



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 04:38 PM EDT

PDB ID : 9CDN / pdb_00009cdn
EMDB ID : EMD-45479
Title : Respiratory supercomplex I+III2 open state
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-06-25
Resolution : 3.47 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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:

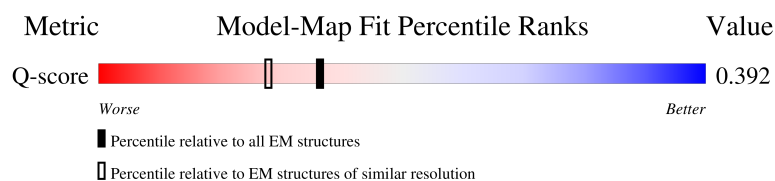
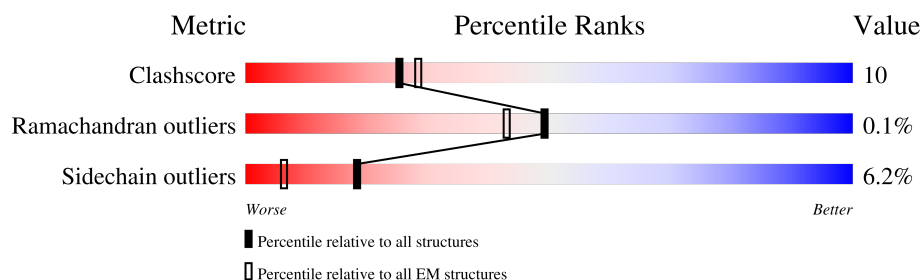
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.47 Å.

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



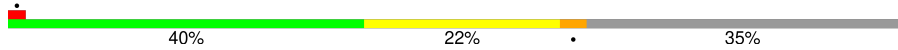
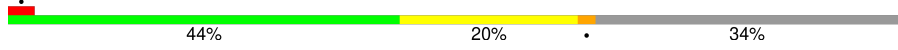
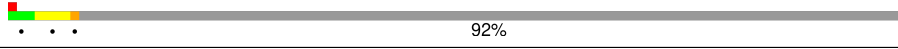
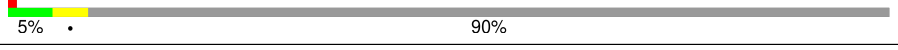
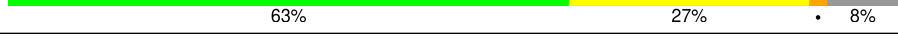
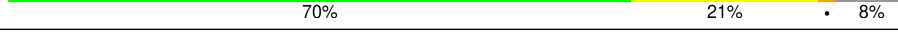
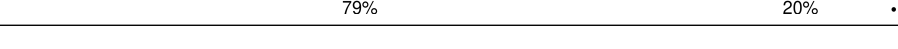
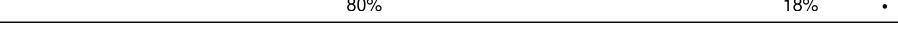
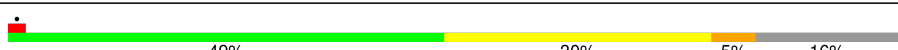
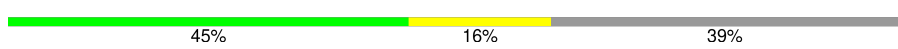
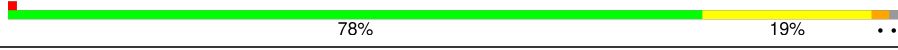
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13733 (2.97 - 3.97)

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

Mol	Chain	Length	Quality of chain
1	0	91	
1	Ab	91	
2	1	64	
2	Ac	64	

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Mol	Chain	Length	Quality of chain
3	2	299	
3	4	299	
3	Ae	299	
3	Af	299	
4	3	56	
4	Ad	56	
5	6	453	
5	v	453	
6	7	379	
6	w	379	
7	8	326	
7	x	326	
8	9	111	
8	y	111	
9	a	189	
10	b	128	
11	c	186	
12	d	176	
13	e	154	
14	f	76	
15	g	122	
16	h	106	
17	i	347	
18	j	115	
19	k	98	

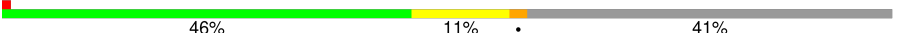
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Mol	Chain	Length	Quality of chain
20	m	175	
21	n	58	
22	o	129	
23	p	221	
24	q	459	
25	r	318	
26	B	464	
27	C	469	
28	D	264	
29	E	249	
30	F	123	
31	H	212	
32	I	196	
33	J	175	
34	K	145	
35	L	372	
36	N	116	
37	O	156	
37	X	156	
38	P	99	
39	Q	154	
40	R	110	
41	S	70	
42	T	169	
43	U	357	

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Mol	Chain	Length	Quality of chain
44	V	141	
45	W	144	
46	Y	105	
47	Z	114	
48	l	606	
49	s	249	
50	t	137	
51	5	480	
51	u	480	
52	Aa	82	
52	z	82	
53	G	727	
54	M	113	

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
55	FES	2	301	-	-	X	-
55	FES	4	301	-	-	X	-
57	HEC	8	401	X	-	-	-
57	HEC	x	401	X	-	-	-
59	SF4	H	301	-	-	X	-
59	SF4	H	302	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 98319 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	68	Total	C	N	O	S	0	0
			557	338	100	114	5		
1	Ab	66	Total	C	N	O	S	0	0
			543	331	99	108	5		

- Molecule 2 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	60	Total	C	N	O	0	0
			493	322	87	84		
2	Ac	59	Total	C	N	O	0	0
			485	318	85	82		

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	195	Total	C	N	O	S	0	0
			1509	951	264	287	7		
3	4	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
3	Ae	23	Total	C	N	O	S	0	0
			143	89	25	28	1		
3	Af	29	Total	C	N	O	S	0	0
			191	118	35	37	1		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	51	Total	C	N	O	S	0	0
			417	279	74	63	1		
4	Ad	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		
5	v	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		

- Molecule 6 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
6	w	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

- Molecule 7 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	238	Total	C	N	O	S	0	0
			1896	1211	326	343	16		
7	x	238	Total	C	N	O	S	0	0
			1896	1211	326	343	16		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	99	Total	C	N	O	S	0	0
			878	563	154	159	2		
8	y	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	b	108	Total	C	N	O	0	0
			900	591	156	153		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	153	Total	C	N	O	S	0	0
			1291	838	208	237	8		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	168	Total	C	N	O	S	0	0
			1417	890	258	261	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	99	Total	C	N	O	S	0	0
			826	530	137	155	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	46	Total	C	N	O	0	0
			391	259	67	65		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	347	Total	C	N	O	S	0	0
			2711	1782	420	463	46		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	100	Total	C	N	O	S	0	0
			793	537	116	135	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	m	175	Total	C	N	O	S	0	0
			1309	873	189	235	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	56	Total	C	N	O	S	0	0
			475	308	87	79	1		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	o	128	Total	C	N	O	0	0
			1058	688	181	189		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	q	459	Total	C	N	O	S	0	0
			3630	2410	572	609	39		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	431	Total	C	N	O	S	0	0
			3318	2095	591	612	20		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	430	Total	C	N	O	S	0	0
			3454	2207	593	630	24		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	208	Total	C	N	O	S	0	0
			1732	1121	297	312	2		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	94	Total	C	N	O	S	0	0
			727	444	136	144	3		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	H	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	I	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	117	Total	C	N	O	S	0	0
			953	602	171	177	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	144	Total	C	N	O	S	0	0
			1203	769	217	212	5		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	340	Total	C	N	O	S	0	0
			2702	1745	473	475	9		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	N	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 37 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	O	84	Total	C	N	O	S	0	0
			680	440	100	135	5		
37	X	85	Total	C	N	O	S	0	0
			689	445	101	138	5		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	P	83	Total	C	N	O	S	0	0
			669	419	125	123	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Q	112	Total	C	N	O	S	0	0
			954	610	176	163	5		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	35	Total	C	N	O	S	0	0
			295	185	55	54	1		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	S	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	T	82	Total	C	N	O	S	0	0
			638	414	109	114	1		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	U	318	Total	C	N	O	S	0	0
			2574	1638	437	489	10		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

- Molecule 45 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	W	140	Total	C	N	O	S	0	0
			1162	749	201	203	9		

- Molecule 46 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	62	Total	C	N	O	S	0	0
			531	352	88	90	1		

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Z	78	Total	C	N	O	S	0	0
			626	410	105	110	1		

- Molecule 48 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	l	603	Total	C	N	O	S	0	0
			4785	3174	741	819	51		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	119	Total	C	N	O	S	0	0
			1019	635	195	180	9		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		
51	5	435	Total	C	N	O	S	0	0
			3374	2105	594	656	19		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	79	Total	C	N	O	S	0	0
			666	434	122	108	2		
52	Aa	78	Total	C	N	O	S	0	0
			662	432	121	107	2		

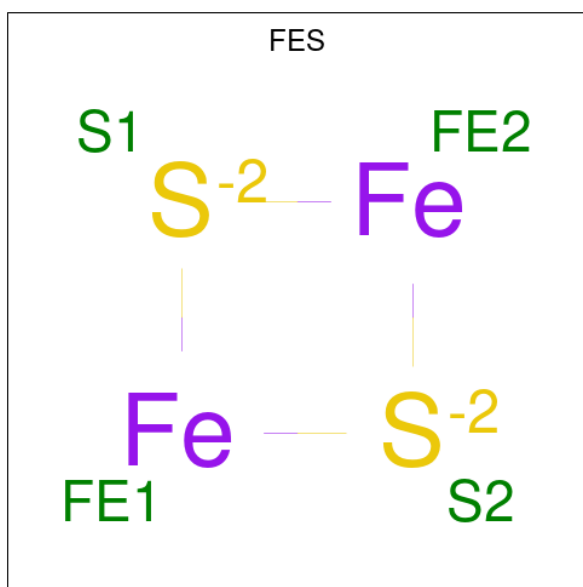
- Molecule 53 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	G	684	Total	C	N	O	S	0	0
			5260	3298	917	1006	39		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

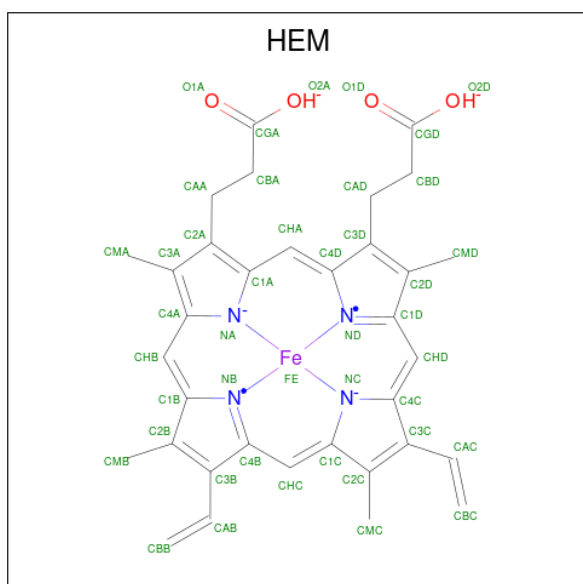
Mol	Chain	Residues	Atoms					AltConf	Trace
54	M	96	Total	C	N	O	S	0	0
			773	487	146	137	3		

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



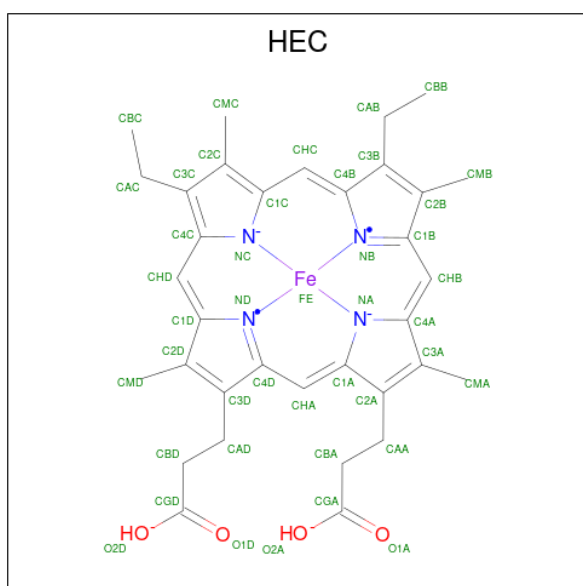
Mol	Chain	Residues	Atoms			AltConf
55	2	1	Total 4	Fe 2	S 2	0
55	4	1	Total 4	Fe 2	S 2	0
55	E	1	Total 4	Fe 2	S 2	0
55	G	1	Total 4	Fe 2	S 2	0

- Molecule 56 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



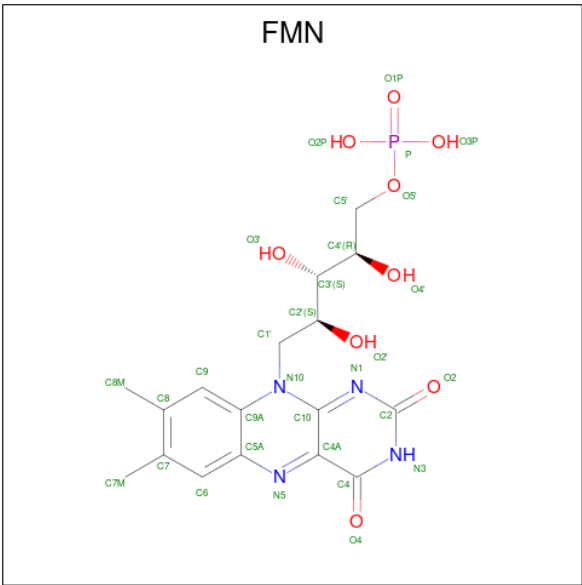
Mol	Chain	Residues	Atoms					AltConf
56	7	1	Total 43	C 34	Fe 1	N 4	O 4	0
56	7	1	Total 43	C 34	Fe 1	N 4	O 4	0
56	w	1	Total 43	C 34	Fe 1	N 4	O 4	0
56	w	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 57 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



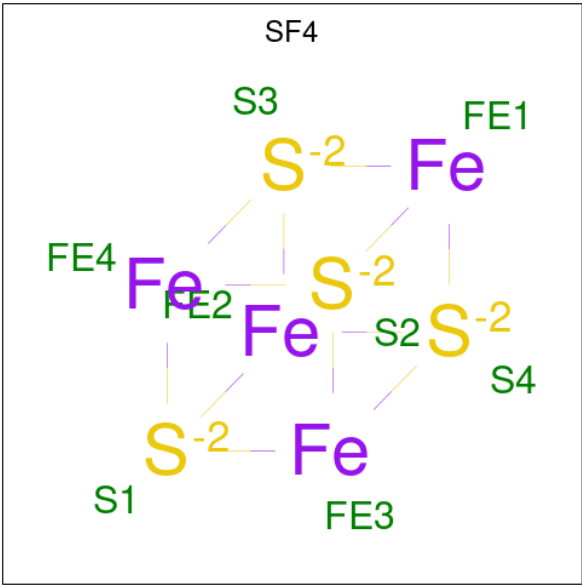
Mol	Chain	Residues	Atoms					AltConf
57	8	1	Total 43	C 34	Fe 1	N 4	O 4	0
57	x	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 58 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



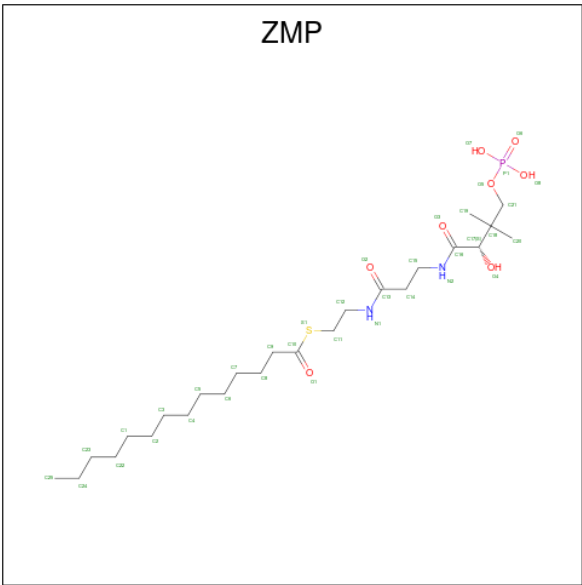
Mol	Chain	Residues	Atoms			AltConf
59	B	1	Total	Fe	S	0
			8	4	4	
59	H	1	Total	Fe	S	0
			8	4	4	
59	H	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Mol	Chain	Residues	Atoms			AltConf
59	I	1	Total 8	Fe 4	S 4	0
59	G	1	Total 8	Fe 4	S 4	0
59	G	1	Total 8	Fe 4	S 4	0

- # NDP

- Molecule 61 is S-[2-($\{N-[(2S)-2\text{-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl}]\text{-beta-alanyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).

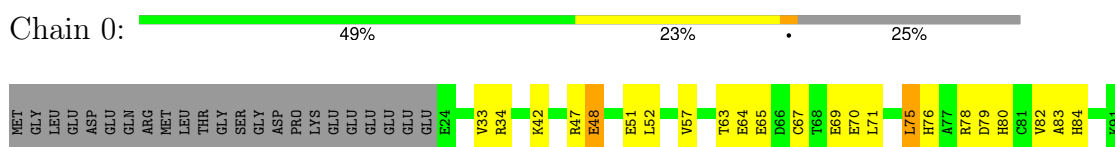


Mol	Chain	Residues	Atoms						AltConf
61	Q	1	Total	C	N	O	P	S	0
			30	18	2	8	1	1	

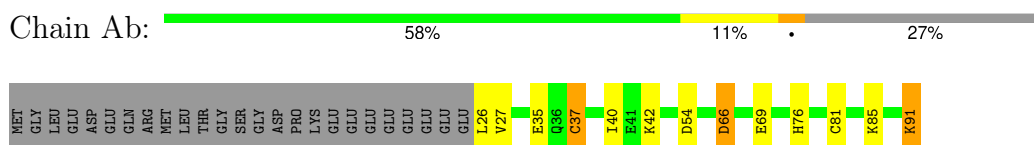
3 Residue-property plots

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 atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

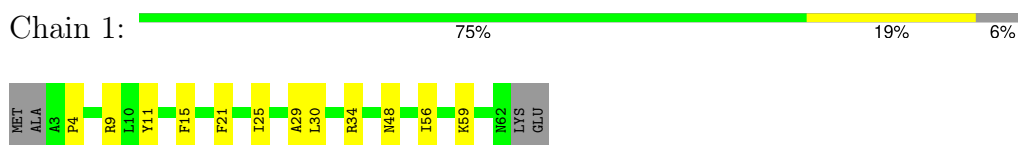
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



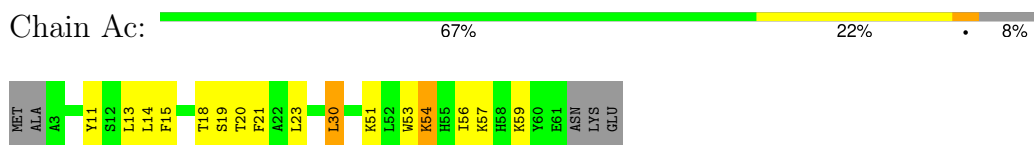
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



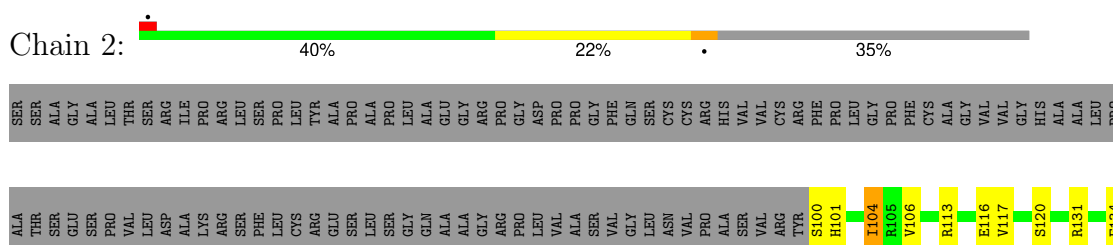
- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

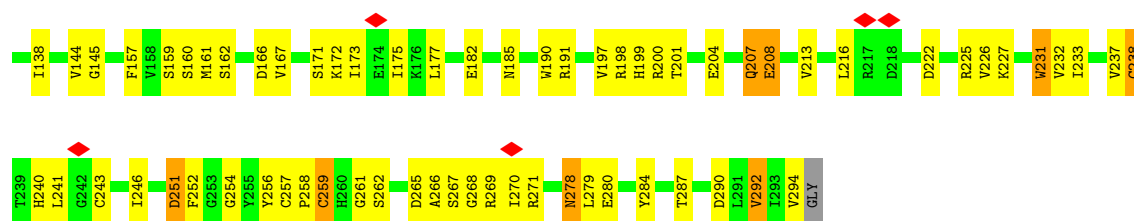


- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



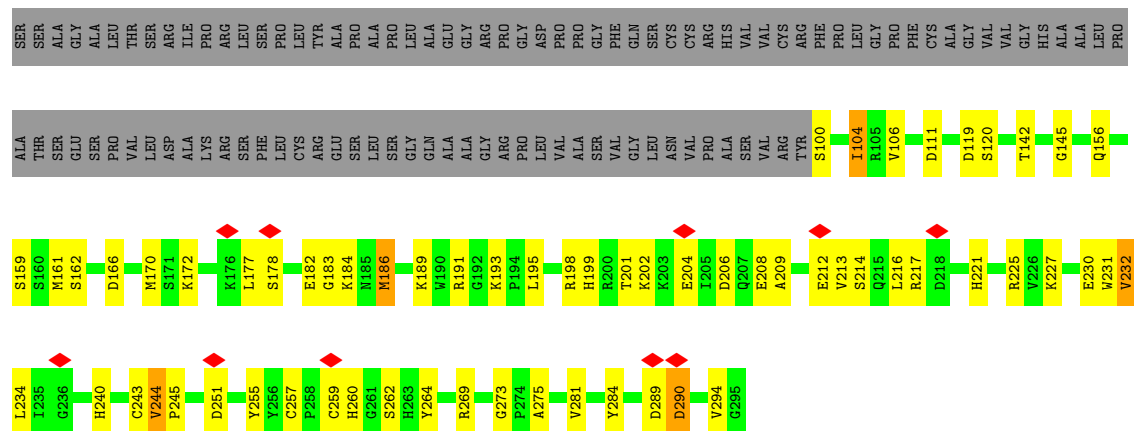
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1





- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain 4: 44% 20% 34%



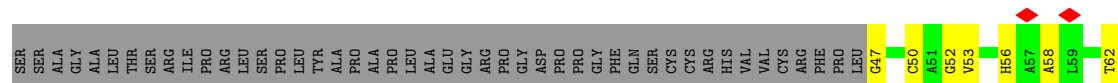
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

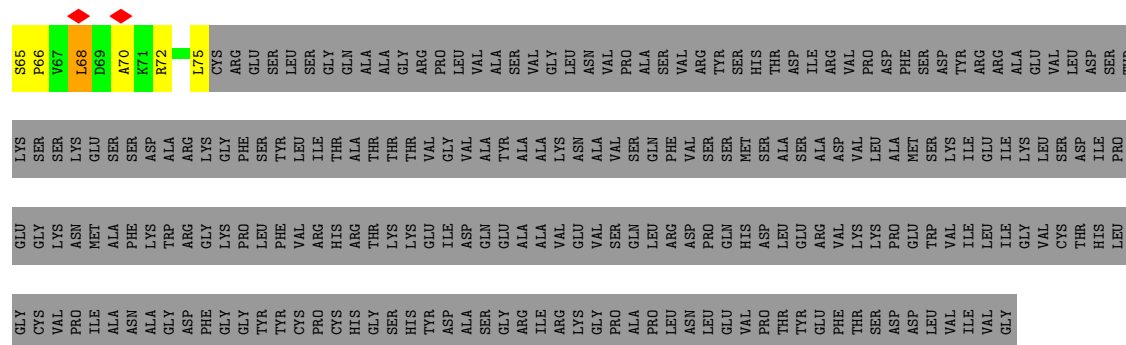
Chain Ae: 92%



- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain Af: 5% 90%





- Molecule 4: Cytochrome b-c1 complex subunit 10

Chain 3: 80% 9% 9%



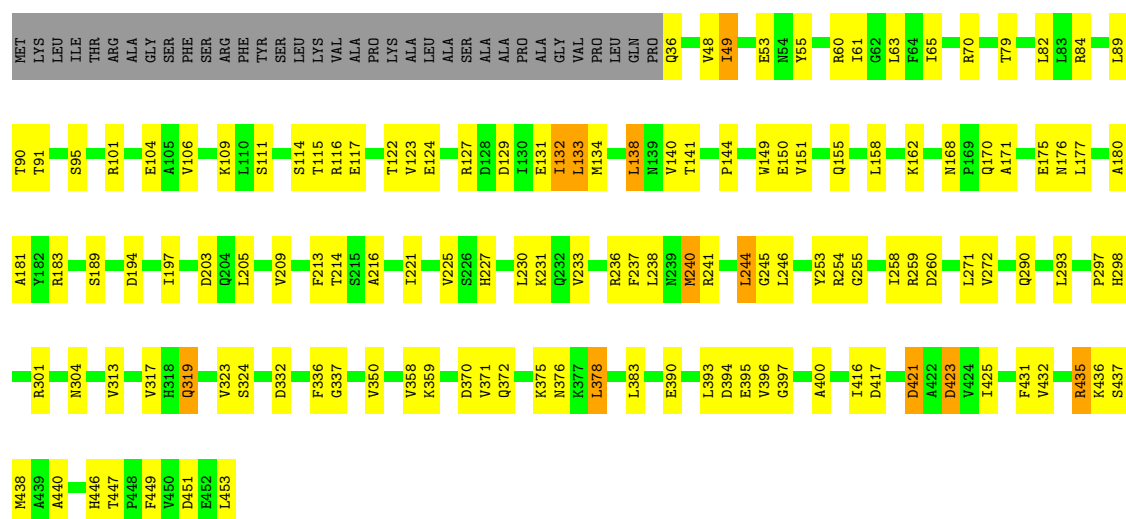
- Molecule 4: Cytochrome b-c1 complex subunit 10

Chain Ad: 86% 5% 9%



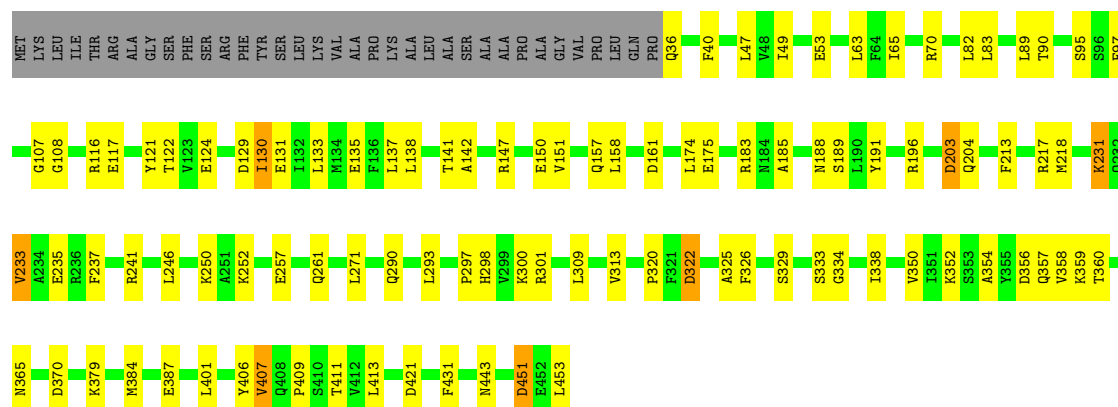
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 6: 63% 27% 8%



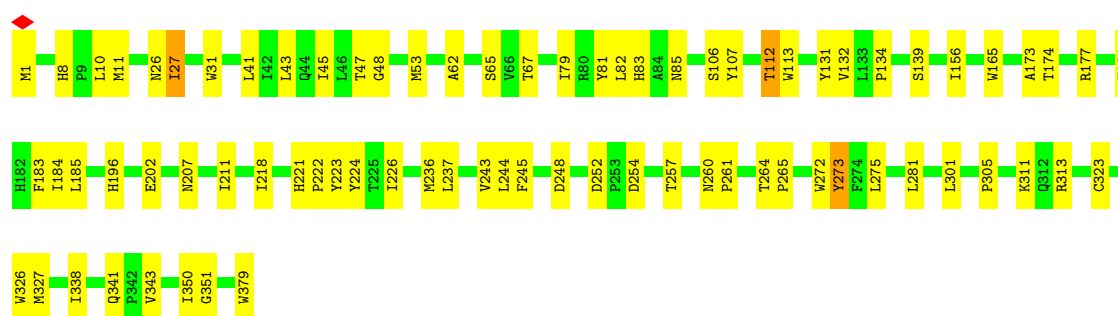
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain v: 70% 21% 8%



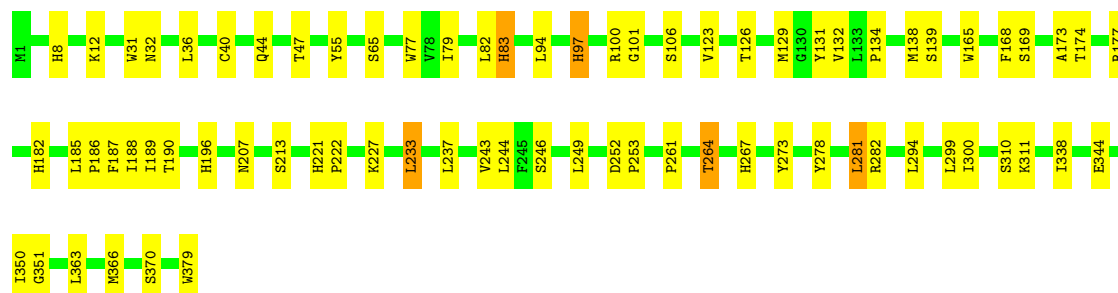
• Molecule 6: Cytochrome b

Chain 7: 79% 20% .



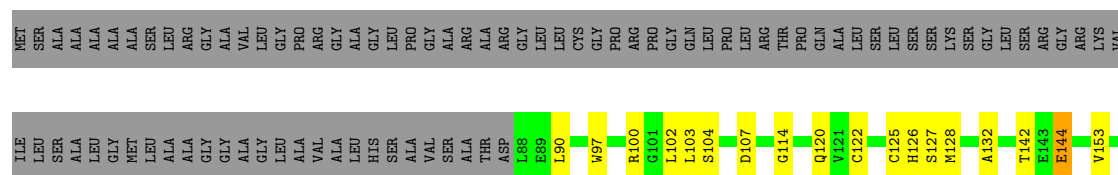
• Molecule 6: Cytochrome b

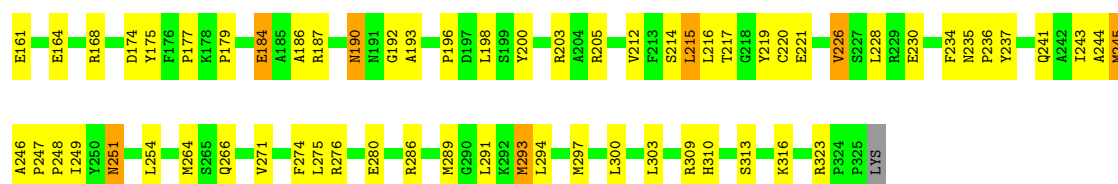
Chain w: 80% 18% .



• Molecule 7: Cytochrome c1

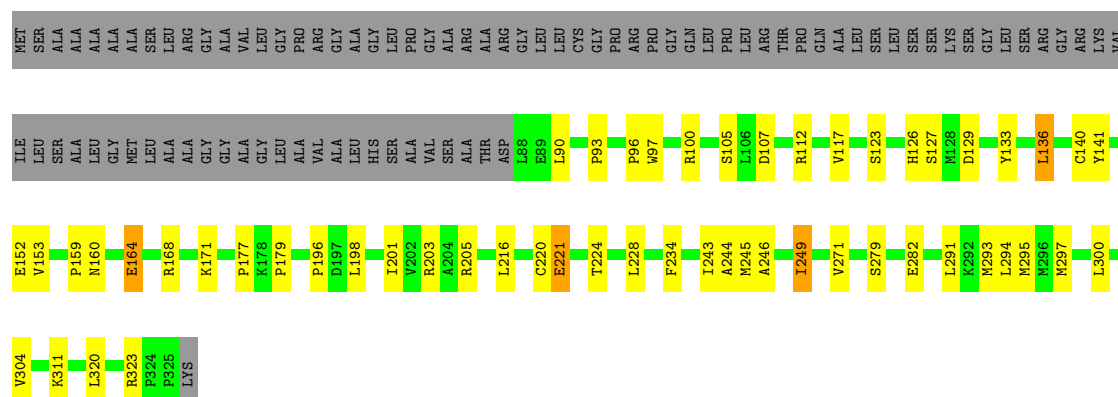
Chain 8: 48% 22% 27% .





- Molecule 7: Cytochrome c1

Chain x: 56% 16% 27%



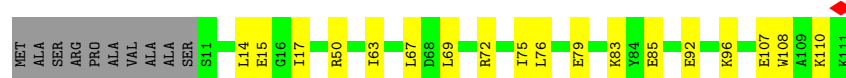
- Molecule 8: Cytochrome b-c1 complex subunit 7

Chain 9: 69% 18% 11%



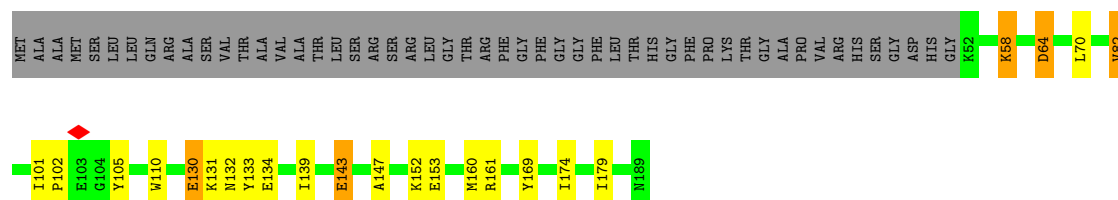
- Molecule 8: Cytochrome b-c1 complex subunit 7

Chain y: 75% 16% 9%

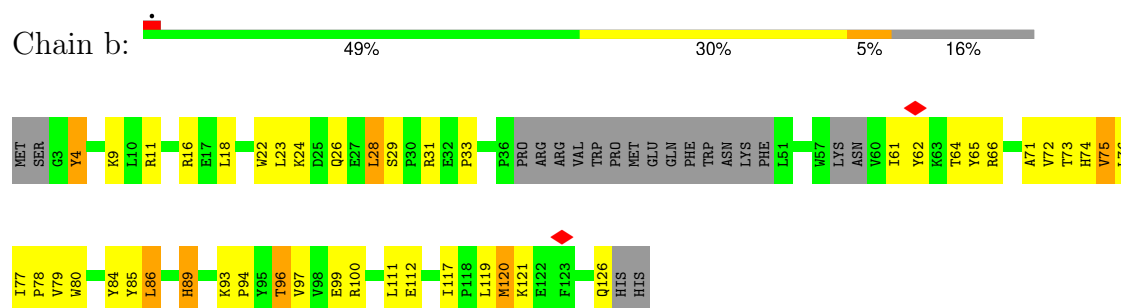


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

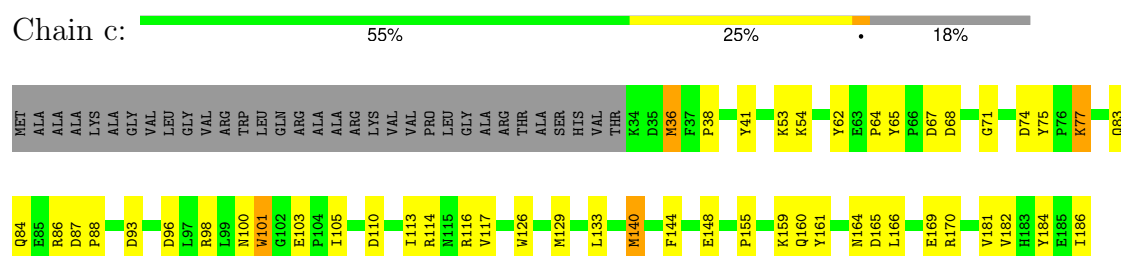
Chain a: 61% 10% 27%



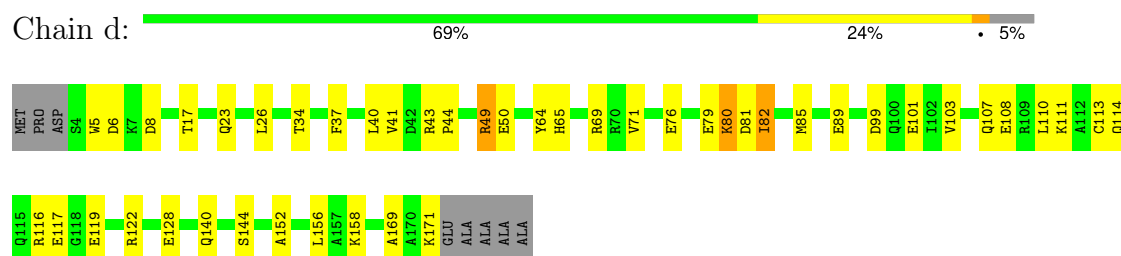
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



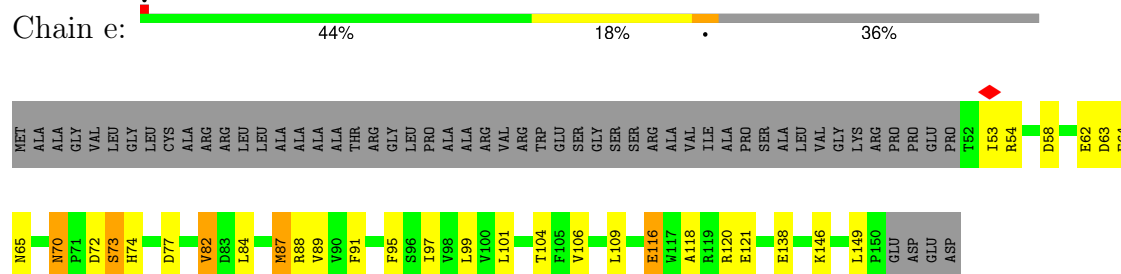
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



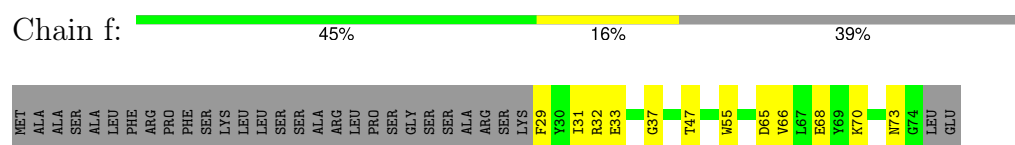
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

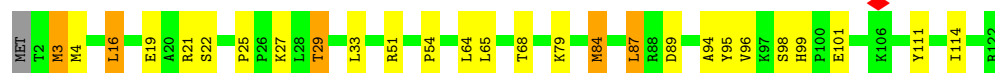


- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 



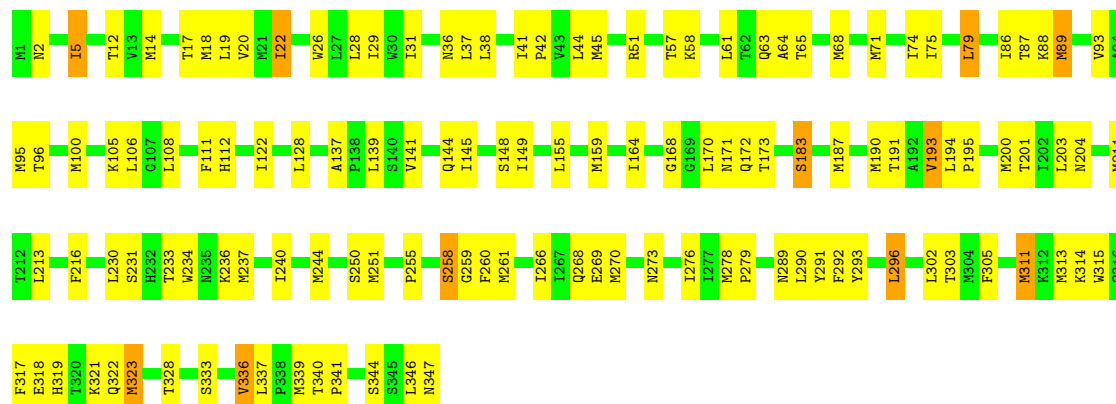
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 



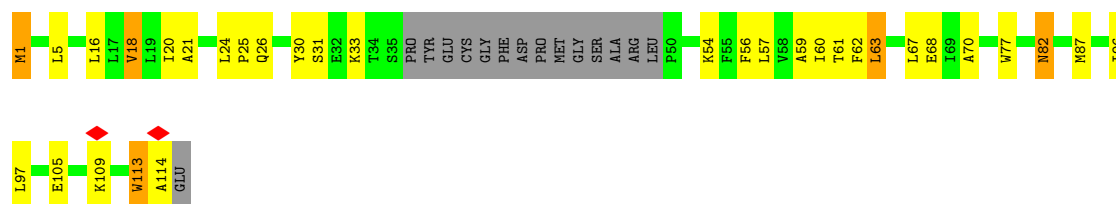
- Molecule 17: NADH-ubiquinone oxidoreductase chain 2

Chain i: 



- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain j: 

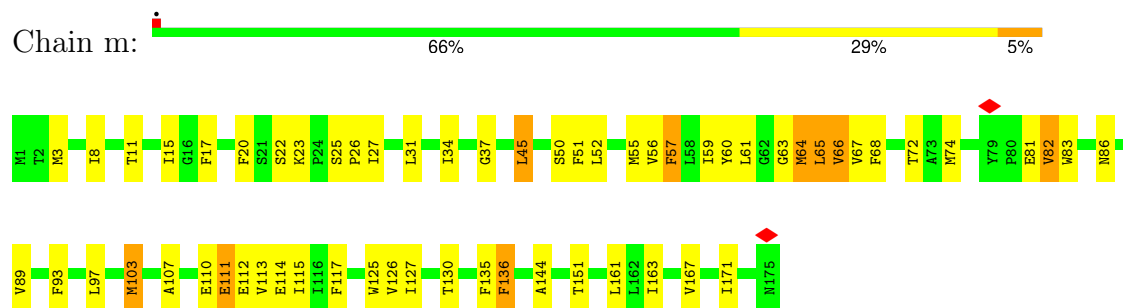


- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

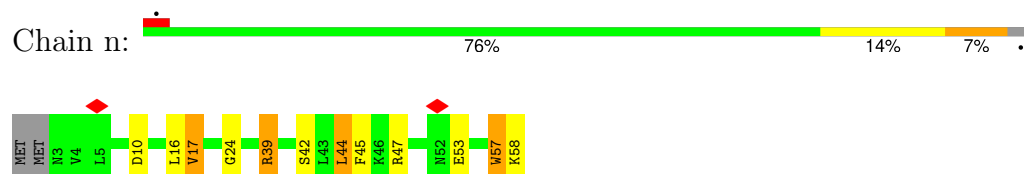
Chain k: 



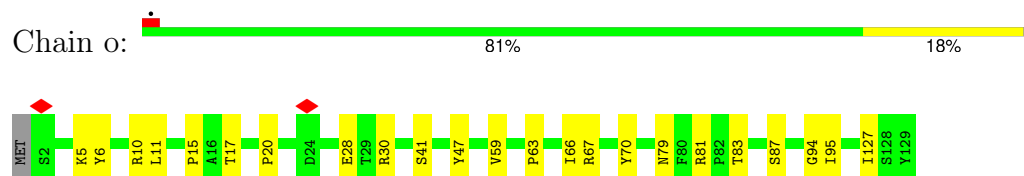
- Molecule 20: NADH-ubiquinone oxidoreductase chain 6



