.60
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.60
22:r:12:ARG:HB3	22:r:20:LEU:HD21	1.84	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
9:I:80:GLU:OE2	22:r:26:LEU:HD11	2.01	0.60
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.15	0.60
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
8:H:311:THR:O	18:Z:51:MET:HG3	2.01	0.60
21:q:85:GLU:HG2	21:q:98:PRO:CB	2.31	0.60
21:q:86:TRP:HA	21:q:98:PRO:HG2	1.84	0.60
2:B:121:PHE:HE1	26:B:302:UQ1:C11	2.14	0.60
4:D:88:HIS:ND1	4:D:90:ALA:HB3	2.16	0.60
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.63	0.60
34:a:101:CDL:HA21	21:q:6:VAL:HG13	1.82	0.60
24:A:401:3PE:H2E1	24:A:401:3PE:H2I2	1.84	0.60
4:D:145:MET:HA	4:D:148:GLU:HG3	1.83	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
19:a:2:TRP:HH2	34:a:101:CDL:H522	1.67	0.60
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
7:G:304:GLU:OE2	10:P:41:ILE:HG12	2.01	0.60
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.60
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.60
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.37	0.60
16:W:122:LEU:HD11	16:W:126:TYR:CZ	2.37	0.60
17:X:16:GLU:CD	17:X:68:LEU:HD13	2.27	0.60
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.31	0.59
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.59
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.59
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.59
5:E:162:THR:CG2	5:E:166:LYS:HA	2.33	0.59
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.82	0.59
18:Z:61:LEU:HA	18:Z:64:ASP:OD2	2.02	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
9:I:63:TRP:CZ2	24:I:301:3PE:H331	2.37	0.59
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.59
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.59
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.37	0.59
4:D:345:GLU:HB2	18:Z:19:ILE:HD12	1.83	0.59
5:E:237:PRO:HG3	6:F:49:HIS:CD2	2.38	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.59
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.67	0.59
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.66	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
10:P:318:LYS:HG2	10:P:322:ILE:HD11	1.84	0.59
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.84	0.59
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.83	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.83	0.59
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.17	0.59
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.37	0.59
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	1.99	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.59
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.85	0.59
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.85	0.59
1:A:108:GLN:HG2	1:A:109:LYS:N	2.16	0.59
3:C:224:GLU:OE2	10:P:45:LYS:HB3	2.01	0.59
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.84	0.59
10:P:96:LEU:HD12	10:P:96:LEU:C	2.28	0.59
21:q:51:ASP:O	21:q:59:HIS:HB2	2.03	0.59
21:q:96:ASP:OD1	21:q:97:PRO:CD	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLU:CD	1:A:98:LEU:HG	2.28	0.59
5:E:190:ASN:HB3	5:E:192:TYR:CD2	2.36	0.59
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.84	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.59
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.59
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.59
8:H:1:MET:CE	19:a:29:PHE:CE2	2.85	0.59
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.38	0.59
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.86	0.58
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.58
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.58
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.58
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.18	0.58
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.85	0.58
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.85	0.58
18:Z:82:ARG:O	18:Z:86:ILE:HG13	2.03	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
5:E:165:ASP:C	5:E:167:LEU:H	2.09	0.58
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.32	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
6:F:382:CYS:SG	25:F:502:SF4:S1	3.02	0.58
8:H:175:LEU:HD21	27:I:302:PC1:H2C1	1.84	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
2:B:124:SER:HB3	2:B:125:PRO:HD2	1.84	0.58
3:C:130:ASN:HD21	3:C:141:ARG:HE	1.51	0.58
5:E:233:LEU:HD11	6:F:289:GLU:OE2	2.02	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.58
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.58
10:P:81:ILE:CD1	12:R:46:VAL:HG11	2.34	0.58
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.58
17:X:124:GLN:O	20:b:70:PRO:HB2	2.04	0.58
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.85	0.58
4:D:128:THR:H	4:D:131:GLN:NE2	2.01	0.58
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.52	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.84	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.58
16:W:67:ARG:HD3	16:W:71:MET:HG2	1.85	0.58
1:A:112:GLU:O	1:A:113:TRP:C	2.47	0.58
6:F:199:ARG:CD	23:s:80:PHE:CE2	2.79	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.86	0.58
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.85	0.58
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.58
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.39	0.58
16:W:42:TRP:CZ2	33:W:201:EHZ:O1	2.56	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58
8:H:85:LEU:CD2	8:H:108:THR:HB	2.33	0.58
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.58
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.58
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.58
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.58
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.58
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.58
16:W:25:SER:CB	16:W:31:ALA:HB2	2.34	0.58
2:B:153:PRO:HB2	2:B:155:PRO:HD2	1.85	0.57
2:B:154:GLU:O	10:P:89:TYR:OH	2.20	0.57
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.57
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.86	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.57
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.57
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	0.57
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.57
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.39	0.57
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.86	0.57
17:X:122:LEU:HD21	20:b:81:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASP:O	2:B:116:ARG:C	2.44	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.39	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.85	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.39	0.57
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.67	0.57
1:A:2:ASN:HB2	18:Z:143:TYR:HE1	1.69	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.57
8:H:318:MET:HG2	19:a:40:ARG:HH22	1.67	0.57
2:B:194:CYS:HB2	9:I:153:ILE:O	2.05	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.57
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
19:a:36:LYS:HA	19:a:59:ARG:NH2	2.19	0.57
19:a:43:TYR:CZ	19:a:47:LEU:HD11	2.40	0.57
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.36	0.57
21:q:65:THR:HG22	21:q:66:THR:N	2.20	0.57
27:B:303:PC1:H131	8:H:39:ILE:HD11	1.87	0.57
5:E:222:PHE:H	5:E:225:GLU:CD	2.13	0.57
10:P:315:THR:HG22	10:P:317:ASP:H	1.69	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.04	0.57
16:W:83:ASP:O	16:W:87:ILE:HG12	2.04	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.83	0.57
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.57
17:X:130:LYS:HE3	20:b:67:PRO:HB3	1.86	0.57
19:a:50:ARG:NH1	19:a:54:ILE:HD11	2.20	0.57
21:q:55:PHE:CG	22:r:26:LEU:HD22	2.40	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.40	0.57
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
17:X:48:TRP:CD1	20:b:55:VAL:HG13	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.35	0.57
2:B:110:PRO:HB3	8:H:33:LEU:O	2.04	0.57
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.57
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.57
16:W:101:LYS:HZ1	16:W:109:PHE:HE2	1.53	0.57
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
18:Z:131:GLU:O	18:Z:132:GLU:C	2.48	0.56
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.56
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.56
2:B:115:ASP:HA	2:B:119:VAL:O	2.05	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.56
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.37	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.89	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.40	0.56
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.56
2:B:81:LEU:HD22	27:B:303:PC1:H352	1.87	0.56
2:B:95:PHE:CZ	2:B:148:VAL:HB	2.27	0.56
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.86	0.56
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.30	0.56
8:H:202:GLU:HA	8:H:206:GLU:OE2	2.05	0.56
10:P:156:SER:CB	10:P:161:VAL:HG21	2.30	0.56
12:R:62:ASP:O	12:R:66:GLN:HG3	2.06	0.56
18:Z:70:ALA:O	18:Z:73:PRO:HD2	2.04	0.56
3:C:124:ARG:HD2	11:Q:140:LYS:HZ2	1.71	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
13:S:23:LEU:HD12	13:S:23:LEU:C	2.29	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.06	0.56
7:G:655:ARG:HH12	13:S:59:SER:N	2.03	0.56
9:I:54:THR:HG21	18:Z:33:TYR:CZ	2.40	0.56
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.56
10:P:323:HIS:ND1	10:P:323:HIS:O	2.39	0.56
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.56
7:G:399:VAL:CG2	7:G:462:PHE:CE1	2.87	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.41	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
8:H:69:SER:C	8:H:71:PHE:H	2.12	0.56
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.05	0.56
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.56
18:Z:122:GLY:O	18:Z:126:GLY:N	2.36	0.56
1:A:52:SER:C	1:A:54:LYS:H	2.11	0.56
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.71	0.56
2:B:173:TYR:O	3:C:203:LEU:HD22	2.05	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
7:G:399:VAL:HG22	7:G:462:PHE:HZ	1.68	0.56
12:R:38:TYR:OH	21:q:127:TYR:HB2	2.05	0.56
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.56
17:X:48:TRP:NE1	20:b:55:VAL:HG22	2.20	0.56
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
20:b:11:ASN:OD1	20:b:12:ALA:N	2.39	0.56
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.87	0.56
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.56
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.41	0.56
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.79	0.56
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
16:W:32:LYS:HZ3	33:W:201:EHZ:C19	2.19	0.56
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.55
3:C:167:ARG:HB3	3:C:186:ILE:HG23	1.86	0.55
4:D:88:HIS:CE1	8:H:205:SER:HA	2.41	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.55
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.41	0.55
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.88	0.55
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.72	0.55
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.88	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.55
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.55
16:W:24:PHE:HB2	16:W:83:ASP:CB	2.37	0.55
1:A:54:LYS:HG3	1:A:55:PHE:N	2.20	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	0.55
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.86	0.55
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.88	0.55
21:q:68:MET:HE1	21:q:81:MET:O	2.06	0.55
1:A:106:TRP:HZ3	20:b:19:LEU:HD21	1.71	0.55
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.88	0.55
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.31	0.55
18:Z:62:ILE:HD12	20:b:81:LEU:HD22	1.88	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.55
16:W:58:THR:HG22	16:W:60:LYS:N	2.21	0.55
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.07	0.55
4:D:80:MET:HG2	8:H:126:LYS:HD3	1.89	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.36	0.55
6:F:382:CYS:SG	25:F:502:SF4:S4	3.05	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.55
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.55
12:R:41:LYS:H	12:R:41:LYS:HD2	1.71	0.55
21:q:64:TYR:CE2	21:q:82:VAL:HG13	2.42	0.55
24:A:401:3PE:H322	24:A:401:3PE:H262	1.88	0.55
8:H:134:ARG:NH2	8:H:200:LEU:CD1	2.70	0.55
34:a:101:CDL:OB7	21:q:3:LEU:HD13	2.06	0.55
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.42	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.55
6:F:392:MET:CE	6:F:419:ILE:CD1	2.60	0.55
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.55
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.72	0.55
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.55
8:H:123:SER:HB3	8:H:214:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.87	0.55
17:X:55:ARG:HB3	17:X:135:ARG:HH22	1.72	0.55
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.55
4:D:79:ASN:HB3	4:D:101:LEU:C	2.32	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.55
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.55
10:P:237:LYS:HE3	10:P:322:ILE:O	2.07	0.55
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.55
1:A:52:SER:C	1:A:54:LYS:N	2.62	0.55
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.70	0.55
3:C:186:ILE:O	4:D:113:ILE:HG13	2.07	0.55
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.55
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.55
10:P:98:GLY:HA3	10:P:103:LEU:HG	1.87	0.55
10:P:236:VAL:HG13	10:P:270:ARG:HH21	1.71	0.55
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.72	0.55
12:R:48:PHE:CD2	12:R:53:LYS:HB2	2.42	0.55
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.54
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
7:G:655:ARG:HH12	13:S:59:SER:H	1.56	0.54
10:P:357:ARG:HB2	10:P:362:LEU:HD23	1.89	0.54
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.54
17:X:22:SER:HB2	19:a:47:LEU:HD23	1.89	0.54
1:A:52:SER:HB3	1:A:54:LYS:HG2	1.88	0.54
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.54
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.54
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.90	0.54
4:D:253:LEU:HD11	22:r:18:GLN:HG3	1.90	0.54
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
2:B:93:MET:HE2	2:B:95:PHE:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
10:P:71:ASN:HA	10:P:97:MET:SD	2.47	0.54
12:R:32:THR:OG1	12:R:33:HIS:N	2.39	0.54
23:s:85:LEU:O	23:s:85:LEU:HD23	2.07	0.54
1:A:2:ASN:HB2	18:Z:143:TYR:CE1	2.41	0.54
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.07	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
9:I:123:CYS:SG	25:I:303:SF4:S3	3.06	0.54
1:A:54:LYS:CG	1:A:55:PHE:N	2.71	0.54
1:A:95:VAL:HG11	8:H:302:MET:CG	2.38	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	2.26	0.54
13:S:44:LEU:HD13	13:S:91:MET:HG2	1.88	0.54
16:W:23:ILE:HG22	16:W:24:PHE:CD2	2.42	0.54
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.54
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.54
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.90	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.54
17:X:130:LYS:CE	20:b:67:PRO:HB3	2.38	0.54
1:A:1:MET:O	1:A:2:ASN:C	2.49	0.54
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.90	0.54
5:E:162:THR:HG22	5:E:166:LYS:HA	1.89	0.54
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.48	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.54
13:S:25:GLN:HG2	13:S:57:GLU:HG2	1.89	0.54
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.73	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.90	0.54
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.43	0.54
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.89	0.54
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.90	0.54
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.54
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.54
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.54
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.54
1:A:72:LEU:HB3	8:H:151:LEU:HD21	1.90	0.54
5:E:187:ILE:O	5:E:188:ASN:C	2.48	0.54
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	0.54
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.54
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.90	0.54
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.54
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.54
9:I:109:GLY:O	12:R:63:LEU:HD12	2.08	0.54
16:W:58:THR:HG22	16:W:60:LYS:H	1.72	0.54
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.53
4:D:92:HIS:H	4:D:458:PHE:HE2	1.57	0.53
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.53
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.44	0.53
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.38	0.53
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.53
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.38	0.53
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.53
18:Z:62:ILE:HG23	20:b:50:PRO:HD3	1.89	0.53
20:b:59:ASP:HA	20:b:63:MET:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.56	0.53
4:D:92:HIS:HB2	4:D:458:PHE:CE2	2.44	0.53
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
10:P:58:VAL:O	10:P:83:PRO:HD2	2.09	0.53
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.53
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.53
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.53
7:G:35:PHE:HB2	7:G:101:ASN:HA	1.90	0.53
7:G:36:VAL:O	7:G:39:GLN:HG2	2.08	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	0.53
10:P:122:HIS:CB	12:R:46:VAL:HG22	2.39	0.53
10:P:262:THR:N	10:P:332:LEU:HD12	2.23	0.53
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.53
5:E:131:ILE:HG13	5:E:187:ILE:HG12	1.89	0.53
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.53
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.53
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.53
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.53
14:T:87:LEU:HD23	14:T:122:MET:HE1	1.91	0.53
21:q:95:ASP:OD1	21:q:96:ASP:N	2.41	0.53
1:A:61:THR:CG2	8:H:290:TRP:CZ3	2.91	0.53
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.24	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.90	0.53
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
6:F:199:ARG:HD3	23:s:80:PHE:CD2	2.41	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.53
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.53
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.74	0.53
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.53
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.74	0.53
5:E:165:ASP:C	5:E:167:LEU:N	2.64	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
9:I:54:THR:HA	20:b:13:TRP:HE1	1.73	0.53
9:I:62:MET:SD	18:Z:35:MET:HG2	2.49	0.53
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.90	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.53
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.53
3:C:234:LEU:O	4:D:387:GLU:HG3	2.08	0.53
4:D:368:ARG:HA	4:D:371:MET:HG2	1.89	0.53
5:E:226:PRO:HD3	6:F:46:TYR:CZ	2.44	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.53
19:a:51:ASP:HA	19:a:54:ILE:HD12	1.91	0.53
1:A:54:LYS:HD2	1:A:113:TRP:CB	2.38	0.53
4:D:101:LEU:HD12	4:D:106:VAL:HA	1.91	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.21	0.53
5:E:81:VAL:CB	5:E:104:LEU:HD11	2.38	0.53
6:F:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
12:R:69:VAL:HG12	12:R:112:LYS:N	2.24	0.53
12:R:98:GLU:HA	12:R:113:GLN:CD	2.33	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
2:B:138:THR:HG21	4:D:116:LEU:HA	1.91	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.53
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.53
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.53
4:D:145:MET:O	4:D:148:GLU:N	2.41	0.52
4:D:170:ILE:HG21	4:D:232:VAL:HG21	1.91	0.52
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.52
10:P:179:LYS:O	10:P:182:ARG:HG2	2.10	0.52
10:P:203:PRO:HG2	31:P:401:NDP:C6N	2.37	0.52
10:P:206:ILE:HG13	31:P:401:NDP:H42N	1.89	0.52
18:Z:68:ARG:O	18:Z:69:ILE:C	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.52
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.45	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
6:F:300:ILE:CG2	6:F:305:GLY:O	2.45	0.52
6:F:392:MET:HE1	6:F:419:ILE:HD12	1.79	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.52
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
10:P:85:ARG:HE	31:P:401:NDP:C2A	2.22	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.52
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.52
4:D:198:THR:OG1	4:D:261:MET:HE1	2.10	0.52
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.52
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.92	0.52
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.52
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.52
10:P:153:ALA:CB	10:P:191:VAL:HG23	2.39	0.52
10:P:305:PHE:CG	10:P:314:THR:HG22	2.45	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
6:F:299:LEU:HD12	6:F:300:ILE:HG13	1.91	0.52
7:G:126:LEU:HD13	12:R:89:PRO:HB3	1.90	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
8:H:307:LEU:HD11	18:Z:47:TYR:CG	2.45	0.52
9:I:80:GLU:OE2	22:r:26:LEU:HD13	2.08	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
17:X:35:GLN:HB2	17:X:70:PHE:CE1	2.44	0.52
18:Z:65:LEU:O	18:Z:69:ILE:HG12	2.09	0.52
19:a:1:MET:HG3	34:a:101:CDL:HB21	1.92	0.52
20:b:66:VAL:HG11	20:b:70:PRO:HA	1.92	0.52
21:q:68:MET:SD	21:q:81:MET:CB	2.95	0.52
23:s:85:LEU:HA	23:s:88:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:O	1:A:20:VAL:C	2.51	0.52
2:B:170:TYR:OH	4:D:131:GLN:O	2.28	0.52
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.91	0.52
3:C:104:ASN:O	22:r:97:PRO:HD3	2.09	0.52
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.52
6:F:296:LEU:HD22	6:F:337:MET:CE	2.39	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
8:H:135:ALA:HB2	8:H:201:THR:OG1	2.09	0.52
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.52
12:R:45:ARG:HD2	12:R:48:PHE:CD1	2.44	0.52
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.51	0.52
19:a:7:PRO:HD3	34:a:101:CDL:H181	1.91	0.52
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.52
4:D:99:LEU:HD12	4:D:99:LEU:O	2.10	0.52
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.52
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.91	0.52
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.23	0.52
7:G:35:PHE:CE1	7:G:40:SER:HB2	2.45	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.52
13:S:16:LEU:O	13:S:16:LEU:CD1	2.51	0.52
16:W:94:GLN:HA	16:W:97:ILE:HG22	1.92	0.52
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.52
2:B:194:CYS:O	25:B:301:SF4:S2	2.67	0.52
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.34	0.52
5:E:87:ARG:HD2	23:s:77:THR:CG2	2.40	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.92	0.52
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.52
8:H:134:ARG:CZ	8:H:200:LEU:HD13	2.39	0.52
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
18:Z:94:GLU:HA	18:Z:97:ILE:CG1	2.39	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.52
1:A:54:LYS:CD	1:A:113:TRP:HB2	2.39	0.52
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.90	0.52
5:E:196:THR:O	5:E:200:ILE:HD12	2.10	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
21:q:138:VAL:HG23	21:q:139:PRO:HD2	1.92	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.92	0.52
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.52
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.91	0.52
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.52
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.52
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.52
9:I:155:CYS:SG	25:I:303:SF4:S2	3.08	0.52
20:b:7:ALA:C	20:b:9:LEU:N	2.68	0.52
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.92	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.91	0.51
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.51
21:q:29:ARG:HD3	21:q:74:PHE:CD1	2.44	0.51
2:B:126:ARG:NH1	8:H:61:MET:SD	2.83	0.51
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.75	0.51
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.51
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.27	0.51
18:Z:99:LYS:HG3	18:Z:100:ASP:N	2.25	0.51
1:A:106:TRP:CZ3	20:b:19:LEU:HD21	2.45	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.46	0.51
7:G:31:LEU:HB3	7:G:42:MET:HE2	1.93	0.51
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.99	0.51
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.51
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.51
8:H:280:PHE:HD2	8:H:284:GLN:CG	2.23	0.51
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.51
18:Z:62:ILE:HG23	20:b:50:PRO:CD	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.51
2:B:87:ARG:HH11	27:B:303:PC1:P	2.34	0.51
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.43	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.51
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
7:G:126:LEU:HD11	12:R:89:PRO:HB3	1.91	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
16:W:71:MET:O	16:W:72:LYS:C	2.51	0.51
20:b:23:PHE:CB	24:b:201:3PE:H2D2	2.37	0.51
1:A:21:ALA:HB2	8:H:218:GLY:HA3	1.91	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.51
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.29	0.51
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.51
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
8:H:212:ASN:HA	8:H:215:TYR:HB2	1.92	0.51
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.51
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.93	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.46	0.51
3:C:84:GLU:CG	3:C:141:ARG:HH11	2.23	0.51
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.51
9:I:48:VAL:O	20:b:10:LYS:NZ	2.42	0.51
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.51
14:T:87:LEU:HD23	14:T:122:MET:CE	2.40	0.51
18:Z:81:ARG:HG3	18:Z:82:ARG:N	2.25	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
6:F:296:LEU:CD1	6:F:337:MET:HE3	2.34	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.51
8:H:200:LEU:HD12	8:H:200:LEU:C	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.51
10:P:172:ALA:H	10:P:202:ARG:NH2	2.08	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
13:S:16:LEU:HD21	13:S:95:LEU:CD1	2.41	0.51
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.51
17:X:78:CYS:C	17:X:81:PRO:HD2	2.36	0.51
18:Z:80:ASP:O	18:Z:84:LEU:HG	2.11	0.51
18:Z:93:GLU:O	18:Z:97:ILE:HG12	2.11	0.51
4:D:271:ARG:CD	8:H:279:ARG:O	2.56	0.51
4:D:279:THR:HA	15:V:12:VAL:HG13	1.93	0.51
6:F:259:GLY:O	6:F:263:ALA:N	2.41	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.51
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.51
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.91	0.51
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.51
6:F:42:PHE:CD1	6:F:137:LYS:HD2	2.46	0.51
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
16:W:28:LEU:HG	16:W:32:LYS:HE2	1.93	0.51
17:X:44:MET:SD	18:Z:73:PRO:HA	2.51	0.51
1:A:57:LEU:O	1:A:58:VAL:C	2.54	0.50
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.76	0.50
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.50
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.50
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
10:P:65:LEU:HD23	10:P:129:LEU:HD22	1.93	0.50
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.50
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.50
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.50
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.50
17:X:141:PRO:HG2	17:X:142:TYR:HD1	1.75	0.50
18:Z:121:ILE:HG23	18:Z:122:GLY:N	2.26	0.50
18:Z:130:LYS:O	18:Z:131:GLU:C	2.52	0.50
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.93	0.50
5:E:75:ALA:O	5:E:78:VAL:HG22	2.11	0.50
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.50
27:H:402:PC1:H3B1	27:H:402:PC1:H261	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.50
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.50
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.50
10:P:374:THR:HG23	10:P:374:THR:O	2.10	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
13:S:54:LEU:HD22	13:S:56:ARG:NH1	2.25	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
20:b:20:VAL:HG22	24:b:201:3PE:H282	1.92	0.50
23:s:85:LEU:HD23	23:s:85:LEU:C	2.36	0.50
4:D:90:ALA:O	4:D:91:ALA:CB	2.59	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
8:H:222:LEU:O	8:H:223:PHE:C	2.51	0.50
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.50
12:R:55:VAL:HG22	12:R:56:ASN:H	1.77	0.50
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.50
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.50
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.26	0.50
22:r:6:ARG:HG2	22:r:6:ARG:O	2.11	0.50
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.50
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.46	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
13:S:21:VAL:CG2	13:S:91:MET:HE1	2.41	0.50
16:W:97:ILE:C	16:W:99:VAL:H	2.18	0.50
17:X:48:TRP:CD1	20:b:55:VAL:HG22	2.46	0.50
19:a:37:ARG:CB	19:a:48:MET:CE	2.90	0.50
1:A:108:GLN:CG	1:A:109:LYS:H	2.18	0.50
1:A:109:LYS:O	1:A:109:LYS:HG2	2.12	0.50
3:C:186:ILE:HG13	3:C:187:LEU:N	2.27	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.93	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.50
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.50
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
10:P:205:ASP:OD1	10:P:205:ASP:O	2.30	0.50
10:P:315:THR:HB	10:P:318:LYS:HB2	1.92	0.50
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.50
19:a:1:MET:HG3	34:a:101:CDL:CB2	2.41	0.50
1:A:1:MET:O	1:A:4:TYR:N	2.45	0.50
2:B:116:ARG:NH2	2:B:117:PHE:CZ	2.79	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.50
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.50
5:E:39:VAL:HG11	7:G:163:LYS:HZ2	1.77	0.50
5:E:199:ASP:O	5:E:202:GLU:HB3	2.11	0.50
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.50
6:F:225:LEU:N	11:Q:160:TYR:HE2	2.07	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
12:R:32:THR:HA	12:R:59:PHE:CZ	2.46	0.50
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.50
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.50
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.27	0.50
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.50
4:D:304:LYS:HE2	9:I:35:THR:N	2.26	0.50
4:D:460:GLU:O	4:D:463:ARG:HG2	2.11	0.50
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.93	0.50
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.50
6:F:225:LEU:HB3	6:F:227:PRO:CD	2.37	0.50
7:G:401:LEU:HD23	7:G:496:MET:HE1	1.92	0.50
8:H:93:HIS:CE1	19:a:24:ALA:CA	2.89	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.50
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.50
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.50
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.50
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.94	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
8:H:66:THR:O	27:H:402:PC1:H153	2.12	0.50
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.50
18:Z:102:PRO:O	18:Z:103:ASN:C	2.53	0.50
1:A:102:LEU:HD11	1:A:106:TRP:HE1	1.77	0.49
2:B:126:ARG:NH2	2:B:151:GLN:HG2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.49
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.47	0.49
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.49
8:H:30:TYR:CE2	19:a:5:ILE:HG23	2.46	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
10:P:70:VAL:HG12	10:P:97:MET:SD	2.52	0.49
2:B:94:THR:CG2	2:B:104:MET:SD	3.00	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
3:C:241:PHE:H	7:G:146:PHE:HE1	1.59	0.49
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.27	0.49
5:E:78:VAL:CG1	5:E:104:LEU:HD13	2.42	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.48	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.92	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
10:P:122:HIS:HB2	12:R:46:VAL:HG22	1.94	0.49
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.49
10:P:359:TYR:CD1	10:P:360:ARG:N	2.80	0.49
18:Z:140:PHE:O	18:Z:141:THR:C	2.56	0.49
1:A:103:ALA:O	1:A:107:THR:HG23	2.12	0.49
2:B:68:ARG:HD3	2:B:70:ARG:CG	2.41	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
6:F:185:ASN:HA	6:F:189:SER:O	2.12	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.94	0.49
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.49
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.94	0.49
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.49
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.49
17:X:48:TRP:HD1	20:b:55:VAL:HG13	1.77	0.49
19:a:51:ASP:O	19:a:54:ILE:HB	2.11	0.49
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.49
4:D:198:THR:HA	8:H:32:GLN:HG2	1.94	0.49
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.13	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
8:H:273:ILE:HD11	24:I:301:3PE:H2A1	1.93	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.48	0.49
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
4:D:79:ASN:O	4:D:80:MET:C	2.53	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:137:ASP:OD1	4:D:148:GLU:HG2	2.11	0.49
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.95	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.49
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.75	0.49
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.95	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.49
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.49
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.42	0.49
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.12	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
11:Q:64:LEU:HG	16:W:84:LEU:HD22	1.94	0.49
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.49
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.49
1:A:51:PHE:CD2	4:D:103:GLY:HA3	2.47	0.49
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.49
2:B:164:CYS:SG	25:B:301:SF4:S4	3.10	0.49
4:D:96:ARG:HG3	4:D:115:LEU:HD21	1.95	0.49
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.49
6:F:163:TYR:CE1	23:s:80:PHE:HB3	2.48	0.49
6:F:379:CYS:SG	25:F:502:SF4:S1	3.11	0.49
8:H:203:GLY:C	8:H:205:SER:H	2.19	0.49
9:I:49:ASP:O	9:I:50:MET:C	2.55	0.49
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.48	0.49
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.49
10:P:315:THR:HB	10:P:318:LYS:H	1.78	0.49
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.49
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.47	0.49
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.94	0.49
26:B:302:UQ1:CM2	4:D:189:THR:HG21	2.43	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.13	0.49
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.42	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.96	0.49
6:F:299:LEU:HD11	6:F:300:ILE:HG13	1.93	0.49
7:G:179:CYS:HG	25:G:802:SF4:FE3	1.28	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
8:H:187:ILE:CD1	24:I:301:3PE:H242	2.41	0.49
10:P:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.49
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.13	0.49
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.49
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.49
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.49
5:E:137:THR:HG22	6:F:370:LEU:HD21	1.95	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.73	0.49
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.49
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.48
2:B:96:GLY:HA3	26:B:302:UQ1:O4	2.13	0.48
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.48	0.48
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.48
4:D:92:HIS:HB2	4:D:458:PHE:HD2	1.78	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.48
10:P:318:LYS:O	10:P:322:ILE:HG13	2.13	0.48
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.48
18:Z:72:MET:O	18:Z:73:PRO:C	2.56	0.48
2:B:68:ARG:HG2	2:B:69:SER:N	2.28	0.48
2:B:175:TYR:OH	4:D:117:HIS:HE1	1.96	0.48
4:D:88:HIS:HE2	8:H:205:SER:HA	1.77	0.48
5:E:81:VAL:HG21	5:E:104:LEU:HD21	1.94	0.48
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.48
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.94	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.48
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.48
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.48
12:R:32:THR:HA	12:R:59:PHE:HZ	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.48
3:C:75:VAL:HG22	3:C:85:ILE:HG23	1.94	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.38	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.95	0.48
10:P:228:LEU:HD11	10:P:288:PHE:HZ	1.78	0.48
12:R:31:ILE:HD11	12:R:37:VAL:HG23	1.95	0.48
16:W:122:LEU:HD11	16:W:126:TYR:CE2	2.47	0.48
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.48
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
6:F:46:TYR:O	6:F:48:ARG:HG2	2.13	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.48
8:H:66:THR:HA	8:H:124:ASN:OD1	2.13	0.48
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.48
16:W:32:LYS:HG2	33:W:201:EHZ:C19	2.44	0.48
16:W:42:TRP:O	16:W:43:TYR:C	2.55	0.48
18:Z:89:GLU:HG2	18:Z:128:ARG:NH1	2.27	0.48
20:b:23:PHE:HD1	24:b:201:3PE:H3B2	1.77	0.48
20:b:26:TRP:CZ3	24:b:201:3PE:H2G2	2.48	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
3:C:107:PHE:CE2	3:C:140:ILE:HD13	2.48	0.48
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.48
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
13:S:31:GLN:CD	13:S:34:ARG:NH2	2.71	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
20:b:19:LEU:HD21	24:b:201:3PE:H332	1.95	0.48
22:r:12:ARG:HE	22:r:20:LEU:HD21	1.78	0.48
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
8:H:93:HIS:HE1	19:a:24:ALA:CA	2.25	0.48
8:H:300:LEU:HD23	20:b:25:VAL:HG11	1.96	0.48
10:P:318:LYS:HA	10:P:321:ARG:HH12	1.78	0.48
12:R:43:TYR:CD1	12:R:44:ARG:HB2	2.49	0.48
1:A:49:LEU:HD23	4:D:80:MET:CB	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TRP:CE3	24:b:201:3PE:H331	2.48	0.48
2:B:96:GLY:HA3	26:B:302:UQ1:HM52	1.96	0.48
3:C:131:LEU:O	3:C:139:ARG:HG3	2.12	0.48
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.44	0.48
4:D:375:MET:HE1	7:G:126:LEU:CA	2.43	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.48
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.48
6:F:226:LYS:O	6:F:227:PRO:C	2.56	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.44	0.48
8:H:296:LEU:HD21	24:I:301:3PE:H351	1.95	0.48
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.48
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.96	0.48
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.48
19:a:3:PHE:CZ	34:a:101:CDL:HA4	2.49	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
5:E:45:GLU:H	5:E:45:GLU:CD	2.21	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.48
6:F:296:LEU:HD13	6:F:337:MET:CE	2.34	0.48
6:F:297:LYS:HB2	6:F:333:GLU:HB3	1.95	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
10:P:79:GLN:NE2	10:P:102:GLN:O	2.47	0.48
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.96	0.48
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.95	0.48
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.78	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
3:C:149:LEU:CD1	16:W:80:ARG:HH21	2.19	0.48
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.73	0.48
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.49	0.48
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	0.48
2:B:121:PHE:CD1	2:B:121:PHE:C	2.89	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
10:P:335:LEU:O	10:P:336:GLU:HB2	2.14	0.48
12:R:79:CYS:O	12:R:88:HIS:CE1	2.67	0.48
14:T:82:ARG:NH1	14:T:126:PHE:HA	2.29	0.48
21:q:23:LEU:HD11	21:q:33:ILE:HG12	1.96	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.47
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.49	0.47
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.47
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.47
3:C:73:GLN:O	3:C:74:GLN:C	2.57	0.47
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.28	0.47
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.47
6:F:233:VAL:HG11	11:Q:164:PHE:HB2	1.95	0.47
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.14	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.47
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.48	0.47
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.47
20:b:68:SER:O	20:b:69:HIS:C	2.56	0.47
21:q:68:MET:SD	21:q:81:MET:HG2	2.55	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	0.47
12:R:32:THR:O	12:R:33:HIS:C	2.57	0.47
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.44	0.47
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.14	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
10:P:108:TRP:CZ2	31:P:401:NDP:H2A	2.49	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
17:X:69:ASN:OD1	17:X:70:PHE:N	2.47	0.47
19:a:3:PHE:HE2	34:a:101:CDL:HA4	1.77	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
2:B:127:GLN:NE2	8:H:215:TYR:O	2.47	0.47
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.49	0.47
6:F:254:ILE:O	6:F:258:GLY:N	2.48	0.47
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.95	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
34:a:101:CDL:HA21	21:q:6:VAL:CG1	2.44	0.47
2:B:95:PHE:CE1	2:B:131:MET:HE2	2.40	0.47
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.12	0.47
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.47
4:D:142:VAL:HG13	4:D:207:ARG:HH12	1.78	0.47
5:E:70:PRO:HG2	6:F:236:PHE:CE2	2.50	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:82:ILE:HG21	7:G:100:TRP:HB3	1.96	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.47
7:G:401:LEU:HD23	7:G:496:MET:CE	2.43	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:1:MET:CB	19:a:30:THR:HG21	2.45	0.47
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.47
14:T:132:ASP:HB3	16:W:40:ARG:HH12	1.78	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.47
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.47
4:D:381:HIS:HE1	9:I:161:ALA:O	1.98	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
6:F:166:ALA:HB1	23:s:80:PHE:CD1	2.50	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:217:GLU:CD	6:F:224:ARG:HH22	2.23	0.47
6:F:425:CYS:SG	25:F:502:SF4:S4	3.13	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.47
9:I:188:GLU:OE1	12:R:56:ASN:CB	2.63	0.47
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.47
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.48	0.47
13:S:16:LEU:HD21	13:S:95:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:116:ILE:O	15:V:116:ILE:CG2	2.61	0.47
16:W:29:ASN:O	16:W:29:ASN:OD1	2.33	0.47
