



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:27 AM EDT

PDB ID : 3IAM / pdb_00003iam
Title : Crystal structure of the hydrophilic domain of respiratory complex I from *Thermus thermophilus*, reduced, 2 mol/ASU, with bound NADH
Authors : Sazanov, L.A.; Berrisford, J.M.
Deposited on : 2009-07-14
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

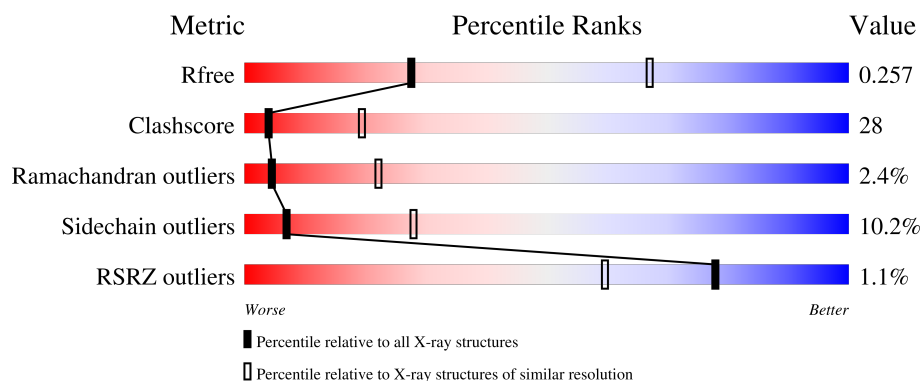
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	438	
1	A	438	
2	2	181	
2	B	181	
3	3	783	

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Mol	Chain	Length	Quality of chain
3	C	783	
4	4	409	
4	D	409	
5	5	207	
5	E	207	
6	6	181	
6	F	181	
7	9	182	
7	G	182	
8	7	129	
8	H	129	

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
9	SF4	9	183	-	-	X	-
9	SF4	F	182	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 37606 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			
1	A	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	179	Total	C	N	O	S	0	0	0
			1410	897	239	266	8			
2	B	179	Total	C	N	O	S	0	0	0
			1410	897	239	266	8			

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			
3	C	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	378	Total	C	N	O	S	0	0	0
			3018	1946	511	550	11			
4	D	378	Total	C	N	O	S	0	0	0
			3018	1946	511	550	11			

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	5	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			
5	E	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			
6	F	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			

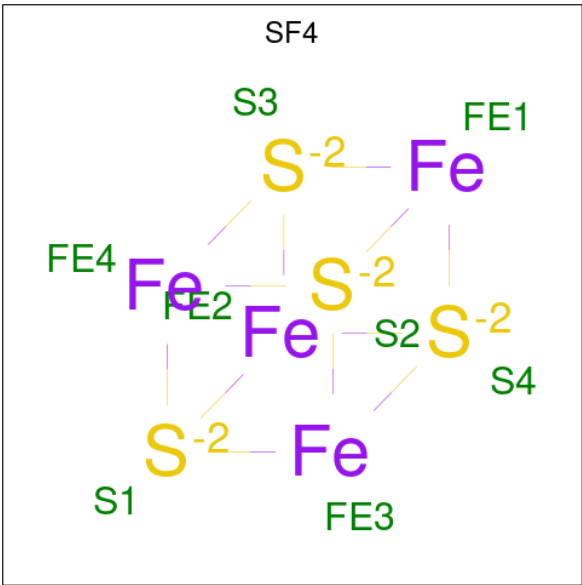
- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			
7	G	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

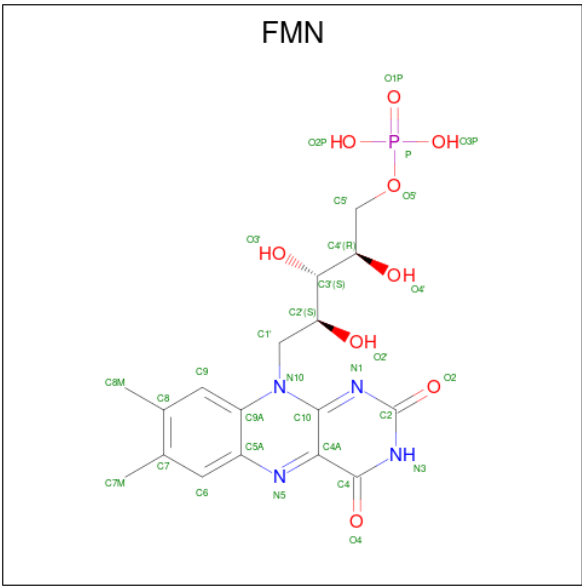
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	H	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



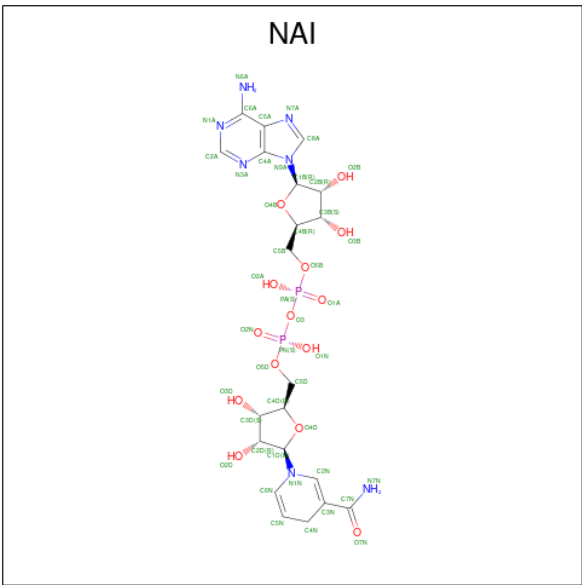
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	1	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	6	1	Total	Fe	S	0	0
			8	4	4		
9	9	1	Total	Fe	S	0	0
			8	4	4		
9	9	1	Total	Fe	S	0	0
			8	4	4		
9	A	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	F	1	Total	Fe	S	0	0
			8	4	4		
9	G	1	Total	Fe	S	0	0
			8	4	4		
9	G	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 11 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).

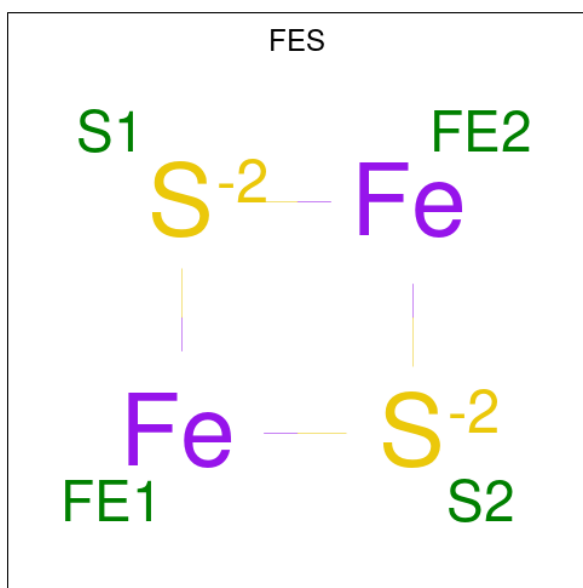


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
11	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	1	1	Total	Mg	0	0
			1	1		
12	2	1	Total	Mg	0	0
			1	1		
12	3	2	Total	Mg	0	0
			2	2		
12	4	1	Total	Mg	0	0
			1	1		
12	5	1	Total	Mg	0	0
			1	1		
12	A	1	Total	Mg	0	0
			1	1		
12	C	2	Total	Mg	0	0
			2	2		
12	E	1	Total	Mg	0	0
			1	1		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	2	1	Total 4	Fe 2	S 2	0	0
13	3	1	Total 4	Fe 2	S 2	0	0
13	B	1	Total 4	Fe 2	S 2	0	0
13	C	1	Total 4	Fe 2	S 2	0	0

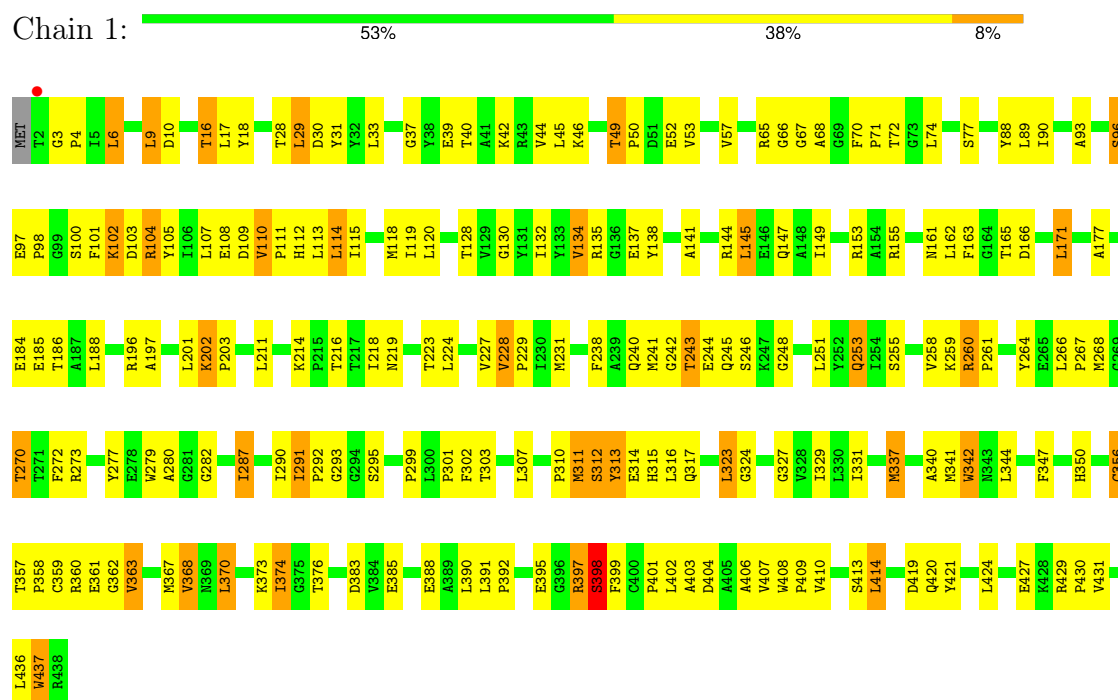
- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	7	1	Total 1	Ca 1	0	0
14	H	1	Total 1	Ca 1	0	0

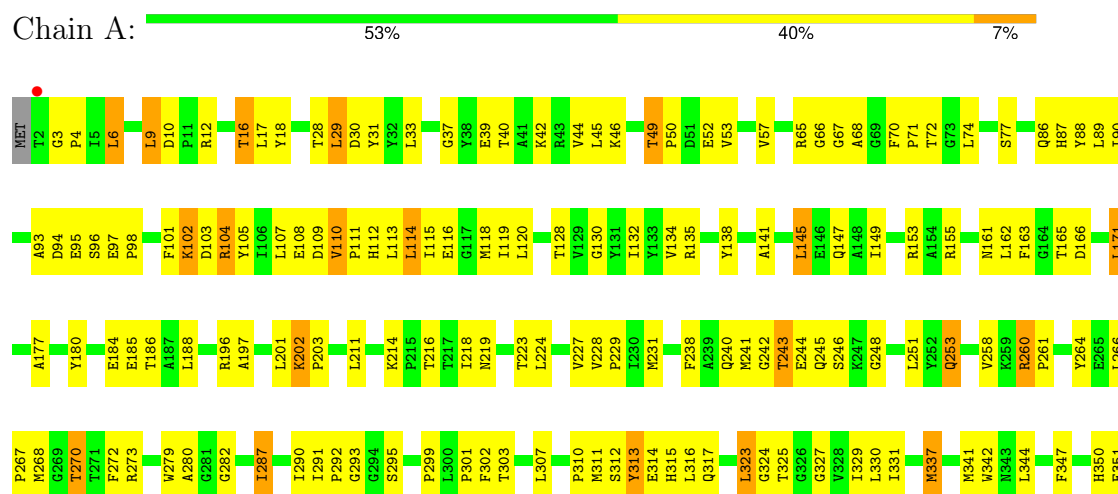
3 Residue-property plots

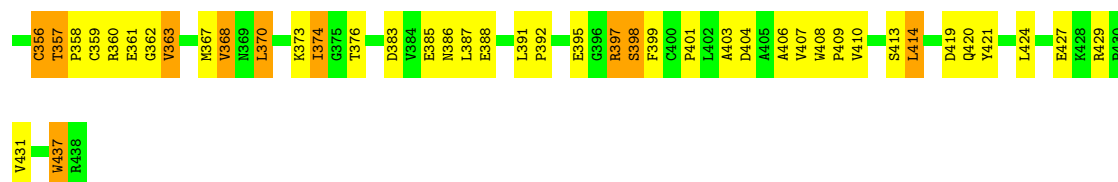
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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-quinone oxidoreductase subunit 1



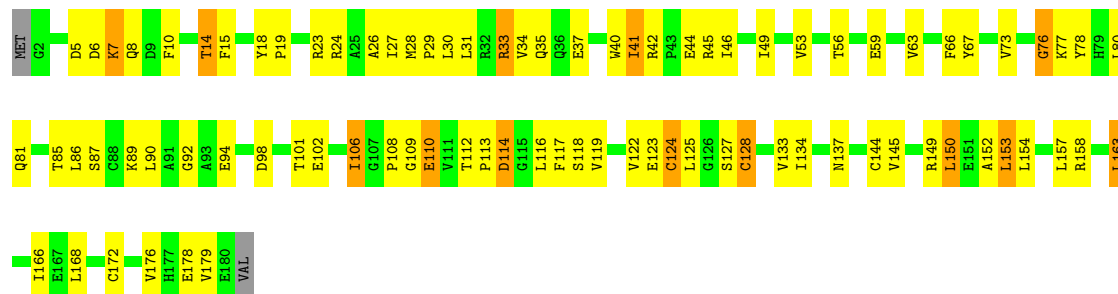
• Molecule 1: NADH-quinone oxidoreductase subunit 1





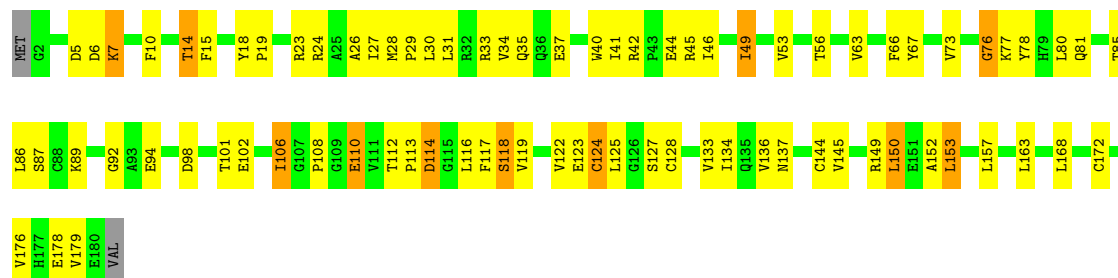
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2: 51% 40% 7% .



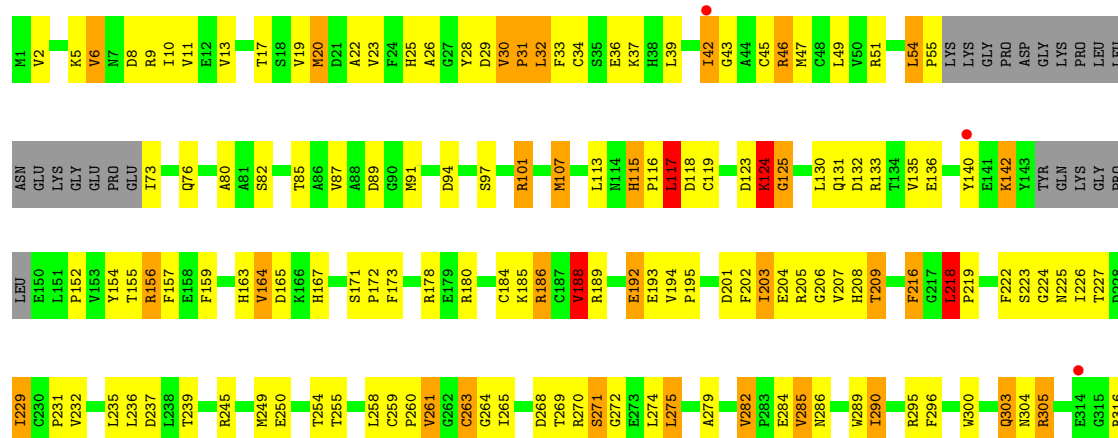
• Molecule 2: NADH-quinone oxidoreductase subunit 2

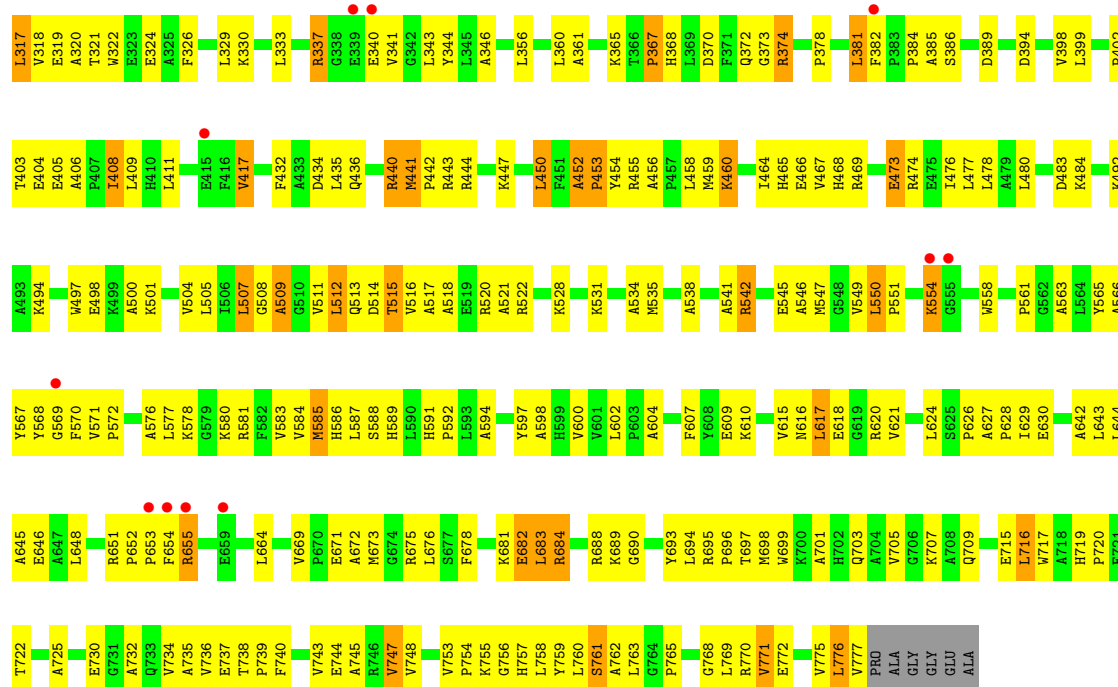
Chain B: 55% 38% 6% .



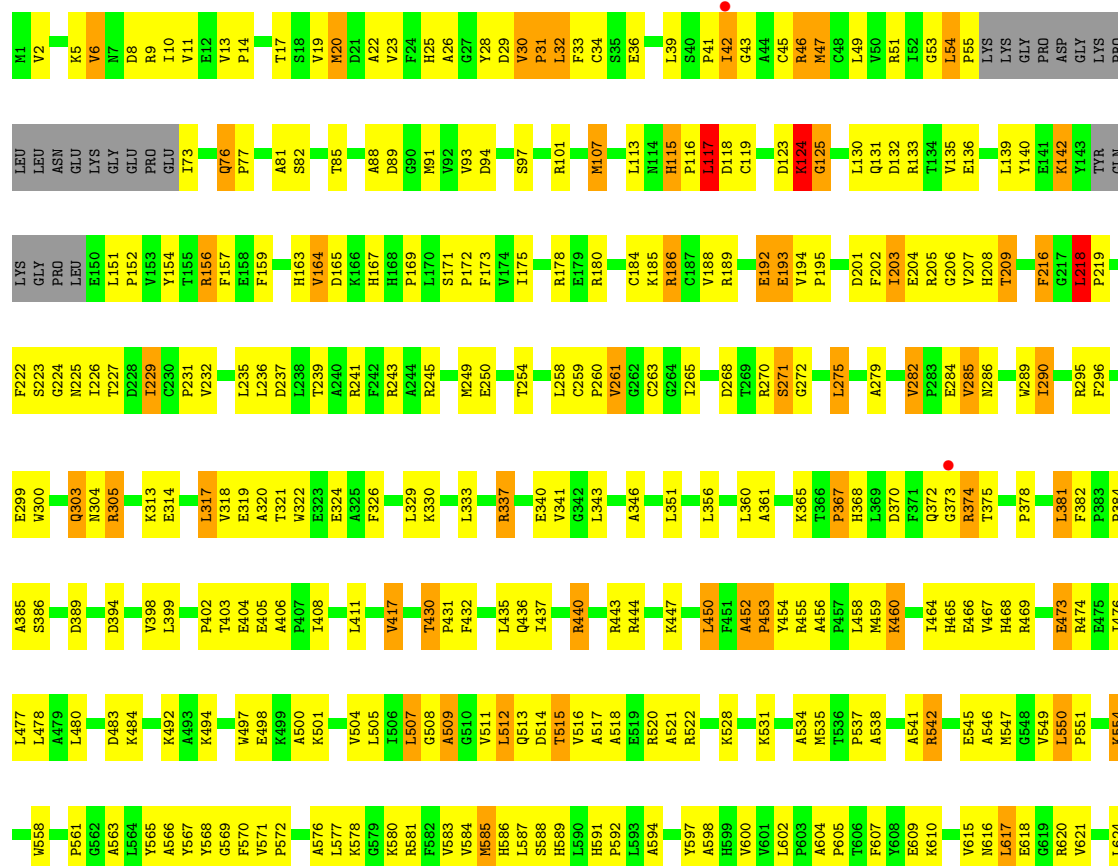
• Molecule 3: NADH-quinone oxidoreductase subunit 3

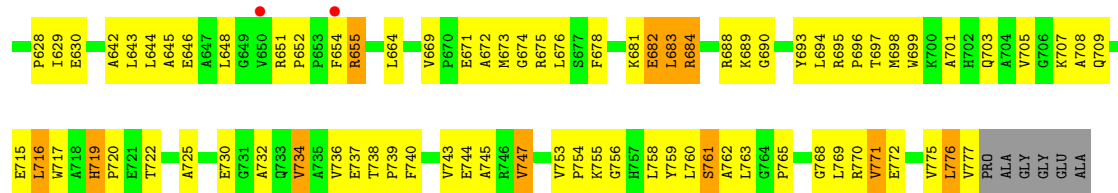
Chain 3: 47% 41% 8% . .



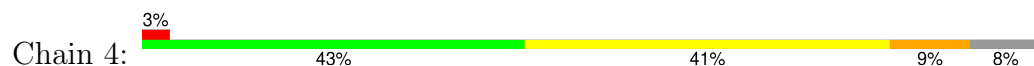
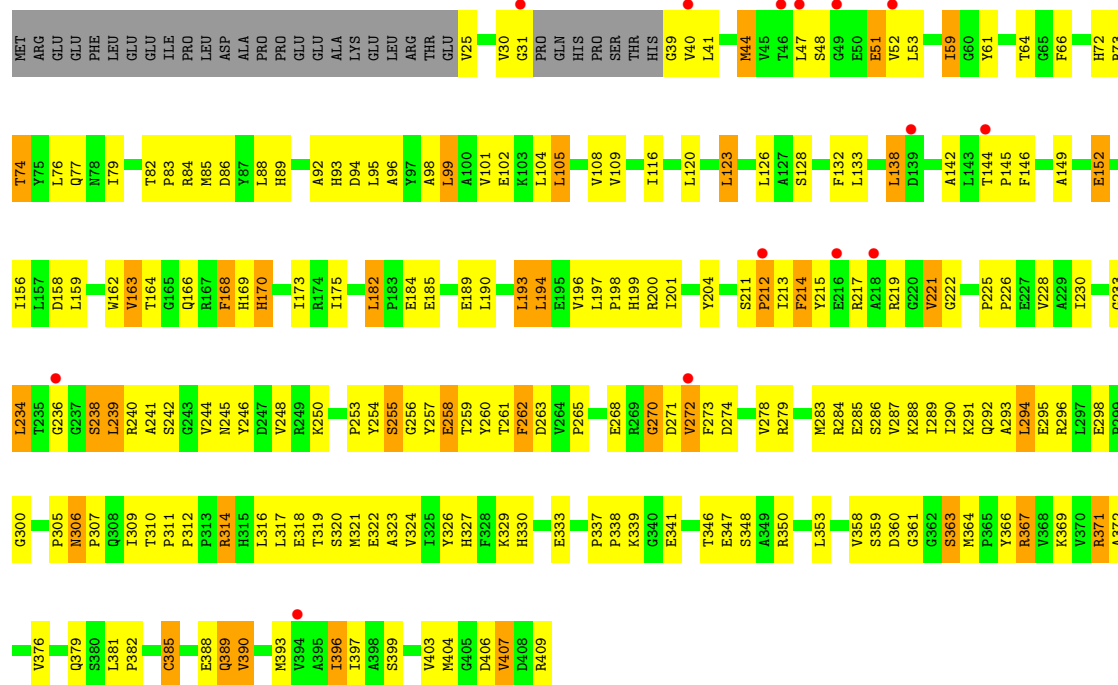


• Molecule 3: NADH-quinone oxidoreductase subunit 3

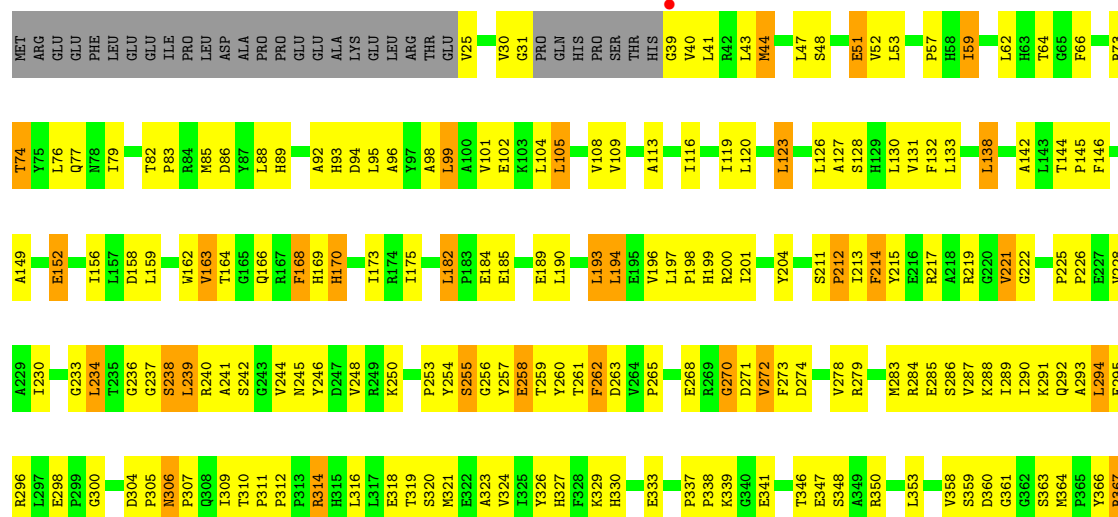




• Molecule 4: NADH-quinone oxidoreductase subunit 4

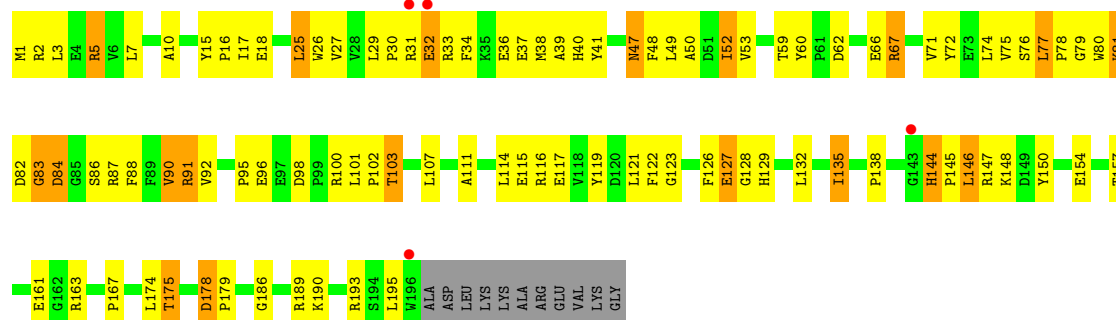


• Molecule 4: NADH-quinone oxidoreductase subunit 4

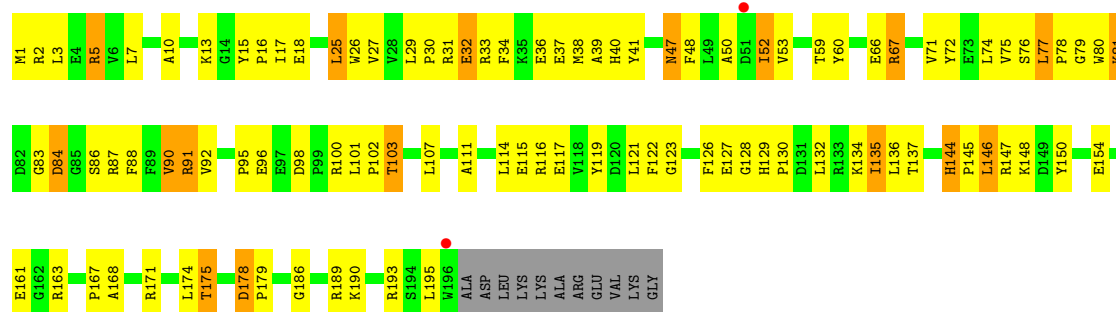




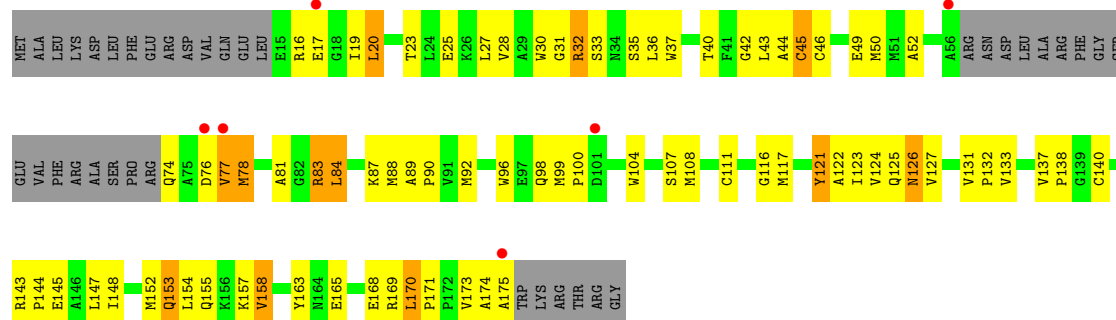
• Molecule 5: NADH-quinone oxidoreductase subunit 5



• Molecule 5: NADH-quinone oxidoreductase subunit 5

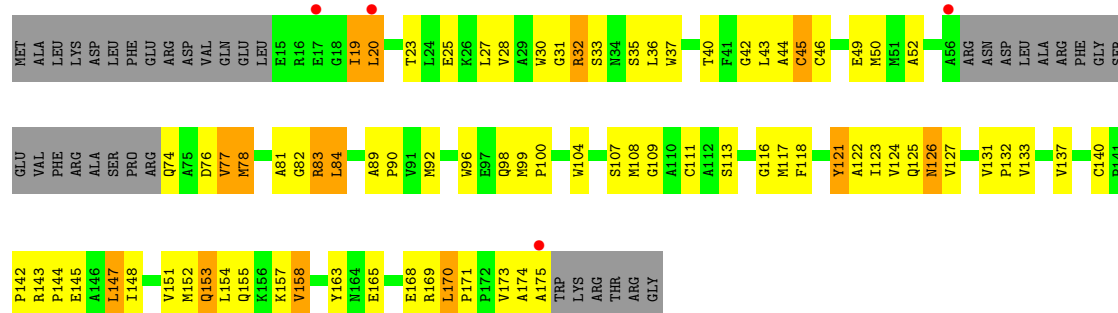


• Molecule 6: NADH-quinone oxidoreductase subunit 6

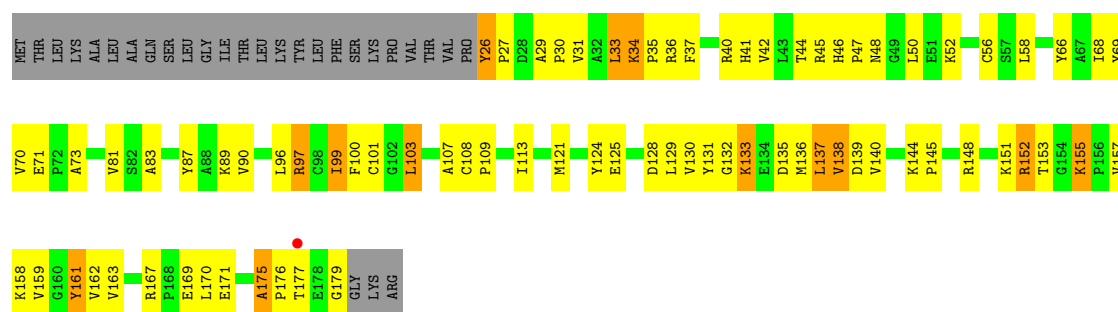


• Molecule 6: NADH-quinone oxidoreductase subunit 6

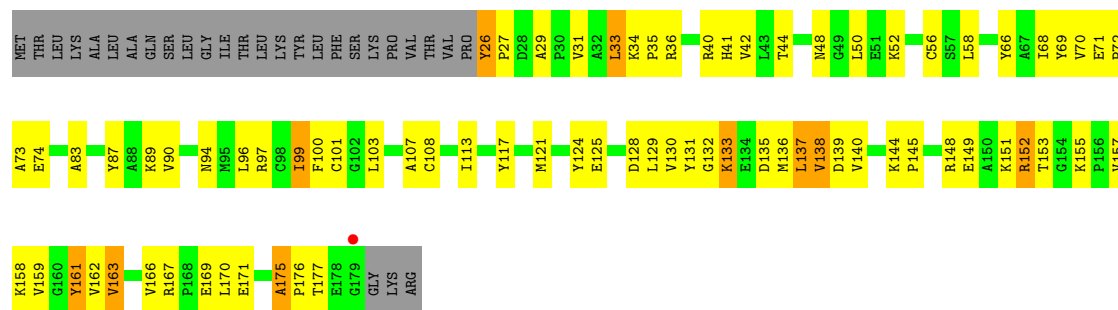




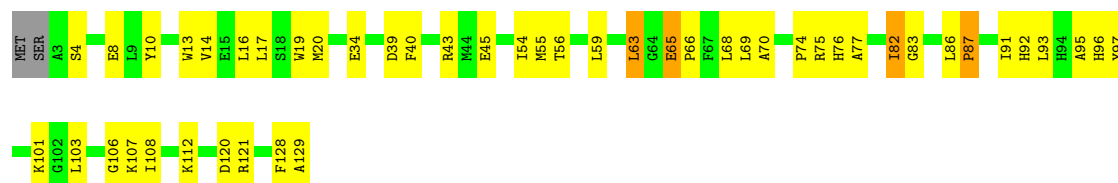
• Molecule 7: NADH-quinone oxidoreductase subunit 9