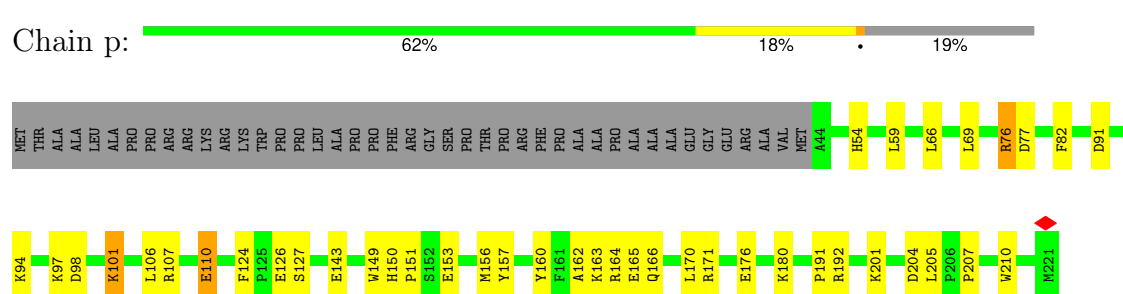
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



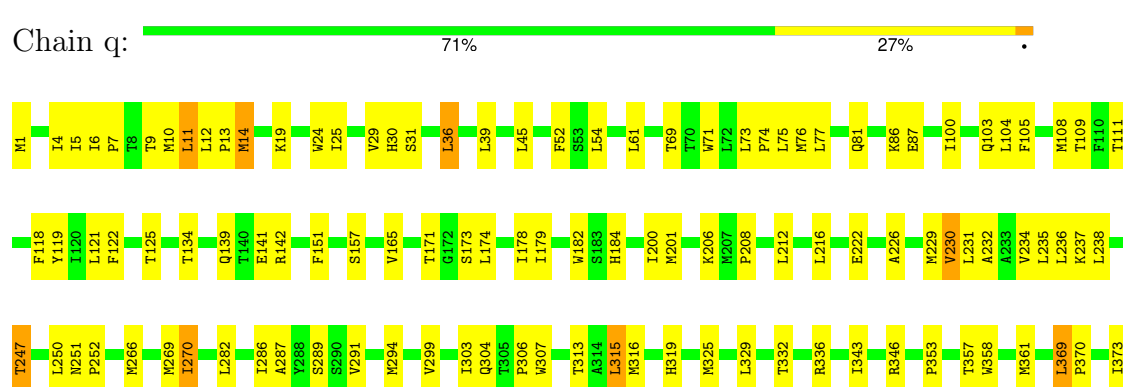
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



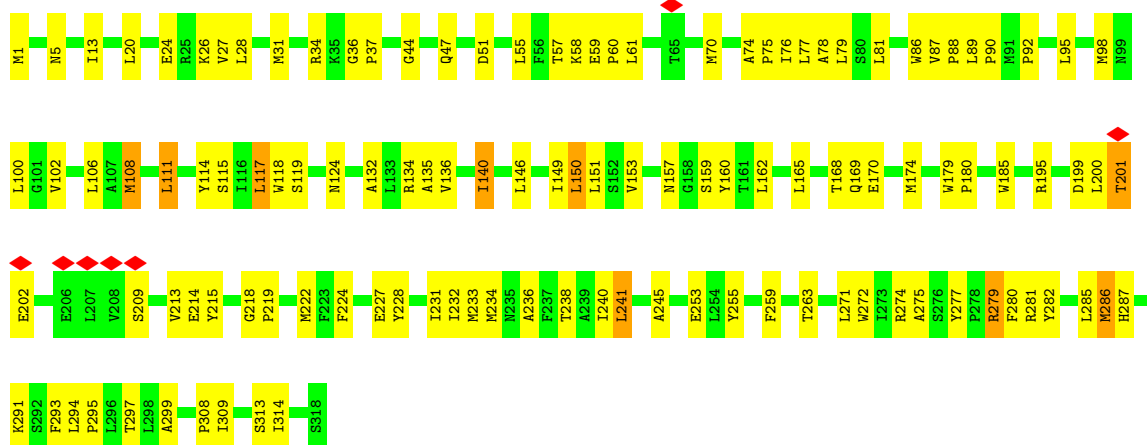
- Molecule 24: NADH-ubiquinone oxidoreductase chain 4





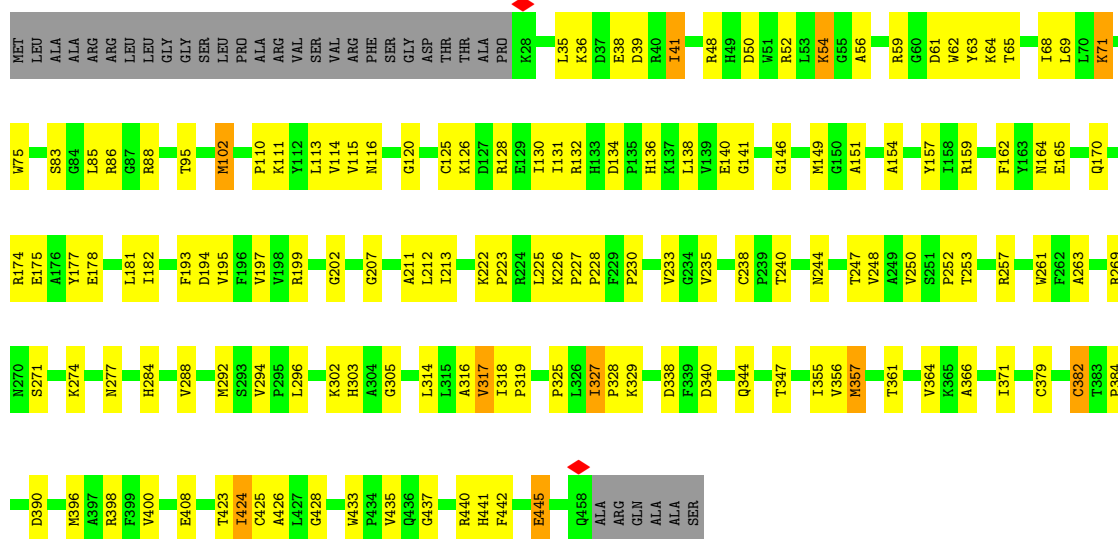
• Molecule 25: NADH-ubiquinone oxidoreductase chain 1

Chain r: 62% 35%



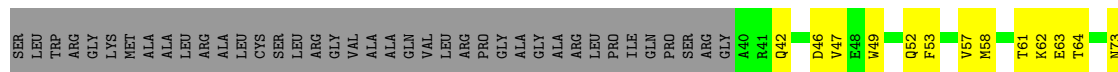
• Molecule 26: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

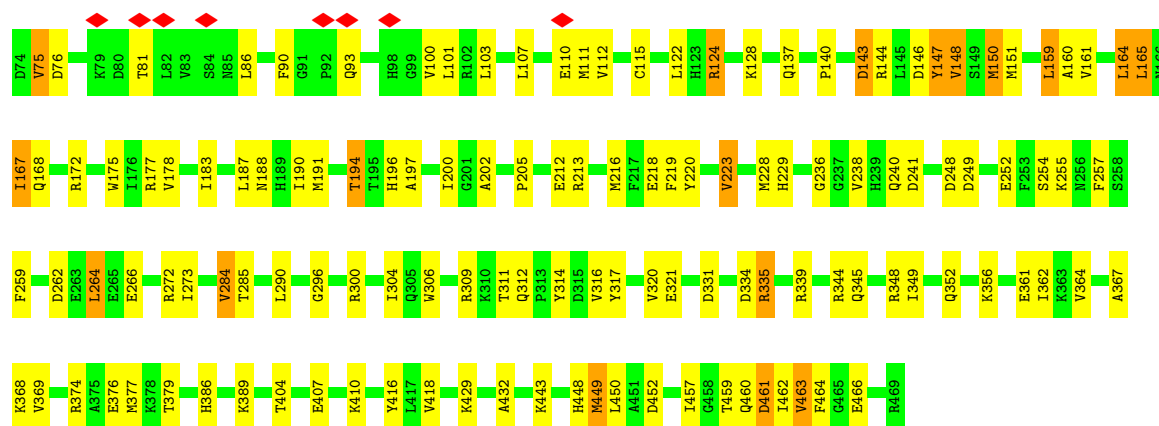
Chain B: 62% 28% 7%



• Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

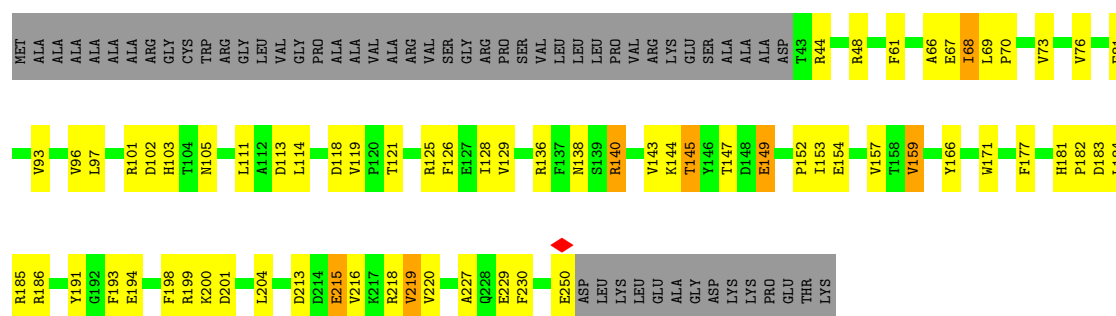
Chain C: 61% 27% 8%





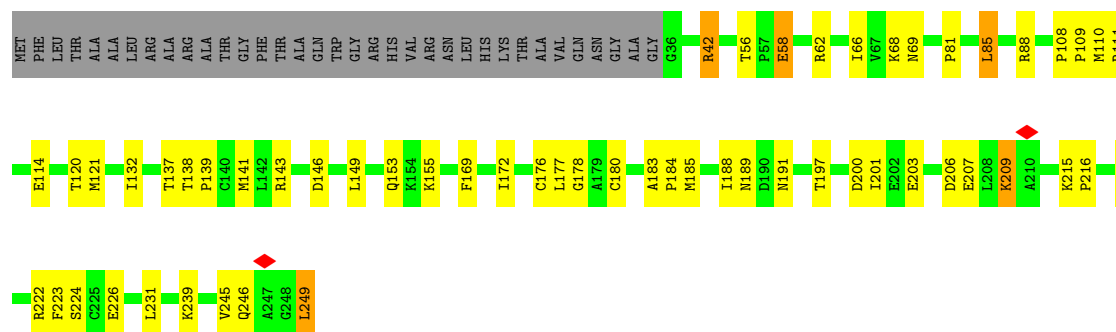
- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain D: 53% 23% 21%



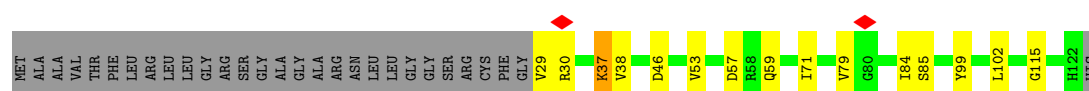
- Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 63% 21% 14%



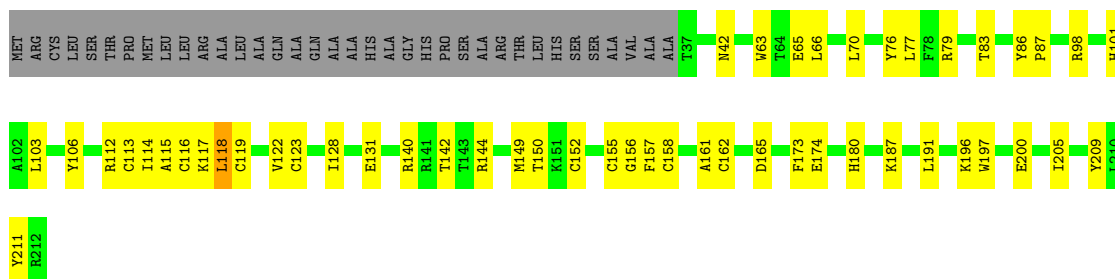
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain F: 64% 11% 24%



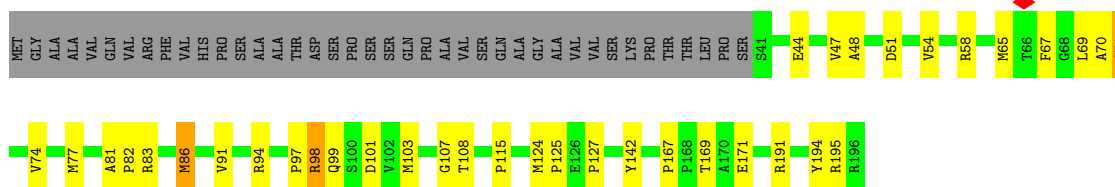
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain H: 



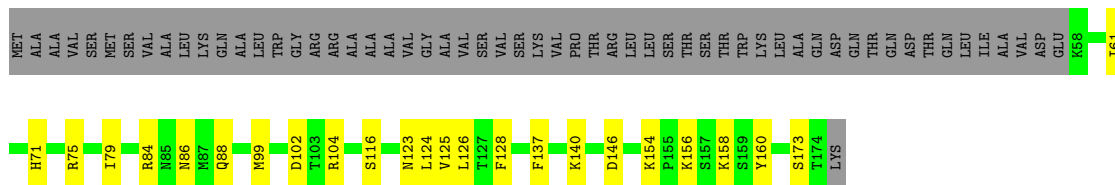
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain I: 



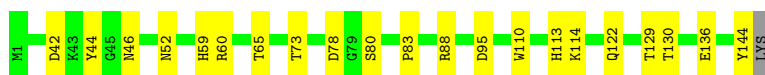
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain J: 



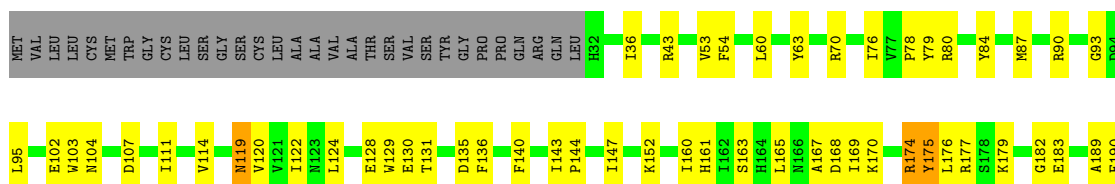
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

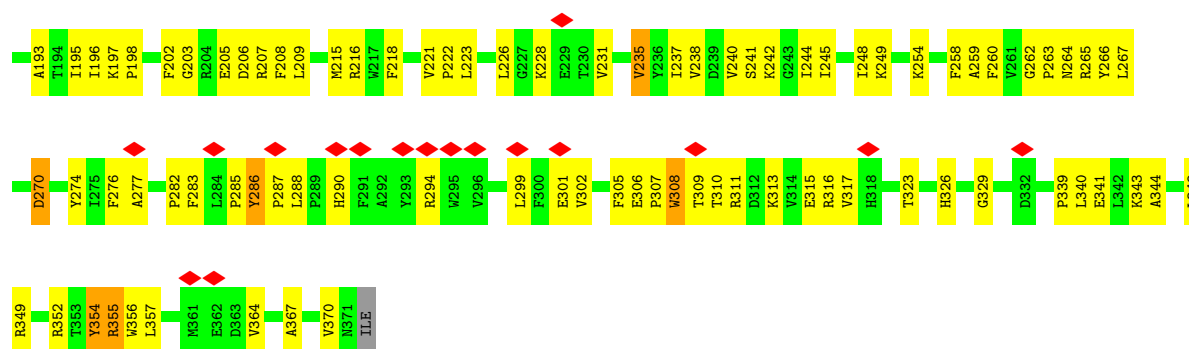
Chain K: 



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain L: 





- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain N: 76% 19%



- Molecule 37: Acyl carrier protein

Chain O: 33% 17% 46%



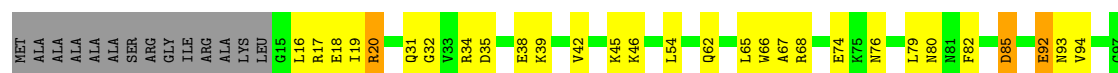
- Molecule 37: Acyl carrier protein

Chain X: 38% 15% 46%

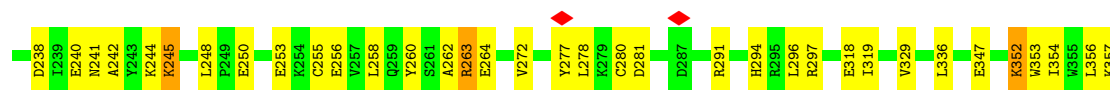


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P: 55% 26% 16%



K104	L110	E117	Y131	Y138	A139	S140	L143	A148	L149	L152	L153	G158	V159	R163	V170	F171	L172	Q178	R182	G185	V186	K193	K194	V195	P203	H204	V211	P212	V213	P214	E215	L216	Q217	S218	K223	G224	N225	E228	M229	T232
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 80% 16% . .



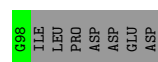
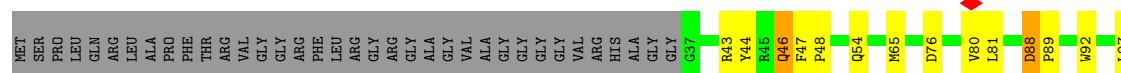
- Molecule 45: NADH:ubiquinone oxidoreductase subunit A13

Chain W: 73% 24% . .



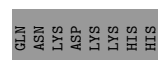
- Molecule 46: NADH:ubiquinone oxidoreductase subunit B2

Chain Y: 46% 11% 41% .



- Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

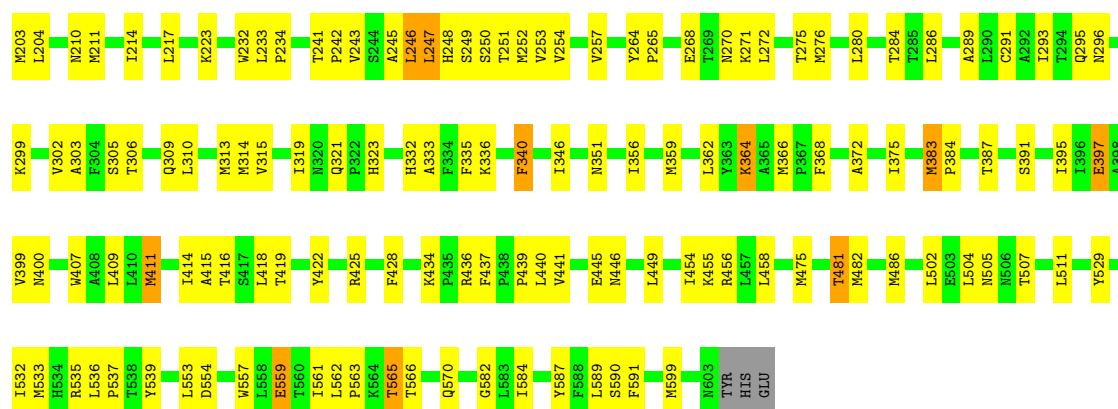
Chain Z: 54% 13% 32% .



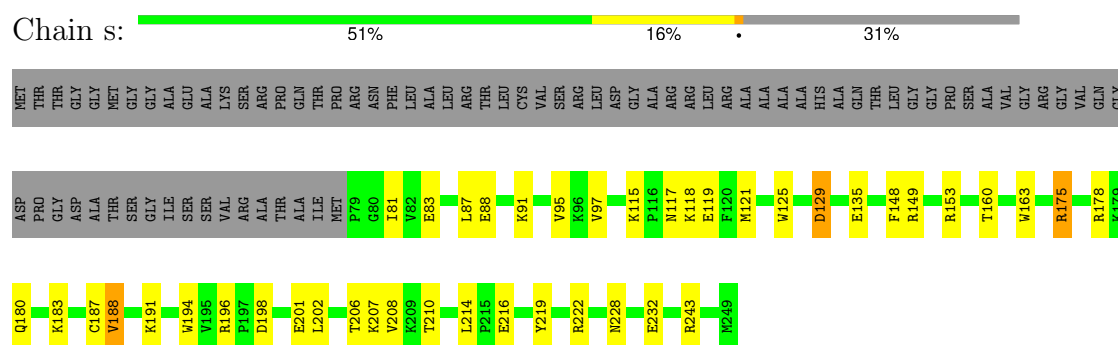
- Molecule 48: NADH-ubiquinone oxidoreductase chain 5

Chain I: 66% 31% .

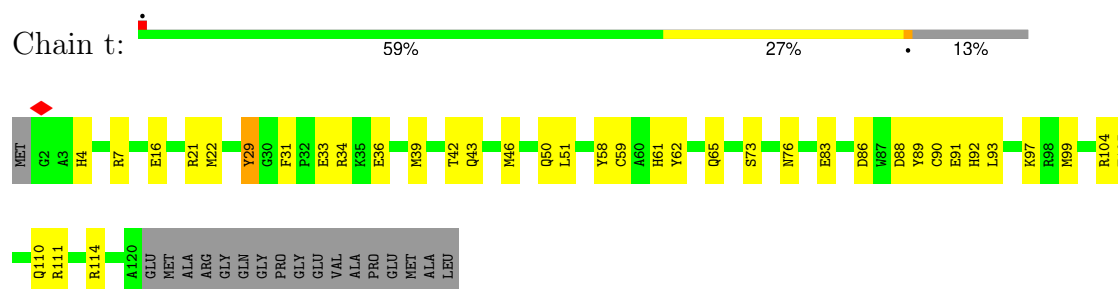




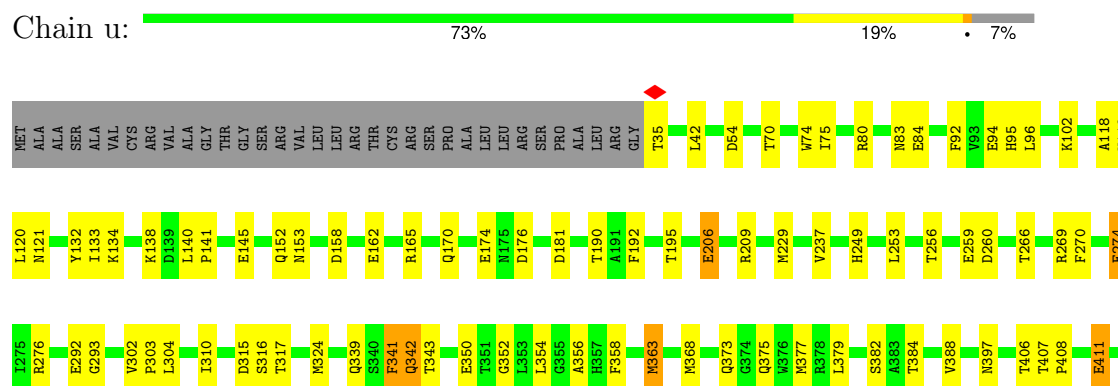
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



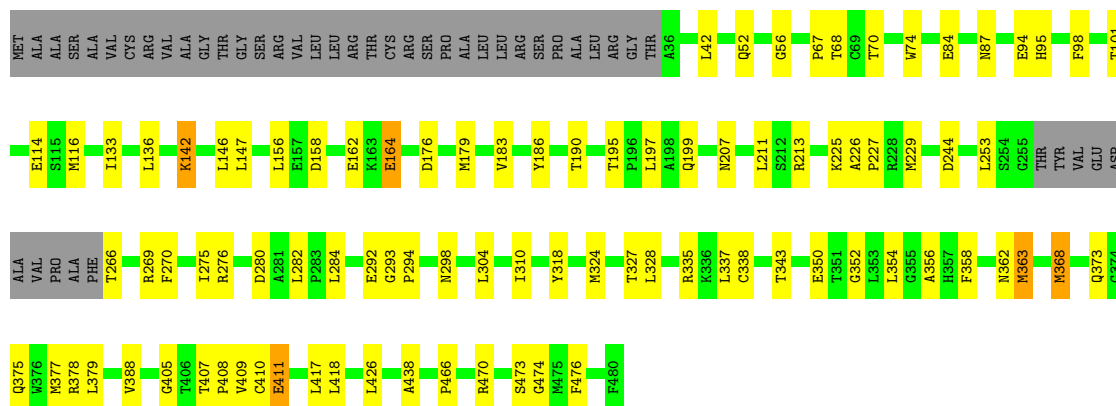
- Molecule 51: Cytochrome b-c1 complex subunit 1, mitochondrial





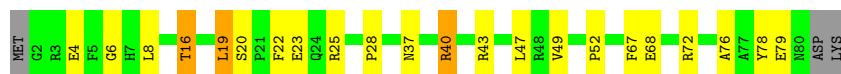
- Molecule 51: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain 5: 71% 18% 9%



- Molecule 52: Cytochrome b-c1 complex subunit 8

Chain z: 70% 23% 7%



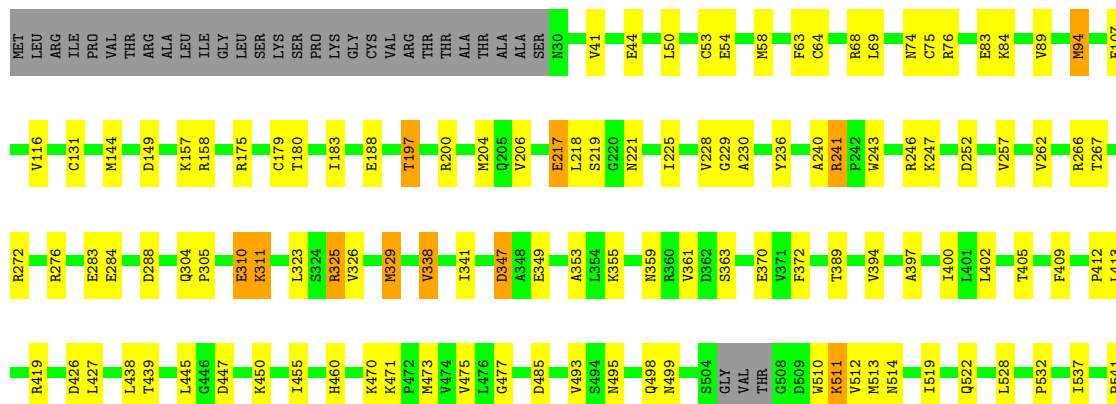
- Molecule 52: Cytochrome b-c1 complex subunit 8

Chain Aa: 71% 23% 6%



- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 73% 19% 8%





- Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11787	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.793	Depositor
Minimum map value	-0.229	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, NDP, HEM, FES, HEC, SF4, FMN

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	0	0.17	0/563	0.32	0/755
1	Ab	0.17	0/549	0.27	0/735
2	1	0.20	0/506	0.30	0/683
2	Ac	0.15	0/498	0.23	0/672
3	2	0.19	0/1542	0.35	0/2088
3	4	0.39	1/1551 (0.1%)	0.48	0/2098
3	Ae	0.28	0/147	0.64	0/203
3	Af	0.25	0/194	0.55	0/265
4	3	0.23	0/433	0.42	0/593
4	Ad	0.14	0/437	0.22	0/598
5	6	0.20	0/3192	0.32	0/4322
5	v	0.17	0/3192	0.29	0/4322
6	7	0.25	0/3123	0.37	0/4269
6	w	0.28	0/3123	0.41	0/4269
7	8	0.50	0/1954	0.64	0/2652
7	x	0.18	0/1954	0.27	0/2652
8	9	0.17	0/898	0.29	0/1204
8	y	0.17	0/913	0.27	0/1223
9	a	0.27	0/1184	0.36	0/1603
10	b	0.38	0/927	0.55	0/1264
11	c	0.18	0/1346	0.30	0/1840
12	d	0.23	0/1449	0.35	0/1953
13	e	0.18	0/849	0.36	0/1153
14	f	0.22	0/404	0.34	0/547
15	g	0.26	0/1031	0.37	0/1394
16	h	0.17	0/889	0.27	0/1190
17	i	0.21	0/2774	0.33	0/3768
18	j	0.42	0/811	0.62	0/1107
19	k	0.38	0/759	0.57	0/1029
20	m	0.56	0/1340	0.75	0/1816
21	n	0.16	0/487	0.32	0/659
22	o	0.17	0/1088	0.31	0/1477

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	p	0.21	0/1590	0.36	0/2155
24	q	0.21	0/3721	0.33	0/5073
25	r	0.45	0/2581	0.61	0/3529
26	B	0.15	0/3393	0.32	0/4584
27	C	0.30	0/3547	0.46	1/4809 (0.0%)
28	D	0.18	0/1783	0.32	0/2428
29	E	0.15	0/1698	0.32	0/2311
30	F	0.14	0/740	0.26	0/998
31	H	0.42	0/1443	0.56	0/1952
32	I	0.22	0/1279	0.35	0/1730
33	J	0.14	0/976	0.26	0/1318
34	K	0.14	0/1244	0.23	0/1693
35	L	0.21	0/2774	0.38	0/3761
36	N	0.15	0/929	0.28	0/1258
37	O	0.14	0/692	0.37	0/934
37	X	0.12	0/701	0.29	0/946
38	P	0.12	0/680	0.28	0/916
39	Q	0.16	0/978	0.30	0/1317
40	R	0.11	0/304	0.25	0/410
41	S	0.18	0/577	0.32	0/777
42	T	0.15	0/659	0.26	0/905
43	U	0.38	0/2634	0.51	0/3565
44	V	0.16	0/1037	0.30	0/1404
45	W	0.20	0/1193	0.32	0/1609
46	Y	0.16	0/555	0.30	0/760
47	Z	0.12	0/645	0.23	0/872
48	l	0.19	0/4914	0.34	0/6683
49	s	0.16	0/1436	0.32	0/1938
50	t	0.28	0/1043	0.40	0/1396
51	5	0.18	0/3442	0.30	0/4667
51	u	0.17	0/3531	0.29	0/4793
52	Aa	0.16	0/684	0.29	0/926
52	z	0.17	0/688	0.33	0/931
53	G	0.15	0/5347	0.30	0/7243
54	M	0.14	0/791	0.29	0/1069
All	All	0.25	1/100336 (0.0%)	0.38	1/136063 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	8	0	1
25	r	0	1
27	C	0	2
32	I	0	1
43	U	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	244	VAL	N-CA	5.10	1.49	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	110	GLU	N-CA-C	-6.42	103.98	113.61

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	8	205	ARG	Sidechain
27	C	335	ARG	Sidechain
27	C	339	ARG	Sidechain
32	I	98	ARG	Sidechain
43	U	297	ARG	Sidechain
25	r	279	ARG	Sidechain