16:W:113:THR:O	16:W:113:THR:HG22	2.15	0.47
17:X:36:CYS:O	17:X:39:THR:HG22	2.15	0.47
17:X:139:GLU:CD	17:X:139:GLU:H	2.22	0.47
19:a:43:TYR:CE1	19:a:47:LEU:HD11	2.50	0.47
20:b:23:PHE:CD1	24:b:201:3PE:H3B2	2.50	0.47
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.50	0.47
23:s:76:ASN:HB3	23:s:79:THR:HB	1.96	0.47
1:A:58:VAL:CG2	8:H:286:MET:HE1	2.45	0.47
2:B:135:GLY:HA2	25:B:301:SF4:S3	2.54	0.47
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
9:I:68:ARG:HH22	18:Z:26:PRO:HD2	1.78	0.47
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.47
19:a:22:SER:O	19:a:23:THR:C	2.57	0.47
20:b:16:GLU:CD	24:b:201:3PE:H12	2.39	0.47
21:q:76:ASP:OD1	21:q:76:ASP:C	2.57	0.47
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.47
1:A:63:LEU:O	1:A:67:LEU:HG	2.14	0.47
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.47
4:D:254:ARG:HH11	22:r:25:GLN:HB2	1.80	0.47
5:E:191:TYR:O	5:E:192:TYR:C	2.58	0.47
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.47
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.47
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
8:H:306:SER:OG	20:b:33:PRO:HG3	2.15	0.47
27:H:402:PC1:O14	27:H:402:PC1:H122	2.15	0.47
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.47
10:P:237:LYS:HZ2	10:P:322:ILE:HG23	1.79	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
20:b:69:HIS:CD2	20:b:71:GLN:H	2.33	0.47
1:A:54:LYS:O	1:A:55:PHE:C	2.58	0.47
3:C:67:ILE:HD11	15:V:47:TYR:CD2	2.50	0.47
8:H:310:PHE:O	20:b:38:TYR:HB2	2.15	0.47
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.47
12:R:47:ARG:HG3	12:R:48:PHE:CD1	2.51	0.47
12:R:54:GLU:HB2	21:q:124:TYR:CD1	2.51	0.47
17:X:120:PRO:CB	17:X:125:LEU:CD1	2.91	0.47
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:LYS:O	2:B:143:PRO:HD2	2.14	0.46
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.48	0.46
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.46
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.46
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.46
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.46
8:H:249:ILE:HD13	17:X:99:HIS:CG	2.50	0.46
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.46
15:V:56:LEU:HD12	15:V:57:ASP:CA	2.44	0.46
16:W:58:THR:HB	16:W:61:GLN:HB3	1.94	0.46
21:q:137:TRP:CH2	21:q:140:PRO:HD3	2.50	0.46
24:A:401:3PE:H262	24:A:401:3PE:C32	2.45	0.46
4:D:359:ASP:O	7:G:150:ARG:NH2	2.48	0.46
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.46
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.46
10:P:318:LYS:O	10:P:319:VAL:C	2.58	0.46
15:V:50:GLN:HE22	22:r:94:ALA:H	1.63	0.46
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.46
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
2:B:93:MET:HE3	4:D:87:GLN:HE21	1.79	0.46
5:E:78:VAL:HG12	5:E:104:LEU:CD1	2.44	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:249:ILE:HG21	17:X:99:HIS:CE1	2.50	0.46
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.46
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.16	0.46
18:Z:99:LYS:HB2	18:Z:99:LYS:HE3	1.77	0.46
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.96	0.46
2:B:174:SER:HA	3:C:203:LEU:CD2	2.46	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
4:D:142:VAL:HG21	4:D:185:MET:HG2	1.98	0.46
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.46
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.46
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.46
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.39	0.46
5:E:221:ARG:HB2	5:E:225:GLU:HG2	1.97	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:201:THR:O	8:H:202:GLU:C	2.58	0.46
8:H:307:LEU:HD11	18:Z:47:TYR:CD1	2.50	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
10:P:153:ALA:HB3	10:P:194:VAL:CG2	2.46	0.46
17:X:35:GLN:O	17:X:36:CYS:CB	2.64	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.46
34:a:101:CDL:H141	34:a:101:CDL:H321	1.97	0.46
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.80	0.46
5:E:62:ILE:HD12	5:E:81:VAL:HG13	1.97	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.98	0.46
5:E:143:ASP:O	5:E:146:SER:N	2.49	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
15:V:72:LEU:C	15:V:72:LEU:CD1	2.89	0.46
17:X:4:ILE:HG22	17:X:5:VAL:N	2.25	0.46
3:C:132:LEU:HD11	4:D:300:TRP:CZ2	2.50	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
6:F:224:ARG:HD3	11:Q:164:PHE:CE1	2.51	0.46
8:H:200:LEU:CD2	8:H:282:TYR:HD1	2.28	0.46
8:H:312:ALA:CB	20:b:38:TYR:HB3	2.44	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.46
17:X:133:THR:HG23	20:b:58:ARG:HH12	1.81	0.46
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.46
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.50	0.46
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.46
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.46
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.46
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
7:G:35:PHE:O	7:G:101:ASN:HA	2.16	0.46
7:G:655:ARG:NH1	13:S:59:SER:H	2.14	0.46
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.46
13:S:25:GLN:NE2	13:S:34:ARG:HH11	2.13	0.46
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.46
16:W:99:VAL:HG13	16:W:99:VAL:O	2.15	0.46
17:X:107:PHE:O	17:X:110:CYS:SG	2.73	0.46
19:a:45:TRP:O	19:a:46:TYR:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.46
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.97	0.46
5:E:136:THR:HB	28:E:301:FES:S2	2.56	0.46
7:G:275:PRO:HB2	11:Q:86:ASN:ND2	2.30	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.46
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	0.46
20:b:19:LEU:CD2	24:b:201:3PE:H332	2.46	0.46
21:q:14:VAL:HA	21:q:23:LEU:HD22	1.98	0.46
4:D:338:ARG:NH1	18:Z:23:ARG:HA	2.31	0.46
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.51	0.46
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.16	0.46
7:G:35:PHE:CE1	7:G:40:SER:CB	2.99	0.46
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.46
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
24:I:301:3PE:H241	24:I:301:3PE:H272	1.60	0.46
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.46
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.46	0.46
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.46
1:A:106:TRP:CH2	8:H:291:LYS:HA	2.51	0.46
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.81	0.46
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.46
5:E:73:HIS:ND1	11:Q:166:TRP:CE3	2.84	0.46
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.46
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.46
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.46
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.46
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.46
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.46
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.98	0.46
9:I:60:ILE:CG2	24:I:301:3PE:H111	2.46	0.46
10:P:66:GLY:O	10:P:69:VAL:N	2.48	0.46
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.46
12:R:54:GLU:HB2	21:q:124:TYR:HD1	1.81	0.46
20:b:38:TYR:O	20:b:39:THR:C	2.59	0.46
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.51	0.45
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.45
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.45
5:E:245:GLN:HB3	6:F:256:ARG:O	2.16	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.30	0.45
7:G:32:ILE:HD11	7:G:45:PRO:HG3	1.98	0.45
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.45
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.45
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.45
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45
17:X:37:ASP:OD2	20:b:70:PRO:HD3	2.16	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.84	0.45
4:D:79:ASN:O	4:D:101:LEU:N	2.49	0.45
5:E:69:TYR:HE2	5:E:80:PRO:HG2	1.81	0.45
6:F:300:ILE:HD13	6:F:307:VAL:HG22	1.96	0.45
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.31	0.45
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.45
8:H:30:TYR:HE2	19:a:5:ILE:CG2	2.16	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.50	0.45
8:H:292:ASN:HD21	24:I:301:3PE:HN2	1.63	0.45
8:H:302:MET:SD	20:b:26:TRP:CD1	3.09	0.45
9:I:53:ALA:O	9:I:54:THR:C	2.56	0.45
9:I:123:CYS:SG	25:I:303:SF4:S4	3.13	0.45
16:W:42:TRP:CZ2	16:W:93:LEU:HB2	2.51	0.45
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.45
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.98	0.45
3:C:100:ARG:NH1	15:V:86:LYS:NZ	2.64	0.45
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	3.05	0.45
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.45
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.47	0.45
7:G:176:CYS:SG	25:G:802:SF4:S1	3.14	0.45
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.16	0.45
21:q:98:PRO:O	21:q:99:THR:C	2.59	0.45
2:B:126:ARG:HG3	8:H:213:VAL:O	2.17	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
7:G:35:PHE:CD1	7:G:40:SER:HB2	2.51	0.45
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.45
13:S:31:GLN:OE1	13:S:34:ARG:NH2	2.49	0.45
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.45
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.45
19:a:45:TRP:O	19:a:48:MET:N	2.50	0.45
2:B:91:TRP:HA	2:B:120:VAL:HG12	1.99	0.45
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.45
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.45
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.45
8:H:140:ILE:HG13	8:H:141:SER:N	2.30	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.45
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.45
16:W:32:LYS:HZ2	33:W:201:EHZ:C19	2.28	0.45
34:a:101:CDL:H321	34:a:101:CDL:C14	2.46	0.45
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.98	0.45
21:q:85:GLU:CG	21:q:98:PRO:HB3	2.36	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
9:I:61:LEU:O	24:I:301:3PE:H332	2.15	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.82	0.45
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.45
13:S:44:LEU:CD1	13:S:91:MET:HG2	2.45	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.97	0.45
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.52	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.45
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.45
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
2:B:94:THR:HG21	2:B:104:MET:SD	2.57	0.45
4:D:266:ARG:NH2	9:I:59:ARG:O	2.50	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45
8:H:224:PHE:CE2	30:H:401:UQ9:C14	3.00	0.45
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.45
14:T:90:TYR:O	14:T:91:ASP:HB2	2.17	0.45
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.45
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.99	0.45
2:B:94:THR:OG1	26:B:302:UQ1:H72	2.17	0.45
4:D:198:THR:HG21	8:H:275:ALA:HB1	1.99	0.45
5:E:52:PHE:O	5:E:99:LYS:HG3	2.17	0.45
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.45
6:F:300:ILE:CG2	6:F:306:GLY:C	2.90	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.45
8:H:179:TRP:CD1	18:Z:43:LEU:HD21	2.52	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.45
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.45
16:W:71:MET:O	16:W:74:ALA:N	2.43	0.45
21:q:55:PHE:CD1	22:r:26:LEU:CD2	2.96	0.45
3:C:98:PHE:HE1	15:V:44:TYR:CE1	2.35	0.45
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.52	0.45
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.45
6:F:382:CYS:HA	7:G:74:ASN:O	2.17	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
9:I:50:MET:O	9:I:51:LYS:C	2.60	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.51	0.45
10:P:238:GLN:HB3	10:P:326:ASP:OD2	2.17	0.45
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
16:W:97:ILE:C	16:W:99:VAL:N	2.73	0.45
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.45
20:b:20:VAL:HA	24:b:201:3PE:H282	1.99	0.45
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.45
1:A:4:TYR:HE2	24:A:401:3PE:H231	1.80	0.44
3:C:78:SER:C	3:C:80:LEU:H	2.24	0.44
4:D:78:THR:O	4:D:100:GLU:HB3	2.17	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.17	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.31	0.44
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.44
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.17	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.34	0.44
10:P:55:VAL:HA	10:P:79:GLN:O	2.18	0.44
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.98	0.44
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.44
10:P:357:ARG:NH2	10:P:364:SER:O	2.47	0.44
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.44
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.44
18:Z:62:ILE:O	18:Z:66:GLU:HG3	2.16	0.44
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.44
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
4:D:94:VAL:HB	4:D:115:LEU:CB	2.48	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.44
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.44
8:H:186:PHE:CE2	24:I:301:3PE:H2B1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.44
8:H:293:PHE:CE1	24:I:301:3PE:H32	2.52	0.44
9:I:48:VAL:HG12	20:b:10:LYS:HZ2	1.82	0.44
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.44
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.44
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.17	0.44
18:Z:94:GLU:HA	18:Z:97:ILE:HG12	1.99	0.44
2:B:90:LEU:O	2:B:119:VAL:HA	2.17	0.44
3:C:107:PHE:CE1	3:C:133:SER:HB3	2.53	0.44
3:C:133:SER:O	3:C:133:SER:OG	2.32	0.44
3:C:149:LEU:O	16:W:23:ILE:HD11	2.17	0.44
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.44
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.51	0.44
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.57	0.44
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.44
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.44
9:I:60:ILE:HG23	24:I:301:3PE:H111	1.99	0.44
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.44
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.44
1:A:48:ARG:C	1:A:49:LEU:HD22	2.43	0.44
2:B:97:LEU:HB2	2:B:134:ALA:O	2.18	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.51	0.44
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.44
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.52	0.44
10:P:305:PHE:CB	10:P:314:THR:HG22	2.47	0.44
17:X:137:LEU:HA	17:X:138:PRO:HD3	1.85	0.44
18:Z:131:GLU:O	18:Z:134:SER:N	2.51	0.44
34:a:101:CDL:CA2	21:q:6:VAL:HG13	2.47	0.44
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.44
3:C:197:PHE:CZ	4:D:121:GLU:HB2	2.53	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
5:E:221:ARG:NH2	5:E:227:ALA:HB2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.32	0.44
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.44
7:G:32:ILE:CG2	7:G:98:LYS:HD2	2.47	0.44
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:93:HIS:NE2	19:a:27:HIS:ND1	2.66	0.44
19:a:43:TYR:O	19:a:47:LEU:HD13	2.18	0.44
19:a:62:VAL:HG23	19:a:62:VAL:O	2.18	0.44
21:q:74:PHE:HD2	21:q:75:TRP:CD1	2.33	0.44
22:r:5:THR:HG22	22:r:5:THR:O	2.18	0.44
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.16	0.44
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.44
4:D:376:GLU:HG2	7:G:121:LEU:HD12	1.98	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
5:E:177:GLY:O	28:E:301:FES:S1	2.75	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
8:H:203:GLY:C	8:H:205:SER:N	2.76	0.44
8:H:277:TYR:CE2	24:I:301:3PE:H271	2.53	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.44
17:X:30:HIS:CE1	18:Z:63:GLU:HG3	2.51	0.44
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.48	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.47	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
10:P:310:PHE:O	10:P:311:GLU:C	2.59	0.44
16:W:58:THR:HB	16:W:61:GLN:H	1.82	0.44
3:C:130:ASN:ND2	3:C:141:ARG:HE	2.13	0.44
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.44
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.44
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.47	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:299:LEU:CD1	6:F:300:ILE:N	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.44
8:H:157:ASN:ND2	8:H:164:THR:OG1	2.49	0.44
8:H:196:ALA:C	8:H:198:PHE:N	2.75	0.44
27:I:302:PC1:H112	18:Z:29:GLY:CA	2.45	0.44
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
18:Z:97:ILE:HG13	18:Z:98:MET:N	2.30	0.44
1:A:105:GLU:OE2	1:A:110:GLY:HA3	2.18	0.44
2:B:114:MET:SD	2:B:121:PHE:HA	2.58	0.44
27:B:303:PC1:H133	27:B:303:PC1:H111	1.72	0.44
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.44
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.44
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.44
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.44
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.44
10:P:169:HIS:CD2	10:P:181:LEU:HD11	2.49	0.44
21:q:21:ARG:HD2	21:q:21:ARG:HA	1.80	0.44
5:E:140:MET:HE1	6:F:366:ALA:HA	2.00	0.43
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.96	0.43
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.43
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.43
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.43
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.43
16:W:47:PRO:HG3	16:W:63:ARG:NH2	2.26	0.43
18:Z:68:ARG:HG3	18:Z:69:ILE:N	2.33	0.43
1:A:4:TYR:O	1:A:5:THR:C	2.61	0.43
2:B:121:PHE:HZ	2:B:122:ARG:HH21	1.65	0.43
2:B:122:ARG:HH11	4:D:89:PRO:CA	2.30	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.43
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.43
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.83	0.43
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.43
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.97	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.59	0.43
8:H:128:SER:HA	8:H:210:GLY:O	2.18	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
17:X:35:GLN:HB2	17:X:70:PHE:CD1	2.53	0.43
1:A:106:TRP:CH2	8:H:295:PRO:HG2	2.53	0.43
4:D:97:LEU:HD21	4:D:109:CYS:HB3	1.99	0.43
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:422:TRP:HZ2	7:G:441:ARG:HB3	1.82	0.43
8:H:63:PRO:HD2	8:H:66:THR:HG21	2.00	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.43
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
17:X:66:CYS:O	17:X:67:ALA:C	2.61	0.43
20:b:82:LYS:HB3	20:b:82:LYS:HE2	1.81	0.43
2:B:96:GLY:CA	26:B:302:UQ1:HM52	2.49	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.43
9:I:35:THR:HG22	22:r:107:SER:HA	1.97	0.43
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.82	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.43
13:S:16:LEU:HD21	13:S:95:LEU:HG	2.00	0.43
16:W:23:ILE:HG22	16:W:24:PHE:HD2	1.81	0.43
17:X:39:THR:HG23	17:X:40:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
3:C:167:ARG:CZ	3:C:186:ILE:HG22	2.49	0.43
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.26	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.51	0.43
5:E:63:GLU:O	5:E:64:ALA:C	2.61	0.43
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.01	0.43
5:E:162:THR:HG21	5:E:166:LYS:HA	2.00	0.43
6:F:44:ASN:HB2	6:F:59:ARG:HD3	1.99	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
7:G:82:ILE:HG22	7:G:100:TRP:HE3	1.83	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.48	0.43
8:H:138:GLN:HG3	8:H:139:THR:N	2.34	0.43
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.18	0.43
8:H:280:PHE:HD2	8:H:284:GLN:HG3	1.81	0.43
8:H:303:TRP:HB2	20:b:25:VAL:CG1	2.49	0.43
10:P:81:ILE:HD13	12:R:46:VAL:HG11	2.00	0.43
10:P:135:GLU:HG3	10:P:140:ASP:HA	2.00	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.43
34:a:101:CDL:H311	21:q:7:LEU:CD2	2.49	0.43
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
4:D:279:THR:HG23	15:V:13:GLY:CA	2.26	0.43
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
8:H:17:MET:HE1	8:H:225:MET:HE3	2.01	0.43
8:H:134:ARG:HH21	8:H:200:LEU:CD1	2.32	0.43
9:I:78:PHE:HB3	22:r:8:ILE:HG22	1.99	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.43
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.43
17:X:50:GLU:OE1	17:X:55:ARG:HB3	2.18	0.43
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.53	0.43
18:Z:62:ILE:CG1	20:b:49:THR:HG22	2.48	0.43
20:b:53:TYR:HA	20:b:54:PRO:HD3	1.92	0.43
1:A:52:SER:O	1:A:55:PHE:N	2.51	0.43
3:C:240:ALA:O	3:C:241:PHE:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.19	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.43
9:I:42:LYS:HD3	9:I:42:LYS:HA	1.84	0.43
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.43
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.43
16:W:36:ARG:O	16:W:39:TYR:N	2.51	0.43
19:a:37:ARG:H	19:a:59:ARG:NH2	2.17	0.43
23:s:87:LEU:HD23	23:s:87:LEU:HA	1.84	0.43
1:A:73:LEU:O	1:A:76:PRO:HD2	2.18	0.43
3:C:78:SER:C	3:C:80:LEU:N	2.76	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
4:D:148:GLU:O	4:D:149:GLN:C	2.62	0.43
4:D:279:THR:HA	15:V:12:VAL:CG1	2.49	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.27	0.43
7:G:651:PRO:HB3	13:S:58:CYS:HA	2.01	0.43
9:I:162:CYS:SG	25:I:304:SF4:S2	3.17	0.43
10:P:81:ILE:HD11	12:R:46:VAL:HG11	2.00	0.43
10:P:315:THR:O	10:P:316:LYS:C	2.57	0.43
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.43
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.43
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.43
16:W:25:SER:OG	16:W:34:ARG:NH2	2.52	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
3:C:180:HIS:CD2	3:C:182:ASP:H	2.37	0.43
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.43
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.43
5:E:70:PRO:HG2	6:F:236:PHE:CD2	2.54	0.43
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
8:H:21:THR:HG21	30:H:401:UQ9:H16	2.01	0.43
10:P:142:GLU:O	10:P:146:VAL:CG1	2.61	0.43
10:P:153:ALA:HB2	10:P:191:VAL:HG23	2.01	0.43
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.43
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.43
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.43
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.43
17:X:52:ASP:HA	18:Z:116:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:121:ILE:HD11	18:Z:136:ALA:HB3	1.98	0.43
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.43
20:b:6:SER:OG	20:b:10:LYS:HD2	2.18	0.43
2:B:81:LEU:CD2	27:B:303:PC1:H352	2.48	0.43
2:B:116:ARG:NH2	9:I:86:TYR:H	2.17	0.43
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.37	0.43
6:F:88:ARG:HA	6:F:88:ARG:HD3	1.85	0.43
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.43
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.43
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.43
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.43
9:I:152:CYS:SG	25:I:303:SF4:S3	3.17	0.43
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.43
11:Q:104:ARG:HA	11:Q:104:ARG:HD3	1.88	0.43
13:S:58:CYS:SG	13:S:59:SER:N	2.92	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
14:T:113:LEU:HD22	16:W:71:MET:HE2	2.01	0.43
16:W:57:ILE:HG23	16:W:107:MET:HE1	2.00	0.43
19:a:50:ARG:O	19:a:54:ILE:HG13	2.18	0.43
1:A:73:LEU:N	1:A:74:PRO:HD2	2.34	0.42
1:A:99:SER:HB3	24:b:201:3PE:C38	2.49	0.42
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.42
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42
6:F:50:ASP:O	6:F:55:GLY:HA3	2.19	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
8:H:33:LEU:HD21	22:r:25:GLN:HG2	2.01	0.42
8:H:200:LEU:CD1	8:H:201:THR:N	2.70	0.42
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.42
10:P:306:GLY:HA2	10:P:312:PRO:HB3	2.01	0.42
10:P:361:TRP:HE3	10:P:364:SER:HB2	1.84	0.42
14:T:87:LEU:HD11	14:T:141:PRO:HB3	2.01	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.62	0.42
16:W:83:ASP:O	16:W:86:VAL:CG2	2.66	0.42
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.42
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	0.42
2:B:69:SER:O	2:B:70:ARG:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ARG:HH22	26:B:302:UQ1:C8	2.32	0.42
2:B:194:CYS:SG	4:D:138:ARG:NE	2.90	0.42
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.44	0.42
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.55	0.42
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.01	0.42
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.42
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.42
1:A:81:THR:O	20:b:46:ASN:ND2	2.52	0.42
3:C:149:LEU:HD21	11:Q:59:LEU:HD22	2.00	0.42
4:D:259:GLU:C	4:D:261:MET:N	2.75	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
5:E:78:VAL:O	5:E:82:LEU:HB2	2.20	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.42
10:P:235:THR:HG21	10:P:323:HIS:CD2	2.55	0.42
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	2.00	0.42
17:X:10:LEU:HD12	17:X:13:LEU:HD12	2.01	0.42
18:Z:10:MET:HE2	18:Z:10:MET:HB3	1.72	0.42
4:D:101:LEU:HD11	4:D:106:VAL:CG2	2.39	0.42
4:D:162:GLN:HB2	4:D:163:PRO:HD2	2.01	0.42
5:E:109:MET:HE2	7:G:196:GLY:CA	2.49	0.42
5:E:179:CYS:C	5:E:181:ASN:N	2.78	0.42
5:E:233:LEU:CD2	6:F:43:THR:HA	2.48	0.42
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.84	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
6:F:296:LEU:HD22	6:F:337:MET:HE1	2.01	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.53	0.42
8:H:39:ILE:HG13	21:q:31:ASN:ND2	2.35	0.42
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.20	0.42
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.42
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
13:S:26:ARG:N	13:S:34:ARG:NH1	2.63	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:130:LYS:HG2	20:b:67:PRO:HA	2.01	0.42
18:Z:129:THR:O	18:Z:130:LYS:C	2.61	0.42
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
6:F:227:PRO:HB3	7:G:95:PRO:HD3	2.01	0.42
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.42
7:G:117:MET:SD	7:G:143:SER:HB2	2.59	0.42
7:G:281:ILE:HD12	7:G:282:ASN:N	2.34	0.42
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.42
8:H:202:GLU:HA	8:H:206:GLU:CD	2.45	0.42
27:H:402:PC1:H342	27:H:402:PC1:C38	2.42	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.42
16:W:38:LEU:O	16:W:39:TYR:C	2.62	0.42
17:X:130:LYS:HG2	20:b:67:PRO:CA	2.50	0.42
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.42
5:E:62:ILE:HG23	5:E:81:VAL:HG22	2.02	0.42
5:E:196:THR:O	5:E:199:ASP:HB2	2.19	0.42
6:F:300:ILE:CG2	6:F:306:GLY:HA2	2.35	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.19	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
10:P:324:ILE:HD13	10:P:324:ILE:HA	1.81	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
12:R:64:ILE:HD12	12:R:64:ILE:HA	1.95	0.42
17:X:127:LYS:HB2	20:b:76:PRO:HD2	2.02	0.42
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.52	0.42
2:B:114:MET:O	2:B:115:ASP:C	2.62	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.42
7:G:404:GLY:HA3	7:G:684:LEU:CD1	2.34	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
9:I:80:GLU:N	19:a:1:MET:HE1	2.34	0.42
10:P:172:ALA:H	10:P:202:ARG:HH21	1.66	0.42
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.42
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.42
17:X:38:LYS:O	17:X:42:GLU:HG3	2.20	0.42
18:Z:120:LEU:HD12	18:Z:121:ILE:H	1.85	0.42
20:b:5:ILE:HD12	20:b:6:SER:N	2.34	0.42
20:b:69:HIS:HD2	20:b:70:PRO:CD	2.26	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
1:A:99:SER:HB3	24:b:201:3PE:C39	2.48	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.42
4:D:264:ASN:O	9:I:65:GLU:OE1	2.38	0.42
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
9:I:92:PRO:HB3	21:q:92:CYS:HB2	2.01	0.42
10:P:316:LYS:O	10:P:320:GLU:HG2	2.19	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
16:W:42:TRP:CE2	16:W:93:LEU:HB2	2.54	0.42
16:W:55:LEU:HB3	16:W:57:ILE:HG12	2.01	0.42
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.42
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.53	0.42
4:D:94:VAL:HB	4:D:115:LEU:HB3	2.02	0.42
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
5:E:39:VAL:HG21	7:G:163:LYS:HZ1	1.85	0.42
5:E:181:ASN:HB3	5:E:193:GLU:HB2	2.01	0.42
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.42
10:P:179:LYS:O	10:P:180:SER:C	2.63	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
13:S:26:ARG:HA	13:S:34:ARG:HH12	1.84	0.42
14:T:132:ASP:O	16:W:40:ARG:NH2	2.53	0.42
16:W:76:VAL:HG13	16:W:82:VAL:HG22	2.02	0.42
19:a:34:LYS:O	19:a:35:GLU:C	2.63	0.42
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.53	0.42
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.42
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.35	0.42
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.42
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.42
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
9:I:152:CYS:SG	25:I:303:SF4:S1	3.17	0.42
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.85	0.42
13:S:31:GLN:CD	13:S:34:ARG:HH21	2.28	0.42
14:T:118:ILE:HD13	14:T:118:ILE:HA	1.83	0.42
18:Z:94:GLU:HA	18:Z:97:ILE:HD11	2.01	0.42
1:A:3:LEU:O	1:A:4:TYR:C	2.60	0.41
1:A:60:ILE:O	1:A:61:THR:C	2.62	0.41
1:A:102:LEU:HD23	24:b:201:3PE:H371	2.02	0.41
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
3:C:102:HIS:CE1	15:V:48:THR:CG2	2.89	0.41
4:D:280:ALA:CB	15:V:11:LEU:CG	2.95	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.41
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.41
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.55	0.41
8:H:16:ALA:HB2	19:a:15:CYS:CB	2.50	0.41
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.41
9:I:50:MET:O	9:I:54:THR:N	2.37	0.41
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.20	0.41
10:P:265:PHE:N	10:P:265:PHE:CD1	2.87	0.41
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.41
16:W:45:GLU:O	16:W:46:VAL:C	2.62	0.41
16:W:93:LEU:HD23	16:W:93:LEU:C	2.45	0.41
20:b:59:ASP:HA	20:b:63:MET:CE	2.50	0.41
21:q:74:PHE:HE2	21:q:75:TRP:HE1	1.68	0.41
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.41
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.35	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
8:H:12:PRO:O	19:a:15:CYS:HB3	2.20	0.41
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.41
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.41
18:Z:91:LEU:HD13	18:Z:91:LEU:C	2.45	0.41
20:b:7:ALA:C	20:b:9:LEU:H	2.27	0.41
20:b:61:GLY:O	20:b:63:MET:HG3	2.20	0.41
1:A:24:LEU:HD13	1:A:24:LEU:O	2.20	0.41
1:A:56:PHE:CZ	1:A:60:ILE:HD11	2.55	0.41
2:B:100:CYS:SG	25:B:301:SF4:S3	3.19	0.41
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.41
26:B:302:UQ1:HM22	4:D:189:THR:HG21	2.03	0.41
4:D:81:THR:HB	4:D:100:GLU:HG2	2.03	0.41
4:D:198:THR:OG1	4:D:261:MET:SD	2.78	0.41
6:F:94:PRO:CG	6:F:97:LEU:HD12	2.45	0.41
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:36:VAL:O	7:G:37:ASP:C	2.63	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:404:GLY:HA2	7:G:684:LEU:HD11	1.99	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.89	0.41
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.81	0.41
10:P:73:LEU:HD23	10:P:73:LEU:HA	1.89	0.41
10:P:156:SER:O	10:P:160:GLY:N	2.45	0.41
12:R:60:ALA:O	12:R:61:ILE:C	2.63	0.41
13:S:21:VAL:HG23	13:S:91:MET:HE1	2.02	0.41
13:S:31:GLN:NE2	13:S:34:ARG:NH2	2.68	0.41
14:T:87:LEU:CD2	14:T:122:MET:CE	2.97	0.41
14:T:115:GLN:O	14:T:116:VAL:C	2.63	0.41
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.41
18:Z:96:ILE:H	18:Z:96:ILE:HG13	1.72	0.41
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.20	0.41
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.84	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
5:E:136:THR:HG21	6:F:122:PRO:HG3	2.01	0.41
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.51	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
10:P:177:SER:O	10:P:182:ARG:NH2	2.53	0.41
10:P:228:LEU:HD11	10:P:288:PHE:CZ	2.54	0.41
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.41
17:X:23:ALA:HB2	17:X:95:GLN:HE22	1.82	0.41
17:X:112:LEU:HD13	17:X:118:VAL:HG22	2.03	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
21:q:5:GLU:HG2	21:q:9:ARG:HE	1.85	0.41
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.55	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
4:D:87:GLN:O	4:D:88:HIS:C	2.61	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
6:F:131:MET:HE3	6:F:131:MET:HB2	1.91	0.41
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.41
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.41
9:I:49:ASP:O	9:I:53:ALA:N	2.41	0.41
10:P:358:THR:HG23	10:P:359:TYR:H	1.81	0.41
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.41
12:R:55:VAL:HG22	12:R:56:ASN:N	2.35	0.41
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.35	0.41
16:W:44:ARG:O	16:W:47:PRO:HG2	2.20	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.41
22:r:12:ARG:HH21	22:r:20:LEU:CD1	2.33	0.41
22:r:24:LEU:HD23	22:r:24:LEU:HA	1.85	0.41
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.41
2:B:210:ARG:NE	21:q:78:ASP:OD1	2.53	0.41
3:C:229:PHE:O	11:Q:123:ASN:ND2	2.54	0.41
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.35	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.55	0.41
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.87	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
11:Q:52:LEU:HD23	16:W:19:SER:O	2.20	0.41
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.03	0.41
12:R:38:TYR:HE2	12:R:44:ARG:NE	2.19	0.41
14:T:87:LEU:HD11	14:T:141:PRO:HG3	2.03	0.41
14:T:100:VAL:O	14:T:141:PRO:HD2	2.20	0.41
16:W:78:ASP:HA	16:W:79:PRO:HD3	1.94	0.41
34:a:101:CDL:CA3	21:q:13:GLN:HE22	2.29	0.41
21:q:56:PHE:HD2	22:r:27:ARG:HH22	1.68	0.41
1:A:61:THR:O	1:A:62:PHE:C	2.64	0.41
1:A:108:GLN:CG	1:A:109:LYS:N	2.80	0.41
3:C:77:VAL:HG22	3:C:83:LEU:HD13	2.03	0.41
5:E:78:VAL:CA	5:E:104:LEU:HD13	2.46	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.41
6:F:296:LEU:HD22	6:F:337:MET:HE3	2.01	0.41
7:G:163:LYS:HD3	7:G:163:LYS:HA	1.84	0.41
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.50	0.41
8:H:75:PRO:HB2	8:H:222:LEU:HB2	2.03	0.41
27:I:302:PC1:H122	18:Z:35:MET:HE1	2.01	0.41
10:P:75:ARG:HH21	16:W:113:THR:HG23	1.86	0.41
10:P:285:HIS:ND1	10:P:361:TRP:HB3	2.36	0.41
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.41
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.41
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.77	0.41
1:A:3:LEU:CA	8:H:96:ILE:HD13	2.45	0.41
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.41
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.03	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
5:E:142:ARG:HB3	5:E:182:ALA:HB3	2.03	0.41
5:E:193:GLU:HG3	5:E:217:PRO:HG3	2.02	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:241:GLY:HA3	6:F:63:TYR:CZ	2.56	0.41
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
8:H:172:MET:HE3	8:H:176:LEU:CB	2.47	0.41
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
20:b:49:THR:HA	20:b:50:PRO:HD3	1.89	0.41
1:A:20:VAL:O	1:A:21:ALA:C	2.63	0.41
1:A:52:SER:O	1:A:55:PHE:HB2	2.21	0.41
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.88	0.41
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.56	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
5:E:145:ASP:OD1	5:E:145:ASP:N	2.54	0.41
6:F:300:ILE:HD13	6:F:307:VAL:CG2	2.51	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.84	0.41
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
8:H:99:ASN:OD1	19:a:40:ARG:HG3	2.21	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
8:H:303:TRP:HZ3	20:b:28:LEU:HG	1.84	0.41
8:H:317:TYR:CZ	19:a:40:ARG:NH1	2.78	0.41
10:P:243:ALA:O	10:P:244:ASP:C	2.63	0.41
12:R:42:ASP:C	12:R:43:TYR:O	2.61	0.41
12:R:48:PHE:CE2	12:R:53:LYS:HB2	2.56	0.41
14:T:99:SER:HB2	14:T:102:SER:HB2	2.02	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
16:W:24:PHE:HB2	16:W:83:ASP:OD2	2.20	0.41
34:a:101:CDL:HA62	21:q:6:VAL:O	2.21	0.41
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.90	0.41
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.85	0.41
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.41
5:E:190:ASN:O	5:E:191:TYR:C	2.63	0.41
5:E:223:CYS:CB	6:F:133:HIS:CE1	3.04	0.41
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:45:LEU:O	6:F:46:TYR:HB2	2.21	0.41
6:F:199:ARG:HD3	23:s:80:PHE:CZ	2.48	0.41
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.41
7:G:357:LEU:HD13	7:G:627:SER:HG	1.84	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
9:I:54:THR:HG21	18:Z:33:TYR:CE2	2.56	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
10:P:96:LEU:HD12	10:P:97:MET:CA	2.51	0.41
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.41
17:X:38:LYS:HD2	17:X:131:VAL:HG12	2.02	0.41
1:A:18:ILE:HG12	8:H:222:LEU:CD2	2.51	0.40
1:A:48:ARG:NE	1:A:48:ARG:HA	2.36	0.40
1:A:60:ILE:HD13	1:A:60:ILE:HA	1.83	0.40
1:A:62:PHE:HD1	8:H:144:VAL:CG2	2.34	0.40
1:A:87:MET:HB3	1:A:87:MET:HE3	1.84	0.40
1:A:111:LEU:HD13	8:H:290:TRP:HB3	2.02	0.40
2:B:84:TRP:CZ3	27:B:303:PC1:H351	2.56	0.40
2:B:117:PHE:CD2	2:B:206:LEU:HD21	2.55	0.40
2:B:120:VAL:HG21	30:H:401:UQ9:C1M	2.36	0.40
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.56	0.40
6:F:208:GLU:OE1	6:F:210:THR:N	2.52	0.40
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.40
6:F:300:ILE:CG2	6:F:306:GLY:CA	2.95	0.40
8:H:87:VAL:HB	8:H:88:PRO:HD3	2.03	0.40
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.40
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.55	0.40
10:P:56:ALA:HA	10:P:125:VAL:O	2.21	0.40
14:T:107:ASP:OD1	14:T:108:LEU:N	2.54	0.40
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.22	0.40
2:B:82:ILE:CG1	8:H:57:MET:CE	2.83	0.40
2:B:147:LYS:HD2	2:B:147:LYS:HA	1.75	0.40
26:B:302:UQ1:HM21	4:D:189:THR:HG21	2.04	0.40
3:C:160:ILE:HB	4:D:286:TYR:CE1	2.56	0.40
3:C:160:ILE:HG13	4:D:285:ASN:ND2	2.36	0.40
3:C:243:ALA:C	7:G:105:ASN:ND2	2.79	0.40
4:D:119:GLY:O	4:D:123:LEU:HD23	2.21	0.40
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.40
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.20	0.40
6:F:47:GLY:O	6:F:48:ARG:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.40
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.40
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.40
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
10:P:180:SER:HB2	10:P:321:ARG:HH21	1.87	0.40
10:P:272:LEU:HD23	10:P:272:LEU:HA	1.92	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
18:Z:59:ARG:HH21	20:b:84:LEU:H	1.68	0.40
19:a:41:VAL:O	19:a:42:GLN:C	2.64	0.40
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.86	0.40
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.86	0.40
7:G:32:ILE:CG2	7:G:98:LYS:HA	2.52	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.09	0.40
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.43	0.40
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.40
8:H:296:LEU:CD2	24:I:301:3PE:H351	2.51	0.40
8:H:306:SER:CB	8:H:310:PHE:HE2	2.34	0.40
9:I:94:SER:HB2	9:I:95:PRO:CD	2.34	0.40
10:P:96:LEU:C	10:P:96:LEU:CD1	2.94	0.40
10:P:120:VAL:O	10:P:121:GLN:C	2.64	0.40
14:T:82:ARG:O	14:T:86:VAL:HG23	2.20	0.40
14:T:120:MET:O	14:T:121:ALA:C	2.63	0.40
17:X:132:LYS:HB3	17:X:132:LYS:HE2	1.84	0.40
19:a:45:TRP:NE1	19:a:49:GLU:HG3	2.36	0.40
3:C:71:TYR:O	3:C:87:ILE:HA	2.21	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
4:D:213:PHE:O	4:D:214:TYR:C	2.65	0.40
4:D:271:ARG:HG2	8:H:281:ARG:CG	2.44	0.40
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.37	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:169:VAL:HG12	7:G:231:LEU:HB2	2.03	0.40
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.87	0.40
8:H:264:LEU:HD21	19:a:12:MET:HE2	2.03	0.40
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.40
9:I:162:CYS:HB3	9:I:165:ASP:HA	2.02	0.40
10:P:40:VAL:HG13	12:R:43:TYR:CZ	2.57	0.40
10:P:300:TRP:CE2	10:P:304:LEU:HD21	2.57	0.40
10:P:315:THR:H	10:P:318:LYS:HB3	1.86	0.40
11:Q:166:TRP:O	11:Q:167:ASN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:38:TYR:HE2	12:R:44:ARG:HE	1.69	0.40
15:V:96:LYS:HE2	15:V:96:LYS:HB2	1.95	0.40
16:W:48:ASN:O	16:W:52:LEU:HG	2.22	0.40
17:X:143:HIS:CG	17:X:143:HIS:O	2.73	0.40
19:a:9:LEU:O	19:a:10:ALA:C	2.64	0.40
21:q:89:TRP:HB2	21:q:98:PRO:HD3	2.03	0.40
2:B:106:HIS:O	2:B:109:ALA:HB3	2.22	0.40
3:C:128:VAL:HG22	3:C:143:LYS:HB3	2.04	0.40
5:E:109:MET:HE2	7:G:196:GLY:HA3	2.04	0.40
6:F:102:MET:HE2	6:F:149:MET:HB2	2.03	0.40
6:F:119:GLU:OE1	6:F:119:GLU:HA	2.21	0.40
6:F:335:VAL:HG12	6:F:336:LEU:N	2.37	0.40
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
8:H:145:THR:HG22	8:H:289:LEU:HD11	2.03	0.40
9:I:149:MET:HE2	9:I:185:TYR:HD2	1.86	0.40
10:P:40:VAL:HG13	12:R:43:TYR:OH	2.22	0.40
12:R:45:ARG:HD2	12:R:48:PHE:CE1	2.57	0.40
14:T:140:CYS:HB2	14:T:143:GLU:HB2	2.02	0.40
24:b:201:3PE:H361	24:b:201:3PE:H391	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	88/115 (76%)	79 (90%)	9 (10%)	0	100 100
2	B	155/224 (69%)	145 (94%)	9 (6%)	1 (1%)	21 52
3	C	196/263 (74%)	185 (94%)	11 (6%)	0	100 100
4	D	384/463 (83%)	357 (93%)	27 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	208/248 (84%)	189 (91%)	19 (9%)	0	100	100
6	F	424/464 (91%)	408 (96%)	16 (4%)	0	100	100
7	G	685/727 (94%)	629 (92%)	56 (8%)	0	100	100
8	H	308/318 (97%)	288 (94%)	19 (6%)	1 (0%)	36	65
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	P	338/377 (90%)	317 (94%)	21 (6%)	0	100	100
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	77 (95%)	4 (5%)	0	100	100
13	S	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
14	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
15	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
16	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100	100
18	Z	137/144 (95%)	129 (94%)	8 (6%)	0	100	100
19	a	65/70 (93%)	57 (88%)	8 (12%)	0	100	100
20	b	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
21	q	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
22	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
23	s	12/104 (12%)	12 (100%)	0	0	100	100
All	All	4124/5036 (82%)	3873 (94%)	249 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
2	B	195	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	73	79
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	333/395 (84%)	332 (100%)	1 (0%)	86	86
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	83
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	88
8	H	276/280 (99%)	276 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	P	297/325 (91%)	296 (100%)	1 (0%)	86	86
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	76
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	73
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	73
14	T	69/135 (51%)	68 (99%)	1 (1%)	59	73
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	129 (100%)	0	100	100
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73	79
19	a	57/60 (95%)	57 (100%)	0	100	100
20	b	71/73 (97%)	71 (100%)	0	100	100
21	q	108/131 (82%)	108 (100%)	0	100	100
22	r	44/96 (46%)	44 (100%)	0	100	100
23	s	14/95 (15%)	14 (100%)	0	100	100
All	All	3622/4292 (84%)	3612 (100%)	10 (0%)	84	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	104	MET
4	D	232	VAL
5	E	244	VAL
7	G	271	MET
10	P	316	LYS
11	Q	96	LYS
12	R	64	ILE