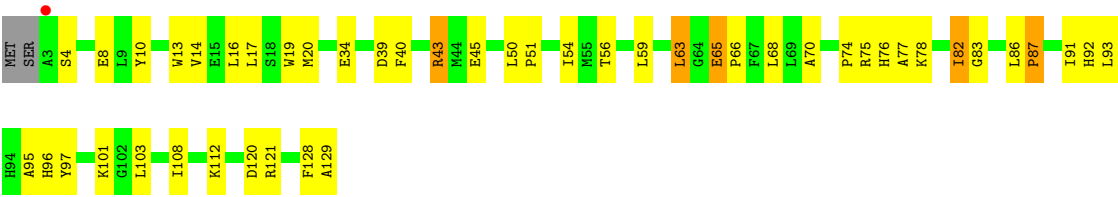
• Molecule 7: NADH-quinone oxidoreductase subunit 9



• Molecule 8: NADH-quinone oxidoreductase subunit 15



• Molecule 8: NADH-quinone oxidoreductase subunit 15



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.00Å 151.01Å 216.62Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	29.57 – 3.10 29.57 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.9 (29.57-3.10) 89.8 (29.57-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.11Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.231 , 0.262 0.226 , 0.257	Depositor DCC
R_{free} test set	2215 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	37606	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, FES, MG, NAI, CA

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	1	0.58	0/3506	1.00	17/4745 (0.4%)
1	A	0.54	0/3506	0.99	14/4745 (0.3%)
2	2	0.55	0/1443	1.03	8/1958 (0.4%)
2	B	0.50	0/1443	1.06	9/1958 (0.5%)
3	3	0.57	1/6019 (0.0%)	0.99	19/8163 (0.2%)
3	C	0.50	0/6019	0.96	24/8163 (0.3%)
4	4	0.55	0/3096	0.93	8/4207 (0.2%)
4	D	0.49	0/3096	0.92	8/4207 (0.2%)
5	5	0.56	0/1656	1.03	13/2246 (0.6%)
5	E	0.48	0/1656	1.04	12/2246 (0.5%)
6	6	0.61	0/1126	1.05	5/1528 (0.3%)
6	F	0.55	0/1126	1.03	5/1528 (0.3%)
7	9	0.59	0/1224	1.10	8/1663 (0.5%)
7	G	0.54	0/1224	1.08	5/1663 (0.3%)
8	7	0.55	0/1059	0.99	3/1429 (0.2%)
8	H	0.53	0/1059	1.00	4/1429 (0.3%)
All	All	0.54	1/38258 (0.0%)	0.99	162/51878 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	188	VAL	CA-CB	5.53	1.60	1.54

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	115	HIS	CA-C-N	11.55	130.99	118.97
3	3	115	HIS	C-N-CA	11.55	130.99	118.97
3	3	218	LEU	CA-C-N	11.52	131.95	119.28
3	3	218	LEU	C-N-CA	11.52	131.95	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	218	LEU	CA-C-N	11.31	131.72	119.28
3	C	218	LEU	C-N-CA	11.31	131.72	119.28
1	1	291	ILE	CA-C-N	10.97	130.38	118.97
1	1	291	ILE	C-N-CA	10.97	130.38	118.97
1	A	291	ILE	CA-C-N	10.70	130.09	118.97
1	A	291	ILE	C-N-CA	10.70	130.09	118.97
2	B	18	TYR	CA-C-N	9.58	126.56	119.66
2	B	18	TYR	C-N-CA	9.58	126.56	119.66
3	C	115	HIS	CA-C-N	8.84	130.89	119.84
3	C	115	HIS	C-N-CA	8.84	130.89	119.84
5	E	144	HIS	CA-C-N	8.39	128.36	119.05
5	E	144	HIS	C-N-CA	8.39	128.36	119.05
1	1	295	SER	N-CA-C	-8.35	103.53	114.31
6	6	123	ILE	N-CA-C	8.09	119.44	108.11
5	5	144	HIS	CA-C-N	8.02	127.96	119.05
5	5	144	HIS	C-N-CA	8.02	127.96	119.05
1	A	295	SER	N-CA-C	-7.97	104.03	114.31
1	A	110	VAL	CA-C-N	7.86	127.14	118.97
1	A	110	VAL	C-N-CA	7.86	127.14	118.97
6	F	123	ILE	N-CA-C	7.72	118.92	108.11
1	1	110	VAL	CA-C-N	7.59	127.48	119.05
1	1	110	VAL	C-N-CA	7.59	127.48	119.05
5	E	60	TYR	CA-C-N	7.42	126.96	119.24
5	E	60	TYR	C-N-CA	7.42	126.96	119.24
4	4	182	LEU	CA-C-N	7.38	127.33	120.03
4	4	182	LEU	C-N-CA	7.38	127.33	120.03
4	D	182	LEU	CA-C-N	7.33	127.29	120.03
4	D	182	LEU	C-N-CA	7.33	127.29	120.03
1	1	282	GLY	CA-C-N	7.30	128.29	120.11
1	1	282	GLY	C-N-CA	7.30	128.29	120.11
6	6	37	TRP	CA-C-N	7.07	128.92	120.23
6	6	37	TRP	C-N-CA	7.07	128.92	120.23
5	5	60	TYR	CA-C-N	7.05	126.57	119.24
5	5	60	TYR	C-N-CA	7.05	126.57	119.24
1	A	260	ARG	CA-C-N	6.81	126.77	120.03
1	A	260	ARG	C-N-CA	6.81	126.77	120.03
3	3	186	ARG	N-CA-C	6.76	119.23	111.11
4	4	39	GLY	N-CA-C	-6.74	93.76	113.30
6	F	37	TRP	CA-C-N	6.68	128.45	120.23
6	F	37	TRP	C-N-CA	6.68	128.45	120.23
3	3	229	ILE	CB-CA-C	-6.66	103.03	112.22
3	3	406	ALA	CA-C-N	6.63	128.13	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	406	ALA	C-N-CA	6.63	128.13	119.84
4	D	39	GLY	N-CA-C	-6.63	94.08	113.30
1	1	260	ARG	CA-C-N	6.56	126.52	120.03
1	1	260	ARG	C-N-CA	6.56	126.52	120.03
1	A	282	GLY	CA-C-N	6.53	128.01	119.84
1	A	282	GLY	C-N-CA	6.53	128.01	119.84
3	C	406	ALA	CA-C-N	6.50	127.96	119.84
3	C	406	ALA	C-N-CA	6.50	127.96	119.84
7	G	175	ALA	CA-C-N	6.32	127.74	119.84
7	G	175	ALA	C-N-CA	6.32	127.74	119.84
3	C	229	ILE	CB-CA-C	-6.30	103.80	112.24
7	G	29	ALA	CA-C-N	6.10	126.12	119.90
7	G	29	ALA	C-N-CA	6.10	126.12	119.90
5	E	178	ASP	CA-C-N	6.09	125.64	119.19
5	E	178	ASP	C-N-CA	6.09	125.64	119.19
7	9	175	ALA	CA-C-N	6.04	127.39	119.84
7	9	175	ALA	C-N-CA	6.04	127.39	119.84
5	5	98	ASP	CA-C-N	6.00	127.35	119.84
5	5	98	ASP	C-N-CA	6.00	127.35	119.84
6	6	170	LEU	CA-C-N	5.97	126.53	120.38
6	6	170	LEU	C-N-CA	5.97	126.53	120.38
3	C	186	ARG	N-CA-C	5.96	118.27	111.11
5	5	178	ASP	CA-C-N	5.93	125.47	119.19
5	5	178	ASP	C-N-CA	5.93	125.47	119.19
4	4	300	GLY	CA-C-N	5.92	125.83	119.85
4	4	300	GLY	C-N-CA	5.92	125.83	119.85
7	9	103	LEU	N-CA-C	-5.86	104.89	111.28
3	C	8	ASP	N-CA-C	-5.84	105.93	114.39
5	E	98	ASP	CA-C-N	5.82	127.12	119.84
5	E	98	ASP	C-N-CA	5.82	127.12	119.84
1	A	331	ILE	CA-C-N	5.77	125.74	120.03
1	A	331	ILE	C-N-CA	5.77	125.74	120.03
8	7	4	SER	N-CA-C	-5.77	105.90	113.17
3	3	441	MET	CA-C-N	5.72	125.91	119.90
3	3	441	MET	C-N-CA	5.72	125.91	119.90
3	C	452	ALA	CA-C-N	5.71	126.98	119.84
3	C	452	ALA	C-N-CA	5.71	126.98	119.84
2	B	73	VAL	CA-C-N	5.71	126.97	119.84
2	B	73	VAL	C-N-CA	5.71	126.97	119.84
4	D	306	ASN	CA-C-N	5.68	125.30	119.56
4	D	306	ASN	C-N-CA	5.68	125.30	119.56
5	5	67	ARG	N-CA-C	5.67	117.46	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	19	PRO	CA-C-N	5.67	126.04	119.47
2	B	19	PRO	C-N-CA	5.67	126.04	119.47
7	G	161	TYR	N-CA-C	5.64	115.99	108.38
2	2	73	VAL	CA-C-N	5.62	126.87	119.84
2	2	73	VAL	C-N-CA	5.62	126.87	119.84
6	F	170	LEU	CA-C-N	5.58	126.12	120.38
6	F	170	LEU	C-N-CA	5.58	126.12	120.38
1	1	331	ILE	CA-C-N	5.57	125.55	120.03
1	1	331	ILE	C-N-CA	5.57	125.55	120.03
8	H	65	GLU	CA-C-N	5.57	125.33	119.76
8	H	65	GLU	C-N-CA	5.57	125.33	119.76
5	E	67	ARG	N-CA-C	5.55	117.33	111.28
7	9	161	TYR	N-CA-C	5.53	115.85	108.38
5	E	77	LEU	CA-C-N	5.52	126.75	119.84
5	E	77	LEU	C-N-CA	5.52	126.75	119.84
1	1	356	CYS	CB-CA-C	-5.52	100.07	109.51
2	2	109	GLY	N-CA-C	5.51	120.51	114.40
5	E	13	LYS	N-CA-C	5.47	116.26	108.54
3	3	30	VAL	CA-C-N	5.46	126.67	119.84
3	3	30	VAL	C-N-CA	5.46	126.67	119.84
5	5	77	LEU	CA-C-N	5.43	126.62	119.84
5	5	77	LEU	C-N-CA	5.43	126.62	119.84
1	1	312	SER	N-CA-C	5.38	117.16	109.14
3	3	76	GLN	CA-C-N	5.36	124.87	119.19
3	3	76	GLN	C-N-CA	5.36	124.87	119.19
1	A	70	PHE	CA-C-N	5.35	126.52	119.84
1	A	70	PHE	C-N-CA	5.35	126.52	119.84
1	A	356	CYS	CB-CA-C	-5.35	100.37	109.51
4	D	300	GLY	CA-C-N	5.34	125.24	119.85
4	D	300	GLY	C-N-CA	5.34	125.24	119.85
2	B	19	PRO	O-C-N	5.33	123.66	121.15
3	3	8	ASP	N-CA-C	-5.32	106.68	114.39
3	C	30	VAL	CA-C-N	5.30	126.47	119.84
3	C	30	VAL	C-N-CA	5.30	126.47	119.84
7	9	155	LYS	CA-C-N	5.30	126.46	119.84
7	9	155	LYS	C-N-CA	5.30	126.46	119.84
3	C	14	PRO	CA-C-N	5.29	125.35	119.32
3	C	14	PRO	C-N-CA	5.29	125.35	119.32
2	B	136	VAL	CA-C-N	-5.29	115.24	121.90
2	B	136	VAL	C-N-CA	-5.29	115.24	121.90
3	C	193	GLU	N-CA-C	5.28	116.84	111.14
3	3	452	ALA	CA-C-N	5.27	126.42	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	452	ALA	C-N-CA	5.27	126.42	119.84
1	1	70	PHE	CA-C-N	5.25	126.40	119.84
1	1	70	PHE	C-N-CA	5.25	126.40	119.84
3	C	719	HIS	CA-C-N	5.24	126.38	119.84
3	C	719	HIS	C-N-CA	5.24	126.38	119.84
2	2	18	TYR	CA-C-N	5.23	125.77	120.38
2	2	18	TYR	C-N-CA	5.23	125.77	120.38
8	H	4	SER	N-CA-C	-5.23	106.58	113.17
3	C	430	THR	CA-C-N	5.22	125.22	119.89
3	C	430	THR	C-N-CA	5.22	125.22	119.89
4	4	306	ASN	CA-C-N	5.21	124.82	119.56
4	4	306	ASN	C-N-CA	5.21	124.82	119.56
3	3	566	ALA	N-CA-C	5.19	117.28	109.23
8	7	65	GLU	CA-C-N	5.17	125.33	119.90
8	7	65	GLU	C-N-CA	5.17	125.33	119.90
3	3	765	PRO	N-CA-C	-5.14	109.33	114.68
3	C	76	GLN	CA-C-N	5.14	124.64	119.19
3	C	76	GLN	C-N-CA	5.14	124.64	119.19
3	C	765	PRO	N-CA-C	-5.14	109.33	114.68
1	1	342	TRP	CA-CB-CG	5.13	123.34	113.60
2	2	19	PRO	CA-C-N	5.12	125.16	119.32
2	2	19	PRO	C-N-CA	5.12	125.16	119.32
4	4	238	SER	N-CA-C	-5.11	106.87	113.01
7	9	34	LYS	CA-C-N	5.11	124.91	119.28
7	9	34	LYS	C-N-CA	5.11	124.91	119.28
5	5	62	ASP	CA-C-N	5.10	125.00	119.85
5	5	62	ASP	C-N-CA	5.10	125.00	119.85
1	1	398	SER	N-CA-C	-5.07	102.08	109.63
2	2	41	ILE	N-CA-C	5.04	115.03	107.51
4	D	238	SER	N-CA-C	-5.03	106.97	113.01
8	H	43	ARG	N-CA-C	-5.02	102.47	109.96
3	C	566	ALA	N-CA-C	5.01	116.99	109.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1	3417	0	3388	180	1
1	A	3417	0	3388	177	0
2	2	1410	0	1376	74	0
2	B	1410	0	1376	68	0
3	3	5880	0	5911	366	1
3	C	5880	0	5911	383	0
4	4	3018	0	3009	203	0
4	D	3018	0	3009	220	0
5	5	1607	0	1574	99	0
5	E	1607	0	1574	99	0
6	6	1102	0	1108	87	0
6	F	1102	0	1108	85	0
7	9	1193	0	1160	66	0
7	G	1193	0	1160	74	0
8	7	1031	0	1029	42	0
8	H	1031	0	1029	42	0
9	1	8	0	0	0	0
9	3	24	0	0	3	0
9	6	8	0	0	1	0
9	9	16	0	0	2	0
9	A	8	0	0	0	0
9	C	24	0	0	3	0
9	F	8	0	0	2	0
9	G	16	0	0	1	0
10	1	31	0	19	6	0
10	A	31	0	19	0	0
11	1	44	0	27	4	0
11	A	44	0	27	7	0
12	1	1	0	0	0	0
12	2	1	0	0	0	0
12	3	2	0	0	0	0
12	4	1	0	0	0	0
12	5	1	0	0	0	0
12	A	1	0	0	0	0
12	C	2	0	0	0	0
12	E	1	0	0	0	0
13	2	4	0	0	0	0
13	3	4	0	0	1	0
13	B	4	0	0	1	0
13	C	4	0	0	1	0
14	7	1	0	0	0	0
14	H	1	0	0	0	0
All	All	37606	0	37202	2093	1

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 28.