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	0	557	0	529	18	0
1	Ab	543	0	528	6	0
2	1	493	0	491	9	0
2	Ac	485	0	485	10	0
3	2	1509	0	1492	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4	1518	0	1499	51	0
3	Ae	143	0	134	10	0
3	Af	191	0	188	8	0
4	3	417	0	414	7	0
4	Ad	421	0	418	4	0
5	6	3140	0	3121	87	0
5	v	3140	0	3121	60	0
6	7	3025	0	3090	55	0
6	w	3025	0	3090	57	0
7	8	1896	0	1844	74	0
7	x	1896	0	1843	38	0
8	9	878	0	870	11	0
8	y	893	0	888	7	0
9	a	1151	0	1164	25	0
10	b	900	0	903	44	0
11	c	1291	0	1185	36	0
12	d	1417	0	1393	35	0
13	e	826	0	789	18	0
14	f	391	0	392	12	0
15	g	1000	0	994	23	0
16	h	867	0	871	18	0
17	i	2711	0	2874	94	0
18	j	793	0	842	27	0
19	k	748	0	799	37	0
20	m	1309	0	1305	70	0
21	n	475	0	475	11	0
22	o	1058	0	1061	19	0
23	p	1534	0	1470	27	0
24	q	3630	0	3837	97	0
25	r	2508	0	2607	91	0
26	B	3318	0	3282	105	0
27	C	3454	0	3383	94	0
28	D	1732	0	1682	47	0
29	E	1658	0	1662	48	0
30	F	727	0	694	7	0
31	H	1412	0	1368	42	0
32	I	1248	0	1254	29	0
33	J	953	0	949	18	0
34	K	1203	0	1161	13	0
35	L	2702	0	2713	89	0
36	N	910	0	950	15	0
37	O	680	0	681	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	X	689	0	687	19	0
38	P	669	0	677	24	0
39	Q	954	0	960	27	0
40	R	295	0	279	14	0
41	S	562	0	557	8	0
42	T	638	0	637	6	0
43	U	2574	0	2532	52	0
44	V	1016	0	1022	19	0
45	W	1162	0	1156	27	0
46	Y	531	0	480	11	0
47	Z	626	0	607	11	0
48	l	4785	0	4935	147	0
49	s	1398	0	1374	31	0
50	t	1019	0	987	22	0
51	5	3374	0	3272	57	0
51	u	3459	0	3350	57	0
52	Aa	662	0	660	14	0
52	z	666	0	663	15	0
53	G	5260	0	5287	92	0
54	M	773	0	801	11	0
55	2	4	0	0	3	0
55	4	4	0	0	3	0
55	E	4	0	0	1	0
55	G	4	0	0	0	0
56	7	86	0	60	14	0
56	w	86	0	60	16	0
57	8	43	0	31	18	0
57	x	43	0	30	4	0
58	B	31	0	19	1	0
59	B	8	0	0	1	0
59	G	16	0	0	1	0
59	H	16	0	0	11	0
59	I	8	0	0	1	0
60	L	48	0	26	1	0
61	Q	30	0	30	3	0
All	All	98319	0	97964	2035	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (2035) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:122:CYS:SG	57:8:401:HEC:CAB	2.22	1.28
31:H:116:CYS:SG	59:H:302:SF4:FE1	1.44	1.07
7:8:122:CYS:SG	57:8:401:HEC:C3B	2.43	1.06
31:H:162:CYS:SG	59:H:302:SF4:FE4	1.59	0.94
31:H:113:CYS:SG	59:H:302:SF4:FE3	1.61	0.92
20:m:26:PRO:HB2	20:m:72:THR:HG21	1.52	0.90
31:H:113:CYS:HG	59:H:302:SF4:FE3	0.67	0.90
16:h:81:ARG:HD2	20:m:111:GLU:HG3	1.57	0.86
24:q:370:PRO:HB3	24:q:375:LEU:HD22	1.59	0.83
17:i:38:LEU:HD23	19:k:73:LEU:HD12	1.59	0.83
20:m:45:LEU:HD22	20:m:50:SER:HA	1.61	0.83
56:7:401:HEM:HHD	56:7:401:HEM:HBC2	1.59	0.83
7:8:219:TYR:HE1	7:8:243:ILE:HG21	1.44	0.82
3:2:213:VAL:HA	3:2:216:LEU:HD12	1.62	0.80
37:X:89:LEU:HD23	47:Z:64:ASN:HA	1.62	0.80
3:2:238:CYS:HB3	3:2:243:CYS:SG	2.21	0.80
7:8:127:SER:HB3	7:8:179:PRO:HD2	1.62	0.80
27:C:367:ALA:HB3	53:G:149:ASP:HB2	1.64	0.78
3:4:262:SER:HA	3:4:273:GLY:HA3	1.65	0.78
56:7:401:HEM:HHC	56:7:401:HEM:HBB2	1.64	0.78
31:H:155:CYS:SG	59:H:301:SF4:FE3	1.75	0.78
19:k:34:GLU:HG3	20:m:64:MET:HE2	1.65	0.78
27:C:183:ILE:HG23	27:C:216:MET:HE2	1.63	0.77
7:8:97:TRP:HB2	7:8:100:ARG:HG3	1.66	0.77
28:D:102:ASP:HB2	36:N:90:LEU:HD22	1.67	0.77
18:j:21:ALA:HB1	25:r:218:GLY:HA3	1.67	0.76
35:L:216:ARG:HE	35:L:282:PRO:HG2	1.48	0.76
17:i:313:MET:HE1	43:U:140:SER:HA	1.67	0.76
17:i:42:PRO:HG3	20:m:167:VAL:HG22	1.68	0.75
7:8:196:PRO:HG2	57:8:401:HEC:HBA2	1.66	0.75
31:H:131:GLU:HB2	31:H:144:ARG:HB3	1.68	0.75
53:G:341:ILE:HD11	53:G:537:ILE:HG13	1.69	0.75
35:L:78:PRO:HB3	35:L:114:VAL:HG21	1.67	0.74
2:Ac:11:TYR:HA	2:Ac:15:PHE:HB2	1.67	0.74
17:i:258:SER:HB2	17:i:336:VAL:HG12	1.67	0.74
3:4:208:GLU:OE1	3:4:269:ARG:NH2	2.21	0.74
11:c:83:GLN:HE22	11:c:86:ARG:HH11	1.33	0.74
6:7:41:LEU:HD12	56:7:401:HEM:HBB1	1.69	0.74
25:r:58:LYS:NZ	32:I:101:ASP:OD1	2.20	0.73
27:C:374:ARG:NH2	31:H:165:ASP:OD1	2.21	0.73
7:8:186:ALA:O	7:8:190:ASN:ND2	2.21	0.73
48:l:359:MET:O	48:l:436:ARG:NH2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:4:MET:HG3	17:i:347:ASN:HD21	1.54	0.73
25:r:185:TRP:HE1	25:r:238:THR:HG22	1.53	0.73
3:4:240:HIS:HB2	3:4:275:ALA:HA	1.71	0.73
26:B:38:GLU:HA	29:E:239:LYS:HE3	1.72	0.72
44:V:69:ILE:HG13	44:V:100:THR:HG21	1.72	0.72
3:4:177:LEU:HB2	3:4:290:ASP:HA	1.72	0.72
51:5:293:GLY:N	51:5:352:GLY:O	2.21	0.72
3:4:255:TYR:HB2	3:4:264:TYR:HB2	1.70	0.72
17:i:58:LYS:HG2	48:l:584:ILE:HD11	1.72	0.72
6:7:338:ILE:HD13	6:7:351:GLY:HA2	1.72	0.71
25:r:79:LEU:HD22	25:r:222:MET:HG2	1.70	0.71
43:U:213:VAL:HG12	43:U:217:GLN:HE21	1.55	0.71
35:L:352:ARG:HG3	35:L:356:TRP:HB3	1.73	0.71
3:4:245:PRO:HB2	3:4:255:TYR:HB3	1.73	0.71
9:a:130:GLU:OE1	9:a:131:LYS:N	2.24	0.71
7:8:186:ALA:O	7:8:190:ASN:CG	2.34	0.70
26:B:288:VAL:HG21	26:B:303:HIS:HB3	1.74	0.70
26:B:50:ASP:O	26:B:59:ARG:NH1	2.24	0.70
44:V:108:TYR:OH	52:z:43:ARG:NH1	2.25	0.70
8:y:14:LEU:HD23	8:y:17:ILE:HD11	1.74	0.70
28:D:186:ARG:NH2	28:D:193:PHE:O	2.25	0.70
5:6:144:PRO:HG2	5:6:209:VAL:HG11	1.74	0.70
6:7:338:ILE:HD11	6:7:350:ILE:HG22	1.74	0.70
25:r:24:GLU:HA	25:r:271:LEU:HD13	1.75	0.69
31:H:76:TYR:HA	31:H:79:ARG:HD3	1.71	0.69
37:X:125:GLU:HG2	48:l:439:PRO:HG2	1.74	0.69
17:i:45:MET:HE1	20:m:171:ILE:HG23	1.73	0.69
28:D:171:TRP:HE1	39:Q:114:MET:HE1	1.56	0.69
51:u:470:ARG:HH21	6:w:222:PRO:HD3	1.57	0.69
53:G:602:ARG:HB2	53:G:659:VAL:HG13	1.74	0.69
14:f:65:ASP:OD2	15:g:79:LYS:NZ	2.25	0.69
7:x:216:LEU:HB3	7:x:249:ILE:HD11	1.73	0.69
12:d:144:SER:O	12:d:158:LYS:NZ	2.26	0.69
18:j:70:ALA:HB2	20:m:59:ILE:HG21	1.74	0.69
25:r:27:VAL:HG12	25:r:31:MET:HE2	1.75	0.68
27:C:143:ASP:OD1	27:C:143:ASP:N	2.26	0.68
29:E:155:LYS:NZ	29:E:206:ASP:OD1	2.22	0.68
17:i:236:LYS:HG2	17:i:237:MET:HG3	1.75	0.68
25:r:157:ASN:ND2	25:r:159:SER:O	2.26	0.68
27:C:457:ILE:HG23	27:C:462:ILE:HD11	1.76	0.68
5:v:65:ILE:HG12	5:v:218:MET:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:53:MET:HB3	6:w:177:ARG:HD3	1.75	0.68
10:b:117:ILE:HG22	10:b:119:LEU:H	1.55	0.68
25:r:90:PRO:HD2	25:r:240:ILE:HD13	1.74	0.68
7:8:103:LEU:HD21	7:8:291:LEU:HB2	1.74	0.68
10:b:80:TRP:HD1	12:d:41:VAL:HG13	1.59	0.68
26:B:296:LEU:HD21	26:B:317:VAL:HG11	1.74	0.68
26:B:382:CYS:HB2	26:B:424:ILE:HG23	1.76	0.68
7:8:104:SER:OG	2:Ac:51:LYS:NZ	2.27	0.68
35:L:163:SER:HA	35:L:179:LYS:HE3	1.76	0.68
51:5:335:ARG:HB2	51:5:337:LEU:HG	1.76	0.68
3:2:225:ARG:NH2	3:2:279:LEU:O	2.25	0.67
27:C:150:MET:SD	27:C:150:MET:N	2.63	0.67
28:D:93:VAL:HG11	28:D:153:ILE:HD11	1.73	0.67
43:U:148:ALA:HB1	43:U:159:VAL:HG11	1.75	0.67
48:l:246:LEU:HB3	48:l:247:LEU:HD23	1.75	0.67
48:l:372:ALA:HA	48:l:458:LEU:HD21	1.76	0.67
3:4:184:LYS:HZ2	3:4:186:MET:HE1	1.58	0.67
5:6:90:THR:HG23	5:6:95:SER:HA	1.77	0.67
20:m:37:GLY:HA3	20:m:61:LEU:HD11	1.75	0.67
51:u:134:LYS:HE3	5:v:384:MET:HE3	1.77	0.67
26:B:318:ILE:HG12	26:B:357:MET:HE1	1.76	0.67
17:i:128:LEU:HD11	17:i:213:LEU:HD23	1.75	0.67
53:G:541:PRO:HB2	53:G:561:PRO:HD3	1.76	0.67
17:i:108:LEU:HD11	17:i:191:THR:HG21	1.75	0.67
31:H:116:CYS:SG	59:H:302:SF4:S3	2.92	0.67
34:K:95:ASP:H	54:M:35:THR:HG23	1.58	0.67
35:L:203:GLY:H	35:L:206:ASP:HB2	1.60	0.67
7:8:216:LEU:HD11	57:8:401:HEC:HMB2	1.77	0.67
10:b:126:GLN:HA	50:t:89:TYR:CE2	2.30	0.67
26:B:357:MET:HG2	26:B:361:THR:HG21	1.75	0.67
46:Y:43:ARG:HB3	46:Y:46:GLN:HG2	1.76	0.66
28:D:181:HIS:HD2	28:D:183:ASP:H	1.43	0.66
14:f:73:ASN:ND2	15:g:22:SER:O	2.27	0.66
7:8:248:PRO:CB	57:8:401:HEC:HHC	2.26	0.66
1:0:69:GLU:OE2	52:z:72:ARG:NH1	2.30	0.65
19:k:75:LEU:HD11	20:m:68:PHE:HD2	1.60	0.65
45:W:105:LYS:HE3	45:W:108:GLU:HB2	1.77	0.65
52:z:76:ALA:HA	52:z:79:GLU:HG2	1.78	0.65
28:D:185:ARG:HA	39:Q:114:MET:HE3	1.78	0.65
17:i:268:GLN:HA	24:q:165:VAL:HG11	1.78	0.65
49:s:198:ASP:N	49:s:201:GLU:OE1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:162:LYS:NZ	5:6:194:ASP:OD1	2.28	0.65
26:B:319:PRO:HB3	26:B:327:ILE:HD11	1.78	0.65
31:H:142:THR:O	31:H:187:LYS:NZ	2.27	0.65
27:C:160:ALA:HA	27:C:404:THR:HG21	1.78	0.65
17:i:18:MET:O	17:i:22:ILE:HB	1.97	0.65
25:r:157:ASN:HA	25:r:168:THR:HG21	1.79	0.64
5:v:217:ARG:NH2	5:v:246:LEU:O	2.29	0.64
23:p:54:HIS:NE2	23:p:106:LEU:HD12	2.12	0.64
12:d:76:GLU:HB3	13:e:146:LYS:HD3	1.79	0.64
24:q:403:THR:HA	24:q:406:TYR:CE2	2.32	0.64
27:C:285:THR:HG23	36:N:13:GLY:HA3	1.79	0.64
8:9:13:TRP:CG	8:9:14:LEU:H	2.14	0.64
9:a:143:GLU:HB3	24:q:178:ILE:HG13	1.79	0.64
3:2:226:VAL:HG11	3:2:232:VAL:HA	1.80	0.64
29:E:177:LEU:N	55:E:301:FES:S1	2.70	0.64
3:4:243:CYS:HA	6:w:264:THR:HG21	1.79	0.64
25:r:169:GLN:HG2	25:r:174:MET:HG3	1.80	0.64
29:E:138:THR:HA	29:E:141:MET:HE2	1.80	0.64
11:c:101:TRP:CD1	22:o:47:TYR:HB2	2.31	0.64
7:8:216:LEU:HB3	7:8:249:ILE:HD11	1.80	0.64
29:E:69:ASN:O	40:R:100:GLN:NE2	2.31	0.64
48:l:5:ALA:HB2	48:l:61:MET:HE1	1.79	0.64
48:l:319:ILE:HG13	48:l:399:VAL:HG22	1.80	0.64
11:c:164:ASN:HA	11:c:181:VAL:HB	1.80	0.63
32:I:94:ARG:NE	32:I:99:GLN:OE1	2.32	0.63
35:L:136:PHE:HD2	35:L:174:ARG:HG2	1.63	0.63
48:l:286:LEU:HD22	48:l:411:MET:HG3	1.80	0.63
11:c:165:ASP:O	11:c:170:ARG:NH1	2.31	0.63
17:i:71:MET:HE3	19:k:59:MET:HE1	1.80	0.63
20:m:26:PRO:CB	20:m:72:THR:HG21	2.27	0.63
25:r:119:SER:HB2	25:r:215:TYR:CE1	2.34	0.63
53:G:389:THR:N	53:G:514:ASN:OD1	2.31	0.63
9:a:101:ILE:HG12	12:d:64:TYR:HB3	1.80	0.63
26:B:88:ARG:HB2	26:B:244:ASN:HD22	1.63	0.63
26:B:211:ALA:HB2	26:B:223:PRO:HG3	1.80	0.63
10:b:100:ARG:HH21	50:t:50:GLN:HB3	1.63	0.63
19:k:27:MET:HG2	20:m:72:THR:HG22	1.80	0.63
25:r:149:ILE:HG21	25:r:185:TRP:HB2	1.80	0.63
43:U:224:GLY:HA2	43:U:229:MET:HE3	1.81	0.63
57:8:401:HEC:HBD1	57:8:401:HEC:HHA	1.78	0.63
18:j:26:GLN:HA	25:r:60:PRO:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:q:36:LEU:HD23	24:q:39:LEU:HD12	1.80	0.63
43:U:72:LYS:HE3	43:U:163:ARG:HG3	1.80	0.63
48:l:10:THR:HA	48:l:13:ILE:HG22	1.79	0.63
56:w:402:HEM:HBC2	56:w:402:HEM:HMC1	1.80	0.63
9:a:179:ILE:HG21	16:h:38:LYS:HG3	1.80	0.63
53:G:338:VAL:HG12	53:G:544:VAL:HB	1.81	0.63
35:L:122:ILE:HG23	35:L:160:ILE:HB	1.81	0.63
5:v:89:LEU:HD22	5:v:150:GLU:HB3	1.81	0.63
5:6:183:ARG:NH2	5:v:451:ASP:OD2	2.32	0.62
53:G:63:PHE:HB2	53:G:75:CYS:HB2	1.81	0.62
7:8:187:ARG:HA	7:8:190:ASN:HD21	1.64	0.62
32:I:86:MET:HB2	32:I:91:VAL:HB	1.81	0.62
6:7:112:THR:HG22	6:7:196:HIS:CE1	2.33	0.62
19:k:18:GLY:O	20:m:23:LYS:NZ	2.21	0.62
19:k:23:ARG:HH21	20:m:86:ASN:HD22	1.47	0.62
52:Aa:19:LEU:HD22	52:Aa:24:GLN:HB3	1.79	0.62
48:l:400:ASN:HA	48:l:409:LEU:HD11	1.80	0.62
8:y:92:GLU:HG2	8:y:96:LYS:HE3	1.81	0.62
48:l:306:THR:HG22	48:l:336:LYS:HG2	1.81	0.62
27:C:187:LEU:HD21	27:C:216:MET:HB2	1.81	0.62
35:L:290:HIS:O	35:L:294:ARG:HB2	2.00	0.62
51:u:120:LEU:HD13	51:u:133:ILE:HG12	1.81	0.62
24:q:208:PRO:HD3	24:q:236:LEU:HD22	1.80	0.62
26:B:164:ASN:HB3	40:R:78:HIS:HB2	1.80	0.62
5:6:216:ALA:HB3	5:6:244:LEU:H	1.65	0.62
5:6:272:VAL:HG12	5:6:337:GLY:HA3	1.81	0.62
42:T:155:PRO:HD3	49:s:206:THR:HG21	1.81	0.62
24:q:11:LEU:HB3	24:q:100:ILE:HD13	1.82	0.61
29:E:188:ILE:HG22	29:E:189:ASN:H	1.64	0.61
29:E:191:ASN:HB3	29:E:216:PRO:HB3	1.81	0.61
50:t:90:CYS:HA	50:t:93:LEU:HD12	1.80	0.61
25:r:31:MET:HG2	31:H:77:LEU:HB2	1.83	0.61
12:d:122:ARG:NH1	48:l:203:MET:O	2.34	0.61
26:B:371:ILE:HD13	26:B:396:MET:HG3	1.83	0.61
37:X:138:LEU:HG	37:X:144:ILE:HG12	1.82	0.61
26:B:314:LEU:HD11	26:B:317:VAL:HG23	1.81	0.61
37:O:104:PHE:CD2	37:O:139:MET:HA	2.35	0.61
39:Q:47:PHE:O	39:Q:57:ARG:NH2	2.34	0.61
27:C:344:ARG:HB3	45:W:21:TYR:O	2.01	0.61
5:6:61:ILE:HD11	5:6:225:VAL:HG11	1.83	0.61
6:7:113:TRP:NE1	6:7:301:LEU:O	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:41:ILE:HG21	19:k:73:LEU:HD21	1.82	0.61
35:L:231:VAL:HB	35:L:265:ARG:HH21	1.66	0.61
17:i:96:THR:O	17:i:100:MET:HG2	2.01	0.61
20:m:26:PRO:HB2	20:m:72:THR:CG2	2.27	0.61
35:L:119:ASN:HD22	35:L:120:VAL:HG23	1.66	0.61
16:h:86:LEU:HD23	16:h:92:TYR:HB2	1.82	0.61
17:i:31:ILE:HD11	19:k:62:ILE:HG21	1.83	0.61
53:G:341:ILE:HG12	53:G:545:LEU:HD11	1.82	0.61
20:m:86:ASN:HB3	20:m:89:VAL:HG23	1.83	0.60
28:D:128:ILE:HB	28:D:145:THR:HG23	1.83	0.60
3:2:198:ARG:HH12	3:2:254:GLY:HA2	1.65	0.60
3:4:230:GLU:HG3	3:4:231:TRP:HD1	1.66	0.60
24:q:370:PRO:HB2	48:l:142:ILE:HG12	1.83	0.60
35:L:198:PRO:HA	35:L:260:PHE:HB2	1.83	0.60
48:l:214:ILE:HG12	48:l:276:MET:HE1	1.83	0.60
10:b:99:GLU:HG2	48:l:61:MET:HG2	1.81	0.60
28:D:218:ARG:HD2	39:Q:127:THR:HA	1.83	0.60
37:O:138:LEU:O	37:O:139:MET:HB2	2.01	0.60
6:w:132:VAL:HA	6:w:139:SER:HB3	1.82	0.60
7:x:96:PRO:HA	7:x:100:ARG:HE	1.66	0.60
20:m:125:TRP:HB2	45:W:137:THR:HG21	1.82	0.60
29:E:246:GLN:HB3	29:E:249:LEU:HD23	1.84	0.60
46:Y:47:PHE:HE1	48:l:364:LYS:HD3	1.66	0.60
52:Aa:21:PRO:HA	52:Aa:24:GLN:HE21	1.65	0.60
7:8:187:ARG:HA	7:8:190:ASN:ND2	2.16	0.60
7:8:228:LEU:HD11	7:8:234:PHE:HB2	1.83	0.60
16:h:59:GLU:OE2	49:s:222:ARG:NH1	2.33	0.60
48:l:504:LEU:O	48:l:507:THR:OG1	2.20	0.60
2:Ac:20:THR:HG22	4:Ad:23:MET:HE2	1.83	0.60
25:r:119:SER:HB2	25:r:215:TYR:HE1	1.66	0.60
48:l:184:LEU:HD21	48:l:211:MET:HG2	1.84	0.60
24:q:104:LEU:HG	24:q:108:MET:HE2	1.84	0.60
24:q:369:LEU:HD13	48:l:149:ILE:HG13	1.84	0.60
51:5:276:ARG:NH2	51:5:466:PRO:O	2.32	0.60
24:q:247:THR:HB	24:q:304:GLN:HE21	1.66	0.60
43:U:110:LEU:HD13	43:U:336:LEU:HD11	1.84	0.60
45:W:82:ARG:HG2	45:W:86:MET:HE2	1.84	0.60
48:l:414:ILE:O	48:l:418:LEU:HG	2.02	0.60
5:6:138:LEU:HD12	5:6:233:VAL:HG22	1.84	0.59
26:B:366:ALA:HA	29:E:141:MET:HE1	1.84	0.59
5:6:151:VAL:O	5:6:155:GLN:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:4:TYR:HD2	10:b:9:LYS:HG2	1.67	0.59
5:6:82:LEU:HD21	5:6:151:VAL:HG13	1.84	0.59
20:m:130:THR:HG21	45:W:124:LEU:HD12	1.84	0.59
35:L:274:TYR:HB2	35:L:367:ALA:HB2	1.85	0.59
27:C:172:ARG:NH1	27:C:241:ASP:OD2	2.36	0.59
8:y:69:LEU:HD11	8:y:76:LEU:HD13	1.84	0.59
5:6:111:SER:HB3	3:Ae:59:LEU:HG	1.84	0.59
5:6:378:LEU:HD13	5:6:416:ILE:HD12	1.84	0.59
26:B:146:GLY:HA3	26:B:193:PHE:CE1	2.37	0.59
1:0:33:VAL:HG12	1:0:82:VAL:HG22	1.85	0.59
19:k:27:MET:HE3	19:k:30:LEU:HB2	1.83	0.59
23:p:76:ARG:HG2	47:Z:65:GLU:HB3	1.85	0.59
1:0:57:VAL:HG22	1:0:65:GLU:HG3	1.84	0.59
3:4:145:GLY:HA3	7:8:300:LEU:HD21	1.85	0.59
17:i:193:VAL:HG13	17:i:266:ILE:HG23	1.85	0.59
24:q:325:MET:HE2	24:q:329:LEU:HD11	1.85	0.59
26:B:116:ASN:ND2	26:B:207:GLY:O	2.36	0.59
6:w:97:HIS:HE1	56:w:401:HEM:C1A	2.21	0.59
51:5:179:MET:HE1	51:5:282:LEU:HD13	1.85	0.59
5:6:60:ARG:NH2	5:6:124:GLU:OE1	2.36	0.59
17:i:171:ASN:ND2	27:C:58:MET:O	2.36	0.59
33:J:75:ARG:NH2	33:J:102:ASP:O	2.35	0.58
53:G:355:LYS:NZ	53:G:528:LEU:O	2.30	0.58
24:q:401:MET:HA	48:l:176:ARG:HG2	1.84	0.58
48:l:250:SER:HB2	48:l:333:ALA:HA	1.85	0.58
6:w:196:HIS:HE1	56:w:401:HEM:ND	2.01	0.58
19:k:75:LEU:HD11	20:m:68:PHE:CD2	2.38	0.58
20:m:17:PHE:HA	20:m:20:PHE:CE2	2.38	0.58
29:E:169:PHE:HE2	29:E:209:LYS:HG3	1.68	0.58
33:J:154:LYS:HZ3	33:J:156:LYS:HE3	1.66	0.58
39:Q:66:TYR:CZ	39:Q:86:ARG:HD3	2.38	0.58
17:i:57:THR:HG22	19:k:77:LEU:HB3	1.86	0.58
23:p:153:GLU:HA	23:p:156:MET:HG3	1.85	0.58
25:r:236:ALA:HA	25:r:263:THR:HG22	1.84	0.58
27:C:228:MET:HG3	32:I:167:PRO:HG3	1.84	0.58
35:L:161:HIS:HB3	35:L:195:ILE:HG12	1.84	0.58
53:G:74:ASN:HD21	53:G:179:CYS:HA	1.67	0.58
25:r:308:PRO:HB2	25:r:314:ILE:HD13	1.84	0.58
28:D:215:GLU:OE1	35:L:70:ARG:NH2	2.37	0.58
5:6:55:TYR:HA	5:6:127:ARG:HH12	1.67	0.58
5:6:240:MET:SD	5:6:241:ARG:N	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:106:VAL:HG13	24:q:453:MET:HE3	1.86	0.58
27:C:460:GLN:O	27:C:461:ASP:C	2.47	0.58
34:K:60:ARG:HH22	34:K:95:ASP:HA	1.69	0.58
17:i:93:VAL:HG13	48:l:599:MET:HE1	1.85	0.58
18:j:1:MET:SD	18:j:1:MET:N	2.64	0.58
26:B:115:VAL:HG22	26:B:248:VAL:HG21	1.85	0.58
26:B:384:PRO:HD2	53:G:76:ARG:HG3	1.85	0.58
46:Y:54:GLN:HE21	48:l:446:ASN:HB2	1.68	0.58
48:l:562:LEU:HB2	48:l:563:PRO:HD3	1.85	0.58
6:w:338:ILE:HD11	6:w:350:ILE:HG22	1.84	0.58
10:b:85:TYR:HE2	48:l:65:ASN:HB2	1.68	0.58
17:i:17:THR:HG22	17:i:137:ALA:HB2	1.86	0.58
20:m:34:ILE:HG12	20:m:65:LEU:HD21	1.86	0.58
28:D:101:ARG:NH1	28:D:159:VAL:O	2.37	0.58
6:7:132:VAL:HA	6:7:139:SER:HB3	1.86	0.58
7:8:271:VAL:O	7:8:275:LEU:HG	2.04	0.58
11:c:159:LYS:NZ	11:c:160:GLN:O	2.37	0.58
7:x:291:LEU:HD11	7:x:295:MET:HE3	1.86	0.58
53:G:257:VAL:HG11	53:G:413:LEU:HB2	1.84	0.58
11:c:166:LEU:HB3	11:c:169:GLU:HB2	1.86	0.57
17:i:20:VAL:HG11	17:i:137:ALA:HB1	1.85	0.57
19:k:27:MET:O	19:k:31:LEU:HG	2.03	0.57
48:l:34:ASN:OD1	48:l:34:ASN:N	2.37	0.57
13:e:82:VAL:HG23	24:q:25:ILE:HD11	1.86	0.57
41:S:69:ILE:HD13	49:s:148:PHE:HB3	1.86	0.57
3:Ae:52:GLY:HA2	3:Ae:61:ALA:HA	1.87	0.57
5:v:90:THR:HG23	5:v:95:SER:HA	1.86	0.57
56:w:401:HEM:HMC2	56:w:401:HEM:HBC2	1.85	0.57
7:8:186:ALA:O	7:8:190:ASN:OD1	2.21	0.57
5:v:82:LEU:HD21	5:v:151:VAL:HG13	1.86	0.57
5:v:290:GLN:HG3	5:v:325:ALA:HB3	1.85	0.57
28:D:215:GLU:HG3	35:L:63:TYR:CD2	2.38	0.57
32:I:65:MET:HE1	32:I:97:PRO:HG3	1.85	0.57
33:J:75:ARG:HH12	33:J:104:ARG:HG3	1.70	0.57
3:4:106:VAL:HG22	51:5:275:ILE:HD11	1.87	0.57
11:c:169:GLU:OE1	11:c:169:GLU:N	2.37	0.57
39:Q:51:MET:HG3	39:Q:55:LYS:HE2	1.87	0.57
48:l:323:HIS:ND1	48:l:475:MET:SD	2.78	0.57
53:G:89:VAL:HB	53:G:94:MET:HG3	1.87	0.57
1:0:34:ARG:HD2	1:0:78:ARG:CZ	2.35	0.57
2:1:56:ILE:HB	2:1:59:LYS:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:7:402:HEM:HMB1	56:7:402:HEM:HBB2	1.86	0.57
9:a:139:ILE:HG12	24:q:54:LEU:HD23	1.87	0.57
11:c:184:TYR:HD1	50:t:36:GLU:HA	1.69	0.57
16:h:16:ARG:O	16:h:19:THR:OG1	2.23	0.57
35:L:206:ASP:CG	35:L:208:PHE:H	2.12	0.57
48:l:223:LYS:HE3	48:l:252:MET:HE3	1.87	0.57
2:1:11:TYR:HA	2:1:15:PHE:HB2	1.86	0.57
5:6:221:ILE:HG12	5:6:396:VAL:HG12	1.86	0.57
26:B:140:GLU:HG3	26:B:252:PRO:HG3	1.86	0.57
51:u:102:LYS:HG2	51:u:153:ASN:HB3	1.86	0.57
5:v:138:LEU:HD11	5:v:233:VAL:HG13	1.87	0.57
16:h:82:GLN:HE21	16:h:82:GLN:HA	1.69	0.56
31:H:118:LEU:HD23	31:H:161:ALA:HB1	1.87	0.56
35:L:165:LEU:HD23	35:L:197:LYS:HE3	1.87	0.56
3:4:260:HIS:HB2	55:4:301:FES:S2	2.45	0.56
7:8:193:ALA:HB1	57:8:401:HEC:HAD1	1.88	0.56
25:r:102:VAL:CG1	25:r:150:LEU:HD21	2.36	0.56
31:H:101:HIS:H	31:H:149:MET:HE1	1.69	0.56
48:l:481:THR:HB	50:t:92:HIS:HD2	1.70	0.56
6:w:101:GLY:HA2	6:w:106:SER:HB2	1.87	0.56
53:G:266:ARG:HG2	53:G:267:THR:HG23	1.85	0.56
9:a:130:GLU:O	9:a:134:GLU:HG2	2.05	0.56
10:b:16:ARG:HD2	37:X:146:ASP:HB2	1.88	0.56
11:c:84:GLN:HA	11:c:98:ARG:HH21	1.69	0.56
21:n:57:TRP:CE3	21:n:57:TRP:HA	2.40	0.56
24:q:266:MET:HE2	24:q:395:LEU:HD12	1.87	0.56
24:q:405:LEU:HD11	48:l:173:LEU:HD13	1.87	0.56
27:C:172:ARG:NH2	45:W:9:ASP:O	2.37	0.56
29:E:85:LEU:HG	40:R:87:LEU:HD13	1.86	0.56
31:H:162:CYS:SG	59:H:302:SF4:S2	3.03	0.56
43:U:178:GLN:NE2	43:U:238:ASP:OD2	2.39	0.56
43:U:263:ARG:HD3	43:U:264:GLU:HG3	1.87	0.56
49:s:160:THR:HA	49:s:163:TRP:CD1	2.41	0.56
50:t:43:GLN:HA	50:t:46:MET:HE2	1.86	0.56
53:G:643:ARG:NH1	53:G:656:TYR:OH	2.38	0.56
49:s:188:VAL:HG13	49:s:194:TRP:HB2	1.87	0.56
6:w:186:PRO:HG2	56:w:402:HEM:HMC3	1.87	0.56
6:w:83:HIS:NE2	56:w:402:HEM:NC	2.54	0.56
52:Aa:19:LEU:HD21	52:Aa:23:GLU:HB2	1.88	0.56
7:8:215:LEU:O	7:8:235:ASN:ND2	2.39	0.56
7:x:153:VAL:HG21	7:x:177:PRO:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:13:TRP:CD1	8:9:14:LEU:H	2.24	0.56
11:c:133:LEU:HD23	48:l:532:ILE:HD11	1.88	0.56
18:j:67:LEU:HD11	19:k:68:ALA:HB3	1.87	0.56
56:w:401:HEM:HBB2	56:w:401:HEM:HMB2	1.87	0.56
5:6:227:HIS:CD2	5:6:231:LYS:HD2	2.40	0.56
7:8:122:CYS:SG	57:8:401:HEC:CBB	2.92	0.56
27:C:124:ARG:HG2	32:I:108:THR:HG21	1.87	0.56
6:w:253:PRO:HB3	7:x:203:ARG:O	2.05	0.56
5:6:84:ARG:HE	5:6:114:SER:HB3	1.71	0.56
32:I:74:VAL:HA	32:I:77:MET:HE2	1.88	0.56
37:O:133:ILE:O	37:O:137:LYS:HG2	2.05	0.56
12:d:140:GLN:HB2	22:o:127:ILE:HG22	1.88	0.56
28:D:220:VAL:HG21	39:Q:136:THR:HG21	1.88	0.56
26:B:114:VAL:HG11	26:B:212:LEU:HD22	1.88	0.55
6:w:94:LEU:HD21	56:w:401:HEM:HAB	1.88	0.55
33:J:71:HIS:HA	33:J:75:ARG:HG3	1.87	0.55
38:P:68:ARG:HA	38:P:74:GLU:HG2	1.88	0.55
10:b:31:ARG:NH1	10:b:33:PRO:HG3	2.21	0.55
14:f:68:GLU:HG2	15:g:21:ARG:HE	1.71	0.55
17:i:95:MET:HE2	17:i:149:ILE:HA	1.88	0.55
25:r:185:TRP:NE1	25:r:238:THR:HG22	2.20	0.55
51:u:276:ARG:NH2	51:u:466:PRO:O	2.30	0.55
53:G:68:ARG:HE	53:G:283:GLU:HB3	1.71	0.55
5:6:89:LEU:HD22	5:6:150:GLU:HB3	1.87	0.55
7:8:122:CYS:SG	57:8:401:HEC:HAB	2.40	0.55
49:s:95:VAL:HG12	49:s:97:VAL:HG22	1.87	0.55
51:5:156:LEU:O	51:5:213:ARG:NH1	2.39	0.55
5:6:36:GLN:HE21	5:6:53:GLU:HB3	1.71	0.55
5:6:63:LEU:HD23	5:6:141:THR:HG21	1.88	0.55
56:7:402:HEM:HBC2	56:7:402:HEM:HMC2	1.89	0.55
15:g:27:LYS:HG2	15:g:29:THR:H	1.71	0.55
26:B:48:ARG:HE	29:E:231:LEU:HD11	1.71	0.55
30:F:53:VAL:HG21	35:L:76:ILE:HD13	1.86	0.55
44:V:62:THR:HG22	44:V:104:ARG:HD3	1.89	0.55
49:s:121:MET:O	49:s:125:TRP:HD1	1.89	0.55
3:2:257:CYS:HB3	3:2:262:SER:HB2	1.89	0.55
3:4:209:ALA:HA	3:4:221:HIS:CE1	2.42	0.55
24:q:329:LEU:HD23	24:q:437:MET:HE3	1.88	0.55
28:D:129:VAL:HG22	28:D:144:LYS:HD2	1.87	0.55
35:L:130:GLU:HG3	35:L:135:ASP:HA	1.88	0.55
6:w:32:ASN:HD21	6:w:227:LYS:HG2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:269:ARG:HA	3:2:278:ASN:HB3	1.89	0.55
6:7:47:THR:HG23	6:7:79:ILE:HG23	1.88	0.55
11:c:96:ASP:OD2	24:q:346:ARG:NH1	2.40	0.55
18:j:59:ALA:HB1	20:m:67:VAL:HG23	1.88	0.55
20:m:65:LEU:HA	20:m:68:PHE:HB2	1.88	0.55
25:r:117:LEU:HG	25:r:136:VAL:HG22	1.88	0.55
27:C:161:VAL:O	27:C:165:LEU:HB2	2.07	0.55
29:E:111:ARG:NH1	33:J:173:SER:OG	2.40	0.55
30:F:71:ILE:HD11	30:F:115:GLY:HA3	1.89	0.55
48:l:65:ASN:H	48:l:65:ASN:HD22	1.54	0.55
5:v:320:PRO:HB3	3:Af:75:LEU:HB3	1.89	0.55
39:Q:48:SER:HB2	39:Q:53:GLU:HB3	1.88	0.55
51:u:152:GLN:HG2	51:u:253:LEU:HD22	1.88	0.55
7:8:245:MET:HE1	7:8:248:PRO:HG3	1.89	0.55
22:o:41:SER:OG	23:p:191:PRO:O	2.23	0.55
26:B:141:GLY:HA2	26:B:252:PRO:HD3	1.87	0.55
39:Q:118:GLU:HB3	39:Q:124:LYS:HG3	1.89	0.55
42:T:141:PRO:HG3	49:s:118:LYS:HD2	1.89	0.55
48:l:97:THR:HG22	48:l:246:LEU:HD21	1.89	0.55
52:z:37:ASN:OD1	52:z:40:ARG:NH1	2.39	0.55
25:r:199:ASP:HB3	25:r:279:ARG:HH21	1.71	0.54
37:O:140:CYS:HB3	37:O:143:GLU:HG3	1.89	0.54
48:l:566:THR:O	48:l:570:GLN:HG2	2.07	0.54
50:t:59:CYS:HA	50:t:61:HIS:CE1	2.42	0.54
22:o:17:THR:HB	23:p:110:GLU:HG2	1.88	0.54
43:U:102:ASP:OD1	43:U:104:LYS:N	2.40	0.54
5:v:231:LYS:O	5:v:235:GLU:HG2	2.07	0.54
3:4:100:SER:N	51:5:176:ASP:OD1	2.40	0.54
18:j:113:TRP:O	18:j:114:ALA:C	2.49	0.54
22:o:28:GLU:OE2	51:u:83:ASN:ND2	2.40	0.54
26:B:174:ARG:O	26:B:178:GLU:HG2	2.06	0.54
38:P:18:GLU:HG3	38:P:68:ARG:HB3	1.89	0.54
6:w:237:LEU:HD13	7:x:297:MET:HG2	1.88	0.54
7:x:112:ARG:HB2	7:x:140:CYS:HB2	1.88	0.54
35:L:43:ARG:NH2	35:L:93:GLY:O	2.41	0.54
48:l:145:GLU:OE2	48:l:176:ARG:NH1	2.40	0.54
48:l:536:LEU:HB3	48:l:537:PRO:HD3	1.89	0.54
4:3:16:ASN:HD22	51:u:382:SER:HA	1.73	0.54
10:b:119:LEU:O	10:b:120:MET:C	2.50	0.54
20:m:103:MET:HE3	20:m:115:ILE:HD12	1.90	0.54
28:D:66:ALA:HA	28:D:73:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:31:TRP:NE1	56:7:402:HEM:O1D	2.39	0.54
13:e:97:ILE:O	13:e:101:LEU:HB2	2.07	0.54
26:B:225:LEU:HD22	26:B:424:ILE:HD12	1.88	0.54
27:C:219:PHE:O	27:C:223:VAL:HG22	2.08	0.54
31:H:116:CYS:HG	59:H:302:SF4:FE1	1.23	0.54
6:w:300:ILE:HD11	6:w:363:LEU:HD21	1.89	0.54
7:8:217:THR:HA	7:8:264:MET:HE2	1.89	0.54
6:w:281:LEU:HB2	6:w:294:LEU:HD12	1.90	0.54
51:5:52:GLN:HE21	51:5:56:GLY:HA2	1.72	0.54
53:G:219:SER:OG	53:G:288:ASP:OD2	2.25	0.54
53:G:347:ASP:N	53:G:347:ASP:OD1	2.40	0.54
5:6:60:ARG:HD3	5:6:393:LEU:HD22	1.89	0.54
17:i:237:MET:HB3	17:i:240:ILE:HD13	1.89	0.54
45:W:73:PRO:HG2	49:s:117:ASN:HB3	1.89	0.54
5:6:317:VAL:HG13	5:6:319:GLN:HE21	1.71	0.54
8:9:69:LEU:HD11	8:9:76:LEU:HD13	1.90	0.54
19:k:27:MET:HG2	20:m:72:THR:CG2	2.38	0.54
24:q:416:ARG:HG2	48:l:159:HIS:HB3	1.90	0.54
35:L:206:ASP:OD1	35:L:207:ARG:N	2.41	0.54
35:L:270:ASP:OD1	35:L:270:ASP:N	2.40	0.54
48:l:302:VAL:O	48:l:306:THR:HG23	2.07	0.54
2:Ac:30:LEU:HG	4:Ad:34:TRP:HB2	1.89	0.54
22:o:30:ARG:NH1	51:u:260:ASP:O	2.41	0.54
48:l:245:ALA:HB2	48:l:340:PHE:HB3	1.89	0.54
48:l:289:ALA:HB1	48:l:418:LEU:HB2	1.89	0.54
6:w:344:GLU:HG3	52:z:67:PHE:HE1	1.71	0.54
3:2:225:ARG:NH1	3:2:267:SER:O	2.41	0.53
7:8:216:LEU:HD21	57:8:401:HEC:C2B	2.38	0.53
17:i:28:LEU:HD23	17:i:31:ILE:HD12	1.90	0.53
24:q:139:GLN:HB2	24:q:222:GLU:OE1	2.08	0.53
25:r:114:TYR:HA	25:r:117:LEU:HB2	1.90	0.53
27:C:416:TYR:HB3	27:C:429:LYS:HB3	1.91	0.53
41:S:52:ARG:NH2	41:S:58:ASN:OD1	2.42	0.53
48:l:247:LEU:HD12	48:l:248:HIS:CE1	2.43	0.53
53:G:83:GLU:HG2	53:G:84:LYS:HG2	1.89	0.53
12:d:107:GLN:OE1	48:l:194:ASN:ND2	2.41	0.53
25:r:26:LYS:HA	25:r:36:GLY:HA3	1.91	0.53
43:U:291:ARG:HH22	43:U:294:HIS:HD2	1.56	0.53
53:G:405:THR:HB	53:G:477:GLY:HA3	1.91	0.53
3:4:216:LEU:HD13	3:4:269:ARG:HD2	1.90	0.53
16:h:50:ILE:O	16:h:54:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:J:154:LYS:NZ	33:J:156:LYS:HE3	2.24	0.53
35:L:165:LEU:HA	35:L:197:LYS:HE3	1.90	0.53
39:Q:97:ALA:HA	61:Q:201:ZMP:O4	2.07	0.53
48:l:8:THR:O	48:l:11:THR:OG1	2.26	0.53
50:t:58:TYR:O	50:t:61:HIS:HE1	1.91	0.53
51:u:377:MET:HE3	51:u:475:MET:HA	1.90	0.53
7:x:244:ALA:HB3	57:x:401:HEC:HBD2	1.90	0.53
52:z:20:SER:HB3	52:z:23:GLU:HG3	1.91	0.53
53:G:218:LEU:HB3	53:G:221:ASN:HD22	1.73	0.53
24:q:12:LEU:HB2	24:q:13:PRO:HD3	1.89	0.53
25:r:26:LYS:HG2	25:r:36:GLY:HA3	1.89	0.53
6:w:94:LEU:HD11	6:w:123:VAL:HG11	1.90	0.53
6:w:246:SER:HB2	6:w:249:LEU:HB2	1.89	0.53
25:r:24:GLU:OE2	25:r:274:ARG:NH1	2.42	0.53
26:B:425:CYS:SG	26:B:426:ALA:N	2.81	0.53
5:v:36:GLN:HG3	5:v:53:GLU:HB3	1.91	0.53
53:G:228:VAL:HG23	53:G:230:ALA:H	1.74	0.53
21:n:57:TRP:HA	21:n:57:TRP:HE3	1.74	0.53
35:L:197:LYS:N	35:L:258:PHE:O	2.40	0.53
47:Z:32:LEU:HD12	47:Z:32:LEU:H	1.73	0.53
3:2:100:SER:OG	3:2:101:HIS:N	2.42	0.53
11:c:110:ASP:OD1	11:c:110:ASP:N	2.42	0.53
35:L:190:PHE:HB3	35:L:193:ALA:HB2	1.90	0.53
51:u:145:GLU:HG2	51:u:249:HIS:CE1	2.44	0.53
5:v:407:VAL:HG23	5:v:411:THR:HB	1.89	0.53
6:w:187:PHE:O	6:w:190:THR:OG1	2.24	0.53
3:2:113:ARG:HH21	3:2:117:VAL:HB	1.74	0.53
24:q:315:LEU:HD12	24:q:381:ILE:HD12	1.91	0.53
31:H:158:CYS:SG	59:H:301:SF4:S1	2.97	0.53
39:Q:92:MET:SD	39:Q:95:LYS:NZ	2.62	0.53
48:l:97:THR:HG21	48:l:125:LEU:HD13	1.90	0.53
51:u:140:LEU:HD22	51:u:237:VAL:HG12	1.89	0.53
5:v:379:LYS:HG2	5:v:413:LEU:HD22	1.91	0.53
7:x:97:TRP:HB2	7:x:100:ARG:HG3	1.91	0.53
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.44	0.53
25:r:100:LEU:HD23	25:r:160:TYR:HB2	1.91	0.53
28:D:213:ASP:OD1	35:L:70:ARG:NH2	2.42	0.53
31:H:115:ALA:HB3	31:H:140:ARG:HG2	1.90	0.53
51:u:388:VAL:HG21	51:u:438:ALA:HA	1.91	0.53
53:G:389:THR:OG1	53:G:511:LYS:O	2.26	0.53
25:r:209:SER:HB3	25:r:213:VAL:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:178:VAL:HG23	27:C:317:TYR:CZ	2.43	0.53
43:U:352:LYS:HD3	43:U:353:TRP:HD1	1.74	0.53
48:l:315:VAL:O	48:l:319:ILE:HG12	2.09	0.53
6:w:182:HIS:HE1	56:w:402:HEM:NB	1.99	0.53
53:G:229:GLY:N	59:G:801:SF4:S2	2.75	0.53
2:1:4:PRO:HB2	2:1:9:ARG:HE	1.74	0.52
3:4:262:SER:HA	3:4:273:GLY:CA	2.39	0.52
14:f:66:VAL:HG12	14:f:70:LYS:HE3	1.90	0.52
6:w:196:HIS:CE1	56:w:401:HEM:ND	2.77	0.52
17:i:2:ASN:HB3	17:i:5:ILE:HD13	1.92	0.52
24:q:5:ILE:HG23	24:q:104:LEU:HD11	1.91	0.52
24:q:269:MET:HG3	24:q:270:ILE:HD12	1.91	0.52
27:C:46:ASP:OD1	27:C:47:VAL:N	2.36	0.52
34:K:52:ASN:HB3	54:M:29:GLN:NE2	2.24	0.52
48:l:559:GLU:O	48:l:563:PRO:HD2	2.08	0.52
53:G:495:ASN:HA	53:G:498:GLN:HG2	1.91	0.52
15:g:89:ASP:OD2	49:s:243:ARG:NH1	2.35	0.52
6:7:112:THR:O	6:7:196:HIS:NE2	2.43	0.52
7:8:248:PRO:HB3	57:8:401:HEC:HHC	1.90	0.52
48:l:419:THR:HA	48:l:422:TYR:CE2	2.45	0.52
21:n:17:VAL:HG11	24:q:30:HIS:CG	2.45	0.52
53:G:131:CYS:SG	53:G:175:ARG:NH1	2.83	0.52
3:2:177:LEU:HB2	3:2:290:ASP:HA	1.92	0.52
3:2:265:ASP:OD1	3:2:269:ARG:N	2.42	0.52
5:6:70:ARG:HH22	5:6:332:ASP:HB2	1.74	0.52
7:8:251:ASN:OD1	7:8:251:ASN:N	2.40	0.52
9:a:152:LYS:HD3	15:g:96:VAL:HG21	1.91	0.52
10:b:97:VAL:HG13	48:l:61:MET:HE3	1.90	0.52
13:e:70:ASN:HD22	13:e:73:SER:HA	1.75	0.52
17:i:44:LEU:HD22	17:i:122:ILE:HG21	1.90	0.52
27:C:321:GLU:O	27:C:352:GLN:NE2	2.41	0.52
27:C:389:LYS:HG3	53:G:144:MET:HG3	1.92	0.52
28:D:76:VAL:HG22	54:M:70:MET:HB3	1.92	0.52
35:L:60:LEU:HA	35:L:237:ILE:HD11	1.91	0.52
43:U:170:VAL:HG13	43:U:242:ALA:HB3	1.92	0.52
49:s:160:THR:HA	49:s:163:TRP:NE1	2.23	0.52
2:Ac:54:LYS:HD3	2:Ac:54:LYS:H	1.73	0.52
6:7:26:ASN:HD21	6:7:207:ASN:HB2	1.74	0.52
19:k:26:LEU:HB3	19:k:78:LEU:HD12	1.91	0.52
7:x:216:LEU:HD11	57:x:401:HEC:HMB2	1.92	0.52
53:G:50:LEU:O	53:G:54:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:122:ARG:NH2	48:l:202:PHE:O	2.42	0.52
18:j:67:LEU:HD21	19:k:68:ALA:HB3	1.92	0.52
25:r:61:LEU:HD23	32:I:125:PRO:HB3	1.91	0.52
27:C:175:TRP:HA	27:C:178:VAL:HG12	1.92	0.52
31:H:157:PHE:O	31:H:158:CYS:HB2	2.08	0.52
53:G:326:VAL:HG23	53:G:626:LEU:HD13	1.92	0.52
33:J:137:PHE:HA	33:J:140:LYS:HE3	1.91	0.52
36:N:36:GLY:O	36:N:45:ARG:NH2	2.43	0.52
48:l:293:ILE:HD11	48:l:418:LEU:HD22	1.91	0.52
3:Ae:47:GLY:C	3:Ae:49:PHE:H	2.18	0.52
17:i:128:LEU:HD13	17:i:216:PHE:HB2	1.92	0.52
11:c:100:ASN:HB2	11:c:103:GLU:CD	2.35	0.51
50:t:62:TYR:CE1	50:t:86:ASP:HB3	2.46	0.51
8:y:107:GLU:HA	8:y:110:LYS:HD3	1.92	0.51
3:2:251:ASP:OD1	3:2:251:ASP:N	2.42	0.51
10:b:76:LEU:O	10:b:79:VAL:HG12	2.10	0.51
19:k:37:MET:HE3	19:k:67:ALA:HA	1.93	0.51
20:m:31:LEU:HD11	25:r:70:MET:SD	2.50	0.51
24:q:122:PHE:HD1	24:q:238:LEU:HD13	1.75	0.51
27:C:93:GLN:NE2	27:C:93:GLN:O	2.44	0.51
31:H:162:CYS:HG	59:H:302:SF4:FE4	0.40	0.51
35:L:349:ARG:O	35:L:352:ARG:HB3	2.10	0.51
43:U:225:ASN:HB3	43:U:228:GLU:HB2	1.93	0.51
37:X:128:PHE:CZ	37:X:148:ILE:HG12	2.45	0.51
48:l:247:LEU:HD12	48:l:248:HIS:HE1	1.76	0.51
3:4:183:GLY:N	3:4:199:HIS:O	2.29	0.51
5:6:421:ASP:N	5:6:421:ASP:OD1	2.40	0.51
11:c:155:PRO:HD3	50:t:4:HIS:CE1	2.46	0.51
17:i:337:LEU:O	17:i:340:THR:HG23	2.11	0.51
18:j:18:VAL:HG11	25:r:76:ILE:HD11	1.92	0.51
33:J:79:ILE:HG12	33:J:99:MET:HG3	1.93	0.51
35:L:203:GLY:N	35:L:206:ASP:HB2	2.25	0.51
38:P:35:ASP:HA	38:P:38:GLU:HG2	1.91	0.51
49:s:187:CYS:SG	49:s:188:VAL:N	2.83	0.51
51:5:375:GLN:OE1	51:5:378:ARG:NH1	2.39	0.51
3:2:120:SER:OG	51:u:269:ARG:NH2	2.44	0.51
4:3:9:ARG:NH1	8:9:109:ALA:O	2.44	0.51
27:C:137:GLN:O	27:C:140:PRO:HD2	2.10	0.51
39:Q:89:VAL:HG22	61:Q:201:ZMP:H7	1.91	0.51
5:v:116:ARG:NH1	5:v:188:ASN:O	2.42	0.51
53:G:64:CYS:HB3	53:G:75:CYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:297:PRO:HB3	5:6:304:ASN:HD21	1.75	0.51
6:7:67:THR:HG22	7:8:200:TYR:HE2	1.75	0.51
6:7:211:ILE:HD12	8:9:37:THR:HA	1.92	0.51
26:B:263:ALA:HA	26:B:271:SER:HB2	1.93	0.51
36:N:89:SER:OG	36:N:93:LYS:NZ	2.42	0.51
6:7:81:TYR:OH	7:8:203:ARG:NH1	2.44	0.51
18:j:20:ILE:O	18:j:25:PRO:HD3	2.11	0.51
25:r:200:LEU:HD21	25:r:280:PHE:O	2.11	0.51
26:B:131:ILE:HG13	26:B:165:GLU:HB3	1.92	0.51
41:S:37:ARG:O	45:W:143:TYR:OH	2.24	0.51
51:5:294:PRO:HB2	51:5:298:ASN:HB3	1.93	0.51
3:4:193:LYS:HE3	6:w:169:SER:HB3	1.91	0.51
3:4:198:ARG:HB3	3:4:232:VAL:HG13	1.93	0.51
6:7:196:HIS:HE1	56:7:402:HEM:ND	2.08	0.51
9:a:130:GLU:HB3	21:n:45:PHE:CG	2.45	0.51
9:a:132:ASN:HD22	24:q:45:LEU:HD12	1.76	0.51
27:C:334:ASP:OD1	31:H:42:ASN:ND2	2.42	0.51
34:K:52:ASN:HB3	54:M:29:GLN:HE22	1.74	0.51
51:u:304:LEU:HD13	51:u:354:LEU:HD22	1.92	0.51
6:7:48:GLY:HA3	56:7:401:HEM:C4C	2.46	0.51
8:9:52:PRO:HD2	8:9:55:LEU:HD12	1.93	0.51
29:E:143:ARG:HG3	29:E:183:ALA:HB3	1.92	0.51
43:U:258:LEU:HD21	43:U:278:LEU:HD21	1.93	0.51
48:l:303:ALA:O	48:l:306:THR:OG1	2.25	0.51
7:x:112:ARG:HG3	7:x:141:TYR:CZ	2.46	0.51
5:6:48:VAL:HG11	5:6:400:ALA:HB1	1.92	0.51
10:b:72:VAL:HG22	10:b:76:LEU:HD12	1.93	0.51
27:C:368:LYS:HG2	27:C:386:HIS:CE1	2.46	0.51
31:H:103:LEU:HB3	31:H:191:LEU:HD23	1.92	0.51
35:L:222:PRO:HB2	35:L:288:LEU:HD11	1.92	0.51
36:N:23:ARG:NH2	43:U:277:TYR:OH	2.44	0.51
37:X:119:ILE:HG21	37:X:135:ALA:HB1	1.92	0.51
26:B:338:ASP:N	26:B:338:ASP:OD1	2.44	0.51
26:B:340:ASP:O	26:B:344:GLN:HG2	2.10	0.51
35:L:167:ALA:HA	35:L:176:LEU:HB3	1.92	0.51
3:Ae:49:PHE:O	3:Ae:51:ALA:N	2.44	0.51
3:2:157:PHE:O	3:2:160:SER:OG	2.22	0.50
3:2:159:SER:O	3:2:162:SER:OG	2.27	0.50
6:7:43:LEU:HD22	6:7:236:MET:HE1	1.94	0.50
6:7:218:ILE:HD11	6:7:224:TYR:CE2	2.47	0.50
11:c:165:ASP:HB3	11:c:170:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:q:358:TRP:CE3	24:q:441:ILE:HD12	2.46	0.50
26:B:423:THR:HB	59:B:502:SF4:S3	2.51	0.50
36:N:59:VAL:HG22	36:N:68:LEU:HD21	1.93	0.50
43:U:131:TYR:CD1	43:U:185:CYS:HB3	2.46	0.50
53:G:402:LEU:HD23	53:G:475:VAL:HB	1.92	0.50
5:6:181:ALA:O	5:6:254:ARG:N	2.42	0.50
10:b:100:ARG:NH2	12:d:119:GLU:HG2	2.26	0.50
30:F:84:ILE:HG12	30:F:102:LEU:HD11	1.94	0.50
31:H:211:TYR:CZ	54:M:39:PRO:HG3	2.47	0.50
5:v:333:SER:OG	5:v:334:GLY:N	2.45	0.50
10:b:31:ARG:HG2	10:b:33:PRO:HD3	1.93	0.50
25:r:200:LEU:HD13	25:r:282:TYR:HA	1.93	0.50
25:r:228:TYR:HA	25:r:231:ILE:HD12	1.93	0.50
27:C:197:ALA:HB1	27:C:202:ALA:HB3	1.93	0.50
29:E:132:ILE:HD11	29:E:169:PHE:HD1	1.76	0.50
31:H:119:CYS:HB3	31:H:158:CYS:SG	2.52	0.50
51:u:170:GLN:O	51:u:174:GLU:HG3	2.10	0.50
3:4:182:GLU:HG2	3:4:201:THR:HG22	1.92	0.50
5:6:194:ASP:HA	5:6:197:ILE:HG12	1.94	0.50
5:6:372:GLN:NE2	5:6:376:ASN:OD1	2.41	0.50
6:7:248:ASP:OD2	7:8:203:ARG:NE	2.44	0.50
10:b:18:LEU:HD21	23:p:205:LEU:HD22	1.92	0.50
11:c:126:TRP:HA	11:c:129:MET:HE2	1.93	0.50
14:f:37:GLY:O	43:U:357:LYS:NZ	2.30	0.50
16:h:105:ARG:HH22	49:s:91:LYS:HA	1.76	0.50
26:B:284:HIS:CD2	26:B:305:GLY:HA3	2.45	0.50
27:C:248:ASP:O	27:C:252:GLU:HG2	2.11	0.50
40:R:78:HIS:HA	40:R:81:TYR:CE2	2.46	0.50
44:V:19:HIS:CD2	44:V:20:ARG:HG3	2.46	0.50
50:t:46:MET:HG2	50:t:51:LEU:HD12	1.94	0.50
6:w:244:LEU:HD12	7:x:293:MET:HG2	1.92	0.50
53:G:323:LEU:HB3	53:G:629:ILE:HD12	1.93	0.50
6:7:260:ASN:HD22	6:7:261:PRO:HD2	1.76	0.50
7:8:184:GLU:OE1	7:x:159:PRO:HB2	2.10	0.50
9:a:169:TYR:OH	44:V:141:VAL:HG11	2.12	0.50
25:r:132:ALA:O	25:r:136:VAL:HG23	2.12	0.50
43:U:182:ARG:NH1	43:U:318:GLU:OE2	2.45	0.50
51:5:87:ASN:ND2	51:5:199:GLN:OE1	2.45	0.50
51:5:195:THR:HG21	51:5:269:ARG:H	1.77	0.50
3:2:116:GLU:OE1	3:2:116:GLU:N	2.32	0.50
5:6:138:LEU:HD13	5:6:237:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:161:ARG:NH2	17:i:195:PRO:O	2.42	0.50
12:d:23:GLN:HE21	50:t:73:SER:HB3	1.75	0.50
24:q:71:TRP:O	24:q:74:PRO:HD2	2.11	0.50
48:l:69:MET:HE3	48:l:71:LEU:HD11	1.93	0.50
51:u:310:ILE:HG21	51:u:379:LEU:HD21	1.93	0.50
53:G:455:ILE:HD13	53:G:460:HIS:HB3	1.93	0.50
3:2:175:ILE:HB	3:2:292:VAL:HG13	1.93	0.50
5:6:116:ARG:HH12	5:6:189:SER:HA	1.75	0.50
35:L:140:PHE:O	35:L:182:GLY:HA3	2.12	0.50
35:L:238:VAL:HG12	35:L:242:LYS:HZ2	1.76	0.50
37:O:143:GLU:HA	37:O:146:ASP:OD2	2.12	0.50
41:S:4:GLU:O	41:S:7:PRO:HD2	2.10	0.50
3:4:161:MET:O	6:w:177:ARG:NH2	2.45	0.50
7:8:293:MET:HG3	7:8:294:LEU:N	2.26	0.50
20:m:15:ILE:HG12	20:m:97:LEU:HD22	1.92	0.50
26:B:257:ARG:HG2	26:B:261:TRP:CD2	2.46	0.50
26:B:284:HIS:HD2	26:B:305:GLY:HA3	1.77	0.50
27:C:90:PHE:HB3	27:C:103:LEU:HB3	1.94	0.50
43:U:153:LEU:HD11	43:U:296:LEU:HD23	1.94	0.50
5:6:255:GLY:HA2	5:6:437:SER:HB3	1.94	0.50
6:7:41:LEU:CD1	56:7:401:HEM:HBB1	2.39	0.50
10:b:28:LEU:HD11	23:p:157:TYR:CD2	2.47	0.50
18:j:33:LYS:HE2	25:r:59:GLU:CD	2.37	0.50
24:q:75:LEU:HD23	24:q:440:HIS:CE1	2.46	0.50
24:q:457:PRO:HG2	24:q:458:LEU:HD12	1.93	0.50
26:B:52:ARG:HB3	26:B:54:LYS:HZ2	1.77	0.50
35:L:263:PRO:HG3	35:L:339:PRO:HA	1.93	0.50
37:O:110:LEU:HB2	37:O:114:ASP:HB3	1.93	0.50
37:O:120:MET:HE1	39:Q:66:TYR:HB3	1.93	0.50
51:u:121:ASN:ND2	51:u:132:TYR:OH	2.45	0.50
51:u:141:PRO:O	51:u:145:GLU:HG3	2.12	0.50
5:v:70:ARG:HD2	5:v:117:GLU:HG2	1.93	0.50
5:v:196:ARG:HH12	5:v:204:GLN:HE22	1.59	0.50
51:5:328:LEU:HB2	51:5:375:GLN:HG3	1.94	0.50
3:4:199:HIS:HB2	3:4:231:TRP:CZ3	2.47	0.49
7:8:212:VAL:HA	7:8:215:LEU:HD23	1.93	0.49
18:j:96:ILE:HD11	42:T:115:ILE:HD11	1.94	0.49
26:B:364:VAL:HG12	26:B:400:VAL:HG12	1.93	0.49
27:C:159:LEU:HD22	27:C:177:ARG:HH21	1.77	0.49
48:l:272:LEU:O	48:l:275:THR:OG1	2.26	0.49
3:4:182:GLU:HA	3:4:199:HIS:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:234:MET:O	25:r:238:THR:HG23	2.12	0.49
38:P:32:GLY:HA3	38:P:82:PHE:O	2.12	0.49
24:q:118:PHE:O	24:q:122:PHE:HB3	2.12	0.49
26:B:41:ILE:HG22	26:B:253:THR:HG21	1.94	0.49
41:S:37:ARG:HD2	41:S:48:MET:HG2	1.94	0.49
53:G:400:ILE:HG13	53:G:427:LEU:HD11	1.93	0.49
3:4:240:HIS:HB3	55:4:301:FES:S1	2.52	0.49
8:9:13:TRP:CG	8:9:14:LEU:N	2.81	0.49
9:a:58:LYS:O	23:p:149:TRP:NE1	2.43	0.49
10:b:89:HIS:NE2	10:b:96:THR:HB	2.27	0.49
11:c:54:LYS:NZ	11:c:74:ASP:OD2	2.43	0.49
14:f:31:ILE:HG13	14:f:32:ARG:H	1.78	0.49
22:o:11:LEU:HD13	48:l:535:ARG:HB3	1.94	0.49
26:B:228:PRO:HG3	33:J:160:TYR:HD2	1.78	0.49
44:V:41:ILE:HD12	44:V:46:PRO:HG3	1.94	0.49
48:l:529:TYR:O	48:l:533:MET:HB2	2.12	0.49
5:6:233:VAL:HG23	5:6:236:ARG:HH12	1.76	0.49
7:8:244:ALA:H	57:8:401:HEC:HBD2	1.77	0.49
11:c:75:TYR:OH	11:c:105:ILE:O	2.30	0.49
17:i:57:THR:HA	19:k:77:LEU:HD13	1.94	0.49
19:k:2:PRO:HG3	20:m:127:ILE:HD13	1.94	0.49
25:r:81:LEU:HD22	25:r:108:MET:HG3	1.94	0.49
25:r:165:LEU:HD23	25:r:241:LEU:HA	1.93	0.49
28:D:68:ILE:HD13	36:N:44:TYR:HA	1.95	0.49
48:l:49:VAL:HB	48:l:50:PRO:HD3	1.95	0.49
48:l:397:GLU:HG3	48:l:482:MET:HE1	1.93	0.49
51:5:388:VAL:HG21	51:5:438:ALA:HA	1.94	0.49
3:4:213:VAL:HA	3:4:216:LEU:HD12	1.95	0.49
5:6:214:THR:HG21	5:6:245:GLY:HA3	1.93	0.49
6:7:196:HIS:HE1	56:7:402:HEM:C1D	2.30	0.49
56:7:402:HEM:HBD1	56:7:402:HEM:HHA	1.93	0.49
7:8:220:CYS:SG	7:8:221:GLU:N	2.86	0.49
10:b:79:VAL:HG23	48:l:10:THR:HG21	1.94	0.49
12:d:85:MET:HE1	24:q:182:TRP:CD1	2.47	0.49
26:B:41:ILE:HD12	26:B:250:VAL:HG12	1.93	0.49
27:C:167:ILE:HD12	27:C:369:VAL:HG21	1.95	0.49
27:C:312:GLN:OE1	28:D:140:ARG:NH1	2.45	0.49
37:O:133:ILE:HG12	37:O:134:ASP:N	2.28	0.49
44:V:90:TYR:CE1	44:V:126:LYS:HD3	2.48	0.49
45:W:108:GLU:HA	49:s:81:ILE:HD13	1.94	0.49
21:n:39:ARG:HD3	21:n:58:LYS:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:73:ASN:HB2	43:U:195:VAL:HG13	1.93	0.49
48:l:90:ILE:HD11	48:l:133:THR:HG21	1.95	0.49
51:u:74:TRP:CZ2	51:u:411:GLU:HA	2.48	0.49
3:Af:47:GLY:C	3:Af:66:PRO:HA	2.37	0.49
15:g:4:MET:HE1	15:g:87:LEU:HB3	1.95	0.49
17:i:12:THR:HG21	20:m:163:ILE:HG21	1.95	0.49
25:r:169:GLN:NE2	25:r:241:LEU:O	2.46	0.49
32:I:81:ALA:HB1	32:I:82:PRO:HD2	1.95	0.49
35:L:286:TYR:HD1	35:L:286:TYR:H	1.60	0.49
48:l:124:PHE:HE1	48:l:252:MET:HB2	1.78	0.49
5:6:324:SER:OG	3:Ae:67:VAL:O	2.31	0.49
6:7:85:ASN:HD22	6:7:243:VAL:HG22	1.78	0.49
18:j:61:THR:HG21	18:j:105:GLU:OE2	2.13	0.49
19:k:35:GLY:HA3	20:m:20:PHE:CZ	2.48	0.49
23:p:149:TRP:CE3	23:p:153:GLU:HB3	2.47	0.49
32:I:71:CYS:HB2	59:I:201:SF4:S2	2.53	0.49
51:u:315:ASP:OD1	51:u:316:SER:N	2.46	0.49
52:z:49:VAL:O	52:z:52:PRO:HD2	2.13	0.49
53:G:471:LYS:HG3	53:G:510:TRP:CD2	2.48	0.49
3:4:284:TYR:HB3	3:4:294:VAL:HA	1.94	0.49
18:j:77:TRP:HB2	20:m:144:ALA:HB2	1.95	0.49
38:P:46:LYS:HZ2	53:G:674:LEU:HD21	1.77	0.49
40:R:95:LYS:HE2	40:R:96:PHE:CZ	2.48	0.49
3:2:182:GLU:HG2	3:2:201:THR:HG22	1.94	0.48
3:4:177:LEU:HD13	3:4:231:TRP:CD2	2.48	0.48
11:c:93:ASP:HB2	11:c:100:ASN:HA	1.95	0.48
12:d:34:THR:HG22	48:l:3:PRO:HG2	1.94	0.48
24:q:108:MET:HB3	24:q:121:LEU:HD13	1.95	0.48
28:D:103:HIS:CE1	28:D:105:ASN:HA	2.48	0.48
43:U:256:GLU:HG3	43:U:278:LEU:HD22	1.95	0.48
48:l:182:PHE:O	48:l:185:SER:OG	2.30	0.48
6:w:32:ASN:O	6:w:36:LEU:HG	2.13	0.48
3:Ae:48:PRO:HA	3:Ae:65:SER:C	2.38	0.48
3:4:217:ARG:HH22	3:4:273:GLY:H	1.61	0.48
17:i:193:VAL:HG23	17:i:201:THR:HG22	1.95	0.48
25:r:57:THR:HB	32:I:58:ARG:HH21	1.78	0.48
48:l:37:LYS:NZ	48:l:102:GLU:OE2	2.41	0.48
48:l:346:ILE:HG12	48:l:366:MET:HE1	1.95	0.48
5:v:121:TYR:HB3	5:v:137:LEU:HD11	1.94	0.48
5:v:131:GLU:O	5:v:135:GLU:HG2	2.13	0.48
14:f:55:TRP:CD1	15:g:68:THR:HG22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:340:THR:N	17:i:341:PRO:HD2	2.29	0.48
24:q:171:THR:HG22	24:q:184:HIS:HE1	1.78	0.48
25:r:136:VAL:HG12	25:r:140:ILE:HD12	1.95	0.48
25:r:287:HIS:HD2	25:r:291:LYS:HB2	1.78	0.48
25:r:299:ALA:HB1	42:T:110:ILE:HB	1.95	0.48
31:H:117:LYS:HE2	53:G:240:ALA:HA	1.95	0.48
36:N:94:MET:HE3	36:N:99:PRO:HG2	1.95	0.48
3:2:161:MET:O	6:7:177:ARG:NH1	2.46	0.48
19:k:64:LEU:HD23	20:m:59:ILE:HD11	1.96	0.48
28:D:126:PHE:HZ	28:D:199:ARG:HE	1.61	0.48
35:L:221:VAL:HG11	35:L:283:PHE:HE1	1.78	0.48
46:Y:47:PHE:CE1	48:l:364:LYS:HD3	2.48	0.48
47:Z:48:VAL:HG22	48:l:511:LEU:HD21	1.95	0.48
53:G:690:THR:OG1	53:G:692:LYS:NZ	2.46	0.48
3:2:225:ARG:HH12	3:2:268:GLY:C	2.22	0.48
9:a:82:VAL:HG11	13:e:104:THR:HG21	1.95	0.48
10:b:28:LEU:CD2	10:b:29:SER:H	2.26	0.48
25:r:81:LEU:HD11	25:r:111:LEU:HD13	1.94	0.48
31:H:200:GLU:HG3	34:K:88:ARG:HD2	1.96	0.48
38:P:38:GLU:HG3	38:P:39:LYS:HG2	1.94	0.48
10:b:84:TYR:HE1	12:d:49:ARG:HG2	1.77	0.48
14:f:29:PHE:CE1	43:U:102:ASP:HB3	2.49	0.48
27:C:218:GLU:OE2	32:I:83:ARG:NH1	2.47	0.48
29:E:132:ILE:HD11	29:E:169:PHE:CD1	2.49	0.48
43:U:152:LEU:HD12	43:U:158:GLY:HA2	1.95	0.48
43:U:204:HIS:CE1	43:U:280:CYS:HB3	2.49	0.48
37:X:115:GLN:O	37:X:118:ILE:HG13	2.13	0.48
6:w:186:PRO:HA	6:w:189:ILE:HD12	1.96	0.48
1:0:67:CYS:SG	7:x:224:THR:OG1	2.68	0.48
7:8:168:ARG:HH22	7:8:174:ASP:CG	2.21	0.48
8:9:106:GLU:O	8:9:110:LYS:HG3	2.14	0.48
25:r:259:PHE:O	25:r:263:THR:HG23	2.14	0.48
28:D:216:VAL:HG13	28:D:218:ARG:HB3	1.94	0.48
53:G:394:VAL:HG13	53:G:400:ILE:HD11	1.96	0.48
2:1:30:LEU:HD11	4:3:48:ILE:HG21	1.94	0.48
3:2:173:ILE:HD13	3:2:190:TRP:HB2	1.96	0.48
3:2:254:GLY:HA3	3:2:265:ASP:C	2.39	0.48
3:4:104:ILE:HG22	7:8:323:ARG:NH1	2.29	0.48
7:8:153:VAL:HG21	7:8:177:PRO:HG2	1.95	0.48
9:a:110:TRP:CD1	9:a:110:TRP:H	2.31	0.48
9:a:134:GLU:OE1	21:n:42:SER:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:161:TYR:HB2	11:c:165:ASP:HA	1.94	0.48
17:i:79:LEU:HD23	19:k:47:ILE:HG12	1.95	0.48
20:m:61:LEU:HA	20:m:65:LEU:HD23	1.96	0.48
20:m:125:TRP:HH2	45:W:126:GLY:HA2	1.78	0.48
25:r:24:GLU:HG3	25:r:271:LEU:HD22	1.96	0.48
26:B:177:TYR:CD1	26:B:182:ILE:HG13	2.49	0.48
35:L:53:VAL:HG22	35:L:122:ILE:HD12	1.95	0.48
43:U:215:GLU:O	43:U:218:SER:OG	2.22	0.48
45:W:100:ASP:OD1	45:W:100:ASP:N	2.41	0.48
51:u:165:ARG:HD3	51:u:209:ARG:HA	1.95	0.48
6:7:326:TRP:NE1	52:Aa:49:VAL:HG22	2.28	0.48
15:g:94:ALA:HB1	49:s:232:GLU:HG3	1.96	0.48
15:g:111:TYR:HA	15:g:114:ILE:HG12	1.94	0.48
25:r:31:MET:HE1	25:r:272:TRP:HA	1.96	0.48
27:C:190:ILE:HD11	27:C:257:PHE:CZ	2.48	0.48
28:D:69:LEU:HD22	28:D:96:VAL:HG22	1.95	0.48
32:I:48:ALA:HA	32:I:191:ARG:HE	1.78	0.48
35:L:183:GLU:HG3	35:L:195:ILE:HG21	1.96	0.48
38:P:92:GLU:HG2	38:P:93:ASN:N	2.27	0.48
39:Q:85:GLY:O	39:Q:89:VAL:HG23	2.14	0.48
48:l:162:THR:O	48:l:166:THR:HG23	2.13	0.48
51:5:42:LEU:HD22	51:5:426:LEU:HB3	1.95	0.48
51:5:74:TRP:CZ2	51:5:411:GLU:HA	2.48	0.48
53:G:241:ARG:HG2	53:G:243:TRP:CH2	2.48	0.48
13:e:74:HIS:ND1	24:q:431:THR:HG21	2.29	0.48
17:i:106:LEU:HD22	17:i:187:MET:HE2	1.95	0.48
25:r:294:LEU:HB3	25:r:295:PRO:HD3	1.96	0.48
48:l:251:THR:O	48:l:254:VAL:HG22	2.14	0.48
50:t:22:MET:HE3	50:t:105:GLU:HG3	1.95	0.48
3:2:100:SER:HB2	51:u:176:ASP:HB2	1.96	0.47
3:2:197:VAL:HG13	3:2:233:ILE:HG12	1.95	0.47
3:2:197:VAL:HG22	3:2:233:ILE:HG23	1.96	0.47
9:a:161:ARG:HH11	44:V:141:VAL:HB	1.78	0.47
16:h:17:TRP:CD1	16:h:17:TRP:H	2.32	0.47
24:q:400:MET:HE1	48:l:183:VAL:HG21	1.95	0.47
26:B:202:GLY:HA3	29:E:121:MET:HG3	1.95	0.47
28:D:200:LYS:O	33:J:126:LEU:HD21	2.13	0.47
35:L:80:ARG:HD2	60:L:401:NDP:C2A	2.43	0.47
35:L:128:GLU:OE2	35:L:313:LYS:HE2	2.14	0.47
38:P:74:GLU:OE2	53:G:645:ARG:NH2	2.47	0.47
48:l:356:ILE:HA	48:l:359:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:368:PHE:HE2	48:l:454:ILE:HB	1.78	0.47
53:G:370:GLU:HB2	53:G:522:GLN:OE1	2.14	0.47
52:Aa:79:GLU:HG2	52:Aa:80:ASN:N	2.27	0.47
3:4:120:SER:HA	51:5:269:ARG:HE	1.79	0.47
17:i:65:THR:HG22	19:k:19:LEU:HD21	1.96	0.47
17:i:111:PHE:HA	48:l:591:PHE:CE1	2.50	0.47
24:q:24:TRP:CD2	24:q:81:GLN:HG2	2.50	0.47
25:r:28:LEU:HD22	25:r:275:ALA:HB2	1.97	0.47
26:B:193:PHE:N	40:R:98:MET:HE1	2.29	0.47
27:C:190:ILE:O	27:C:194:THR:HB	2.13	0.47
35:L:84:TYR:HA	35:L:87:MET:HE2	1.95	0.47
5:v:271:LEU:HD22	5:v:453:LEU:HD13	1.95	0.47
56:7:402:HEM:HHA	56:7:402:HEM:HBA1	1.95	0.47
7:8:187:ARG:HB3	7:8:192:GLY:HA2	1.96	0.47
9:a:169:TYR:CE2	15:g:3:MET:HG2	2.49	0.47
17:i:200:MET:HG3	17:i:269:GLU:HG3	1.95	0.47
25:r:219:PRO:HA	25:r:222:MET:HE3	1.96	0.47
27:C:122:LEU:HD11	32:I:70:ALA:HB2	1.97	0.47
27:C:410:LYS:NZ	27:C:461:ASP:HB2	2.29	0.47
32:I:98:ARG:HA	32:I:125:PRO:HD3	1.95	0.47
39:Q:65:TRP:O	39:Q:69:VAL:HG23	2.14	0.47
44:V:22:ALA:O	44:V:26:THR:OG1	2.31	0.47
45:W:66:GLU:OE2	49:s:201:GLU:N	2.46	0.47
5:6:446:HIS:H	5:6:446:HIS:CD2	2.32	0.47
10:b:62:TYR:HA	10:b:66:ARG:HB2	1.97	0.47
17:i:311:MET:HE3	17:i:314:LYS:HD3	1.95	0.47
24:q:11:LEU:HA	24:q:14:MET:HE3	1.96	0.47
25:r:58:LYS:HD2	32:I:127:PRO:HD2	1.96	0.47
28:D:61:PHE:CE1	54:M:97:PRO:HD3	2.49	0.47
28:D:230:PHE:O	33:J:123:ASN:ND2	2.47	0.47
42:T:167:LYS:HA	45:W:59:ARG:HD3	1.96	0.47
45:W:30:LEU:HD23	45:W:34:SER:OG	2.14	0.47
48:l:8:THR:HB	48:l:82:MET:HE3	1.96	0.47
48:l:296:ASN:O	48:l:356:ILE:HG12	2.14	0.47
2:Ac:18:THR:HA	2:Ac:21:PHE:HB3	1.96	0.47
3:2:240:HIS:HB3	55:2:301:FES:S2	2.55	0.47
17:i:112:HIS:CE1	17:i:164:ILE:HD13	2.49	0.47
23:p:201:LYS:HE2	23:p:201:LYS:HB3	1.74	0.47
25:r:168:THR:HG22	45:W:57:ARG:NH2	2.29	0.47
32:I:51:ASP:HA	32:I:54:VAL:HG22	1.96	0.47
35:L:226:LEU:HB3	35:L:228:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:W:10:MET:HE3	45:W:11:PRO:HD2	1.97	0.47
48:l:428:PHE:CE2	48:l:505:ASN:HB3	2.50	0.47
10:b:84:TYR:CE1	12:d:49:ARG:HG2	2.50	0.47
24:q:208:PRO:HG3	24:q:216:LEU:HD13	1.96	0.47
35:L:277:ALA:HB1	35:L:364:VAL:HG11	1.97	0.47
51:u:192:PHE:HB3	51:u:195:THR:OG1	2.14	0.47
3:2:100:SER:HB2	51:u:176:ASP:OD2	2.15	0.47
7:8:216:LEU:HD11	57:8:401:HEC:CMB	2.45	0.47
17:i:250:SER:O	17:i:259:GLY:HA3	2.15	0.47
23:p:124:PHE:O	23:p:127:SER:OG	2.29	0.47
23:p:150:HIS:CD2	23:p:151:PRO:HD2	2.50	0.47
24:q:358:TRP:HE3	24:q:441:ILE:HD12	1.80	0.47
26:B:52:ARG:HG2	26:B:175:GLU:OE2	2.15	0.47
26:B:445:GLU:H	26:B:445:GLU:HG2	1.47	0.47
27:C:53:PHE:HD1	27:C:58:MET:HE1	1.79	0.47
34:K:44:TYR:HE2	34:K:83:PRO:HB3	1.80	0.47
35:L:163:SER:O	35:L:197:LYS:HA	2.14	0.47
37:O:104:PHE:HD2	37:O:139:MET:HA	1.75	0.47
38:P:31:GLN:OE1	38:P:34:ARG:NH1	2.48	0.47
44:V:90:TYR:CD1	44:V:126:LYS:HD3	2.49	0.47
46:Y:44:TYR:HD2	47:Z:33:PRO:HD2	1.79	0.47
48:l:362:LEU:HD22	48:l:366:MET:HE2	1.96	0.47
48:l:587:TYR:O	48:l:590:SER:OG	2.25	0.47
5:v:63:LEU:HD11	5:v:218:MET:HB3	1.96	0.47
6:w:182:HIS:HE1	56:w:402:HEM:C1B	2.33	0.47
8:y:63:ILE:O	8:y:67:LEU:HG	2.14	0.47
53:G:310:GLU:OE1	53:G:311:LYS:HG2	2.14	0.47
53:G:438:LEU:O	53:G:439:THR:OG1	2.31	0.47
53:G:575:VAL:O	53:G:578:PRO:HD2	2.15	0.47
3:2:190:TRP:CE2	3:2:191:ARG:HG2	2.49	0.47
3:4:199:HIS:HE1	3:4:230:GLU:HB2	1.80	0.47
5:6:131:GLU:HA	5:6:134:MET:HE3	1.97	0.47
7:8:246:ALA:O	7:8:247:PRO:C	2.57	0.47
26:B:85:LEU:HD21	26:B:247:THR:HG23	1.95	0.47
28:D:118:ASP:OD1	28:D:125:ARG:NE	2.42	0.47
35:L:349:ARG:NH1	39:Q:77:GLN:O	2.47	0.47
36:N:23:ARG:NH2	36:N:27:LEU:HD21	2.30	0.47
41:S:16:LEU:O	41:S:19:PRO:HD2	2.14	0.47
48:l:95:PHE:CZ	48:l:456:ARG:HB3	2.50	0.47
51:u:276:ARG:HB2	52:z:16:THR:HG23	1.96	0.47
3:2:284:TYR:HB3	3:2:294:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:87:MET:HE3	13:e:88:ARG:HG3	1.97	0.47
24:q:6:ILE:O	24:q:9:THR:OG1	2.27	0.47
24:q:73:LEU:HD22	24:q:103:GLN:OE1	2.14	0.47
26:B:86:ARG:NH1	26:B:269:ARG:O	2.46	0.47
27:C:147:TYR:HB3	32:I:71:CYS:HB3	1.96	0.47
31:H:106:TYR:CE2	31:H:112:ARG:HA	2.49	0.47
3:2:177:LEU:HD22	3:2:231:TRP:CD2	2.49	0.47
5:6:358:VAL:HG11	5:6:431:PHE:CD2	2.50	0.47
7:8:198:LEU:HD13	7:8:275:LEU:HD21	1.96	0.47
9:a:147:ALA:HB2	24:q:173:SER:HB2	1.97	0.47
10:b:4:TYR:CD2	10:b:9:LYS:HG2	2.48	0.47
11:c:41:TYR:CG	11:c:67:ASP:HB2	2.50	0.47
16:h:26:PRO:HD3	19:k:55:LEU:HD13	1.97	0.47
20:m:64:MET:O	20:m:67:VAL:HG12	2.14	0.47
22:o:87:SER:HA	48:l:557:TRP:CZ2	2.49	0.47
26:B:102:MET:HG2	26:B:149:MET:HB3	1.97	0.47
27:C:212:GLU:O	27:C:216:MET:HG3	2.14	0.47
38:P:42:VAL:HG12	38:P:46:LYS:HE2	1.97	0.47
48:l:391:SER:O	48:l:395:ILE:HG12	2.15	0.47
53:G:397:ALA:HA	53:G:471:LYS:HB3	1.96	0.47
53:G:624:ARG:NH1	53:G:628:GLU:HB2	2.30	0.47
5:6:176:ASN:ND2	5:6:260:ASP:OD2	2.48	0.46
10:b:28:LEU:HD23	10:b:29:SER:H	1.79	0.46
12:d:37:PHE:CD2	48:l:3:PRO:HG3	2.50	0.46
20:m:8:ILE:O	20:m:11:THR:OG1	2.30	0.46
23:p:171:ARG:HD2	23:p:210:TRP:CD2	2.50	0.46
24:q:216:LEU:HD22	24:q:291:VAL:HG23	1.97	0.46
26:B:325:PRO:HG3	26:B:433:TRP:HB3	1.97	0.46
27:C:432:ALA:HB1	27:C:466:GLU:HB3	1.97	0.46
31:H:128:ILE:CD1	31:H:158:CYS:SG	3.03	0.46
35:L:104:ASN:HB3	35:L:107:ASP:HB3	1.97	0.46
43:U:263:ARG:HD3	43:U:264:GLU:N	2.30	0.46
51:u:80:ARG:NH2	51:u:266:THR:O	2.48	0.46
6:w:126:THR:HA	6:w:129:MET:HE2	1.96	0.46
3:Ae:56:HIS:C	3:Ae:58:ALA:H	2.23	0.46
5:6:70:ARG:NH1	5:6:117:GLU:OE2	2.47	0.46
5:6:221:ILE:HD13	5:6:397:GLY:HA2	1.97	0.46
5:6:233:VAL:HG23	5:6:236:ARG:NH1	2.30	0.46
6:7:165:TRP:O	6:7:174:THR:OG1	2.26	0.46
7:8:219:TYR:CE1	7:8:243:ILE:HG21	2.35	0.46
17:i:137:ALA:O	17:i:141:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:p:91:ASP:HA	23:p:94:LYS:HB2	1.96	0.46
24:q:226:ALA:O	24:q:230:VAL:HG22	2.15	0.46
29:E:66:ILE:HD13	29:E:81:PRO:HB2	1.97	0.46
43:U:241:ASN:O	43:U:245:LYS:HB2	2.16	0.46
45:W:23:ARG:HG3	45:W:25:LEU:HD13	1.97	0.46