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Mol	Chain	Res	Type
13	S	68	ARG
14	T	103	HIS
18	Z	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
3	C	88	HIS
3	C	123	ASN
3	C	130	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	313	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	132	GLN
5	E	152	GLN
5	E	190	ASN
5	E	245	GLN
6	F	44	ASN
6	F	168	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	277	ASN
6	F	346	GLN
7	G	59	GLN

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Mol	Chain	Res	Type
7	G	74	ASN
7	G	101	ASN
7	G	105	ASN
7	G	140	GLN
7	G	164	ASN
7	G	205	GLN
7	G	444	HIS
7	G	495	ASN
7	G	498	GLN
7	G	569	GLN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	32	GLN
8	H	47	GLN
8	H	97	ASN
8	H	169	GLN
8	H	171	HIS
8	H	258	ASN
8	H	284	GLN
8	H	292	ASN
9	I	126	GLN
10	P	43	HIS
10	P	71	ASN
10	P	79	GLN
10	P	169	HIS
10	P	216	HIS
10	P	251	ASN
10	P	269	ASN
10	P	275	HIS
10	P	323	HIS
10	P	341	GLN
11	Q	51	GLN
11	Q	88	GLN
13	S	25	GLN
15	V	41	HIS
15	V	50	GLN
16	W	29	ASN
16	W	54	GLN
17	X	30	HIS