All (2093) 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)
1:A:104:ARG:HH21	2:B:127:SER:HB3	1.09	1.17
3:3:474:ARG:HH21	3:3:516:VAL:HG21	1.03	1.17
6:6:83:ARG:HH11	6:6:83:ARG:HG3	1.13	1.13
1:1:104:ARG:HH21	2:2:127:SER:HB3	1.04	1.12
3:3:11:VAL:HG11	3:3:25:HIS:HD2	1.16	1.11
3:C:474:ARG:HH21	3:C:516:VAL:HG21	1.03	1.09
5:E:66:GLU:HG2	5:E:95:PRO:HA	1.37	1.06
3:3:31:PRO:HB3	3:3:47:MET:HE3	1.38	1.05
3:C:31:PRO:HB3	3:C:47:MET:HE3	1.38	1.04
1:1:97:GLU:HB2	11:1:441:NAI:H42N	1.37	1.04
3:C:11:VAL:HG11	3:C:25:HIS:HD2	1.17	1.04
1:1:104:ARG:NH2	2:2:127:SER:HB3	1.73	1.03
5:E:175:THR:HG23	5:E:178:ASP:HB2	1.40	1.01
3:3:474:ARG:NH2	3:3:516:VAL:HG21	1.75	1.01
5:5:34:PHE:HE1	5:5:38:MET:HE2	1.22	1.01
6:F:83:ARG:HH11	6:F:83:ARG:HG3	1.23	1.00
3:C:474:ARG:NH2	3:C:516:VAL:HG21	1.77	1.00
5:5:66:GLU:HG2	5:5:95:PRO:HA	1.40	1.00
1:A:97:GLU:HB2	11:A:441:NAI:H42N	1.39	1.00
4:D:40:VAL:HG13	4:D:404:MET:HG3	1.43	1.00
5:E:34:PHE:HE1	5:E:38:MET:HE2	1.24	0.99
5:5:52:ILE:CG2	5:5:114:LEU:HB3	1.92	0.99
5:E:52:ILE:CG2	5:E:114:LEU:HB3	1.93	0.99
5:5:175:THR:HG23	5:5:178:ASP:HB2	1.42	0.98
1:A:104:ARG:NH2	2:B:127:SER:HB3	1.78	0.97
3:C:373:GLY:HA3	3:C:538:ALA:HB2	1.47	0.96
3:3:373:GLY:HA3	3:3:538:ALA:HB2	1.48	0.96
2:B:114:ASP:HB2	2:B:116:LEU:HD22	1.47	0.96
1:A:16:THR:HG21	1:A:229:PRO:HB3	1.48	0.95
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.48	0.95
3:C:459:MET:HE2	3:C:465:HIS:HB2	1.48	0.95
6:F:46:CYS:HB3	6:F:81:ALA:HB1	1.48	0.95
5:E:121:LEU:HB3	5:E:146:LEU:HB2	1.49	0.94
3:C:522:ARG:HH12	3:C:681:LYS:HE3	1.33	0.94
3:C:405:GLU:HB2	3:C:535:MET:HE2	1.49	0.93
3:3:405:GLU:HB2	3:3:535:MET:HE2	1.50	0.93
3:3:701:ALA:HB2	3:3:763:LEU:HB2	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:LEU:N	4:D:321:MET:HE1	1.83	0.93
3:3:117:LEU:N	4:4:321:MET:HE1	1.84	0.92
1:1:16:THR:HG21	1:1:229:PRO:HB3	1.50	0.92
3:3:459:MET:HE2	3:3:465:HIS:HB2	1.51	0.92
1:1:184:GLU:OE1	1:1:186:THR:HG22	1.69	0.92
3:C:701:ALA:HB2	3:C:763:LEU:HB2	1.49	0.92
6:6:117:MET:HE3	7:9:99:ILE:HG12	1.49	0.92
4:4:40:VAL:HG13	4:4:404:MET:HG3	1.52	0.91
2:2:114:ASP:HB2	2:2:116:LEU:HD22	1.52	0.91
3:3:11:VAL:HG11	3:3:25:HIS:CD2	2.06	0.91
3:C:55:PRO:HB3	3:C:73:ILE:CA	2.01	0.91
3:3:165:ASP:HB3	3:3:178:ARG:HD2	1.52	0.90
3:3:522:ARG:HH12	3:3:681:LYS:HE3	1.35	0.90
1:A:184:GLU:OE1	1:A:186:THR:HG22	1.72	0.90
4:D:341:GLU:HG2	4:D:358:VAL:HG22	1.54	0.90
5:5:5:ARG:HH11	5:5:5:ARG:HG3	1.37	0.90
5:E:5:ARG:HH11	5:E:5:ARG:HG3	1.37	0.89
3:3:117:LEU:HD12	4:4:321:MET:HE2	1.52	0.89
3:C:738:THR:HG22	3:C:740:PHE:H	1.38	0.89
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.55	0.89
1:A:185:GLU:HB2	1:A:218:ILE:HD12	1.55	0.89
5:5:121:LEU:HB3	5:5:146:LEU:HB2	1.52	0.89
4:D:250:LYS:HE2	4:D:262:PHE:HB3	1.51	0.89
3:3:115:HIS:CG	3:3:116:PRO:HD2	2.07	0.89
3:C:11:VAL:HG11	3:C:25:HIS:CD2	2.07	0.89
3:C:165:ASP:HB3	3:C:178:ARG:HD2	1.55	0.89
5:E:52:ILE:HG21	5:E:114:LEU:HB3	1.54	0.88
6:F:117:MET:HE3	7:G:99:ILE:HG12	1.53	0.88
3:C:116:PRO:O	3:C:117:LEU:HB2	1.74	0.88
3:3:237:ASP:OD1	3:3:239:THR:HG22	1.75	0.87
3:C:522:ARG:NH1	3:C:681:LYS:HE3	1.89	0.87
3:3:738:THR:HG22	3:3:740:PHE:H	1.39	0.86
3:3:20:MET:HE1	3:3:432:PHE:HB2	1.55	0.86
1:A:149:ILE:HD13	1:A:171:LEU:HB3	1.58	0.86
4:4:250:LYS:HE2	4:4:262:PHE:HB3	1.54	0.86
3:C:186:ARG:HD3	3:C:229:ILE:HG22	1.58	0.86
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.55	0.85
3:3:494:LYS:O	3:3:498:GLU:HG2	1.76	0.85
4:4:96:ALA:HB2	4:4:346:THR:HG21	1.57	0.85
3:C:115:HIS:CG	3:C:116:PRO:HD2	2.10	0.85
6:6:46:CYS:HB3	6:6:81:ALA:HB1	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:384:PRO:HG3	3:C:542:ARG:HH21	1.42	0.85
5:5:34:PHE:CE1	5:5:38:MET:HE2	2.11	0.85
5:5:52:ILE:HG21	5:5:114:LEU:HB3	1.58	0.85
1:1:242:GLY:HA2	1:1:268:MET:O	1.76	0.84
3:3:561:PRO:HB3	3:3:576:ALA:HA	1.57	0.84
1:A:242:GLY:HA2	1:A:268:MET:O	1.77	0.84
3:C:20:MET:HE1	3:C:432:PHE:HB2	1.59	0.84
3:C:501:LYS:H	3:C:501:LYS:HD2	1.42	0.84
3:C:561:PRO:HB3	3:C:576:ALA:HA	1.56	0.84
1:1:337:MET:HE2	1:1:337:MET:HA	1.59	0.84
8:7:101:LYS:HE2	8:7:101:LYS:HA	1.60	0.84
4:D:96:ALA:HB2	4:D:346:THR:HG21	1.58	0.84
1:1:293:GLY:HA3	1:1:324:GLY:H	1.42	0.83
3:C:237:ASP:OD1	3:C:239:THR:HG22	1.76	0.83
3:C:515:THR:HG23	3:C:683:LEU:HD12	1.59	0.83
1:1:149:ILE:HD13	1:1:171:LEU:HB3	1.57	0.83
3:3:116:PRO:O	3:3:117:LEU:HB2	1.77	0.83
3:3:522:ARG:NH1	3:3:681:LYS:HE3	1.92	0.83
1:A:337:MET:HE2	1:A:337:MET:HA	1.57	0.83
4:D:104:LEU:O	5:E:193:ARG:HD2	1.79	0.82
1:1:185:GLU:HB2	1:1:218:ILE:HD12	1.61	0.82
1:A:293:GLY:HA3	1:A:324:GLY:H	1.42	0.82
1:A:437:TRP:HB3	2:B:92:GLY:HA3	1.60	0.82
4:4:367:ARG:HG2	4:4:367:ARG:HH11	1.43	0.82
3:C:642:ALA:HB1	3:C:652:PRO:HG3	1.61	0.82
5:E:34:PHE:CE1	5:E:38:MET:HE2	2.13	0.82
3:C:55:PRO:HB3	3:C:73:ILE:HA	1.61	0.82
3:3:515:THR:HG23	3:3:683:LEU:HD12	1.60	0.81
1:1:246:SER:HB3	1:1:268:MET:HG2	1.62	0.81
3:C:55:PRO:HB3	3:C:73:ILE:N	1.95	0.81
3:C:494:LYS:O	3:C:498:GLU:HG2	1.79	0.81
4:D:222:GLY:HA3	4:D:396:ILE:HD11	1.61	0.81
8:H:101:LYS:HE2	8:H:101:LYS:HA	1.60	0.81
1:1:118:MET:HG2	1:1:224:LEU:HD13	1.60	0.81
3:3:501:LYS:H	3:3:501:LYS:HD2	1.43	0.81
1:1:344:LEU:O	1:1:347:PHE:HB3	1.80	0.81
1:A:118:MET:HG2	1:A:224:LEU:HD13	1.62	0.81
3:C:117:LEU:HD12	4:D:321:MET:HE2	1.63	0.81
7:G:26:TYR:N	7:G:27:PRO:HD3	1.96	0.80
4:D:367:ARG:HG2	4:D:367:ARG:HH11	1.46	0.80
3:3:384:PRO:HG3	3:3:542:ARG:HH21	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:642:ALA:HB1	3:3:652:PRO:HG3	1.63	0.80
3:3:370:ASP:OD1	3:3:551:PRO:HD3	1.82	0.80
4:4:363:SER:HB2	5:5:174:LEU:H	1.46	0.80
4:4:212:PRO:HB2	4:4:213:ILE:HD12	1.63	0.79
4:4:222:GLY:HA3	4:4:396:ILE:HD11	1.63	0.79
4:4:310:THR:HG22	4:4:311:PRO:O	1.83	0.79
1:A:246:SER:HB3	1:A:268:MET:HG2	1.62	0.79
4:D:105:LEU:HD13	4:D:309:ILE:HD13	1.64	0.79
4:D:310:THR:HG22	4:D:311:PRO:O	1.82	0.79
7:G:40:ARG:HB2	7:G:121:MET:HE1	1.64	0.79
4:D:261:THR:N	4:D:292:GLN:HE22	1.80	0.79
5:E:66:GLU:HG2	5:E:95:PRO:CA	2.12	0.79
6:F:83:ARG:HG3	6:F:83:ARG:NH1	1.98	0.79
4:D:212:PRO:HB2	4:D:213:ILE:HD12	1.64	0.78
4:D:213:ILE:HD12	4:D:213:ILE:H	1.49	0.78
8:H:8:GLU:HG2	8:H:97:TYR:CZ	2.18	0.78
3:3:19:VAL:HG22	3:3:91:MET:HE1	1.66	0.78
3:C:194:VAL:HB	3:C:195:PRO:HD3	1.65	0.78
3:3:171:SER:HB2	3:3:172:PRO:HD2	1.64	0.78
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.66	0.78
3:3:655:ARG:HB2	3:3:655:ARG:HH11	1.47	0.78
5:5:47:ASN:ND2	5:5:47:ASN:H	1.80	0.78
3:C:370:ASP:OD1	3:C:551:PRO:HD3	1.83	0.78
4:D:318:GLU:HB2	8:H:39:ASP:HA	1.65	0.78
3:3:279:ALA:HB2	3:3:290:ILE:HG12	1.64	0.78
3:C:655:ARG:HB2	3:C:655:ARG:HH11	1.49	0.78
3:C:171:SER:HB2	3:C:172:PRO:HD2	1.65	0.78
4:D:363:SER:HB2	5:E:174:LEU:H	1.49	0.78
5:E:145:PRO:HA	5:E:150:TYR:CD2	2.19	0.78
6:F:148:ILE:HG21	7:G:27:PRO:HG3	1.65	0.78
8:7:8:GLU:HG2	8:7:97:TYR:CZ	2.19	0.78
1:1:162:LEU:O	1:1:165:THR:HG22	1.84	0.77
5:E:186:GLY:HA2	5:E:190:LYS:HD3	1.66	0.77
8:H:121:ARG:HH11	8:H:121:ARG:HG3	1.47	0.77
5:5:47:ASN:H	5:5:47:ASN:HD22	1.32	0.77
5:5:186:GLY:HA2	5:5:190:LYS:HD3	1.65	0.77
3:C:384:PRO:HG3	3:C:542:ARG:NH2	2.00	0.77
3:3:194:VAL:HB	3:3:195:PRO:HD3	1.66	0.77
7:9:26:TYR:N	7:9:27:PRO:HD3	1.98	0.77
5:E:47:ASN:H	5:E:47:ASN:HD22	1.33	0.77
4:4:213:ILE:HD12	4:4:213:ILE:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:104:LEU:O	5:5:193:ARG:HD2	1.84	0.77
4:D:254:TYR:HD1	4:D:255:SER:H	1.32	0.76
3:C:542:ARG:HB2	3:C:542:ARG:HH11	1.49	0.76
3:3:55:PRO:HB3	3:3:73:ILE:HA	1.66	0.76
3:C:405:GLU:HB2	3:C:535:MET:CE	2.16	0.76
5:E:47:ASN:H	5:E:47:ASN:ND2	1.83	0.76
6:F:77:VAL:HG22	6:F:104:TRP:HB2	1.67	0.76
3:3:542:ARG:HB2	3:3:542:ARG:HH11	1.51	0.75
5:5:66:GLU:HG2	5:5:95:PRO:CA	2.16	0.75
3:3:218:LEU:N	3:3:219:PRO:HD3	2.01	0.75
4:4:254:TYR:HD1	4:4:255:SER:H	1.30	0.75
3:C:194:VAL:HG12	3:C:411:LEU:HD22	1.67	0.75
3:C:386:SER:HB2	3:C:675:ARG:HH12	1.51	0.75
4:4:261:THR:N	4:4:292:GLN:HE22	1.83	0.75
1:1:358:PRO:HD3	3:3:107:MET:CE	2.16	0.75
1:A:50:PRO:O	1:A:53:VAL:HG12	1.87	0.75
4:D:274:ASP:O	4:D:278:VAL:HG23	1.86	0.75
2:2:101:THR:HG23	2:2:106:ILE:O	1.87	0.75
3:C:509:ALA:HB1	3:C:768:GLY:HA3	1.69	0.75
4:D:261:THR:H	4:D:292:GLN:HE22	1.33	0.75
1:A:162:LEU:O	1:A:165:THR:HG22	1.85	0.74
6:6:77:VAL:HG22	6:6:104:TRP:HB2	1.69	0.74
7:9:131:TYR:CB	7:9:136:MET:HE2	2.17	0.74
1:A:16:THR:CG2	1:A:229:PRO:HB3	2.17	0.74
2:B:101:THR:HG22	8:H:108:ILE:HD11	1.69	0.74
3:3:402:PRO:HA	3:3:535:MET:CE	2.17	0.74
4:4:105:LEU:HD13	4:4:309:ILE:HD13	1.67	0.74
4:4:346:THR:HG23	4:4:353:LEU:HB3	1.69	0.74
2:2:81:GLN:HB3	2:2:122:VAL:HG21	1.70	0.74
2:B:106:ILE:HG23	2:B:110:GLU:HB2	1.69	0.74
7:G:131:TYR:CB	7:G:136:MET:HE2	2.17	0.74
3:3:101:ARG:NH1	3:3:140:TYR:CD1	2.55	0.74
8:7:121:ARG:HH11	8:7:121:ARG:HG3	1.50	0.74
2:B:81:GLN:HB3	2:B:122:VAL:HG21	1.69	0.74
1:1:40:THR:O	1:1:44:VAL:HG23	1.87	0.74
4:4:261:THR:H	4:4:292:GLN:HE22	1.34	0.74
3:3:184:CYS:O	3:3:184:CYS:SG	2.45	0.74
4:4:47:LEU:HD12	4:4:48:SER:N	2.03	0.74
4:4:274:ASP:O	4:4:278:VAL:HG23	1.87	0.74
1:A:344:LEU:O	1:A:347:PHE:HB3	1.87	0.74
2:B:101:THR:HG23	2:B:106:ILE:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:GLU:CG	5:E:95:PRO:HA	2.16	0.74
1:A:40:THR:O	1:A:44:VAL:HG23	1.88	0.74
3:3:384:PRO:HG3	3:3:542:ARG:NH2	2.01	0.73
3:C:42:ILE:HD11	3:C:189:ARG:CD	2.18	0.73
3:3:509:ALA:HB1	3:3:768:GLY:HA3	1.69	0.73
3:3:55:PRO:HB3	3:3:73:ILE:CA	2.18	0.73
2:2:101:THR:HG22	8:7:108:ILE:HD11	1.69	0.73
5:5:5:ARG:HG3	5:5:5:ARG:NH1	2.00	0.73
4:D:346:THR:HG23	4:D:353:LEU:HB3	1.68	0.73
2:B:134:ILE:HG13	2:B:145:VAL:HG21	1.71	0.73
3:C:101:ARG:NH1	3:C:140:TYR:CD1	2.57	0.73
1:1:50:PRO:O	1:1:53:VAL:HG12	1.89	0.73
3:3:405:GLU:HB2	3:3:535:MET:CE	2.17	0.73
3:3:156:ARG:HH11	3:3:156:ARG:HG3	1.53	0.73
3:3:567:TYR:HA	3:3:584:VAL:HG23	1.69	0.73
1:A:115:ILE:O	1:A:119:ILE:HG13	1.89	0.73
3:C:279:ALA:HB2	3:C:290:ILE:HG12	1.69	0.73
4:4:262:PHE:CE1	4:4:289:ILE:HD11	2.24	0.73
7:9:40:ARG:HB2	7:9:121:MET:HE1	1.69	0.72
6:6:148:ILE:HG21	7:9:27:PRO:HG3	1.71	0.72
1:1:253:GLN:N	1:1:253:GLN:HE21	1.87	0.72
3:C:55:PRO:CB	3:C:73:ILE:HA	2.19	0.72
4:4:126:LEU:HD21	4:4:286:SER:HB2	1.71	0.72
10:1:440:FMN:N1	10:1:440:FMN:O3'	2.20	0.72
1:A:358:PRO:HD3	3:C:107:MET:CE	2.19	0.72
3:C:19:VAL:HG22	3:C:91:MET:HE1	1.70	0.72
3:C:218:LEU:N	3:C:219:PRO:HD3	2.05	0.72
3:C:402:PRO:HA	3:C:535:MET:CE	2.19	0.72
3:3:20:MET:CE	3:3:432:PHE:HB2	2.19	0.72
5:5:10:ALA:HB1	5:5:15:TYR:HB2	1.72	0.71
1:1:90:ILE:HD11	1:1:211:LEU:HD22	1.71	0.71
1:1:395:GLU:HB2	1:1:407:VAL:HG21	1.72	0.71
4:D:47:LEU:HD12	4:D:48:SER:N	2.05	0.71
5:E:5:ARG:HG3	5:E:5:ARG:NH1	1.99	0.71
6:6:108:MET:HA	6:6:137:VAL:CG1	2.21	0.71
1:A:395:GLU:HB2	1:A:407:VAL:HG21	1.72	0.71
3:C:583:VAL:CG2	3:C:598:ALA:HA	2.20	0.71
6:F:163:TYR:HB2	7:G:152:ARG:NH1	2.06	0.71
6:6:163:TYR:HB2	7:9:152:ARG:NH1	2.05	0.71
7:9:96:LEU:HD21	7:9:129:LEU:HD13	1.71	0.71
1:A:90:ILE:HD11	1:A:211:LEU:HD22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:371:ARG:NH1	5:5:50:ALA:O	2.24	0.71
6:6:83:ARG:HH11	6:6:83:ARG:CG	1.97	0.71
6:F:163:TYR:HD1	7:G:152:ARG:HH11	1.38	0.71
2:2:106:ILE:HG23	2:2:110:GLU:HB2	1.73	0.70
7:G:71:GLU:HB2	7:G:90:VAL:HB	1.72	0.70
3:C:737:GLU:HB2	3:C:776:LEU:HD21	1.73	0.70
3:3:583:VAL:CG2	3:3:598:ALA:HA	2.21	0.70
5:5:47:ASN:HD22	5:5:47:ASN:N	1.87	0.70
6:F:77:VAL:HA	6:F:104:TRP:O	1.91	0.70
3:3:31:PRO:CB	3:3:47:MET:HE3	2.18	0.70
3:C:31:PRO:CB	3:C:47:MET:HE3	2.18	0.70
1:1:253:GLN:HE21	1:1:253:GLN:H	1.38	0.70
1:A:253:GLN:HE21	1:A:253:GLN:H	1.40	0.70
4:4:318:GLU:HB2	8:7:39:ASP:HA	1.74	0.70
1:A:253:GLN:HE21	1:A:253:GLN:N	1.89	0.70
3:C:20:MET:CE	3:C:432:PHE:HB2	2.20	0.70
5:E:47:ASN:HD22	5:E:47:ASN:N	1.88	0.70
6:F:108:MET:HA	6:F:137:VAL:CG1	2.22	0.70
4:4:272:VAL:HG23	4:4:399:SER:HB3	1.74	0.70
6:6:83:ARG:HG3	6:6:83:ARG:NH1	1.93	0.70
1:A:341:MET:HE3	1:A:413:SER:HB3	1.74	0.70
4:D:272:VAL:HG23	4:D:399:SER:HB3	1.73	0.70
6:F:108:MET:HA	6:F:137:VAL:HG13	1.74	0.70
3:C:538:ALA:HB3	3:C:541:ALA:HB2	1.73	0.69
3:C:567:TYR:HA	3:C:584:VAL:HG23	1.74	0.69
4:D:254:TYR:CE2	4:D:346:THR:HA	2.27	0.69
2:2:27:ILE:O	2:2:31:LEU:HD23	1.92	0.69
1:A:49:THR:HG23	1:A:52:GLU:HG3	1.74	0.69
4:D:126:LEU:HD21	4:D:286:SER:HB2	1.72	0.69
7:9:131:TYR:HB2	7:9:136:MET:HE2	1.72	0.69
3:C:378:PRO:O	3:C:381:LEU:HB2	1.92	0.69
3:C:738:THR:HG23	3:C:739:PRO:HD2	1.74	0.69
3:3:11:VAL:CG1	3:3:25:HIS:HD2	2.00	0.69
5:5:66:GLU:CG	5:5:95:PRO:HA	2.19	0.69
5:E:10:ALA:HB1	5:E:15:TYR:HB2	1.73	0.69
6:6:77:VAL:HA	6:6:104:TRP:O	1.92	0.69
1:A:270:THR:O	1:A:311:MET:HG3	1.92	0.69
4:D:85:MET:CE	4:D:409:ARG:HB2	2.23	0.69
3:C:184:CYS:O	3:C:184:CYS:SG	2.51	0.69
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.75	0.69
3:3:737:GLU:HB2	3:3:776:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:254:TYR:CE2	4:4:346:THR:HA	2.27	0.69
2:B:27:ILE:O	2:B:31:LEU:HD23	1.91	0.69
4:D:372:ALA:HB1	4:D:406:ASP:OD1	1.92	0.69
7:G:96:LEU:HD21	7:G:129:LEU:HD13	1.75	0.69
5:5:145:PRO:HA	5:5:150:TYR:CD2	2.27	0.69
3:C:216:PHE:CZ	8:H:128:PHE:HD2	2.11	0.69
5:5:29:LEU:O	5:5:92:VAL:HG12	1.93	0.68
6:F:163:TYR:HD1	7:G:152:ARG:NH1	1.91	0.68
1:1:272:PHE:CE2	1:1:311:MET:HE3	2.29	0.68
1:1:363:VAL:HA	1:1:367:MET:HB2	1.76	0.68
7:9:71:GLU:HB2	7:9:90:VAL:HB	1.74	0.68
1:1:267:PRO:O	1:1:270:THR:HG23	1.92	0.68
3:C:55:PRO:HG3	3:C:73:ILE:HA	1.74	0.68
1:1:49:THR:HG23	1:1:52:GLU:HG3	1.75	0.68
4:4:85:MET:CE	4:4:409:ARG:HB2	2.24	0.68
1:1:341:MET:HE3	1:1:413:SER:HB3	1.76	0.68
5:5:123:GLY:H	5:5:147:ARG:NH1	1.91	0.68
1:A:16:THR:HG21	1:A:229:PRO:CB	2.22	0.68
3:C:31:PRO:HB3	3:C:47:MET:CE	2.19	0.68
3:C:42:ILE:HD11	3:C:189:ARG:HD2	1.74	0.68
2:2:144:CYS:O	2:2:149:ARG:HD2	1.93	0.68
3:3:378:PRO:O	3:3:381:LEU:HB2	1.93	0.68
3:C:2:VAL:CG1	3:C:89:ASP:HA	2.24	0.68
3:3:386:SER:HB2	3:3:675:ARG:HH12	1.57	0.68
7:G:40:ARG:HB2	7:G:121:MET:CE	2.24	0.68
1:1:18:TYR:OH	1:1:105:TYR:HB2	1.94	0.68
3:3:261:VAL:HG22	9:3:786:SF4:S2	2.33	0.68
8:H:10:TYR:O	8:H:14:VAL:HG23	1.94	0.68
3:3:2:VAL:CG1	3:3:89:ASP:HA	2.24	0.68
5:E:29:LEU:O	5:E:92:VAL:HG12	1.94	0.68
1:A:370:LEU:O	1:A:374:ILE:HG22	1.93	0.67
3:C:282:VAL:HG22	3:C:285:VAL:HG12	1.76	0.67
3:3:20:MET:HE1	3:3:432:PHE:CB	2.23	0.67
3:3:31:PRO:HB3	3:3:47:MET:CE	2.20	0.67
3:3:402:PRO:HA	3:3:535:MET:HE1	1.74	0.67
4:D:393:MET:HA	4:D:396:ILE:HG22	1.76	0.67
1:1:219:ASN:ND2	10:1:440:FMN:O2P	2.26	0.67
1:A:18:TYR:OH	1:A:105:TYR:HB2	1.95	0.67
6:F:154:LEU:O	6:F:158:VAL:HG13	1.95	0.67
4:D:85:MET:HE2	4:D:409:ARG:HB2	1.77	0.67
3:C:402:PRO:HA	3:C:535:MET:HE1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:216:PHE:CZ	8:7:128:PHE:HD2	2.13	0.67
1:1:16:THR:CG2	1:1:229:PRO:HB3	2.22	0.67
6:6:108:MET:HA	6:6:137:VAL:HG13	1.75	0.67
1:A:267:PRO:O	1:A:270:THR:HG23	1.94	0.67
2:B:106:ILE:CG2	2:B:110:GLU:HB2	2.24	0.67
4:4:367:ARG:HG2	4:4:367:ARG:NH1	2.10	0.67
3:C:739:PRO:HG2	3:C:771:VAL:HG12	1.76	0.67
7:G:131:TYR:HB2	7:G:136:MET:HE2	1.76	0.67
7:9:40:ARG:HB2	7:9:121:MET:CE	2.25	0.67
4:D:190:LEU:O	4:D:194:LEU:HB2	1.95	0.67
3:C:722:THR:HG21	3:C:756:GLY:N	2.09	0.66
1:1:104:ARG:HD2	1:1:108:GLU:OE2	1.94	0.66
2:2:110:GLU:HA	8:7:121:ARG:HH12	1.59	0.66
2:B:144:CYS:O	2:B:149:ARG:HD2	1.94	0.66
3:C:20:MET:HE1	3:C:432:PHE:CB	2.25	0.66
7:G:73:ALA:HB2	7:G:89:LYS:HB2	1.76	0.66
1:1:104:ARG:NH2	2:2:127:SER:CB	2.57	0.66
4:4:279:ARG:HH11	4:4:279:ARG:HG3	1.60	0.66
3:C:739:PRO:HG2	3:C:771:VAL:CG1	2.25	0.66
3:3:42:ILE:HD11	3:3:189:ARG:CD	2.25	0.66
3:3:405:GLU:OE1	3:3:508:GLY:HA3	1.96	0.66
2:B:122:VAL:HG12	2:B:123:GLU:N	2.11	0.66
4:D:262:PHE:CE1	4:D:289:ILE:HD11	2.30	0.66
4:4:372:ALA:HB1	4:4:406:ASP:OD1	1.94	0.66
1:A:110:VAL:N	1:A:111:PRO:HD3	2.11	0.66
3:C:156:ARG:HH11	3:C:156:ARG:HG3	1.60	0.66
4:D:149:ALA:HA	4:D:152:GLU:OE2	1.95	0.66
1:A:104:ARG:HD2	1:A:108:GLU:OE2	1.96	0.66
5:E:47:ASN:HD21	5:E:76:SER:HA	1.61	0.66
5:E:59:THR:HG22	5:E:59:THR:O	1.96	0.66
3:3:305:ARG:HH22	3:3:609:GLU:CD	2.04	0.65
3:3:738:THR:HG23	3:3:739:PRO:HD2	1.77	0.65
3:C:304:ASN:O	3:C:589:HIS:CD2	2.49	0.65
3:3:249:MET:HE3	3:3:268:ASP:HB3	1.77	0.65
2:B:44:GLU:CD	2:B:44:GLU:H	2.04	0.65
2:2:134:ILE:HG13	2:2:145:VAL:HG21	1.77	0.65
3:3:722:THR:HG21	3:3:756:GLY:N	2.12	0.65
3:3:578:LYS:HG2	3:3:597:TYR:HE2	1.62	0.65
1:1:370:LEU:O	1:1:374:ILE:HG22	1.96	0.65
2:2:106:ILE:CG2	2:2:110:GLU:HB2	2.27	0.65
4:4:236:GLY:C	4:4:238:SER:H	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:47:ASN:HD21	5:5:76:SER:HA	1.60	0.65
1:A:363:VAL:HA	1:A:367:MET:HB2	1.77	0.65
3:C:305:ARG:HH22	3:C:609:GLU:CD	2.05	0.65
1:A:177:ALA:O	2:B:67:TYR:HB3	1.96	0.65
3:C:346:ALA:HB2	3:C:569:GLY:O	1.96	0.65
1:1:110:VAL:N	1:1:111:PRO:HD3	2.11	0.65
1:1:437:TRP:CB	2:2:92:GLY:HA3	2.26	0.65
3:3:285:VAL:HG22	3:3:286:ASN:H	1.62	0.65
3:3:739:PRO:HG2	3:3:771:VAL:CG1	2.27	0.65
3:C:115:HIS:C	4:D:321:MET:HE3	2.22	0.65
1:1:16:THR:HG21	1:1:229:PRO:CB	2.25	0.65
3:3:591:HIS:ND1	3:3:592:PRO:HD2	2.11	0.65
4:4:59:ILE:HD11	5:5:135:ILE:HG23	1.79	0.65
2:B:26:ALA:O	2:B:29:PRO:HG2	1.97	0.65
3:C:545:GLU:HA	3:C:550:LEU:HD11	1.79	0.64
3:C:671:GLU:HG2	3:C:672:ALA:H	1.61	0.64
3:C:385:ALA:HB2	3:C:531:LYS:HB3	1.80	0.64
3:C:736:VAL:HG22	3:C:775:VAL:HG22	1.79	0.64
4:D:279:ARG:HG3	4:D:279:ARG:HH11	1.63	0.64
5:E:123:GLY:H	5:E:147:ARG:NH1	1.96	0.64
1:1:115:ILE:O	1:1:119:ILE:HG13	1.97	0.64
1:1:350:HIS:O	3:3:205:ARG:NH1	2.31	0.64
2:2:26:ALA:O	2:2:29:PRO:HG2	1.97	0.64
1:1:357:THR:N	1:1:358:PRO:HD2	2.13	0.64
7:9:44:THR:HA	7:9:138:VAL:HG13	1.80	0.64
3:C:55:PRO:CG	3:C:73:ILE:HA	2.27	0.64
3:3:279:ALA:CB	3:3:290:ILE:HG12	2.28	0.64
4:4:98:ALA:O	4:4:102:GLU:HG3	1.97	0.64
3:C:583:VAL:HG21	3:C:598:ALA:HA	1.78	0.64
4:D:234:LEU:HD21	4:D:238:SER:HB2	1.79	0.64
4:D:236:GLY:C	4:D:238:SER:H	2.05	0.64
1:1:53:VAL:HG23	1:1:231:MET:HE2	1.80	0.64
3:3:671:GLU:HG2	3:3:672:ALA:H	1.62	0.64
7:G:133:LYS:O	7:G:137:LEU:HD13	1.98	0.64
3:3:739:PRO:HG2	3:3:771:VAL:HG12	1.79	0.64
2:B:110:GLU:HA	8:H:121:ARG:HH12	1.62	0.64
3:C:54:LEU:N	3:C:55:PRO:CD	2.60	0.64
3:C:226:ILE:HD12	3:C:235:LEU:HD13	1.79	0.64
4:D:225:PRO:HG2	4:D:228:VAL:HB	1.80	0.64
1:A:120:LEU:HD13	1:A:227:VAL:HG12	1.79	0.64
7:G:44:THR:HA	7:G:138:VAL:HG13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:397:ARG:HD2	1:1:397:ARG:N	2.13	0.64
2:2:33:ARG:HH21	2:2:37:GLU:HG2	1.63	0.64
7:9:73:ALA:HB2	7:9:89:LYS:HB2	1.80	0.64
8:7:10:TYR:O	8:7:14:VAL:HG23	1.98	0.64
3:3:54:LEU:N	3:3:55:PRO:CD	2.60	0.63
3:C:216:PHE:HZ	8:H:128:PHE:HD2	1.46	0.63
5:5:18:GLU:HB2	5:5:26:TRP:HB2	1.81	0.63
6:6:36:LEU:HD22	6:6:77:VAL:HG21	1.79	0.63
7:9:56:CYS:SG	7:9:58:LEU:HB2	2.39	0.63
1:1:358:PRO:HD3	3:3:107:MET:HE1	1.79	0.63
2:2:122:VAL:HG12	2:2:123:GLU:N	2.12	0.63
4:4:47:LEU:HD12	4:4:48:SER:H	1.63	0.63
4:4:393:MET:HA	4:4:396:ILE:HG22	1.81	0.63
3:C:11:VAL:CG1	3:C:25:HIS:HD2	2.03	0.63
3:3:184:CYS:O	9:3:785:SF4:S4	2.57	0.63
3:3:206:GLY:O	3:3:209:THR:HG23	1.98	0.63
3:3:282:VAL:HG22	3:3:285:VAL:HG12	1.80	0.63
3:3:285:VAL:HG22	3:3:286:ASN:N	2.14	0.63
6:6:154:LEU:O	6:6:158:VAL:HG13	1.99	0.63
1:1:120:LEU:HD13	1:1:227:VAL:HG12	1.79	0.63
3:3:30:VAL:CG2	3:3:31:PRO:HD2	2.28	0.63
3:3:583:VAL:HG21	3:3:598:ALA:HA	1.80	0.63
1:A:357:THR:N	1:A:358:PRO:HD2	2.14	0.63
1:A:97:GLU:HB2	11:A:441:NAI:C4N	2.23	0.63
1:A:253:GLN:HG2	1:A:327:GLY:HA2	1.80	0.63
2:B:78:TYR:HA	2:B:137:ASN:HD21	1.63	0.63
4:D:83:PRO:HB2	4:D:169:HIS:HA	1.81	0.63
1:1:253:GLN:HG2	1:1:327:GLY:HA2	1.81	0.63
1:A:145:LEU:O	1:A:149:ILE:HG13	1.99	0.63
3:C:583:VAL:HG21	3:C:597:TYR:O	1.99	0.63
4:D:47:LEU:HD12	4:D:48:SER:H	1.64	0.63
4:D:73:ARG:O	4:D:364:MET:HB3	1.99	0.63
5:5:59:THR:O	5:5:59:THR:HG22	1.99	0.62
3:3:55:PRO:CB	3:3:73:ILE:HA	2.29	0.62
2:B:10:PHE:CZ	2:B:33:ARG:HG3	2.34	0.62
3:C:405:GLU:OE1	3:C:508:GLY:HA3	1.98	0.62
4:D:250:LYS:CE	4:D:262:PHE:HB3	2.25	0.62
4:D:389:GLN:HG3	4:D:390:VAL:H	1.64	0.62
3:3:154:TYR:CZ	4:4:312:PRO:HB3	2.34	0.62
3:3:545:GLU:HA	3:3:550:LEU:HD11	1.81	0.62
3:C:116:PRO:O	3:C:117:LEU:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:ARG:C	3:C:209:THR:HG22	2.23	0.62
4:4:85:MET:HE2	4:4:409:ARG:HB2	1.80	0.62
3:C:343:LEU:HD12	3:C:361:ALA:HB2	1.82	0.62
3:3:346:ALA:HB2	3:3:569:GLY:O	1.99	0.62
4:4:64:THR:OG1	6:6:83:ARG:NH1	2.32	0.62
6:F:36:LEU:HD22	6:F:77:VAL:HG21	1.81	0.62
3:C:30:VAL:CG2	3:C:31:PRO:HD2	2.29	0.62
3:C:249:MET:HE3	3:C:268:ASP:HB3	1.80	0.62
3:C:333:LEU:HB3	3:C:648:LEU:HD21	1.81	0.62
3:C:578:LYS:HG2	3:C:597:TYR:HE2	1.62	0.62
5:E:80:TRP:HA	5:E:80:TRP:CE3	2.34	0.62
3:3:205:ARG:C	3:3:209:THR:HG22	2.24	0.62
1:A:397:ARG:HD2	1:A:397:ARG:N	2.15	0.62
2:B:114:ASP:HB2	2:B:116:LEU:CD2	2.24	0.62
3:C:435:LEU:HD22	3:C:435:LEU:H	1.64	0.62
4:D:371:ARG:NH1	5:E:50:ALA:O	2.32	0.62
2:2:10:PHE:CZ	2:2:33:ARG:HG3	2.34	0.62
3:3:259:CYS:SG	3:3:261:VAL:HG13	2.40	0.62
3:3:736:VAL:HG22	3:3:775:VAL:HG22	1.80	0.62
3:C:591:HIS:ND1	3:C:592:PRO:HD2	2.15	0.62
3:3:185:LYS:HG3	3:3:202:PHE:HE2	1.65	0.62
6:6:76:ASP:O	6:6:77:VAL:HB	2.00	0.62
3:C:2:VAL:HG13	3:C:89:ASP:HA	1.82	0.62
4:4:149:ALA:HA	4:4:152:GLU:OE2	2.00	0.61
3:3:435:LEU:HD22	3:3:435:LEU:H	1.65	0.61
4:4:190:LEU:O	4:4:194:LEU:HB2	1.99	0.61
1:A:272:PHE:CE2	1:A:311:MET:HE3	2.34	0.61
2:B:33:ARG:HH21	2:B:37:GLU:HG2	1.64	0.61
5:E:175:THR:HG23	5:E:178:ASP:CB	2.24	0.61
2:2:114:ASP:HB2	2:2:116:LEU:CD2	2.26	0.61
1:A:350:HIS:O	3:C:205:ARG:NH1	2.33	0.61
3:C:6:VAL:HG13	3:C:23:VAL:HG22	1.83	0.61
3:3:304:ASN:O	3:3:589:HIS:CD2	2.54	0.61
3:C:469:ARG:HG2	3:C:754:PRO:HB3	1.81	0.61
1:1:270:THR:O	1:1:311:MET:HG3	2.00	0.61
4:D:64:THR:OG1	6:F:83:ARG:NH1	2.33	0.61
3:3:333:LEU:HB3	3:3:648:LEU:HD21	1.82	0.61
1:A:267:PRO:HG2	1:A:270:THR:HG22	1.82	0.61
3:3:117:LEU:HD12	4:4:321:MET:CE	2.28	0.61
3:3:216:PHE:HZ	8:7:128:PHE:HD2	1.47	0.61
4:4:89:HIS:CE1	4:4:92:ALA:HB2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:367:ARG:HG2	4:D:367:ARG:NH1	2.12	0.61
6:6:143:ARG:HG2	6:6:144:PRO:HD2	1.82	0.61
2:B:77:LYS:H	2:B:116:LEU:HA	1.65	0.61
3:C:279:ALA:CB	3:C:290:ILE:HG12	2.30	0.61
4:4:230:ILE:HG22	4:4:230:ILE:O	2.00	0.61
8:7:34:GLU:HB3	8:7:56:THR:HG22	1.82	0.61
3:C:259:CYS:SG	3:C:261:VAL:HG13	2.41	0.61
1:1:66:GLY:O	11:1:441:NAI:H2N	2.01	0.61
1:A:358:PRO:HD3	3:C:107:MET:HE3	1.82	0.61
1:A:385:GLU:O	1:A:388:GLU:HB3	2.00	0.61
4:D:89:HIS:CE1	4:D:92:ALA:HB2	2.35	0.61
4:D:200:ARG:HG3	4:D:204:TYR:HE1	1.66	0.61
1:1:266:LEU:HB3	1:1:270:THR:HG21	1.82	0.60
3:3:11:VAL:CG1	3:3:25:HIS:CD2	2.81	0.60
4:4:83:PRO:HB2	4:4:169:HIS:HA	1.82	0.60
3:C:206:GLY:O	3:C:209:THR:HG23	2.00	0.60
3:C:722:THR:HG21	3:C:756:GLY:H	1.65	0.60
4:D:226:PRO:HG3	4:D:242:SER:O	2.00	0.60
1:1:385:GLU:O	1:1:388:GLU:HB3	2.00	0.60
3:C:152:PRO:HG3	4:D:305:PRO:O	1.99	0.60
2:2:44:GLU:CD	2:2:44:GLU:H	2.08	0.60
3:3:453:PRO:HD3	3:3:468:HIS:CE1	2.36	0.60
1:A:397:ARG:HD2	1:A:397:ARG:H	1.65	0.60
5:E:18:GLU:HB2	5:E:26:TRP:HB2	1.83	0.60
3:3:2:VAL:HG13	3:3:89:ASP:HA	1.83	0.60
4:4:226:PRO:HG3	4:4:242:SER:O	2.02	0.60
6:6:153:GLN:HG3	7:9:124:TYR:OH	2.00	0.60
3:C:285:VAL:HG22	3:C:286:ASN:H	1.66	0.60
4:4:164:THR:OG1	4:4:170:HIS:HB3	2.02	0.60
1:A:266:LEU:HB3	1:A:270:THR:HG21	1.83	0.60
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.84	0.60
1:A:356:CYS:HB3	1:A:358:PRO:HD2	1.83	0.60
1:1:138:TYR:HB3	1:1:141:ALA:HB3	1.84	0.60
2:2:149:ARG:NH1	2:2:168:LEU:HD13	2.16	0.60
6:6:99:MET:HG2	6:6:100:PRO:HD2	1.84	0.60
3:C:47:MET:SD	3:C:107:MET:HB3	2.41	0.60
3:C:469:ARG:HG2	3:C:754:PRO:CB	2.31	0.60
5:E:37:GLU:O	5:E:41:TYR:HD1	1.85	0.60
6:F:99:MET:HG2	6:F:100:PRO:HD2	1.83	0.60
1:1:145:LEU:O	1:1:149:ILE:HG13	2.01	0.60
7:9:175:ALA:O	7:9:177:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:153:GLN:HG3	7:G:124:TYR:OH	2.00	0.60
3:3:615:VAL:HG22	3:3:621:VAL:HG12	1.82	0.60
4:4:234:LEU:HD21	4:4:238:SER:HB2	1.84	0.60
4:4:389:GLN:HG3	4:4:390:VAL:H	1.67	0.60
3:C:55:PRO:CB	3:C:73:ILE:N	2.65	0.60
3:C:101:ARG:NH1	3:C:140:TYR:CE1	2.69	0.60
4:D:144:THR:HB	4:D:145:PRO:HD3	1.83	0.60
6:F:163:TYR:CD1	7:G:152:ARG:HD2	2.37	0.60
4:4:144:THR:HB	4:4:145:PRO:HD3	1.84	0.60
4:4:200:ARG:HG3	4:4:204:TYR:HE1	1.67	0.60
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.37	0.60
6:F:83:ARG:HD3	9:F:182:SF4:S4	2.42	0.60
3:3:385:ALA:HB2	3:3:531:LYS:HB3	1.84	0.59
3:3:583:VAL:HG21	3:3:597:TYR:O	2.02	0.59
4:4:222:GLY:CA	4:4:396:ILE:HD11	2.31	0.59
6:F:143:ARG:HG2	6:F:144:PRO:HD2	1.84	0.59
8:H:121:ARG:HG3	8:H:121:ARG:NH1	2.16	0.59
1:1:358:PRO:HD3	3:3:107:MET:HE3	1.83	0.59
5:5:37:GLU:O	5:5:41:TYR:HD1	1.84	0.59
1:A:437:TRP:CB	2:B:92:GLY:HA3	2.30	0.59
3:C:385:ALA:HB2	3:C:531:LYS:CB	2.32	0.59
3:C:655:ARG:HB2	3:C:655:ARG:NH1	2.17	0.59
4:D:337:PRO:O	4:D:361:GLY:HA2	2.02	0.59
3:3:132:ASP:OD1	4:4:329:LYS:HE2	2.02	0.59
3:3:156:ARG:HG3	3:3:156:ARG:NH1	2.16	0.59
3:3:722:THR:HA	3:3:725:ALA:HB3	1.84	0.59
4:4:363:SER:HB2	5:5:174:LEU:N	2.17	0.59
7:G:131:TYR:HB3	7:G:136:MET:HE2	1.84	0.59
1:1:356:CYS:HB3	1:1:358:PRO:HD2	1.84	0.59
2:2:77:LYS:H	2:2:116:LEU:HA	1.68	0.59
4:4:74:THR:HB	4:4:77:GLN:H	1.67	0.59
1:A:104:ARG:NH2	2:B:127:SER:CB	2.61	0.59
3:3:511:VAL:O	3:3:518:ALA:HB2	2.03	0.59
1:1:267:PRO:HG2	1:1:270:THR:HG22	1.83	0.59
3:3:655:ARG:HB2	3:3:655:ARG:NH1	2.16	0.59
3:3:722:THR:HG21	3:3:756:GLY:H	1.66	0.59
1:1:301:PRO:HB2	1:1:303:THR:HG23	1.85	0.59
3:3:101:ARG:NH1	3:3:140:TYR:CE1	2.67	0.59
3:3:337:ARG:HH12	3:3:581:ARG:NH1	2.00	0.59
6:6:92:MET:HE1	6:6:127:VAL:HG13	1.84	0.59
1:A:184:GLU:CD	1:A:186:THR:HG22	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ALA:O	1:A:410:VAL:HG23	2.03	0.59
4:D:74:THR:HB	4:D:77:GLN:H	1.66	0.59
4:D:230:ILE:HG22	4:D:230:ILE:O	2.02	0.59
4:D:263:ASP:O	4:D:265:PRO:HD3	2.02	0.59
4:D:366:TYR:CZ	5:E:148:LYS:HE3	2.38	0.59
8:H:34:GLU:HB3	8:H:56:THR:HG22	1.83	0.59
2:2:78:TYR:HA	2:2:137:ASN:HD21	1.66	0.59
1:A:28:THR:HG22	1:A:30:ASP:H	1.67	0.59
1:A:374:ILE:O	1:A:374:ILE:HG12	2.02	0.59
6:F:78:MET:HE2	6:F:99:MET:HE1	1.84	0.59
6:F:81:ALA:HB1	6:F:108:MET:HE2	1.85	0.59
3:3:586:HIS:CD2	3:3:604:ALA:HB2	2.38	0.59
3:C:30:VAL:HG22	3:C:31:PRO:HD2	1.84	0.59
3:C:227:THR:HG21	3:C:237:ASP:HB2	1.84	0.59
3:C:689:LYS:HB2	3:C:772:GLU:HG2	1.85	0.59
3:3:42:ILE:HD11	3:3:189:ARG:HD2	1.85	0.59
3:3:440:ARG:HG2	3:3:440:ARG:HH11	1.67	0.59
4:4:221:VAL:O	4:4:272:VAL:HG12	2.02	0.58
1:A:96:SER:HA	1:A:135:ARG:NH1	2.18	0.58
3:C:474:ARG:HA	3:C:517:ALA:HB2	1.85	0.58
3:3:279:ALA:HB2	3:3:290:ILE:CG1	2.31	0.58
3:3:515:THR:HG23	3:3:683:LEU:CD1	2.31	0.58
5:5:123:GLY:H	5:5:147:ARG:HH11	1.51	0.58
1:A:363:VAL:O	1:A:368:VAL:HG12	2.02	0.58
3:C:285:VAL:HG22	3:C:286:ASN:N	2.18	0.58
6:F:163:TYR:CD1	7:G:152:ARG:NH1	2.71	0.58
8:H:63:LEU:HD13	8:H:129:ALA:HB3	1.85	0.58
1:1:184:GLU:CD	1:1:186:THR:HG22	2.28	0.58
1:1:214:LYS:O	1:1:216:THR:HG23	2.03	0.58
3:C:515:THR:HG23	3:C:683:LEU:CD1	2.31	0.58
1:1:397:ARG:HD2	1:1:397:ARG:H	1.67	0.58
4:4:163:VAL:HG22	4:4:164:THR:HG22	1.85	0.58
6:6:163:TYR:HB2	7:9:152:ARG:HH11	1.68	0.58
1:A:88:TYR:HB2	1:A:216:THR:HG22	1.84	0.58
1:A:358:PRO:HD3	3:C:107:MET:HE1	1.85	0.58
3:C:184:CYS:O	9:C:785:SF4:S4	2.61	0.58
3:C:444:ARG:NH2	3:C:447:LYS:HG3	2.18	0.58
1:1:33:LEU:HA	1:1:37:GLY:HA2	1.85	0.58
3:3:123:ASP:HB2	3:3:236:LEU:HD13	1.85	0.58
3:C:550:LEU:HD12	3:C:550:LEU:N	2.18	0.58
3:C:583:VAL:HG23	3:C:598:ALA:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:513:GLN:HG2	3:3:769:LEU:HD23	1.84	0.58
3:C:398:VAL:HB	3:C:450:LEU:HD22	1.85	0.58
4:D:98:ALA:O	4:D:102:GLU:HG3	2.02	0.58
4:D:239:LEU:HD22	4:D:244:VAL:HB	1.84	0.58
4:D:261:THR:H	4:D:292:GLN:NE2	2.01	0.58
5:5:5:ARG:HH11	5:5:5:ARG:CG	2.15	0.58
2:B:149:ARG:NH1	2:B:168:LEU:HD13	2.18	0.58
3:3:370:ASP:OD1	3:3:374:ARG:HD3	2.03	0.58
8:7:63:LEU:HD13	8:7:129:ALA:HB3	1.86	0.58
2:B:31:LEU:HD12	2:B:41:ILE:HD13	1.86	0.58
3:C:225:ASN:ND2	3:C:289:TRP:HB3	2.19	0.58
3:C:337:ARG:HH12	3:C:581:ARG:NH1	2.02	0.58
6:F:145:GLU:HG2	7:G:31:VAL:CG2	2.34	0.58
3:3:343:LEU:HD12	3:3:361:ALA:HB2	1.84	0.58
5:5:53:VAL:HG13	5:5:71:VAL:HB	1.86	0.58
8:7:121:ARG:HG3	8:7:121:ARG:NH1	2.18	0.58
1:A:6:LEU:HB2	1:A:241:MET:HA	1.85	0.58
3:C:511:VAL:O	3:C:518:ALA:HB2	2.03	0.58
5:E:37:GLU:O	5:E:41:TYR:CD1	2.57	0.58
7:G:56:CYS:SG	7:G:58:LEU:HB2	2.43	0.58
3:3:167:HIS:ND1	3:3:167:HIS:O	2.36	0.57
4:4:225:PRO:HG2	4:4:228:VAL:HB	1.85	0.57
3:C:320:ALA:HB1	3:C:324:GLU:HB2	1.86	0.57
4:D:95:LEU:HG	4:D:99:LEU:HD23	1.85	0.57
4:D:164:THR:OG1	4:D:170:HIS:HB3	2.03	0.57
6:F:121:TYR:HD1	6:F:121:TYR:H	1.51	0.57
1:1:374:ILE:HG12	1:1:374:ILE:O	2.02	0.57
3:C:326:PHE:CZ	3:C:330:LYS:HE3	2.39	0.57
3:3:185:LYS:HG2	3:3:188:VAL:HG22	1.86	0.57
3:3:226:ILE:HD12	3:3:235:LEU:HD13	1.85	0.57
6:6:78:MET:O	6:6:78:MET:HG3	2.03	0.57
6:6:121:TYR:HD1	6:6:121:TYR:H	1.52	0.57
3:C:34:CYS:HA	3:C:184:CYS:HB2	1.85	0.57
6:F:76:ASP:O	6:F:77:VAL:HB	2.04	0.57
1:1:337:MET:HA	1:1:337:MET:CE	2.33	0.57
4:4:40:VAL:O	4:4:40:VAL:HG22	2.03	0.57
1:A:359:CYS:HA	1:A:363:VAL:HG13	1.85	0.57
3:3:385:ALA:HB2	3:3:531:LYS:CB	2.35	0.57
3:C:615:VAL:HG22	3:C:621:VAL:HG12	1.86	0.57
3:C:722:THR:HA	3:C:725:ALA:HB3	1.86	0.57
4:D:221:VAL:O	4:D:272:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:5:ARG:HH11	5:E:5:ARG:CG	2.14	0.57
3:C:386:SER:HB2	3:C:675:ARG:NH1	2.19	0.57
4:4:250:LYS:CE	4:4:262:PHE:HB3	2.31	0.57
6:6:50:MET:C	6:6:52:ALA:H	2.12	0.57
4:D:248:VAL:HB	4:D:347:GLU:HB2	1.86	0.57
6:F:163:TYR:HB2	7:G:152:ARG:HH11	1.68	0.57
1:1:93:ALA:O	1:1:134:VAL:HA	2.05	0.57
1:1:177:ALA:O	2:2:67:TYR:HB3	2.05	0.57
3:3:116:PRO:O	3:3:117:LEU:CB	2.49	0.57
3:3:469:ARG:HG2	3:3:754:PRO:CB	2.35	0.57
1:A:93:ALA:O	1:A:134:VAL:HA	2.05	0.57
3:C:370:ASP:OD1	3:C:374:ARG:HD3	2.04	0.57
1:A:98:PRO:HA	2:B:124:CYS:SG	2.44	0.57
3:C:11:VAL:CG1	3:C:25:HIS:CD2	2.83	0.57
3:C:453:PRO:HD3	3:C:468:HIS:CE1	2.40	0.57
3:3:469:ARG:HG2	3:3:754:PRO:HB3	1.85	0.57
5:5:37:GLU:O	5:5:41:TYR:CD1	2.58	0.57
3:C:507:LEU:HD22	3:C:511:VAL:HG11	1.87	0.57
1:1:28:THR:HG22	1:1:30:ASP:H	1.70	0.56
3:3:101:ARG:NH1	3:3:140:TYR:HD1	2.00	0.56
3:3:583:VAL:HG23	3:3:598:ALA:HA	1.87	0.56
2:B:112:THR:OG1	2:B:113:PRO:HD2	2.05	0.56
6:F:49:GLU:OE1	6:F:49:GLU:HA	2.05	0.56
3:3:466:GLU:CD	3:3:467:VAL:H	2.13	0.56
3:3:689:LYS:HB2	3:3:772:GLU:HG2	1.85	0.56
6:F:23:THR:O	6:F:27:LEU:HD13	2.05	0.56
2:2:112:THR:OG1	2:2:113:PRO:HD2	2.05	0.56
3:3:47:MET:SD	3:3:107:MET:HB3	2.46	0.56
3:3:394:ASP:OD2	3:3:501:LYS:HB2	2.05	0.56
4:4:211:SER:HB2	4:4:214:PHE:HB3	1.87	0.56
7:9:131:TYR:HB3	7:9:136:MET:HE2	1.85	0.56
2:B:27:ILE:HG12	2:B:53:VAL:HG21	1.88	0.56
4:D:138:LEU:HD13	4:D:146:PHE:CD1	2.40	0.56
5:E:53:VAL:HG13	5:E:71:VAL:HB	1.86	0.56
3:3:567:TYR:HA	3:3:584:VAL:CG2	2.35	0.56
3:C:154:TYR:CZ	4:D:312:PRO:HB3	2.41	0.56
4:D:211:SER:HB2	4:D:214:PHE:HB3	1.87	0.56
1:1:6:LEU:HB2	1:1:241:MET:HA	1.86	0.56
3:3:140:TYR:CE2	3:3:142:LYS:HB3	2.41	0.56
3:3:204:GLU:O	3:3:209:THR:HB	2.06	0.56
3:3:440:ARG:HH11	3:3:440:ARG:CG	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:HIS:ND1	3:C:116:PRO:HD2	2.20	0.56
3:C:607:PHE:HA	3:C:610:LYS:HE2	1.85	0.56
7:G:175:ALA:O	7:G:177:THR:HG23	2.06	0.56
3:3:270:ARG:O	3:3:271:SER:HB2	2.06	0.56
4:4:95:LEU:HG	4:4:99:LEU:HD23	1.87	0.56
4:4:288:LYS:O	4:4:292:GLN:HB2	2.05	0.56
3:C:101:ARG:NH1	3:C:140:TYR:HD1	2.02	0.56
3:C:546:ALA:O	3:C:547:MET:HE2	2.05	0.56
4:D:327:HIS:HE1	7:G:107:ALA:O	1.88	0.56
3:3:607:PHE:HA	3:3:610:LYS:HE2	1.87	0.56
4:4:138:LEU:HD13	4:4:146:PHE:CD1	2.41	0.56
6:6:81:ALA:HB1	6:6:108:MET:HE2	1.87	0.56
3:C:136:GLU:HG2	5:E:189:ARG:HG3	1.88	0.56
3:C:715:GLU:H	3:C:761:SER:HB2	1.71	0.56
4:D:320:SER:O	4:D:324:VAL:HG23	2.06	0.56
4:D:363:SER:HB2	5:E:174:LEU:N	2.19	0.56
3:3:707:LYS:C	3:3:709:GLN:H	2.14	0.56
3:C:115:HIS:HB3	4:D:321:MET:HE3	1.88	0.56
3:C:167:HIS:ND1	3:C:167:HIS:O	2.38	0.56
3:C:456:ALA:HB3	3:C:459:MET:HG3	1.87	0.56
3:C:600:VAL:HG12	3:C:602:LEU:CD1	2.36	0.56
4:D:222:GLY:CA	4:D:396:ILE:HD11	2.32	0.56
6:F:83:ARG:HA	6:F:111:CYS:HB3	1.88	0.56
3:3:227:THR:HG21	3:3:237:ASP:HB2	1.86	0.56
4:4:233:GLY:HA2	5:5:48:PHE:HE1	1.71	0.56
5:5:32:GLU:CD	5:5:32:GLU:H	2.13	0.56
1:A:437:TRP:C	1:A:437:TRP:CD1	2.83	0.56
3:C:513:GLN:HG2	3:C:769:LEU:HD23	1.87	0.56
4:D:241:ALA:HB2	4:D:278:VAL:HG21	1.88	0.56
6:F:50:MET:C	6:F:52:ALA:H	2.14	0.56
10:1:440:FMN:HO3'	10:1:440:FMN:C2	2.15	0.56
3:3:398:VAL:HB	3:3:450:LEU:HD22	1.87	0.56
4:4:239:LEU:HD22	4:4:244:VAL:HB	1.87	0.56
5:5:175:THR:HG23	5:5:178:ASP:CB	2.26	0.56
6:6:83:ARG:HD3	6:6:83:ARG:H	1.71	0.56
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.88	0.56
3:C:156:ARG:HG3	3:C:156:ARG:NH1	2.20	0.56
5:E:161:GLU:CG	5:E:163:ARG:HH22	2.19	0.56
6:F:42:GLY:O	6:F:43:LEU:HD23	2.06	0.56
7:G:132:GLY:H	7:G:135:ASP:HB2	1.71	0.56
3:3:115:HIS:ND1	3:3:116:PRO:HD2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:248:VAL:HB	4:4:347:GLU:HB2	1.89	0.55
1:A:214:LYS:O	1:A:216:THR:HG23	2.06	0.55
3:C:135:VAL:HG23	4:D:326:TYR:CE1	2.41	0.55
3:C:318:VAL:HG12	3:C:319:GLU:N	2.21	0.55
3:3:6:VAL:HG13	3:3:23:VAL:HG22	1.88	0.55
3:3:456:ALA:HB3	3:3:459:MET:HG3	1.88	0.55
1:A:161:ASN:ND2	1:A:166:ASP:HA	2.21	0.55
1:A:258:VAL:HG21	1:A:280:ALA:HB1	1.87	0.55
3:C:117:LEU:HG	4:D:324:VAL:HG21	1.88	0.55
4:D:123:LEU:HD13	4:D:290:ILE:HD12	1.88	0.55
6:6:49:GLU:OE1	6:6:49:GLU:HA	2.05	0.55
8:7:8:GLU:HG2	8:7:97:TYR:CE2	2.42	0.55
4:D:25:VAL:HA	4:D:48:SER:HB3	1.88	0.55
1:1:359:CYS:HA	1:1:363:VAL:HG13	1.87	0.55
3:3:320:ALA:HB1	3:3:324:GLU:HB2	1.87	0.55
4:4:409:ARG:NH2	5:5:117:GLU:OE2	2.40	0.55
1:A:33:LEU:HA	1:A:37:GLY:HA2	1.86	0.55
3:C:586:HIS:CD2	3:C:604:ALA:HB2	2.41	0.55
3:3:30:VAL:HG22	3:3:31:PRO:HD2	1.87	0.55
4:4:193:LEU:HD22	4:4:197:LEU:HG	1.87	0.55
4:4:261:THR:H	4:4:292:GLN:NE2	2.04	0.55
4:D:44:MET:HE2	4:D:44:MET:HA	1.88	0.55
4:D:288:LYS:O	4:D:292:GLN:HB2	2.07	0.55
1:A:219:ASN:ND2	1:A:223:THR:HG21	2.22	0.55
1:A:272:PHE:HZ	1:A:316:LEU:HD21	1.72	0.55
3:C:440:ARG:HG2	3:C:440:ARG:HH11	1.71	0.55
4:4:320:SER:O	4:4:324:VAL:HG23	2.07	0.55
8:7:108:ILE:HD12	8:7:108:ILE:N	2.22	0.55
1:A:37:GLY:C	1:A:39:GLU:H	2.14	0.55
3:C:185:LYS:HG2	3:C:188:VAL:HG22	1.89	0.55
4:D:133:LEU:HD21	4:D:204:TYR:CD2	2.42	0.55
5:E:37:GLU:O	5:E:40:HIS:HB3	2.06	0.55
7:G:137:LEU:O	7:G:140:VAL:HG12	2.06	0.55
7:G:151:LYS:C	7:G:153:THR:H	2.14	0.55
3:3:386:SER:HB2	3:3:675:ARG:NH1	2.22	0.55
3:3:550:LEU:HD12	3:3:550:LEU:N	2.21	0.55
4:4:263:ASP:O	4:4:265:PRO:HD3	2.07	0.55
6:6:83:ARG:HD3	9:6:182:SF4:S4	2.46	0.55
7:9:26:TYR:N	7:9:27:PRO:CD	2.69	0.55
5:E:32:GLU:CD	5:E:32:GLU:H	2.13	0.55
1:1:437:TRP:C	1:1:437:TRP:CD1	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:507:LEU:HD22	3:3:511:VAL:HG11	1.88	0.55
4:4:246:TYR:CD1	5:5:77:LEU:HD22	2.42	0.55
3:C:270:ARG:O	3:C:271:SER:HB2	2.05	0.55
4:D:371:ARG:HH22	4:D:376:VAL:HG21	1.72	0.55
6:F:92:MET:HE1	6:F:127:VAL:HG13	1.89	0.55
7:G:144:LYS:HB2	7:G:145:PRO:HD2	1.89	0.55
3:3:34:CYS:HA	3:3:184:CYS:HB2	1.89	0.55
3:3:715:GLU:H	3:3:761:SER:HB2	1.72	0.55
3:3:225:ASN:ND2	3:3:289:TRP:HB3	2.21	0.54
3:3:444:ARG:NH2	3:3:447:LYS:HG3	2.22	0.54
4:4:25:VAL:HA	4:4:48:SER:HB3	1.88	0.54
3:3:546:ALA:O	3:3:547:MET:HE2	2.07	0.54
4:4:337:PRO:O	4:4:361:GLY:HA2	2.07	0.54
5:5:37:GLU:O	5:5:40:HIS:HB3	2.07	0.54
7:9:48:ASN:HB2	7:9:50:LEU:HD23	1.89	0.54
1:A:311:MET:HA	1:A:316:LEU:HD11	1.89	0.54
8:H:8:GLU:HG2	8:H:97:TYR:CE2	2.42	0.54
3:3:546:ALA:HA	3:3:678:PHE:CE2	2.43	0.54
3:3:629:ILE:HG22	3:3:630:GLU:N	2.23	0.54
1:A:373:LYS:HD3	1:A:383:ASP:OD2	2.07	0.54
3:C:567:TYR:HA	3:C:584:VAL:CG2	2.37	0.54
2:2:98:ASP:O	2:2:102:GLU:HB2	2.06	0.54
4:4:193:LEU:CD2	4:4:197:LEU:HG	2.38	0.54
1:A:337:MET:HA	1:A:337:MET:CE	2.31	0.54
3:C:694:LEU:HB3	3:C:762:ALA:HB2	1.90	0.54
6:F:163:TYR:CD2	6:F:169:ARG:HA	2.43	0.54
5:5:53:VAL:CG1	5:5:71:VAL:HB	2.37	0.54
3:C:123:ASP:HB2	3:C:236:LEU:HD13	1.89	0.54
3:C:477:LEU:CD2	3:C:521:ALA:HB2	2.37	0.54
3:C:546:ALA:HA	3:C:678:PHE:CE2	2.42	0.54
4:D:254:TYR:O	4:D:256:GLY:N	2.36	0.54
5:E:87:ARG:O	5:E:88:PHE:HB3	2.07	0.54
1:1:376:THR:O	1:1:376:THR:HG22	2.07	0.54
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.88	0.54
6:6:42:GLY:O	6:6:43:LEU:HD23	2.07	0.54
6:6:165:GLU:HG2	7:9:148:ARG:NH1	2.22	0.54
7:9:151:LYS:C	7:9:153:THR:H	2.16	0.54
3:C:466:GLU:CD	3:C:467:VAL:H	2.16	0.54
4:D:271:ASP:OD1	4:D:274:ASP:N	2.37	0.54
8:H:82:ILE:HG23	8:H:95:ALA:HB3	1.90	0.54
3:3:113:LEU:HD12	3:3:157:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:318:VAL:HG12	3:3:319:GLU:N	2.23	0.54
3:3:474:ARG:HA	3:3:517:ALA:HB2	1.89	0.54
3:3:501:LYS:HD2	3:3:501:LYS:N	2.19	0.54
1:A:301:PRO:HB2	1:A:303:THR:HG23	1.89	0.54
3:C:113:LEU:HD12	3:C:157:PHE:HB2	1.90	0.54
1:1:373:LYS:HD3	1:1:383:ASP:OD2	2.06	0.54
2:B:98:ASP:O	2:B:102:GLU:HB2	2.07	0.54
3:C:132:ASP:OD1	4:D:329:LYS:HE2	2.08	0.54
3:C:405:GLU:CB	3:C:535:MET:HE2	2.31	0.54
3:C:501:LYS:H	3:C:501:LYS:CD	2.19	0.54
1:1:98:PRO:HA	2:2:124:CYS:SG	2.48	0.54
1:1:161:ASN:ND2	1:1:166:ASP:HA	2.23	0.54
3:3:664:LEU:O	3:3:669:VAL:HG12	2.08	0.54
4:4:369:LYS:HG3	5:5:53:VAL:HG23	1.90	0.54
6:6:83:ARG:CG	6:6:83:ARG:NH1	2.64	0.54
1:A:29:LEU:HD22	1:A:29:LEU:O	2.08	0.54
3:C:394:ASP:OD2	3:C:501:LYS:HB2	2.08	0.54
1:1:312:SER:C	1:1:314:GLU:H	2.15	0.54
1:1:406:ALA:O	1:1:410:VAL:HG23	2.08	0.54
3:3:55:PRO:HB3	3:3:73:ILE:N	2.22	0.54
1:A:188:LEU:HD23	1:A:188:LEU:C	2.33	0.54
4:D:163:VAL:HG22	4:D:164:THR:HG22	1.89	0.54
4:D:193:LEU:CD2	4:D:197:LEU:HG	2.38	0.54
3:3:550:LEU:HD23	3:3:684:ARG:HH21	1.73	0.53
4:4:213:ILE:H	4:4:213:ILE:CD1	2.20	0.53
1:A:397:ARG:HG3	3:C:49:LEU:HD13	1.88	0.53
3:C:204:GLU:O	3:C:209:THR:HB	2.07	0.53
3:C:440:ARG:HH11	3:C:440:ARG:CG	2.21	0.53
3:C:664:LEU:O	3:C:669:VAL:HG12	2.08	0.53
5:5:121:LEU:HD13	5:5:146:LEU:HD23	1.91	0.53
6:6:163:TYR:CD2	6:6:169:ARG:HA	2.44	0.53
1:A:53:VAL:HG23	1:A:231:MET:HE2	1.89	0.53
1:A:188:LEU:HD23	1:A:188:LEU:O	2.09	0.53
3:3:452:ALA:O	3:3:454:TYR:N	2.42	0.53
4:4:44:MET:HE2	4:4:44:MET:HA	1.89	0.53
4:4:283:MET:O	4:4:287:VAL:HG23	2.08	0.53
1:A:197:ALA:HB3	2:B:66:PHE:CE1	2.43	0.53
4:D:233:GLY:HA2	5:E:48:PHE:HE1	1.73	0.53
1:1:363:VAL:O	1:1:368:VAL:HG12	2.09	0.53
3:3:218:LEU:H	3:3:219:PRO:HD3	1.71	0.53
8:7:82:ILE:HG23	8:7:95:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:26:TYR:N	7:G:27:PRO:CD	2.68	0.53
8:H:66:PRO:O	8:H:87:PRO:HG2	2.08	0.53
3:3:356:LEU:HD13	3:3:654:PHE:HB2	1.91	0.53
4:4:241:ALA:HB2	4:4:278:VAL:HG21	1.90	0.53
6:F:83:ARG:NH1	6:F:83:ARG:CG	2.71	0.53
1:A:138:TYR:HB3	1:A:141:ALA:HB3	1.91	0.53
7:G:48:ASN:HB2	7:G:50:LEU:HD23	1.91	0.53
8:H:39:ASP:OD2	8:H:75:ARG:HD3	2.09	0.53
2:2:153:LEU:O	2:2:153:LEU:HD22	2.09	0.53
7:9:132:GLY:H	7:9:135:ASP:HB2	1.74	0.53
1:A:74:LEU:O	1:A:77:SER:HB3	2.09	0.53
3:C:261:VAL:HG22	9:C:786:SF4:S2	2.49	0.53
3:C:402:PRO:HA	3:C:535:MET:HE3	1.91	0.53
4:D:283:MET:O	4:D:287:VAL:HG23	2.09	0.53
1:1:313:TYR:CE1	1:1:323:LEU:HD13	2.44	0.53
4:4:250:LYS:HE2	4:4:262:PHE:CB	2.33	0.53
6:6:96:TRP:O	6:6:99:MET:HB2	2.09	0.53
6:6:116:GLY:O	7:9:97:ARG:NH1	2.42	0.53
7:9:137:LEU:O	7:9:140:VAL:HG12	2.08	0.53
1:A:184:GLU:OE1	1:A:186:THR:CG2	2.52	0.53
3:C:51:ARG:HB3	3:C:94:ASP:HB3	1.90	0.53
3:C:185:LYS:HG3	3:C:202:PHE:HE2	1.74	0.53
4:D:59:ILE:HD11	5:E:135:ILE:HG23	1.91	0.53
4:D:257:TYR:C	4:D:259:THR:H	2.17	0.53
6:F:163:TYR:H	7:G:152:ARG:HH12	1.56	0.53
1:1:188:LEU:HD23	1:1:188:LEU:C	2.34	0.53
4:4:245:ASN:O	5:5:79:GLY:HA3	2.09	0.53
4:4:381:LEU:HD11	4:4:397:ILE:HG12	1.91	0.53
5:5:36:GLU:HG3	5:5:37:GLU:N	2.24	0.53
6:6:163:TYR:HD1	7:9:152:ARG:NH1	2.05	0.53
1:A:219:ASN:HD22	1:A:223:THR:HG21	1.74	0.53
1:A:310:PRO:O	1:A:315:HIS:HB2	2.09	0.53
1:A:376:THR:O	1:A:376:THR:HG22	2.08	0.53
3:C:572:PRO:HG2	3:C:577:LEU:HD21	1.90	0.53
4:D:193:LEU:HD22	4:D:197:LEU:HG	1.89	0.53
3:3:688:ARG:HB3	3:3:770:ARG:HB2	1.91	0.53
4:4:213:ILE:HD12	4:4:213:ILE:N	2.20	0.53
1:A:29:LEU:HD23	1:A:112:HIS:CE1	2.44	0.53
1:A:238:PHE:CZ	1:A:248:GLY:HA3	2.44	0.53
1:A:243:THR:HG21	1:A:315:HIS:HE1	1.74	0.53
3:C:707:LYS:C	3:C:709:GLN:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:358:PRO:O	1:1:362:GLY:HA3	2.08	0.52
3:3:405:GLU:CB	3:3:535:MET:HE2	2.33	0.52
3:3:572:PRO:HG2	3:3:577:LEU:HD21	1.91	0.52
2:B:6:ASP:HB3	2:B:7:LYS:HD2	1.90	0.52
3:C:568:TYR:CD1	3:C:572:PRO:HG3	2.45	0.52
5:E:53:VAL:CG1	5:E:71:VAL:HB	2.39	0.52
1:1:74:LEU:O	1:1:77:SER:HB3	2.09	0.52
2:2:28:MET:HB2	2:2:29:PRO:CD	2.38	0.52
3:3:224:GLY:O	3:3:227:THR:HB	2.09	0.52
3:3:337:ARG:HD3	3:3:340:GLU:HG3	1.92	0.52
1:A:260:ARG:HG3	1:A:264:TYR:OH	2.09	0.52
3:C:688:ARG:HB3	3:C:770:ARG:HB2	1.91	0.52
6:F:104:TRP:NE1	6:F:173:VAL:HG22	2.24	0.52
3:3:205:ARG:HH11	3:3:205:ARG:HG3	1.72	0.52
6:6:23:THR:O	6:6:27:LEU:HD13	2.09	0.52
6:F:96:TRP:O	6:F:99:MET:HB2	2.09	0.52
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.91	0.52
4:4:254:TYR:O	4:4:256:GLY:N	2.35	0.52
1:A:437:TRP:CD1	1:A:437:TRP:O	2.62	0.52
2:B:145:VAL:CG1	2:B:150:LEU:HB2	2.40	0.52
3:3:645:ALA:HB3	3:3:652:PRO:HD3	1.91	0.52
4:4:257:TYR:C	4:4:259:THR:H	2.18	0.52
5:5:80:TRP:CD1	5:5:81:LYS:HG2	2.44	0.52
3:C:19:VAL:HG23	3:C:85:THR:O	2.09	0.52
4:D:40:VAL:O	4:D:40:VAL:HG22	2.10	0.52
7:G:125:GLU:O	7:G:128:ASP:HB2	2.10	0.52
1:1:196:ARG:NH2	3:3:203:ILE:O	2.42	0.52
2:2:76:GLY:H	2:2:118:SER:HB2	1.74	0.52
2:B:28:MET:HB2	2:B:29:PRO:CD	2.40	0.52
4:4:327:HIS:HE1	7:9:107:ALA:O	1.92	0.52
6:6:78:MET:HE2	6:6:99:MET:HE1	1.91	0.52
1:A:313:TYR:CE1	1:A:323:LEU:HD13	2.45	0.52
3:C:224:GLY:O	3:C:227:THR:HB	2.09	0.52
3:C:254:THR:OG1	3:C:624:LEU:HD12	2.10	0.52
3:C:550:LEU:HB3	3:C:684:ARG:HH21	1.75	0.52
6:F:145:GLU:HG2	7:G:31:VAL:HG21	1.90	0.52
3:3:115:HIS:C	4:4:321:MET:HE3	2.33	0.52
3:3:192:GLU:HG3	3:3:193:GLU:HG3	1.92	0.52
3:3:458:LEU:C	3:3:460:LYS:H	2.18	0.52
3:3:600:VAL:HG12	3:3:602:LEU:CD1	2.40	0.52
4:D:393:MET:HA	4:D:396:ILE:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:7:LEU:HD22	5:E:17:ILE:HD12	1.90	0.52
1:1:29:LEU:O	1:1:29:LEU:HD22	2.10	0.52
3:3:132:ASP:O	3:3:135:VAL:HG12	2.09	0.52
3:3:136:GLU:HG2	5:5:189:ARG:HG3	1.91	0.52
5:5:87:ARG:O	5:5:88:PHE:HB3	2.09	0.52
3:C:501:LYS:HD2	3:C:501:LYS:N	2.20	0.52
3:C:629:ILE:HG22	3:C:630:GLU:N	2.24	0.52
3:C:642:ALA:CB	3:C:652:PRO:HG3	2.37	0.52
7:G:73:ALA:HB3	7:G:87:TYR:CE2	2.44	0.52
2:2:31:LEU:HD12	2:2:41:ILE:HD13	1.92	0.52
2:2:40:TRP:CH2	2:2:42:ARG:HG2	2.45	0.52
3:3:402:PRO:HA	3:3:535:MET:HE3	1.89	0.52
5:5:52:ILE:HG22	5:5:114:LEU:HB3	1.86	0.52
6:6:83:ARG:HA	6:6:111:CYS:HB3	1.92	0.52
4:D:245:ASN:O	5:E:79:GLY:HA3	2.10	0.52
1:1:29:LEU:HD23	1:1:112:HIS:CE1	2.45	0.51
1:1:93:ALA:HB1	1:1:107:LEU:HD11	1.91	0.51
8:7:34:GLU:HB3	8:7:56:THR:CG2	2.40	0.51
1:A:49:THR:HG23	1:A:52:GLU:CG	2.40	0.51
1:A:312:SER:C	1:A:314:GLU:H	2.17	0.51
4:D:250:LYS:HE2	4:D:262:PHE:CB	2.32	0.51
5:E:80:TRP:CD1	5:E:81:LYS:HG2	2.45	0.51
3:3:501:LYS:H	3:3:501:LYS:CD	2.21	0.51
5:5:161:GLU:CG	5:5:163:ARG:HH22	2.23	0.51
7:9:144:LYS:HB2	7:9:145:PRO:HD2	1.92	0.51
1:A:358:PRO:O	1:A:362:GLY:HA3	2.10	0.51
3:C:33:PHE:HB2	3:C:45:CYS:SG	2.50	0.51
4:D:213:ILE:HD12	4:D:213:ILE:N	2.21	0.51
4:D:284:ARG:HH11	4:D:284:ARG:HG3	1.74	0.51
5:E:161:GLU:HB2	5:E:163:ARG:CZ	2.41	0.51
3:3:135:VAL:HG23	4:4:326:TYR:CE1	2.46	0.51
8:7:20:MET:HE3	8:7:59:LEU:HG	1.91	0.51
1:1:397:ARG:HG3	3:3:49:LEU:HD13	1.91	0.51
6:6:32:ARG:HA	6:6:35:SER:OG	2.10	0.51
6:6:74:GLN:OE1	6:6:74:GLN:HA	2.09	0.51
3:C:192:GLU:HG3	3:C:193:GLU:HG3	1.93	0.51
4:D:215:TYR:CE2	4:D:219:ARG:HG2	2.45	0.51
4:D:369:LYS:HG3	5:E:53:VAL:HG23	1.93	0.51
6:F:78:MET:O	6:F:78:MET:HG3	2.10	0.51
3:3:117:LEU:CA	4:4:321:MET:HE1	2.41	0.51
4:D:132:PHE:CE2	4:D:279:ARG:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:PRO:HG2	5:E:33:ARG:HB2	1.92	0.51
1:1:96:SER:HA	1:1:135:ARG:NH1	2.26	0.51
2:2:6:ASP:HB3	2:2:7:LYS:HD2	1.92	0.51
2:2:27:ILE:HG12	2:2:53:VAL:HG21	1.91	0.51
8:7:66:PRO:O	8:7:87:PRO:HG2	2.11	0.51
1:A:120:LEU:HD22	1:A:231:MET:HG3	1.91	0.51
3:C:458:LEU:C	3:C:460:LYS:H	2.18	0.51
4:D:381:LEU:HD11	4:D:397:ILE:HG12	1.91	0.51
5:E:36:GLU:HG3	5:E:37:GLU:N	2.26	0.51
5:E:101:LEU:O	5:E:126:PHE:HA	2.11	0.51
2:2:112:THR:HG22	2:2:117:PHE:H	1.75	0.51
3:3:94:ASP:OD2	3:3:97:SER:HB2	2.10	0.51
3:C:645:ALA:HB3	3:C:652:PRO:HD3	1.93	0.51
1:1:310:PRO:O	1:1:315:HIS:HB2	2.10	0.51
3:3:568:TYR:CD1	3:3:572:PRO:HG3	2.46	0.51
4:4:404:MET:HA	4:4:407:VAL:CG1	2.40	0.51
5:5:7:LEU:HD22	5:5:17:ILE:HD12	1.93	0.51
1:A:132:ILE:HG21	1:A:145:LEU:HD11	1.93	0.51
3:C:154:TYR:CE1	4:D:307:PRO:HB3	2.46	0.51
3:C:326:PHE:CE2	3:C:330:LYS:HE3	2.45	0.51
3:C:715:GLU:HA	3:C:745:ALA:HB1	1.93	0.51
4:D:219:ARG:NH1	4:D:273:PHE:CD2	2.79	0.51
4:D:240:ARG:C	4:D:242:SER:H	2.18	0.51
6:F:30:TRP:O	6:F:30:TRP:CD1	2.64	0.51
1:1:97:GLU:O	1:1:100:SER:HB3	2.10	0.51
1:1:114:LEU:HD22	1:1:118:MET:HG3	1.93	0.51
7:9:83:ALA:HB2	8:7:40:PHE:HE1	1.75	0.51
4:D:381:LEU:N	4:D:382:PRO:CD	2.74	0.51
1:1:197:ALA:HB3	2:2:66:PHE:CE1	2.46	0.51
2:2:149:ARG:O	2:2:152:ALA:HB3	2.11	0.51
4:4:123:LEU:HD13	4:4:290:ILE:HD12	1.92	0.51
3:C:19:VAL:O	3:C:22:ALA:HB3	2.11	0.51
3:C:367:PRO:CG	3:C:554:LYS:HB2	2.41	0.51
4:D:88:LEU:HD12	4:D:403:VAL:HG22	1.92	0.51
4:D:346:THR:CG2	4:D:353:LEU:HB3	2.39	0.51
8:H:14:VAL:HA	8:H:17:LEU:HD12	1.92	0.51
1:1:258:VAL:HG21	1:1:280:ALA:HB1	1.91	0.50
3:3:43:GLY:HA2	13:3:787:FES:S1	2.52	0.50
4:4:233:GLY:HA2	5:5:48:PHE:CE1	2.46	0.50
4:4:333:GLU:OE2	5:5:189:ARG:HD2	2.11	0.50
1:A:398:SER:C	3:C:46:ARG:HD2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:734:VAL:HG12	3:C:736:VAL:HG23	1.93	0.50
4:D:320:SER:HB3	4:D:323:ALA:HB3	1.91	0.50
8:H:34:GLU:HB3	8:H:56:THR:CG2	2.41	0.50
1:1:37:GLY:C	1:1:39:GLU:H	2.18	0.50
3:3:55:PRO:HG3	3:3:73:ILE:HA	1.92	0.50
6:6:163:TYR:HD1	7:9:152:ARG:HH11	1.59	0.50
3:C:42:ILE:HG22	3:C:43:GLY:H	1.76	0.50
3:C:356:LEU:HD13	3:C:654:PHE:HB2	1.94	0.50
4:4:133:LEU:HD21	4:4:204:TYR:CD2	2.46	0.50
4:4:381:LEU:N	4:4:382:PRO:CD	2.74	0.50
7:9:68:ILE:HD11	9:9:183:SF4:S1	2.51	0.50
1:A:66:GLY:O	11:A:441:NAI:H2N	2.10	0.50
1:A:149:ILE:O	1:A:153:ARG:HG3	2.11	0.50
1:A:367:MET:HE1	1:A:410:VAL:HG21	1.94	0.50
4:D:126:LEU:HD21	4:D:286:SER:CB	2.41	0.50
1:1:149:ILE:O	1:1:153:ARG:HG3	2.11	0.50
1:1:359:CYS:HB2	1:1:403:ALA:HB2	1.93	0.50
1:A:67:GLY:HA2	1:A:324:GLY:O	2.12	0.50
2:B:40:TRP:CH2	2:B:42:ARG:HG2	2.47	0.50
5:E:31:ARG:O	5:E:34:PHE:HB3	2.11	0.50