46:Y:97:LEU:H	50:t:111:ARG:HH21	1.62	0.46
51:u:447:LYS:HE3	51:u:448:TYR:CE2	2.50	0.46
53:G:372:PHE:H	53:G:532:PRO:HB2	1.79	0.46
52:Aa:73:LYS:NZ	1:Ab:66:ASP:H	2.13	0.46
3:4:243:CYS:SG	3:4:244:VAL:N	2.88	0.46
7:8:245:MET:HG2	57:8:401:HEC:C4D	2.46	0.46
11:c:96:ASP:N	11:c:96:ASP:OD1	2.47	0.46
19:k:21:MET:O	20:m:23:LYS:NZ	2.44	0.46
20:m:25:SER:HB3	20:m:81:GLU:N	2.30	0.46
25:r:153:VAL:HB	25:r:174:MET:HE1	1.98	0.46
26:B:71:LYS:HG2	26:B:75:TRP:CD2	2.49	0.46
28:D:67:GLU:O	28:D:70:PRO:HD3	2.15	0.46
32:I:191:ARG:O	32:I:195:ARG:HG3	2.16	0.46
35:L:152:LYS:HG3	35:L:189:ALA:O	2.15	0.46
46:Y:65:MET:HE2	48:l:375:ILE:HG12	1.98	0.46
48:l:76:LEU:HD21	48:l:196:TRP:HE3	1.80	0.46
6:w:165:TRP:O	6:w:174:THR:OG1	2.28	0.46
6:w:278:TYR:CE2	6:w:282:ARG:HD3	2.51	0.46
53:G:445:LEU:HD22	53:G:460:HIS:HE1	1.79	0.46
3:2:256:TYR:CZ	3:2:258:PRO:HA	2.51	0.46
5:6:109:LYS:HE2	5:6:124:GLU:HG3	1.97	0.46
10:b:94:PRO:HB3	12:d:5:TRP:CG	2.50	0.46
11:c:38:PRO:HD2	22:o:70:TYR:CD1	2.51	0.46
17:i:230:LEU:O	17:i:233:THR:OG1	2.31	0.46
18:j:113:TRP:HB2	25:r:286:MET:HE3	1.98	0.46
19:k:22:TYR:HA	20:m:23:LYS:HE2	1.97	0.46
24:q:7:PRO:O	24:q:11:LEU:HD23	2.15	0.46
25:r:61:LEU:HD13	32:I:98:ARG:HH11	1.79	0.46
27:C:317:TYR:HA	27:C:320:VAL:HG22	1.97	0.46
35:L:221:VAL:HB	35:L:285:PRO:HA	1.97	0.46
37:O:115:GLN:O	37:O:119:ILE:HG12	2.15	0.46
43:U:50:ARG:HA	43:U:50:ARG:HD3	1.79	0.46
48:l:118:PHE:O	48:l:122:VAL:HG23	2.16	0.46
5:v:338:ILE:HG21	5:v:354:ALA:HB1	1.97	0.46
51:5:275:ILE:HG12	52:Aa:17:TYR:HD2	1.80	0.46
5:6:421:ASP:O	5:6:425:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:245:PHE:HE2	7:8:102:LEU:HB3	1.81	0.46
11:c:65:TYR:CE1	11:c:77:LYS:HG2	2.51	0.46
13:e:101:LEU:O	13:e:104:THR:OG1	2.33	0.46
20:m:83:TRP:HA	20:m:89:VAL:HG12	1.98	0.46
24:q:119:TYR:HE1	24:q:157:SER:HB2	1.81	0.46
24:q:134:THR:O	24:q:142:ARG:NH1	2.49	0.46
26:B:68:ILE:HG23	26:B:75:TRP:HZ3	1.80	0.46
43:U:291:ARG:HH22	43:U:294:HIS:CD2	2.33	0.46
45:W:66:GLU:OE2	49:s:202:LEU:N	2.48	0.46
5:v:65:ILE:HG21	5:v:213:PHE:CD1	2.51	0.46
51:5:133:ILE:HG13	51:5:147:LEU:HD21	1.96	0.46
53:G:669:ASN:O	53:G:672:SER:OG	2.29	0.46
1:0:34:ARG:HG2	1:0:82:VAL:HG21	1.96	0.46
1:0:80:HIS:CE1	1:0:84:HIS:HE2	2.34	0.46
3:2:200:ARG:NH1	3:2:222:ASP:OD1	2.48	0.46
5:6:171:ALA:O	5:6:175:GLU:HG2	2.15	0.46
10:b:89:HIS:CD2	10:b:96:THR:HB	2.51	0.46
19:k:97:GLN:HA	48:l:582:GLY:HA3	1.96	0.46
24:q:1:MET:HG2	24:q:52:PHE:CD2	2.50	0.46
24:q:122:PHE:HE1	24:q:206:LYS:HG3	1.81	0.46
26:B:442:PHE:HB3	26:B:445:GLU:HG3	1.97	0.46
27:C:128:LYS:HB2	28:D:198:PHE:CE1	2.51	0.46
48:l:154:LEU:HD13	48:l:243:VAL:HG22	1.97	0.46
51:u:42:LEU:HD22	51:u:426:LEU:HB3	1.98	0.46
51:5:186:TYR:O	51:5:190:THR:HG22	2.16	0.46
51:5:318:TYR:CE1	3:Ae:55:GLY:HA2	2.51	0.46
3:4:142:THR:OG1	7:8:303:LEU:HB3	2.16	0.46
3:4:159:SER:O	3:4:162:SER:OG	2.29	0.46
11:c:36:MET:HG2	22:o:67:ARG:HE	1.81	0.46
17:i:26:TRP:CE2	17:i:86:ILE:HG13	2.51	0.46
17:i:244:MET:HE2	17:i:244:MET:HB3	1.76	0.46
26:B:355:ILE:HD13	29:E:139:PRO:HG3	1.97	0.46
29:E:222:ARG:NH2	29:E:226:GLU:O	2.49	0.46
38:P:68:ARG:HH11	53:G:359:ASN:HD21	1.63	0.46
48:l:86:SER:HB3	48:l:133:THR:HG22	1.98	0.46
49:s:115:LYS:HE3	49:s:119:GLU:CD	2.41	0.46
51:u:316:SER:N	51:u:339:GLN:O	2.48	0.46
6:w:82:LEU:HD23	6:w:243:VAL:HG21	1.98	0.46
1:0:76:HIS:HB2	7:x:90:LEU:HD11	1.98	0.46
1:0:79:ASP:HB3	7:x:93:PRO:HG2	1.98	0.46
3:2:227:LYS:HG3	3:2:284:TYR:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:241:LEU:HB2	55:2:301:FES:S1	2.56	0.46
5:6:449:PHE:CZ	5:v:183:ARG:HB2	2.51	0.46
20:m:107:ALA:HA	20:m:113:VAL:HB	1.98	0.46
24:q:174:LEU:HA	24:q:179:ILE:HD11	1.97	0.46
29:E:146:ASP:OD1	29:E:146:ASP:N	2.49	0.46
35:L:209:LEU:HD21	35:L:340:LEU:HD11	1.97	0.46
38:P:42:VAL:O	38:P:46:LYS:HG3	2.16	0.46
51:u:270:PHE:CG	51:u:292:GLU:HB2	2.51	0.46
3:2:182:GLU:HA	3:2:199:HIS:HB3	1.98	0.46
5:6:271:LEU:HD11	5:6:436:LYS:HB3	1.97	0.46
7:8:236:PRO:HA	7:8:241:GLN:HG3	1.97	0.46
9:a:169:TYR:CZ	15:g:3:MET:HG2	2.50	0.46
11:c:113:ILE:HD11	11:c:116:ARG:HG3	1.98	0.46
13:e:91:PHE:HA	13:e:95:PHE:HD2	1.81	0.46
17:i:173:THR:HG22	27:C:58:MET:HE2	1.98	0.46
24:q:121:LEU:O	24:q:125:THR:HG23	2.16	0.46
35:L:111:ILE:HG21	35:L:147:ILE:HA	1.97	0.46
35:L:264:ASN:HB2	35:L:266:TYR:CZ	2.51	0.46
39:Q:55:LYS:HZ2	61:Q:201:ZMP:H21	1.81	0.46
39:Q:63:ARG:O	39:Q:67:ARG:HG2	2.16	0.46
43:U:353:TRP:HZ3	43:U:356:LEU:HD12	1.81	0.46
48:l:253:VAL:HB	48:l:310:LEU:HD11	1.98	0.46
51:u:343:THR:HG22	51:u:356:ALA:HB2	1.98	0.46
6:w:77:TRP:CD2	7:x:282:GLU:HG3	2.51	0.46
7:x:198:LEU:HA	7:x:201:ILE:HB	1.98	0.46
51:5:142:LYS:O	51:5:146:LEU:HG	2.15	0.46
53:G:262:VAL:HG23	53:G:276:ARG:HB2	1.98	0.46
3:2:270:ILE:HG22	3:2:278:ASN:OD1	2.16	0.46
7:8:216:LEU:HD21	57:8:401:HEC:HMB2	1.96	0.46
17:i:63:GLN:OE1	17:i:105:LYS:HG2	2.15	0.46
17:i:270:MET:HE1	17:i:278:MET:HG2	1.98	0.46
23:p:160:TYR:HA	23:p:163:LYS:HE2	1.97	0.46
28:D:152:PRO:HD3	39:Q:46:ILE:HG12	1.97	0.46
28:D:171:TRP:HH2	39:Q:111:LYS:HZ2	1.63	0.46
29:E:143:ARG:O	29:E:184:PRO:HG3	2.16	0.46
44:V:59:TYR:O	44:V:62:THR:OG1	2.31	0.46
7:x:117:VAL:HG11	7:x:271:VAL:HB	1.97	0.46
53:G:75:CYS:SG	53:G:76:ARG:N	2.89	0.46
3:Af:50:CYS:O	3:Af:52:GLY:N	2.49	0.46
3:2:106:VAL:HG21	51:u:190:THR:HA	1.97	0.45
3:2:145:GLY:HA3	7:x:300:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:91:THR:HG21	5:6:140:VAL:HA	1.98	0.45
5:6:104:GLU:OE2	51:5:324:MET:HG3	2.17	0.45
5:6:375:LYS:HD3	5:6:417:ASP:HA	1.97	0.45
17:i:170:LEU:HD22	17:i:291:TYR:HD2	1.81	0.45
22:o:20:PRO:HA	23:p:107:ARG:HH12	1.81	0.45
26:B:317:VAL:HG22	26:B:356:VAL:HG22	1.98	0.45
27:C:101:LEU:HB2	27:C:464:PHE:CZ	2.51	0.45
30:F:99:TYR:CD1	53:G:157:LYS:HB2	2.50	0.45
51:u:342:GLN:HE21	51:u:342:GLN:HB2	1.62	0.45
6:w:97:HIS:CE1	6:w:100:ARG:HH22	2.34	0.45
53:G:236:TYR:CZ	53:G:272:ARG:HD3	2.51	0.45
3:4:227:LYS:NZ	3:4:284:TYR:O	2.39	0.45
5:6:129:ASP:OD1	5:6:129:ASP:N	2.48	0.45
5:6:155:GLN:O	5:6:158:LEU:HB2	2.17	0.45
7:8:122:CYS:SG	57:8:401:HEC:C4B	3.04	0.45
7:8:132:ALA:HB2	7:8:175:TYR:CD2	2.51	0.45
17:i:64:ALA:O	17:i:68:MET:HG2	2.17	0.45
24:q:122:PHE:CE1	24:q:206:LYS:HG3	2.52	0.45
24:q:216:LEU:HD23	24:q:287:ALA:HB1	1.98	0.45
25:r:20:LEU:HD13	41:S:12:MET:HE1	1.98	0.45
34:K:65:THR:O	34:K:73:THR:OG1	2.31	0.45
35:L:168:ASP:OD1	35:L:169:ILE:N	2.50	0.45
48:l:232:TRP:HZ3	48:l:248:HIS:HD2	1.64	0.45
48:l:249:SER:O	48:l:332:HIS:HE1	1.99	0.45
5:v:142:ALA:HA	5:v:241:ARG:HH22	1.81	0.45
53:G:338:VAL:O	53:G:363:SER:OG	2.30	0.45
54:M:46:SER:O	54:M:52:ASN:ND2	2.50	0.45
3:4:225:ARG:HH12	3:4:269:ARG:HG2	1.81	0.45
6:7:1:MET:O	51:5:335:ARG:NH1	2.50	0.45
6:7:244:LEU:O	7:8:286:ARG:NH1	2.33	0.45
13:e:65:ASN:HB3	24:q:427:LYS:HE3	1.97	0.45
17:i:211:MET:HG2	17:i:333:SER:HB2	1.98	0.45
17:i:302:LEU:HD13	24:q:134:THR:OG1	2.16	0.45
18:j:67:LEU:HD21	19:k:68:ALA:CB	2.47	0.45
20:m:3:MET:HE1	45:W:133:ILE:HG21	1.97	0.45
23:p:98:ASP:HB3	23:p:101:LYS:HB2	1.98	0.45
23:p:180:LYS:HE3	23:p:180:LYS:HB3	1.87	0.45
26:B:314:LEU:HB3	26:B:329:LYS:HG3	1.98	0.45
31:H:86:TYR:CD1	31:H:87:PRO:HA	2.51	0.45
44:V:18:CYS:SG	44:V:75:CYS:HB3	2.56	0.45
47:Z:49:GLN:HE22	47:Z:59:ASP:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:v:138:LEU:HD13	5:v:237:PHE:HB2	1.97	0.45
6:w:338:ILE:HD13	6:w:351:GLY:HA2	1.99	0.45
7:x:245:MET:HG2	7:x:246:ALA:O	2.16	0.45
51:5:417:LEU:HD23	51:5:417:LEU:HA	1.82	0.45
3:2:171:SER:O	3:2:190:TRP:NE1	2.48	0.45
3:2:204:GLU:O	3:2:207:GLN:HG3	2.17	0.45
6:7:27:ILE:HG12	6:7:224:TYR:CZ	2.51	0.45
7:8:310:HIS:CE1	52:Aa:21:PRO:HB2	2.52	0.45
13:e:116:GLU:HB3	13:e:120:ARG:NH1	2.31	0.45
24:q:373:ILE:HA	24:q:376:ILE:HD12	1.99	0.45
27:C:103:LEU:HD22	27:C:457:ILE:HD11	1.99	0.45
37:O:138:LEU:HB3	37:O:139:MET:H	1.66	0.45
51:u:92:PHE:O	51:u:96:LEU:HG	2.16	0.45
5:v:189:SER:OG	5:v:191:TYR:O	2.27	0.45
3:4:156:GLN:HE22	7:8:289:MET:HE3	1.81	0.45
20:m:34:ILE:HG23	20:m:61:LEU:HD23	1.98	0.45
25:r:34:ARG:HG2	32:I:82:PRO:HA	1.98	0.45
26:B:174:ARG:HA	40:R:93:LEU:HD21	1.98	0.45
26:B:235:VAL:HG12	26:B:240:THR:OG1	2.17	0.45
27:C:196:HIS:O	27:C:200:ILE:HG12	2.16	0.45
43:U:69:CYS:HG	43:U:223:LYS:HZ3	1.61	0.45
46:Y:47:PHE:HA	47:Z:73:PHE:CZ	2.52	0.45
48:l:419:THR:HA	48:l:422:TYR:CZ	2.52	0.45
7:8:103:LEU:HD11	7:8:291:LEU:HD13	1.99	0.45
23:p:170:LEU:HG	23:p:205:LEU:HD11	1.98	0.45
24:q:232:ALA:O	24:q:237:LYS:NZ	2.49	0.45
24:q:353:PRO:O	24:q:357:THR:HG23	2.17	0.45
25:r:200:LEU:CD1	25:r:282:TYR:HA	2.47	0.45
34:K:78:ASP:OD1	34:K:80:SER:OG	2.28	0.45
48:l:375:ILE:HD12	48:l:458:LEU:HD22	1.99	0.45
49:s:178:ARG:HD3	49:s:178:ARG:HA	1.68	0.45
51:u:54:ASP:OD1	51:u:54:ASP:N	2.49	0.45
5:v:49:ILE:HD13	5:v:231:LYS:HA	1.99	0.45
7:x:160:ASN:OD1	7:x:164:GLU:HG3	2.16	0.45
51:5:280:ASP:OD2	52:Aa:10:ARG:HA	2.17	0.45
2:Ac:56:ILE:HB	2:Ac:59:LYS:HE2	1.99	0.45
7:8:309:ARG:HG3	52:Aa:27:PHE:CE1	2.52	0.45
10:b:11:ARG:NH2	23:p:207:PRO:O	2.49	0.45
25:r:281:ARG:HD2	27:C:449:MET:HE3	1.98	0.45
32:I:103:MET:HB2	32:I:124:MET:HE1	1.99	0.45
48:l:37:LYS:HD2	48:l:105:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:u:341:PHE:HB2	51:u:358:PHE:HB3	1.99	0.45
53:G:627:SER:HB3	53:G:632:MET:O	2.15	0.45
16:h:3:PHE:HB2	17:i:144:GLN:CD	2.41	0.45
20:m:34:ILE:HD11	20:m:65:LEU:HD11	1.98	0.45
21:n:24:GLY:HA2	24:q:6:ILE:HD12	1.99	0.45
27:C:107:LEU:HD23	27:C:112:VAL:HA	1.98	0.45
36:N:38:ILE:O	36:N:45:ARG:NH2	2.48	0.45
42:T:151:VAL:O	49:s:207:LYS:NZ	2.40	0.45
48:l:62:ILE:HG21	48:l:199:GLN:HE22	1.81	0.45
48:l:561:ILE:O	48:l:565:THR:OG1	2.35	0.45
51:5:116:MET:SD	51:5:142:LYS:HG2	2.57	0.45
3:2:131:ARG:NH1	52:z:22:PHE:O	2.48	0.45
6:7:106:SER:HA	6:7:313:ARG:HH21	1.82	0.45
16:h:38:LYS:HE2	49:s:219:TYR:CZ	2.52	0.45
24:q:251:ASN:HB2	24:q:252:PRO:HD3	1.99	0.45
26:B:213:ILE:HG23	26:B:235:VAL:HA	1.98	0.45
26:B:257:ARG:HG2	26:B:261:TRP:CG	2.52	0.45
26:B:327:ILE:HG12	26:B:347:THR:HG21	1.98	0.45
26:B:371:ILE:HD11	26:B:435:VAL:HG22	1.99	0.45
27:C:236:GLY:O	27:C:364:VAL:HG23	2.17	0.45
39:Q:47:PHE:HB3	39:Q:57:ARG:CZ	2.47	0.45
43:U:138:TYR:OH	43:U:193:LYS:HA	2.16	0.45
48:l:241:THR:HG22	48:l:299:LYS:HD2	1.99	0.45
5:v:322:ASP:C	3:Af:68:LEU:HD11	2.42	0.45
53:G:485:ASP:HA	53:G:677:GLN:NE2	2.32	0.45
3:4:259:CYS:SG	3:4:260:HIS:N	2.89	0.45
6:7:183:PHE:CE2	56:7:401:HEM:HBC1	2.52	0.45
7:8:243:ILE:HD11	57:8:401:HEC:HHA	1.98	0.45
9:a:174:ILE:HG21	16:h:20:ILE:HG21	1.99	0.45
14:f:33:GLU:OE1	14:f:33:GLU:N	2.48	0.45
17:i:51:ARG:HH11	27:C:75:VAL:HG22	1.81	0.45
17:i:313:MET:HE2	43:U:143:LEU:HD22	1.99	0.45
25:r:74:ALA:HB3	25:r:75:PRO:HD3	1.99	0.45
35:L:326:HIS:H	35:L:326:HIS:CD2	2.35	0.45
48:l:15:LEU:O	48:l:18:PRO:HD2	2.16	0.45
48:l:416:THR:O	48:l:419:THR:OG1	2.26	0.45
48:l:428:PHE:CD2	48:l:505:ASN:HB3	2.52	0.45
51:u:206:GLU:CD	51:u:206:GLU:H	2.24	0.45
5:v:108:GLY:HA3	5:v:133:LEU:HD21	1.99	0.45
5:v:360:THR:HG22	5:v:365:ASN:HB3	1.98	0.45
6:w:131:TYR:O	6:w:134:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:x:168:ARG:NH1	7:x:171:LYS:HE3	2.32	0.45
51:5:304:LEU:HD23	51:5:304:LEU:HA	1.86	0.45
1:0:34:ARG:HD2	1:0:78:ARG:NE	2.31	0.44
5:6:254:ARG:O	5:6:435:ARG:NH1	2.50	0.44
17:i:251:MET:HE2	17:i:293:TYR:OH	2.17	0.44
20:m:51:PHE:CZ	20:m:55:MET:HE2	2.53	0.44
22:o:59:VAL:HG22	24:q:423:ILE:HG23	1.99	0.44
24:q:77:LEU:O	24:q:81:GLN:HG3	2.17	0.44
26:B:120:GLY:HA2	26:B:159:ARG:HH21	1.81	0.44
28:D:227:ALA:O	33:J:116:SER:OG	2.22	0.44
35:L:87:MET:HA	35:L:90:ARG:HE	1.81	0.44
35:L:267:LEU:HG	35:L:370:VAL:HG21	1.99	0.44
36:N:35:LEU:HD23	36:N:38:ILE:HD12	2.00	0.44
43:U:172:LEU:HD21	43:U:186:VAL:HG13	1.99	0.44
45:W:129:THR:HG23	45:W:132:GLU:H	1.82	0.44
2:1:34:ARG:HH21	4:3:50:GLY:HA3	1.83	0.44
17:i:255:PRO:HG3	17:i:260:PHE:CD1	2.52	0.44
18:j:82:ASN:OD1	18:j:82:ASN:N	2.50	0.44
24:q:1:MET:HE2	24:q:111:THR:HG21	1.99	0.44
24:q:25:ILE:O	24:q:29:VAL:HG23	2.16	0.44
24:q:306:PRO:HA	24:q:458:LEU:HD22	1.98	0.44
26:B:423:THR:HG21	26:B:428:GLY:HA3	1.99	0.44
27:C:187:LEU:HD22	27:C:213:ARG:HE	1.82	0.44
33:J:158:LYS:NZ	53:G:69:LEU:O	2.35	0.44
35:L:54:PHE:O	35:L:124:LEU:HB2	2.18	0.44
36:N:77:ILE:O	36:N:81:ILE:HG23	2.17	0.44
37:O:112:SER:O	37:O:116:VAL:HG23	2.16	0.44
43:U:66:GLY:O	43:U:163:ARG:NH2	2.43	0.44
48:l:332:HIS:HA	48:l:335:PHE:CZ	2.51	0.44
5:v:203:ASP:OD1	5:v:203:ASP:N	2.47	0.44
51:5:407:THR:HB	51:5:408:PRO:HD3	2.00	0.44
3:2:104:ILE:HG23	7:x:323:ARG:HE	1.81	0.44
3:2:134:PHE:CZ	3:2:138:ILE:HD11	2.53	0.44
7:8:214:SER:HB3	7:8:237:TYR:CE2	2.52	0.44
10:b:86:LEU:HD21	48:l:9:LEU:HD12	2.00	0.44
11:c:36:MET:HE3	11:c:36:MET:HB3	1.69	0.44
17:i:61:LEU:O	17:i:65:THR:HG23	2.17	0.44
17:i:75:ILE:HD12	19:k:40:LEU:HD22	1.99	0.44
17:i:89:MET:HB2	17:i:95:MET:HG2	1.98	0.44
26:B:126:LYS:HB3	26:B:277:ASN:HD21	1.81	0.44
27:C:463:VAL:HG13	27:C:466:GLU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:185:MET:HE3	29:E:185:MET:HB3	1.70	0.44
5:v:138:LEU:HD12	5:v:233:VAL:HG22	1.99	0.44
5:v:196:ARG:NH2	5:v:204:GLN:OE1	2.42	0.44
5:v:358:VAL:HG11	5:v:431:PHE:CD2	2.53	0.44
51:5:253:LEU:HD12	51:5:253:LEU:HA	1.81	0.44
53:G:325:ARG:HE	53:G:325:ARG:HB2	1.53	0.44
5:6:313:VAL:HG11	5:6:350:VAL:HG13	1.99	0.44
12:d:40:LEU:HD23	12:d:40:LEU:HA	1.87	0.44
12:d:110:LEU:HD21	48:l:204:LEU:HD21	2.00	0.44
20:m:57:PHE:HD1	20:m:57:PHE:HA	1.72	0.44
22:o:87:SER:HA	48:l:557:TRP:HZ2	1.81	0.44
28:D:219:VAL:HG21	32:I:115:PRO:HG3	2.00	0.44
29:E:42:ARG:HB2	29:E:42:ARG:HH11	1.83	0.44
37:O:110:LEU:HD13	37:O:114:ASP:HB3	1.98	0.44
37:O:147:TYR:O	37:O:151:LYS:HG2	2.17	0.44
43:U:149:LEU:HD13	43:U:296:LEU:HD21	1.99	0.44
5:v:70:ARG:HG3	5:v:185:ALA:HB1	2.00	0.44
56:w:402:HEM:HBB2	56:w:402:HEM:HMB1	2.00	0.44
53:G:305:PRO:HA	53:G:585:PRO:HD3	1.99	0.44
5:6:49:ILE:HB	5:6:230:LEU:HD23	2.00	0.44
6:7:8:HIS:ND1	6:7:11:MET:HG2	2.32	0.44
10:b:28:LEU:HD11	23:p:157:TYR:HD2	1.82	0.44
25:r:162:LEU:HA	25:r:165:LEU:HD13	1.99	0.44
26:B:111:LYS:HB2	26:B:151:ALA:HA	1.99	0.44
26:B:128:ARG:HG2	26:B:132:ARG:NH1	2.31	0.44
35:L:129:TRP:CZ3	35:L:131:THR:HG22	2.53	0.44
6:w:310:SER:HB2	6:w:370:SER:HB3	1.99	0.44
51:5:310:ILE:HG21	51:5:379:LEU:HD21	1.99	0.44
6:7:131:TYR:O	6:7:134:PRO:HD2	2.18	0.44
6:7:275:LEU:HD23	6:7:275:LEU:HA	1.82	0.44
57:8:401:HEC:HBD1	57:8:401:HEC:CHA	2.48	0.44
16:h:82:GLN:OE1	45:W:101:VAL:HG23	2.17	0.44
17:i:203:LEU:HD21	17:i:261:MET:HE2	1.99	0.44
20:m:3:MET:HE3	20:m:125:TRP:NE1	2.32	0.44
20:m:56:VAL:O	20:m:60:TYR:HB3	2.17	0.44
23:p:59:LEU:HD21	37:X:112:SER:HB2	1.99	0.44
23:p:66:LEU:HB3	37:X:120:MET:HE1	1.99	0.44
24:q:76:MET:SD	24:q:230:VAL:HG13	2.58	0.44
24:q:231:LEU:O	24:q:236:LEU:HG	2.17	0.44
24:q:329:LEU:O	24:q:332:THR:OG1	2.35	0.44
27:C:103:LEU:HD11	27:C:115:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:223:PHE:H	29:E:226:GLU:CD	2.26	0.44
35:L:216:ARG:HB2	35:L:276:PHE:CE2	2.53	0.44
47:Z:46:GLU:HG2	47:Z:50:GLU:OE2	2.18	0.44
50:t:34:ARG:NH1	50:t:104:ARG:HH12	2.14	0.44
50:t:99:MET:HE2	50:t:99:MET:HB3	1.87	0.44
7:x:196:PRO:HG2	57:x:401:HEC:HBA1	1.99	0.44
51:5:207:ASN:O	51:5:211:LEU:HG	2.17	0.44
51:5:473:SER:HA	51:5:476:PHE:CE1	2.53	0.44
53:G:68:ARG:NH1	53:G:284:GLU:OE2	2.51	0.44
53:G:600:GLU:OE1	53:G:602:ARG:NH2	2.48	0.44
3:4:161:MET:HE2	3:4:161:MET:HB3	1.82	0.44
6:7:45:ILE:HA	56:7:401:HEM:HMC2	2.00	0.44
6:7:47:THR:HB	6:7:83:HIS:HD1	1.83	0.44
7:8:249:ILE:O	7:8:264:MET:HG3	2.17	0.44
11:c:88:PRO:HA	11:c:98:ARG:HD3	2.00	0.44
11:c:184:TYR:HB3	50:t:34:ARG:HB3	1.98	0.44
26:B:52:ARG:HB3	26:B:54:LYS:NZ	2.32	0.44
26:B:62:TRP:CZ3	26:B:181:LEU:HB3	2.53	0.44
31:H:211:TYR:CE2	54:M:39:PRO:HG3	2.52	0.44
35:L:240:VAL:HG13	35:L:260:PHE:HD2	1.83	0.44
43:U:244:LYS:HA	43:U:248:LEU:HD12	1.99	0.44
51:u:397:ASN:ND2	5:v:107:GLY:O	2.51	0.44
53:G:217:GLU:HG2	53:G:412:PRO:HB3	1.99	0.44
3:4:177:LEU:O	3:4:178:SER:OG	2.32	0.44
5:6:106:VAL:HG21	5:6:133:LEU:HD13	1.99	0.44
6:7:223:TYR:O	6:7:226:ILE:HG22	2.17	0.44
12:d:80:LYS:HD2	24:q:182:TRP:CE2	2.53	0.44
20:m:103:MET:N	20:m:103:MET:SD	2.91	0.44
24:q:375:LEU:HD11	48:l:141:PHE:HE2	1.83	0.44
26:B:199:ARG:NH1	29:E:88:ARG:HH12	2.16	0.44
27:C:140:PRO:HB2	32:I:142:TYR:CE2	2.53	0.44
27:C:144:ARG:NH1	27:C:229:HIS:HB3	2.33	0.44
39:Q:88:LYS:HD3	39:Q:132:PHE:HB3	2.00	0.44
7:x:123:SER:O	7:x:179:PRO:HB3	2.18	0.44
51:5:362:ASN:ND2	51:5:363:MET:SD	2.90	0.44
53:G:498:GLN:HG3	53:G:499:ASN:N	2.32	0.44
1:0:71:LEU:HG	1:0:75:LEU:HD12	2.00	0.44
6:7:173:ALA:O	6:7:177:ARG:HG3	2.17	0.44
6:7:272:TRP:HA	6:7:275:LEU:HD12	2.00	0.44
7:8:294:LEU:HD23	7:8:294:LEU:HA	1.88	0.44
16:h:47:ILE:HA	49:s:228:ASN:HD21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:88:LYS:HD2	17:i:148:SER:HB3	1.99	0.44
17:i:231:SER:O	17:i:234:TRP:HD1	1.99	0.44
20:m:82:VAL:HG12	20:m:83:TRP:H	1.82	0.44
20:m:110:GLU:O	20:m:111:GLU:C	2.61	0.44
24:q:357:THR:O	24:q:361:MET:HG3	2.18	0.44
27:C:284:VAL:HG22	27:C:335:ARG:NH2	2.33	0.44
29:E:177:LEU:HD12	29:E:185:MET:SD	2.58	0.44
34:K:110:TRP:CZ3	34:K:114:LYS:HE2	2.53	0.44
50:t:29:TYR:HD1	50:t:29:TYR:HA	1.69	0.44
5:v:130:ILE:HD13	5:v:130:ILE:HA	1.85	0.44
6:w:31:TRP:NE1	56:w:401:HEM:O2D	2.51	0.44
7:x:220:CYS:SG	7:x:221:GLU:N	2.91	0.44
51:5:304:LEU:HD13	51:5:354:LEU:HD22	2.00	0.44
53:G:338:VAL:HG23	53:G:363:SER:HB2	2.00	0.44
53:G:562:LYS:HA	53:G:562:LYS:HD3	1.85	0.44
1:0:65:GLU:HB3	52:z:78:TYR:CG	2.52	0.43
6:7:221:HIS:HB3	6:7:222:PRO:HD3	1.99	0.43
10:b:73:THR:HA	10:b:77:ILE:HD12	2.00	0.43
10:b:74:HIS:O	10:b:78:PRO:HG2	2.18	0.43
11:c:62:TYR:CE2	11:c:64:PRO:HD3	2.53	0.43
11:c:186:ILE:HB	50:t:97:LYS:HG3	1.99	0.43
24:q:313:THR:HA	24:q:316:MET:HE2	2.00	0.43
25:r:77:LEU:HD22	25:r:118:TRP:CZ3	2.53	0.43
27:C:205:PRO:HB3	27:C:264:LEU:HD12	1.99	0.43
29:E:203:GLU:O	29:E:207:GLU:HG3	2.17	0.43
31:H:63:TRP:HB3	31:H:66:LEU:HD12	1.99	0.43
31:H:65:GLU:OE1	31:H:65:GLU:N	2.51	0.43
37:O:100:VAL:HG12	37:O:142:GLN:HB2	1.99	0.43
37:O:120:MET:HA	37:O:123:GLU:HG2	2.00	0.43
38:P:68:ARG:HD2	53:G:359:ASN:ND2	2.33	0.43
43:U:245:LYS:HB2	43:U:245:LYS:HE3	1.85	0.43
48:l:79:SER:OG	48:l:135:ASN:HB3	2.18	0.43
3:2:252:PHE:CZ	3:2:271:ARG:HB2	2.53	0.43
5:6:79:THR:HG23	5:6:205:LEU:HD23	2.00	0.43
5:6:438:MET:HE2	5:6:440:ALA:HB2	1.99	0.43
7:8:316:LYS:HA	7:8:316:LYS:HD3	1.79	0.43
25:r:280:PHE:CZ	27:C:273:ILE:HG12	2.53	0.43
37:X:120:MET:O	37:X:123:GLU:HG2	2.18	0.43
6:w:8:HIS:O	6:w:12:LYS:N	2.46	0.43
1:Ab:40:ILE:HG22	1:Ab:42:LYS:HD2	2.01	0.43
10:b:22:TRP:O	10:b:26:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:71:ALA:O	10:b:75:VAL:HG22	2.18	0.43
12:d:82:ILE:H	12:d:82:ILE:HG13	1.46	0.43
14:f:31:ILE:HG13	14:f:32:ARG:N	2.33	0.43
15:g:98:SER:OG	15:g:99:HIS:ND1	2.49	0.43
19:k:64:LEU:HD12	19:k:64:LEU:HA	1.83	0.43
21:n:47:ARG:HH22	21:n:53:GLU:CD	2.26	0.43
25:r:92:PRO:HB3	25:r:255:TYR:CD1	2.53	0.43
26:B:194:ASP:OD2	40:R:98:MET:HG2	2.17	0.43
27:C:296:GLY:O	27:C:300:ARG:HG3	2.18	0.43
29:E:219:ARG:HD2	29:E:219:ARG:HA	1.78	0.43
36:N:88:LEU:HD22	36:N:92:ARG:NH1	2.33	0.43
43:U:211:VAL:HG22	43:U:262:ALA:HB2	1.99	0.43
48:l:124:PHE:CD2	48:l:247:LEU:HD22	2.53	0.43
49:s:208:VAL:HG12	49:s:210:THR:HG23	2.00	0.43
5:v:63:LEU:HD23	5:v:141:THR:HG21	1.99	0.43
3:2:256:TYR:HE1	3:2:261:GLY:HA2	1.82	0.43
5:6:359:LYS:HA	5:6:432:VAL:HG21	2.00	0.43
5:6:371:VAL:HG12	5:6:375:LYS:HE3	2.01	0.43
5:6:383:LEU:HD13	51:5:67:PRO:HB2	2.00	0.43
9:a:70:LEU:HD22	13:e:87:MET:HE1	2.01	0.43
17:i:273:ASN:HD21	44:V:141:VAL:HG23	1.84	0.43
24:q:299:VAL:O	24:q:303:ILE:HG13	2.19	0.43
26:B:157:TYR:CB	26:B:212:LEU:HD21	2.48	0.43
48:l:190:LEU:HD22	48:l:196:TRP:CZ2	2.54	0.43
5:v:40:PHE:CE1	5:v:406:TYR:HB2	2.53	0.43
1:Ab:37:CYS:O	1:Ab:40:ILE:N	2.51	0.43
10:b:77:ILE:HB	10:b:78:PRO:HD3	2.00	0.43
17:i:139:LEU:HD23	17:i:139:LEU:HA	1.86	0.43
17:i:291:TYR:HA	24:q:151:PHE:HZ	1.83	0.43
20:m:110:GLU:O	20:m:112:GLU:N	2.51	0.43
25:r:233:MET:HE3	25:r:233:MET:HB3	1.74	0.43
26:B:62:TRP:HE1	26:B:136:HIS:HB3	1.84	0.43
35:L:129:TRP:H	35:L:129:TRP:CD1	2.37	0.43
48:l:37:LYS:NZ	48:l:98:TRP:HE1	2.16	0.43
7:x:228:LEU:HD11	7:x:234:PHE:HB2	1.99	0.43
7:x:311:LYS:HD3	7:x:311:LYS:HA	1.86	0.43
51:5:318:TYR:CD1	3:Ae:55:GLY:HA2	2.54	0.43
3:2:278:ASN:OD1	3:2:278:ASN:N	2.50	0.43
20:m:126:VAL:HG13	45:W:122:GLY:HA3	2.00	0.43
24:q:31:SER:HB2	24:q:74:PRO:HG3	2.01	0.43
26:B:115:VAL:HG11	26:B:138:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:226:LYS:O	26:B:227:PRO:C	2.62	0.43
26:B:292:MET:HE3	26:B:292:MET:HB3	1.84	0.43
27:C:309:ARG:HG3	27:C:407:GLU:HB3	2.01	0.43
37:X:133:ILE:HD13	37:X:133:ILE:H	1.82	0.43
51:u:317:THR:HA	5:v:157:GLN:NE2	2.34	0.43
51:u:406:THR:HG1	5:v:387:GLU:CD	2.25	0.43
51:5:225:LYS:O	51:5:229:MET:HG3	2.19	0.43
51:5:373:GLN:O	51:5:377:MET:HG2	2.18	0.43
53:G:76:ARG:O	53:G:116:VAL:HG21	2.18	0.43
5:6:301:ARG:HH22	51:5:94:GLU:HG2	1.83	0.43
7:8:128:MET:HE3	7:8:198:LEU:HB3	2.01	0.43
9:a:160:MET:HE2	15:g:95:TYR:CD1	2.54	0.43
18:j:87:MET:HE1	25:r:309:ILE:HD11	2.01	0.43
19:k:23:ARG:HD3	20:m:23:LYS:HB2	2.00	0.43
20:m:63:GLY:O	20:m:66:VAL:HG12	2.18	0.43
20:m:66:VAL:HG23	25:r:114:TYR:CZ	2.54	0.43
24:q:336:ARG:NH2	24:q:429:SER:HA	2.33	0.43
26:B:371:ILE:CD1	26:B:396:MET:HG3	2.47	0.43
31:H:98:ARG:HD2	31:H:156:GLY:CA	2.49	0.43
31:H:196:LYS:HD3	34:K:113:HIS:CE1	2.54	0.43
35:L:120:VAL:HG11	35:L:248:ILE:HD13	2.01	0.43
35:L:306:GLU:O	35:L:308:TRP:N	2.45	0.43
38:P:85:ASP:OD1	38:P:85:ASP:N	2.41	0.43
51:u:407:THR:HB	51:u:408:PRO:HD3	1.99	0.43
7:x:205:ARG:NE	57:x:401:HEC:O2A	2.43	0.43
3:2:166:ASP:OD1	3:2:167:VAL:N	2.52	0.43
3:4:257:CYS:SG	3:4:259:CYS:SG	3.17	0.43
5:6:65:ILE:HG21	5:6:213:PHE:CD1	2.53	0.43
16:h:85:LYS:O	16:h:89:GLU:HG2	2.19	0.43
17:i:190:MET:HG2	17:i:204:ASN:HB3	2.01	0.43
17:i:337:LEU:C	17:i:339:MET:H	2.27	0.43
20:m:55:MET:O	20:m:59:ILE:HG12	2.18	0.43
22:o:10:ARG:NH2	48:l:539:TYR:OH	2.51	0.43
23:p:162:ALA:O	23:p:166:GLN:HG3	2.18	0.43
24:q:10:MET:O	24:q:13:PRO:HD2	2.19	0.43
24:q:14:MET:HE3	24:q:14:MET:HB3	1.80	0.43
24:q:231:LEU:HA	24:q:235:LEU:HB2	2.01	0.43
26:B:325:PRO:HD2	26:B:347:THR:HA	1.99	0.43
27:C:63:GLU:H	27:C:63:GLU:CD	2.26	0.43
27:C:345:GLN:O	27:C:349:ILE:HG13	2.18	0.43
28:D:149:GLU:HG3	33:J:61:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:224:SER:C	29:E:226:GLU:H	2.27	0.43
30:F:30:ARG:O	30:F:38:VAL:HG12	2.19	0.43
37:O:110:LEU:HB2	37:O:114:ASP:CB	2.48	0.43
5:v:261:GLN:NE2	5:v:443:ASN:O	2.48	0.43
51:5:343:THR:HG22	51:5:356:ALA:HB2	1.99	0.43
3:4:212:GLU:HG2	3:4:214:SER:H	1.82	0.43
12:d:79:GLU:C	12:d:81:ASP:H	2.27	0.43
12:d:79:GLU:C	12:d:81:ASP:N	2.76	0.43
14:f:47:THR:HG23	15:g:65:LEU:HD22	2.01	0.43
16:h:81:ARG:HD2	20:m:111:GLU:CG	2.40	0.43
18:j:87:MET:HE3	18:j:87:MET:HB3	1.92	0.43
24:q:235:LEU:HD23	24:q:235:LEU:HA	1.84	0.43
26:B:225:LEU:HB2	33:J:160:TYR:CE2	2.54	0.43
27:C:62:LYS:HE3	27:C:62:LYS:HB2	1.78	0.43
29:E:149:LEU:HG	29:E:153:GLN:HE21	1.82	0.43
31:H:116:CYS:SG	59:H:302:SF4:S2	3.11	0.43
38:P:62:GLN:HB2	38:P:80:ASN:HB2	2.01	0.43
38:P:65:LEU:HB2	38:P:79:LEU:HD11	2.01	0.43
37:X:82:ARG:HH21	37:X:125:GLU:CD	2.27	0.43
46:Y:88:ASP:N	46:Y:89:PRO:HD2	2.34	0.43
49:s:121:MET:HE2	49:s:121:MET:HA	2.00	0.43
51:u:75:ILE:HG12	51:u:229:MET:HG2	2.01	0.43
51:u:453:CYS:HA	51:u:472:ARG:HD3	1.99	0.43
53:G:587:ALA:O	53:G:592:LYS:NZ	2.49	0.43
5:6:149:TRP:CE2	8:y:50:ARG:HD3	2.54	0.43
14:f:65:ASP:HB3	15:g:25:PRO:HB3	2.01	0.43
26:B:424:ILE:HG22	53:G:76:ARG:CZ	2.49	0.43
26:B:437:GLY:HA2	26:B:440:ARG:NH2	2.34	0.43
27:C:229:HIS:NE2	32:I:71:CYS:HB3	2.34	0.43
27:C:259:PHE:CD1	54:M:23:LYS:HD2	2.54	0.43
27:C:448:HIS:HB3	27:C:452:ASP:HB2	2.01	0.43
48:l:88:MET:O	48:l:91:PRO:HD2	2.19	0.43
7:8:313:SER:HA	7:8:316:LYS:HB2	2.00	0.42
10:b:16:ARG:HD3	37:X:150:ASP:OD2	2.18	0.42
10:b:93:LYS:HD2	10:b:94:PRO:HD2	2.00	0.42
12:d:113:CYS:SG	12:d:116:ARG:NH2	2.92	0.42
17:i:317:PHE:HZ	43:U:143:LEU:HD21	1.84	0.42
21:n:10:ASP:HB2	24:q:19:LYS:HD2	2.01	0.42
24:q:69:THR:HG22	24:q:234:VAL:HG21	2.00	0.42
26:B:398:ARG:HH22	26:B:408:GLU:CD	2.27	0.42
28:D:125:ARG:NH2	28:D:199:ARG:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:184:LEU:HA	28:D:184:LEU:HD23	1.80	0.42
31:H:180:HIS:CE1	35:L:95:LEU:HD21	2.54	0.42
43:U:61:VAL:HG12	43:U:203:PRO:HB3	2.01	0.42
7:x:203:ARG:HG3	7:x:279:SER:HB3	1.99	0.42
5:6:317:VAL:HG13	5:6:319:GLN:NE2	2.35	0.42
6:7:27:ILE:HG12	6:7:224:TYR:CE1	2.54	0.42
6:7:207:ASN:ND2	6:7:211:ILE:O	2.48	0.42
15:g:51:ARG:HD3	17:i:322:GLN:HG3	1.99	0.42
30:F:59:GLN:HG2	34:K:122:GLN:HA	2.01	0.42
31:H:205:ILE:O	31:H:209:TYR:HB3	2.19	0.42
35:L:355:ARG:HA	35:L:355:ARG:HD2	1.61	0.42
38:P:16:LEU:HD11	38:P:94:VAL:HG12	2.01	0.42
43:U:256:GLU:OE2	43:U:278:LEU:HB3	2.19	0.42
37:X:140:CYS:HB3	37:X:143:GLU:HG2	1.99	0.42
48:l:59:GLN:HE22	48:l:61:MET:HG3	1.84	0.42
48:l:241:THR:OG1	48:l:242:PRO:HD3	2.19	0.42
51:u:119:HIS:ND1	5:v:384:MET:HE1	2.33	0.42
6:w:47:THR:HG23	6:w:79:ILE:CG2	2.49	0.42
51:5:158:ASP:O	51:5:162:GLU:HG2	2.18	0.42
53:G:310:GLU:H	53:G:310:GLU:HG3	1.57	0.42
53:G:598:ASN:OD1	53:G:602:ARG:N	2.49	0.42
3:4:189:LYS:HE2	3:4:189:LYS:HB2	1.89	0.42
17:i:68:MET:HE2	19:k:36:MET:HB3	2.00	0.42
17:i:231:SER:HB2	17:i:305:PHE:HB2	2.01	0.42
25:r:179:TRP:CG	25:r:180:PRO:HD3	2.54	0.42
26:B:328:PRO:HD3	26:B:441:HIS:CG	2.54	0.42
26:B:340:ASP:OD1	26:B:340:ASP:N	2.51	0.42
58:B:501:FMN:HM81	58:B:501:FMN:HM73	1.84	0.42
27:C:168:GLN:HB2	28:D:48:ARG:HA	2.01	0.42
28:D:44:ARG:NH2	54:M:62:GLU:OE1	2.45	0.42
31:H:196:LYS:HD2	31:H:197:TRP:NE1	2.34	0.42
38:P:17:ARG:HB3	38:P:68:ARG:HH21	1.84	0.42
45:W:63:GLU:OE2	49:s:196:ARG:NH1	2.46	0.42
37:X:128:PHE:HZ	37:X:148:ILE:HG12	1.84	0.42
48:l:60:GLU:OE1	48:l:84:TYR:N	2.51	0.42
48:l:76:LEU:HD23	48:l:76:LEU:HA	1.91	0.42
48:l:415:ALA:O	48:l:419:THR:HG23	2.19	0.42
5:v:352:LYS:HD2	5:v:352:LYS:HA	1.84	0.42
52:z:25:ARG:NH1	52:z:28:PRO:HA	2.34	0.42
2:Ac:23:LEU:HD22	4:Ad:23:MET:HE3	2.01	0.42
2:1:29:ALA:HA	3:2:144:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:47:TYR:N	4:3:49:ASN:OD1	2.52	0.42
5:6:259:ARG:NH2	5:6:447:THR:O	2.52	0.42
6:7:185:LEU:HD23	6:7:185:LEU:HA	1.73	0.42
7:8:216:LEU:HB3	7:8:249:ILE:CD1	2.47	0.42
18:j:77:TRP:CH2	25:r:100:LEU:HD21	2.55	0.42
25:r:195:ARG:HD3	25:r:231:ILE:HD11	2.01	0.42
26:B:56:ALA:HB1	26:B:61:ASP:HB2	2.02	0.42
27:C:190:ILE:HG21	27:C:213:ARG:HG3	2.01	0.42
36:N:78:GLU:O	36:N:81:ILE:HG12	2.18	0.42
37:O:114:ASP:O	37:O:118:ILE:HG23	2.18	0.42
51:5:405:GLY:O	51:5:409:VAL:HG23	2.19	0.42
51:5:418:LEU:HD23	51:5:418:LEU:HA	1.84	0.42
2:Ac:53:TRP:O	2:Ac:57:LYS:N	2.51	0.42
1:0:65:GLU:HB3	52:z:78:TYR:CD1	2.54	0.42
3:2:226:VAL:HA	3:2:284:TYR:OH	2.19	0.42
5:6:298:HIS:HB2	51:5:114:GLU:HG2	2.01	0.42
20:m:52:LEU:O	20:m:55:MET:HB2	2.19	0.42
20:m:114:GLU:HA	20:m:117:PHE:O	2.19	0.42
23:p:54:HIS:CD2	23:p:106:LEU:HD12	2.54	0.42
25:r:89:LEU:HD22	25:r:240:ILE:HD12	2.01	0.42
26:B:35:LEU:HD11	26:B:39:ASP:HB2	2.02	0.42
26:B:316:ALA:HA	26:B:327:ILE:O	2.19	0.42
27:C:146:ASP:HB2	27:C:466:GLU:HG3	2.00	0.42
35:L:175:TYR:CE1	35:L:316:ARG:HD2	2.55	0.42
35:L:241:SER:O	35:L:245:ILE:HG12	2.20	0.42
35:L:311:ARG:O	35:L:315:GLU:HG2	2.18	0.42
43:U:131:TYR:CG	43:U:185:CYS:HB3	2.54	0.42
48:l:63:ILE:O	48:l:79:SER:HA	2.20	0.42
52:z:4:GLU:O	52:z:8:LEU:HG	2.20	0.42
51:5:276:ARG:O	52:Aa:15:ILE:HA	2.20	0.42
3:2:237:VAL:HA	3:2:243:CYS:O	2.19	0.42
5:6:123:VAL:HB	5:6:133:LEU:HD23	2.01	0.42
9:a:64:ASP:OD1	9:a:64:ASP:N	2.50	0.42
17:i:145:ILE:O	17:i:149:ILE:HG13	2.19	0.42
17:i:313:MET:HE3	43:U:96:ALA:HB2	2.01	0.42
18:j:68:GLU:HG3	20:m:161:LEU:HD13	2.00	0.42
19:k:26:LEU:O	19:k:29:SER:OG	2.28	0.42
25:r:146:LEU:HG	25:r:185:TRP:CZ3	2.54	0.42
26:B:63:TYR:CE2	29:E:245:VAL:HG21	2.54	0.42
26:B:88:ARG:HD2	26:B:274:LYS:HE2	2.02	0.42
26:B:230:PRO:HA	26:B:233:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:L:79:TYR:CZ	35:L:102:GLU:HB2	2.54	0.42
39:Q:124:LYS:HE3	39:Q:129:ILE:HD13	2.00	0.42
48:l:291:CYS:O	48:l:295:GLN:HG2	2.19	0.42
48:l:383:MET:SD	48:l:384:PRO:HD2	2.59	0.42
5:v:300:LYS:HG2	5:v:301:ARG:HG3	2.01	0.42
5:v:326:PHE:CE2	3:Af:65:SER:HB2	2.55	0.42
6:7:237:LEU:HD13	7:8:297:MET:HG2	2.01	0.42
6:7:327:MET:HA	52:Aa:52:PRO:HB3	2.02	0.42
7:8:120:GLN:NE2	7:8:254:LEU:HB2	2.35	0.42
7:8:245:MET:HB2	7:8:245:MET:HE3	1.54	0.42
9:a:102:PRO:HG2	9:a:105:TYR:HB3	2.02	0.42
15:g:33:LEU:HD12	15:g:33:LEU:HA	1.83	0.42
18:j:16:LEU:O	18:j:20:ILE:HG13	2.19	0.42
26:B:170:GLN:OE1	26:B:197:VAL:HB	2.20	0.42
27:C:348:ARG:HB2	45:W:21:TYR:CD2	2.54	0.42
29:E:56:THR:OG1	29:E:58:GLU:HG3	2.19	0.42
31:H:173:PHE:CE1	32:I:171:GLU:HB3	2.55	0.42
32:I:70:ALA:H	32:I:107:GLY:HA3	1.85	0.42
37:O:104:PHE:CE1	37:O:141:PRO:HG3	2.55	0.42
37:O:104:PHE:HD1	37:O:108:LEU:HD12	1.84	0.42
44:V:118:MET:HE3	44:V:118:MET:HB2	1.95	0.42
48:l:264:TYR:N	48:l:265:PRO:HD2	2.35	0.42
49:s:180:GLN:HA	49:s:183:LYS:HD3	2.02	0.42
6:w:138:MET:HE3	6:w:252:ASP:CG	2.45	0.42
1:0:83:ALA:HB2	7:x:93:PRO:HB2	2.00	0.42
5:6:55:TYR:HA	5:6:127:ARG:NH1	2.34	0.42
10:b:93:LYS:HB3	10:b:96:THR:HG23	2.01	0.42
20:m:60:TYR:HA	20:m:64:MET:CG	2.50	0.42
27:C:306:TRP:CE3	27:C:311:THR:HG21	2.55	0.42
27:C:410:LYS:HZ2	27:C:461:ASP:HB2	1.83	0.42
28:D:114:LEU:HB3	28:D:166:TYR:HB3	2.02	0.42
29:E:111:ARG:HD2	33:J:173:SER:HB2	2.02	0.42
33:J:84:ARG:NH2	33:J:88:GLN:O	2.45	0.42
43:U:223:LYS:HZ1	43:U:228:GLU:CD	2.27	0.42
37:X:122:MET:HG3	37:X:144:ILE:HD13	2.01	0.42
49:s:87:LEU:O	49:s:91:LYS:HG3	2.20	0.42
49:s:149:ARG:O	49:s:153:ARG:HG3	2.19	0.42
5:v:370:ASP:N	5:v:370:ASP:OD1	2.53	0.42
6:w:196:HIS:HE1	56:w:401:HEM:NA	2.18	0.42
7:x:126:HIS:HE1	7:x:196:PRO:HD2	1.85	0.42
5:6:168:ASN:H	5:6:168:ASN:HD22	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:254:ARG:HH21	5:v:257:GLU:HG3	1.85	0.42
6:7:222:PRO:HG3	51:5:470:ARG:HE	1.84	0.42
10:b:61:ILE:HB	10:b:65:TYR:HB3	2.01	0.42
18:j:18:VAL:HA	25:r:222:MET:HE1	2.02	0.42
25:r:294:LEU:O	25:r:297:THR:OG1	2.33	0.42
26:B:64:LYS:HZ3	29:E:245:VAL:HG11	1.85	0.42
26:B:65:THR:O	26:B:69:LEU:HG	2.19	0.42
26:B:110:PRO:O	26:B:238:CYS:HB3	2.20	0.42
27:C:252:GLU:O	27:C:255:LYS:HG2	2.20	0.42
43:U:258:LEU:HD11	43:U:278:LEU:HD11	2.02	0.42
6:7:272:TRP:CE2	6:7:273:TYR:HD1	2.37	0.42
10:b:61:ILE:HG22	10:b:64:THR:H	1.85	0.42
11:c:140:MET:HE3	48:l:286:LEU:HD23	2.01	0.42
17:i:26:TRP:HB3	17:i:74:ILE:HD13	2.01	0.42
24:q:75:LEU:HB3	24:q:229:MET:HE1	2.01	0.42
24:q:141:GLU:HB2	24:q:222:GLU:CD	2.45	0.42
24:q:307:TRP:CZ3	48:l:190:LEU:HD21	2.54	0.42
26:B:225:LEU:HB3	26:B:227:PRO:HD2	2.01	0.42
28:D:183:ASP:OD2	28:D:185:ARG:NH1	2.50	0.42
35:L:313:LYS:O	35:L:317:VAL:HG23	2.19	0.42
48:l:217:LEU:HD13	48:l:276:MET:HE3	2.02	0.42
51:u:70:THR:HG21	51:u:407:THR:HA	2.02	0.42
6:w:182:HIS:CD2	56:w:402:HEM:C4C	3.08	0.42
2:Ac:19:SER:HB3	4:Ad:23:MET:HB3	2.01	0.42
2:1:21:PHE:O	2:1:25:ILE:HG13	2.20	0.41
3:4:191:ARG:HG2	6:w:168:PHE:CD2	2.55	0.41
16:h:103:ASP:OD1	16:h:103:ASP:N	2.52	0.41
17:i:37:LEU:O	17:i:41:ILE:HG12	2.20	0.41
17:i:296:LEU:HD23	17:i:296:LEU:HA	1.85	0.41
20:m:22:SER:HB2	20:m:89:VAL:HG13	2.02	0.41
23:p:143:GLU:HB2	23:p:164:ARG:HH12	1.85	0.41
25:r:47:GLN:HE21	25:r:51:ASP:CG	2.28	0.41
25:r:55:LEU:HA	25:r:55:LEU:HD23	1.84	0.41
25:r:228:TYR:O	25:r:232:ILE:HG13	2.19	0.41
25:r:313:SER:HB3	45:W:51:MET:HA	2.01	0.41
26:B:162:PHE:CZ	29:E:178:GLY:HA3	2.55	0.41
31:H:144:ARG:HB2	34:K:130:THR:HG23	2.01	0.41
39:Q:101:ASP:O	39:Q:105:VAL:HG23	2.20	0.41
46:Y:47:PHE:CD1	46:Y:48:PRO:HD2	2.54	0.41
48:l:280:LEU:O	48:l:284:THR:HG23	2.20	0.41
3:2:185:ASN:HB2	3:2:198:ARG:HE	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:101:GLU:HG3	13:e:118:ALA:HB1	2.02	0.41
17:i:276:ILE:C	17:i:279:PRO:HD2	2.45	0.41
25:r:135:ALA:O	25:r:136:VAL:C	2.63	0.41
25:r:201:THR:OG1	25:r:202:GLU:N	2.53	0.41
27:C:151:MET:HG3	27:C:220:TYR:CE2	2.55	0.41
29:E:215:LYS:HE2	29:E:215:LYS:HB2	1.91	0.41
32:I:67:PHE:CZ	32:I:69:LEU:HD21	2.54	0.41
35:L:143:ILE:HB	35:L:144:PRO:HD3	2.02	0.41
47:Z:41:GLU:H	47:Z:41:GLU:HG3	1.67	0.41
48:l:21:MET:O	48:l:24:SER:OG	2.31	0.41
51:u:302:VAL:HB	51:u:303:PRO:HD3	2.01	0.41
5:v:183:ARG:HG2	5:v:252:LYS:HB2	2.03	0.41
5:v:356:ASP:HA	5:v:359:LYS:HD3	2.02	0.41
51:5:358:PHE:CD2	51:5:368:MET:HG2	2.56	0.41
53:G:53:CYS:O	53:G:58:MET:N	2.53	0.41
53:G:217:GLU:OE2	53:G:409:PHE:HA	2.20	0.41
1:0:63:THR:OG1	1:0:65:GLU:HG2	2.20	0.41
3:4:204:GLU:O	3:4:208:GLU:HG2	2.19	0.41
7:8:90:LEU:HD11	1:Ab:76:HIS:HB2	2.02	0.41
7:8:168:ARG:NH1	7:8:174:ASP:OD2	2.53	0.41
9:a:133:TYR:CZ	21:n:44:LEU:HD12	2.55	0.41
11:c:71:GLY:HA2	22:o:79:ASN:O	2.20	0.41
13:e:65:ASN:OD1	13:e:65:ASN:N	2.53	0.41
17:i:323:MET:HE2	17:i:323:MET:HB3	1.89	0.41
27:C:331:ASP:OD1	27:C:331:ASP:N	2.53	0.41
28:D:186:ARG:NH1	28:D:191:TYR:O	2.54	0.41
29:E:141:MET:HE2	29:E:141:MET:HB3	1.87	0.41
35:L:216:ARG:HH11	35:L:216:ARG:HG3	1.85	0.41
37:O:130:ILE:HG12	37:O:147:TYR:HE2	1.85	0.41
37:X:138:LEU:HD13	37:X:138:LEU:HA	1.85	0.41
48:l:437:PHE:HE1	48:l:441:VAL:HG22	1.85	0.41
51:u:304:LEU:HD23	51:u:304:LEU:HA	1.78	0.41
53:G:183:ILE:HD11	53:G:206:VAL:HG13	2.01	0.41
5:6:60:ARG:CZ	5:6:390:GLU:HG2	2.49	0.41
5:6:253:TYR:HE2	5:6:435:ARG:HB3	1.85	0.41
6:7:338:ILE:HD13	6:7:351:GLY:CA	2.46	0.41
15:g:16:LEU:HD13	15:g:16:LEU:HA	1.80	0.41
17:i:155:LEU:HD22	17:i:278:MET:HE2	2.01	0.41
18:j:54:LYS:HD2	18:j:54:LYS:HA	1.87	0.41
18:j:60:ILE:O	18:j:63:LEU:HB2	2.21	0.41
27:C:352:GLN:O	27:C:356:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:44:GLU:HG2	32:I:194:TYR:CE2	2.55	0.41
37:O:113:LEU:HD12	39:Q:94:MET:HE2	2.01	0.41
48:l:54:PHE:CZ	48:l:84:TYR:HB2	2.56	0.41
48:l:257:VAL:HG11	48:l:313:MET:HB3	2.02	0.41
48:l:305:SER:O	48:l:309:GLN:HG2	2.19	0.41
48:l:368:PHE:HZ	48:l:455:LYS:HG3	1.85	0.41
50:t:7:ARG:NH1	50:t:16:GLU:OE2	2.52	0.41
6:w:299:LEU:HD23	6:w:299:LEU:HA	1.86	0.41
51:5:373:GLN:OE1	51:5:474:GLY:HA3	2.20	0.41
6:7:264:THR:HG22	6:7:265:PRO:O	2.21	0.41
6:7:323:CYS:SG	6:7:327:MET:HE3	2.61	0.41
10:b:75:VAL:HG12	48:l:14:ILE:HD13	2.03	0.41
10:b:93:LYS:NZ	12:d:108:GLU:OE2	2.49	0.41
12:d:89:GLU:CD	12:d:152:ALA:H	2.28	0.41
12:d:169:ALA:O	12:d:171:LYS:HG3	2.20	0.41
17:i:168:GLY:O	17:i:172:GLN:HG2	2.19	0.41
22:o:94:GLY:HA2	48:l:553:LEU:HD21	2.01	0.41
24:q:105:PHE:O	24:q:109:THR:HG23	2.19	0.41
25:r:1:MET:HE2	25:r:1:MET:HB3	1.80	0.41
25:r:245:ALA:HB3	25:r:255:TYR:CE2	2.54	0.41
25:r:293:PHE:O	25:r:294:LEU:C	2.63	0.41
26:B:125:CYS:SG	29:E:180:CYS:N	2.93	0.41
29:E:197:THR:H	29:E:200:ASP:HB2	1.84	0.41
35:L:223:LEU:O	35:L:287:PRO:HA	2.21	0.41
38:P:16:LEU:HD21	38:P:67:ALA:HB1	2.03	0.41
40:R:87:LEU:O	40:R:91:VAL:HG23	2.20	0.41
43:U:319:ILE:H	43:U:319:ILE:HG13	1.75	0.41
44:V:17:GLU:HB3	44:V:20:ARG:HD3	2.03	0.41
46:Y:54:GLN:NE2	48:l:446:ASN:HB2	2.34	0.41
48:l:12:LEU:HD22	48:l:129:MET:HB3	2.03	0.41
48:l:94:LEU:HD23	48:l:125:LEU:HD21	2.01	0.41
48:l:100:ILE:O	48:l:104:SER:OG	2.31	0.41
49:s:175:ARG:H	49:s:175:ARG:HG3	1.53	0.41
51:u:293:GLY:N	51:u:352:GLY:O	2.51	0.41
51:u:373:GLN:HE22	51:u:471:ILE:HG23	1.86	0.41
6:w:207:ASN:ND2	6:w:213:SER:HB3	2.36	0.41
51:5:70:THR:HB	51:5:410:CYS:SG	2.61	0.41
51:5:95:HIS:HB3	51:5:164:GLU:HG3	2.03	0.41
53:G:710:CYS:O	53:G:714:VAL:HG12	2.20	0.41
1:0:47:ARG:O	1:0:51:GLU:HG2	2.20	0.41
6:7:82:LEU:HD23	6:7:243:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:65:HIS:CE1	13:e:121:GLU:HG2	2.55	0.41
12:d:79:GLU:O	12:d:81:ASP:N	2.54	0.41
19:k:65:VAL:HG13	20:m:161:LEU:HD21	2.03	0.41
22:o:6:TYR:CE2	22:o:15:PRO:HD3	2.55	0.41
25:r:87:VAL:HG13	25:r:95:LEU:HD23	2.03	0.41
27:C:61:THR:N	27:C:64:THR:OG1	2.53	0.41
27:C:164:LEU:HD12	27:C:164:LEU:HA	1.82	0.41
30:F:37:LYS:HE3	30:F:37:LYS:HB2	1.78	0.41
31:H:122:VAL:O	31:H:123:CYS:C	2.64	0.41
34:K:42:ASP:OD1	34:K:46:ASN:N	2.54	0.41
35:L:78:PRO:HB2	35:L:103:TRP:CD1	2.55	0.41
38:P:65:LEU:O	38:P:76:ASN:HA	2.21	0.41
38:P:68:ARG:NH1	53:G:359:ASN:HD21	2.18	0.41
39:Q:67:ARG:HE	39:Q:67:ARG:HB3	1.28	0.41
43:U:83:LEU:HG	43:U:272:VAL:HG13	2.02	0.41
45:W:95:ALA:HA	45:W:106:VAL:HG11	2.02	0.41
47:Z:40:ILE:O	47:Z:43:THR:OG1	2.37	0.41
48:l:233:LEU:HB3	48:l:234:PRO:HD3	2.01	0.41
48:l:336:LYS:HA	48:l:336:LYS:HD3	1.71	0.41
3:2:213:VAL:O	3:2:216:LEU:HB2	2.20	0.41
5:6:180:ALA:HB2	5:6:258:ILE:HG13	2.03	0.41
7:8:142:THR:HG23	7:8:144:GLU:HG2	2.02	0.41
10:b:119:LEU:O	10:b:121:LYS:N	2.53	0.41
12:d:43:ARG:HB3	12:d:44:PRO:HD3	2.02	0.41
12:d:113:CYS:O	12:d:117:GLU:HG2	2.21	0.41
17:i:315:TRP:HZ3	43:U:329:VAL:HG12	1.85	0.41
20:m:27:ILE:O	20:m:31:LEU:HG	2.20	0.41
20:m:136:PHE:HD1	20:m:136:PHE:HA	1.77	0.41
25:r:37:PRO:O	25:r:44:GLY:HA3	2.20	0.41
27:C:262:ASP:CG	27:C:344:ARG:HH22	2.29	0.41
27:C:449:MET:HE3	27:C:449:MET:HB2	1.80	0.41
35:L:36:ILE:HD11	53:G:304:GLN:HE21	1.84	0.41
35:L:235:VAL:HG22	35:L:262:GLY:N	2.34	0.41
35:L:245:ILE:O	35:L:249:LYS:HG3	2.20	0.41
35:L:259:ALA:O	35:L:329:GLY:HA2	2.20	0.41
38:P:20:ARG:HB2	38:P:66:TRP:HB2	2.02	0.41
38:P:20:ARG:NH2	38:P:74:GLU:OE1	2.43	0.41
47:Z:52:LEU:HA	47:Z:55:ARG:HG2	2.02	0.41
51:u:477:TRP:HB3	51:u:479:ARG:HG2	2.02	0.41
5:v:309:LEU:HD23	5:v:357:GLN:HB3	2.03	0.41
51:5:197:LEU:HD23	51:5:197:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:5:338:CYS:SG	51:5:358:PHE:HB2	2.60	0.41
53:G:179:CYS:O	53:G:180:THR:OG1	2.33	0.41
2:1:48:ASN:OD1	7:x:105:SER:N	2.53	0.41
5:6:423:ASP:OD1	5:6:423:ASP:N	2.52	0.41
6:7:181:PHE:HA	6:7:184:ILE:HG22	2.02	0.41
8:9:83:LYS:H	8:9:86:GLU:HG2	1.85	0.41
12:d:26:LEU:HD12	50:t:76:ASN:HB2	2.02	0.41
12:d:128:GLU:H	12:d:128:GLU:HG2	1.64	0.41
17:i:14:MET:O	17:i:18:MET:HG2	2.20	0.41
21:n:16:LEU:HB3	24:q:10:MET:HE3	2.02	0.41
22:o:63:PRO:O	22:o:67:ARG:HG3	2.20	0.41
25:r:88:PRO:HB3	25:r:98:MET:HE3	2.03	0.41
26:B:63:TYR:CE2	26:B:64:LYS:HG3	2.55	0.41
26:B:63:TYR:CZ	26:B:64:LYS:HG3	2.56	0.41
27:C:290:LEU:HD23	27:C:290:LEU:HA	1.90	0.41
28:D:177:PHE:CE1	39:Q:110:ILE:HD13	2.55	0.41
35:L:36:ILE:HG23	53:G:615:LEU:HG	2.02	0.41
44:V:9:TYR:CE1	44:V:21:LYS:HE3	2.55	0.41
51:u:118:ALA:O	5:v:298:HIS:HB3	2.20	0.41
51:u:470:ARG:NH2	6:w:221:HIS:HB3	2.36	0.41
5:v:293:LEU:HB3	5:v:309:LEU:HG	2.02	0.41
5:v:313:VAL:HG11	5:v:350:VAL:HG13	2.03	0.41
52:z:19:LEU:HD23	52:z:19:LEU:HA	1.93	0.41
53:G:197:THR:HB	53:G:204:MET:HE3	2.03	0.41
53:G:445:LEU:HD22	53:G:460:HIS:CE1	2.55	0.41
3:2:207:GLN:HE21	3:2:207:GLN:HB2	1.61	0.41
4:3:9:ARG:HH11	4:3:9:ARG:HB3	1.86	0.41
3:4:195:LEU:HD21	3:4:294:VAL:HG21	2.03	0.41
3:4:257:CYS:SG	55:4:301:FES:S2	3.19	0.41
5:6:394:ASP:OD1	5:6:395:GLU:N	2.54	0.41
6:7:107:TYR:HB2	6:7:305:PRO:HG3	2.03	0.41
11:c:96:ASP:O	11:c:114:ARG:HD3	2.21	0.41
12:d:107:GLN:O	12:d:111:LYS:HG3	2.21	0.41
13:e:53:ILE:H	13:e:53:ILE:HG12	1.70	0.41
15:g:84:MET:HB3	17:i:344:SER:HB3	2.03	0.41
17:i:31:ILE:HG23	19:k:66:PHE:CZ	2.56	0.41
17:i:204:ASN:HD22	17:i:204:ASN:C	2.27	0.41
18:j:30:TYR:HB3	18:j:31:SER:H	1.72	0.41
19:k:75:LEU:CD1	20:m:67:VAL:HG13	2.51	0.41
20:m:83:TRP:HA	20:m:89:VAL:CG1	2.51	0.41
23:p:69:LEU:HD21	23:p:82:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:q:86:LYS:HE2	24:q:86:LYS:HB3	1.89	0.41
24:q:405:LEU:HD23	24:q:405:LEU:HA	1.78	0.41
26:B:136:HIS:O	26:B:140:GLU:HG2	2.21	0.41
27:C:49:TRP:NE1	27:C:53:PHE:HE2	2.19	0.41
27:C:443:LYS:HE2	27:C:443:LYS:HB2	1.93	0.41
28:D:157:VAL:HG11	28:D:182:PRO:HG2	2.02	0.41
28:D:181:HIS:CD2	28:D:183:ASP:H	2.32	0.41
35:L:60:LEU:HD21	35:L:244:ILE:HD11	2.02	0.41
35:L:161:HIS:O	35:L:196:ILE:N	2.54	0.41
35:L:215:MET:HA	35:L:218:PHE:CD2	2.56	0.41
37:X:104:PHE:HA	37:X:108:LEU:HB2	2.01	0.41
48:l:210:ASN:OD1	48:l:270:ASN:ND2	2.43	0.41
50:t:110:GLN:O	50:t:114:ARG:HG2	2.21	0.41
51:u:363:MET:HE3	52:z:6:GLY:HA3	2.03	0.41
6:w:138:MET:HE1	6:w:267:HIS:O	2.21	0.41
7:x:127:SER:HB2	7:x:179:PRO:HD2	2.03	0.41
53:G:188:GLU:O	53:G:419:ARG:NE	2.50	0.41
53:G:353:ALA:HA	53:G:636:TYR:OH	2.21	0.41
17:i:100:MET:HE3	17:i:111:PHE:CZ	2.56	0.41
20:m:61:LEU:HA	20:m:65:LEU:CD2	2.50	0.41
24:q:201:MET:HE1	24:q:212:LEU:HD11	2.03	0.41
29:E:68:LYS:HE2	29:E:68:LYS:HB3	1.78	0.41
29:E:108:PRO:HA	29:E:109:PRO:HD3	1.97	0.41
41:S:1:MET:HB2	41:S:3:PHE:CZ	2.56	0.41
44:V:95:CYS:HA	44:V:115:CYS:HA	2.02	0.41
45:W:116:TRP:HB2	49:s:129:ASP:OD2	2.21	0.41
6:w:40:CYS:O	6:w:44:GLN:HG2	2.21	0.41
6:w:55:TYR:HA	6:w:65:SER:OG	2.21	0.41
6:w:185:LEU:HD23	6:w:185:LEU:HA	1.79	0.41
51:5:68:THR:HG22	51:5:136:LEU:HD23	2.02	0.41
53:G:329:MET:HG2	53:G:565:PHE:CD2	2.56	0.41
53:G:400:ILE:HD12	53:G:427:LEU:HD21	2.03	0.41
2:1:34:ARG:NH2	4:3:50:GLY:HA3	2.36	0.40
3:2:259:CYS:HB2	55:2:301:FES:S1	2.60	0.40
5:6:293:LEU:HD12	5:6:336:PHE:HZ	1.85	0.40
7:8:114:GLY:HA3	7:8:274:PHE:HB2	2.02	0.40
7:8:203:ARG:CZ	7:8:280:GLU:HG2	2.52	0.40
7:8:266:GLN:HE22	1:Ab:91:LYS:H	1.69	0.40
10:b:79:VAL:HA	48:l:10:THR:HG21	2.03	0.40
15:g:87:LEU:HD23	15:g:87:LEU:HA	1.87	0.40
17:i:112:HIS:CE1	17:i:164:ILE:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:128:LEU:HD11	17:i:213:LEU:HA	2.02	0.40
25:r:78:ALA:HB2	25:r:115:SER:HB2	2.02	0.40
25:r:134:ARG:NH2	25:r:282:TYR:HB2	2.36	0.40
26:B:170:GLN:HE22	40:R:93:LEU:HD12	1.86	0.40
29:E:110:MET:O	29:E:114:GLU:HG3	2.20	0.40
29:E:169:PHE:CE2	29:E:209:LYS:HG3	2.51	0.40
35:L:183:GLU:HG3	35:L:195:ILE:HD13	2.03	0.40
35:L:222:PRO:HA	35:L:288:LEU:HD21	2.04	0.40
48:l:154:LEU:HD23	48:l:154:LEU:HA	1.91	0.40
5:v:409:PRO:O	5:v:413:LEU:HG	2.21	0.40
6:w:173:ALA:O	6:w:177:ARG:HG2	2.21	0.40
6:w:185:LEU:HD23	6:w:188:ILE:HD12	2.03	0.40
53:G:400:ILE:HG12	53:G:473:MET:HB3	2.02	0.40
53:G:618:GLU:O	53:G:622:ILE:HG13	2.20	0.40
1:0:79:ASP:HA	1:0:82:VAL:HB	2.03	0.40
3:4:189:LYS:HZ1	6:w:261:PRO:HB2	1.85	0.40
5:6:138:LEU:HD22	5:6:238:LEU:HD21	2.03	0.40
6:7:62:ALA:O	6:7:65:SER:OG	2.24	0.40
7:8:226:VAL:HG23	1:Ab:66:ASP:OD2	2.22	0.40
8:9:59:ARG:O	8:9:63:ILE:HG13	2.22	0.40
13:e:109:LEU:HD12	13:e:109:LEU:HA	1.91	0.40
17:i:89:MET:HE3	17:i:89:MET:HB3	1.91	0.40
17:i:183:SER:O	17:i:187:MET:HG2	2.21	0.40
24:q:142:ARG:NH2	27:C:42:GLN:HE21	2.20	0.40
28:D:121:THR:OG1	33:J:128:PHE:HA	2.22	0.40
28:D:229:GLU:OE2	53:G:246:ARG:NH2	2.55	0.40
29:E:66:ILE:HD11	40:R:87:LEU:HD22	2.04	0.40
35:L:340:LEU:O	35:L:344:ALA:N	2.54	0.40
35:L:354:TYR:HA	35:L:357:LEU:HB3	2.03	0.40
37:O:104:PHE:HE2	37:O:144:ILE:HD11	1.87	0.40
37:O:115:GLN:O	37:O:118:ILE:HG13	2.21	0.40
43:U:67:ASN:OD1	43:U:68:ILE:N	2.45	0.40
43:U:258:LEU:HB3	43:U:260:TYR:CE2	2.57	0.40
6:w:97:HIS:HE1	56:w:401:HEM:CHA	2.34	0.40
7:x:294:LEU:HD23	7:x:294:LEU:HA	1.95	0.40
51:5:426:LEU:HD23	51:5:426:LEU:HA	1.91	0.40
54:M:9:GLN:HA	54:M:12:ARG:HG2	2.03	0.40
1:0:48:GLU:O	1:0:52:LEU:HG	2.21	0.40
3:4:202:LYS:NZ	3:4:206:ASP:OD1	2.47	0.40
5:6:132:ILE:H	5:6:132:ILE:HG13	1.64	0.40
5:6:168:ASN:HB2	5:6:170:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:177:LEU:HD21	5:6:272:VAL:HG11	2.02	0.40
5:6:290:GLN:HB2	5:6:336:PHE:HE1	1.86	0.40
8:9:105:ARG:HG2	5:v:97:PHE:CE1	2.57	0.40
17:i:273:ASN:HA	44:V:140:LYS:HD2	2.02	0.40
20:m:93:PHE:O	20:m:97:LEU:HG	2.21	0.40
25:r:86:TRP:NE1	25:r:233:MET:HB2	2.36	0.40
25:r:277:TYR:HB3	27:C:273:ILE:HD12	2.04	0.40
26:B:36:LYS:HE3	26:B:36:LYS:HB3	1.88	0.40
26:B:85:LEU:HD23	26:B:95:THR:HG21	2.03	0.40
26:B:154:ALA:HB3	26:B:195:VAL:HG12	2.04	0.40
27:C:159:LEU:HD13	27:C:159:LEU:HA	1.91	0.40
27:C:272:ARG:HH22	31:H:63:TRP:HA	1.87	0.40
27:C:285:THR:HA	36:N:12:VAL:HG23	2.04	0.40
28:D:93:VAL:O	28:D:97:LEU:HB2	2.21	0.40
29:E:69:ASN:OD1	40:R:90:ASN:ND2	2.48	0.40
35:L:301:GLU:HA	35:L:307:PRO:HB3	2.02	0.40
40:R:98:MET:HE2	40:R:98:MET:HB3	1.74	0.40
37:X:93:ILE:HD11	37:X:110:LEU:HD11	2.03	0.40
48:l:13:ILE:HD12	48:l:13:ILE:HA	1.93	0.40
48:l:293:ILE:O	48:l:425:ARG:HD2	2.22	0.40
5:v:297:PRO:CD	3:Af:70:ALA:HB1	2.51	0.40
5:v:297:PRO:HD3	3:Af:70:ALA:HB1	2.04	0.40
6:w:129:MET:HE3	6:w:129:MET:HB2	1.91	0.40
6:w:233:LEU:CD1	7:x:304:VAL:HG21	2.52	0.40
3:2:208:GLU:OE1	3:2:266:ALA:HB3	2.21	0.40
5:6:101:ARG:HB3	8:y:108:TRP:CZ2	2.56	0.40
5:6:168:ASN:H	5:6:168:ASN:ND2	2.19	0.40
5:6:170:GLN:HG2	3:Ae:67:VAL:HG11	2.04	0.40
18:j:62:PHE:CG	25:r:140:ILE:HG23	2.55	0.40
22:o:81:ARG:O	22:o:83:THR:HG23	2.22	0.40
24:q:286:ILE:O	24:q:289:SER:OG	2.27	0.40
24:q:294:MET:HE3	24:q:319:HIS:ND1	2.37	0.40
26:B:62:TRP:CD2	26:B:181:LEU:HD13	2.57	0.40
26:B:113:LEU:HD13	26:B:149:MET:HE1	2.02	0.40
26:B:126:LYS:O	26:B:130:ILE:HG13	2.21	0.40
26:B:222:LYS:HG2	26:B:379:CYS:SG	2.62	0.40
29:E:120:THR:HG23	53:G:200:ARG:HH11	1.86	0.40
35:L:202:PHE:HE2	35:L:343:LYS:HB2	1.86	0.40
35:L:209:LEU:HB3	35:L:348:LEU:HD21	2.04	0.40
44:V:140:LYS:HE2	44:V:140:LYS:HB2	1.92	0.40
48:l:105:MET:HB3	48:l:449:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:u:158:ASP:O	51:u:162:GLU:HG2	2.21	0.40
51:u:274:GLU:CD	51:u:276:ARG:HE	2.28	0.40
51:u:324:MET:HE3	51:u:324:MET:HB2	1.91	0.40
51:5:226:ALA:N	51:5:227:PRO:HD2	2.36	0.40
53:G:679:LEU:H	53:G:679:LEU:HG	1.61	0.40
3:4:111:ASP:OD1	52:Aa:29:HIS:NE2	2.55	0.40
3:4:201:THR:HG1	3:4:204:GLU:HG3	1.87	0.40
5:6:168:ASN:HB2	5:6:170:GLN:NE2	2.36	0.40
11:c:117:VAL:HG21	48:l:539:TYR:HA	2.04	0.40
11:c:144:PHE:O	11:c:148:GLU:HG2	2.21	0.40
12:d:99:ASP:O	12:d:103:VAL:HG23	2.21	0.40
15:g:54:PRO:HG2	43:U:354:ILE:HG21	2.03	0.40
20:m:57:PHE:HA	20:m:61:LEU:HD13	2.04	0.40
27:C:148:VAL:HG12	27:C:188:ASN:HA	2.04	0.40
27:C:376:GLU:HA	27:C:379:THR:HG22	2.04	0.40
28:D:138:ASN:ND2	28:D:138:ASN:O	2.54	0.40
29:E:62:ARG:HD3	40:R:87:LEU:HB2	2.03	0.40
31:H:205:ILE:O	31:H:209:TYR:N	2.55	0.40
35:L:356:TRP:O	35:L:356:TRP:CD1	2.74	0.40
38:P:20:ARG:HG3	38:P:54:LEU:HB2	2.04	0.40
48:l:7:LEU:HD13	48:l:7:LEU:HA	1.83	0.40
7:x:133:TYR:HA	7:x:136:LEU:HD12	2.03	0.40
51:5:270:PHE:CG	51:5:292:GLU:HB2	2.56	0.40
3:Af:56:HIS:C	3:Af:58:ALA:H	2.30	0.40
52:Aa:68:GLU:O	52:Aa:72:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	66/91 (72%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ab	64/91 (70%)	64 (100%)	0	0	100	100
2	1	58/64 (91%)	58 (100%)	0	0	100	100
2	Ac	57/64 (89%)	55 (96%)	2 (4%)	0	100	100
3	2	193/299 (64%)	188 (97%)	5 (3%)	0	100	100
3	4	194/299 (65%)	184 (95%)	9 (5%)	1 (0%)	24	58
3	Ae	21/299 (7%)	13 (62%)	7 (33%)	1 (5%)	2	16
3	Af	27/299 (9%)	20 (74%)	7 (26%)	0	100	100
4	3	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
4	Ad	49/56 (88%)	46 (94%)	3 (6%)	0	100	100
5	6	416/453 (92%)	412 (99%)	4 (1%)	0	100	100
5	v	416/453 (92%)	412 (99%)	4 (1%)	0	100	100
6	7	377/379 (100%)	365 (97%)	12 (3%)	0	100	100
6	w	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
7	8	236/326 (72%)	227 (96%)	8 (3%)	1 (0%)	30	62
7	x	236/326 (72%)	231 (98%)	5 (2%)	0	100	100
8	9	97/111 (87%)	97 (100%)	0	0	100	100
8	y	99/111 (89%)	99 (100%)	0	0	100	100
9	a	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
10	b	102/128 (80%)	93 (91%)	8 (8%)	1 (1%)	12	44
11	c	151/186 (81%)	147 (97%)	4 (3%)	0	100	100
12	d	166/176 (94%)	165 (99%)	0	1 (1%)	21	53
13	e	97/154 (63%)	90 (93%)	7 (7%)	0	100	100
14	f	44/76 (58%)	44 (100%)	0	0	100	100
15	g	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
16	h	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
17	i	345/347 (99%)	341 (99%)	4 (1%)	0	100	100
18	j	96/115 (84%)	92 (96%)	4 (4%)	0	100	100
19	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
20	m	173/175 (99%)	162 (94%)	10 (6%)	1 (1%)	21	53
21	n	54/58 (93%)	49 (91%)	5 (9%)	0	100	100
22	o	126/129 (98%)	122 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	p	176/221 (80%)	175 (99%)	1 (1%)	0	100	100
24	q	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
25	r	316/318 (99%)	298 (94%)	17 (5%)	1 (0%)	36	67
26	B	429/464 (92%)	418 (97%)	11 (3%)	0	100	100
27	C	428/469 (91%)	411 (96%)	16 (4%)	1 (0%)	43	74
28	D	206/264 (78%)	197 (96%)	9 (4%)	0	100	100
29	E	212/249 (85%)	204 (96%)	8 (4%)	0	100	100
30	F	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
31	H	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
32	I	154/196 (79%)	151 (98%)	3 (2%)	0	100	100
33	J	115/175 (66%)	115 (100%)	0	0	100	100
34	K	142/145 (98%)	142 (100%)	0	0	100	100
35	L	338/372 (91%)	324 (96%)	14 (4%)	0	100	100
36	N	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
37	O	82/156 (53%)	79 (96%)	2 (2%)	1 (1%)	10	41
37	X	83/156 (53%)	80 (96%)	3 (4%)	0	100	100
38	P	81/99 (82%)	80 (99%)	1 (1%)	0	100	100
39	Q	110/154 (71%)	108 (98%)	2 (2%)	0	100	100
40	R	33/110 (30%)	33 (100%)	0	0	100	100
41	S	68/70 (97%)	68 (100%)	0	0	100	100
42	T	80/169 (47%)	78 (98%)	2 (2%)	0	100	100
43	U	316/357 (88%)	307 (97%)	9 (3%)	0	100	100
44	V	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
45	W	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
46	Y	60/105 (57%)	55 (92%)	5 (8%)	0	100	100
47	Z	76/114 (67%)	76 (100%)	0	0	100	100
48	l	601/606 (99%)	578 (96%)	23 (4%)	0	100	100
49	s	169/249 (68%)	167 (99%)	2 (1%)	0	100	100
50	t	117/137 (85%)	115 (98%)	2 (2%)	0	100	100
51	5	431/480 (90%)	423 (98%)	8 (2%)	0	100	100
51	u	444/480 (92%)	437 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	Aa	76/82 (93%)	76 (100%)	0	0	100	100
52	z	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
53	G	680/727 (94%)	668 (98%)	12 (2%)	0	100	100
54	M	92/113 (81%)	89 (97%)	3 (3%)	0	100	100
All	All	12140/14729 (82%)	11826 (97%)	305 (2%)	9 (0%)	49	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	b	120	MET
25	r	201	THR
27	C	461	ASP
3	Ae	50	CYS
12	d	80	LYS
20	m	111	GLU
3	4	289	ASP
7	8	126	HIS
37	O	138	LEU