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Mol	Chain	Res	Type
17	X	77	HIS
19	a	58	ASN
20	b	69	HIS
20	b	83	ASN
21	q	13	GLN
21	q	31	ASN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS
21	q	91	HIS
22	r	21	GLN
22	r	110	GLN
23	s	84	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.08	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	SF4	F	502	6	0,12,12	-	-	-		
29	FMN	F	501	-	33,33,33	1.40	5 (15%)	48,50,50	1.22	7 (14%)
28	FES	G	803	7	0,4,4	-	-	-		
27	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.16	3 (7%)
28	FES	E	301	5	0,4,4	-	-	-		
25	SF4	G	802	7	0,12,12	-	-	-		
31	NDP	P	401	-	49,52,52	1.21	5 (10%)	66,80,80	1.68	11 (16%)
30	UQ9	H	401	-	35,35,58	0.81	2 (5%)	42,45,73	0.49	0
24	3PE	I	301	-	50,50,50	0.89	2 (4%)	53,55,55	1.03	4 (7%)
24	3PE	b	201	-	45,45,50	0.95	2 (4%)	48,50,55	1.10	3 (6%)
26	UQ1	B	302	-	18,18,18	1.07	2 (11%)	22,25,25	0.70	0
25	SF4	B	301	2	0,12,12	-	-	-		
24	3PE	A	401	-	45,45,50	0.94	2 (4%)	48,50,55	1.01	2 (4%)
25	SF4	G	801	7	0,12,12	-	-	-		
27	PC1	H	402	-	41,41,53	1.07	2 (4%)	47,49,61	1.08	4 (8%)
25	SF4	I	303	9	0,12,12	-	-	-		
34	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)
33	EHZ	W	201	-	27,31,37	1.89	7 (25%)	37,41,47	1.86	11 (29%)
25	SF4	I	304	9	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PC1	I	302	-	-	13/50/50/57	-
25	SF4	F	502	6	-	-	0/6/5/5
29	FMN	F	501	-	-	4/18/18/18	0/3/3/3
28	FES	G	803	7	-	-	0/1/1/1
27	PC1	B	303	-	-	11/38/38/57	-
28	FES	E	301	5	-	-	0/1/1/1
25	SF4	G	802	7	-	-	0/6/5/5
31	NDP	P	401	-	-	6/34/77/77	0/5/5/5
30	UQ9	H	401	-	-	13/30/54/81	0/1/1/1
24	3PE	I	301	-	-	17/54/54/54	-
24	3PE	b	201	-	-	8/49/49/54	-
26	UQ1	B	302	-	-	3/9/33/33	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SF4	B	301	2	-	-	0/6/5/5
24	3PE	A	401	-	-	14/49/49/54	-
25	SF4	G	801	7	-	-	0/6/5/5
27	PC1	H	402	-	-	14/45/45/57	-
25	SF4	I	303	9	-	-	0/6/5/5
34	CDL	a	101	-	-	14/67/67/110	-
33	EHZ	W	201	-	-	22/39/39/45	-
25	SF4	I	304	9	-	-	0/6/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	W	201	EHZ	C15-N2	5.38	1.45	1.33
33	W	201	EHZ	C12-N1	5.11	1.45	1.33
29	F	501	FMN	C9A-C5A	4.79	1.49	1.41
31	P	401	NDP	C5A-C4A	4.27	1.47	1.39
27	H	402	PC1	O31-C31	4.24	1.45	1.33
34	a	101	CDL	OB8-CB7	4.20	1.45	1.33
27	B	303	PC1	O31-C31	4.17	1.45	1.33
27	I	302	PC1	O31-C31	4.17	1.45	1.33
34	a	101	CDL	OB6-CB5	4.14	1.46	1.34
24	b	201	3PE	O31-C31	4.14	1.45	1.33
34	a	101	CDL	OA8-CA7	4.11	1.45	1.33
24	A	401	3PE	O31-C31	4.10	1.45	1.33
27	H	402	PC1	O21-C21	4.10	1.45	1.34
27	I	302	PC1	O21-C21	4.09	1.45	1.34
24	I	301	3PE	O31-C31	4.08	1.45	1.33
34	a	101	CDL	OA6-CA5	4.05	1.45	1.34
27	B	303	PC1	O21-C21	4.04	1.45	1.34
24	b	201	3PE	O21-C21	4.01	1.45	1.34
24	I	301	3PE	O21-C21	3.97	1.45	1.34
24	A	401	3PE	O21-C21	3.96	1.45	1.34
31	P	401	NDP	C6N-C5N	3.26	1.39	1.33
29	F	501	FMN	C8-C7	3.15	1.48	1.40
26	B	302	UQ1	C3-C4	-2.96	1.40	1.48
29	F	501	FMN	C4-N3	-2.75	1.33	1.38
30	H	401	UQ9	C4-C5	-2.68	1.41	1.48
30	H	401	UQ9	C3-C2	-2.61	1.41	1.48
33	W	201	EHZ	P1-O7	2.55	1.64	1.54
31	P	401	NDP	C5A-C6A	2.52	1.48	1.41
33	W	201	EHZ	O4-C15	-2.48	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	501	FMN	C5A-N5	-2.41	1.34	1.39
33	W	201	EHZ	C9-S1	2.40	1.81	1.76
26	B	302	UQ1	C2-C1	-2.40	1.42	1.48
31	P	401	NDP	C8A-N7A	2.34	1.36	1.31
31	P	401	NDP	C5A-N7A	-2.34	1.34	1.39
33	W	201	EHZ	O3-C12	-2.33	1.18	1.23
33	W	201	EHZ	P1-OP3	-2.22	1.46	1.54
29	F	501	FMN	C4A-N5	2.05	1.34	1.30

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	W	201	EHZ	C8-C9-S1	6.32	121.44	113.63
31	P	401	NDP	C5A-C4A-N3A	-6.05	118.85	126.75
31	P	401	NDP	N3A-C4A-N9A	4.76	134.92	127.08
34	a	101	CDL	OA6-CA5-C11	4.33	120.84	111.50
27	I	302	PC1	O21-C21-C22	4.23	120.61	111.50
34	a	101	CDL	OB6-CB5-C51	4.07	120.28	111.50
27	H	402	PC1	O21-C21-C22	4.01	120.13	111.50
27	B	303	PC1	O21-C21-C22	3.81	119.71	111.50
31	P	401	NDP	C2A-N3A-C4A	3.81	120.74	111.75
24	A	401	3PE	O21-C21-C22	3.76	119.61	111.50
24	I	301	3PE	O21-C21-C22	3.68	119.43	111.50
31	P	401	NDP	PN-O3-PA	-3.56	120.62	132.83
24	b	201	3PE	O21-C21-C22	3.51	119.07	111.50
24	b	201	3PE	C2-O21-C21	-3.48	109.22	117.79
31	P	401	NDP	C4A-C5A-N7A	-3.31	106.59	110.62
33	W	201	EHZ	C13-C12-N1	3.10	121.64	116.42
31	P	401	NDP	N3A-C2A-N1A	-3.09	123.78	128.60
33	W	201	EHZ	C14-C13-C12	-3.02	107.33	112.36
33	W	201	EHZ	OP3-P1-O9	-2.90	99.33	110.68
33	W	201	EHZ	C7-C8-C9	-2.89	107.30	113.89
31	P	401	NDP	C4A-N9A-C8A	2.86	108.83	105.73
27	I	302	PC1	C2-O21-C21	-2.83	110.83	117.79
31	P	401	NDP	C5A-N7A-C8A	2.79	107.47	103.51
27	B	303	PC1	O31-C31-C32	2.78	120.62	111.91
34	a	101	CDL	OA8-CA7-C31	2.74	120.50	111.91
34	a	101	CDL	CA4-OA6-CA5	-2.74	111.06	117.79
27	B	303	PC1	C2-O21-C21	-2.69	111.16	117.79
24	I	301	3PE	O31-C31-C32	2.67	120.28	111.91
29	F	501	FMN	C4A-C10-N1	-2.63	118.62	124.73
27	I	302	PC1	O31-C31-C32	2.59	120.04	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	401	3PE	O31-C31-C32	2.56	119.95	111.91
29	F	501	FMN	O4-C4-C4A	-2.53	119.90	126.60
24	b	201	3PE	O31-C31-C32	2.49	119.74	111.91
31	P	401	NDP	C3D-C2D-C1D	2.47	106.11	101.43
33	W	201	EHZ	C5-C6-C7	-2.39	107.98	114.85
34	a	101	CDL	OB8-CB7-C71	2.39	119.40	111.91
27	H	402	PC1	C2-O21-C21	-2.33	112.04	117.79
27	H	402	PC1	O31-C31-C32	2.33	119.23	111.91
33	W	201	EHZ	C10-S1-C9	2.27	108.93	101.87
34	a	101	CDL	CB4-OB6-CB5	-2.23	112.30	117.79
31	P	401	NDP	C6A-C5A-N7A	2.21	136.15	132.02
31	P	401	NDP	N9A-C8A-N7A	-2.21	110.89	113.91
29	F	501	FMN	C4-C4A-N5	2.19	121.35	118.23
33	W	201	EHZ	C11-N1-C12	-2.18	118.79	122.84
29	F	501	FMN	C4A-C10-N10	2.12	119.58	116.48
33	W	201	EHZ	O2-C9-S1	-2.12	119.86	122.61
33	W	201	EHZ	O6-P1-O9	2.10	112.36	106.47
33	W	201	EHZ	O3-C12-N1	-2.07	119.11	123.01
29	F	501	FMN	O2-C2-N1	-2.06	118.41	121.83
29	F	501	FMN	C10-N1-C2	2.06	121.02	116.90
24	I	301	3PE	O31-C31-O32	-2.03	118.47	123.59
27	H	402	PC1	C11-C12-N	-2.01	109.05	115.78
24	I	301	3PE	C2-O21-C21	-2.01	112.85	117.79
29	F	501	FMN	C4A-C4-N3	2.00	118.28	113.19

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	401	3PE	C12-C11-O13-P
24	A	401	3PE	O32-C31-O31-C3
24	A	401	3PE	C32-C31-O31-C3
24	I	301	3PE	C11-O13-P-O12
24	b	201	3PE	O22-C21-O21-C2
24	b	201	3PE	C22-C21-O21-C2
26	B	302	UQ1	C7-C8-C9-C11
27	B	303	PC1	C1-O11-P-O12
27	B	303	PC1	C1-O11-P-O14
27	B	303	PC1	C1-O11-P-O13
27	B	303	PC1	C22-C21-O21-C2
27	H	402	PC1	C11-O13-P-O12
27	H	402	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
27	H	402	PC1	C1-O11-P-O12
27	H	402	PC1	C1-O11-P-O13
27	H	402	PC1	C12-C11-O13-P
27	I	302	PC1	C11-O13-P-O12
27	I	302	PC1	C11-O13-P-O14
27	I	302	PC1	C11-O13-P-O11
27	I	302	PC1	C1-O11-P-O12
29	F	501	FMN	N10-C1'-C2'-O2'
29	F	501	FMN	C5'-O5'-P-O1P
29	F	501	FMN	C5'-O5'-P-O3P
30	H	401	UQ9	C22-C23-C24-C26
30	H	401	UQ9	C22-C23-C24-C25
30	H	401	UQ9	C20-C19-C21-C22
30	H	401	UQ9	C7-C8-C9-C11
30	H	401	UQ9	C7-C8-C9-C10
31	P	401	NDP	C2N-C3N-C7N-N7N
33	W	201	EHZ	O1-C7-C8-C9
33	W	201	EHZ	C6-C7-C8-C9
33	W	201	EHZ	C7-C8-C9-S1
33	W	201	EHZ	S1-C10-C11-N1
33	W	201	EHZ	C11-C10-S1-C9
33	W	201	EHZ	C16-C17-C20-O6
33	W	201	EHZ	C20-O6-P1-O7
33	W	201	EHZ	C20-O6-P1-O9
33	W	201	EHZ	C20-O6-P1-OP3
34	a	101	CDL	CA3-OA5-PA1-OA2
34	a	101	CDL	CA3-OA5-PA1-OA3
34	a	101	CDL	CA3-OA5-PA1-OA4
27	I	302	PC1	O32-C31-O31-C3
27	I	302	PC1	C32-C31-O31-C3
27	H	402	PC1	O32-C31-O31-C3
27	B	303	PC1	O22-C21-O21-C2
27	H	402	PC1	C32-C31-O31-C3
30	H	401	UQ9	C18-C19-C21-C22
26	B	302	UQ1	C7-C8-C9-C10
30	H	401	UQ9	C25-C24-C26-C27
30	H	401	UQ9	C15-C14-C16-C17
30	H	401	UQ9	C23-C24-C26-C27
30	H	401	UQ9	C13-C14-C16-C17
24	A	401	3PE	C22-C21-O21-C2
27	H	402	PC1	C11-C12-N-C13
24	I	301	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
24	b	201	3PE	C32-C31-O31-C3
34	a	101	CDL	C12-C13-C14-C15
27	I	302	PC1	C11-C12-N-C15
24	I	301	3PE	O32-C31-O31-C3
24	b	201	3PE	O32-C31-O31-C3
30	H	401	UQ9	C19-C21-C22-C23
24	A	401	3PE	O22-C21-O21-C2
24	A	401	3PE	C11-O13-P-O11
24	I	301	3PE	C1-O11-P-O13
24	I	301	3PE	C11-O13-P-O11
27	H	402	PC1	C11-O13-P-O11
27	I	302	PC1	C1-O11-P-O13
34	a	101	CDL	C31-CA7-OA8-CA6
27	H	402	PC1	C11-C12-N-C15
34	a	101	CDL	OA9-CA7-OA8-CA6
27	H	402	PC1	C11-C12-N-C14
27	I	302	PC1	C11-C12-N-C13
24	A	401	3PE	C31-C32-C33-C34
34	a	101	CDL	C51-CB5-OB6-CB4
34	a	101	CDL	OB7-CB5-OB6-CB4
27	I	302	PC1	C11-C12-N-C14
24	I	301	3PE	C22-C21-O21-C2
24	I	301	3PE	C24-C25-C26-C27
24	b	201	3PE	C2A-C2B-C2C-C2D
24	I	301	3PE	O22-C21-O21-C2
27	B	303	PC1	C2-C1-O11-P
27	B	303	PC1	C32-C33-C34-C35
33	W	201	EHZ	N2-C15-C16-C17
33	W	201	EHZ	C3-C4-C5-C6
33	W	201	EHZ	C5-C6-C7-O1
27	B	303	PC1	C32-C31-O31-C3
33	W	201	EHZ	O2-C9-S1-C10
24	A	401	3PE	C3-C2-O21-C21
31	P	401	NDP	C2B-O2B-P2B-O2X
27	B	303	PC1	O32-C31-O31-C3
24	A	401	3PE	C2E-C2F-C2G-C2H
24	A	401	3PE	C2-C1-O11-P
34	a	101	CDL	CA4-CA3-OA5-PA1
24	A	401	3PE	C11-O13-P-O14
24	I	301	3PE	C1-O11-P-O12
24	I	301	3PE	C1-O11-P-O14
24	I	301	3PE	C11-O13-P-O14

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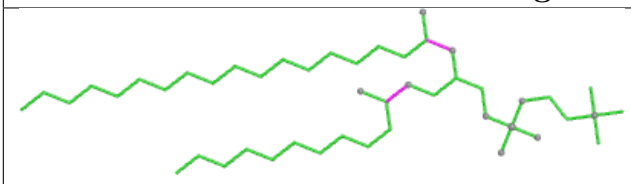
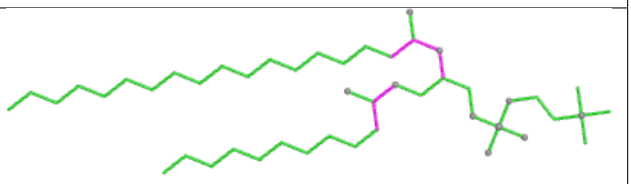
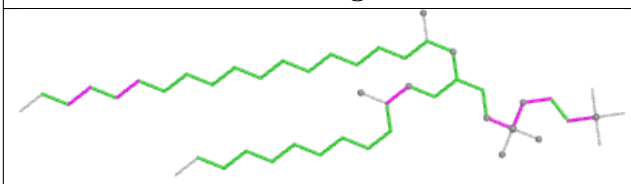
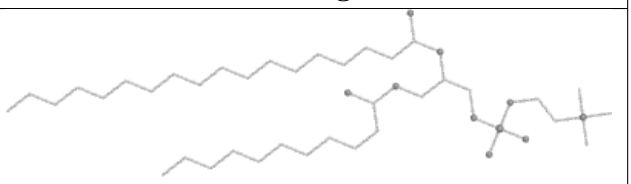
Mol	Chain	Res	Type	Atoms
27	H	402	PC1	C1-O11-P-O14
24	A	401	3PE	O11-C1-C2-C3
24	A	401	3PE	O11-C1-C2-O21
27	B	303	PC1	O13-C11-C12-N
27	H	402	PC1	O13-C11-C12-N
24	I	301	3PE	O21-C2-C3-O31
33	W	201	EHZ	O4-C15-C16-O5
33	W	201	EHZ	C19-C17-C20-O6
24	b	201	3PE	C2B-C2C-C2D-C2E
34	a	101	CDL	CB2-OB2-PB2-OB5
33	W	201	EHZ	C2-C3-C4-C5
31	P	401	NDP	O4D-C1D-N1N-C6N
26	B	302	UQ1	C1-C2-O2-CM2
34	a	101	CDL	C1-CB2-OB2-PB2
27	B	303	PC1	C34-C35-C36-C37
31	P	401	NDP	C2D-C1D-N1N-C6N
24	I	301	3PE	C37-C38-C39-C3A
27	H	402	PC1	C34-C35-C36-C37
24	b	201	3PE	C24-C25-C26-C27
27	I	302	PC1	C2E-C2F-C2G-C2H
31	P	401	NDP	PN-O3-PA-O2A
30	H	401	UQ9	C12-C11-C9-C10
24	I	301	3PE	C35-C36-C37-C38
24	I	301	3PE	C33-C34-C35-C36
29	F	501	FMN	C5'-O5'-P-O2P
33	W	201	EHZ	N2-C15-C16-O5
33	W	201	EHZ	C18-C17-C20-O6
33	W	201	EHZ	C8-C9-S1-C10
33	W	201	EHZ	C15-C16-C17-C18
31	P	401	NDP	C2B-O2B-P2B-O3X
33	W	201	EHZ	O5-C16-C17-C18
34	a	101	CDL	C32-C31-CA7-OA8
30	H	401	UQ9	C12-C11-C9-C8
24	I	301	3PE	C1-C2-C3-O31
24	A	401	3PE	O13-C11-C12-N
27	I	302	PC1	C12-C11-O13-P
33	W	201	EHZ	O4-C15-C16-C17
34	a	101	CDL	OA7-CA5-OA6-CA4
24	I	301	3PE	C2-C1-O11-P
34	a	101	CDL	C32-C31-CA7-OA9
24	b	201	3PE	C39-C3A-C3B-C3C
27	I	302	PC1	C2C-C2D-C2E-C2F

There are no ring outliers.