1:1:132:ILE:HG21	1:1:145:LEU:HD11	1.94	0.50
1:1:260:ARG:HG3	1:1:264:TYR:OH	2.11	0.50
3:3:326:PHE:CZ	3:3:330:LYS:HE3	2.47	0.50
3:3:617:LEU:HD23	3:3:618:GLU:N	2.26	0.50
5:5:163:ARG:HD2	7:9:69:TYR:CD1	2.47	0.50
3:C:130:LEU:HD23	9:C:784:SF4:S4	2.51	0.50
4:D:102:GLU:HG2	4:D:175:ILE:O	2.12	0.50
4:D:339:LYS:HA	4:D:359:SER:O	2.12	0.50
3:3:42:ILE:HG22	3:3:43:GLY:H	1.76	0.50
3:3:629:ILE:HG22	3:3:630:GLU:H	1.77	0.50
1:A:45:LEU:HD12	1:A:163:PHE:HD1	1.77	0.50
3:C:716:LEU:HD21	3:C:758:LEU:HB3	1.94	0.50
4:D:260:TYR:HE2	4:D:293:ALA:HB2	1.76	0.50
4:D:291:LYS:O	4:D:295:GLU:HG3	2.12	0.50
5:E:123:GLY:H	5:E:147:ARG:HH11	1.58	0.50
6:F:121:TYR:CG	6:F:122:ALA:N	2.80	0.50
1:1:184:GLU:OE1	1:1:186:THR:CG2	2.52	0.50
2:2:113:PRO:HG2	2:2:114:ASP:OD1	2.11	0.50
3:3:549:VAL:HG12	3:3:549:VAL:O	2.12	0.50
4:4:271:ASP:OD1	4:4:274:ASP:N	2.39	0.50
4:4:385:CYS:HB3	4:4:396:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:30:PRO:HG2	5:5:33:ARG:HB2	1.93	0.50
7:9:73:ALA:HB3	7:9:87:TYR:CE2	2.46	0.50
3:C:218:LEU:H	3:C:219:PRO:HD3	1.77	0.50
3:C:279:ALA:HB2	3:C:290:ILE:CG1	2.40	0.50
3:C:337:ARG:HD3	3:C:340:GLU:HG3	1.92	0.50
1:1:272:PHE:HZ	1:1:316:LEU:HD21	1.77	0.50
2:2:89:LYS:HE3	2:2:94:GLU:OE1	2.11	0.50
3:3:208:HIS:ND1	8:7:92:HIS:CE1	2.80	0.50
7:9:45:ARG:NH2	7:9:137:LEU:HD23	2.26	0.50
1:A:114:LEU:HD22	1:A:118:MET:HG3	1.93	0.50
3:C:508:GLY:O	3:C:512:LEU:HB2	2.12	0.50
3:C:697:THR:OG1	3:C:763:LEU:HD23	2.11	0.50
7:G:83:ALA:HB2	8:H:40:PHE:HE1	1.77	0.50
1:1:243:THR:HG21	1:1:315:HIS:HE1	1.77	0.50
3:3:42:ILE:HG22	3:3:43:GLY:N	2.27	0.50
3:3:697:THR:OG1	3:3:763:LEU:HD23	2.12	0.50
4:4:73:ARG:O	4:4:364:MET:HB3	2.12	0.50
4:4:371:ARG:HH22	4:4:376:VAL:HG21	1.76	0.50
2:B:113:PRO:HG2	2:B:114:ASP:OD1	2.12	0.50
3:C:33:PHE:O	3:C:186:ARG:NH2	2.45	0.50
3:C:518:ALA:O	3:C:521:ALA:HB3	2.12	0.50
2:2:24:ARG:HA	2:2:53:VAL:CG1	2.42	0.49
3:3:19:VAL:O	3:3:22:ALA:HB3	2.12	0.49
4:4:132:PHE:CE2	4:4:279:ARG:HG3	2.47	0.49
4:4:284:ARG:HH11	4:4:284:ARG:HG3	1.77	0.49
1:A:93:ALA:HB1	1:A:107:LEU:HD11	1.94	0.49
1:A:359:CYS:HB2	1:A:403:ALA:HB2	1.94	0.49
3:C:42:ILE:HG22	3:C:43:GLY:N	2.27	0.49
3:C:717:TRP:HB2	3:C:759:TYR:HB2	1.94	0.49
3:C:719:HIS:ND1	3:C:720:PRO:HD2	2.27	0.49
1:1:219:ASN:ND2	1:1:223:THR:HG21	2.27	0.49
2:2:24:ARG:HA	2:2:53:VAL:HG13	1.95	0.49
3:3:130:LEU:HD23	9:3:784:SF4:S4	2.53	0.49
5:5:101:LEU:O	5:5:126:PHE:HA	2.11	0.49
3:C:561:PRO:CB	3:C:576:ALA:HA	2.35	0.49
4:D:233:GLY:HA2	5:E:48:PHE:CE1	2.46	0.49
6:F:74:GLN:OE1	6:F:74:GLN:HA	2.12	0.49
6:F:81:ALA:CB	6:F:108:MET:HE2	2.42	0.49
1:1:311:MET:HA	1:1:316:LEU:HD11	1.94	0.49
3:3:188:VAL:CG1	3:3:201:ASP:HA	2.42	0.49
3:3:452:ALA:C	3:3:454:TYR:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:30:TRP:O	6:6:30:TRP:CD1	2.65	0.49
1:A:358:PRO:HB3	3:C:107:MET:HE1	1.94	0.49
1:A:397:ARG:O	3:C:46:ARG:HD3	2.13	0.49
6:F:28:VAL:O	6:F:32:ARG:HG2	2.12	0.49
5:5:161:GLU:HB2	5:5:163:ARG:CZ	2.43	0.49
2:B:122:VAL:CG1	2:B:123:GLU:N	2.75	0.49
2:B:149:ARG:O	2:B:152:ALA:HB3	2.13	0.49
4:D:200:ARG:O	4:D:204:TYR:HD1	1.96	0.49
4:D:320:SER:HB3	4:D:323:ALA:CB	2.43	0.49
5:E:52:ILE:HG22	5:E:114:LEU:HB3	1.88	0.49
1:1:292:PRO:HB2	1:1:316:LEU:CD2	2.41	0.49
1:1:437:TRP:CD1	1:1:437:TRP:O	2.64	0.49
4:4:341:GLU:OE1	5:5:91:ARG:NH2	2.46	0.49
5:5:31:ARG:O	5:5:34:PHE:HB3	2.12	0.49
4:D:197:LEU:O	4:D:198:PRO:C	2.56	0.49
4:D:409:ARG:NH2	5:E:117:GLU:OE2	2.45	0.49
1:1:9:LEU:HD13	1:1:279:TRP:CZ2	2.48	0.49
3:3:693:TYR:HB3	3:3:759:TYR:CD2	2.48	0.49
4:4:126:LEU:HD21	4:4:286:SER:CB	2.40	0.49
4:4:240:ARG:C	4:4:242:SER:H	2.19	0.49
8:7:45:GLU:CD	8:7:45:GLU:H	2.21	0.49
8:H:108:ILE:N	8:H:108:ILE:HD12	2.27	0.49
1:1:356:CYS:SG	1:1:399:PHE:HB2	2.53	0.49
1:1:358:PRO:HB3	3:3:107:MET:HE1	1.95	0.49
2:2:33:ARG:HH21	2:2:37:GLU:CG	2.26	0.49
3:3:123:ASP:C	3:3:125:GLY:H	2.19	0.49
3:3:719:HIS:HB2	3:3:753:VAL:O	2.12	0.49
4:4:53:LEU:N	4:4:53:LEU:HD22	2.28	0.49
7:9:153:THR:HG22	7:9:155:LYS:H	1.76	0.49
1:A:68:ALA:HB1	11:A:441:NAI:H51A	1.93	0.49
1:A:391:LEU:HB2	1:A:392:PRO:CD	2.42	0.49
3:C:382:PHE:N	3:C:382:PHE:CD1	2.80	0.49
7:G:153:THR:HG22	7:G:155:LYS:H	1.76	0.49
8:H:45:GLU:CD	8:H:45:GLU:H	2.21	0.49
1:1:188:LEU:HD23	1:1:188:LEU:O	2.13	0.49
3:3:113:LEU:CD1	3:3:157:PHE:HB2	2.43	0.49
3:3:477:LEU:CD2	3:3:521:ALA:HB2	2.42	0.49
1:A:28:THR:HB	1:A:31:TYR:H	1.78	0.49
2:B:89:LYS:HE3	2:B:94:GLU:OE1	2.12	0.49
4:D:263:ASP:HB2	4:D:285:GLU:OE1	2.13	0.49
5:E:3:LEU:HB2	5:E:86:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:163:TYR:CE1	7:G:152:ARG:HD2	2.47	0.49
8:H:20:MET:HE3	8:H:59:LEU:HG	1.95	0.49
1:1:391:LEU:HB2	1:1:392:PRO:CD	2.43	0.49
1:1:401:PRO:O	1:1:404:ASP:HB2	2.11	0.49
2:2:122:VAL:CG1	2:2:123:GLU:N	2.75	0.49
3:3:367:PRO:CG	3:3:554:LYS:HB2	2.43	0.49
1:A:9:LEU:HD13	1:A:279:TRP:CZ2	2.48	0.49
3:C:94:ASP:OD2	3:C:97:SER:HB2	2.13	0.49
3:C:123:ASP:C	3:C:125:GLY:H	2.20	0.49
3:C:205:ARG:HH11	3:C:205:ARG:HG3	1.78	0.49
4:D:93:HIS:CE1	4:D:353:LEU:HD11	2.48	0.49
4:D:385:CYS:HB3	4:D:396:ILE:HG21	1.94	0.49
4:D:404:MET:HA	4:D:407:VAL:CG1	2.43	0.49
1:1:49:THR:HG23	1:1:52:GLU:CG	2.43	0.49
3:3:341:VAL:HA	3:3:565:TYR:O	2.13	0.49
3:3:382:PHE:CD1	3:3:382:PHE:N	2.81	0.49
1:A:72:THR:HG21	1:A:223:THR:HG23	1.94	0.49
1:A:161:ASN:HD22	1:A:166:ASP:HA	1.78	0.49
3:C:333:LEU:HB3	3:C:648:LEU:CD2	2.43	0.49
4:D:234:LEU:O	4:D:239:LEU:HG	2.12	0.49
4:D:234:LEU:CD2	4:D:238:SER:HB2	2.42	0.49
1:1:238:PHE:CZ	1:1:248:GLY:HA3	2.47	0.48
3:3:20:MET:HE2	3:3:20:MET:HB3	1.69	0.48
4:4:197:LEU:O	4:4:198:PRO:C	2.56	0.48
4:4:219:ARG:NH1	4:4:273:PHE:CD2	2.81	0.48
4:4:381:LEU:HB3	4:4:382:PRO:HD3	1.95	0.48
3:C:188:VAL:CG1	3:C:201:ASP:HA	2.43	0.48
4:D:409:ARG:HG2	4:D:409:ARG:HH11	1.77	0.48
1:1:299:PRO:HG3	1:1:341:MET:CE	2.43	0.48
1:1:398:SER:C	3:3:46:ARG:HD2	2.38	0.48
4:4:88:LEU:HD12	4:4:403:VAL:HG22	1.94	0.48
4:4:234:LEU:O	4:4:239:LEU:HG	2.12	0.48
3:C:113:LEU:CD1	3:C:157:PHE:HB2	2.42	0.48
3:C:452:ALA:O	3:C:454:TYR:N	2.46	0.48
3:3:333:LEU:HB3	3:3:648:LEU:CD2	2.43	0.48
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.94	0.48
3:3:734:VAL:HG12	3:3:736:VAL:HG23	1.94	0.48
4:4:61:TYR:HB3	6:6:88:MET:HE2	1.95	0.48
5:5:163:ARG:HD2	7:9:69:TYR:CE1	2.48	0.48
2:B:33:ARG:HH21	2:B:37:GLU:CG	2.26	0.48
3:C:300:TRP:HB3	3:C:705:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:549:VAL:HG12	3:C:549:VAL:O	2.13	0.48
3:C:617:LEU:HD23	3:C:618:GLU:N	2.28	0.48
3:C:629:ILE:HG22	3:C:630:GLU:H	1.77	0.48
3:C:693:TYR:HB3	3:C:759:TYR:CD2	2.48	0.48
7:G:163:VAL:HG22	7:G:177:THR:HG22	1.96	0.48
1:1:72:THR:HG21	1:1:223:THR:HG23	1.94	0.48
1:1:219:ASN:HD22	1:1:223:THR:HG21	1.78	0.48
1:1:273:ARG:HB2	1:1:307:LEU:O	2.13	0.48
3:3:254:THR:OG1	3:3:624:LEU:HD12	2.12	0.48
3:3:550:LEU:HB3	3:3:684:ARG:HH21	1.77	0.48
4:4:82:THR:N	4:4:83:PRO:HD2	2.29	0.48
3:C:117:LEU:HD12	4:D:321:MET:CE	2.39	0.48
3:C:452:ALA:C	3:C:454:TYR:H	2.22	0.48
4:D:246:TYR:CD1	5:E:77:LEU:HD22	2.48	0.48
6:F:32:ARG:HA	6:F:35:SER:OG	2.12	0.48
1:1:211:LEU:H	1:1:216:THR:HG21	1.78	0.48
3:3:250:GLU:CD	3:3:628:PRO:HG2	2.39	0.48
8:7:86:LEU:HD12	8:7:91:ILE:HD12	1.95	0.48
1:A:211:LEU:H	1:A:216:THR:HG21	1.78	0.48
3:C:225:ASN:HD21	3:C:289:TRP:HB3	1.78	0.48
5:E:71:VAL:HG22	5:E:91:ARG:HB2	1.95	0.48
5:E:175:THR:O	5:E:175:THR:OG1	2.29	0.48
2:2:28:MET:HB2	2:2:29:PRO:HD2	1.95	0.48
4:4:93:HIS:CE1	4:4:353:LEU:HD11	2.49	0.48
5:5:167:PRO:HB3	7:9:66:TYR:CE2	2.48	0.48
8:7:14:VAL:HA	8:7:17:LEU:HD12	1.95	0.48
3:C:337:ARG:H	3:C:337:ARG:HD2	1.78	0.48
3:C:550:LEU:HD23	3:C:684:ARG:HH21	1.79	0.48
3:C:694:LEU:HD23	3:C:760:LEU:HB3	1.94	0.48
3:C:719:HIS:HB2	3:C:753:VAL:O	2.13	0.48
1:1:120:LEU:HD22	1:1:231:MET:HG3	1.96	0.48
3:3:518:ALA:O	3:3:521:ALA:HB3	2.14	0.48
3:3:719:HIS:ND1	3:3:720:PRO:HD2	2.28	0.48
4:4:163:VAL:HG22	4:4:164:THR:CG2	2.43	0.48
2:B:28:MET:HB2	2:B:29:PRO:HD2	1.95	0.48
3:C:140:TYR:CE2	3:C:142:LYS:HB3	2.48	0.48
4:D:236:GLY:C	4:D:238:SER:N	2.71	0.48
8:H:13:TRP:O	8:H:17:LEU:HG	2.14	0.48
3:3:512:LEU:HD21	3:3:534:ALA:HB1	1.96	0.48
3:3:695:ARG:O	3:3:697:THR:HG23	2.14	0.48
4:4:215:TYR:CE2	4:4:219:ARG:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:366:TYR:CZ	5:5:148:LYS:HE3	2.49	0.48
6:6:50:MET:C	6:6:52:ALA:N	2.71	0.48
6:6:121:TYR:CG	6:6:122:ALA:N	2.81	0.48
5:E:135:ILE:HG22	5:E:136:LEU:HG	1.95	0.48
1:1:367:MET:HE1	1:1:410:VAL:HG21	1.94	0.48
1:1:420:GLN:O	1:1:424:LEU:HD13	2.14	0.48
2:2:145:VAL:CG1	2:2:150:LEU:HB2	2.44	0.48
4:4:168:PHE:N	4:4:168:PHE:CD1	2.81	0.48
2:B:31:LEU:HD22	2:B:49:ILE:HD12	1.96	0.48
2:B:145:VAL:HG12	2:B:150:LEU:HB2	1.95	0.48
3:C:43:GLY:HA2	13:C:787:FES:S1	2.53	0.48
3:C:465:HIS:O	3:C:465:HIS:CG	2.67	0.48
3:C:732:ALA:O	3:C:747:VAL:HG12	2.14	0.48
5:E:119:TYR:O	5:E:122:PHE:O	2.31	0.48
6:F:99:MET:CG	6:F:100:PRO:HD2	2.43	0.48
3:3:473:GLU:O	3:3:477:LEU:HD12	2.14	0.48
3:3:508:GLY:O	3:3:512:LEU:HB2	2.13	0.48
3:3:591:HIS:ND1	3:3:592:PRO:CD	2.76	0.48
4:4:238:SER:OG	4:4:279:ARG:NH2	2.47	0.48
4:4:320:SER:HB3	4:4:323:ALA:HB3	1.95	0.48
6:6:104:TRP:NE1	6:6:173:VAL:HG22	2.29	0.48
6:6:140:CYS:SG	7:9:99:ILE:HG13	2.54	0.48
7:9:133:LYS:O	7:9:137:LEU:HD13	2.14	0.48
7:9:170:LEU:O	7:9:171:GLU:C	2.56	0.48
1:A:42:LYS:O	1:A:46:LYS:HG3	2.14	0.48
1:A:401:PRO:O	1:A:404:ASP:HB2	2.14	0.48
2:B:76:GLY:H	2:B:118:SER:HB2	1.78	0.48
3:C:341:VAL:HA	3:C:565:TYR:O	2.14	0.48
4:D:381:LEU:HB3	4:D:382:PRO:HD3	1.96	0.48
6:F:165:GLU:HG2	7:G:148:ARG:NH1	2.29	0.48
2:B:112:THR:HG22	2:B:117:PHE:H	1.79	0.47
3:C:192:GLU:HG3	3:C:193:GLU:N	2.28	0.47
6:F:84:LEU:HD12	6:F:124:VAL:HG21	1.96	0.47
3:3:113:LEU:HD12	3:3:157:PHE:CB	2.44	0.47
3:3:117:LEU:HG	4:4:324:VAL:HG21	1.96	0.47
3:C:223:SER:O	3:C:226:ILE:HG12	2.14	0.47
4:D:30:VAL:HG12	4:D:31:GLY:N	2.29	0.47
4:D:200:ARG:O	4:D:204:TYR:CD1	2.67	0.47
4:D:314:ARG:NH2	7:G:108:CYS:O	2.47	0.47
7:G:73:ALA:HB3	7:G:87:TYR:CZ	2.48	0.47
1:1:109:ASP:O	1:1:110:VAL:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:386:SER:HB3	3:3:389:ASP:CG	2.40	0.47
3:3:571:VAL:HG11	3:3:591:HIS:CD2	2.50	0.47
3:3:732:ALA:O	3:3:747:VAL:HG12	2.15	0.47
3:C:20:MET:HB3	3:C:20:MET:HE2	1.70	0.47
3:C:222:PHE:CD1	3:C:411:LEU:HD11	2.49	0.47
4:D:44:MET:HA	4:D:44:MET:CE	2.43	0.47
4:D:348:SER:C	4:D:350:ARG:H	2.22	0.47
6:F:89:ALA:N	6:F:90:PRO:HD2	2.30	0.47
8:7:39:ASP:OD2	8:7:75:ARG:HD3	2.14	0.47
1:A:180:TYR:N	1:A:351:GLU:OE1	2.44	0.47
3:C:326:PHE:CD1	3:C:643:LEU:HG	2.49	0.47
4:D:108:VAL:HG23	4:D:108:VAL:O	2.14	0.47
4:D:168:PHE:N	4:D:168:PHE:CD1	2.82	0.47
1:1:272:PHE:CD2	1:1:311:MET:HE3	2.49	0.47
1:1:370:LEU:HD12	1:1:370:LEU:HA	1.56	0.47
3:3:465:HIS:O	3:3:465:HIS:CG	2.66	0.47
7:G:41:HIS:HB3	7:G:113:ILE:HD11	1.97	0.47
8:H:96:HIS:O	8:H:103:LEU:HD12	2.15	0.47
4:4:236:GLY:C	4:4:238:SER:N	2.70	0.47
1:A:356:CYS:SG	1:A:399:PHE:HB2	2.55	0.47
4:D:211:SER:OG	4:D:215:TYR:HB2	2.14	0.47
4:D:213:ILE:H	4:D:213:ILE:CD1	2.21	0.47
1:1:243:THR:HG22	1:1:244:GLU:H	1.79	0.47
3:3:55:PRO:CG	3:3:73:ILE:HA	2.45	0.47
3:3:321:THR:HG22	3:3:322:TRP:N	2.29	0.47
4:4:30:VAL:HG12	4:4:31:GLY:N	2.29	0.47
4:4:102:GLU:HG2	4:4:175:ILE:O	2.14	0.47
5:5:25:LEU:CD2	5:5:25:LEU:N	2.78	0.47
1:A:292:PRO:HB2	1:A:316:LEU:CD2	2.44	0.47
3:C:469:ARG:HG2	3:C:754:PRO:HG3	1.96	0.47
3:C:497:TRP:O	3:C:500:ALA:HB3	2.15	0.47
4:D:221:VAL:HG12	4:D:388:GLU:OE1	2.15	0.47
4:D:296:ARG:O	4:D:298:GLU:HG3	2.15	0.47
5:E:15:TYR:OH	5:E:33:ARG:HD3	2.14	0.47
5:E:161:GLU:CG	5:E:163:ARG:NH2	2.78	0.47
1:1:9:LEU:HD13	1:1:279:TRP:HZ2	1.78	0.47
3:3:326:PHE:CD1	3:3:643:LEU:HG	2.49	0.47
4:4:94:ASP:HB3	4:4:173:ILE:HG21	1.96	0.47
7:9:44:THR:HA	7:9:138:VAL:CG1	2.44	0.47
1:A:45:LEU:HD12	1:A:163:PHE:CD1	2.50	0.47
1:A:420:GLN:O	1:A:424:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:LEU:HD12	2:B:133:VAL:HG12	1.96	0.47
3:3:561:PRO:CB	3:3:576:ALA:HA	2.37	0.47
4:4:234:LEU:CD2	4:4:238:SER:HB2	2.45	0.47
1:A:149:ILE:HD13	1:A:171:LEU:CB	2.39	0.47
3:C:351:LEU:HD13	3:C:615:VAL:HG23	1.97	0.47
3:C:478:LEU:HD22	3:C:484:LYS:HB2	1.96	0.47
4:D:341:GLU:OE1	5:E:91:ARG:NH2	2.47	0.47
1:1:161:ASN:HD22	1:1:166:ASP:HA	1.80	0.47
1:1:361:GLU:H	1:1:361:GLU:HG2	1.53	0.47
2:2:10:PHE:O	2:2:14:THR:OG1	2.33	0.47
2:2:122:VAL:HG12	2:2:123:GLU:H	1.77	0.47
3:3:33:PHE:O	3:3:186:ARG:NH2	2.48	0.47
4:4:86:ASP:OD2	4:4:350:ARG:HD2	2.14	0.47
4:4:211:SER:OG	4:4:215:TYR:HB2	2.15	0.47
4:4:291:LYS:O	4:4:295:GLU:HG3	2.14	0.47
5:5:15:TYR:OH	5:5:33:ARG:HD3	2.15	0.47
6:6:99:MET:CG	6:6:100:PRO:HD2	2.44	0.47
7:9:100:PHE:HA	9:9:183:SF4:S4	2.55	0.47
1:A:17:LEU:HD12	1:A:251:LEU:HD11	1.97	0.47
3:C:208:HIS:ND1	8:H:92:HIS:CE1	2.83	0.47
3:C:300:TRP:N	3:C:705:VAL:HG21	2.30	0.47
4:D:86:ASP:OD2	4:D:350:ARG:HD2	2.15	0.47
4:D:333:GLU:OE2	5:E:189:ARG:HD2	2.15	0.47
6:F:84:LEU:HD11	6:F:89:ALA:HA	1.97	0.47
8:H:75:ARG:NE	8:H:76:HIS:NE2	2.57	0.47
2:2:81:GLN:HB3	2:2:122:VAL:CG2	2.43	0.46
3:3:722:THR:CG2	3:3:755:LYS:HB3	2.45	0.46
4:4:348:SER:C	4:4:350:ARG:H	2.22	0.46
5:5:71:VAL:HG22	5:5:91:ARG:HB2	1.97	0.46
7:9:34:LYS:HB3	7:9:35:PRO:HD2	1.97	0.46
2:B:30:LEU:O	2:B:34:VAL:HG23	2.15	0.46
4:D:190:LEU:HG	4:D:194:LEU:HD22	1.96	0.46
5:E:121:LEU:HD13	5:E:146:LEU:HD23	1.98	0.46
6:F:50:MET:C	6:F:52:ALA:N	2.73	0.46
6:F:83:ARG:HD3	6:F:83:ARG:H	1.80	0.46
3:3:469:ARG:HG2	3:3:754:PRO:HG3	1.98	0.46
3:3:652:PRO:HA	3:3:653:PRO:HD3	1.82	0.46
5:5:195:LEU:HD22	5:5:195:LEU:N	2.30	0.46
2:B:101:THR:HG22	8:H:108:ILE:CD1	2.44	0.46
3:C:370:ASP:OD2	3:C:558:TRP:HD1	1.97	0.46
3:C:585:MET:HG3	3:C:598:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:185:GLU:O	4:D:189:GLU:HG2	2.16	0.46
4:D:238:SER:OG	4:D:279:ARG:NH2	2.48	0.46
6:F:163:TYR:HD2	6:F:168:GLU:O	1.98	0.46
1:1:110:VAL:O	1:1:113:LEU:HB3	2.15	0.46
3:3:478:LEU:HD22	3:3:484:LYS:HB2	1.97	0.46
3:3:717:TRP:HB2	3:3:759:TYR:HB2	1.97	0.46
6:6:104:TRP:NE1	6:6:158:VAL:HG12	2.30	0.46
1:A:427:GLU:OE2	1:A:429:ARG:HD3	2.14	0.46
3:C:20:MET:HG3	3:C:82:SER:OG	2.15	0.46
3:C:113:LEU:HD12	3:C:157:PHE:CB	2.45	0.46
1:1:245:GLN:HB2	1:1:314:GLU:OE2	2.15	0.46
4:4:257:TYR:C	4:4:259:THR:N	2.72	0.46
4:4:393:MET:HA	4:4:396:ILE:CG2	2.44	0.46
6:6:28:VAL:O	6:6:32:ARG:HG2	2.15	0.46
2:B:112:THR:HG21	2:B:116:LEU:HD23	1.95	0.46
4:D:66:PHE:CG	4:D:85:MET:HE3	2.50	0.46
1:1:65:ARG:HA	1:1:65:ARG:HD3	1.76	0.46
3:3:101:ARG:NH1	3:3:101:ARG:HB3	2.31	0.46
3:3:224:GLY:HA3	3:3:295:ARG:HD2	1.96	0.46
3:3:642:ALA:CB	3:3:652:PRO:HG3	2.39	0.46
8:7:13:TRP:O	8:7:17:LEU:HG	2.16	0.46
2:B:81:GLN:HB3	2:B:122:VAL:CG2	2.43	0.46
3:C:186:ARG:HD2	3:C:231:PRO:HD3	1.97	0.46
3:C:218:LEU:HD22	3:C:218:LEU:HA	1.77	0.46
4:D:52:VAL:HG23	4:D:388:GLU:O	2.15	0.46
4:D:350:ARG:NE	4:D:403:VAL:HG23	2.30	0.46
5:E:144:HIS:O	5:E:147:ARG:HG2	2.15	0.46
6:F:82:GLY:HA2	9:F:182:SF4:S4	2.55	0.46
7:G:101:CYS:SG	7:G:103:LEU:HB2	2.56	0.46
7:G:163:VAL:O	7:G:177:THR:HB	2.15	0.46
1:1:149:ILE:HD13	1:1:171:LEU:CB	2.37	0.46
1:1:228:VAL:HB	1:1:229:PRO:CD	2.45	0.46
1:1:356:CYS:SG	1:1:399:PHE:CB	3.03	0.46
2:2:153:LEU:O	2:2:157:LEU:HG	2.15	0.46
3:3:269:THR:HG22	3:3:274:LEU:HA	1.97	0.46
3:3:715:GLU:HA	3:3:745:ALA:HB1	1.97	0.46
4:4:108:VAL:HG23	4:4:108:VAL:O	2.16	0.46
4:4:279:ARG:HG3	4:4:279:ARG:NH1	2.29	0.46
5:5:3:LEU:HB2	5:5:86:SER:HB3	1.96	0.46
5:5:116:ARG:HB3	5:5:135:ILE:HG13	1.97	0.46
2:B:10:PHE:O	2:B:14:THR:OG1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:ASP:O	3:C:119:CYS:C	2.58	0.46
3:C:616:ASN:HB3	3:C:620:ARG:H	1.80	0.46
3:3:171:SER:CB	3:3:172:PRO:HD2	2.39	0.46
3:3:337:ARG:H	3:3:337:ARG:HD2	1.80	0.46
3:3:398:VAL:C	3:3:399:LEU:HD12	2.41	0.46
3:3:417:VAL:CG1	3:3:443:ARG:HB3	2.46	0.46
7:9:96:LEU:CD2	7:9:129:LEU:HD13	2.45	0.46
1:A:243:THR:HG22	1:A:244:GLU:H	1.81	0.46
2:B:24:ARG:HA	2:B:53:VAL:CG1	2.46	0.46
3:C:124:LYS:HA	3:C:124:LYS:HD3	1.69	0.46
3:C:473:GLU:O	3:C:477:LEU:HD12	2.16	0.46
5:E:80:TRP:HA	5:E:80:TRP:HE3	1.81	0.46
6:F:143:ARG:HG2	6:F:145:GLU:OE1	2.16	0.46
3:3:587:LEU:HD13	3:3:589:HIS:O	2.16	0.46
1:A:53:VAL:O	1:A:57:VAL:HG23	2.16	0.46
1:A:180:TYR:OH	11:A:441:NAI:H5N	2.16	0.46
3:C:132:ASP:O	3:C:135:VAL:HG12	2.16	0.46
4:D:53:LEU:N	4:D:53:LEU:HD22	2.30	0.46
4:D:369:LYS:C	4:D:369:LYS:HD3	2.41	0.46
1:1:42:LYS:O	1:1:46:LYS:HG3	2.15	0.46
3:3:19:VAL:HG23	3:3:85:THR:O	2.15	0.46
3:3:616:ASN:HB3	3:3:620:ARG:H	1.81	0.46
3:3:694:LEU:HD23	3:3:760:LEU:HB3	1.98	0.46
4:4:369:LYS:C	4:4:369:LYS:HD3	2.40	0.46
1:A:42:LYS:HG3	1:A:163:PHE:CD2	2.51	0.46
3:C:13:VAL:HG21	3:C:17:THR:HG21	1.98	0.46
3:C:321:THR:HG22	3:C:322:TRP:N	2.31	0.46
3:C:504:VAL:HG12	3:C:505:LEU:N	2.30	0.46
4:D:64:THR:HG21	6:F:118:PHE:CE1	2.51	0.46
3:3:115:HIS:HB3	4:4:321:MET:HE3	1.98	0.46
3:3:370:ASP:OD2	3:3:558:TRP:HD1	1.98	0.46
3:3:476:ILE:O	3:3:480:LEU:HG	2.16	0.46
4:4:44:MET:HA	4:4:44:MET:CE	2.46	0.46
4:4:200:ARG:O	4:4:204:TYR:HD1	1.99	0.46
4:4:320:SER:HB3	4:4:323:ALA:CB	2.46	0.46
6:6:163:TYR:CD1	7:9:152:ARG:HD2	2.50	0.46
5:E:195:LEU:HD22	5:E:195:LEU:N	2.31	0.46
4:4:346:THR:CG2	4:4:353:LEU:HB3	2.40	0.45
5:5:161:GLU:CG	5:5:163:ARG:NH2	2.79	0.45
1:A:273:ARG:HB2	1:A:307:LEU:O	2.15	0.45
3:C:91:MET:HE3	3:C:93:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:368:HIS:HE2	3:C:554:LYS:HG2	1.82	0.45
4:D:253:PRO:HB2	4:D:258:GLU:HG3	1.97	0.45
4:D:339:LYS:HG2	4:D:360:ASP:HA	1.98	0.45
5:E:15:TYR:HA	5:E:16:PRO:HD3	1.76	0.45
5:E:77:LEU:HA	5:E:78:PRO:HD3	1.61	0.45
7:G:34:LYS:HB3	7:G:35:PRO:HD2	1.98	0.45
1:1:28:THR:HB	1:1:31:TYR:H	1.81	0.45
1:1:53:VAL:O	1:1:57:VAL:HG23	2.16	0.45
1:1:101:PHE:CZ	1:1:253:GLN:HB2	2.51	0.45
4:4:314:ARG:NH2	7:9:108:CYS:O	2.50	0.45
6:6:31:GLY:C	6:6:33:SER:H	2.24	0.45
1:A:9:LEU:HD13	1:A:279:TRP:HZ2	1.82	0.45
3:C:317:LEU:HD22	3:C:317:LEU:N	2.31	0.45
3:C:386:SER:HB3	3:C:389:ASP:CG	2.41	0.45
5:E:47:ASN:ND2	5:E:76:SER:HA	2.30	0.45
6:F:143:ARG:HE	7:G:31:VAL:HG11	1.82	0.45
1:1:45:LEU:HD12	1:1:163:PHE:HD1	1.81	0.45
6:6:89:ALA:N	6:6:90:PRO:HD2	2.31	0.45
3:C:224:GLY:HA3	3:C:295:ARG:HD2	1.96	0.45
3:C:250:GLU:CD	3:C:628:PRO:HG2	2.41	0.45
3:C:417:VAL:CG1	3:C:443:ARG:HB3	2.46	0.45
3:C:584:VAL:HG12	3:C:600:VAL:HB	1.97	0.45
6:F:145:GLU:HA	6:F:148:ILE:HD13	1.97	0.45
7:G:163:VAL:HG22	7:G:177:THR:CG2	2.47	0.45
4:4:101:VAL:CG1	4:4:175:ILE:HD12	2.47	0.45
1:A:102:LYS:HE3	1:A:103:ASP:CG	2.41	0.45
2:B:122:VAL:HG12	2:B:123:GLU:H	1.79	0.45
3:C:54:LEU:HD13	3:C:91:MET:HG3	1.97	0.45
3:C:672:ALA:O	3:C:673:MET:HB2	2.16	0.45
1:1:68:ALA:HB1	11:1:441:NAI:H51A	1.98	0.45
3:3:541:ALA:O	3:3:545:GLU:HG3	2.15	0.45
4:4:185:GLU:O	4:4:189:GLU:HG2	2.17	0.45
4:4:200:ARG:O	4:4:204:TYR:CD1	2.70	0.45
8:7:74:PRO:HG2	8:7:77:ALA:HB2	1.99	0.45
1:A:6:LEU:HD21	1:A:12:ARG:HG3	1.98	0.45
1:A:6:LEU:HD12	1:A:240:GLN:HG3	1.98	0.45
1:A:361:GLU:H	1:A:361:GLU:HG2	1.56	0.45
3:C:241:ARG:HH11	7:G:74:GLU:CD	2.24	0.45
3:C:722:THR:CG2	3:C:755:LYS:HB3	2.45	0.45
4:D:101:VAL:CG1	4:D:175:ILE:HD12	2.47	0.45
4:D:327:HIS:CE1	7:G:107:ALA:O	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:31:GLY:C	6:F:33:SER:N	2.74	0.45
6:F:31:GLY:C	6:F:33:SER:H	2.24	0.45
3:3:2:VAL:HG13	3:3:89:ASP:CA	2.47	0.45
4:4:88:LEU:HD12	4:4:403:VAL:CG2	2.45	0.45
4:4:101:VAL:HG11	4:4:175:ILE:HD12	1.98	0.45
4:4:190:LEU:HG	4:4:194:LEU:HD22	1.98	0.45
5:5:72:TYR:HB2	5:5:90:VAL:HG13	1.98	0.45
6:6:25:GLU:HA	6:6:28:VAL:HG23	1.98	0.45
11:A:441:NAI:O1N	11:A:441:NAI:H52A	2.17	0.45
2:B:24:ARG:HA	2:B:53:VAL:HG13	1.98	0.45
3:C:403:THR:OG1	3:C:458:LEU:HD11	2.17	0.45
3:C:474:ARG:NH2	3:C:516:VAL:CG2	2.65	0.45
4:D:213:ILE:HG21	4:D:217:ARG:HH11	1.82	0.45
4:D:409:ARG:HG2	4:D:409:ARG:NH1	2.31	0.45
5:E:2:ARG:HB2	5:E:84:ASP:OD2	2.17	0.45
5:E:168:ALA:HA	5:E:171:ARG:NH1	2.31	0.45
3:3:192:GLU:HG3	3:3:193:GLU:N	2.31	0.45
3:3:695:ARG:HA	3:3:696:PRO:HD2	1.87	0.45
5:5:75:VAL:HG12	5:5:76:SER:N	2.31	0.45
3:C:117:LEU:CA	4:D:321:MET:HE1	2.47	0.45
4:D:257:TYR:C	4:D:259:THR:N	2.72	0.45
7:G:162:VAL:HA	7:G:176:PRO:O	2.17	0.45
8:H:121:ARG:NH1	8:H:121:ARG:CG	2.77	0.45
1:1:408:TRP:HB2	1:1:409:PRO:HD2	1.99	0.45
3:3:29:ASP:OD2	5:5:186:GLY:HA3	2.17	0.45
3:3:36:GLU:HG3	3:3:37:LYS:N	2.32	0.45
3:3:588:SER:C	3:3:589:HIS:ND1	2.75	0.45
4:4:47:LEU:HD13	4:4:52:VAL:HA	1.98	0.45
4:4:262:PHE:CD1	4:4:289:ILE:HD11	2.51	0.45
6:6:125:GLN:O	6:6:126:ASN:CB	2.64	0.45
6:6:145:GLU:HG2	7:9:31:VAL:CG2	2.47	0.45
7:9:33:LEU:HD11	7:9:161:TYR:HB2	1.98	0.45
7:9:125:GLU:O	7:9:128:ASP:HB2	2.16	0.45
3:C:47:MET:HE3	3:C:47:MET:HB3	1.67	0.45
3:C:403:THR:HG22	3:C:404:GLU:OE2	2.17	0.45
3:C:459:MET:HE2	3:C:465:HIS:CB	2.32	0.45
4:D:128:SER:OG	4:D:350:ARG:NH1	2.45	0.45
5:E:116:ARG:HB3	5:E:135:ILE:HG13	1.99	0.45
5:5:119:TYR:O	5:5:122:PHE:O	2.35	0.45
4:D:82:THR:N	4:D:83:PRO:HD2	2.30	0.45
1:1:102:LYS:HE3	1:1:103:ASP:CG	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:8:GLN:HE21	2:2:8:GLN:HB3	1.66	0.45
2:2:26:ALA:O	2:2:30:LEU:HG	2.18	0.45
3:3:124:LYS:HD3	3:3:124:LYS:HA	1.76	0.45
3:3:514:ASP:OD1	3:3:516:VAL:HB	2.17	0.45
1:A:95:GLU:OE2	1:A:102:LYS:HD3	2.17	0.45
1:A:299:PRO:HG3	1:A:341:MET:CE	2.46	0.45
1:A:314:GLU:HA	1:A:317:GLN:HB3	1.99	0.45
1:A:325:THR:HG21	11:A:441:NAI:N7N	2.32	0.45
4:D:47:LEU:HD13	4:D:52:VAL:HA	1.99	0.45
5:E:52:ILE:HG23	5:E:52:ILE:O	2.16	0.45
5:E:178:ASP:OD1	5:E:179:PRO:HD2	2.17	0.45
6:F:125:GLN:O	6:F:126:ASN:CB	2.65	0.45
2:2:45:ARG:O	2:2:49:ILE:HG13	2.17	0.44
3:3:440:ARG:CG	3:3:440:ARG:NH1	2.77	0.44
6:6:84:LEU:HD12	6:6:124:VAL:HG21	1.99	0.44
6:6:163:TYR:HD2	6:6:168:GLU:O	1.99	0.44
3:C:54:LEU:N	3:C:55:PRO:HD3	2.31	0.44
3:C:151:LEU:HD23	3:C:151:LEU:HA	1.81	0.44
3:C:476:ILE:O	3:C:480:LEU:HG	2.16	0.44
4:D:94:ASP:HB3	4:D:173:ILE:HG21	1.98	0.44
4:D:262:PHE:CD1	4:D:289:ILE:HD11	2.52	0.44
4:D:290:ILE:O	4:D:294:LEU:HB2	2.17	0.44
5:E:7:LEU:CD2	5:E:17:ILE:HD12	2.47	0.44
5:E:103:THR:HG22	5:E:127:GLU:O	2.17	0.44
1:1:397:ARG:O	1:1:397:ARG:HG2	2.16	0.44
3:3:303:GLN:HE21	3:3:303:GLN:HB3	1.65	0.44
3:3:736:VAL:HG11	3:3:760:LEU:HD22	1.98	0.44
4:4:333:GLU:CD	5:5:189:ARG:HH11	2.25	0.44
6:6:145:GLU:HG2	7:9:31:VAL:HG21	1.98	0.44
1:A:356:CYS:SG	1:A:399:PHE:CB	3.06	0.44
3:C:305:ARG:NH2	3:C:609:GLU:OE1	2.51	0.44
3:C:458:LEU:C	3:C:460:LYS:N	2.73	0.44
4:D:163:VAL:HG13	4:D:164:THR:HG23	1.99	0.44
6:F:132:PRO:HB3	6:F:174:ALA:HB1	1.99	0.44
7:G:44:THR:HA	7:G:138:VAL:CG1	2.46	0.44
8:H:19:TRP:CD1	8:H:112:LYS:HE3	2.53	0.44
2:2:31:LEU:HD22	2:2:49:ILE:HD12	1.99	0.44
3:3:36:GLU:HB3	3:3:39:LEU:HD12	1.98	0.44
3:3:54:LEU:N	3:3:55:PRO:HD3	2.30	0.44
3:3:458:LEU:C	3:3:460:LYS:N	2.73	0.44
4:4:339:LYS:HA	4:4:359:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:77:LEU:HA	5:5:78:PRO:HD3	1.61	0.44
5:5:144:HIS:O	5:5:147:ARG:HG2	2.17	0.44
3:C:46:ARG:NH2	3:C:81:ALA:HB2	2.32	0.44
3:C:512:LEU:HD21	3:C:534:ALA:HB1	1.99	0.44
4:D:241:ALA:O	4:D:270:GLY:HA2	2.18	0.44
4:D:279:ARG:HG3	4:D:279:ARG:NH1	2.30	0.44
6:F:104:TRP:NE1	6:F:158:VAL:HG12	2.32	0.44
2:2:125:LEU:HD12	2:2:133:VAL:HG12	2.00	0.44
3:3:222:PHE:CD1	3:3:411:LEU:HD11	2.52	0.44
3:3:317:LEU:HD22	3:3:317:LEU:N	2.32	0.44
5:5:103:THR:HG22	5:5:127:GLU:O	2.17	0.44
5:5:132:LEU:HA	5:5:132:LEU:HD23	1.58	0.44
3:C:375:THR:CG2	3:C:537:PRO:HD2	2.47	0.44
3:C:497:TRP:O	3:C:528:LYS:HE3	2.17	0.44
1:1:299:PRO:HG3	1:1:341:MET:HE1	2.00	0.44
4:4:142:ALA:HB1	4:4:145:PRO:HD2	1.99	0.44
4:4:158:ASP:OD1	7:9:34:LYS:HE3	2.17	0.44
4:4:263:ASP:HB2	4:4:285:GLU:OE1	2.16	0.44
5:5:39:ALA:HA	5:5:107:LEU:HD13	1.99	0.44
1:A:101:PHE:CZ	1:A:253:GLN:HB2	2.52	0.44
3:C:169:PRO:HA	3:C:175:ILE:HA	1.98	0.44
4:D:88:LEU:HD12	4:D:403:VAL:CG2	2.47	0.44
5:E:132:LEU:HD23	5:E:132:LEU:HA	1.65	0.44
5:E:161:GLU:HG3	5:E:163:ARG:HH22	1.83	0.44
6:F:140:CYS:SG	7:G:99:ILE:HG13	2.57	0.44
7:G:117:TYR:HE2	7:G:166:VAL:HG12	1.82	0.44
3:3:497:TRP:O	3:3:500:ALA:HB3	2.17	0.44
6:6:46:CYS:HB3	6:6:108:MET:HE2	2.00	0.44
6:6:84:LEU:HD11	6:6:89:ALA:HA	1.98	0.44
1:A:260:ARG:HA	1:A:261:PRO:HD2	1.71	0.44
3:C:9:ARG:HD2	3:C:26:ALA:O	2.17	0.44
3:C:329:LEU:HD21	3:C:644:LEU:HD12	1.99	0.44
3:C:550:LEU:N	3:C:550:LEU:CD1	2.81	0.44
4:D:194:LEU:HD21	4:D:290:ILE:HG22	2.00	0.44
7:G:33:LEU:HD11	7:G:161:TYR:HB2	1.99	0.44
2:2:87:SER:HB3	2:2:128:CYS:HB3	2.00	0.44
2:2:123:GLU:O	2:2:124:CYS:C	2.61	0.44
3:3:13:VAL:HG21	3:3:17:THR:HG21	1.99	0.44
3:3:459:MET:HE2	3:3:465:HIS:CB	2.35	0.44
3:3:627:ALA:HA	3:3:628:PRO:HD3	1.81	0.44
4:4:396:ILE:HD12	4:4:396:ILE:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:LEU:O	2:B:153:LEU:HD22	2.18	0.44
3:C:587:LEU:HD13	3:C:589:HIS:O	2.18	0.44
6:F:155:GLN:C	6:F:157:LYS:N	2.75	0.44
1:1:391:LEU:HB2	1:1:392:PRO:HD3	2.00	0.44
1:1:414:LEU:HD13	1:1:421:TYR:CE1	2.53	0.44
2:2:163:LEU:HA	2:2:166:ILE:HD11	2.00	0.44
2:B:45:ARG:O	2:B:49:ILE:HG13	2.18	0.44
3:C:372:GLN:HB2	3:C:570:PHE:CD1	2.53	0.44
3:C:689:LYS:H	3:C:689:LYS:HG2	1.47	0.44
4:D:213:ILE:O	4:D:214:PHE:C	2.61	0.44
4:D:213:ILE:HG22	4:D:217:ARG:CG	2.48	0.44
6:F:163:TYR:CB	7:G:152:ARG:NH1	2.77	0.44
7:G:68:ILE:HD11	9:G:183:SF4:S1	2.58	0.44
3:3:305:ARG:NH2	3:3:609:GLU:OE1	2.51	0.44
3:3:646:GLU:C	3:3:648:LEU:H	2.26	0.44
4:4:306:ASN:HA	4:4:307:PRO:HD3	1.81	0.44
5:5:111:ALA:O	5:5:115:GLU:HG3	2.17	0.44
6:6:155:GLN:C	6:6:157:LYS:H	2.26	0.44
3:C:368:HIS:CE1	3:C:563:ALA:HA	2.52	0.44
4:D:169:HIS:O	4:D:170:HIS:C	2.60	0.44
2:2:33:ARG:O	2:2:34:VAL:C	2.61	0.43
3:3:300:TRP:N	3:3:705:VAL:HG21	2.33	0.43
4:4:253:PRO:HB2	4:4:258:GLU:HG3	1.99	0.43
4:4:257:TYR:O	4:4:259:THR:N	2.51	0.43
6:6:155:GLN:C	6:6:157:LYS:N	2.75	0.43
6:6:163:TYR:CD1	7:9:152:ARG:NH1	2.85	0.43
8:7:70:ALA:HA	8:7:83:GLY:O	2.17	0.43
1:A:110:VAL:O	1:A:113:LEU:HB3	2.18	0.43
3:C:259:CYS:CB	3:C:260:PRO:CD	2.96	0.43
5:E:39:ALA:HA	5:E:107:LEU:HD13	2.00	0.43
7:G:94:ASN:C	7:G:94:ASN:HD22	2.25	0.43
3:3:186:ARG:HD2	3:3:231:PRO:HD3	1.99	0.43
3:3:550:LEU:CD2	3:3:684:ARG:HH21	2.31	0.43
4:4:221:VAL:HG12	4:4:388:GLU:OE1	2.17	0.43
4:4:350:ARG:NE	4:4:403:VAL:HG23	2.32	0.43
5:5:138:PRO:HA	6:6:87:LYS:HD2	2.00	0.43
6:6:31:GLY:C	6:6:33:SER:N	2.74	0.43
6:6:145:GLU:HA	6:6:148:ILE:HD13	1.99	0.43
7:9:73:ALA:HB3	7:9:87:TYR:CZ	2.53	0.43
8:7:17:LEU:HD22	8:7:54:ILE:HD11	2.00	0.43
4:D:363:SER:CB	5:E:174:LEU:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:86:LEU:HD12	8:H:91:ILE:HD12	2.00	0.43
1:1:397:ARG:O	3:3:46:ARG:HD3	2.18	0.43
3:3:368:HIS:CE1	3:3:563:ALA:HA	2.53	0.43
6:6:174:ALA:O	6:6:175:ALA:HB2	2.19	0.43
3:C:36:GLU:HB3	3:C:39:LEU:HD12	2.00	0.43
3:C:343:LEU:CD1	3:C:360:LEU:HD23	2.48	0.43
3:C:753:VAL:HA	3:C:754:PRO:HD2	1.84	0.43
5:E:74:LEU:O	5:E:87:ARG:HA	2.18	0.43
7:G:129:LEU:HD23	7:G:129:LEU:HA	1.85	0.43
3:3:49:LEU:HA	3:3:80:ALA:O	2.19	0.43
3:3:125:GLY:HA2	3:3:245:ARG:HH21	1.84	0.43
3:3:173:PHE:HB3	3:3:296:PHE:CE2	2.54	0.43
3:3:505:LEU:HD21	3:3:507:LEU:CD2	2.48	0.43
4:4:128:SER:OG	4:4:350:ARG:NH1	2.47	0.43
1:A:391:LEU:HB2	1:A:392:PRO:HD3	1.99	0.43
3:C:101:ARG:NH1	3:C:101:ARG:HB3	2.33	0.43
4:D:48:SER:H	4:D:53:LEU:HD23	1.83	0.43
4:D:101:VAL:HG11	4:D:175:ILE:HD12	1.99	0.43
3:3:152:PRO:HG3	4:4:305:PRO:O	2.18	0.43
3:3:585:MET:HG3	3:3:598:ALA:CB	2.48	0.43
1:A:228:VAL:HB	1:A:229:PRO:CD	2.49	0.43
1:A:287:ILE:HG13	1:A:330:LEU:HB3	2.01	0.43
1:A:414:LEU:HD13	1:A:421:TYR:CE1	2.54	0.43
3:C:300:TRP:CA	3:C:705:VAL:HG21	2.48	0.43
3:C:504:VAL:CG1	3:C:505:LEU:N	2.82	0.43
3:C:513:GLN:NE2	3:C:769:LEU:HD21	2.33	0.43
3:C:600:VAL:HG12	3:C:602:LEU:HD12	2.00	0.43
4:D:86:ASP:HB3	4:D:93:HIS:CD2	2.53	0.43
1:1:42:LYS:HG3	1:1:163:PHE:CD2	2.53	0.43
3:3:305:ARG:NH2	3:3:609:GLU:CD	2.74	0.43
4:4:51:GLU:HB3	4:4:52:VAL:H	1.65	0.43
4:4:213:ILE:O	4:4:214:PHE:C	2.60	0.43
6:6:132:PRO:HB3	6:6:174:ALA:HB1	2.00	0.43
7:9:29:ALA:HA	7:9:30:PRO:HD2	1.72	0.43
1:A:109:ASP:O	1:A:110:VAL:HG13	2.18	0.43
3:C:173:PHE:HB3	3:C:296:PHE:CE2	2.54	0.43
3:C:719:HIS:CD2	3:C:755:LYS:HG2	2.54	0.43
4:D:51:GLU:HB3	4:D:52:VAL:H	1.65	0.43
2:2:26:ALA:C	2:2:29:PRO:HG2	2.44	0.43
3:3:587:LEU:O	3:3:604:ALA:HB3	2.17	0.43
4:4:213:ILE:HG22	4:4:217:ARG:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:260:TYR:HE2	4:4:293:ALA:HB2	1.82	0.43
4:4:338:PRO:HG2	5:5:193:ARG:HD3	2.01	0.43
5:5:47:ASN:ND2	5:5:76:SER:HA	2.31	0.43
8:7:96:HIS:O	8:7:103:LEU:HD12	2.19	0.43
1:A:89:LEU:O	1:A:130:GLY:HA2	2.19	0.43
3:C:272:GLY:HA2	3:C:628:PRO:O	2.19	0.43
3:C:317:LEU:HD22	3:C:317:LEU:H	1.84	0.43
3:C:460:LYS:HD3	3:C:460:LYS:HA	1.85	0.43
3:C:591:HIS:ND1	3:C:592:PRO:CD	2.80	0.43
4:D:304:ASP:HA	4:D:305:PRO:HD2	1.87	0.43
6:F:145:GLU:CD	6:F:145:GLU:H	2.26	0.43
6:F:152:MET:HE2	6:F:152:MET:HB3	1.82	0.43
8:H:34:GLU:CB	8:H:56:THR:HG22	2.49	0.43
1:1:102:LYS:H	1:1:102:LYS:HD3	1.84	0.43
1:1:401:PRO:HG2	10:1:440:FMN:C8M	2.49	0.43
2:2:28:MET:HB3	2:2:28:MET:HE2	1.75	0.43
3:3:344:TYR:CD1	3:3:568:TYR:CE1	3.07	0.43
3:3:719:HIS:CD2	3:3:755:LYS:HG2	2.54	0.43
6:6:32:ARG:HG2	6:6:32:ARG:H	1.54	0.43
3:C:163:HIS:C	3:C:164:VAL:HG13	2.44	0.43
4:D:163:VAL:HG22	4:D:164:THR:CG2	2.48	0.43
4:D:306:ASN:HA	4:D:307:PRO:HD3	1.79	0.43
6:F:121:TYR:N	6:F:121:TYR:CD1	2.86	0.43
1:1:6:LEU:HD12	1:1:240:GLN:HG3	2.01	0.43
1:1:53:VAL:HG23	1:1:231:MET:CE	2.45	0.43
3:3:225:ASN:O	3:3:229:ILE:HG13	2.19	0.43
3:3:504:VAL:HG12	3:3:505:LEU:N	2.34	0.43
3:3:563:ALA:HB3	3:3:580:LYS:HE3	2.01	0.43
3:3:716:LEU:HD21	3:3:758:LEU:HB3	1.99	0.43
3:3:717:TRP:CD1	3:3:748:VAL:HB	2.54	0.43
7:9:46:HIS:HB3	7:9:47:PRO:HD2	2.01	0.43
1:A:110:VAL:N	1:A:111:PRO:CD	2.81	0.43
1:A:245:GLN:HB2	1:A:314:GLU:OE2	2.19	0.43
3:C:370:ASP:OD2	3:C:558:TRP:CD1	2.72	0.43
4:D:62:LEU:HD23	4:D:62:LEU:HA	1.64	0.43
6:F:174:ALA:O	6:F:175:ALA:HB2	2.19	0.43
3:3:118:ASP:O	3:3:119:CYS:C	2.62	0.43
3:3:343:LEU:CD1	3:3:360:LEU:HD23	2.49	0.43
5:5:178:ASP:OD1	5:5:179:PRO:HD2	2.19	0.43
8:7:121:ARG:NH1	8:7:121:ARG:CG	2.78	0.43
1:A:53:VAL:HG23	1:A:231:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:440:ARG:CG	3:C:440:ARG:NH1	2.79	0.43
4:D:374:SER:HB2	4:D:406:ASP:HB3	2.01	0.43
8:H:16:LEU:HD13	8:H:20:MET:HG3	2.01	0.43
8:H:65:GLU:HA	8:H:66:PRO:HD3	1.72	0.43
3:3:483:ASP:O	3:3:484:LYS:HG2	2.19	0.42
3:3:594:ALA:O	3:3:598:ALA:HB3	2.19	0.42
6:6:81:ALA:CB	6:6:108:MET:HE2	2.48	0.42
7:9:81:VAL:HG11	7:9:87:TYR:CD1	2.54	0.42
1:A:65:ARG:HA	1:A:65:ARG:HD3	1.75	0.42
1:A:293:GLY:HA3	1:A:324:GLY:N	2.23	0.42
3:C:505:LEU:HD21	3:C:507:LEU:CD2	2.48	0.42
5:E:75:VAL:HG12	5:E:76:SER:N	2.34	0.42
5:E:163:ARG:HD2	7:G:69:TYR:CD1	2.54	0.42
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.59	0.42
3:3:223:SER:O	3:3:226:ILE:HG12	2.19	0.42
3:3:403:THR:HG22	3:3:404:GLU:OE2	2.19	0.42
1:A:211:LEU:H	1:A:216:THR:CG2	2.32	0.42
3:C:305:ARG:NH2	3:C:609:GLU:CD	2.74	0.42
3:C:469:ARG:HG2	3:C:754:PRO:CG	2.49	0.42
6:F:147:LEU:O	6:F:151:VAL:HG13	2.19	0.42
7:G:149:GLU:O	7:G:153:THR:HB	2.20	0.42
8:H:75:ARG:HE	8:H:76:HIS:CD2	2.33	0.42
1:1:135:ARG:C	1:1:137:GLU:H	2.26	0.42
3:3:586:HIS:NE2	3:3:604:ALA:HB2	2.35	0.42
4:4:241:ALA:O	4:4:270:GLY:HA2	2.18	0.42
5:5:74:LEU:O	5:5:87:ARG:HA	2.19	0.42
1:A:357:THR:N	1:A:358:PRO:CD	2.82	0.42
3:C:115:HIS:O	4:D:321:MET:HE3	2.18	0.42
3:C:605:PRO:HB3	3:C:609:GLU:HG3	2.01	0.42
3:C:695:ARG:O	3:C:697:THR:HG23	2.18	0.42
3:C:695:ARG:HA	3:C:696:PRO:HD2	1.85	0.42
3:C:736:VAL:HG11	3:C:760:LEU:HD22	2.01	0.42
4:D:230:ILE:HD11	4:D:244:VAL:CG1	2.49	0.42
5:E:116:ARG:CG	5:E:129:HIS:CE1	3.02	0.42
7:G:48:ASN:HB2	7:G:50:LEU:CD2	2.50	0.42
10:1:440:FMN:H9	10:1:440:FMN:H1'1	1.63	0.42
3:3:254:THR:HG23	3:3:255:THR:N	2.34	0.42
3:3:743:VAL:HG12	3:3:744:GLU:N	2.34	0.42
5:5:116:ARG:CG	5:5:129:HIS:CE1	3.02	0.42
5:5:161:GLU:HG3	5:5:163:ARG:HH22	1.85	0.42
7:9:101:CYS:SG	7:9:103:LEU:HB2	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HH11	1:A:65:ARG:HG3	1.83	0.42
3:C:130:LEU:O	3:C:131:GLN:C	2.62	0.42
3:C:587:LEU:O	3:C:604:ALA:HB3	2.20	0.42
4:D:311:PRO:HD3	4:D:330:HIS:CE1	2.54	0.42
5:E:67:ARG:HB3	5:E:96:GLU:HB2	2.00	0.42
5:E:103:THR:HG21	5:E:128:GLY:C	2.43	0.42
5:E:167:PRO:HB3	7:G:66:TYR:CE2	2.54	0.42
7:G:44:THR:OG1	7:G:52:LYS:HD2	2.18	0.42
1:1:171:LEU:HD12	1:1:171:LEU:HA	1.73	0.42
1:1:260:ARG:HA	1:1:261:PRO:HD2	1.75	0.42
1:1:429:ARG:HA	1:1:430:PRO:HD2	1.92	0.42
2:2:15:PHE:HE1	2:2:23:ARG:HB3	1.84	0.42
2:2:33:ARG:NH2	2:2:37:GLU:CG	2.83	0.42
2:2:87:SER:CB	2:2:128:CYS:HB3	2.50	0.42
4:4:72:HIS:O	4:4:73:ARG:HD3	2.19	0.42
4:4:221:VAL:HG23	4:4:272:VAL:CG1	2.50	0.42
8:7:55:MET:HE2	8:7:55:MET:HB3	1.90	0.42
3:C:139:LEU:HD12	4:D:326:TYR:CZ	2.55	0.42
3:C:282:VAL:CG2	3:C:285:VAL:HG12	2.47	0.42
3:C:483:ASP:O	3:C:484:LYS:HG2	2.19	0.42
3:C:689:LYS:HD2	3:C:772:GLU:CG	2.49	0.42
4:D:83:PRO:CB	4:D:169:HIS:HA	2.49	0.42
4:D:257:TYR:O	4:D:259:THR:N	2.52	0.42
4:D:350:ARG:HE	4:D:403:VAL:HG23	1.84	0.42
1:1:67:GLY:HA2	1:1:324:GLY:O	2.20	0.42
1:1:408:TRP:CB	1:1:409:PRO:CD	2.98	0.42
3:3:5:LYS:HB2	3:3:10:ILE:HG13	2.01	0.42
3:3:249:MET:HE3	3:3:268:ASP:CB	2.48	0.42
3:3:258:LEU:HD11	3:3:703:GLN:NE2	2.34	0.42
3:3:513:GLN:NE2	3:3:769:LEU:HD21	2.34	0.42
4:4:48:SER:H	4:4:53:LEU:HD23	1.85	0.42
4:4:169:HIS:O	4:4:170:HIS:C	2.63	0.42
5:5:15:TYR:HA	5:5:16:PRO:HD3	1.75	0.42
6:6:137:VAL:HA	6:6:138:PRO:HD2	1.90	0.42
1:A:86:GLN:O	1:A:87:HIS:HD2	2.03	0.42
1:A:202:LYS:N	1:A:203:PRO:CD	2.83	0.42
4:D:196:VAL:O	4:D:200:ARG:HB2	2.20	0.42
5:E:111:ALA:O	5:E:115:GLU:HG3	2.20	0.42
1:1:358:PRO:CD	3:3:107:MET:HE1	2.46	0.42
3:3:9:ARG:HD2	3:3:26:ALA:O	2.19	0.42
3:3:116:PRO:HG3	3:3:180:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:373:GLY:O	3:3:374:ARG:C	2.63	0.42
4:4:230:ILE:O	4:4:230:ILE:CG2	2.67	0.42
6:6:76:ASP:O	6:6:77:VAL:CB	2.65	0.42
7:9:100:PHE:N	7:9:100:PHE:CD1	2.87	0.42
2:B:33:ARG:NH2	2:B:37:GLU:CG	2.82	0.42
3:C:113:LEU:HD11	3:C:157:PHE:CD1	2.55	0.42
3:C:249:MET:HE1	3:C:275:LEU:HB3	2.02	0.42
3:C:398:VAL:C	3:C:399:LEU:HD12	2.45	0.42
4:D:233:GLY:CA	5:E:48:PHE:HE1	2.32	0.42
5:E:72:TYR:HB2	5:E:90:VAL:HG13	2.00	0.42
7:G:71:GLU:HA	7:G:72:PRO:HD3	1.75	0.42
7:G:170:LEU:O	7:G:171:GLU:C	2.61	0.42
1:1:314:GLU:HA	1:1:317:GLN:HB3	1.99	0.42
1:1:437:TRP:O	1:1:437:TRP:HD1	2.03	0.42
3:3:155:THR:HB	4:4:322:GLU:OE1	2.19	0.42
3:3:216:PHE:HZ	8:7:128:PHE:CD2	2.33	0.42
3:3:326:PHE:CE2	3:3:330:LYS:HE3	2.55	0.42
3:3:368:HIS:HE2	3:3:554:LYS:HG2	1.85	0.42
3:3:651:ARG:HD2	3:3:651:ARG:C	2.44	0.42
4:4:66:PHE:CG	4:4:85:MET:HE3	2.55	0.42
4:4:211:SER:HA	4:4:212:PRO:HD2	1.93	0.42
5:5:82:ASP:O	5:5:83:GLY:C	2.63	0.42
6:6:163:TYR:OH	6:6:169:ARG:NH2	2.52	0.42
8:7:75:ARG:NE	8:7:76:HIS:NE2	2.62	0.42
2:B:153:LEU:O	2:B:157:LEU:HG	2.20	0.42
3:C:10:ILE:HD12	3:C:10:ILE:N	2.34	0.42
1:1:9:LEU:HD12	1:1:9:LEU:HA	1.74	0.42
4:4:317:LEU:HD12	4:4:317:LEU:HA	1.91	0.42
5:5:25:LEU:N	5:5:25:LEU:HD23	2.34	0.42
6:6:140:CYS:SG	6:6:140:CYS:O	2.77	0.42
1:A:211:LEU:CB	1:A:216:THR:HG21	2.50	0.42
1:A:299:PRO:HG3	1:A:341:MET:HE1	2.02	0.42
3:C:299:GLU:O	3:C:303:GLN:HG3	2.20	0.42
3:C:477:LEU:HD21	3:C:521:ALA:HB2	2.02	0.42
3:C:683:LEU:N	3:C:683:LEU:HD23	2.35	0.42
3:C:698:MET:CE	3:C:699:TRP:NE1	2.82	0.42
4:D:236:GLY:O	4:D:238:SER:N	2.51	0.42
4:D:241:ALA:CB	4:D:278:VAL:HG21	2.49	0.42
7:G:144:LYS:HB2	7:G:145:PRO:CD	2.49	0.42
7:G:144:LYS:CB	7:G:145:PRO:CD	2.97	0.42
7:G:153:THR:HG22	7:G:155:LYS:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:122:VAL:CG1	2:2:123:GLU:H	2.32	0.42
3:3:249:MET:HE1	3:3:275:LEU:HB3	2.02	0.42
3:3:263:CYS:HB3	3:3:264:GLY:H	1.57	0.42
3:3:272:GLY:HA2	3:3:628:PRO:O	2.20	0.42
2:B:123:GLU:O	2:B:124:CYS:C	2.63	0.42
3:C:571:VAL:HG11	3:C:591:HIS:CD2	2.55	0.42
4:D:105:LEU:HD13	4:D:309:ILE:CD1	2.43	0.42
8:H:50:LEU:HA	8:H:51:PRO:HD3	1.93	0.42
1:1:45:LEU:HD12	1:1:163:PHE:CD1	2.54	0.41
3:3:54:LEU:HD12	3:3:54:LEU:HA	1.80	0.41
3:3:157:PHE:CZ	3:3:159:PHE:HB2	2.55	0.41
3:3:163:HIS:C	3:3:164:VAL:HG13	2.44	0.41
3:3:441:MET:HA	3:3:442:PRO:HD2	1.87	0.41
4:4:404:MET:HA	4:4:407:VAL:HG12	2.02	0.41
1:A:408:TRP:HB2	1:A:409:PRO:HD2	2.02	0.41
1:A:437:TRP:O	1:A:437:TRP:HD1	2.01	0.41
2:B:87:SER:HB3	2:B:128:CYS:HB3	2.01	0.41
3:C:125:GLY:HA2	3:C:245:ARG:HH21	1.84	0.41
3:C:154:TYR:CZ	4:D:307:PRO:HB3	2.55	0.41
6:F:155:GLN:C	6:F:157:LYS:H	2.27	0.41
3:3:130:LEU:O	3:3:131:GLN:C	2.64	0.41
3:3:681:LYS:O	3:3:682:GLU:HB3	2.20	0.41
4:4:84:ARG:O	6:6:83:ARG:NH2	2.54	0.41
4:4:163:VAL:HG13	4:4:164:THR:HG23	2.02	0.41
4:4:290:ILE:O	4:4:294:LEU:HB2	2.20	0.41
7:9:144:LYS:HB2	7:9:145:PRO:CD	2.50	0.41
8:7:16:LEU:HD13	8:7:20:MET:HG3	2.02	0.41
3:C:171:SER:CB	3:C:172:PRO:HD2	2.41	0.41
3:C:225:ASN:O	3:C:229:ILE:HG13	2.19	0.41
4:D:109:VAL:HG12	4:D:113:ALA:HB3	2.01	0.41
4:D:127:ALA:O	4:D:131:VAL:HG23	2.19	0.41
1:1:184:GLU:HG2	10:1:440:FMN:HM82	2.03	0.41
1:1:287:ILE:HG22	1:1:302:PHE:HB2	2.03	0.41
3:3:47:MET:HE3	3:3:47:MET:HB3	1.66	0.41
3:3:689:LYS:HD2	3:3:772:GLU:CG	2.51	0.41
4:4:52:VAL:HG23	4:4:388:GLU:O	2.20	0.41
4:4:350:ARG:HE	4:4:403:VAL:HG23	1.85	0.41
6:6:36:LEU:HD22	6:6:77:VAL:CG2	2.46	0.41
1:A:184:GLU:O	1:A:185:GLU:C	2.63	0.41
3:C:76:GLN:HA	3:C:77:PRO:HD3	1.84	0.41
3:C:313:LYS:HB3	3:C:314:GLU:H	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:318:VAL:CG1	3:C:319:GLU:N	2.82	0.41
3:C:681:LYS:O	3:C:682:GLU:HB3	2.21	0.41
4:D:101:VAL:HB	4:D:175:ILE:HD12	2.01	0.41
5:E:25:LEU:N	5:E:25:LEU:CD2	2.84	0.41
8:H:75:ARG:HE	8:H:76:HIS:CE1	2.38	0.41
1:1:357:THR:N	1:1:358:PRO:CD	2.80	0.41
3:3:205:ARG:HH11	3:3:205:ARG:CG	2.33	0.41
3:3:683:LEU:N	3:3:683:LEU:HD23	2.35	0.41
3:3:689:LYS:HD2	3:3:772:GLU:HG2	2.03	0.41
4:4:30:VAL:CG1	4:4:31:GLY:N	2.83	0.41
4:4:159:LEU:O	4:4:162:TRP:HB2	2.19	0.41
6:6:44:ALA:O	6:6:46:CYS:N	2.53	0.41
6:6:121:TYR:CD1	6:6:121:TYR:N	2.87	0.41
1:A:287:ILE:HG22	1:A:302:PHE:HB2	2.02	0.41
3:C:435:LEU:HD22	3:C:435:LEU:N	2.33	0.41
3:C:444:ARG:HH21	3:C:447:LYS:HG3	1.83	0.41
4:D:119:ILE:O	4:D:123:LEU:HB2	2.20	0.41
4:D:159:LEU:O	4:D:162:TRP:HB2	2.21	0.41
6:F:113:SER:HB3	7:G:96:LEU:HD22	2.02	0.41
6:F:163:TYR:HB3	6:F:168:GLU:O	2.20	0.41
1:1:202:LYS:N	1:1:203:PRO:CD	2.84	0.41
3:3:321:THR:HG22	3:3:322:TRP:H	1.85	0.41
3:3:329:LEU:HD21	3:3:644:LEU:HD12	2.01	0.41
4:4:105:LEU:HD13	4:4:309:ILE:CD1	2.44	0.41
4:4:279:ARG:O	4:4:283:MET:HG3	2.20	0.41
2:B:15:PHE:HE1	2:B:23:ARG:HB3	1.85	0.41
3:C:54:LEU:HD11	3:C:88:ALA:HB3	2.02	0.41
3:C:188:VAL:CG2	3:C:189:ARG:N	2.83	0.41
3:C:430:THR:HA	3:C:431:PRO:HD2	1.83	0.41
4:D:62:LEU:HD12	4:D:404:MET:HB2	2.02	0.41
4:D:158:ASP:OD1	7:G:34:LYS:HE3	2.21	0.41
4:D:389:GLN:HG3	4:D:391:PRO:HD2	2.02	0.41
5:E:134:LYS:HD3	5:E:137:THR:OG1	2.20	0.41
6:F:170:LEU:HA	6:F:171:PRO:HD2	1.82	0.41
1:1:427:GLU:OE2	1:1:429:ARG:HD3	2.20	0.41
3:3:409:LEU:HA	3:3:409:LEU:HD23	1.80	0.41
3:3:434:ASP:C	3:3:436:GLN:H	2.29	0.41
4:4:318:GLU:OE2	8:7:75:ARG:NH2	2.54	0.41
6:6:143:ARG:HG2	6:6:145:GLU:OE1	2.20	0.41
7:9:44:THR:OG1	7:9:52:LYS:HD2	2.21	0.41
3:C:243:ARG:HD3	3:C:243:ARG:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:507:LEU:HB2	3:C:511:VAL:HG11	2.03	0.41
3:C:651:ARG:HD2	3:C:651:ARG:C	2.45	0.41
4:D:142:ALA:HB1	4:D:145:PRO:HD2	2.01	0.41
4:D:372:ALA:HA	4:D:373:PRO:HD2	1.91	0.41
6:F:25:GLU:HA	6:F:28:VAL:HG23	2.01	0.41
8:H:59:LEU:HB2	8:H:68:LEU:HB3	2.02	0.41
8:H:70:ALA:HA	8:H:83:GLY:O	2.20	0.41
8:H:74:PRO:HG2	8:H:77:ALA:HB2	2.02	0.41
1:1:89:LEU:O	1:1:130:GLY:HA2	2.21	0.41
3:3:5:LYS:HA	3:3:10:ILE:HA	2.03	0.41
3:3:285:VAL:HG13	3:3:286:ASN:H	1.86	0.41
3:3:672:ALA:O	3:3:673:MET:HB2	2.19	0.41
4:4:196:VAL:O	4:4:200:ARG:HB2	2.21	0.41
4:4:339:LYS:HG2	4:4:360:ASP:HA	2.01	0.41
6:6:163:TYR:HB3	6:6:168:GLU:O	2.21	0.41
7:9:108:CYS:HA	7:9:109:PRO:HD2	1.78	0.41
3:C:621:VAL:HG22	3:C:674:GLY:O	2.21	0.41
3:C:743:VAL:HG12	3:C:744:GLU:N	2.35	0.41
4:D:239:LEU:O	4:D:242:SER:HB3	2.20	0.41
6:F:107:SER:HB2	6:F:133:VAL:HG11	2.03	0.41
6:F:116:GLY:O	7:G:97:ARG:NH1	2.53	0.41
2:2:30:LEU:O	2:2:34:VAL:HG23	2.20	0.41
3:3:259:CYS:CB	3:3:260:PRO:CD	2.98	0.41
3:3:317:LEU:HD22	3:3:317:LEU:H	1.85	0.41
3:3:370:ASP:OD2	3:3:558:TRP:CD1	2.73	0.41
3:3:469:ARG:HD2	3:3:757:HIS:HE1	1.85	0.41
3:3:473:GLU:O	3:3:477:LEU:CD1	2.69	0.41
3:3:497:TRP:O	3:3:528:LYS:HE3	2.20	0.41
5:5:116:ARG:HG3	5:5:129:HIS:CE1	2.55	0.41
6:6:16:ARG:NH1	6:6:17:GLU:OE2	2.54	0.41
1:A:6:LEU:HD12	1:A:240:GLN:CG	2.51	0.41
1:A:94:ASP:OD1	1:A:135:ARG:HB3	2.21	0.41
2:B:26:ALA:O	2:B:30:LEU:HG	2.21	0.41
3:C:594:ALA:O	3:C:598:ALA:HB3	2.21	0.41
4:D:221:VAL:HG23	4:D:272:VAL:CG1	2.50	0.41
6:F:109:GLY:HA2	6:F:142:PRO:HD3	2.02	0.41
1:1:65:ARG:HH11	1:1:65:ARG:HG3	1.85	0.41
1:1:109:ASP:O	1:1:110:VAL:CG1	2.69	0.41
1:1:258:VAL:O	1:1:259:LYS:C	2.64	0.41
2:2:145:VAL:HG12	2:2:150:LEU:HB2	2.03	0.41
3:3:10:ILE:HD12	3:3:10:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:87:VAL:HG23	3:3:87:VAL:O	2.21	0.41
3:3:218:LEU:HD22	3:3:218:LEU:HA	1.72	0.41
3:3:571:VAL:HA	3:3:572:PRO:HD3	1.73	0.41
4:4:379:GLN:O	4:4:382:PRO:HD2	2.21	0.41
5:5:49:LEU:HD23	5:5:111:ALA:HB2	2.02	0.41
5:5:52:ILE:O	5:5:52:ILE:HG23	2.20	0.41
5:5:67:ARG:HB3	5:5:96:GLU:HB2	2.02	0.41
6:6:170:LEU:HA	6:6:171:PRO:HD2	1.82	0.41
7:9:33:LEU:HD22	7:9:37:PHE:CD2	2.55	0.41
7:9:153:THR:HG22	7:9:155:LYS:N	2.36	0.41
7:9:167:ARG:HD2	7:9:169:GLU:OE1	2.21	0.41
8:7:75:ARG:HE	8:7:76:HIS:CE1	2.39	0.41
1:A:102:LYS:HD3	1:A:102:LYS:H	1.86	0.41
1:A:116:GLU:HG2	1:A:228:VAL:HG13	2.03	0.41
1:A:397:ARG:O	1:A:397:ARG:HG2	2.20	0.41
2:B:30:LEU:HB2	2:B:49:ILE:HD13	2.02	0.41
2:B:87:SER:HB2	13:B:182:FES:S2	2.61	0.41
3:C:5:LYS:HB2	3:C:10:ILE:HG13	2.03	0.41
3:C:29:ASP:OD2	5:E:186:GLY:HA3	2.21	0.41
3:C:258:LEU:HA	3:C:258:LEU:HD23	1.85	0.41
3:C:340:GLU:HA	3:C:340:GLU:OE1	2.21	0.41
3:C:436:GLN:HE21	3:C:436:GLN:HB3	1.62	0.41
3:C:437:ILE:H	3:C:437:ILE:HG13	1.72	0.41
3:C:577:LEU:HA	3:C:580:LYS:HD2	2.03	0.41
3:C:588:SER:C	3:C:589:HIS:ND1	2.79	0.41
3:C:646:GLU:C	3:C:648:LEU:H	2.28	0.41
4:D:64:THR:CG2	6:F:118:PHE:CD1	3.04	0.41
4:D:86:ASP:HB3	4:D:93:HIS:HD2	1.86	0.41
4:D:184:GLU:H	4:D:184:GLU:CD	2.29	0.41
4:D:338:PRO:HG2	5:E:193:ARG:HD3	2.03	0.41
5:E:144:HIS:HA	5:E:145:PRO:HD2	1.71	0.41
6:F:163:TYR:OH	6:F:169:ARG:NH2	2.54	0.41
7:G:100:PHE:N	7:G:100:PHE:CD1	2.89	0.41
7:G:167:ARG:HD2	7:G:169:GLU:OE1	2.21	0.41
1:1:291:ILE:HA	1:1:292:PRO:HD2	1.84	0.41
1:1:337:MET:HE2	1:1:340:ALA:HB3	2.03	0.41
3:3:460:LYS:HD3	3:3:460:LYS:HA	1.88	0.41
4:4:225:PRO:HA	4:4:226:PRO:HD3	1.98	0.41
4:4:289:ILE:O	4:4:290:ILE:C	2.64	0.41
5:5:2:ARG:HB2	5:5:84:ASP:OD2	2.21	0.41
5:5:103:THR:HG21	5:5:128:GLY:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:75:ARG:HE	8:7:76:HIS:CD2	2.38	0.41
1:A:196:ARG:NH2	3:C:203:ILE:O	2.45	0.41
1:A:272:PHE:CD2	1:A:311:MET:HE3	2.55	0.41
2:B:30:LEU:CB	2:B:49:ILE:HD13	2.50	0.41
3:C:2:VAL:HG13	3:C:89:ASP:CA	2.47	0.41
3:C:36:GLU:OE1	3:C:36:GLU:HA	2.21	0.41
3:C:514:ASP:OD1	3:C:516:VAL:HB	2.20	0.41
4:D:43:LEU:HD23	4:D:57:PRO:HA	2.03	0.41
4:D:130:LEU:HG	4:D:283:MET:HE1	2.03	0.41
4:D:366:TYR:CE1	5:E:148:LYS:HE3	2.56	0.41
1:1:141:ALA:O	1:1:145:LEU:HB2	2.21	0.40
1:1:224:LEU:HD23	1:1:224:LEU:HA	1.88	0.40
1:1:436:LEU:HD23	2:2:90:LEU:HA	2.03	0.40
2:2:59:GLU:O	2:2:63:VAL:HG23	2.20	0.40
2:2:112:THR:HG21	2:2:116:LEU:HD23	2.03	0.40
3:3:408:ILE:HG23	3:3:408:ILE:O	2.21	0.40
6:6:96:TRP:HA	6:6:99:MET:HE3	2.04	0.40
6:6:145:GLU:CD	6:6:145:GLU:H	2.28	0.40
7:9:162:VAL:HA	7:9:176:PRO:O	2.21	0.40
3:C:157:PHE:CZ	3:C:159:PHE:HB2	2.56	0.40
3:C:258:LEU:HD11	3:C:703:GLN:NE2	2.36	0.40
3:C:478:LEU:HD12	3:C:520:ARG:CZ	2.51	0.40
4:D:279:ARG:O	4:D:283:MET:HG3	2.21	0.40
4:D:379:GLN:O	4:D:382:PRO:HD2	2.21	0.40
5:E:101:LEU:HA	5:E:102:PRO:HD2	1.84	0.40
6:F:44:ALA:O	6:F:46:CYS:N	2.54	0.40
6:F:163:TYR:H	7:G:152:ARG:NH1	2.20	0.40
1:1:196:ARG:HG2	2:2:63:VAL:HA	2.04	0.40
1:1:402:LEU:HD23	1:1:402:LEU:C	2.46	0.40
3:3:478:LEU:HD12	3:3:520:ARG:CZ	2.52	0.40
3:3:698:MET:CE	3:3:699:TRP:NE1	2.85	0.40
4:4:184:GLU:CD	4:4:184:GLU:H	2.28	0.40
4:4:213:ILE:HG21	4:4:217:ARG:HH11	1.86	0.40
4:4:241:ALA:CB	4:4:278:VAL:HG21	2.51	0.40
5:5:175:THR:O	5:5:175:THR:OG1	2.31	0.40
8:7:68:LEU:HD13	8:7:69:LEU:N	2.36	0.40
1:A:370:LEU:HA	1:A:370:LEU:HD12	1.58	0.40
3:C:116:PRO:HG3	3:C:180:ARG:HG2	2.03	0.40
3:C:689:LYS:HD2	3:C:772:GLU:HG2	2.03	0.40
4:D:213:ILE:HG22	4:D:217:ARG:HG3	2.03	0.40
8:H:17:LEU:HD22	8:H:54:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:390:LEU:HA	1:1:390:LEU:HD23	1.85	0.40
3:3:20:MET:HG3	3:3:82:SER:OG	2.20	0.40
3:3:542:ARG:HH11	3:3:542:ARG:CB	2.27	0.40
3:3:550:LEU:N	3:3:550:LEU:CD1	2.83	0.40
4:4:88:LEU:HD23	4:4:88:LEU:HA	1.95	0.40
7:9:177:THR:C	7:9:179:GLY:N	2.79	0.40
8:7:59:LEU:HB2	8:7:68:LEU:HB3	2.02	0.40
2:B:87:SER:CB	2:B:128:CYS:HB3	2.51	0.40
3:C:53:GLY:C	3:C:55:PRO:CD	2.95	0.40
3:C:216:PHE:HZ	8:H:128:PHE:CD2	2.32	0.40
3:C:375:THR:HG21	3:C:537:PRO:HD2	2.03	0.40
3:C:452:ALA:HA	3:C:453:PRO:HD2	1.82	0.40
4:D:62:LEU:HD12	4:D:404:MET:CB	2.52	0.40
4:D:130:LEU:HD23	4:D:130:LEU:HA	1.92	0.40
4:D:253:PRO:HB2	4:D:258:GLU:CG	2.51	0.40
4:D:390:VAL:H	4:D:391:PRO:CD	2.35	0.40
8:H:78:LYS:HD3	8:H:78:LYS:HA	1.83	0.40
2:2:24:ARG:HG2	2:2:53:VAL:HG11	2.03	0.40
2:2:125:LEU:HA	2:2:125:LEU:HD23	1.87	0.40
3:3:372:GLN:HB2	3:3:570:PHE:CD1	2.57	0.40
3:3:688:ARG:CB	3:3:770:ARG:HD3	2.51	0.40
4:4:200:ARG:HD2	4:4:200:ARG:HA	1.86	0.40
4:4:311:PRO:HD3	4:4:330:HIS:CE1	2.56	0.40
4:4:409:ARG:HG2	4:4:409:ARG:HH11	1.87	0.40
5:5:101:LEU:HA	5:5:102:PRO:HD2	1.84	0.40
8:7:19:TRP:CD1	8:7:112:LYS:HE3	2.56	0.40
8:7:65:GLU:HA	8:7:66:PRO:HD3	1.73	0.40
1:A:29:LEU:HD12	1:A:155:ARG:CZ	2.52	0.40
1:A:386:ASN:O	1:A:387:LEU:C	2.65	0.40
2:B:33:ARG:O	2:B:34:VAL:C	2.63	0.40
3:C:41:PRO:HD2	3:C:437:ILE:O	2.21	0.40
3:C:54:LEU:HD12	3:C:54:LEU:HA	1.79	0.40
1:1:17:LEU:HD12	1:1:251:LEU:HD11	2.03	0.40
1:1:97:GLU:HB2	11:1:441:NAI:C4N	2.27	0.40
1:1:273:ARG:O	1:1:277:TYR:HB2	2.21	0.40
2:2:154:LEU:O	2:2:158:ARG:HB2	2.21	0.40
3:3:735:ALA:O	3:3:775:VAL:HG13	2.22	0.40
4:4:53:LEU:N	4:4:53:LEU:CD2	2.83	0.40
4:4:296:ARG:O	4:4:298:GLU:HG3	2.20	0.40
4:4:333:GLU:OE1	5:5:189:ARG:NH1	2.54	0.40
5:5:75:VAL:HG22	5:5:87:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:107:SER:HB2	6:6:133:VAL:HG11	2.03	0.40
6:6:152:MET:HE2	6:6:152:MET:HB3	1.83	0.40
6:6:163:TYR:HD2	6:6:169:ARG:HA	1.85	0.40
8:7:106:GLY:O	8:7:107:LYS:HG2	2.22	0.40
1:A:196:ARG:HG2	2:B:63:VAL:HA	2.03	0.40
3:C:218:LEU:N	3:C:219:PRO:CD	2.78	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:427:GLU:O	3:3:316:ARG:NH1[2_545]	2.12	0.08