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	64/85 (75%)	59 (92%)	5 (8%)	11	37
1	Ab	63/85 (74%)	53 (84%)	10 (16%)	2	14
2	1	49/52 (94%)	49 (100%)	0	100	100
2	Ac	48/52 (92%)	44 (92%)	4 (8%)	10	35
3	2	165/245 (67%)	152 (92%)	13 (8%)	11	36
3	4	166/245 (68%)	155 (93%)	11 (7%)	15	42
3	Ae	14/245 (6%)	12 (86%)	2 (14%)	3	18
3	Af	19/245 (8%)	15 (79%)	4 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	40/46 (87%)	39 (98%)	1 (2%)	42	63
4	Ad	41/46 (89%)	40 (98%)	1 (2%)	43	64
5	6	329/355 (93%)	310 (94%)	19 (6%)	18	45
5	v	329/355 (93%)	308 (94%)	21 (6%)	16	43
6	7	332/332 (100%)	318 (96%)	14 (4%)	26	52
6	w	332/332 (100%)	323 (97%)	9 (3%)	39	62
7	8	203/259 (78%)	189 (93%)	14 (7%)	14	40
7	x	203/259 (78%)	194 (96%)	9 (4%)	25	51
8	9	91/99 (92%)	82 (90%)	9 (10%)	7	29
8	y	93/99 (94%)	87 (94%)	6 (6%)	15	42
9	a	121/158 (77%)	115 (95%)	6 (5%)	22	48
10	b	97/121 (80%)	87 (90%)	10 (10%)	7	28
11	c	138/160 (86%)	130 (94%)	8 (6%)	18	45
12	d	152/156 (97%)	142 (93%)	10 (7%)	15	42
13	e	91/129 (70%)	74 (81%)	17 (19%)	1	9
14	f	42/66 (64%)	42 (100%)	0	100	100
15	g	108/109 (99%)	100 (93%)	8 (7%)	13	38
16	h	93/94 (99%)	88 (95%)	5 (5%)	20	47
17	i	311/311 (100%)	287 (92%)	24 (8%)	12	37
18	j	87/100 (87%)	76 (87%)	11 (13%)	4	21
19	k	85/85 (100%)	80 (94%)	5 (6%)	18	45
20	m	136/141 (96%)	125 (92%)	11 (8%)	11	35
21	n	52/55 (94%)	48 (92%)	4 (8%)	12	37
22	o	112/114 (98%)	109 (97%)	3 (3%)	39	62
23	p	159/190 (84%)	149 (94%)	10 (6%)	16	43
24	q	409/409 (100%)	391 (96%)	18 (4%)	25	51
25	r	275/275 (100%)	257 (94%)	18 (6%)	15	42
26	B	345/368 (94%)	330 (96%)	15 (4%)	26	52
27	C	370/398 (93%)	332 (90%)	38 (10%)	7	28
28	D	188/228 (82%)	169 (90%)	19 (10%)	7	28
29	E	183/207 (88%)	174 (95%)	9 (5%)	22	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	F	78/97 (80%)	72 (92%)	6 (8%)	12	37
31	H	151/176 (86%)	144 (95%)	7 (5%)	24	50
32	I	132/163 (81%)	128 (97%)	4 (3%)	36	60
33	J	106/152 (70%)	102 (96%)	4 (4%)	29	56
34	K	130/131 (99%)	126 (97%)	4 (3%)	35	60
35	L	289/320 (90%)	269 (93%)	20 (7%)	14	40
36	N	99/101 (98%)	94 (95%)	5 (5%)	21	48
37	O	78/132 (59%)	69 (88%)	9 (12%)	5	24
37	X	79/132 (60%)	74 (94%)	5 (6%)	16	43
38	P	74/82 (90%)	69 (93%)	5 (7%)	14	41
39	Q	105/134 (78%)	100 (95%)	5 (5%)	23	49
40	R	34/92 (37%)	32 (94%)	2 (6%)	18	45
41	S	58/58 (100%)	57 (98%)	1 (2%)	53	69
42	T	69/134 (52%)	64 (93%)	5 (7%)	13	38
43	U	281/307 (92%)	266 (95%)	15 (5%)	20	47
44	V	101/102 (99%)	95 (94%)	6 (6%)	18	45
45	W	122/124 (98%)	117 (96%)	5 (4%)	27	53
46	Y	54/84 (64%)	48 (89%)	6 (11%)	6	26
47	Z	60/90 (67%)	56 (93%)	4 (7%)	15	41
48	l	537/540 (99%)	503 (94%)	34 (6%)	16	43
49	s	153/206 (74%)	144 (94%)	9 (6%)	18	45
50	t	107/120 (89%)	97 (91%)	10 (9%)	8	31
51	5	363/397 (91%)	349 (96%)	14 (4%)	28	55
51	u	372/397 (94%)	353 (95%)	19 (5%)	21	48
52	Aa	70/73 (96%)	65 (93%)	5 (7%)	13	39
52	z	70/73 (96%)	65 (93%)	5 (7%)	13	39
53	G	576/610 (94%)	539 (94%)	37 (6%)	16	43
54	M	86/98 (88%)	80 (93%)	6 (7%)	14	40
All	All	10569/12435 (85%)	9911 (94%)	658 (6%)	18	44