19 monomers are involved in 158 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	I	302	PC1	9	0
25	F	502	SF4	10	0
29	F	501	FMN	1	0
28	G	803	FES	4	0
27	B	303	PC1	7	0
28	E	301	FES	5	0
25	G	802	SF4	5	0
31	P	401	NDP	7	0
30	H	401	UQ9	4	0
24	I	301	3PE	14	0
24	b	201	3PE	16	0
26	B	302	UQ1	13	0
25	B	301	SF4	6	0
24	A	401	3PE	6	0
27	H	402	PC1	6	0
25	I	303	SF4	11	0
34	a	101	CDL	22	0
33	W	201	EHZ	7	0
25	I	304	SF4	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PC1 I 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

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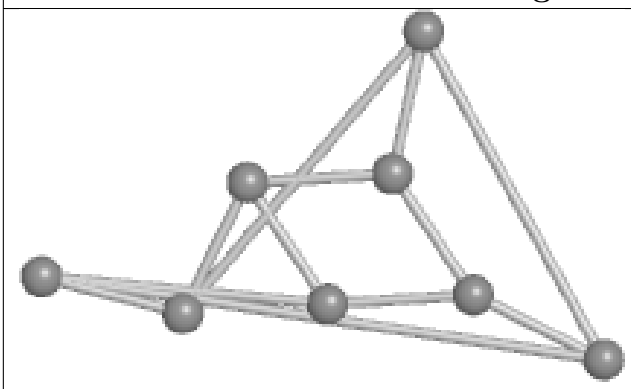
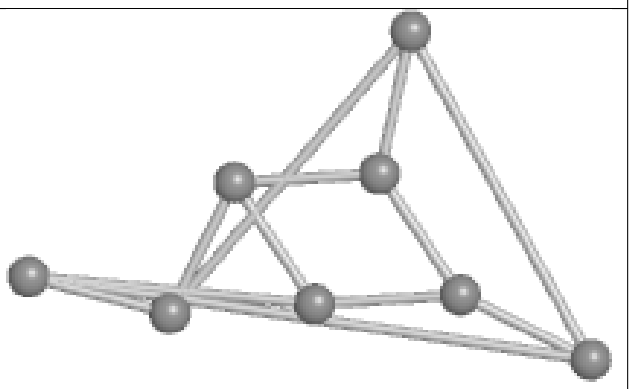
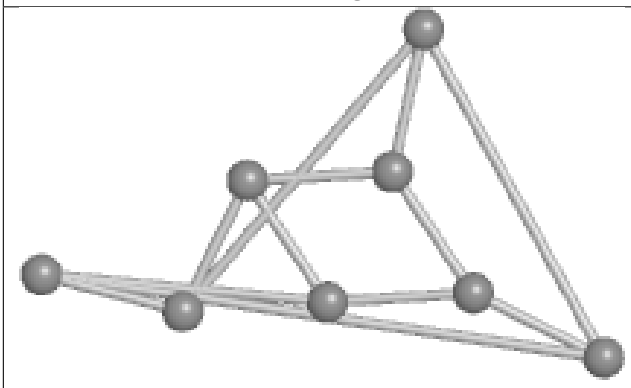
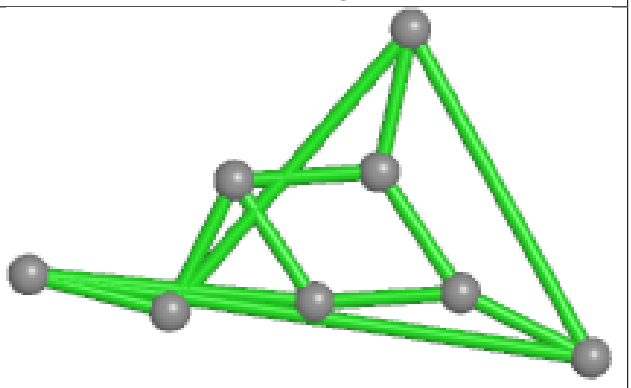
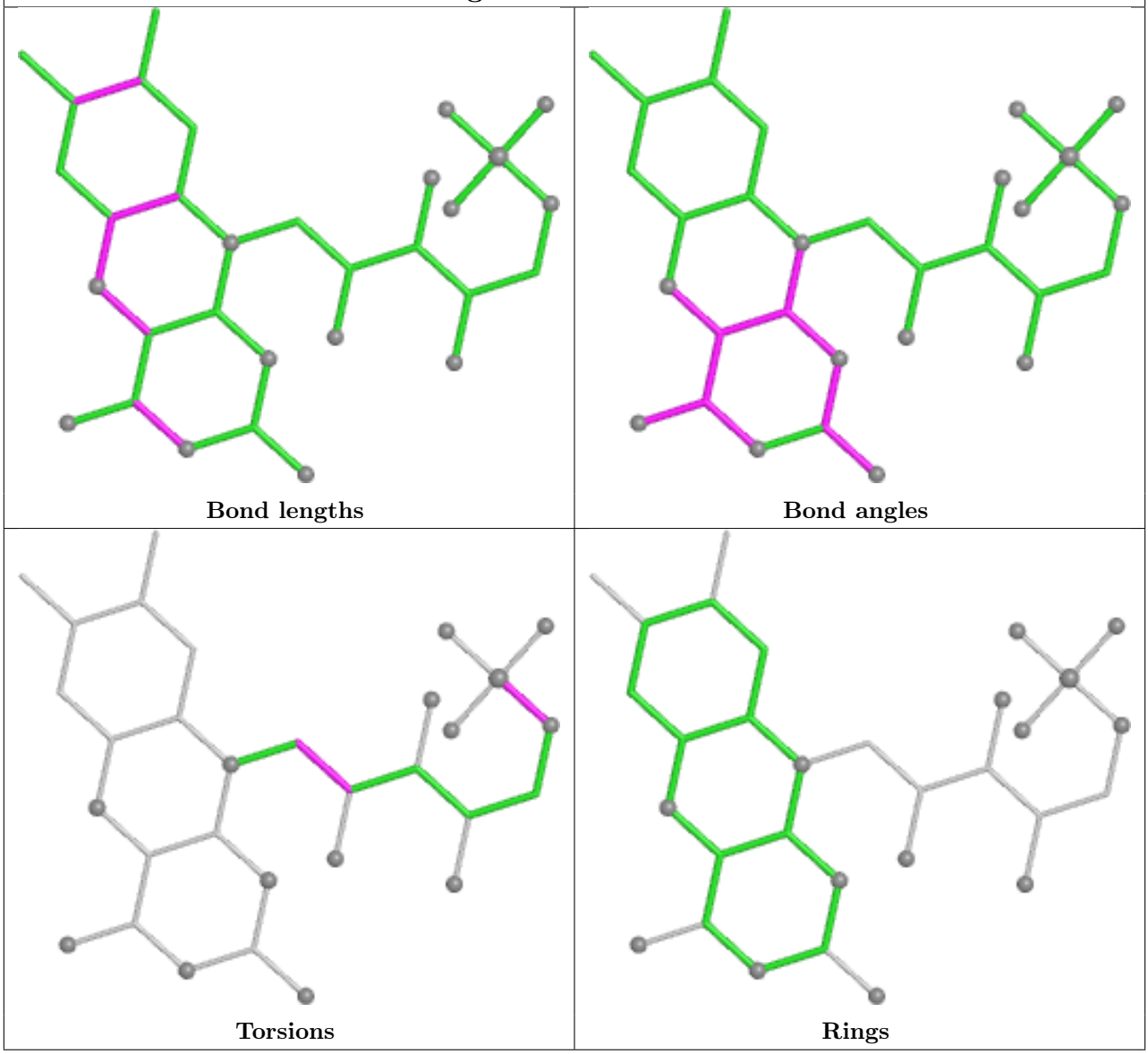
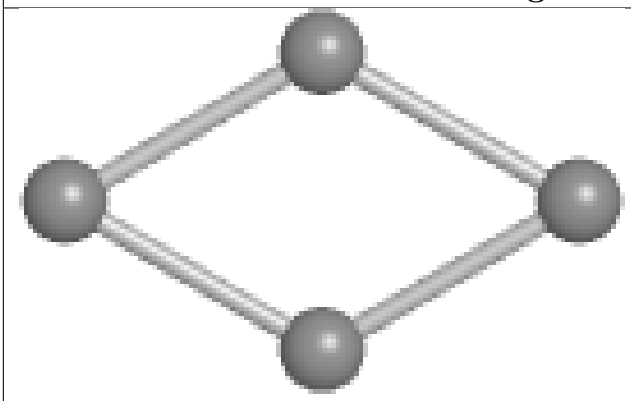
 Bond lengths	 Bond angles
 Torsions	 Rings

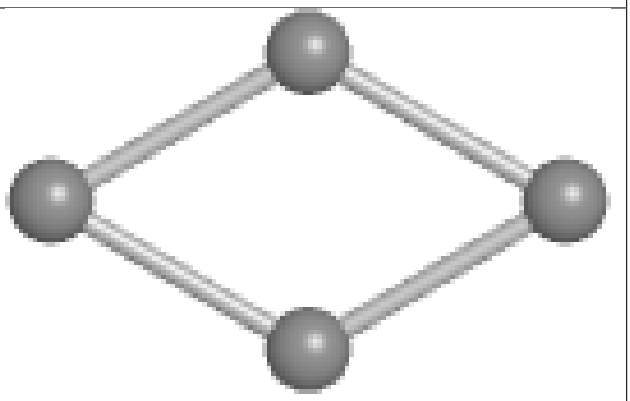
Ligand FMN F 501



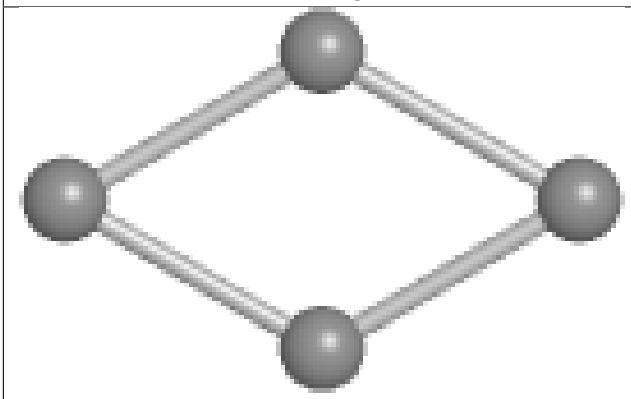
Ligand FES G 803



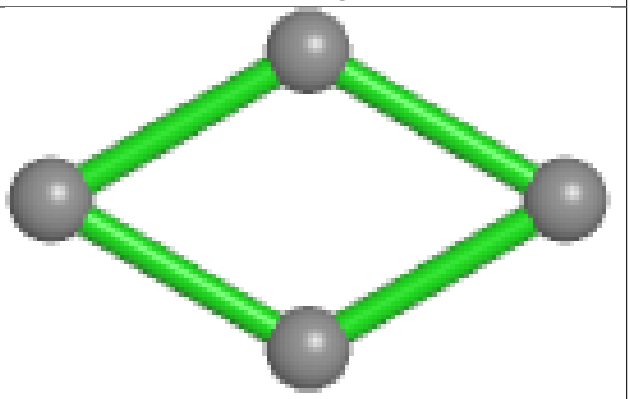
Bond lengths



Bond angles

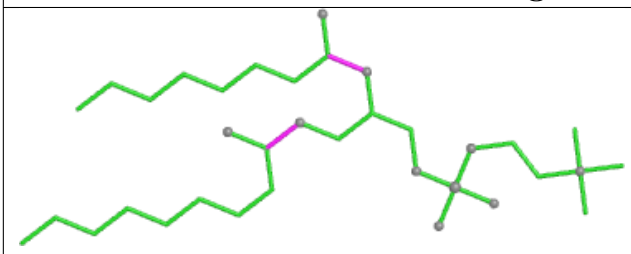


Torsions

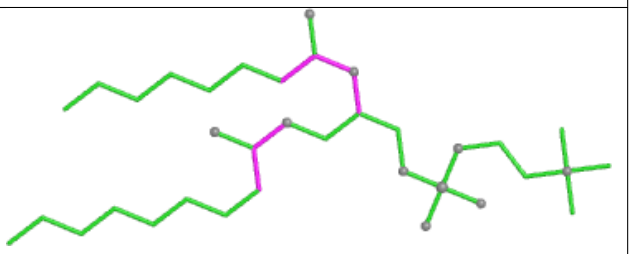


Rings

Ligand PC1 B 303



Bond lengths



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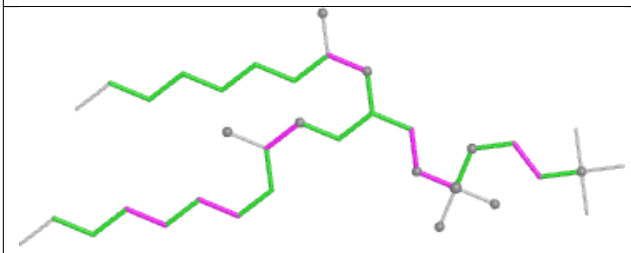
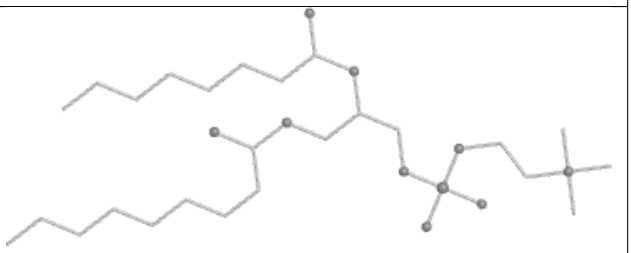
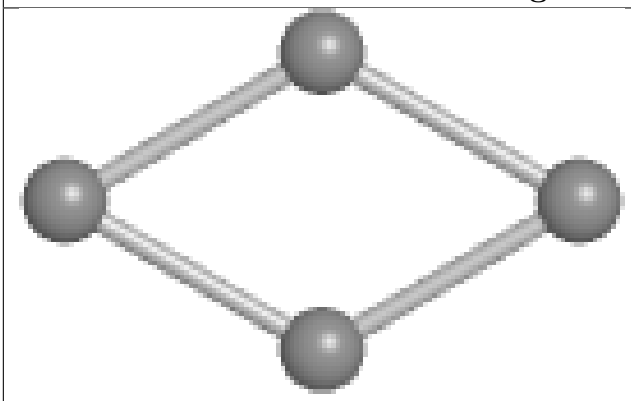
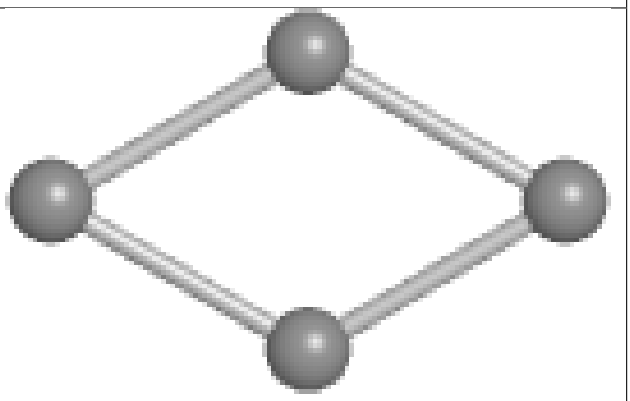
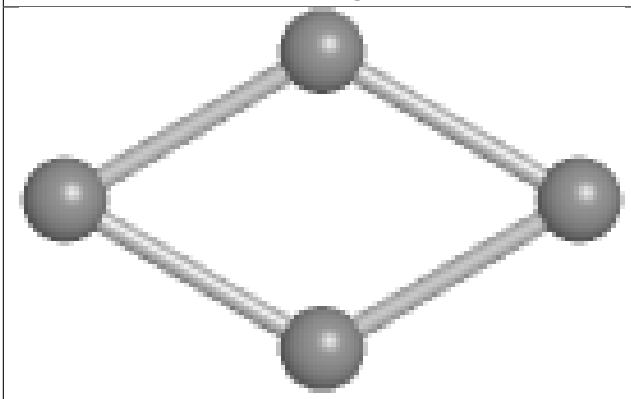
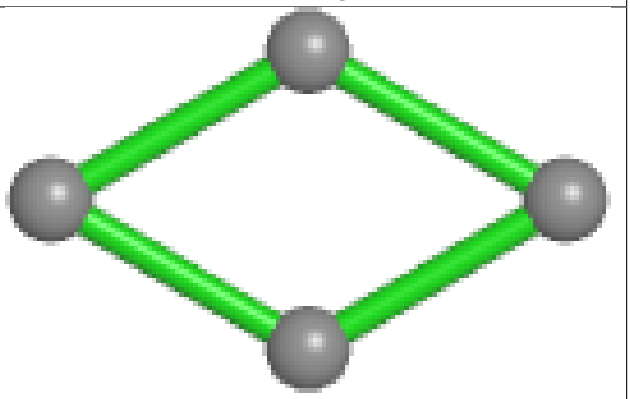