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1	435/438 (99%)	380 (87%)	48 (11%)	7 (2%)	7	30
1	A	435/438 (99%)	379 (87%)	50 (12%)	6 (1%)	9	34
2	2	177/181 (98%)	152 (86%)	21 (12%)	4 (2%)	5	23
2	B	177/181 (98%)	151 (85%)	22 (12%)	4 (2%)	5	23
3	3	748/783 (96%)	624 (83%)	100 (13%)	24 (3%)	3	18
3	C	748/783 (96%)	626 (84%)	98 (13%)	24 (3%)	3	18
4	4	374/409 (91%)	331 (88%)	34 (9%)	9 (2%)	4	22
4	D	374/409 (91%)	332 (89%)	32 (9%)	10 (3%)	4	20
5	5	194/207 (94%)	167 (86%)	23 (12%)	4 (2%)	5	25
5	E	194/207 (94%)	166 (86%)	24 (12%)	4 (2%)	5	25
6	6	140/181 (77%)	114 (81%)	21 (15%)	5 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	140/181 (77%)	113 (81%)	21 (15%)	6 (4%)	2	12
7	9	152/182 (84%)	129 (85%)	22 (14%)	1 (1%)	18	49
7	G	152/182 (84%)	132 (87%)	19 (12%)	1 (1%)	18	49
8	7	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	16	47
8	H	125/129 (97%)	112 (90%)	12 (10%)	1 (1%)	16	47
All	All	4690/5020 (93%)	4019 (86%)	560 (12%)	111 (2%)	4	22