All (658) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	42	LYS
1	0	48	GLU
1	0	64	GLU
1	0	70	GLU
1	0	75	LEU
3	2	104	ILE
3	2	172	LYS
3	2	207	GLN
3	2	208	GLU
3	2	231	TRP
3	2	238	CYS
3	2	246	ILE
3	2	251	ASP
3	2	259	CYS
3	2	278	ASN
3	2	280	GLU
3	2	287	THR
3	2	292	VAL
4	3	9	ARG
3	4	104	ILE
3	4	119	ASP
3	4	166	ASP
3	4	170	MET
3	4	172	LYS
3	4	186	MET
3	4	232	VAL
3	4	234	LEU
3	4	251	ASP
3	4	281	VAL
3	4	290	ASP
5	6	49	ILE
5	6	115	THR
5	6	122	THR
5	6	132	ILE
5	6	133	LEU
5	6	138	LEU
5	6	203	ASP
5	6	240	MET
5	6	244	LEU
5	6	246	LEU
5	6	319	GLN
5	6	323	VAL
5	6	370	ASP

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Mol	Chain	Res	Type
5	6	378	LEU
5	6	421	ASP
5	6	423	ASP
5	6	435	ARG
5	6	451	ASP
5	6	453	LEU
6	7	10	LEU
6	7	27	ILE
6	7	112	THR
6	7	156	ILE
6	7	202	GLU
6	7	252	ASP
6	7	254	ASP
6	7	257	THR
6	7	273	TYR
6	7	281	LEU
6	7	311	LYS
6	7	341	GLN
6	7	343	VAL
6	7	379	TRP
7	8	107	ASP
7	8	125	CYS
7	8	144	GLU
7	8	161	GLU
7	8	164	GLU
7	8	184	GLU
7	8	190	ASN
7	8	215	LEU
7	8	226	VAL
7	8	230	GLU
7	8	245	MET
7	8	251	ASN
7	8	276	ARG
7	8	293	MET
8	9	14	LEU
8	9	15	GLU
8	9	40	GLU
8	9	53	GLU
8	9	72	ARG
8	9	75	ILE
8	9	83	LYS
8	9	85	GLU

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Mol	Chain	Res	Type
8	9	92	GLU
9	a	58	LYS
9	a	64	ASP
9	a	82	VAL
9	a	130	GLU
9	a	143	GLU
9	a	153	GLU
10	b	4	TYR
10	b	23	LEU
10	b	24	LYS
10	b	28	LEU
10	b	75	VAL
10	b	86	LEU
10	b	89	HIS
10	b	96	THR
10	b	111	LEU
10	b	112	GLU
11	c	36	MET
11	c	53	LYS
11	c	68	ASP
11	c	77	LYS
11	c	87	ASP
11	c	101	TRP
11	c	140	MET
11	c	182	VAL
12	d	6	ASP
12	d	8	ASP
12	d	17	THR
12	d	49	ARG
12	d	50	GLU
12	d	69	ARG
12	d	71	VAL
12	d	82	ILE
12	d	114	GLN
12	d	156	LEU
13	e	54	ARG
13	e	58	ASP
13	e	62	GLU
13	e	63	ASP
13	e	64	GLU
13	e	70	ASN
13	e	72	ASP

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Mol	Chain	Res	Type
13	e	73	SER
13	e	77	ASP
13	e	82	VAL
13	e	84	LEU
13	e	87	MET
13	e	89	VAL
13	e	99	LEU
13	e	116	GLU
13	e	138	GLU
13	e	149	LEU
15	g	3	MET
15	g	16	LEU
15	g	19	GLU
15	g	29	THR
15	g	64	LEU
15	g	84	MET
15	g	87	LEU
15	g	101	GLU
16	h	75	ARG
16	h	82	GLN
16	h	86	LEU
16	h	91	LYS
16	h	101	LYS
17	i	5	ILE
17	i	19	LEU
17	i	22	ILE
17	i	29	ILE
17	i	36	ASN
17	i	79	LEU
17	i	87	THR
17	i	89	MET
17	i	159	MET
17	i	183	SER
17	i	193	VAL
17	i	194	LEU
17	i	258	SER
17	i	290	LEU
17	i	296	LEU
17	i	303	THR
17	i	311	MET
17	i	318	GLU
17	i	319	HIS

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Mol	Chain	Res	Type
17	i	321	LYS
17	i	323	MET
17	i	328	THR
17	i	336	VAL
17	i	346	LEU
18	j	1	MET
18	j	5	LEU
18	j	18	VAL
18	j	24	LEU
18	j	56	PHE
18	j	57	LEU
18	j	63	LEU
18	j	82	ASN
18	j	97	LEU
18	j	109	LYS
18	j	113	TRP
19	k	3	LEU
19	k	4	VAL
19	k	26	LEU
19	k	43	MET
19	k	59	MET
20	m	45	LEU
20	m	57	PHE
20	m	64	MET
20	m	65	LEU
20	m	66	VAL
20	m	74	MET
20	m	82	VAL
20	m	103	MET
20	m	135	PHE
20	m	136	PHE
20	m	151	THR
21	n	17	VAL
21	n	39	ARG
21	n	44	LEU
21	n	57	TRP
22	o	5	LYS
22	o	66	ILE
22	o	95	ILE
23	p	76	ARG
23	p	77	ASP
23	p	97	LYS

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Mol	Chain	Res	Type
23	p	101	LYS
23	p	110	GLU
23	p	126	GLU
23	p	165	GLU
23	p	176	GLU
23	p	192	ARG
23	p	204	ASP
24	q	4	ILE
24	q	11	LEU
24	q	14	MET
24	q	36	LEU
24	q	61	LEU
24	q	87	GLU
24	q	200	ILE
24	q	230	VAL
24	q	247	THR
24	q	250	LEU
24	q	270	ILE
24	q	282	LEU
24	q	315	LEU
24	q	343	ILE
24	q	369	LEU
24	q	375	LEU
24	q	426	ILE
24	q	454	ILE
25	r	5	ASN
25	r	13	ILE
25	r	106	LEU
25	r	108	MET
25	r	111	LEU
25	r	117	LEU
25	r	124	ASN
25	r	140	ILE
25	r	150	LEU
25	r	151	LEU
25	r	170	GLU
25	r	214	GLU
25	r	224	PHE
25	r	227	GLU
25	r	241	LEU
25	r	253	GLU
25	r	285	LEU

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Mol	Chain	Res	Type
25	r	286	MET
26	B	41	ILE
26	B	54	LYS
26	B	71	LYS
26	B	83	SER
26	B	102	MET
26	B	134	ASP
26	B	294	VAL
26	B	302	LYS
26	B	317	VAL
26	B	327	ILE
26	B	357	MET
26	B	382	CYS
26	B	390	ASP
26	B	424	ILE
26	B	445	GLU
27	C	52	GLN
27	C	57	VAL
27	C	75	VAL
27	C	76	ASP
27	C	81	THR
27	C	86	LEU
27	C	100	VAL
27	C	111	MET
27	C	124	ARG
27	C	143	ASP
27	C	147	TYR
27	C	148	VAL
27	C	150	MET
27	C	159	LEU
27	C	164	LEU
27	C	165	LEU
27	C	167	ILE
27	C	191	MET
27	C	194	THR
27	C	223	VAL
27	C	238	VAL
27	C	240	GLN
27	C	249	ASP
27	C	254	SER
27	C	264	LEU
27	C	266	GLU

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Mol	Chain	Res	Type
27	C	284	VAL
27	C	304	ILE
27	C	314	TYR
27	C	316	VAL
27	C	361	GLU
27	C	362	ILE
27	C	377	MET
27	C	418	VAL
27	C	449	MET
27	C	450	LEU
27	C	459	THR
27	C	463	VAL
28	D	68	ILE
28	D	81	PHE
28	D	111	LEU
28	D	113	ASP
28	D	119	VAL
28	D	136	ARG
28	D	140	ARG
28	D	143	VAL
28	D	145	THR
28	D	147	THR
28	D	149	GLU
28	D	154	GLU
28	D	159	VAL
28	D	194	GLU
28	D	201	ASP
28	D	204	LEU
28	D	215	GLU
28	D	219	VAL
28	D	250	GLU
29	E	42	ARG
29	E	58	GLU
29	E	85	LEU
29	E	137	THR
29	E	172	ILE
29	E	176	CYS
29	E	201	ILE
29	E	209	LYS
29	E	249	LEU
30	F	29	VAL
30	F	37	LYS

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Mol	Chain	Res	Type
30	F	46	ASP
30	F	57	ASP
30	F	79	VAL
30	F	85	SER
31	H	70	LEU
31	H	83	THR
31	H	114	ILE
31	H	118	LEU
31	H	150	THR
31	H	152	CYS
31	H	174	GLU
32	I	47	VAL
32	I	71	CYS
32	I	86	MET
32	I	169	THR
33	J	86	ASN
33	J	124	LEU
33	J	125	VAL
33	J	146	ASP
34	K	59	HIS
34	K	129	THR
34	K	136	GLU
34	K	144	TYR
35	L	119	ASN
35	L	170	LYS
35	L	174	ARG
35	L	175	TYR
35	L	177	ARG
35	L	205	GLU
35	L	235	VAL
35	L	254	LYS
35	L	270	ASP
35	L	286	TYR
35	L	299	LEU
35	L	302	VAL
35	L	305	PHE
35	L	308	TRP
35	L	309	THR
35	L	310	THR
35	L	323	THR
35	L	341	GLU
35	L	354	TYR

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Mol	Chain	Res	Type
35	L	355	ARG
36	N	5	LEU
36	N	40	LYS
36	N	87	GLU
36	N	88	LEU
36	N	94	MET
37	O	76	LEU
37	O	96	GLU
37	O	98	LEU
37	O	106	LYS
37	O	114	ASP
37	O	115	GLN
37	O	118	ILE
37	O	124	ASP
37	O	133	ILE
38	P	19	ILE
38	P	20	ARG
38	P	45	LYS
38	P	85	ASP
38	P	92	GLU
39	Q	67	ARG
39	Q	108	LEU
39	Q	117	GLU
39	Q	122	VAL
39	Q	127	THR
40	R	76	LEU
40	R	80	GLU
41	S	3	PHE
42	T	100	LYS
42	T	134	THR
42	T	142	LEU
42	T	151	VAL
42	T	166	LEU
43	U	43	LEU
43	U	69	CYS
43	U	117	GLU
43	U	152	LEU
43	U	172	LEU
43	U	232	THR
43	U	240	GLU
43	U	245	LYS
43	U	250	GLU