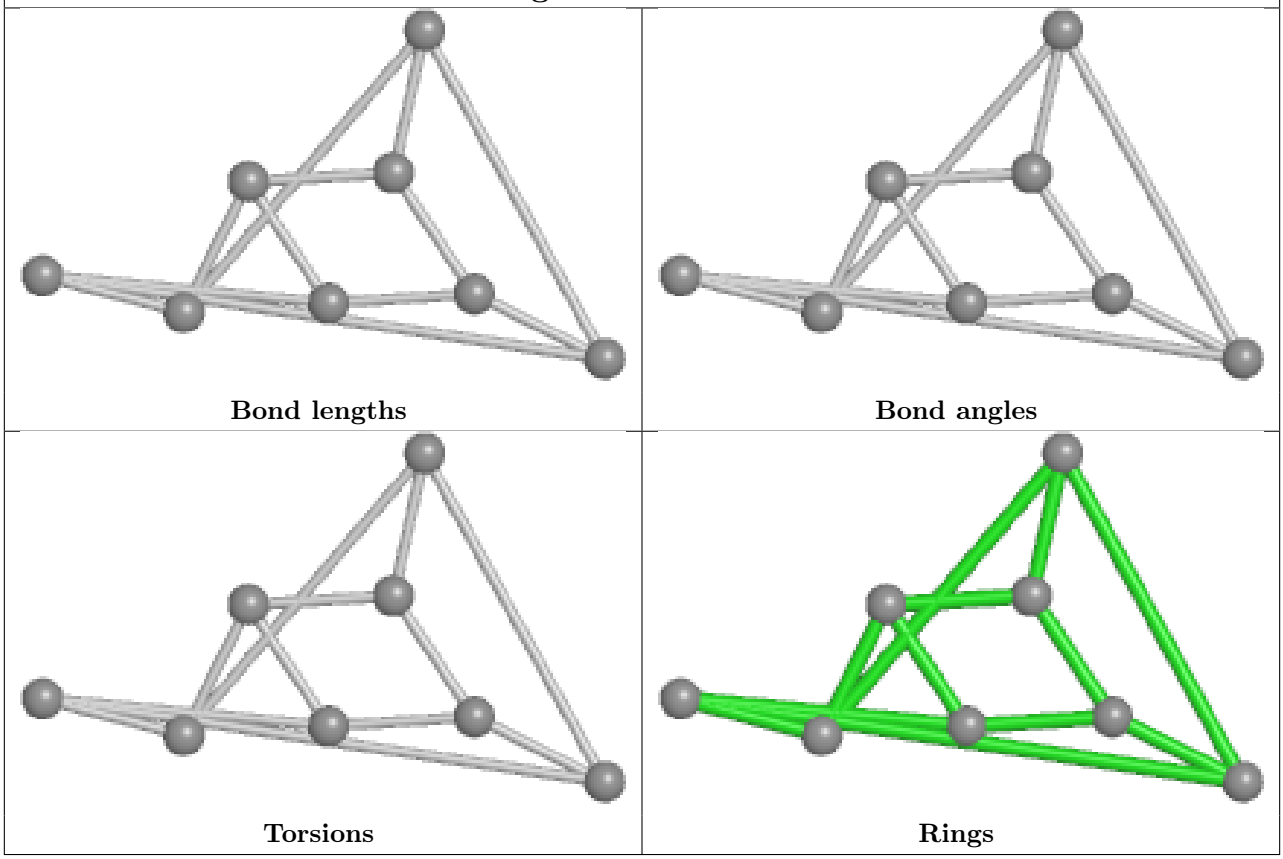
Torsions



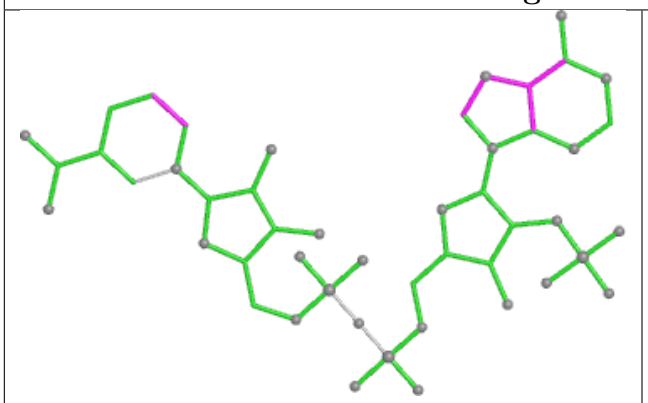
Rings

Ligand FES E 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

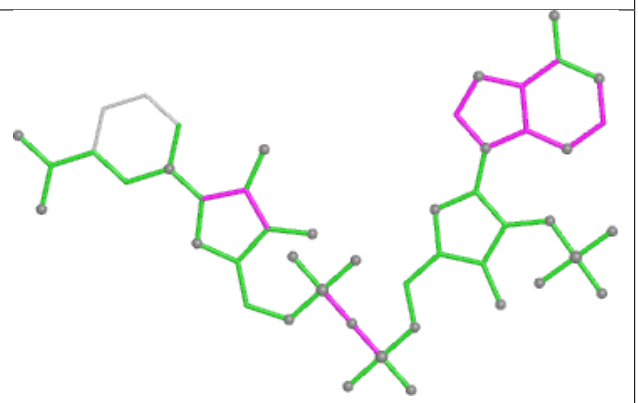
Ligand SF4 G 802



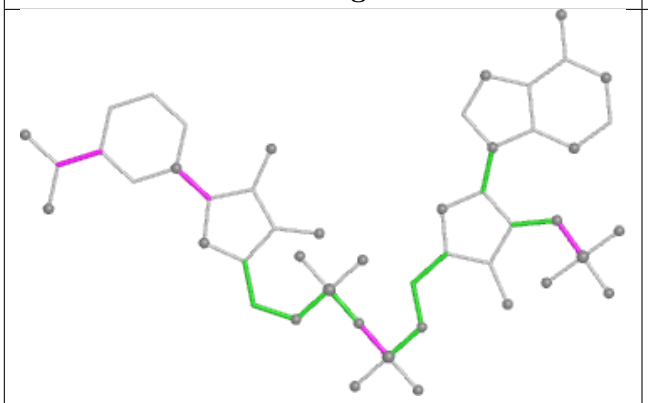
Ligand NDP P 401



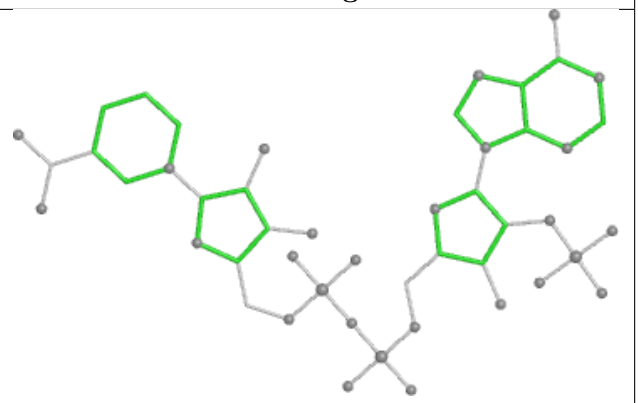
Bond lengths



Bond angles

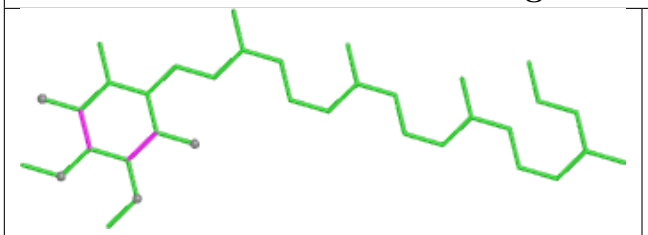


Torsions

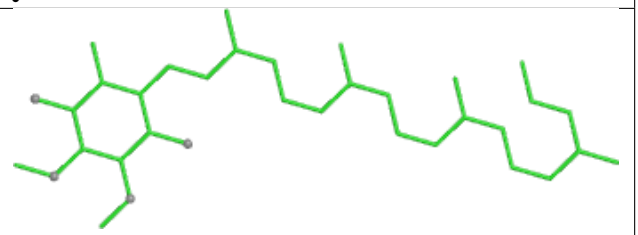


Rings

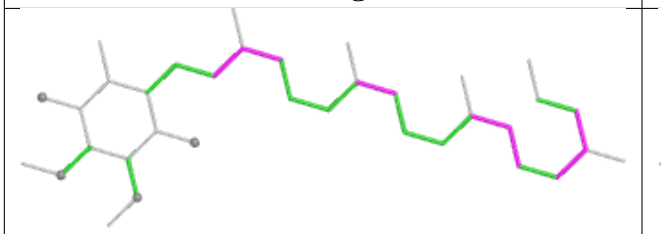
Ligand UQ9 H 401



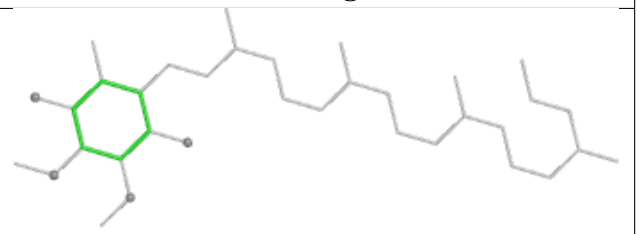
Bond lengths



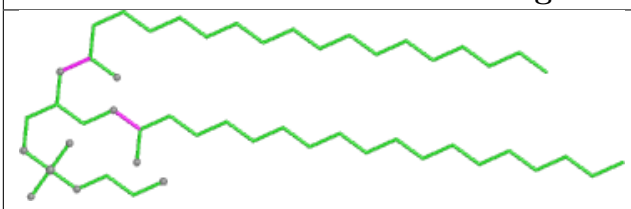
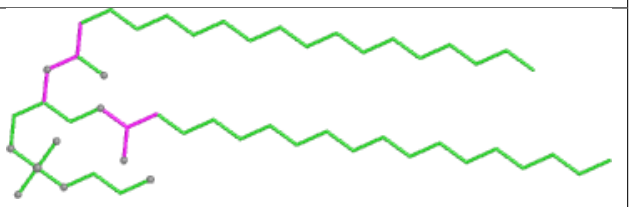
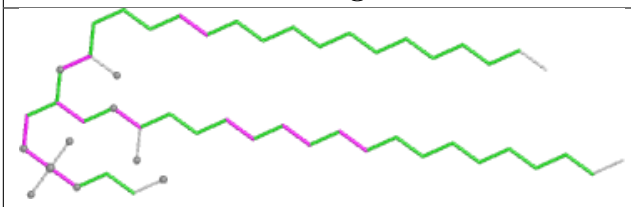
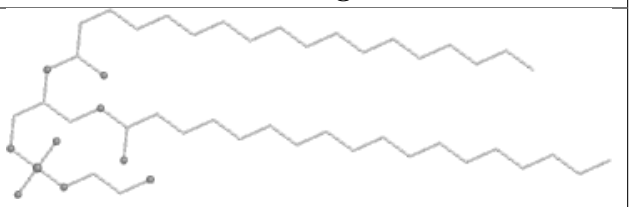
Bond angles

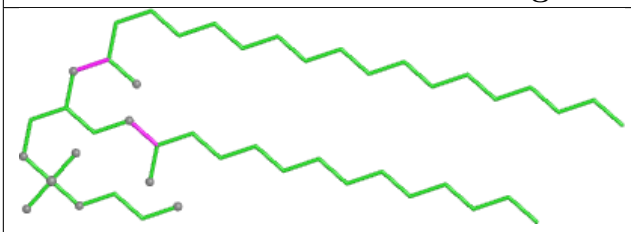
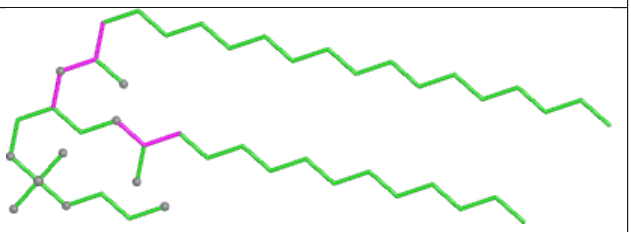
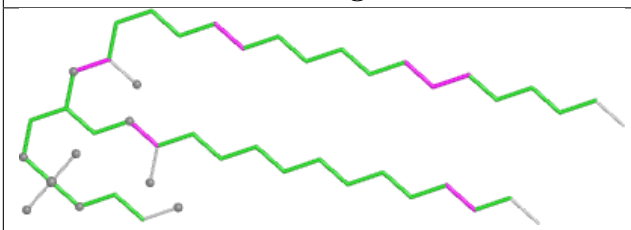
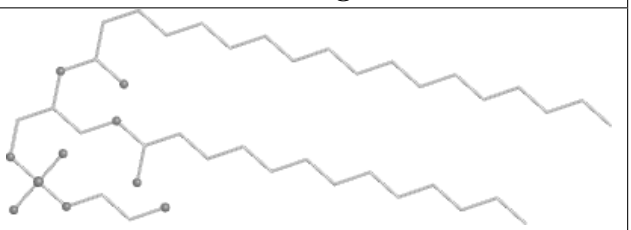


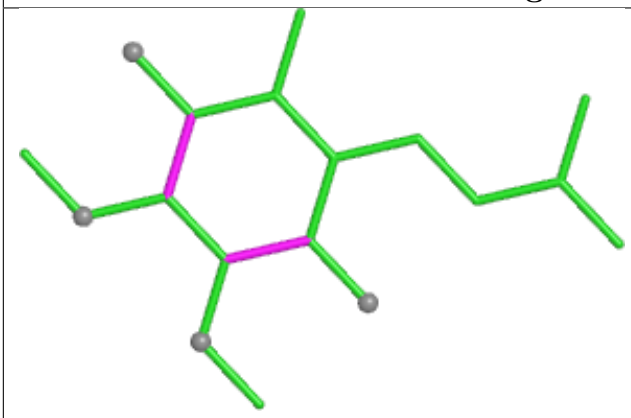
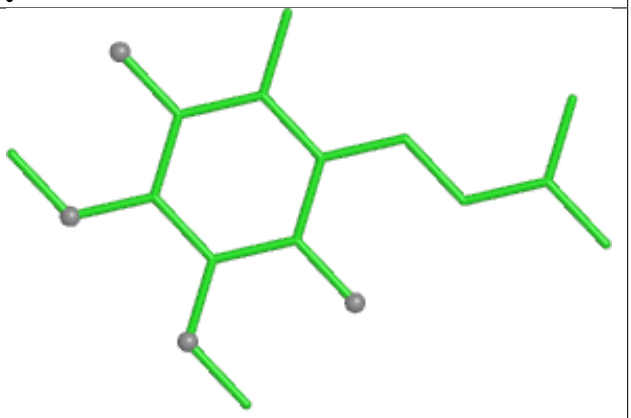
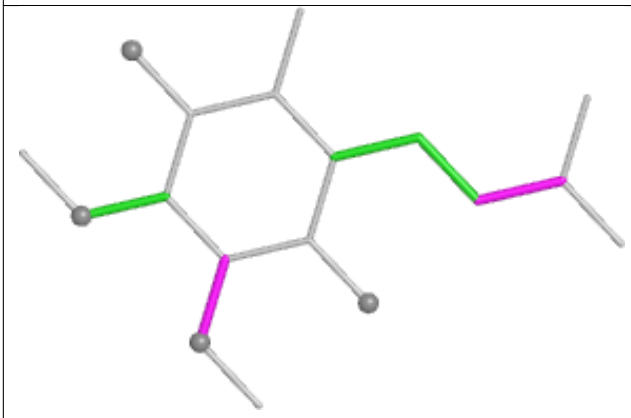
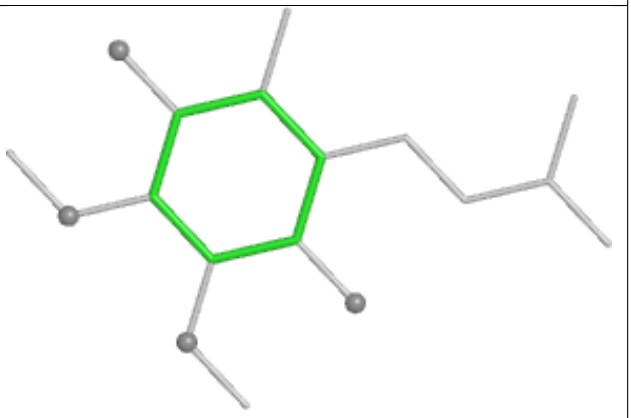
Torsions



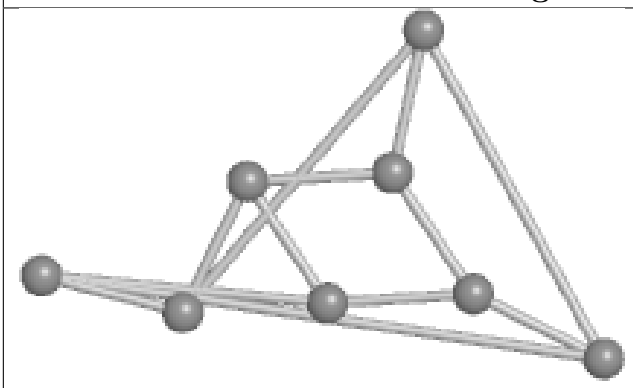
Rings

Ligand 3PE I 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

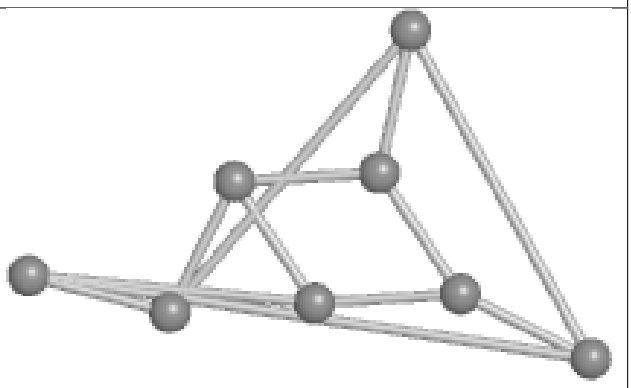
Ligand 3PE b 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ1 B 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