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
2	2	108	PRO
3	3	6	VAL
3	3	117	LEU
3	3	216	PHE
3	3	367	PRO
3	3	509	ALA
4	4	212	PRO
4	4	255	SER
5	5	81	LYS
8	7	87	PRO
1	A	4	PRO
2	B	108	PRO
3	C	6	VAL
3	C	117	LEU
3	C	216	PHE
3	C	367	PRO
3	C	509	ALA
4	D	212	PRO
5	E	81	LYS
8	H	87	PRO
1	1	360	ARG
2	2	86	LEU
2	2	124	CYS
3	3	31	PRO
3	3	32	LEU
3	3	125	GLY
3	3	164	VAL
3	3	263	CYS
3	3	453	PRO

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Mol	Chain	Res	Type
3	3	554	LYS
4	4	51	GLU
4	4	258	GLU
5	5	83	GLY
6	6	45	CYS
7	9	152	ARG
1	A	71	PRO
1	A	360	ARG
2	B	76	GLY
2	B	86	LEU
2	B	124	CYS
3	C	31	PRO
3	C	32	LEU
3	C	125	GLY
3	C	263	CYS
3	C	453	PRO
3	C	554	LYS
3	C	690	GLY
4	D	255	SER
4	D	258	GLU
4	D	389	GLN
5	E	83	GLY
6	F	45	CYS
7	G	152	ARG
1	1	71	PRO
2	2	76	GLY
3	3	28	TYR
3	3	271	SER
3	3	285	VAL
3	3	365	LYS
3	3	374	ARG
3	3	690	GLY
4	4	214	PHE
4	4	389	GLN
6	6	98	GLN
6	6	126	ASN
3	C	28	TYR
3	C	164	VAL
3	C	271	SER
3	C	682	GLU
3	C	730	GLU
4	D	51	GLU