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Mol	Chain	Res	Type
43	U	253	GLU
43	U	255	CYS
43	U	263	ARG
43	U	281	ASP
43	U	347	GLU
43	U	352	LYS
44	V	3	LYS
44	V	6	LEU
44	V	104	ARG
44	V	115	CYS
44	V	140	LYS
44	V	141	VAL
45	W	80	ASP
45	W	99	LYS
45	W	101	VAL
45	W	110	VAL
45	W	131	GLU
37	X	76	LEU
37	X	89	LEU
37	X	129	GLU
37	X	133	ILE
37	X	138	LEU
46	Y	46	GLN
46	Y	76	ASP
46	Y	80	VAL
46	Y	81	LEU
46	Y	88	ASP
46	Y	92	TRP
47	Z	41	GLU
47	Z	59	ASP
47	Z	67	TRP
47	Z	101	GLU
48	l	7	LEU
48	l	34	ASN
48	l	36	VAL
48	l	59	GLN
48	l	60	GLU
48	l	62	ILE
48	l	65	ASN
48	l	70	THR
48	l	105	MET
48	l	169	LEU

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Mol	Chain	Res	Type
48	l	246	LEU
48	l	247	LEU
48	l	268	GLU
48	l	271	LYS
48	l	314	MET
48	l	321	GLN
48	l	340	PHE
48	l	351	ASN
48	l	364	LYS
48	l	383	MET
48	l	387	THR
48	l	397	GLU
48	l	407	TRP
48	l	411	MET
48	l	434	LYS
48	l	440	LEU
48	l	445	GLU
48	l	481	THR
48	l	486	MET
48	l	502	LEU
48	l	554	ASP
48	l	559	GLU
48	l	565	THR
48	l	589	LEU
49	s	83	GLU
49	s	88	GLU
49	s	129	ASP
49	s	135	GLU
49	s	175	ARG
49	s	188	VAL
49	s	191	LYS
49	s	214	LEU
49	s	216	GLU
50	t	21	ARG
50	t	29	TYR
50	t	31	PHE
50	t	33	GLU
50	t	39	MET
50	t	42	THR
50	t	65	GLN
50	t	83	GLU
50	t	88	ASP

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Mol	Chain	Res	Type
50	t	91	GLU
51	u	35	THR
51	u	84	GLU
51	u	94	GLU
51	u	95	HIS
51	u	138	LYS
51	u	181	ASP
51	u	206	GLU
51	u	256	THR
51	u	259	GLU
51	u	274	GLU
51	u	341	PHE
51	u	342	GLN
51	u	350	GLU
51	u	363	MET
51	u	368	MET
51	u	375	GLN
51	u	384	THR
51	u	411	GLU
51	u	467	ASP
5	v	47	LEU
5	v	83	LEU
5	v	122	THR
5	v	124	GLU
5	v	129	ASP
5	v	130	ILE
5	v	147	ARG
5	v	158	LEU
5	v	161	ASP
5	v	174	LEU
5	v	175	GLU
5	v	203	ASP
5	v	231	LYS
5	v	233	VAL
5	v	250	LYS
5	v	322	ASP
5	v	329	SER
5	v	401	LEU
5	v	407	VAL
5	v	421	ASP
5	v	451	ASP
6	w	83	HIS

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Mol	Chain	Res	Type
6	w	97	HIS
6	w	233	LEU
6	w	264	THR
6	w	273	TYR
6	w	281	LEU
6	w	311	LYS
6	w	366	MET
6	w	379	TRP
7	x	107	ASP
7	x	129	ASP
7	x	136	LEU
7	x	152	GLU
7	x	164	GLU
7	x	221	GLU
7	x	243	ILE
7	x	249	ILE
7	x	320	LEU
8	y	15	GLU
8	y	72	ARG
8	y	75	ILE
8	y	79	GLU
8	y	83	LYS
8	y	85	GLU
52	z	16	THR
52	z	19	LEU
52	z	40	ARG
52	z	47	LEU
52	z	68	GLU
51	5	84	GLU
51	5	98	PHE
51	5	101	THR
51	5	142	LYS
51	5	164	GLU
51	5	183	VAL
51	5	244	ASP
51	5	266	THR
51	5	284	LEU
51	5	327	THR
51	5	350	GLU
51	5	363	MET
51	5	368	MET
51	5	411	GLU

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Mol	Chain	Res	Type
53	G	41	VAL
53	G	44	GLU
53	G	94	MET
53	G	107	GLU
53	G	158	ARG
53	G	197	THR
53	G	217	GLU
53	G	225	ILE
53	G	241	ARG
53	G	247	LYS
53	G	252	ASP
53	G	310	GLU
53	G	311	LYS
53	G	325	ARG
53	G	329	MET
53	G	338	VAL
53	G	347	ASP
53	G	349	GLU
53	G	361	VAL
53	G	426	ASP
53	G	447	ASP
53	G	450	LYS
53	G	470	LYS
53	G	493	VAL
53	G	511	LYS
53	G	512	VAL
53	G	513	MET
53	G	519	ILE
53	G	592	LYS
53	G	617	ARG
53	G	632	MET
53	G	636	TYR
53	G	657	ASP
53	G	659	VAL
53	G	671	LEU
53	G	679	LEU
53	G	680	LEU
54	M	10	LEU
54	M	25	GLN
54	M	31	ILE
54	M	64	MET
54	M	69	VAL

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Mol	Chain	Res	Type
54	M	91	GLU
3	Ae	50	CYS
3	Ae	59	LEU
3	Af	53	VAL
3	Af	62	THR
3	Af	68	LEU
3	Af	72	ARG
52	Aa	5	PHE
52	Aa	32	THR
52	Aa	47	LEU
52	Aa	48	ARG
52	Aa	79	GLU
1	Ab	26	LEU
1	Ab	27	VAL
1	Ab	35	GLU
1	Ab	37	CYS
1	Ab	54	ASP
1	Ab	66	ASP
1	Ab	69	GLU
1	Ab	81	CYS
1	Ab	85	LYS
1	Ab	91	LYS
2	Ac	13	LEU
2	Ac	14	LEU
2	Ac	30	LEU
2	Ac	54	LYS
4	Ad	13	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	39	GLN
1	0	62	GLN
3	2	156	GLN
3	2	207	GLN
4	3	16	ASN
3	4	156	GLN
3	4	215	GLN
3	4	240	HIS
5	6	36	GLN
5	6	139	ASN
5	6	168	ASN

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Mol	Chain	Res	Type
5	6	170	GLN
5	6	176	ASN
5	6	268	HIS
5	6	291	HIS
5	6	304	ASN
5	6	311	GLN
5	6	318	HIS
5	6	319	GLN
5	6	446	HIS
6	7	85	ASN
6	7	137	GLN
6	7	196	HIS
6	7	201	HIS
6	7	260	ASN
6	7	286	ASN
6	7	312	GLN
6	7	374	ASN
7	8	116	GLN
7	8	120	GLN
7	8	126	HIS
7	8	190	ASN
7	8	191	ASN
7	8	206	HIS
7	8	283	HIS
7	8	310	HIS
8	9	23	ASN
9	a	170	GLN
11	c	83	GLN
11	c	94	HIS
12	d	23	GLN
12	d	55	GLN
12	d	114	GLN
13	e	70	ASN
15	g	81	GLN
16	h	25	GLN
16	h	82	GLN
16	h	97	HIS
17	i	49	ASN
17	i	112	HIS
17	i	171	ASN
17	i	197	ASN
17	i	221	HIS

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Mol	Chain	Res	Type
17	i	289	ASN
18	j	26	GLN
20	m	86	ASN
21	n	40	ASN
23	p	75	HIS
23	p	93	HIS
24	q	180	HIS
24	q	184	HIS
24	q	279	GLN
24	q	304	GLN
24	q	338	HIS
24	q	366	ASN
24	q	390	ASN
25	r	247	HIS
25	r	287	HIS
26	B	133	HIS
26	B	170	GLN
26	B	244	ASN
26	B	376	HIS
26	B	418	GLN
26	B	456	GLN
27	C	240	GLN
27	C	305	GLN
27	C	386	HIS
27	C	448	HIS
28	D	51	ASN
28	D	77	GLN
28	D	124	ASN
28	D	138	ASN
28	D	181	HIS
28	D	228	GLN
29	E	87	GLN
29	E	123	ASN
29	E	133	GLN
29	E	153	GLN
30	F	63	ASN
30	F	120	GLN
32	I	111	ASN
33	J	86	ASN
35	L	32	HIS
35	L	74	GLN
35	L	117	HIS

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Mol	Chain	Res	Type
35	L	123	ASN
35	L	264	ASN
35	L	326	HIS
36	N	21	HIS
36	N	73	GLN
39	Q	74	HIS
39	Q	96	ASN
39	Q	98	HIS
40	R	79	HIS
41	S	25	HIS
41	S	44	GLN
41	S	68	ASN
42	T	125	ASN
43	U	204	HIS
43	U	217	GLN
45	W	8	GLN
45	W	76	GLN
46	Y	54	GLN
48	l	56	HIS
48	l	59	GLN
48	l	65	ASN
48	l	72	GLN
48	l	135	ASN
48	l	170	GLN
48	l	309	GLN
48	l	354	GLN
48	l	470	ASN
48	l	506	ASN
49	s	108	HIS
49	s	112	GLN
49	s	181	GLN
49	s	240	HIS
50	t	4	HIS
50	t	44	GLN
50	t	61	HIS
50	t	82	HIS
50	t	92	HIS
51	u	160	GLN
51	u	323	HIS
51	u	342	GLN
51	u	397	ASN
5	v	157	GLN

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Mol	Chain	Res	Type
5	v	168	ASN
5	v	212	HIS
5	v	268	HIS
5	v	311	GLN
5	v	372	GLN
6	w	3	ASN
6	w	196	HIS
6	w	255	ASN
7	x	120	GLN
7	x	241	GLN
7	x	283	HIS
8	y	23	ASN
51	5	52	GLN
51	5	119	HIS
51	5	277	HIS
51	5	362	ASN
53	G	30	ASN
53	G	74	ASN
53	G	123	ASN
53	G	142	GLN
53	G	278	HIS
53	G	304	GLN
53	G	359	ASN
53	G	425	ASN
53	G	569	GLN
53	G	604	GLN
53	G	666	GLN
53	G	678	GLN
3	Af	56	HIS
52	Aa	13	HIS
1	Ab	76	HIS
2	Ac	48	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

19 ligands are modelled in this entry.

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
56	HEM	7	401	6	50,50,50	1.61	9 (18%)	67,82,82	1.67	12 (17%)
59	SF4	G	802	53	0,12,12	-	-	-		
55	FES	4	301	3	0,4,4	-	-	-		
59	SF4	G	801	53	0,12,12	-	-	-		
56	HEM	7	402	-	50,50,50	1.41	7 (14%)	67,82,82	1.06	6 (8%)
55	FES	E	301	29	0,4,4	-	-	-		
57	HEC	8	401	7	50,50,50	3.06	29 (58%)	68,82,82	2.30	29 (42%)
59	SF4	B	502	26	0,12,12	-	-	-		
55	FES	G	803	53	0,4,4	-	-	-		
58	FMN	B	501	-	33,33,33	1.11	3 (9%)	48,50,50	1.23	8 (16%)
59	SF4	H	302	31	0,12,12	-	-	-		
60	NDP	L	401	-	51,52,52	0.50	0	71,80,80	0.84	2 (2%)
57	HEC	x	401	7	50,50,50	1.72	6 (12%)	68,82,82	1.32	4 (5%)
61	ZMP	Q	201	-	27,29,36	1.86	5 (18%)	34,38,45	1.74	8 (23%)
56	HEM	w	402	6	50,50,50	1.29	7 (14%)	67,82,82	0.95	0
59	SF4	I	201	32	0,12,12	-	-	-		
55	FES	2	301	3	0,4,4	-	-	-		
56	HEM	w	401	-	50,50,50	1.29	5 (10%)	67,82,82	1.08	3 (4%)
59	SF4	H	301	31	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
56	HEM	7	401	6	-	5/14/54/54	-
59	SF4	G	802	53	-	-	0/6/5/5
55	FES	4	301	3	-	-	0/1/1/1
59	SF4	G	801	53	-	-	0/6/5/5
56	HEM	7	402	-	-	6/14/54/54	-
55	FES	E	301	29	-	-	0/1/1/1
57	HEC	8	401	7	1/1/3/7	11/14/54/54	-
59	SF4	B	502	26	-	-	0/6/5/5
55	FES	G	803	53	-	-	0/1/1/1
58	FMN	B	501	-	-	0/18/18/18	0/3/3/3
60	NDP	L	401	-	-	4/34/77/77	0/5/5/5
59	SF4	H	302	31	-	-	0/6/5/5
57	HEC	x	401	7	1/1/3/7	6/14/54/54	-
61	ZMP	Q	201	-	-	11/36/36/43	-
56	HEM	w	402	6	-	1/14/54/54	-
59	SF4	I	201	32	-	-	0/6/5/5
55	FES	2	301	3	-	-	0/1/1/1
56	HEM	w	401	-	-	0/14/54/54	-
59	SF4	H	301	31	-	-	0/6/5/5

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	x	401	HEC	C3D-C2D	7.62	1.53	1.36
56	7	401	HEM	FE-NB	5.54	2.11	1.94
57	8	401	HEC	C3B-C2B	5.53	1.48	1.36
61	Q	201	ZMP	C13-N1	5.36	1.46	1.33
57	8	401	HEC	CHC-C4B	5.31	1.49	1.38
57	8	401	HEC	C3D-C2D	5.27	1.48	1.36
57	8	401	HEC	C2A-C3A	5.27	1.48	1.36
61	Q	201	ZMP	C16-N2	5.17	1.45	1.33
57	8	401	HEC	CHA-C1A	5.15	1.48	1.38
57	8	401	HEC	CHC-C1C	4.99	1.50	1.39
57	8	401	HEC	CHB-C4A	4.90	1.48	1.38
57	8	401	HEC	CHD-C1D	4.74	1.48	1.38
57	8	401	HEC	FE-NB	4.54	2.08	1.94
57	8	401	HEC	CHA-C4D	4.43	1.49	1.39
56	7	401	HEM	FE-NC	4.42	2.09	1.95
57	8	401	HEC	FE-ND	4.35	2.08	1.94
57	8	401	HEC	FE-NC	4.32	2.09	1.95
57	8	401	HEC	FE-NA	4.30	2.09	1.95
57	8	401	HEC	C3C-C2C	3.96	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	8	401	HEC	CHB-C1B	3.94	1.48	1.39
57	8	401	HEC	CHD-C4C	3.90	1.48	1.39
57	8	401	HEC	C1D-ND	-3.89	1.33	1.40
57	x	401	HEC	FE-NA	3.52	2.06	1.95
57	8	401	HEC	C4B-NB	-3.44	1.34	1.40
58	B	501	FMN	C4A-N5	3.41	1.38	1.30
57	x	401	HEC	FE-NB	3.37	2.05	1.94
56	7	401	HEM	C1B-NB	-3.29	1.34	1.40
56	7	401	HEM	C4D-ND	-3.21	1.34	1.40
57	8	401	HEC	C1C-C2C	3.20	1.50	1.43
56	7	402	HEM	FE-ND	3.07	2.04	1.94
56	7	402	HEM	CAC-C3C	3.02	1.55	1.47
56	w	401	HEM	CAB-C3B	3.01	1.55	1.47
56	w	401	HEM	CAC-C3C	3.01	1.55	1.47
56	7	402	HEM	CAB-C3B	2.99	1.55	1.47
57	x	401	HEC	FE-NC	2.98	2.05	1.95
57	x	401	HEC	FE-ND	2.98	2.04	1.94
56	7	402	HEM	FE-NB	2.97	2.04	1.94
56	w	402	HEM	CAC-C3C	2.87	1.55	1.47
56	w	402	HEM	CAB-C3B	2.86	1.55	1.47
57	8	401	HEC	C4A-NA	-2.79	1.34	1.39
56	w	402	HEM	FE-NC	2.68	2.04	1.95
57	8	401	HEC	C4D-C3D	2.68	1.49	1.45
57	8	401	HEC	C4B-C3B	2.66	1.49	1.45
56	7	402	HEM	FE-NC	2.66	2.03	1.95
61	Q	201	ZMP	O2-C13	-2.65	1.18	1.23
57	8	401	HEC	C1A-NA	-2.60	1.34	1.39
61	Q	201	ZMP	C10-S1	2.56	1.82	1.76
56	w	401	HEM	FE-ND	2.55	2.02	1.94
56	7	402	HEM	FE-NA	2.55	2.03	1.95
61	Q	201	ZMP	O3-C16	-2.53	1.18	1.23
56	7	401	HEM	C1C-C2C	-2.50	1.40	1.45
57	8	401	HEC	C1C-NC	-2.47	1.35	1.39
56	w	402	HEM	FE-ND	2.45	2.02	1.94
57	8	401	HEC	C1A-C2A	2.43	1.49	1.45
57	8	401	HEC	C4C-NC	-2.40	1.35	1.39
56	w	401	HEM	FE-NB	2.32	2.02	1.94
56	7	401	HEM	C1D-ND	-2.28	1.34	1.38
57	8	401	HEC	C4C-C3C	2.23	1.49	1.44
56	7	401	HEM	FE-ND	-2.21	1.88	1.94
56	w	402	HEM	FE-NB	2.20	2.01	1.94
56	7	401	HEM	C3B-C4B	2.19	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	401	HEM	FE-NA	2.19	2.02	1.95
57	x	401	HEC	C3C-C2C	-2.13	1.33	1.38
56	w	402	HEM	C2A-C3A	-2.11	1.33	1.38
56	7	402	HEM	C2A-C3A	-2.10	1.33	1.38
58	B	501	FMN	C10-N1	2.10	1.37	1.33
56	7	401	HEM	C4B-NB	-2.06	1.34	1.38
57	8	401	HEC	C4D-ND	-2.05	1.34	1.38
56	w	402	HEM	CMB-C2B	2.03	1.54	1.50
57	8	401	HEC	C1B-NB	-2.03	1.34	1.38
58	B	501	FMN	C4A-C10	-2.01	1.38	1.44

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	8	401	HEC	C1B-C2B-C3B	-5.67	101.02	106.98
60	L	401	NDP	P2B-O2B-C2B	-5.38	109.06	123.43
57	x	401	HEC	C1D-ND-C4D	5.15	111.30	105.21
61	Q	201	ZMP	C9-C10-S1	4.81	119.13	113.40
57	8	401	HEC	C2B-C1B-NB	4.56	115.18	109.90
57	8	401	HEC	CBC-CAC-C3C	4.48	124.55	112.42
56	7	401	HEM	CHD-C1D-ND	4.45	129.22	124.42
56	7	401	HEM	CHC-C4B-NB	4.18	128.92	124.42
57	8	401	HEC	CBB-CAB-C3B	4.16	123.70	112.42
57	8	401	HEC	CHA-C4D-ND	-3.87	120.26	124.42
57	8	401	HEC	CHB-C4A-NA	-3.80	120.32	124.45
57	8	401	HEC	C2A-C1A-NA	3.79	113.98	110.32
56	7	401	HEM	CHB-C1B-NB	3.76	129.02	124.37
57	8	401	HEC	C2D-C1D-ND	3.70	114.10	109.84
57	8	401	HEC	CHA-C1A-NA	-3.66	120.47	124.45
61	Q	201	ZMP	O1-C10-C9	-3.62	119.81	123.98
56	7	401	HEM	C1B-NB-C4B	3.51	109.36	105.21
57	8	401	HEC	CHC-C4B-NB	-3.42	120.13	124.37
57	8	401	HEC	C1D-C2D-C3D	-3.33	103.48	106.98
57	8	401	HEC	CHB-C1B-NB	-3.29	120.88	124.42
57	x	401	HEC	CHA-C4D-ND	3.28	127.95	124.42
58	B	501	FMN	C4-N3-C2	-3.25	119.86	125.64
57	8	401	HEC	C1C-C2C-C3C	-3.25	103.10	106.82
56	7	401	HEM	CHA-C4D-ND	3.20	128.32	124.37
57	8	401	HEC	CAD-C3D-C4D	3.19	130.25	124.70
57	8	401	HEC	C1A-C2A-C3A	-3.15	102.96	107.11
57	8	401	HEC	C3C-C4C-NC	3.08	113.57	110.15
56	7	401	HEM	C3B-C4B-NB	-2.98	107.33	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	Q	201	ZMP	O3-C16-N2	-2.97	116.69	122.98
61	Q	201	ZMP	C11-S1-C10	2.95	110.57	101.84
57	8	401	HEC	C4D-C3D-C2D	-2.95	102.59	106.89
57	8	401	HEC	C3D-C4D-ND	2.91	113.16	110.35
58	B	501	FMN	C4A-C10-N10	2.88	120.61	116.48
57	8	401	HEC	C4A-C3A-C2A	-2.88	102.69	106.97
56	7	401	HEM	CHD-C1D-C2D	-2.85	120.52	125.03
57	8	401	HEC	C3A-C4A-NA	2.76	114.73	109.64
57	8	401	HEC	CAC-C3C-C4C	2.72	128.66	124.91
61	Q	201	ZMP	C14-C15-N2	-2.71	106.23	112.00
57	8	401	HEC	CAA-C2A-C1A	2.50	129.93	124.85
58	B	501	FMN	C4A-C4-N3	2.49	119.60	113.25
56	w	401	HEM	C4D-ND-C1D	2.45	108.11	105.21
57	8	401	HEC	CAD-CBD-CGD	-2.43	107.23	113.67
57	x	401	HEC	CHB-C1B-NB	2.42	127.03	124.42
57	8	401	HEC	CMB-C2B-C3B	2.42	132.69	126.15
58	B	501	FMN	O4-C4-C4A	-2.39	120.22	126.53
61	Q	201	ZMP	C15-C14-C13	-2.39	108.42	112.39
57	8	401	HEC	C4C-C3C-C2C	-2.38	103.19	106.87
56	7	402	HEM	CAD-C3D-C2D	-2.35	123.46	127.87
58	B	501	FMN	C5A-C9A-N10	2.34	120.08	117.97
57	x	401	HEC	CAA-CBA-CGA	-2.33	107.48	113.67
56	w	401	HEM	C3D-C4D-ND	-2.30	107.64	110.17
61	Q	201	ZMP	C12-N1-C13	-2.27	118.59	122.82
58	B	501	FMN	C10-C4A-N5	-2.26	120.19	124.81
56	7	401	HEM	CHA-C1A-NA	2.24	127.93	123.86
57	8	401	HEC	CHD-C1D-ND	-2.24	121.59	124.37
56	7	402	HEM	CAD-C3D-C4D	2.24	128.60	124.70
57	8	401	HEC	CHD-C4C-NC	-2.23	119.81	123.86
57	8	401	HEC	CHC-C1C-NC	-2.17	119.92	123.86
56	7	402	HEM	CAD-CBD-CGD	-2.17	107.90	113.67
57	8	401	HEC	CMA-C3A-C4A	2.14	128.50	124.73
56	7	401	HEM	C1A-CHA-C4D	-2.13	121.23	126.25
56	7	401	HEM	CHB-C1B-C2B	-2.10	120.97	126.95
56	7	402	HEM	C3D-C4D-ND	-2.09	107.88	110.17
60	L	401	NDP	O4D-C1D-C2D	-2.07	102.20	106.62
58	B	501	FMN	C9A-C5A-N5	-2.06	120.27	122.45
56	7	402	HEM	C3B-C2B-C1B	2.05	107.95	106.41
56	7	401	HEM	CAC-C3C-C4C	2.04	129.69	124.82
56	w	401	HEM	C2A-C1A-NA	-2.04	107.89	110.15
61	Q	201	ZMP	C17-C16-N2	2.04	120.34	116.48
58	B	501	FMN	C4'-C3'-C2'	-2.02	110.21	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	7	402	HEM	C4D-ND-C1D	2.02	107.60	105.21
56	7	401	HEM	CAD-C3D-C4D	2.02	128.21	124.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	8	401	HEC	NA
57	x	401	HEC	NA

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	7	402	HEM	C1A-C2A-CAA-CBA
61	Q	201	ZMP	C17-C16-N2-C15
61	Q	201	ZMP	S1-C11-C12-N1
61	Q	201	ZMP	C12-C11-S1-C10
57	8	401	HEC	C2C-C3C-CAC-CBC
57	8	401	HEC	C4C-C3C-CAC-CBC
57	8	401	HEC	C4B-C3B-CAB-CBB
57	8	401	HEC	C2B-C3B-CAB-CBB
61	Q	201	ZMP	O3-C16-N2-C15
57	8	401	HEC	C4D-C3D-CAD-CBD
57	x	401	HEC	C2B-C3B-CAB-CBB
60	L	401	NDP	O4D-C1D-N1N-C6N
57	8	401	HEC	C3D-CAD-CBD-CGD
60	L	401	NDP	O4B-C4B-C5B-O5B
57	8	401	HEC	C2D-C3D-CAD-CBD
57	x	401	HEC	C4B-C3B-CAB-CBB
56	7	402	HEM	C3A-C2A-CAA-CBA
56	7	402	HEM	C4D-C3D-CAD-CBD
61	Q	201	ZMP	O3-C16-C17-O4
56	7	402	HEM	C2D-C3D-CAD-CBD
56	7	401	HEM	C3D-CAD-CBD-CGD
61	Q	201	ZMP	N2-C16-C17-O4
61	Q	201	ZMP	O1-C10-S1-C11
60	L	401	NDP	C3B-C4B-C5B-O5B
61	Q	201	ZMP	C9-C10-S1-C11
56	7	401	HEM	C4B-C3B-CAB-CBB
56	7	401	HEM	C4C-C3C-CAC-CBC
60	L	401	NDP	O4D-C4D-C5D-O5D
61	Q	201	ZMP	C6-C7-C8-C9
61	Q	201	ZMP	O3-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
61	Q	201	ZMP	N2-C16-C17-C18
56	7	401	HEM	CAA-CBA-CGA-O1A
56	w	402	HEM	C3D-CAD-CBD-CGD
57	8	401	HEC	CAD-CBD-CGD-O2D
56	7	401	HEM	CAA-CBA-CGA-O2A
57	8	401	HEC	CAA-CBA-CGA-O2A
57	x	401	HEC	CAD-CBD-CGD-O2D
57	x	401	HEC	CAA-CBA-CGA-O2A
57	8	401	HEC	CAD-CBD-CGD-O1D
57	x	401	HEC	CAA-CBA-CGA-O1A
57	x	401	HEC	CAD-CBD-CGD-O1D
57	8	401	HEC	CAA-CBA-CGA-O1A
56	7	402	HEM	CAD-CBD-CGD-O1D
56	7	402	HEM	CAA-CBA-CGA-O2A

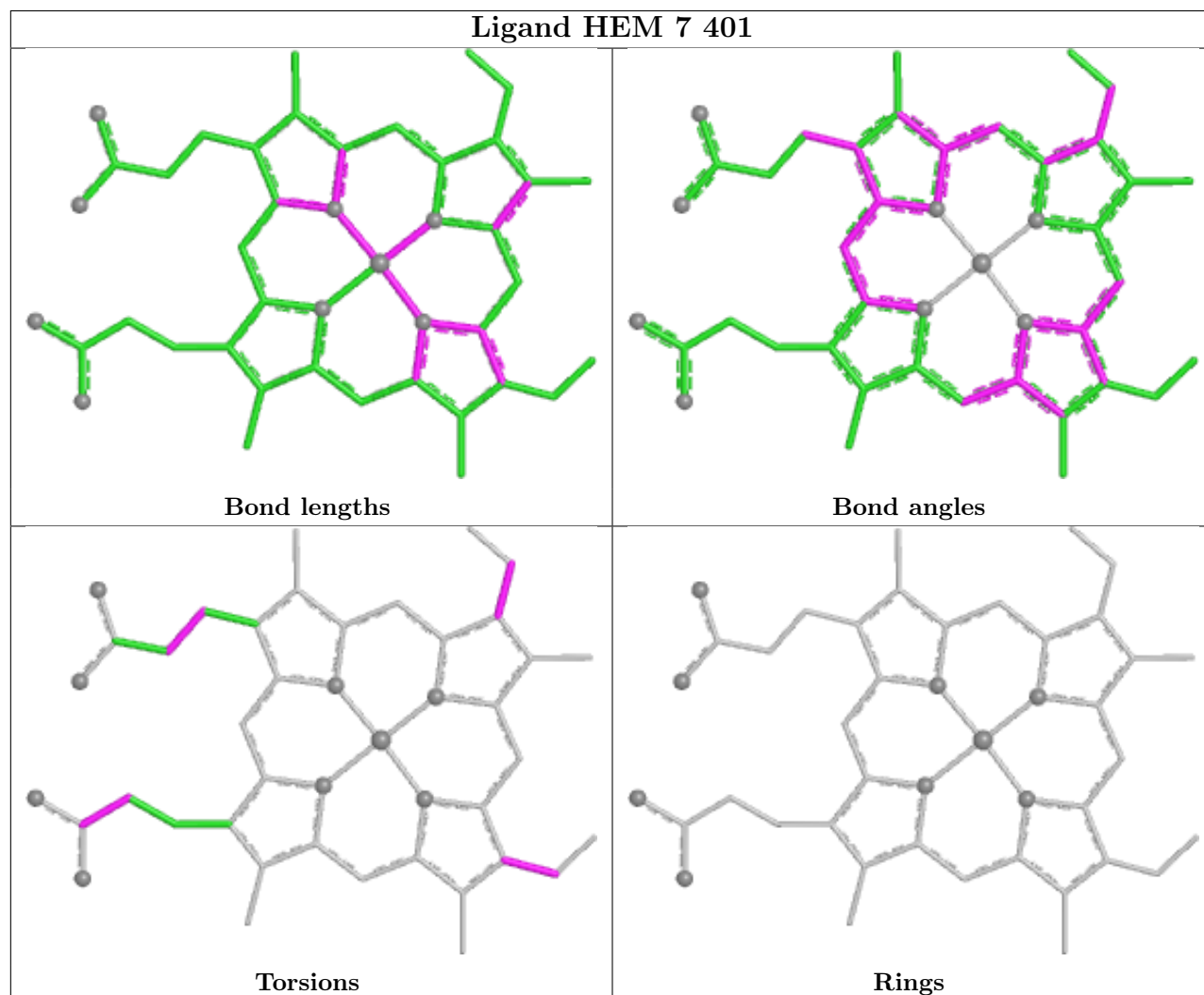
There are no ring outliers.

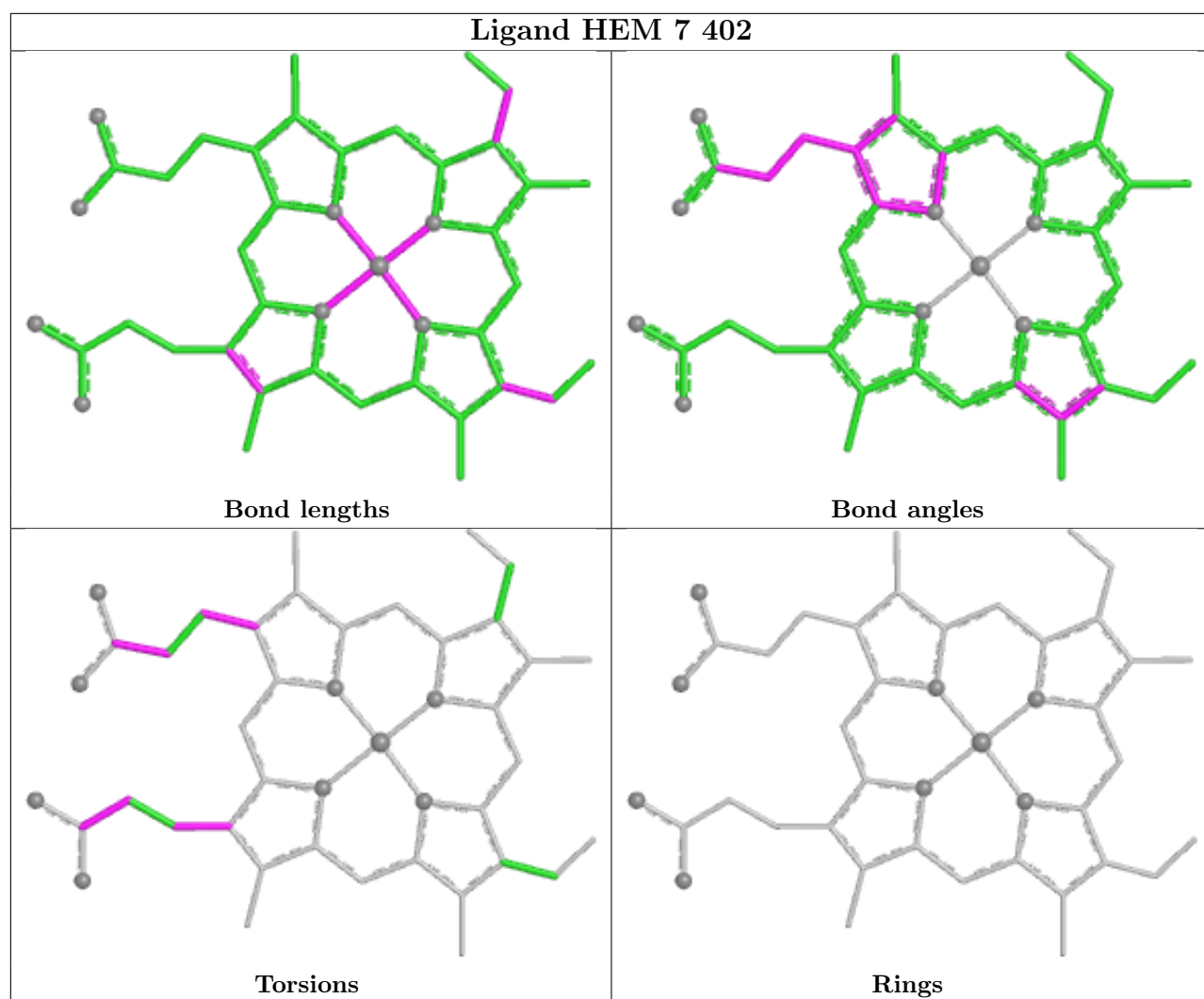
17 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	7	401	HEM	7	0
55	4	301	FES	3	0
59	G	801	SF4	1	0
56	7	402	HEM	7	0
55	E	301	FES	1	0
57	8	401	HEC	18	0
59	B	502	SF4	1	0
58	B	501	FMN	1	0
59	H	302	SF4	9	0
60	L	401	NDP	1	0
57	x	401	HEC	4	0
61	Q	201	ZMP	3	0
56	w	402	HEM	7	0
59	I	201	SF4	1	0
55	2	301	FES	3	0
56	w	401	HEM	9	0
59	H	301	SF4	2	0

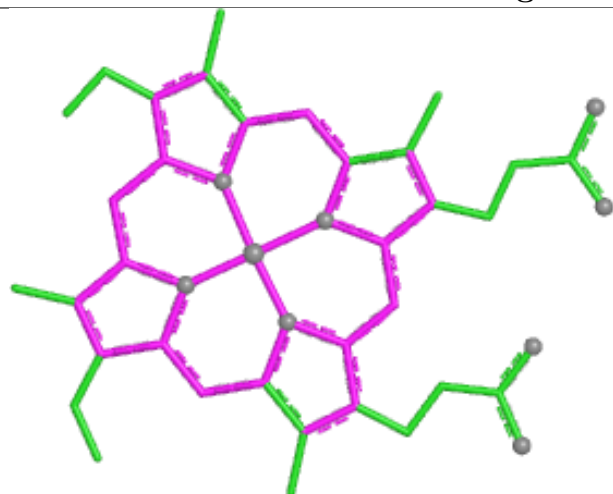
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