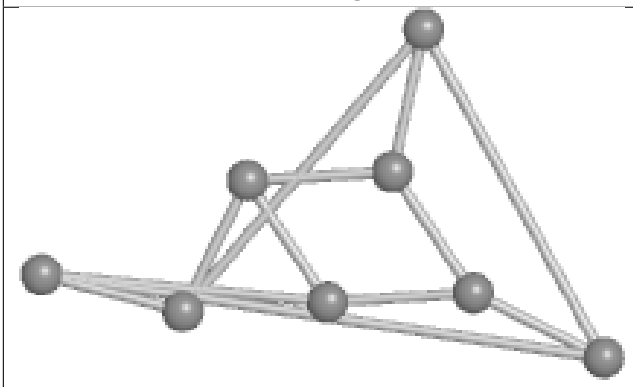
Ligand SF4 B 301



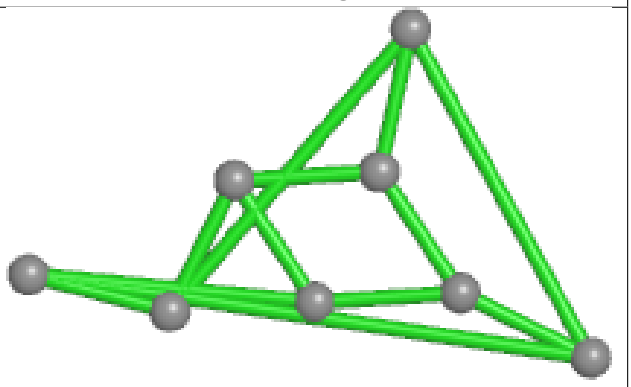
Bond lengths



Bond angles

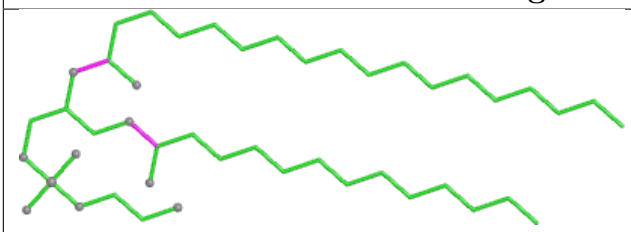


Torsions

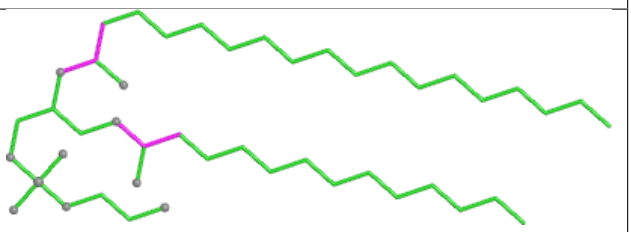


Rings

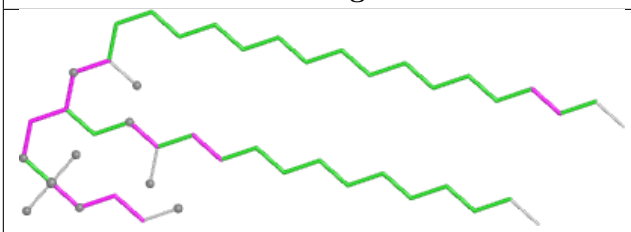
Ligand 3PE A 401



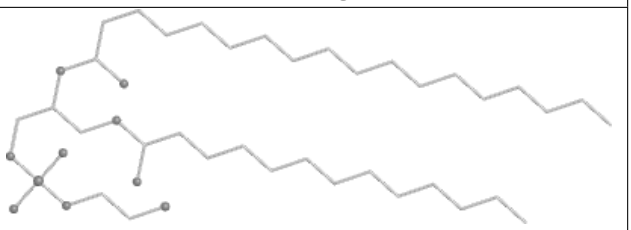
Bond lengths



Bond angles

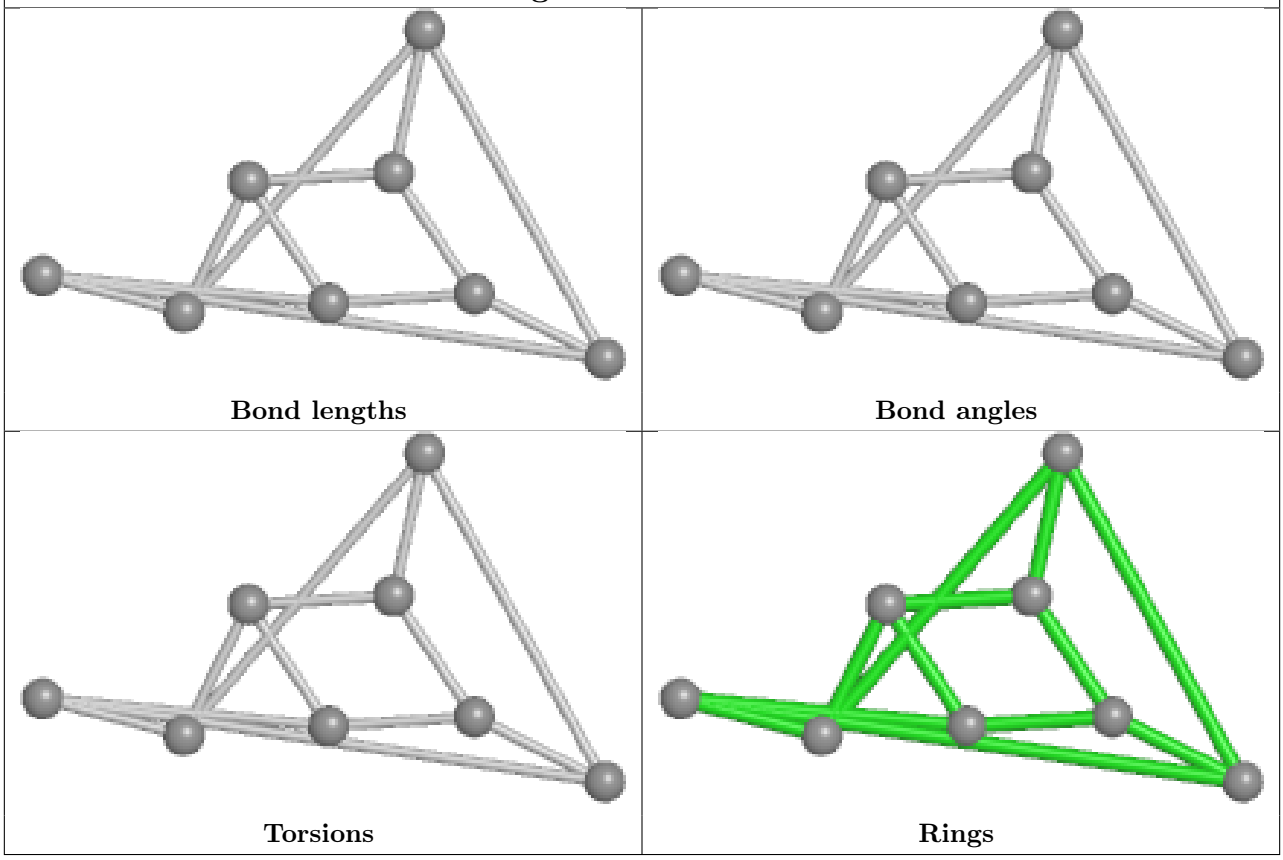


Torsions

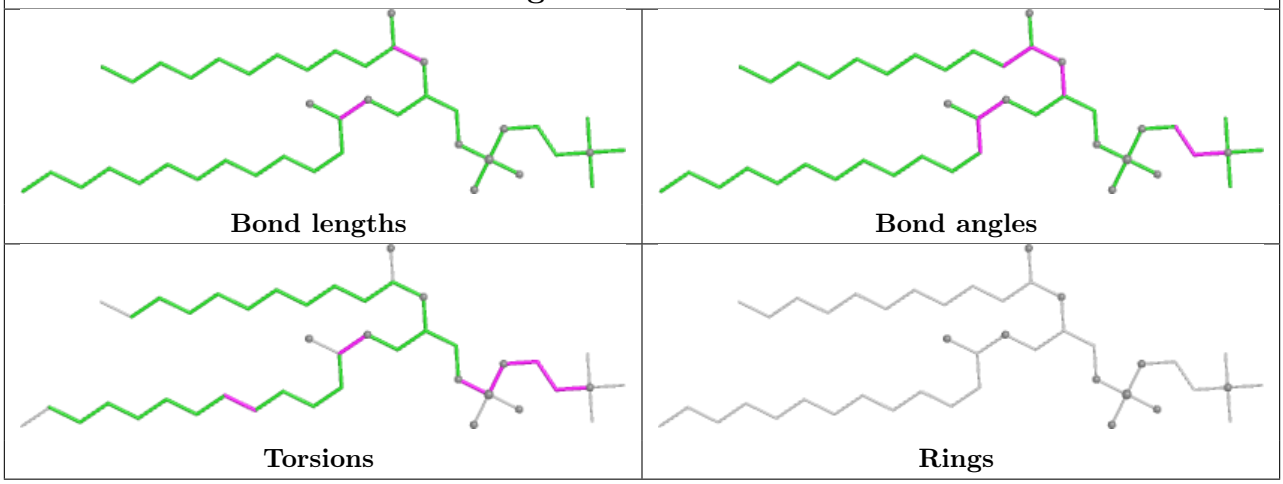


Rings

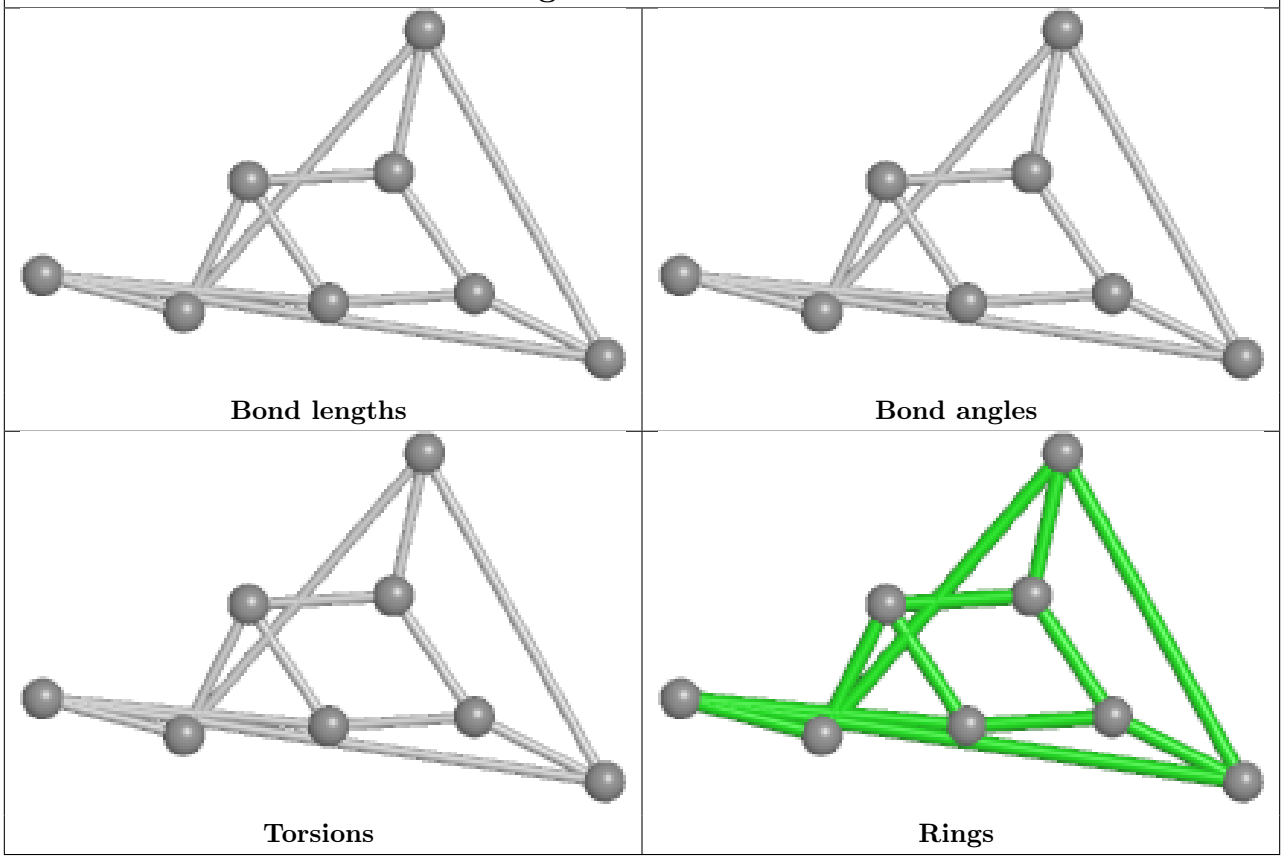
Ligand SF4 G 801



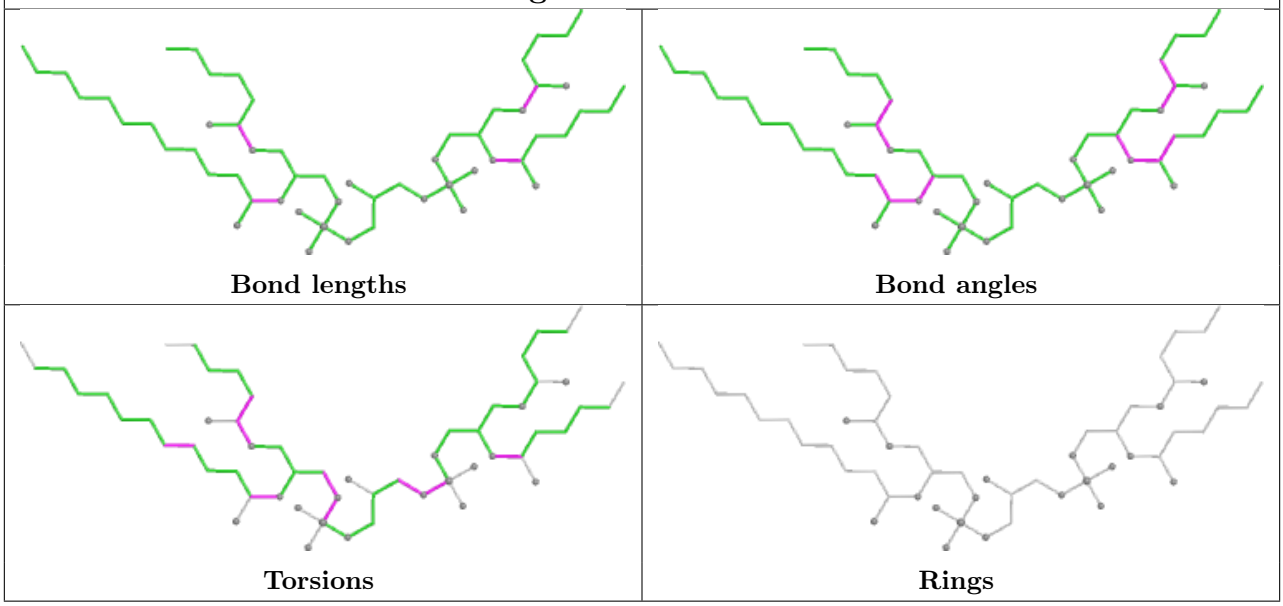
Ligand PC1 H 402



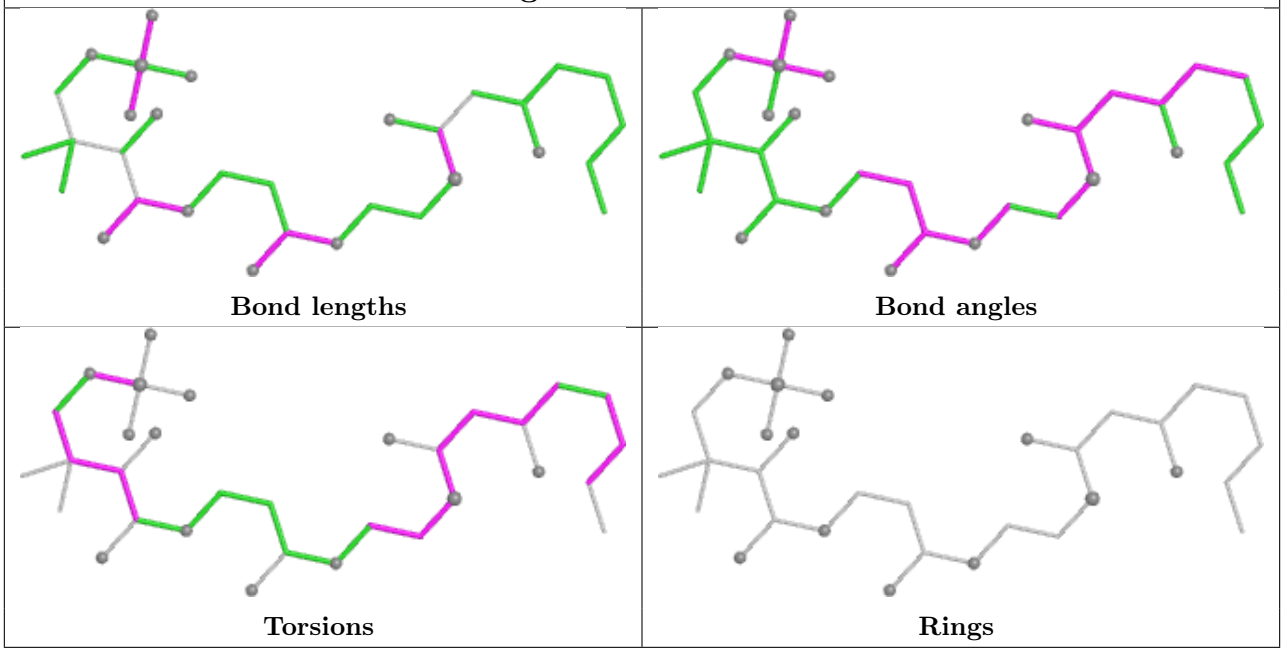
Ligand SF4 I 303



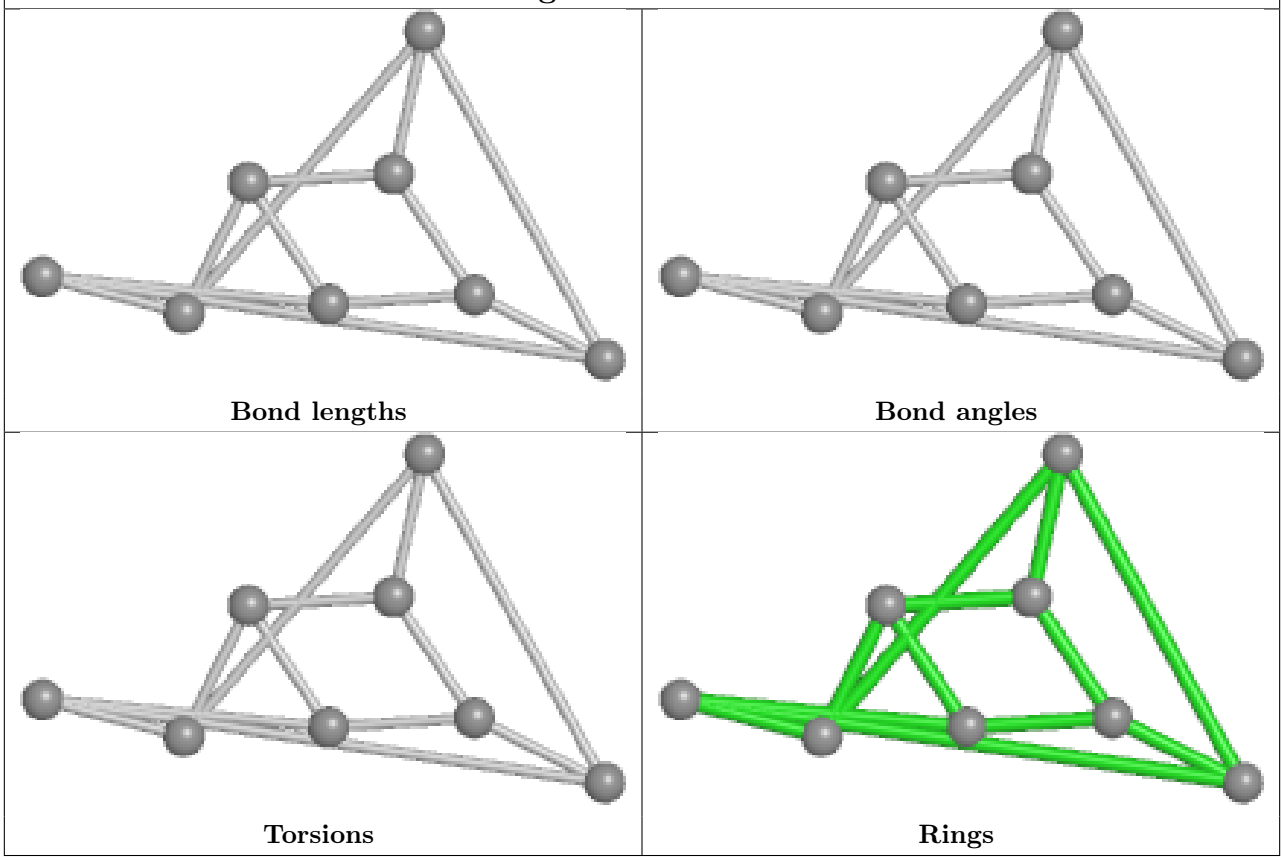
Ligand CDL a 101



Ligand EHZ W 201



Ligand SF4 I 304



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

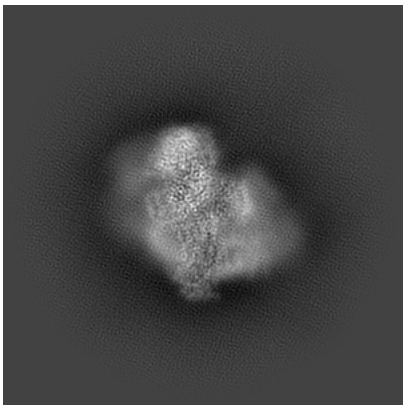
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35332. These allow visual inspection of the internal detail of the map and identification of artifacts.

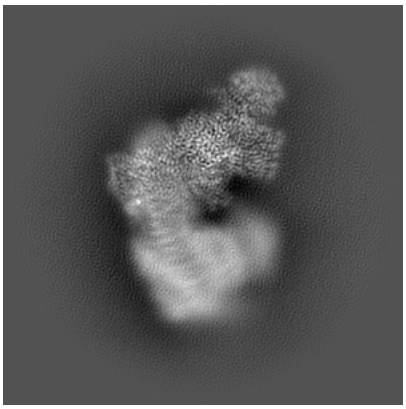
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

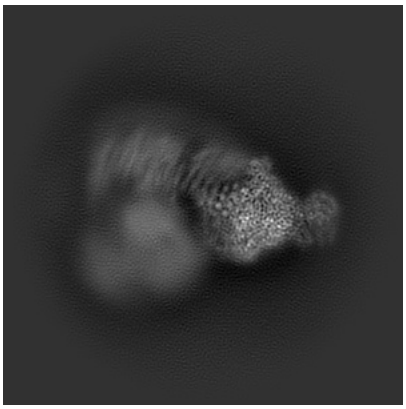
6.1.1 Primary map



X

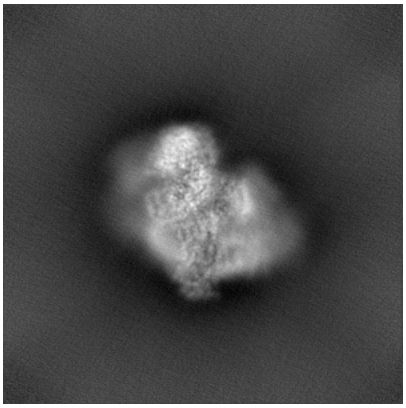


Y

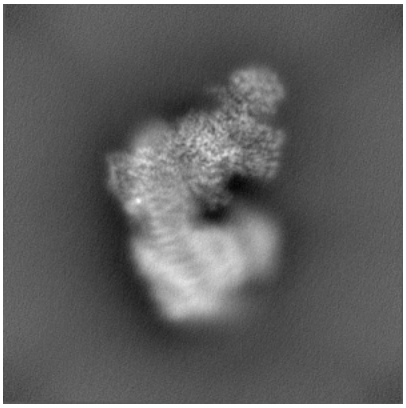


Z

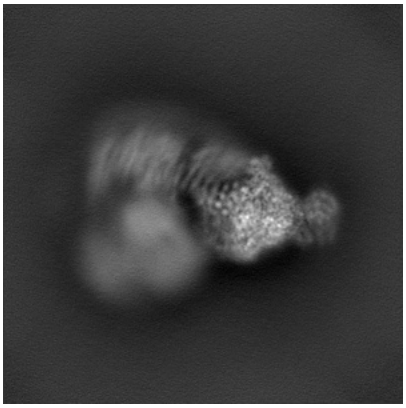
6.1.2 Raw map



X



Y

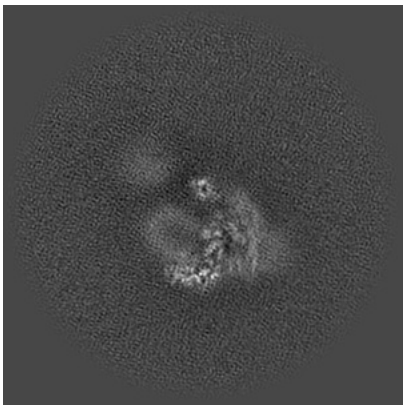


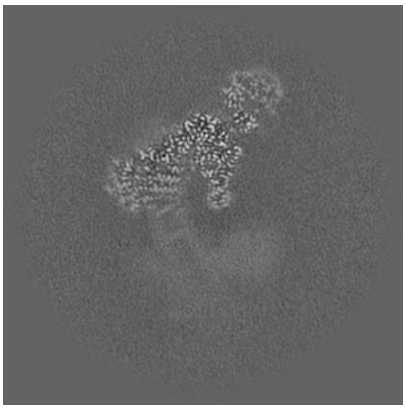
Z

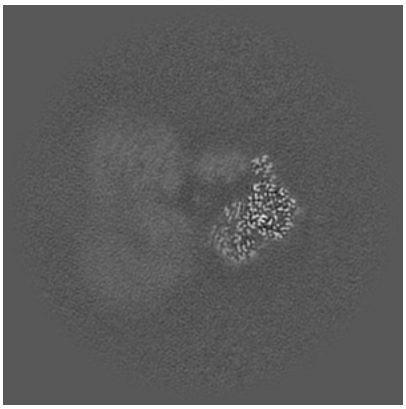
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

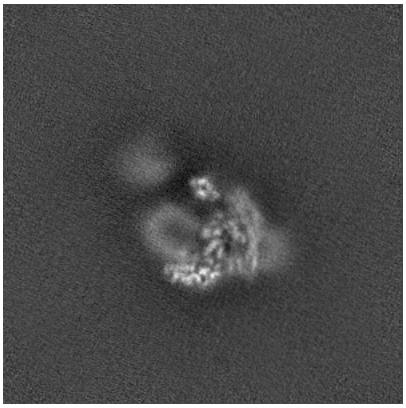
6.2.1 Primary map

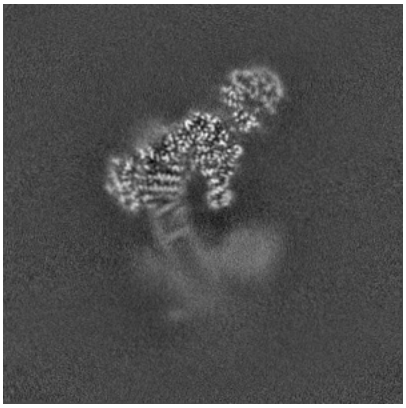

X Index: 192

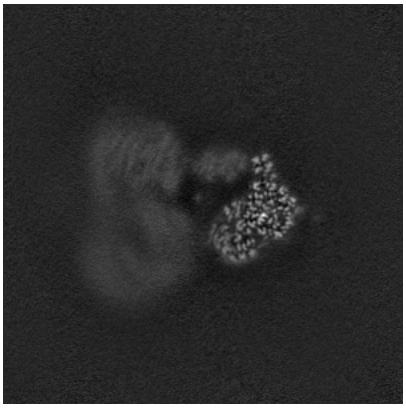

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

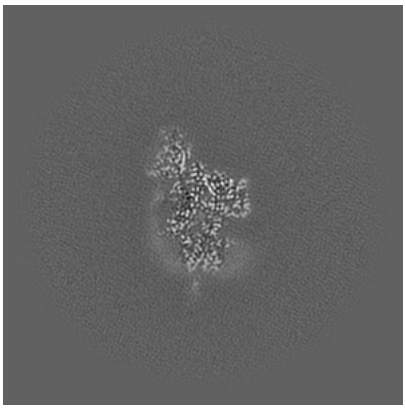

Y Index: 192

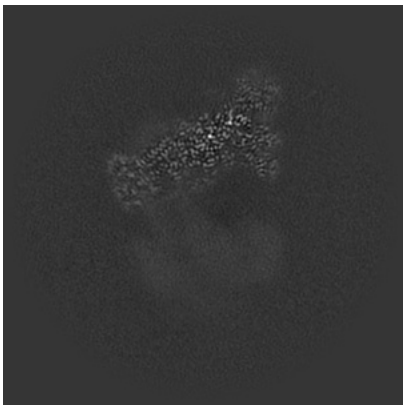

Z Index: 192

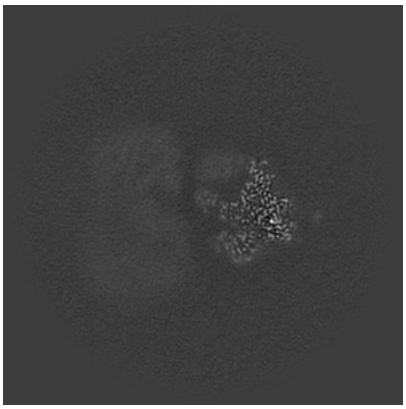
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

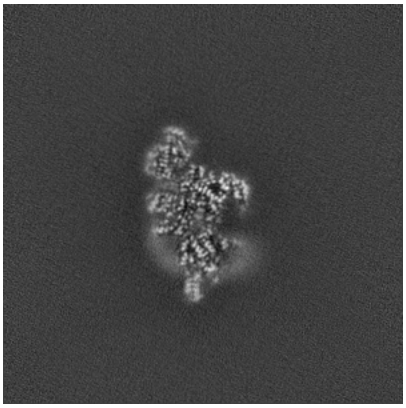
6.3.1 Primary map

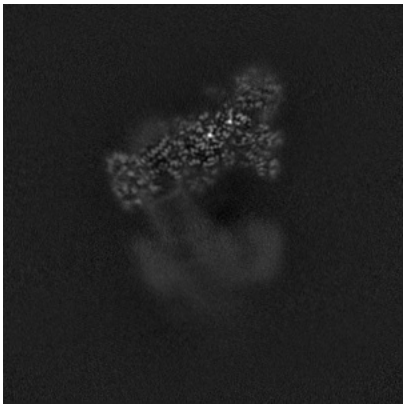

X Index: 243

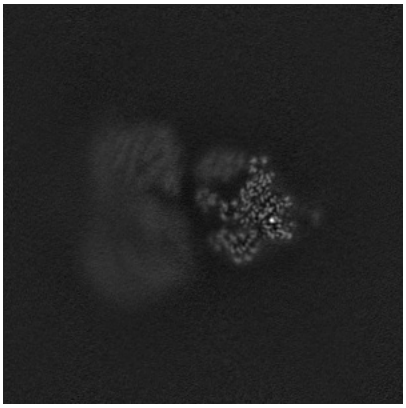

Y Index: 176


Z Index: 199

6.3.2 Raw map


X Index: 238

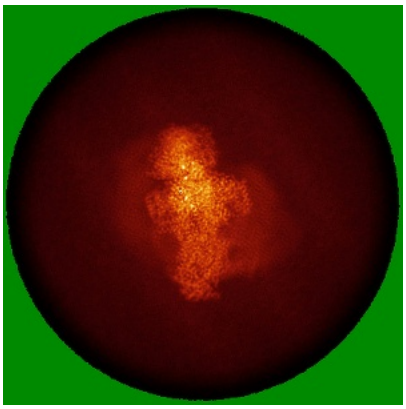

Y Index: 176

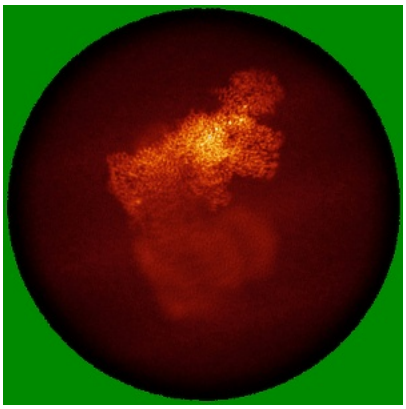

Z Index: 198

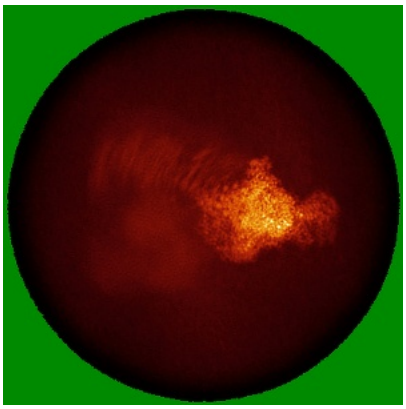
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

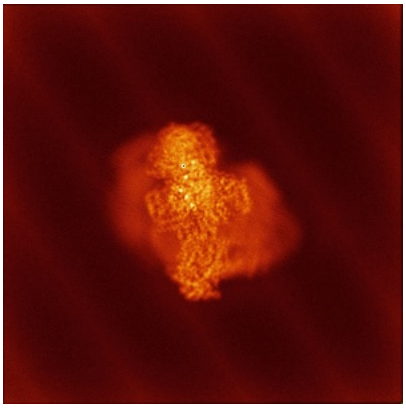
6.4.1 Primary map

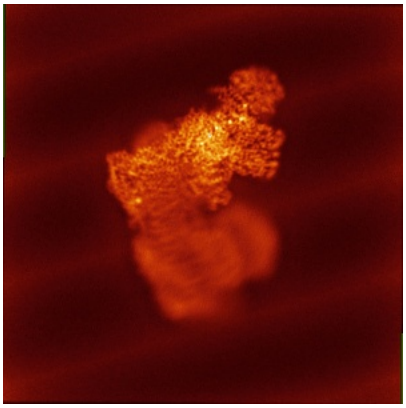

X

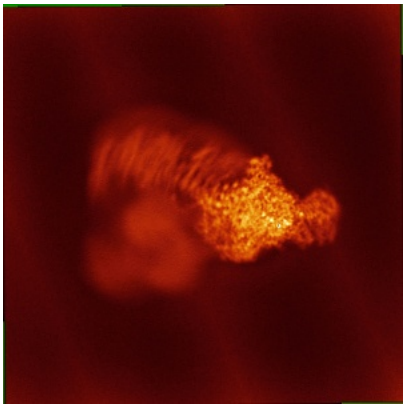

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

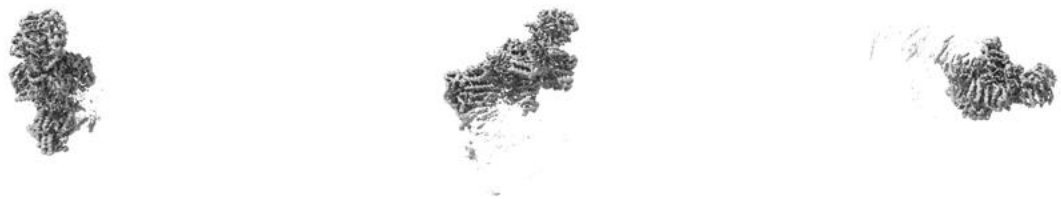
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

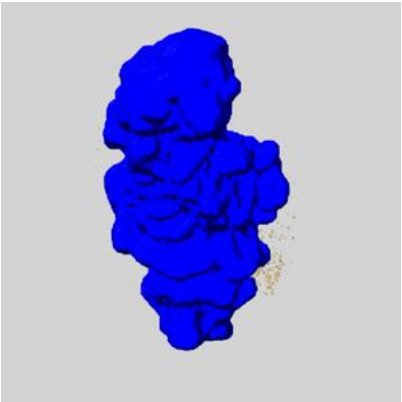
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

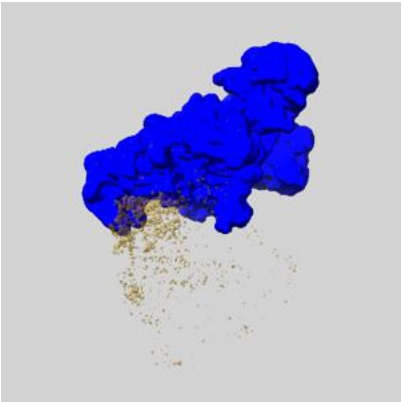
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

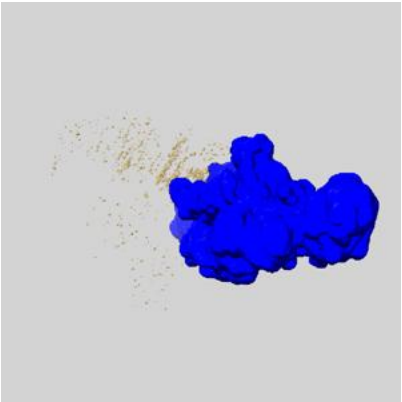
6.6.1 emd_35332_msk_1.map (i)