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Mol	Chain	Res	Type
4	D	214	PHE
4	D	268	GLU
6	F	98	GLN
6	F	126	ASN
1	1	313	TYR
3	3	682	GLU
3	3	730	GLU
4	4	268	GLU
4	4	270	GLY
6	6	77	VAL
1	A	313	TYR
3	C	285	VAL
3	C	365	LYS
3	C	374	ARG
3	C	455	ARG
6	F	77	VAL
3	3	203	ILE
3	3	455	ARG
5	5	127	GLU
3	C	203	ILE
4	D	270	GLY
6	F	20	LEU
1	1	311	MET
3	3	124	LYS
4	4	390	VAL
6	6	20	LEU
3	C	124	LYS
3	C	708	ALA
4	D	390	VAL
1	1	202	LYS
5	5	52	ILE
1	A	3	GLY
1	1	3	GLY
1	A	202	LYS
5	E	52	ILE
6	F	19	ILE
3	3	626	PRO
5	E	130	PRO
4	D	237	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	1	355/356 (100%)	316 (89%)	39 (11%)	6	24
1	A	355/356 (100%)	321 (90%)	34 (10%)	8	30
2	2	150/152 (99%)	129 (86%)	21 (14%)	3	15
2	B	150/152 (99%)	129 (86%)	21 (14%)	3	15
3	3	607/628 (97%)	553 (91%)	54 (9%)	9	33
3	C	607/628 (97%)	553 (91%)	54 (9%)	9	33
4	4	326/355 (92%)	287 (88%)	39 (12%)	5	21
4	D	326/355 (92%)	289 (89%)	37 (11%)	5	23
5	5	167/175 (95%)	151 (90%)	16 (10%)	8	30
5	E	167/175 (95%)	152 (91%)	15 (9%)	9	33
6	6	117/149 (78%)	104 (89%)	13 (11%)	6	24
6	F	117/149 (78%)	104 (89%)	13 (11%)	6	24
7	9	126/150 (84%)	110 (87%)	16 (13%)	4	18
7	G	126/150 (84%)	111 (88%)	15 (12%)	5	21
8	7	104/106 (98%)	99 (95%)	5 (5%)	23	54
8	H	104/106 (98%)	99 (95%)	5 (5%)	23	54
All	All	3904/4142 (94%)	3507 (90%)	397 (10%)	7	28

All (397) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	6	LEU
1	1	9	LEU
1	1	10	ASP
1	1	16	THR
1	1	29	LEU
1	1	49	THR
1	1	96	SER
1	1	102	LYS

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Mol	Chain	Res	Type
1	1	104	ARG
1	1	114	LEU
1	1	128	THR
1	1	134	VAL
1	1	144	ARG
1	1	145	LEU
1	1	147	GLN
1	1	155	ARG
1	1	171	LEU
1	1	201	LEU
1	1	228	VAL
1	1	243	THR
1	1	253	GLN
1	1	255	SER
1	1	270	THR
1	1	287	ILE
1	1	290	ILE
1	1	323	LEU
1	1	329	ILE
1	1	337	MET
1	1	342	TRP
1	1	363	VAL
1	1	368	VAL
1	1	370	LEU
1	1	374	ILE
1	1	397	ARG
1	1	398	SER
1	1	414	LEU
1	1	419	ASP
1	1	431	VAL
1	1	437	TRP
2	2	5	ASP
2	2	7	LYS
2	2	14	THR
2	2	33	ARG
2	2	35	GLN
2	2	46	ILE
2	2	56	THR
2	2	80	LEU
2	2	85	THR
2	2	106	ILE
2	2	110	GLU

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Mol	Chain	Res	Type
2	2	114	ASP
2	2	119	VAL
2	2	128	CYS
2	2	150	LEU
2	2	153	LEU
2	2	163	LEU
2	2	172	CYS
2	2	176	VAL
2	2	178	GLU
2	2	179	VAL
3	3	20	MET
3	3	32	LEU
3	3	42	ILE
3	3	46	ARG
3	3	54	LEU
3	3	101	ARG
3	3	107	MET
3	3	117	LEU
3	3	124	LYS
3	3	133	ARG
3	3	142	LYS
3	3	156	ARG
3	3	188	VAL
3	3	192	GLU
3	3	207	VAL
3	3	209	THR
3	3	218	LEU
3	3	232	VAL
3	3	261	VAL
3	3	265	ILE
3	3	275	LEU
3	3	282	VAL
3	3	284	GLU
3	3	290	ILE
3	3	303	GLN
3	3	305	ARG
3	3	317	LEU
3	3	337	ARG
3	3	381	LEU
3	3	408	ILE
3	3	417	VAL
3	3	440	ARG

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Mol	Chain	Res	Type
3	3	450	LEU
3	3	460	LYS
3	3	464	ILE
3	3	473	GLU
3	3	492	LYS
3	3	507	LEU
3	3	512	LEU
3	3	515	THR
3	3	542	ARG
3	3	550	LEU
3	3	585	MET
3	3	617	LEU
3	3	655	ARG
3	3	676	LEU
3	3	683	LEU
3	3	684	ARG
3	3	716	LEU
3	3	747	VAL
3	3	761	SER
3	3	771	VAL
3	3	776	LEU
3	3	777	VAL
4	4	41	LEU
4	4	44	MET
4	4	59	ILE
4	4	74	THR
4	4	76	LEU
4	4	79	ILE
4	4	99	LEU
4	4	105	LEU
4	4	109	VAL
4	4	116	ILE
4	4	120	LEU
4	4	123	LEU
4	4	138	LEU
4	4	152	GLU
4	4	156	ILE
4	4	163	VAL
4	4	166	GLN
4	4	168	PHE
4	4	170	HIS
4	4	182	LEU

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Mol	Chain	Res	Type
4	4	193	LEU
4	4	194	LEU
4	4	199	HIS
4	4	201	ILE
4	4	221	VAL
4	4	234	LEU
4	4	239	LEU
4	4	262	PHE
4	4	272	VAL
4	4	294	LEU
4	4	314	ARG
4	4	316	LEU
4	4	319	THR
4	4	363	SER
4	4	367	ARG
4	4	371	ARG
4	4	385	CYS
4	4	396	ILE
4	4	407	VAL
5	5	1	MET
5	5	5	ARG
5	5	25	LEU
5	5	27	VAL
5	5	32	GLU
5	5	47	ASN
5	5	84	ASP
5	5	90	VAL
5	5	91	ARG
5	5	100	ARG
5	5	103	THR
5	5	135	ILE
5	5	146	LEU
5	5	154	GLU
5	5	157	THR
5	5	175	THR
6	6	19	ILE
6	6	20	LEU
6	6	32	ARG
6	6	40	THR
6	6	45	CYS
6	6	78	MET
6	6	83	ARG

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Mol	Chain	Res	Type
6	6	84	LEU
6	6	121	TYR
6	6	131	VAL
6	6	147	LEU
6	6	153	GLN
6	6	158	VAL
7	9	26	TYR
7	9	33	LEU
7	9	36	ARG
7	9	42	VAL
7	9	70	VAL
7	9	97	ARG
7	9	99	ILE
7	9	130	VAL
7	9	133	LYS
7	9	137	LEU
7	9	138	VAL
7	9	139	ASP
7	9	157	VAL
7	9	158	LYS
7	9	159	VAL
7	9	163	VAL
8	7	43	ARG
8	7	63	LEU
8	7	82	ILE
8	7	93	LEU
8	7	120	ASP
1	A	6	LEU
1	A	9	LEU
1	A	10	ASP
1	A	16	THR
1	A	29	LEU
1	A	49	THR
1	A	102	LYS
1	A	104	ARG
1	A	114	LEU
1	A	128	THR
1	A	145	LEU
1	A	147	GLN
1	A	171	LEU
1	A	201	LEU
1	A	243	THR

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Mol	Chain	Res	Type
1	A	253	GLN
1	A	270	THR
1	A	287	ILE
1	A	290	ILE
1	A	323	LEU
1	A	329	ILE
1	A	337	MET
1	A	342	TRP
1	A	357	THR
1	A	363	VAL
1	A	368	VAL
1	A	370	LEU
1	A	374	ILE
1	A	397	ARG
1	A	398	SER
1	A	414	LEU
1	A	419	ASP
1	A	431	VAL
1	A	437	TRP
2	B	5	ASP
2	B	7	LYS
2	B	14	THR
2	B	35	GLN
2	B	46	ILE
2	B	49	ILE
2	B	56	THR
2	B	80	LEU
2	B	85	THR
2	B	106	ILE
2	B	110	GLU
2	B	114	ASP
2	B	118	SER
2	B	119	VAL
2	B	150	LEU
2	B	153	LEU
2	B	163	LEU
2	B	172	CYS
2	B	176	VAL
2	B	178	GLU
2	B	179	VAL
3	C	20	MET
3	C	32	LEU

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Mol	Chain	Res	Type
3	C	42	ILE
3	C	46	ARG
3	C	47	MET
3	C	54	LEU
3	C	107	MET
3	C	117	LEU
3	C	124	LYS
3	C	133	ARG
3	C	142	LYS
3	C	156	ARG
3	C	192	GLU
3	C	207	VAL
3	C	209	THR
3	C	218	LEU
3	C	232	VAL
3	C	261	VAL
3	C	265	ILE
3	C	275	LEU
3	C	282	VAL
3	C	284	GLU
3	C	290	ILE
3	C	303	GLN
3	C	305	ARG
3	C	317	LEU
3	C	337	ARG
3	C	381	LEU
3	C	408	ILE
3	C	417	VAL
3	C	440	ARG
3	C	450	LEU
3	C	460	LYS
3	C	464	ILE
3	C	473	GLU
3	C	492	LYS
3	C	507	LEU
3	C	512	LEU
3	C	515	THR
3	C	542	ARG
3	C	550	LEU
3	C	585	MET
3	C	617	LEU
3	C	655	ARG

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Mol	Chain	Res	Type
3	C	676	LEU
3	C	683	LEU
3	C	684	ARG
3	C	716	LEU
3	C	734	VAL
3	C	747	VAL
3	C	761	SER
3	C	771	VAL
3	C	776	LEU
3	C	777	VAL
4	D	41	LEU
4	D	44	MET
4	D	59	ILE
4	D	74	THR
4	D	76	LEU
4	D	79	ILE
4	D	99	LEU
4	D	105	LEU
4	D	116	ILE
4	D	120	LEU
4	D	123	LEU
4	D	138	LEU
4	D	152	GLU
4	D	156	ILE
4	D	163	VAL
4	D	166	GLN
4	D	168	PHE
4	D	170	HIS
4	D	182	LEU
4	D	193	LEU
4	D	194	LEU
4	D	199	HIS
4	D	201	ILE
4	D	221	VAL
4	D	234	LEU
4	D	239	LEU
4	D	262	PHE
4	D	272	VAL
4	D	294	LEU
4	D	314	ARG
4	D	316	LEU
4	D	319	THR

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Mol	Chain	Res	Type
4	D	367	ARG
4	D	371	ARG
4	D	385	CYS
4	D	396	ILE
4	D	407	VAL
5	E	1	MET
5	E	5	ARG
5	E	25	LEU
5	E	27	VAL
5	E	32	GLU
5	E	47	ASN
5	E	84	ASP
5	E	90	VAL
5	E	91	ARG
5	E	100	ARG
5	E	103	THR
5	E	135	ILE
5	E	146	LEU
5	E	154	GLU
5	E	175	THR
6	F	19	ILE
6	F	20	LEU
6	F	32	ARG
6	F	40	THR
6	F	45	CYS
6	F	78	MET
6	F	83	ARG
6	F	84	LEU
6	F	121	TYR
6	F	131	VAL
6	F	147	LEU
6	F	153	GLN
6	F	158	VAL
7	G	26	TYR
7	G	33	LEU
7	G	36	ARG
7	G	42	VAL
7	G	70	VAL
7	G	99	ILE
7	G	130	VAL
7	G	133	LYS
7	G	137	LEU

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Mol	Chain	Res	Type
7	G	138	VAL
7	G	139	ASP
7	G	157	VAL
7	G	158	LYS
7	G	159	VAL
7	G	163	VAL
8	H	43	ARG
8	H	63	LEU
8	H	82	ILE
8	H	93	LEU
8	H	120	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	87	HIS
1	1	161	ASN
1	1	219	ASN
1	1	220	ASN
1	1	240	GLN
1	1	369	ASN
1	1	416	HIS
2	2	137	ASN
3	3	303	GLN
3	3	613	HIS
3	3	757	HIS
4	4	93	HIS
4	4	171	ASN
4	4	199	HIS
4	4	292	GLN
4	4	327	HIS
4	4	330	HIS
5	5	47	ASN
6	6	161	GLN
7	9	94	ASN
8	7	92	HIS
1	A	87	HIS
1	A	161	ASN
1	A	219	ASN
1	A	220	ASN
1	A	240	GLN
1	A	369	ASN

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Mol	Chain	Res	Type
1	A	416	HIS
2	B	137	ASN
3	C	38	HIS
3	C	303	GLN
3	C	613	HIS
3	C	757	HIS
4	D	93	HIS
4	D	199	HIS
4	D	292	GLN
4	D	327	HIS
4	D	330	HIS
5	E	47	ASN
6	F	161	GLN
7	G	94	ASN
8	H	92	HIS

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 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 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
13	FES	C	787	3	0,4,4	-	-	-		
13	FES	B	182	2	0,4,4	-	-	-		
9	SF4	F	182	6	0,12,12	-	-	-		
9	SF4	3	784	3	0,12,12	-	-	-		
9	SF4	G	184	7	0,12,12	-	-	-		
9	SF4	6	182	6	0,12,12	-	-	-		
9	SF4	C	786	3	0,12,12	-	-	-		
13	FES	2	182	2	0,4,4	-	-	-		
9	SF4	3	786	3	0,12,12	-	-	-		
10	FMN	A	440	-	33,33,33	1.10	3 (9%)	48,50,50	1.54	10 (20%)
9	SF4	C	785	3	0,12,12	-	-	-		
13	FES	3	787	3	0,4,4	-	-	-		
11	NAI	1	441	-	47,48,48	3.97	32 (68%)	64,73,73	1.76	16 (25%)
9	SF4	A	439	1	0,12,12	-	-	-		
11	NAI	A	441	-	47,48,48	4.08	31 (65%)	64,73,73	1.80	16 (25%)
9	SF4	3	785	3	0,12,12	-	-	-		
9	SF4	C	784	3	0,12,12	-	-	-		
9	SF4	9	184	7	0,12,12	-	-	-		
9	SF4	9	183	7	0,12,12	-	-	-		
10	FMN	1	440	-	33,33,33	1.24	2 (6%)	48,50,50	1.88	12 (25%)
9	SF4	G	183	7	0,12,12	-	-	-		
9	SF4	1	439	1	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
13	FES	C	787	3	-	-	0/1/1/1
13	FES	B	182	2	-	-	0/1/1/1
9	SF4	F	182	6	-	-	0/6/5/5
9	SF4	3	784	3	-	-	0/6/5/5
9	SF4	G	184	7	-	-	0/6/5/5
9	SF4	6	182	6	-	-	0/6/5/5
9	SF4	C	786	3	-	-	0/6/5/5
13	FES	2	182	2	-	-	0/1/1/1
9	SF4	3	786	3	-	-	0/6/5/5
10	FMN	A	440	-	-	8/18/18/18	0/3/3/3
9	SF4	C	785	3	-	-	0/6/5/5
13	FES	3	787	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAI	1	441	-	-	7/29/72/72	0/5/5/5
9	SF4	A	439	1	-	-	0/6/5/5
11	NAI	A	441	-	-	10/29/72/72	0/5/5/5
9	SF4	3	785	3	-	-	0/6/5/5
9	SF4	C	784	3	-	-	0/6/5/5
9	SF4	9	184	7	-	-	0/6/5/5
9	SF4	9	183	7	-	-	0/6/5/5
10	FMN	1	440	-	-	6/18/18/18	0/3/3/3
9	SF4	G	183	7	-	-	0/6/5/5
9	SF4	1	439	1	-	-	0/6/5/5

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	441	NAI	C2A-N1A	11.91	1.55	1.33
11	A	441	NAI	C2A-N1A	11.78	1.54	1.33
11	A	441	NAI	PA-O3	8.55	1.68	1.59
11	A	441	NAI	C5A-N7A	7.92	1.53	1.39
11	1	441	NAI	PA-O3	7.67	1.67	1.59
11	A	441	NAI	PN-O3	7.56	1.67	1.59
11	A	441	NAI	C8A-N9A	7.46	1.50	1.37
11	1	441	NAI	C5A-N7A	7.39	1.52	1.39
11	1	441	NAI	C8A-N9A	7.29	1.49	1.37
11	1	441	NAI	PN-O3	6.36	1.66	1.59
11	A	441	NAI	C3D-C4D	-6.34	1.36	1.53
11	1	441	NAI	C3D-C4D	-5.82	1.38	1.53
11	1	441	NAI	C2B-C3B	-5.67	1.38	1.53
11	A	441	NAI	C6A-N6A	5.66	1.48	1.34
11	A	441	NAI	C2B-C3B	-5.44	1.38	1.53
11	A	441	NAI	C5A-C6A	5.36	1.55	1.41
11	1	441	NAI	C3B-C4B	-5.29	1.39	1.53
11	A	441	NAI	C2D-C1D	-5.22	1.37	1.53
11	1	441	NAI	C6A-N6A	5.18	1.47	1.34
11	1	441	NAI	C2D-C1D	-5.16	1.37	1.53
11	1	441	NAI	C5A-C6A	5.03	1.55	1.41
11	A	441	NAI	C4A-N9A	4.83	1.47	1.37
11	A	441	NAI	C3B-C4B	-4.80	1.40	1.53
11	1	441	NAI	C2B-C1B	-4.66	1.38	1.53
11	A	441	NAI	C2B-C1B	-4.58	1.39	1.53
11	1	441	NAI	C6A-N1A	-4.30	1.23	1.35
11	1	441	NAI	C7N-N7N	4.16	1.45	1.33
11	1	441	NAI	C4A-N9A	4.15	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	441	NAI	C7N-C3N	3.91	1.57	1.48
11	A	441	NAI	C6A-N1A	-3.87	1.25	1.35
10	1	440	FMN	C4A-N5	3.77	1.38	1.30
11	A	441	NAI	C7N-N7N	3.76	1.44	1.33
11	A	441	NAI	C7N-C3N	3.75	1.56	1.48
10	A	440	FMN	C4A-N5	3.63	1.38	1.30
11	1	441	NAI	C4N-C5N	3.56	1.58	1.49
11	A	441	NAI	C2D-C3D	-3.47	1.44	1.53
11	A	441	NAI	C4A-N3A	3.32	1.40	1.34
11	1	441	NAI	C2D-C3D	-3.29	1.44	1.53
11	1	441	NAI	O4D-C4D	-3.24	1.37	1.45
11	A	441	NAI	C4N-C5N	3.24	1.57	1.49
11	1	441	NAI	O4B-C4B	-3.00	1.38	1.45
10	1	440	FMN	C9A-N10	-2.91	1.36	1.41
11	A	441	NAI	O4D-C4D	-2.89	1.38	1.45
11	1	441	NAI	C1D-N1N	-2.74	1.38	1.46
11	A	441	NAI	PN-O5D	2.66	1.69	1.59
10	A	440	FMN	C10-N1	2.59	1.38	1.33
11	A	441	NAI	O4B-C1B	-2.57	1.36	1.42
11	1	441	NAI	O4D-C1D	-2.52	1.36	1.42
11	A	441	NAI	C1D-N1N	-2.49	1.39	1.46
11	1	441	NAI	PN-O5D	2.48	1.69	1.59
11	A	441	NAI	PN-O1N	2.46	1.66	1.55
11	1	441	NAI	O4B-C1B	-2.43	1.36	1.42
11	1	441	NAI	O3B-C3B	-2.41	1.37	1.43
11	A	441	NAI	C4N-C3N	2.37	1.54	1.50
11	1	441	NAI	C4A-N3A	2.37	1.38	1.34
11	A	441	NAI	O4B-C4B	-2.29	1.39	1.45
11	A	441	NAI	C8A-N7A	2.25	1.36	1.31
11	A	441	NAI	O4D-C1D	-2.24	1.36	1.42
11	1	441	NAI	PA-O2A	2.21	1.65	1.55
11	A	441	NAI	O2B-C2B	-2.20	1.37	1.43
11	1	441	NAI	C4N-C3N	2.17	1.54	1.50
11	1	441	NAI	PN-O1N	2.14	1.65	1.55
11	1	441	NAI	O2B-C2B	-2.13	1.37	1.43
10	A	440	FMN	C4A-C10	-2.13	1.37	1.44
11	A	441	NAI	O7N-C7N	-2.06	1.19	1.24
11	A	441	NAI	PA-O2A	2.06	1.64	1.55
11	1	441	NAI	PN-O2N	-2.05	1.43	1.50
11	1	441	NAI	C8A-N7A	2.03	1.35	1.31