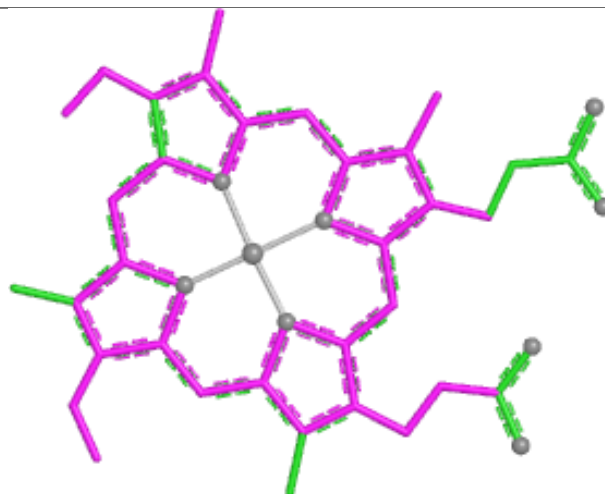




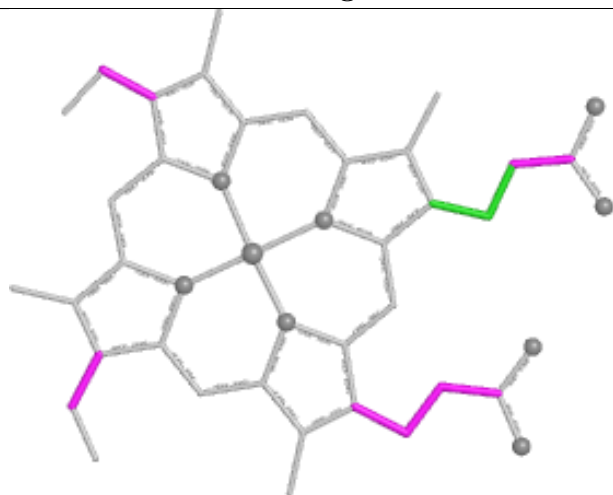
Ligand HEC 8 401



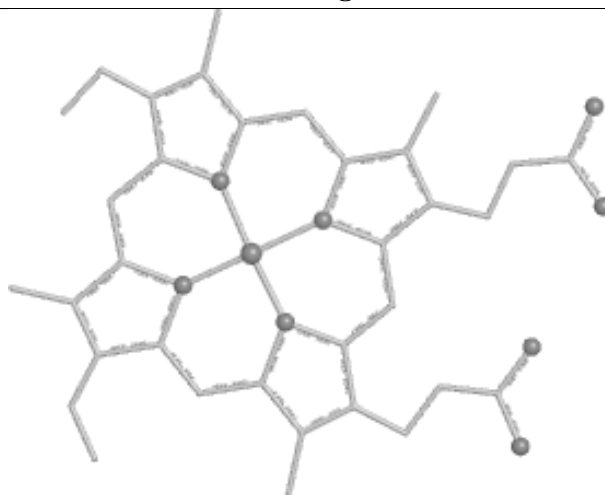
Bond lengths



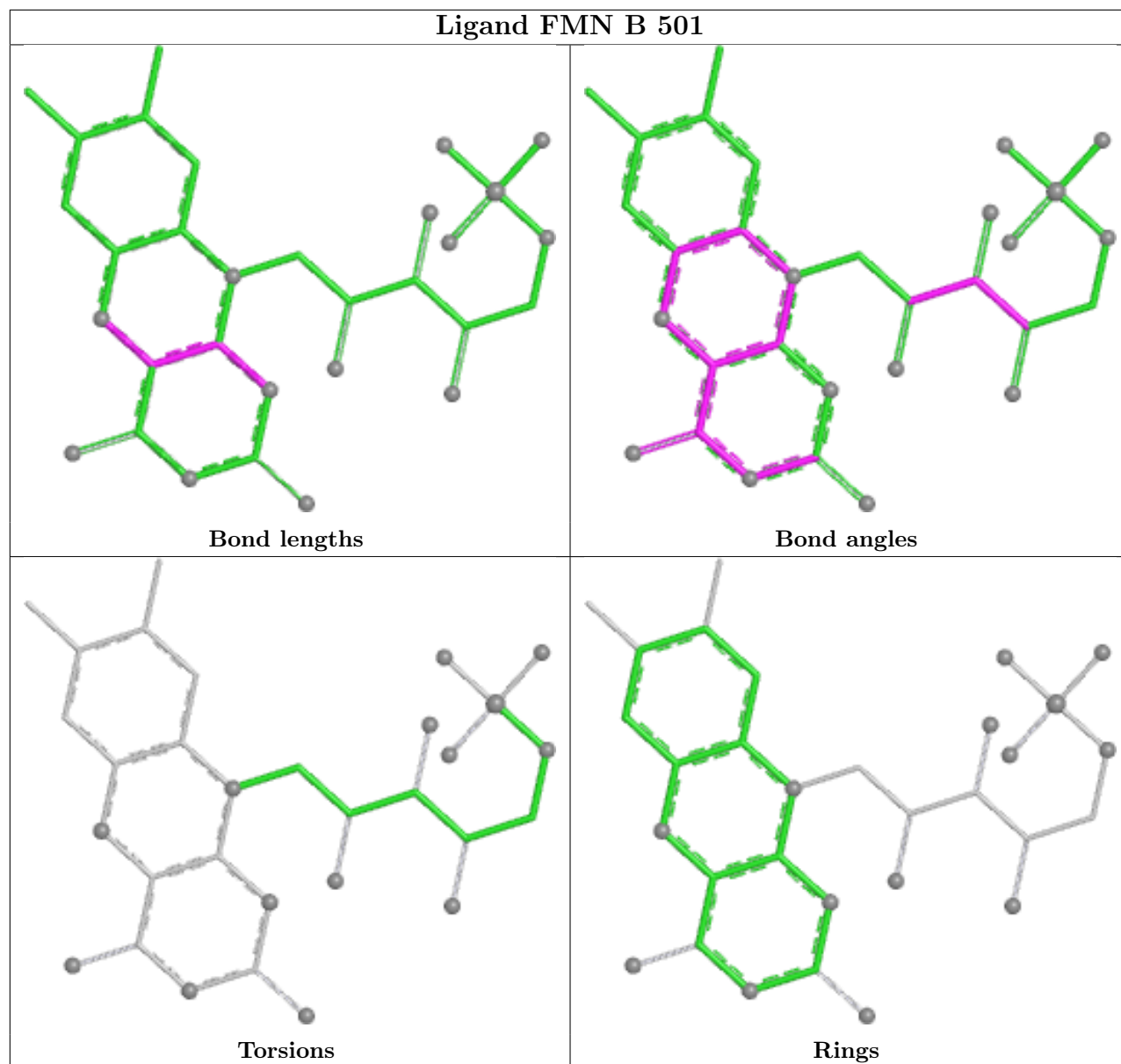
Bond angles

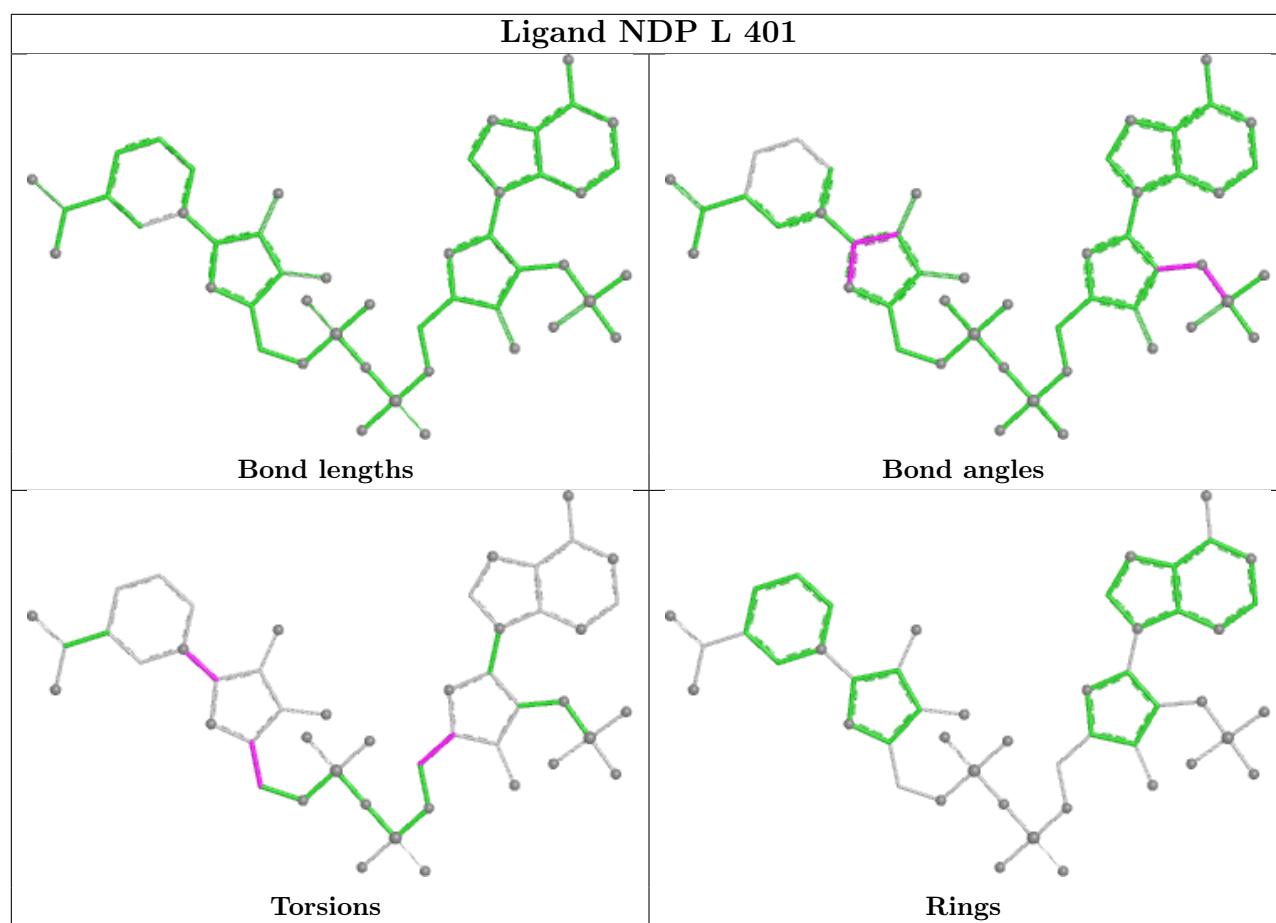


Torsions

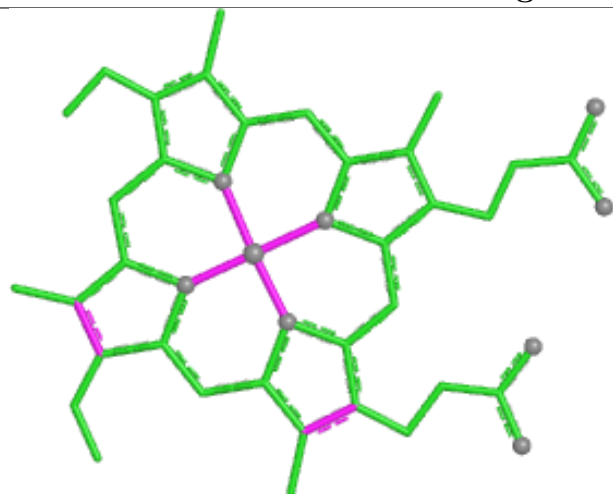


Rings

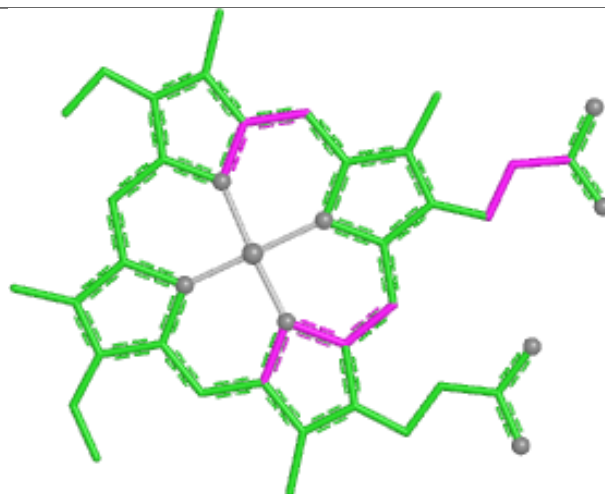




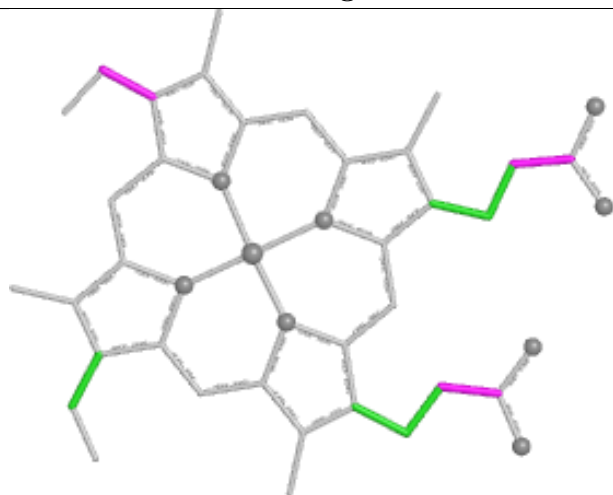
Ligand HEC x 401



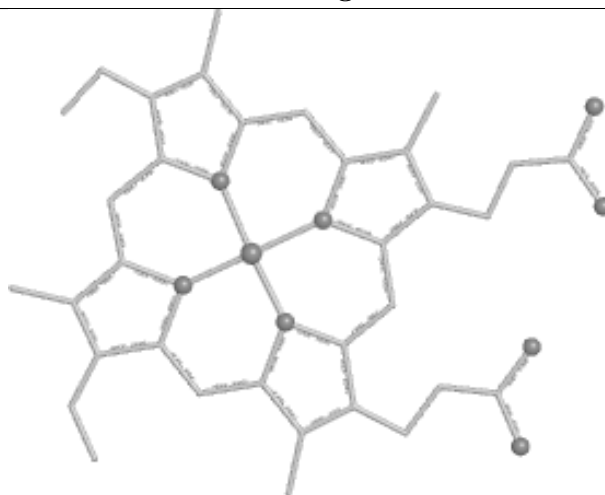
Bond lengths



Bond angles

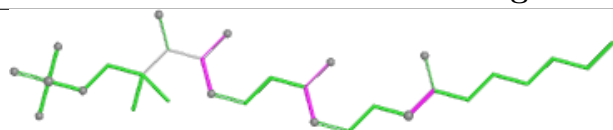


Torsions



Rings

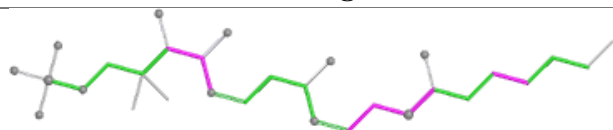
Ligand ZMP Q 201



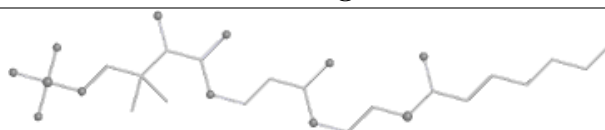
Bond lengths



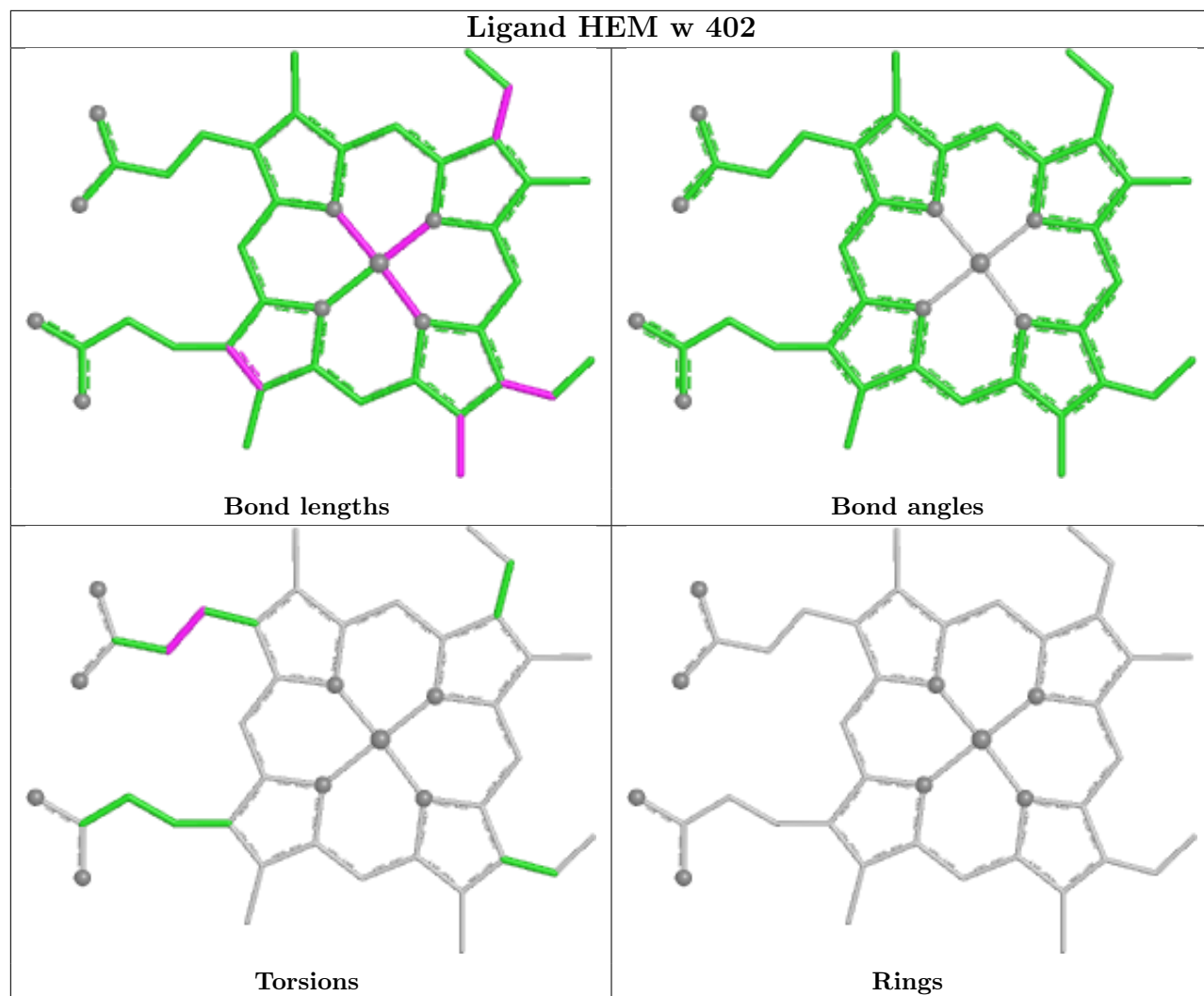
Bond angles

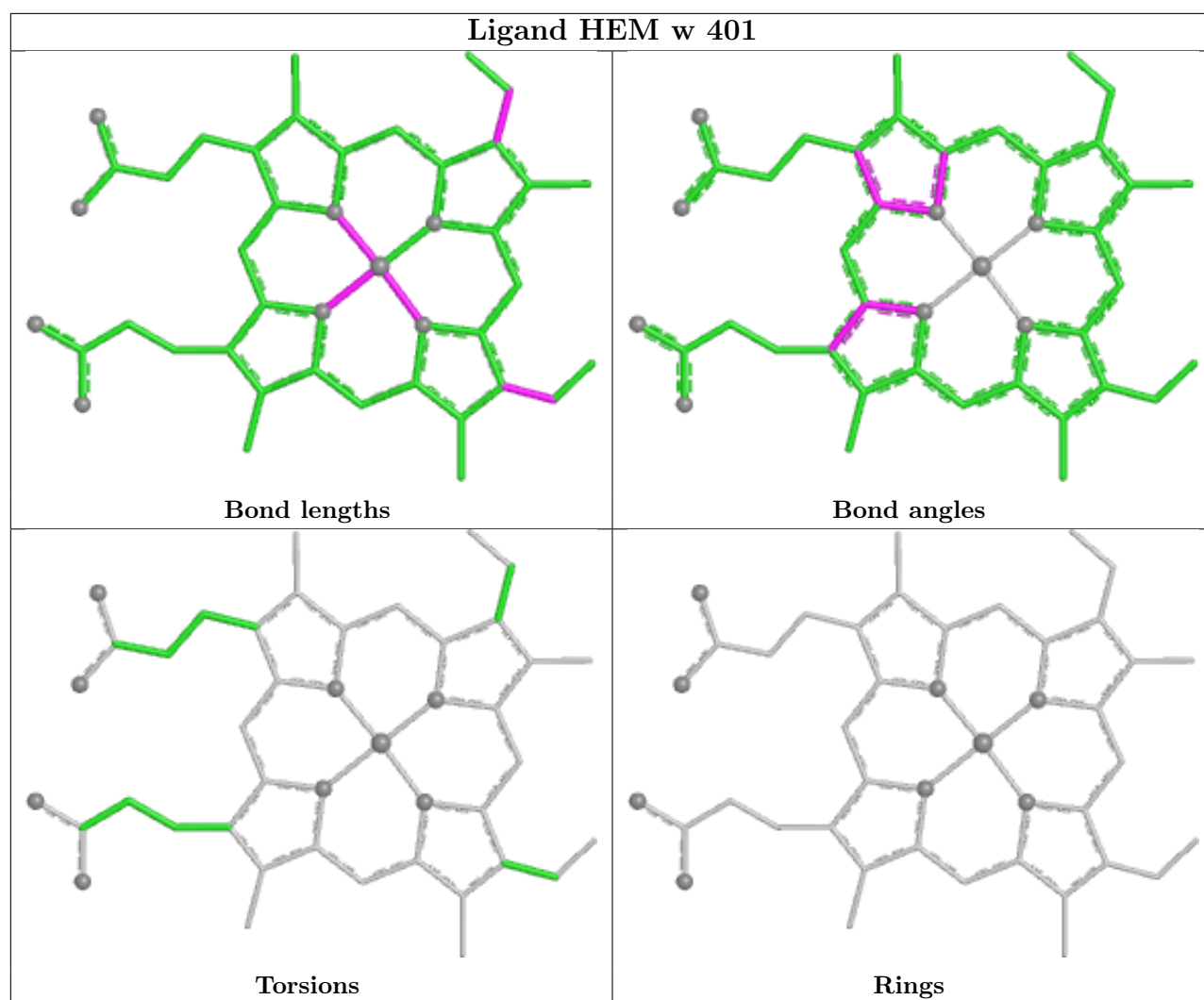


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

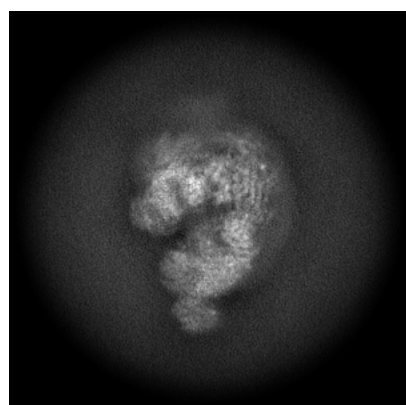
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45479. These allow visual inspection of the internal detail of the map and identification of artifacts.

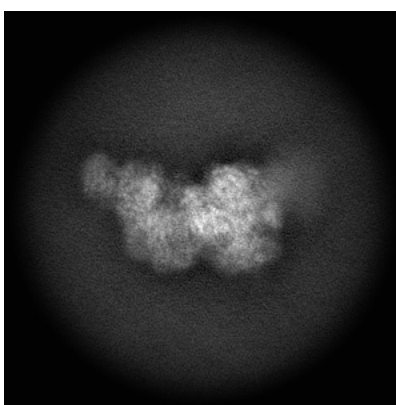
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

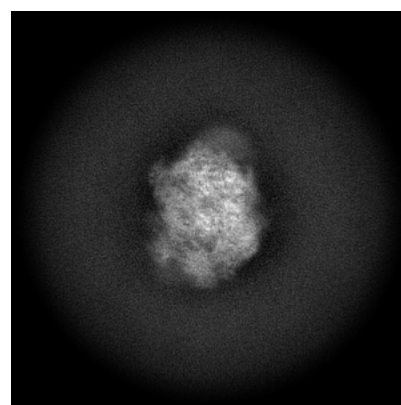
6.1.1 Primary map



X



Y

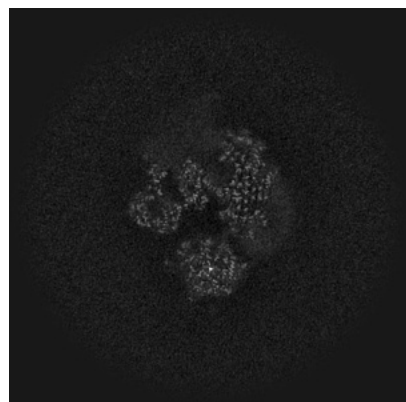


Z

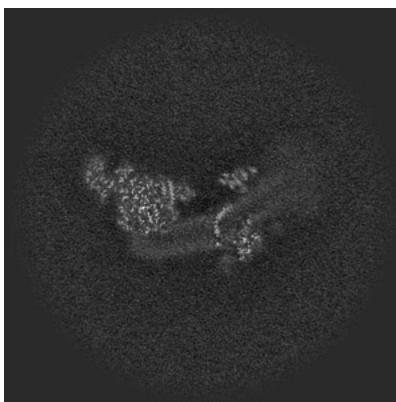
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

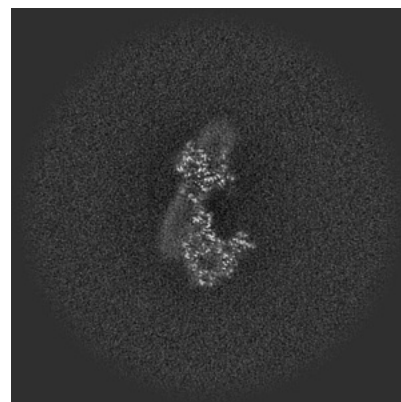
6.2.1 Primary map



X Index: 256



Y Index: 256

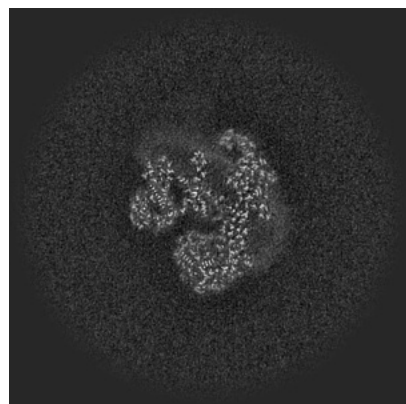


Z Index: 256

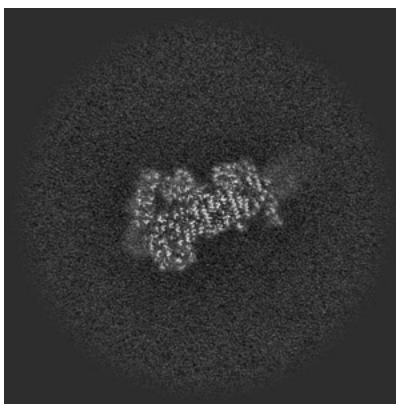
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

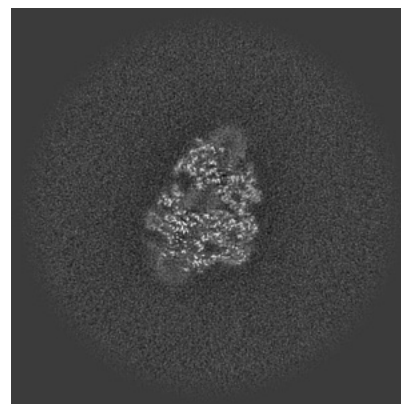
6.3.1 Primary map



X Index: 244



Y Index: 291

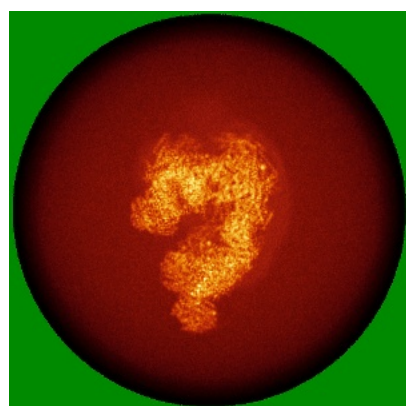


Z Index: 294

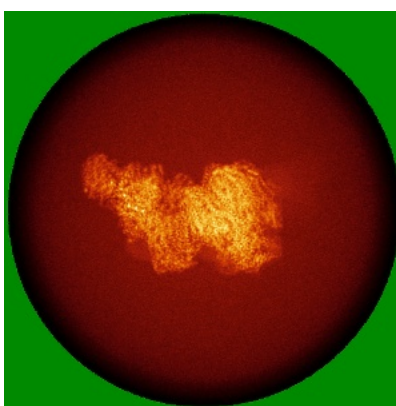
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

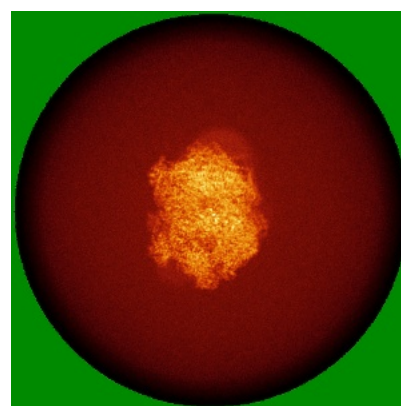
6.4.1 Primary map



X



Y

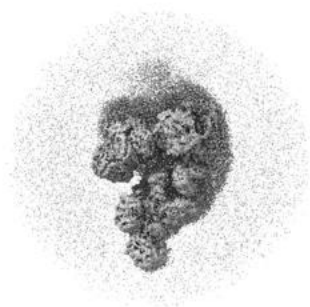


Z

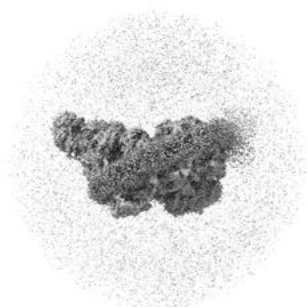
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

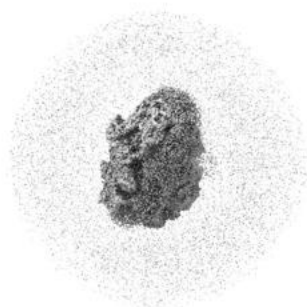
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

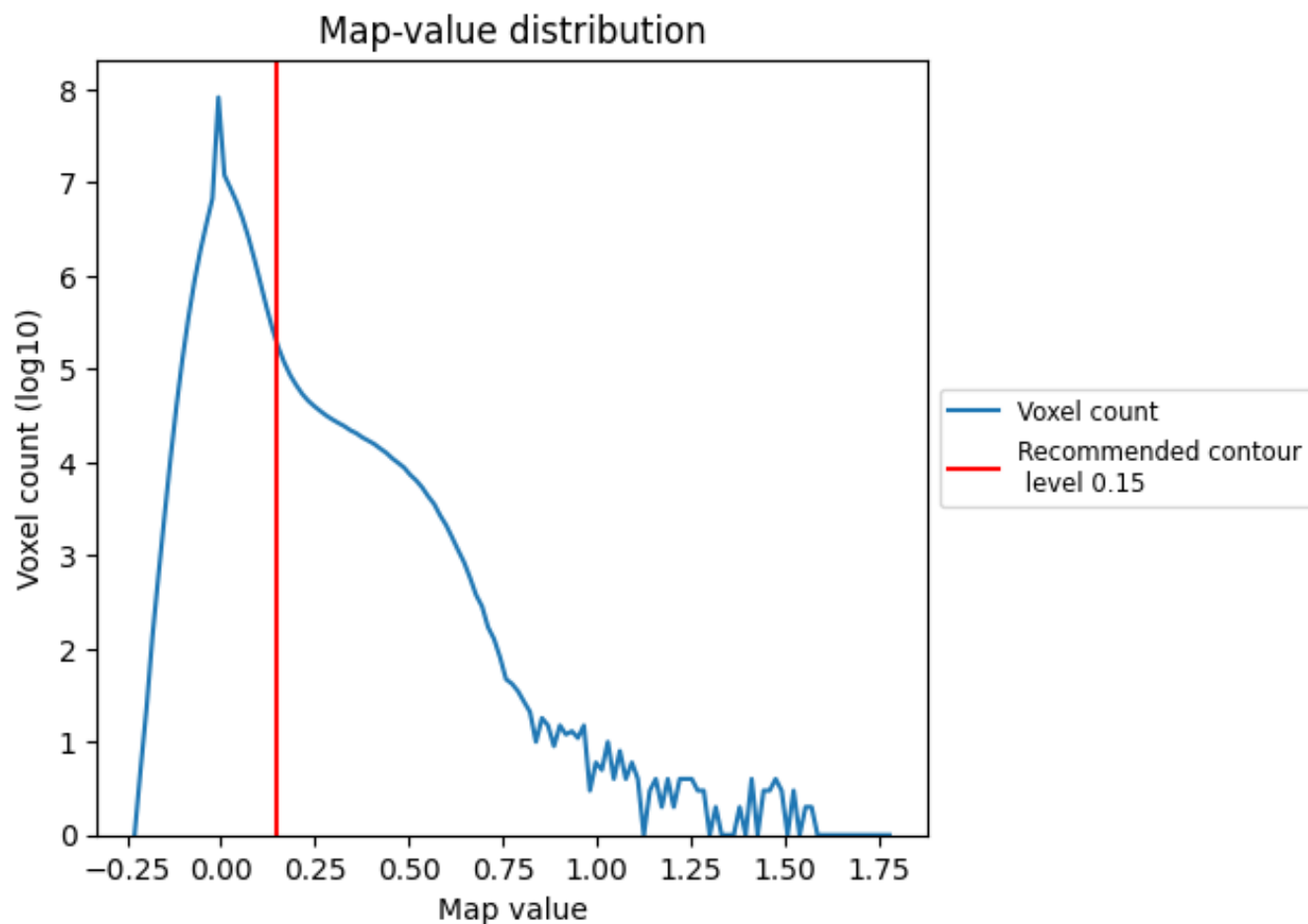
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

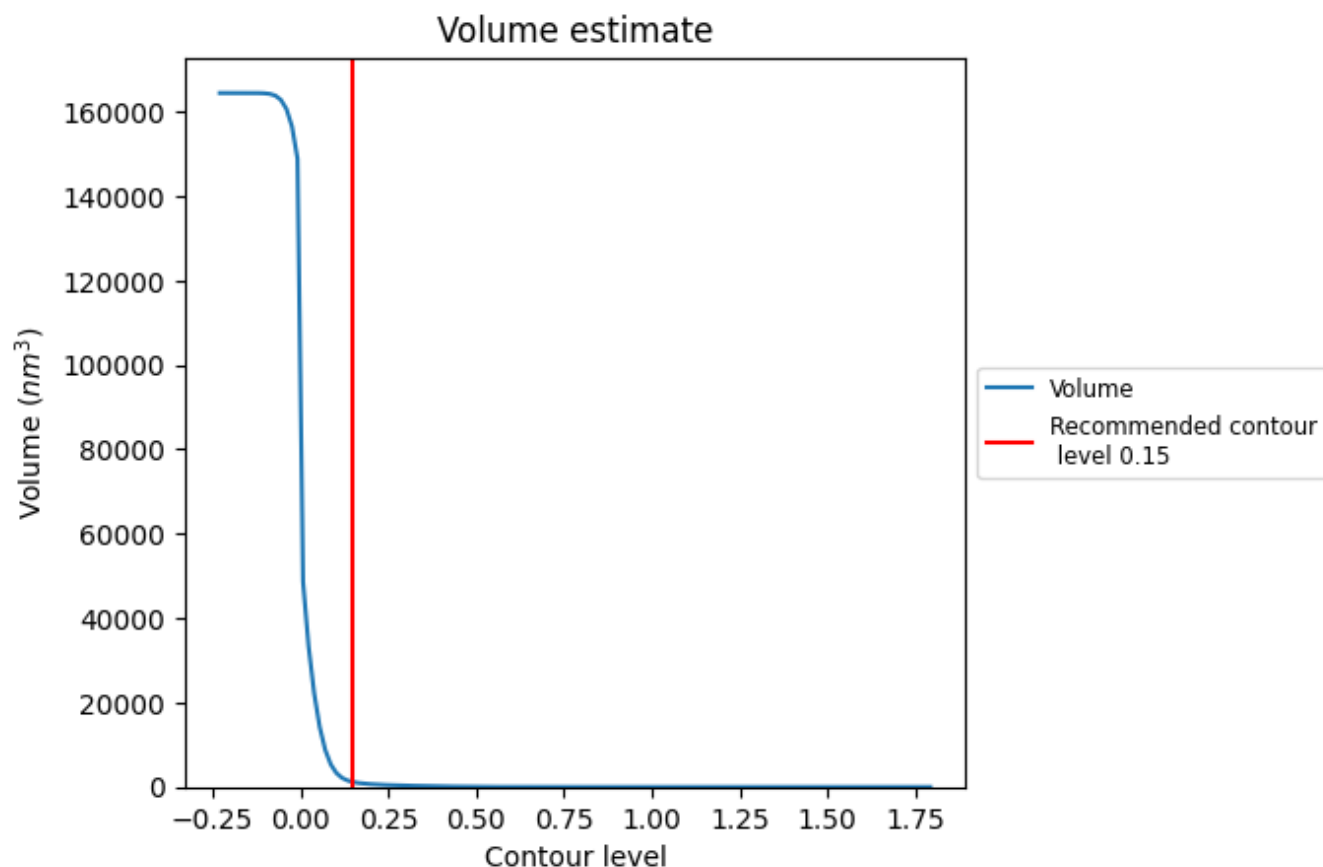
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

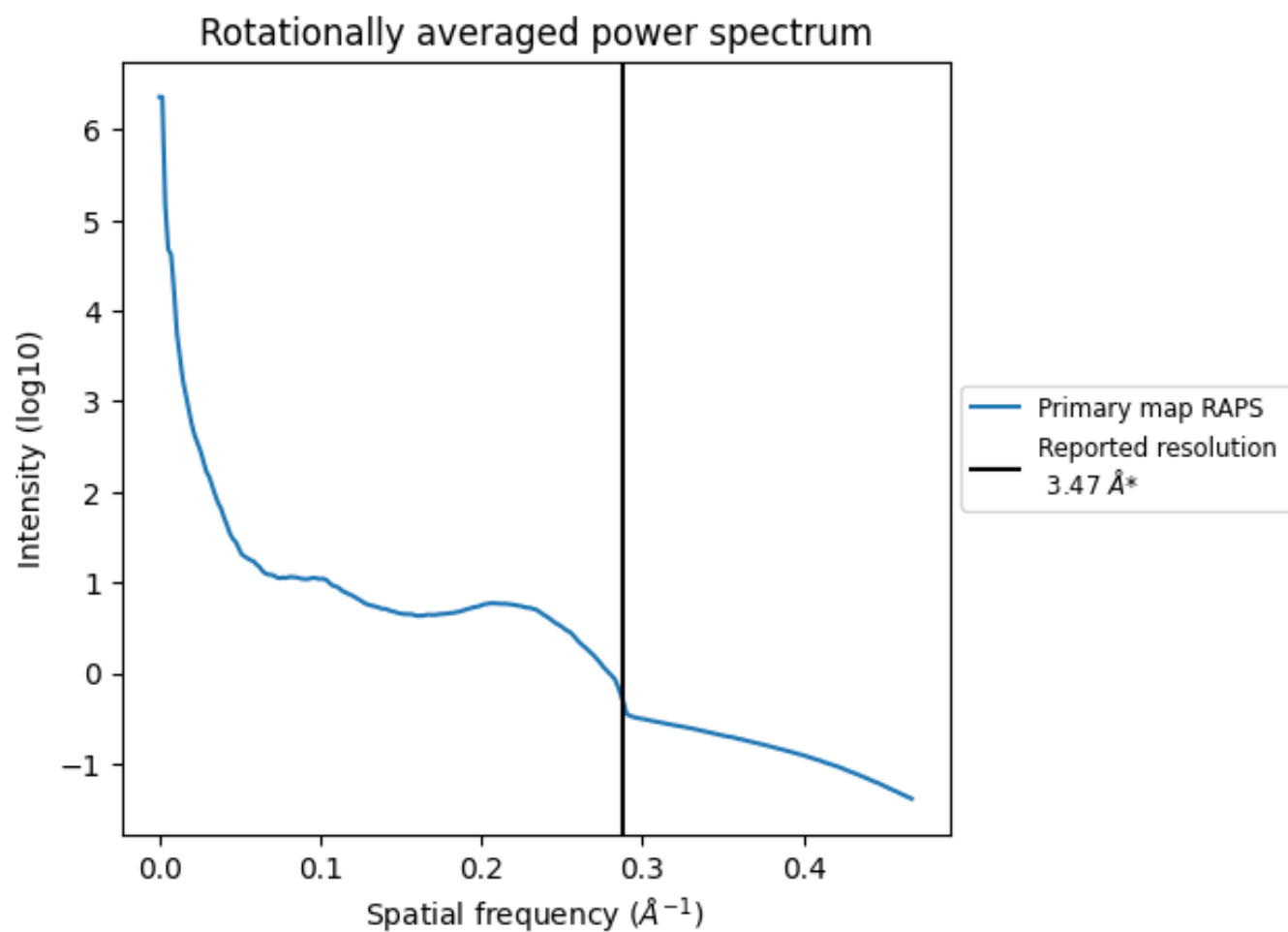
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1168 nm^3 ; this corresponds to an approximate mass of 1055 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.288 Å⁻¹

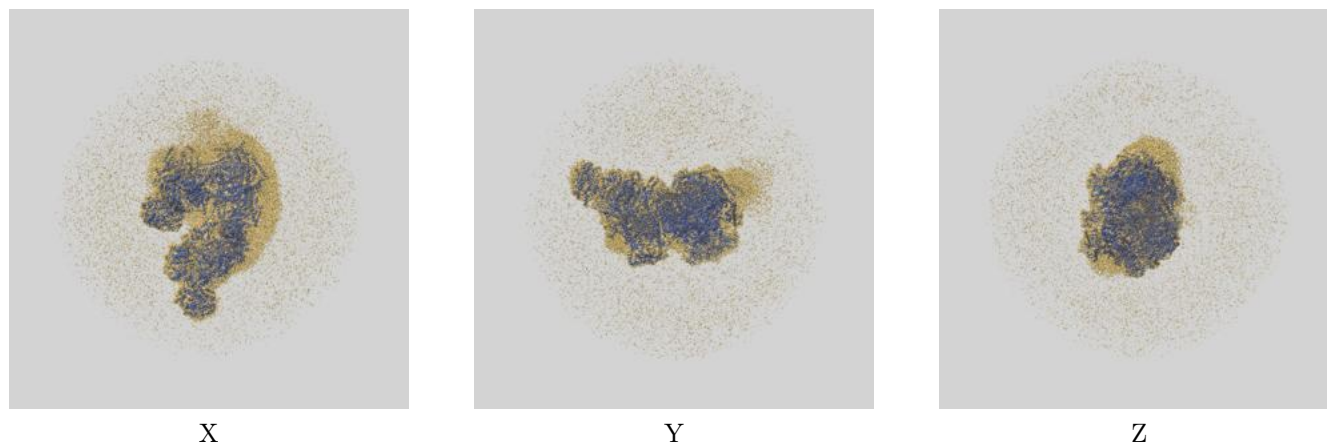
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

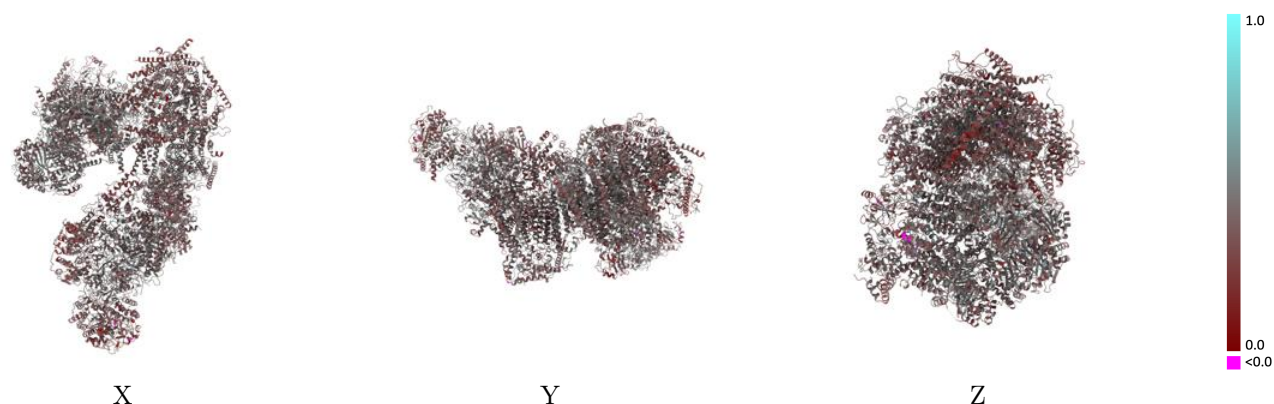
This section contains information regarding the fit between EMDB map EMD-45479 and PDB model 9CDN. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



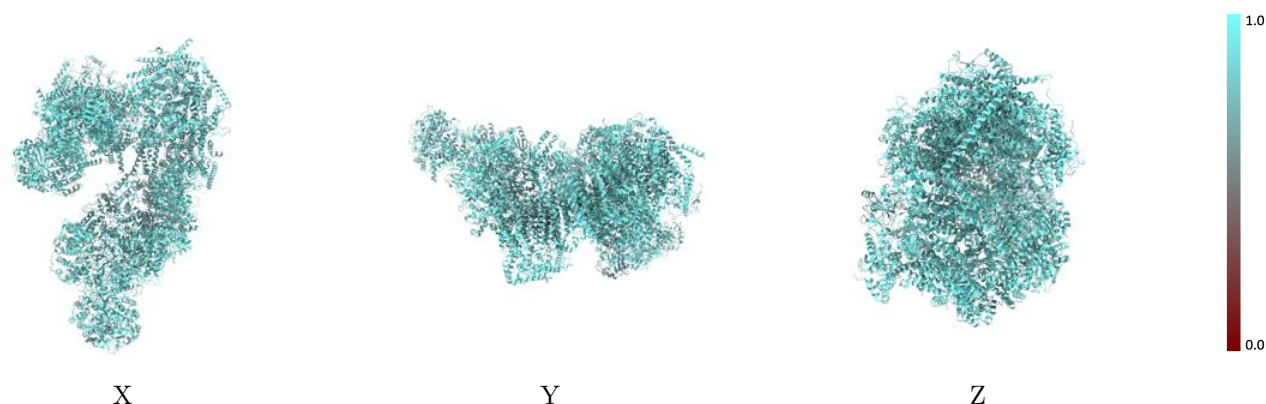
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



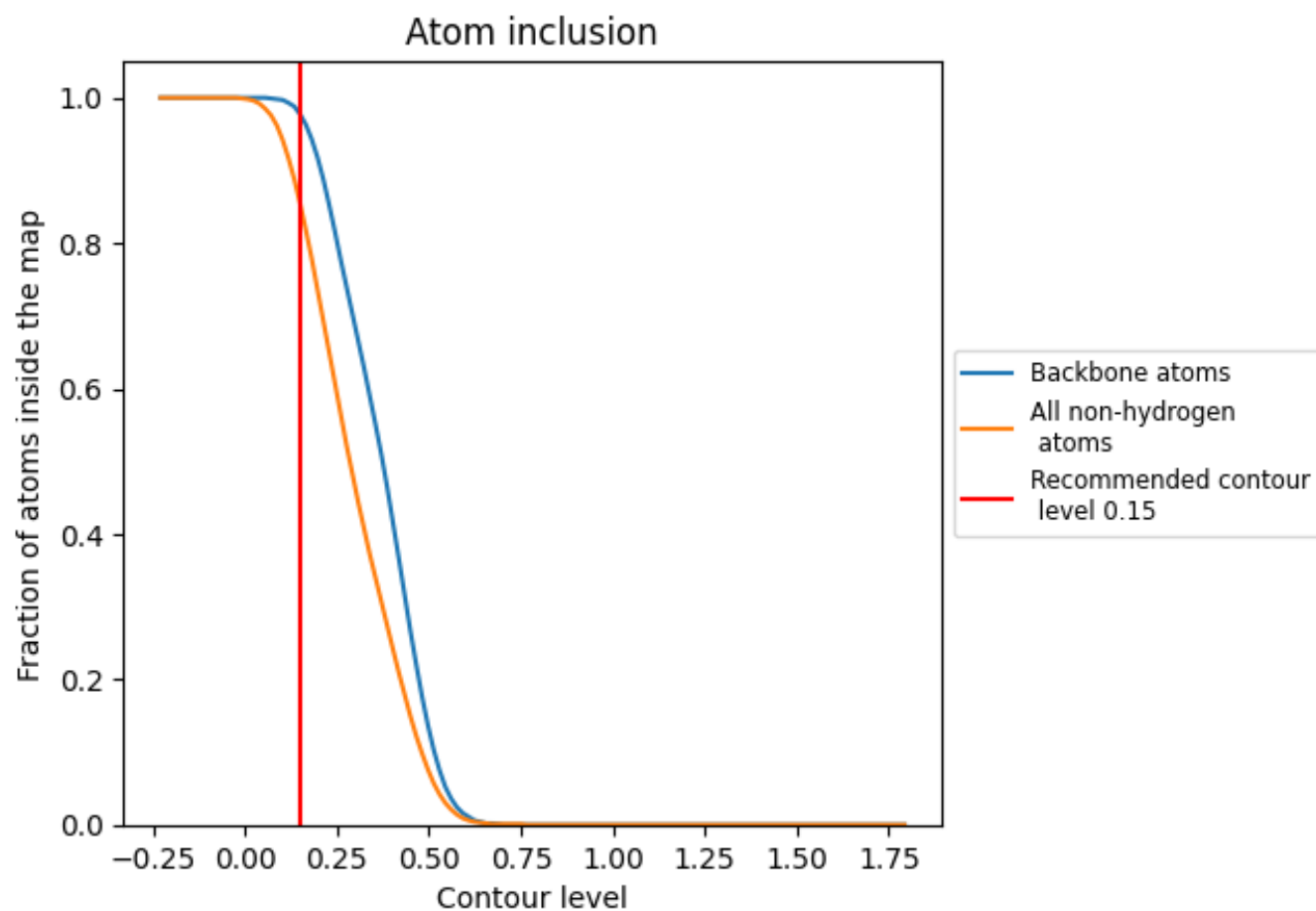
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8540	 0.3920
0	 0.8330	 0.3460
1	 0.8810	 0.3980
2	 0.7930	 0.3530
3	 0.8900	 0.4090
4	 0.7490	 0.3420
5	 0.8900	 0.4250
6	 0.8730	 0.4220
7	 0.8850	 0.4340
8	 0.8860	 0.4220
9	 0.8750	 0.4170
Aa	 0.8720	 0.4260
Ab	 0.8290	 0.3390
Ac	 0.8250	 0.3840
Ad	 0.8590	 0.4140
Ae	 0.7060	 0.2910
Af	 0.7040	 0.3210
B	 0.8240	 0.3410
C	 0.8710	 0.4090
D	 0.8850	 0.4230
E	 0.8250	 0.3620
F	 0.8160	 0.4170
G	 0.8470	 0.3850
H	 0.8980	 0.4290
I	 0.8800	 0.4120
J	 0.8540	 0.4240
K	 0.8360	 0.4160
L	 0.7840	 0.3420
M	 0.8600	 0.4160
N	 0.8510	 0.3720
O	 0.7540	 0.2820
P	 0.7980	 0.3090
Q	 0.8090	 0.3610
R	 0.7730	 0.3480
S	 0.8940	 0.4280



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Chain	Atom inclusion	Q-score
T	 0.8770	 0.4100
U	 0.8420	 0.3610
V	 0.8460	 0.3630
W	 0.8790	 0.3790
X	 0.8240	 0.3320
Y	 0.8510	 0.3340
Z	 0.8440	 0.3300
a	 0.8690	 0.3640
b	 0.8480	 0.3240
c	 0.8770	 0.3890
d	 0.8670	 0.3560
e	 0.8120	 0.3640
f	 0.8000	 0.3520
g	 0.8910	 0.4140
h	 0.8690	 0.4010
i	 0.8750	 0.4290
j	 0.7880	 0.3740
k	 0.8420	 0.3990
l	 0.8400	 0.3940
m	 0.7880	 0.3420
n	 0.8150	 0.3460
o	 0.8250	 0.3500
p	 0.8710	 0.3620
q	 0.8620	 0.4250
r	 0.8290	 0.3930
s	 0.8710	 0.3890
t	 0.8560	 0.2930
u	 0.8910	 0.4220
v	 0.8890	 0.4220
w	 0.8890	 0.4370
x	 0.9040	 0.4310
y	 0.8850	 0.4220
z	 0.9100	 0.4220