X



Y

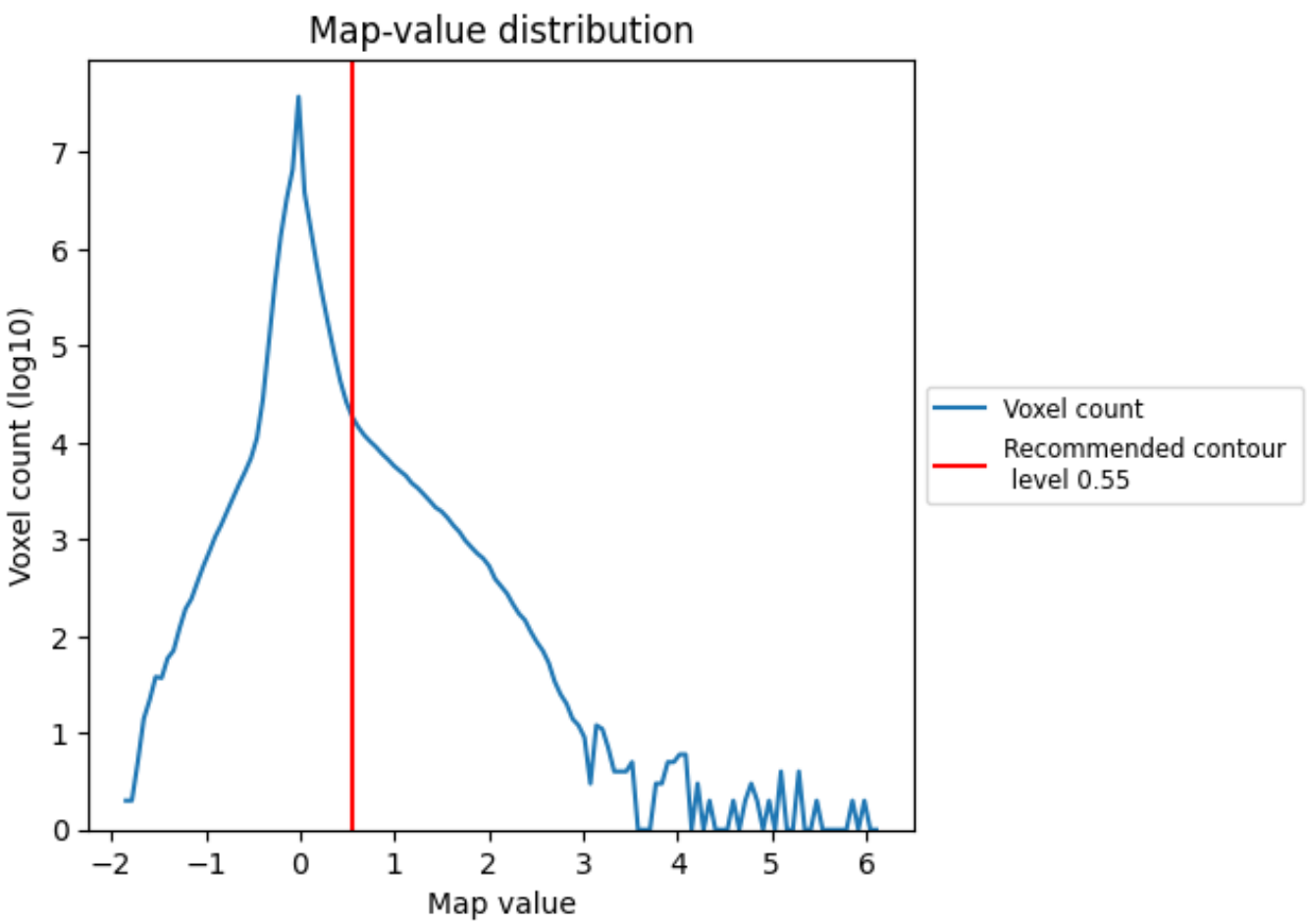


Z

7 Map analysis (i)

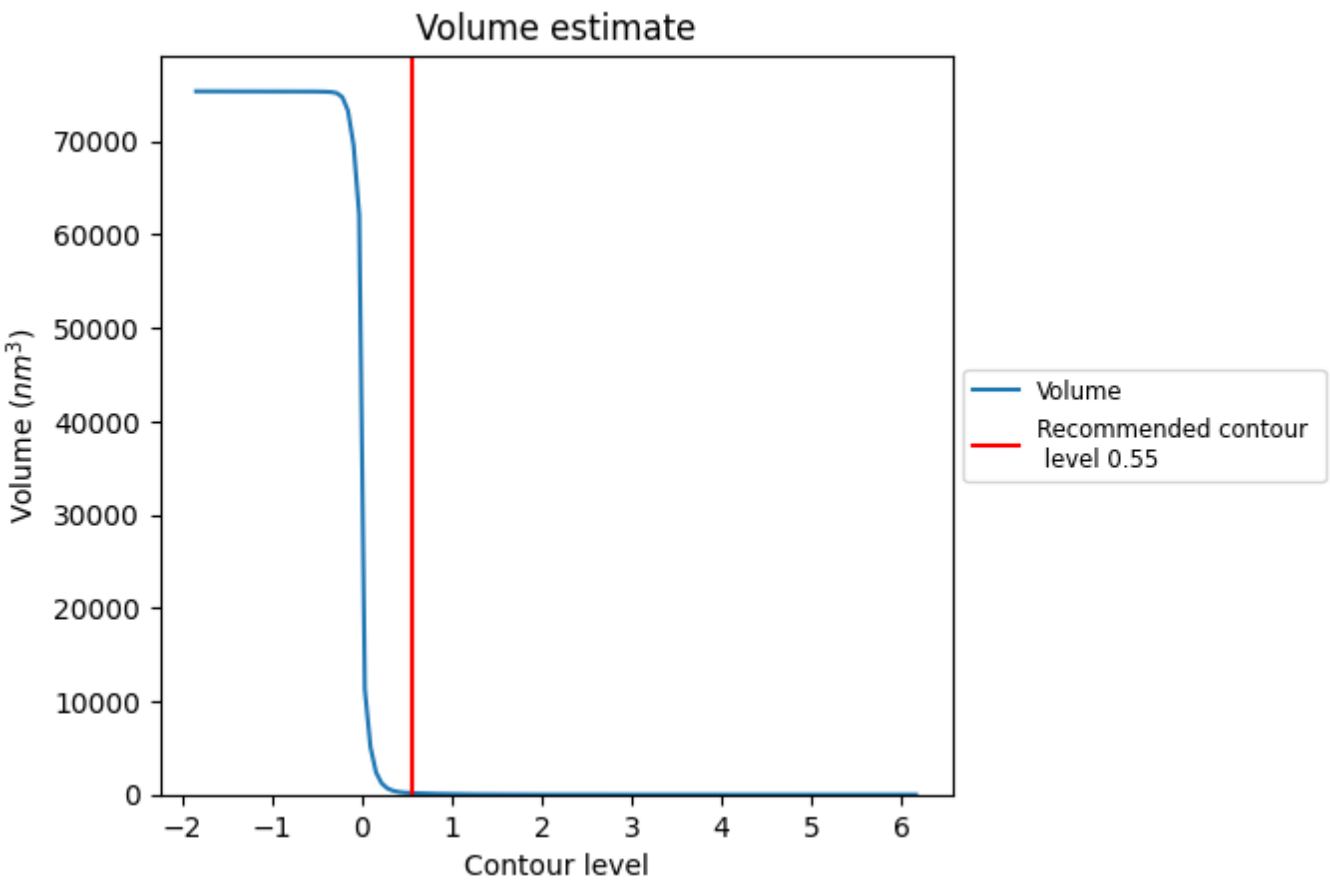
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

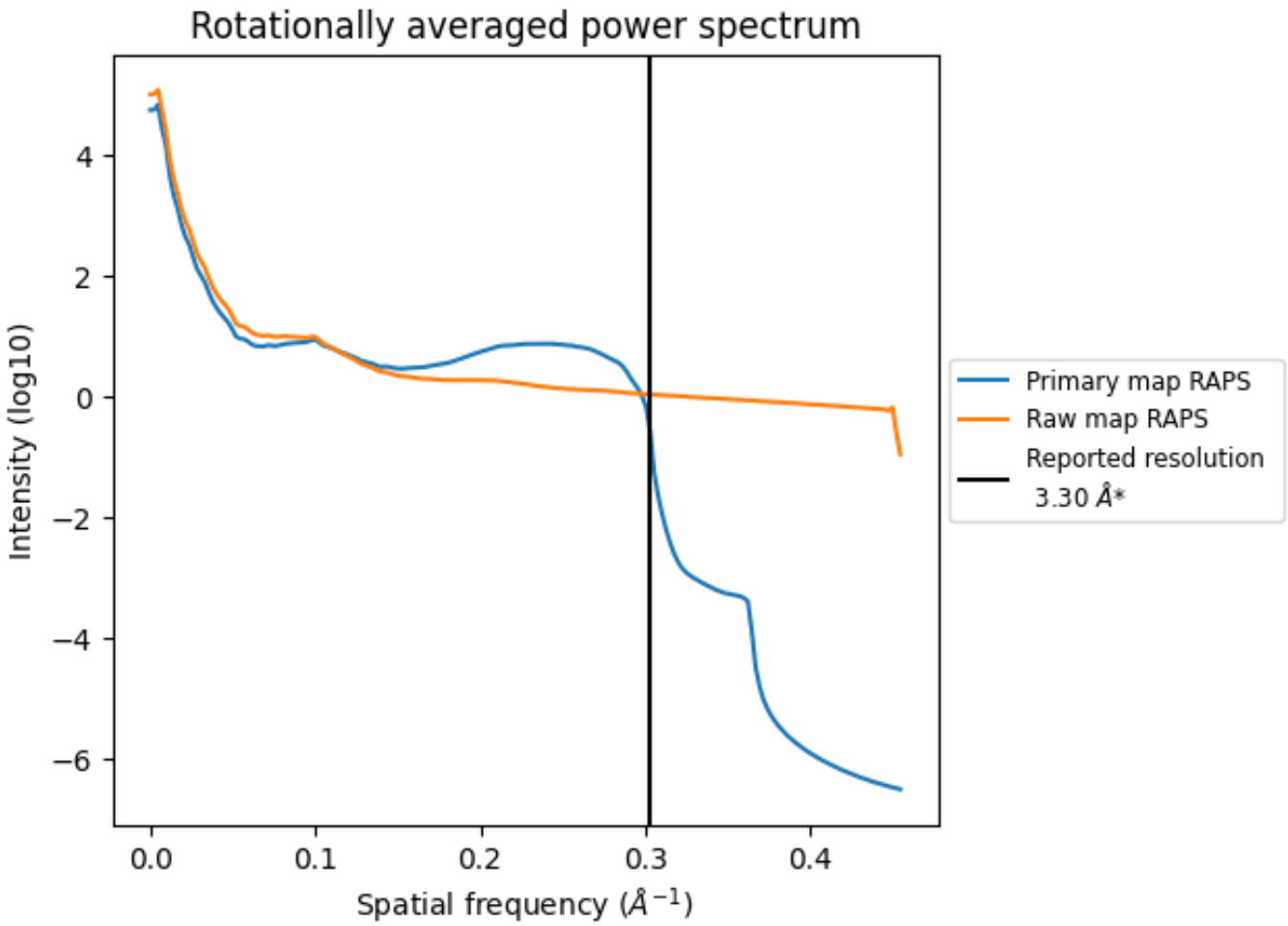
7.2 Volume estimate (i)



The volume at the recommended contour level is 163 nm^3; this corresponds to an approximate mass of 148 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

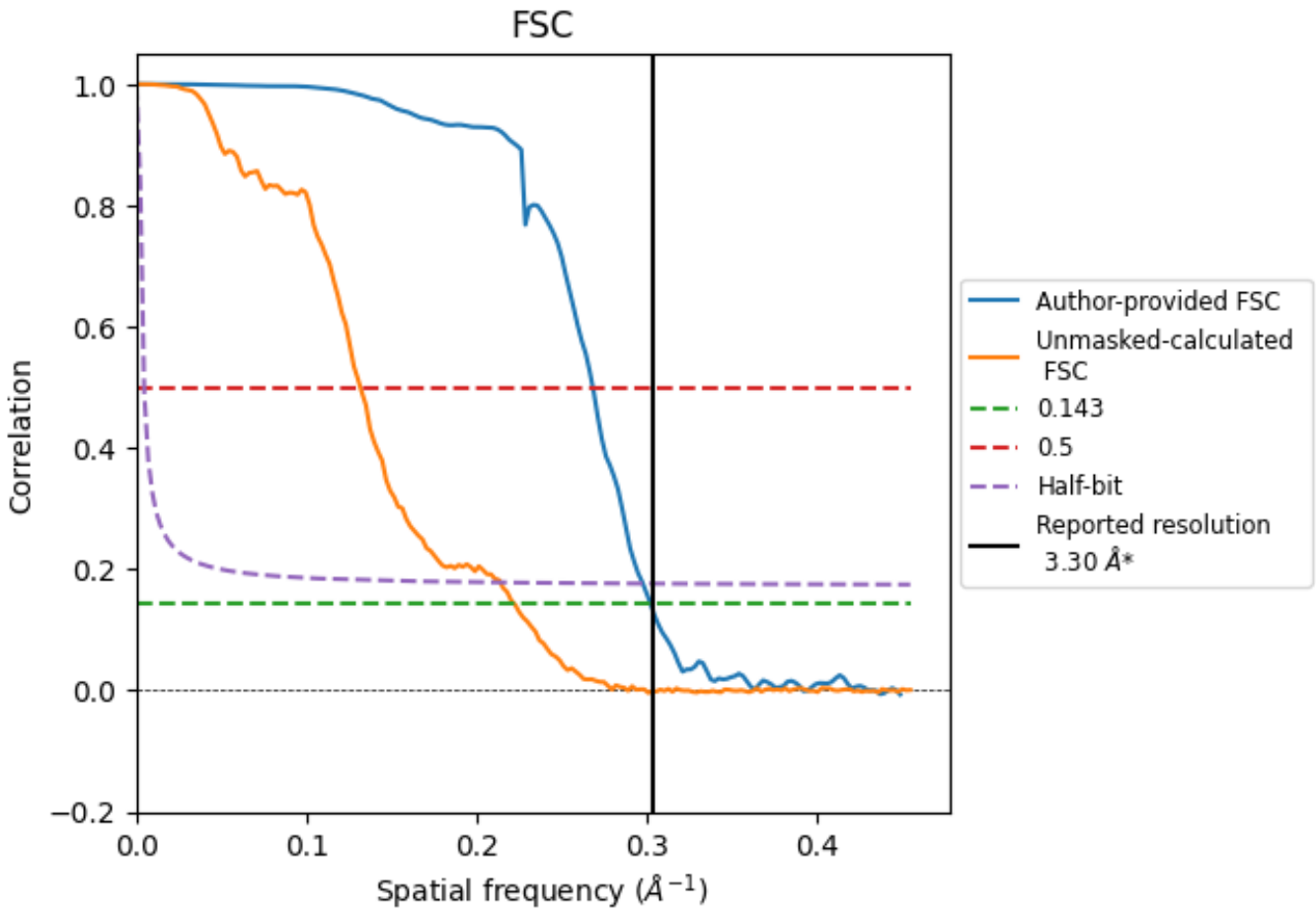


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

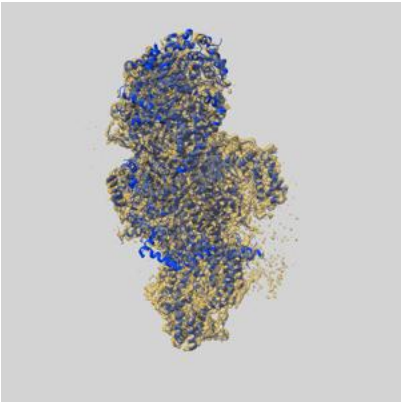
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.73	3.36
Unmasked-calculated*	4.50	7.60	4.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.3 by more than 10 %

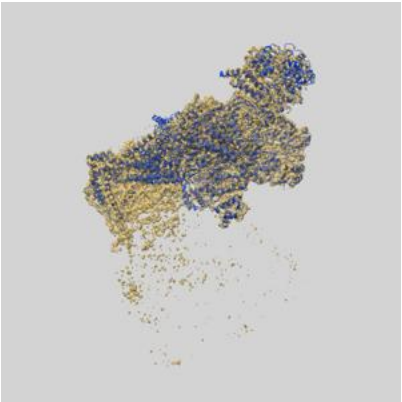
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35332 and PDB model 8IB5. Per-residue inclusion information can be found in section 3 on page 16.

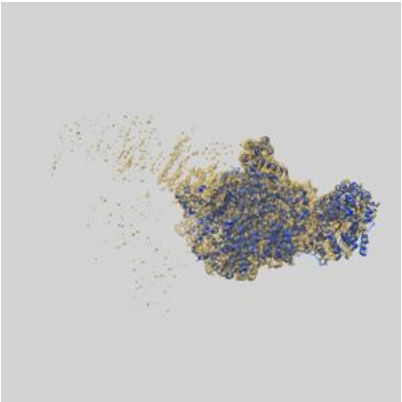
9.1 Map-model overlay (i)



X



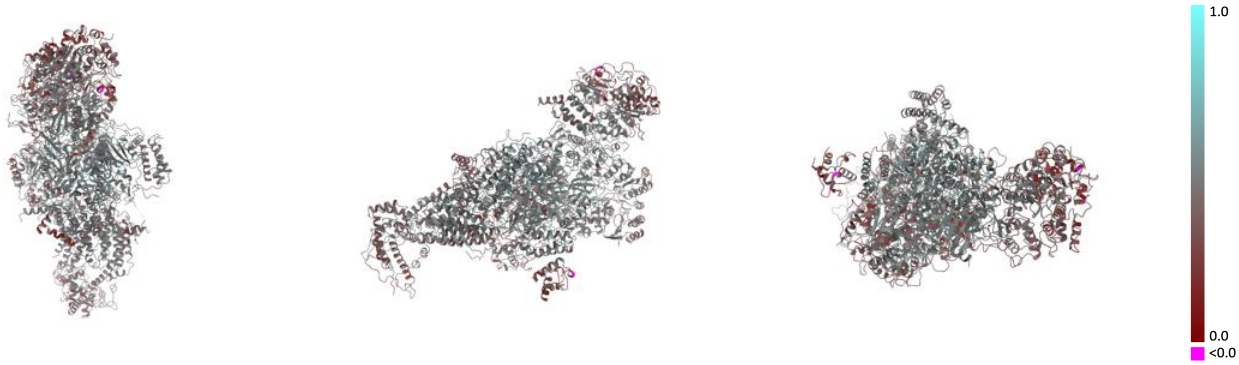
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

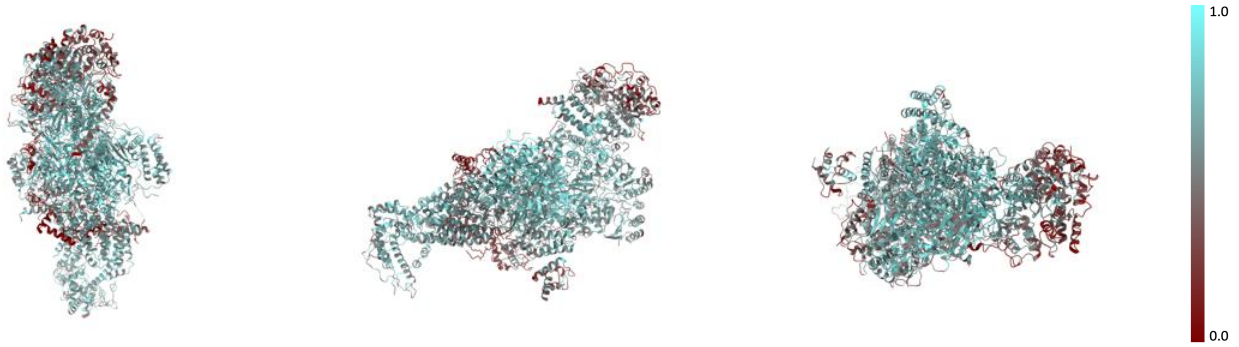
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

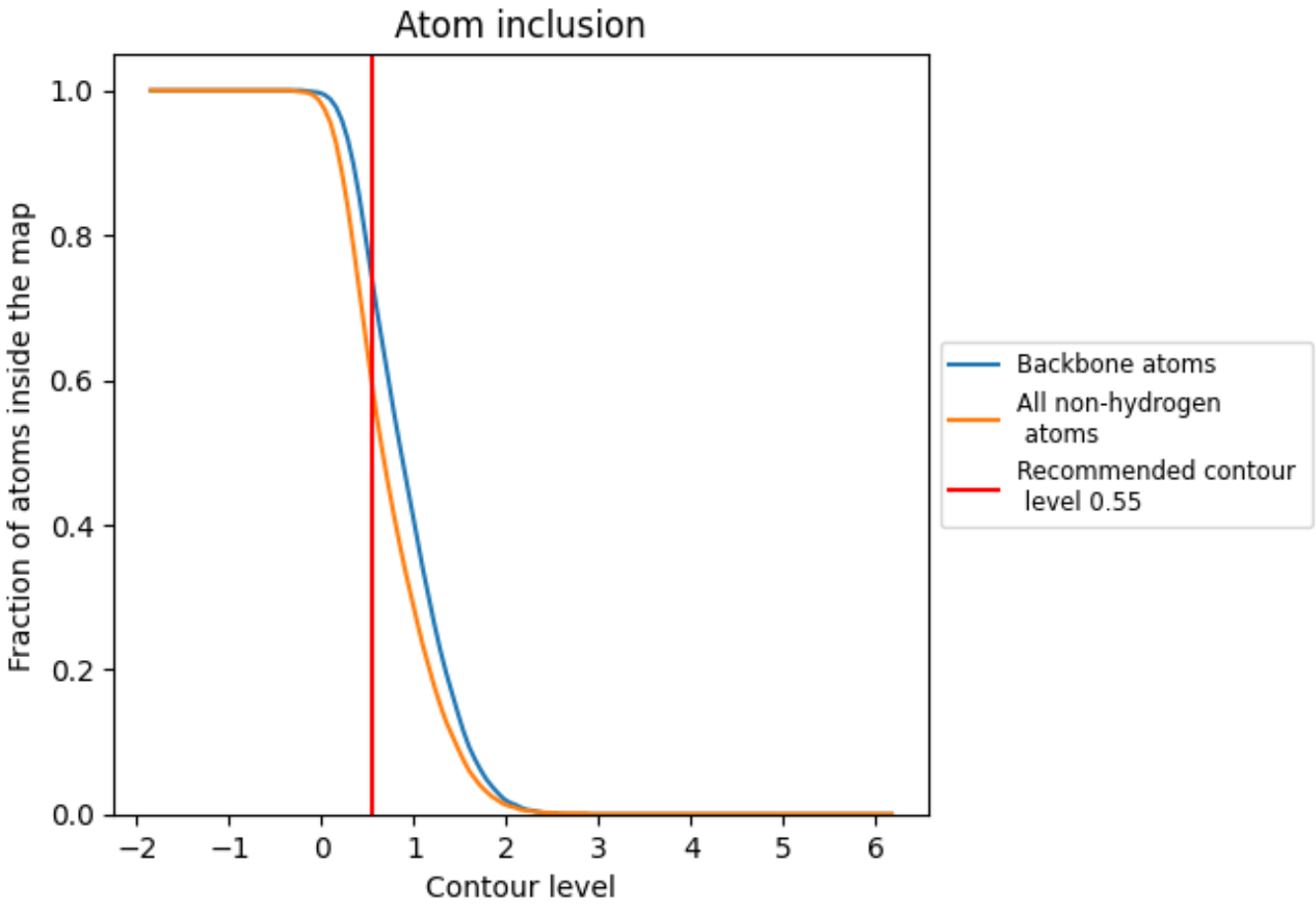
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5900	0.4470
A	0.5110	0.4430
B	0.7060	0.5030
C	0.7550	0.5190
D	0.7540	0.5140
E	0.3690	0.3900
F	0.4820	0.3970
G	0.6830	0.4660
H	0.6260	0.4750
I	0.7400	0.5030
P	0.4820	0.4230
Q	0.6150	0.4940
R	0.2630	0.3910
S	0.5990	0.3990
T	0.4110	0.2890
V	0.6620	0.4510
W	0.6020	0.4650
X	0.6160	0.3900
Z	0.6250	0.4130
a	0.6430	0.4470
b	0.5260	0.4310
q	0.2690	0.3810
r	0.3250	0.3660
s	0.0790	0.2480