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	441	NAI	N3A-C2A-N1A	-5.55	120.18	128.58
10	1	440	FMN	O2'-C2'-C3'	5.24	121.52	109.25
10	1	440	FMN	C5'-C4'-C3'	-5.23	102.34	112.22
11	1	441	NAI	N3A-C2A-N1A	-4.89	121.18	128.58
11	A	441	NAI	C5A-C4A-N3A	-4.83	120.06	126.72
10	A	440	FMN	C5'-C4'-C3'	-4.58	103.58	112.22
11	1	441	NAI	C5A-C4A-N3A	-4.32	120.77	126.72
10	1	440	FMN	C4'-C3'-C2'	3.86	120.00	113.57
11	1	441	NAI	C4D-O4D-C1D	-3.85	100.97	109.47
11	A	441	NAI	O4D-C1D-N1N	3.66	115.07	108.08
11	A	441	NAI	N9A-C8A-N7A	-3.59	108.85	113.94
11	A	441	NAI	C2A-N3A-C4A	3.56	120.52	111.83
10	A	440	FMN	C4'-C3'-C2'	3.55	119.48	113.57
10	1	440	FMN	C1'-C2'-C3'	-3.51	100.15	109.66
11	1	441	NAI	N9A-C8A-N7A	-3.46	109.03	113.94
10	A	440	FMN	O4-C4-C4A	-3.22	118.04	126.53
11	1	441	NAI	C5A-C4A-N9A	3.15	109.25	105.81
10	1	440	FMN	O4-C4-C4A	-3.13	118.27	126.53
11	1	441	NAI	O4D-C1D-N1N	3.11	114.01	108.08
11	A	441	NAI	C5A-N7A-C8A	3.09	108.30	103.45
11	1	441	NAI	C2A-N3A-C4A	3.06	119.29	111.83
10	1	440	FMN	C4-N3-C2	-3.03	120.26	125.64
10	A	440	FMN	C4-N3-C2	-2.92	120.46	125.64
11	1	441	NAI	C5A-N7A-C8A	2.92	108.03	103.45
11	1	441	NAI	O5B-C5B-C4B	2.89	118.84	108.99
10	A	440	FMN	O2'-C2'-C3'	2.85	115.93	109.25
11	1	441	NAI	C3N-C7N-N7N	2.83	122.70	117.67
10	A	440	FMN	C4A-C4-N3	2.80	120.37	113.25
11	A	441	NAI	C3B-C2B-C1B	2.70	106.58	101.46
11	A	441	NAI	C5A-C4A-N9A	2.62	108.67	105.81
11	A	441	NAI	C3D-C2D-C1D	2.60	106.39	101.46
10	1	440	FMN	C10-C4A-N5	-2.53	119.65	124.81
11	A	441	NAI	O7N-C7N-N7N	-2.52	117.25	122.89
11	1	441	NAI	O1N-PN-O3	2.50	114.04	107.27
11	1	441	NAI	C4A-C5A-N7A	-2.49	107.73	110.58
11	A	441	NAI	C4A-C5A-N7A	-2.45	107.78	110.58
11	A	441	NAI	C3N-C7N-N7N	2.43	121.98	117.67
11	A	441	NAI	N3A-C4A-N9A	2.41	131.27	127.17
10	1	440	FMN	O2-C2-N1	-2.37	117.87	121.80
10	A	440	FMN	C9A-C5A-N5	-2.36	119.95	122.45
11	A	441	NAI	O2A-PA-O3	2.34	113.59	107.27
11	1	441	NAI	O2A-PA-O3	2.33	113.57	107.27
10	A	440	FMN	C1'-C2'-C3'	-2.30	103.41	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	441	NAI	C4D-O4D-C1D	-2.27	104.45	109.47
10	1	440	FMN	C4A-C4-N3	2.27	119.02	113.25
10	A	440	FMN	O4'-C4'-C5'	2.23	114.89	109.99
11	A	441	NAI	O5B-C5B-C4B	2.18	116.41	108.99
11	1	441	NAI	O7N-C7N-N7N	-2.16	118.06	122.89
10	1	440	FMN	C4A-C10-N10	2.14	119.55	116.48
11	1	441	NAI	C6A-C5A-C4A	2.12	120.07	117.18
10	1	440	FMN	O5'-C5'-C4'	2.09	114.95	109.36
10	A	440	FMN	O5'-C5'-C4'	2.06	114.87	109.36
10	1	440	FMN	C4-C4A-N5	2.06	121.05	118.21
11	1	441	NAI	C2B-C1B-N9A	2.03	118.34	113.30

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1	440	FMN	N10-C1'-C2'-O2'
10	1	440	FMN	N10-C1'-C2'-C3'
10	1	440	FMN	C1'-C2'-C3'-O3'
10	1	440	FMN	C1'-C2'-C3'-C4'
10	A	440	FMN	N10-C1'-C2'-O2'
10	A	440	FMN	N10-C1'-C2'-C3'
10	A	440	FMN	C1'-C2'-C3'-O3'
10	A	440	FMN	C1'-C2'-C3'-C4'
10	A	440	FMN	O2'-C2'-C3'-O3'
10	A	440	FMN	O2'-C2'-C3'-C4'
10	A	440	FMN	C3'-C4'-C5'-O5'
10	A	440	FMN	O4'-C4'-C5'-O5'
11	1	441	NAI	O4B-C4B-C5B-O5B
11	1	441	NAI	C5D-O5D-PN-O3
11	1	441	NAI	C5D-O5D-PN-O2N
11	A	441	NAI	O4B-C4B-C5B-O5B
10	1	440	FMN	O2'-C2'-C3'-C4'
11	1	441	NAI	C3B-C4B-C5B-O5B
11	A	441	NAI	C3B-C4B-C5B-O5B
10	1	440	FMN	O2'-C2'-C3'-O3'
11	1	441	NAI	PN-O3-PA-O1A
11	A	441	NAI	PN-O3-PA-O1A
11	A	441	NAI	C3D-C4D-C5D-O5D
11	A	441	NAI	O4D-C4D-C5D-O5D
11	A	441	NAI	C5D-O5D-PN-O3
11	A	441	NAI	C5D-O5D-PN-O1N

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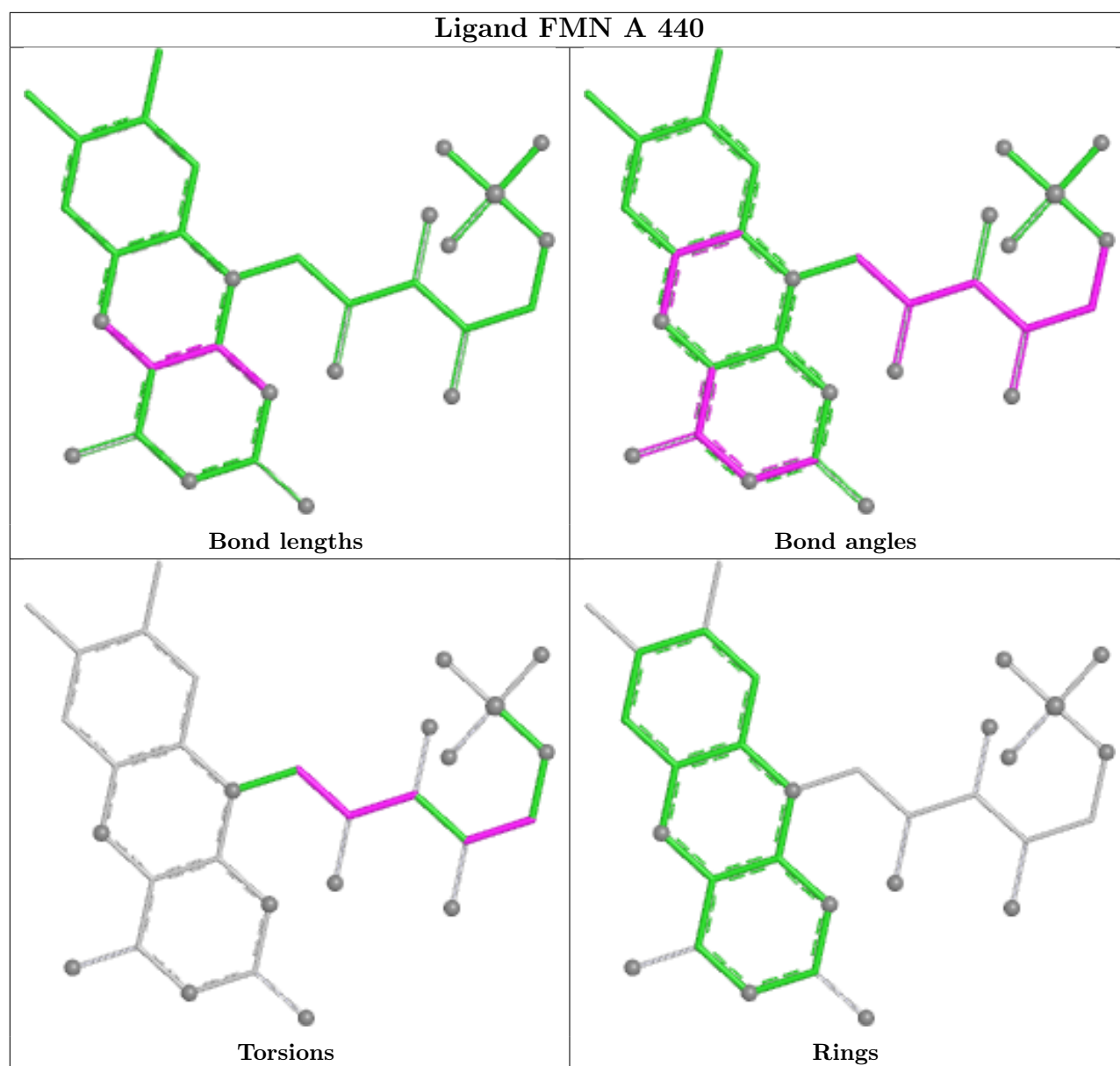
Mol	Chain	Res	Type	Atoms
11	A	441	NAI	C5D-O5D-PN-O2N
11	1	441	NAI	O4D-C1D-N1N-C2N
11	A	441	NAI	O4D-C1D-N1N-C2N
11	1	441	NAI	C2N-C3N-C7N-N7N
11	A	441	NAI	C2N-C3N-C7N-N7N

There are no ring outliers.

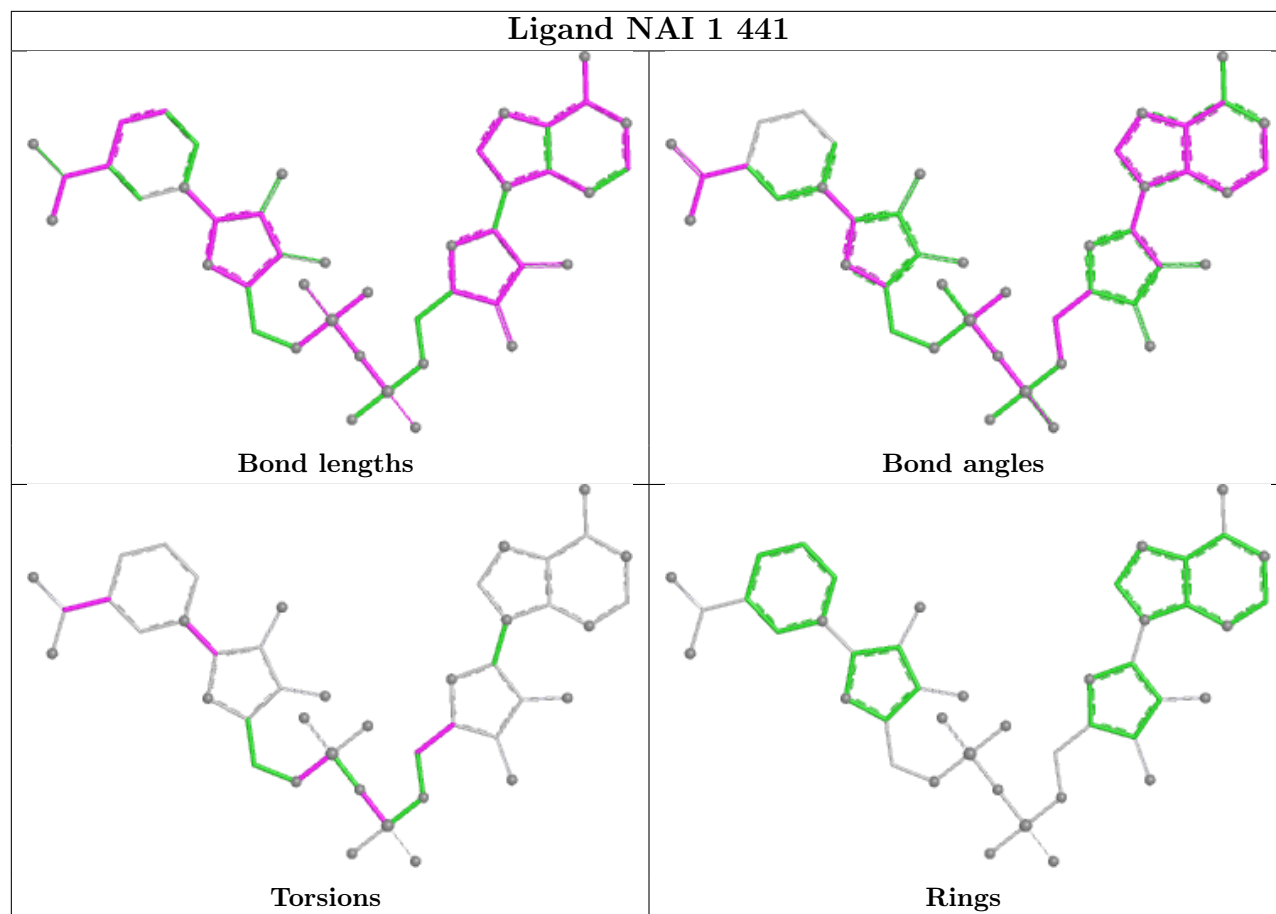
16 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	787	FES	1	0
13	B	182	FES	1	0
9	F	182	SF4	2	0
9	3	784	SF4	1	0
9	6	182	SF4	1	0
9	C	786	SF4	1	0
9	3	786	SF4	1	0
9	C	785	SF4	1	0
13	3	787	FES	1	0
11	1	441	NAI	4	0
11	A	441	NAI	7	0
9	3	785	SF4	1	0
9	C	784	SF4	1	0
9	9	183	SF4	2	0
10	1	440	FMN	6	0
9	G	183	SF4	1	0

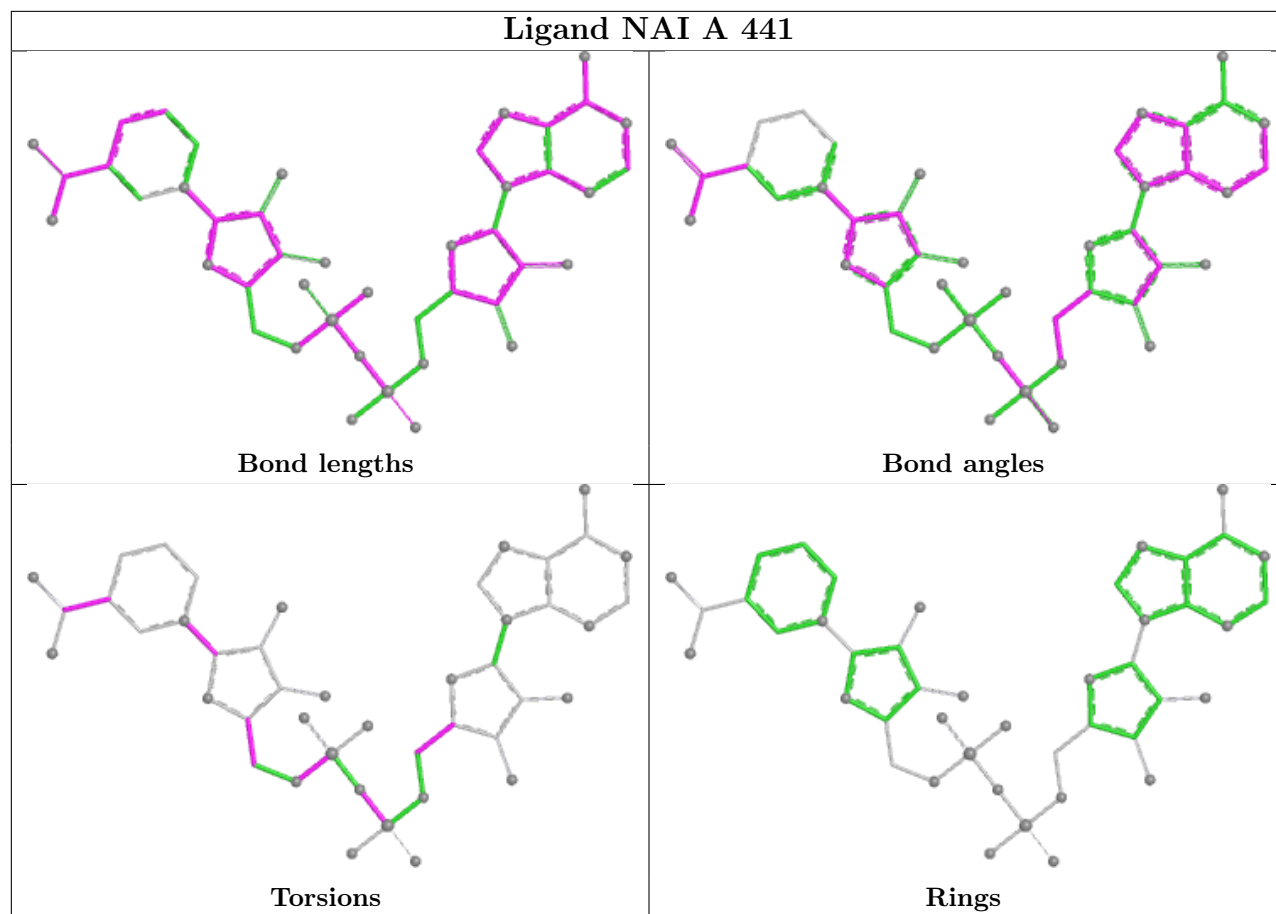
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

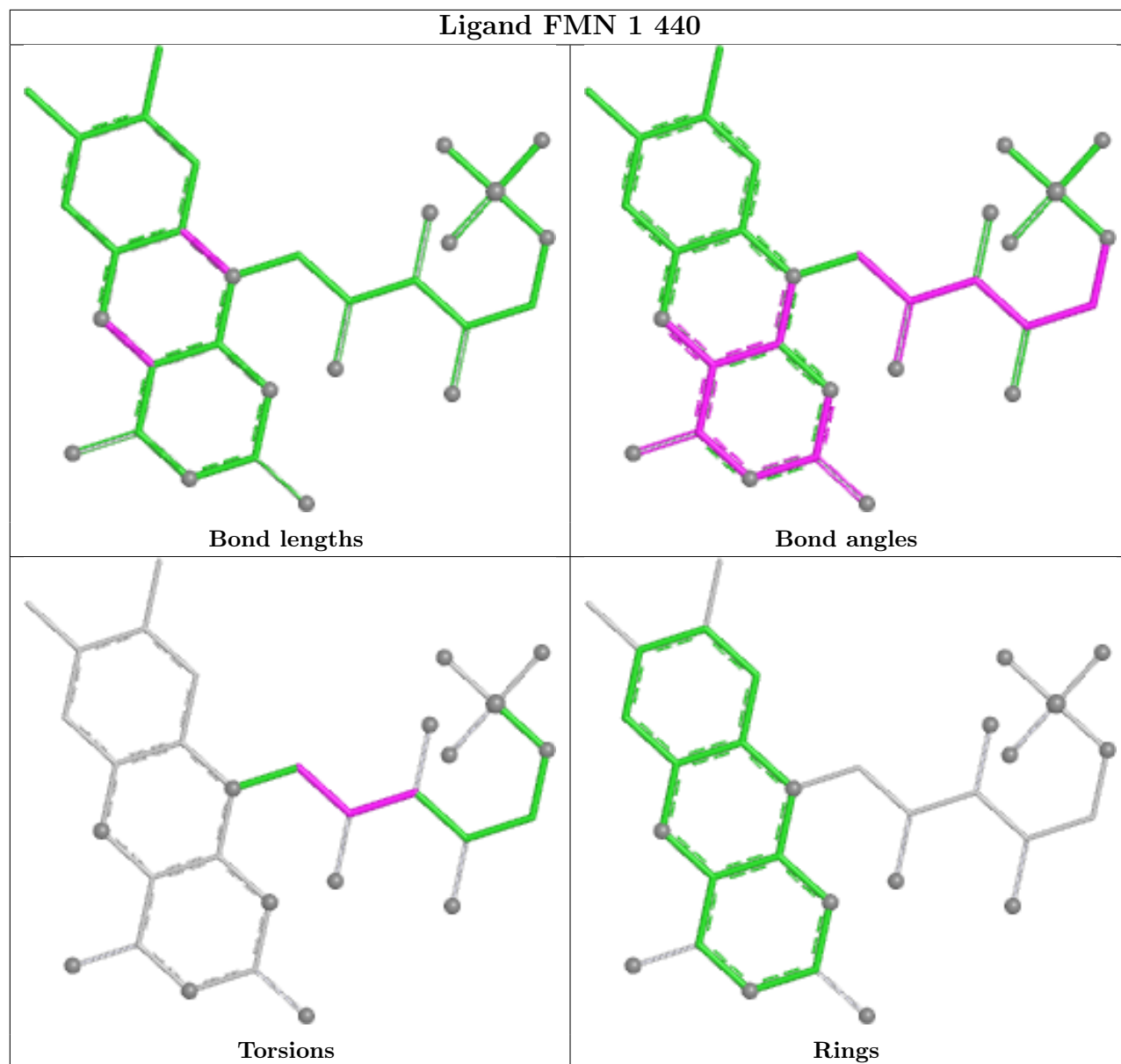


Ligand NAI 1 441



Ligand NAI A 441





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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	437/438 (99%)	-0.22	1 (0%) 91 83	28, 49, 71, 111	0
1	A	437/438 (99%)	-0.28	1 (0%) 91 83	29, 49, 72, 111	0
2	2	179/181 (98%)	-0.19	0 100 100	32, 48, 78, 118	0
2	B	179/181 (98%)	-0.25	0 100 100	33, 48, 79, 118	0
3	3	754/783 (96%)	0.21	14 (1%) 66 45	25, 68, 106, 126	0
3	C	754/783 (96%)	0.11	4 (0%) 87 73	26, 69, 107, 127	0
4	4	378/409 (92%)	0.27	14 (3%) 45 25	33, 66, 103, 119	0
4	D	378/409 (92%)	0.08	1 (0%) 90 80	33, 67, 103, 119	0
5	5	196/207 (94%)	0.55	4 (2%) 65 44	34, 66, 102, 116	0
5	E	196/207 (94%)	0.12	2 (1%) 79 61	35, 68, 103, 117	0
6	6	144/181 (79%)	0.38	6 (4%) 40 22	36, 62, 93, 135	0
6	F	144/181 (79%)	0.22	4 (2%) 55 34	37, 63, 93, 135	0
7	9	154/182 (84%)	-0.05	1 (0%) 85 70	30, 48, 86, 120	0
7	G	154/182 (84%)	-0.09	1 (0%) 85 70	31, 48, 86, 120	0
8	7	127/129 (98%)	-0.08	0 100 100	43, 55, 91, 115	0
8	H	127/129 (98%)	-0.13	1 (0%) 82 65	43, 56, 91, 114	0
All	All	4738/5020 (94%)	0.05	54 (1%) 78 59	25, 58, 101, 135	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	4	236	GLY	3.5
6	6	175	ALA	3.4
6	6	76	ASP	3.2
3	3	654	PHE	3.1
3	3	554	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
7	G	179	GLY	2.9
4	4	212	PRO	2.7
5	5	32	GLU	2.7
6	F	56	ALA	2.6
4	D	39	GLY	2.6
5	5	143	GLY	2.6
4	4	144	THR	2.6
6	6	17	GLU	2.6
8	H	3	ALA	2.6
4	4	31	GLY	2.4
6	F	17	GLU	2.4
3	3	140	TYR	2.4
3	3	339	GLU	2.4
3	3	659	GLU	2.3
4	4	216	GLU	2.3
5	E	196	TRP	2.3
1	A	2	THR	2.3
3	3	340	GLU	2.3
4	4	47	LEU	2.3
3	C	650	VAL	2.2
4	4	272	VAL	2.2
6	6	77	VAL	2.2
4	4	49	GLY	2.2
6	F	175	ALA	2.2
7	9	177	THR	2.2
3	3	415	GLU	2.2
6	F	20	LEU	2.1
3	3	314	GLU	2.1
3	3	653	PRO	2.1
3	3	42	ILE	2.1
3	3	382	PHE	2.1
4	4	139	ASP	2.1
6	6	101	ASP	2.1
1	1	2	THR	2.1
3	C	42	ILE	2.1
4	4	218	ALA	2.1
3	3	569	GLY	2.1
6	6	56	ALA	2.1
5	5	196	TRP	2.1
4	4	46	THR	2.1
4	4	40	VAL	2.0
3	C	654	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
4	4	394	VAL	2.0
5	E	51	ASP	2.0
3	3	555	GLY	2.0
3	C	373	GLY	2.0
3	3	655	ARG	2.0
4	4	52	VAL	2.0
5	5	31	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	MG	C	789	1/1	0.88	0.09	44,44,44,44	0
12	MG	A	442	1/1	0.90	0.12	54,54,54,54	0
12	MG	E	208	1/1	0.90	0.14	44,44,44,44	0
12	MG	3	789	1/1	0.91	0.17	42,42,42,42	0
11	NAI	A	441	44/44	0.91	0.10	45,59,68,71	0
10	FMN	A	440	31/31	0.93	0.10	39,44,47,51	0
10	FMN	1	440	31/31	0.93	0.11	34,42,46,48	0
12	MG	2	206	1/1	0.94	0.06	32,32,32,32	0
11	NAI	1	441	44/44	0.94	0.09	39,50,62,65	0
12	MG	4	410	1/1	0.94	0.23	59,59,59,59	0
12	MG	5	208	1/1	0.96	0.13	26,26,26,26	0
12	MG	1	442	1/1	0.97	0.18	40,40,40,40	0
12	MG	3	788	1/1	0.98	0.17	23,23,23,23	0
12	MG	C	788	1/1	0.98	0.19	35,35,35,35	0
14	CA	H	204	1/1	0.98	0.12	32,32,32,32	0
9	SF4	6	182	8/8	0.99	0.04	0,23,42,50	0

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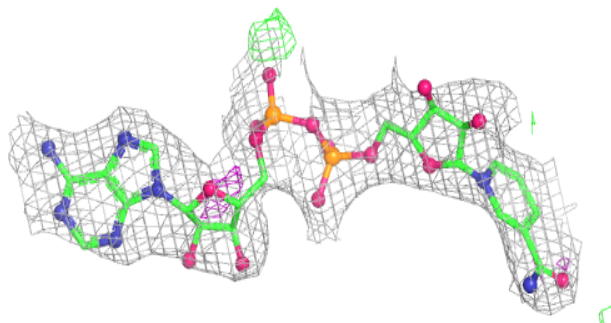
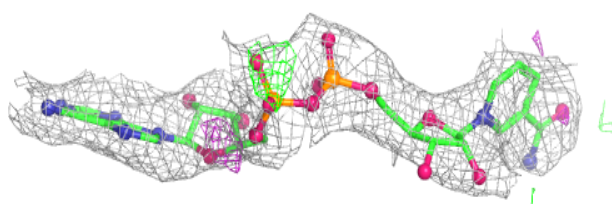
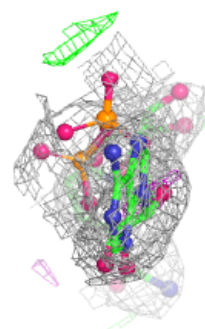
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SF4	9	183	8/8	0.99	0.04	2,19,36,39	0
9	SF4	9	184	8/8	0.99	0.04	8,12,33,34	0
9	SF4	A	439	8/8	0.99	0.04	0,22,31,38	0
9	SF4	C	785	8/8	0.99	0.03	10,13,29,33	0
9	SF4	C	786	8/8	0.99	0.05	19,27,45,47	0
9	SF4	F	182	8/8	0.99	0.05	22,32,48,55	0
9	SF4	G	183	8/8	0.99	0.04	11,15,32,36	0
9	SF4	G	184	8/8	0.99	0.05	13,20,37,39	0
9	SF4	1	439	8/8	0.99	0.04	0,12,24,25	0
9	SF4	3	784	8/8	0.99	0.03	0,9,26,36	0
13	FES	2	182	4/4	0.99	0.05	11,20,27,33	0
13	FES	3	787	4/4	0.99	0.05	9,14,30,34	0
13	FES	B	182	4/4	0.99	0.04	22,22,37,45	0
13	FES	C	787	4/4	0.99	0.05	19,26,32,33	0
14	CA	7	204	1/1	0.99	0.11	36,36,36,36	0
9	SF4	3	786	8/8	0.99	0.04	3,15,43,48	0
9	SF4	C	784	8/8	1.00	0.03	6,11,31,36	0
9	SF4	3	785	8/8	1.00	0.02	0,11,22,22	0

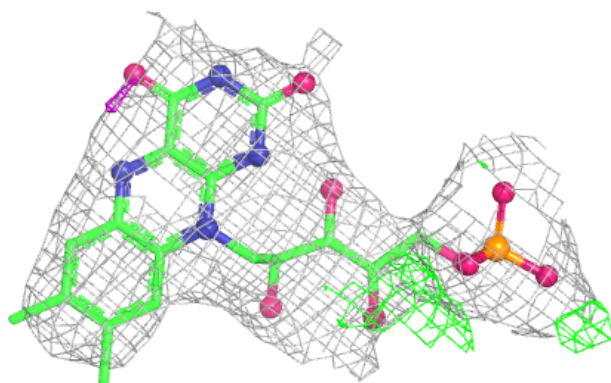
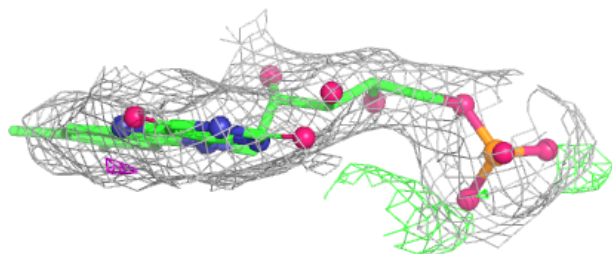
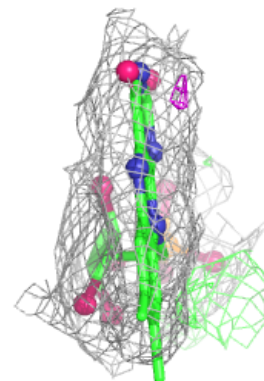
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAI A 441:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

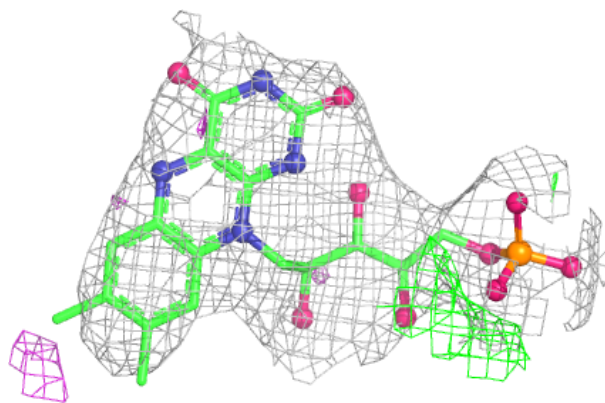
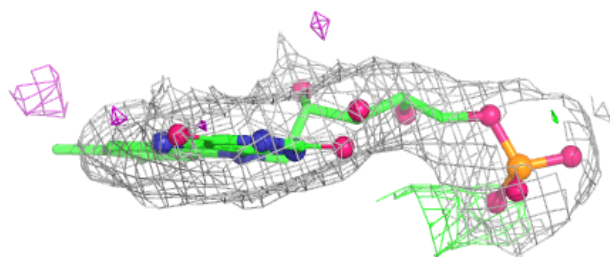
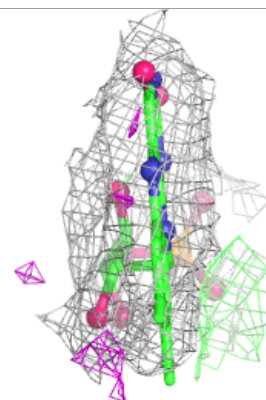
**Electron density around FMN A 440:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

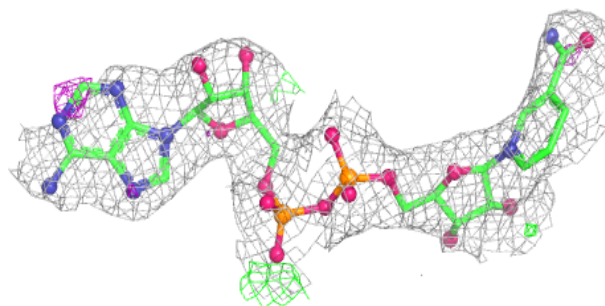
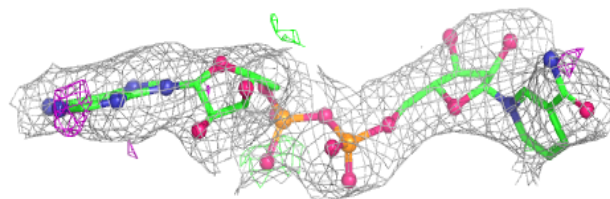
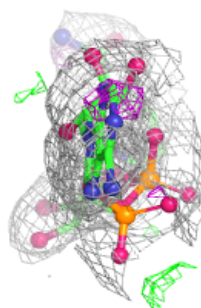


Electron density around FMN 1 440:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAI 1 441:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.