



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 01:26 PM EDT

PDB ID : 9BUH / pdb_00009buh
EMDB ID : EMD-44908
Title : Cryo-EM structure of respiratory supercomplex I III IV
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-05-17
Resolution : 2.80 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

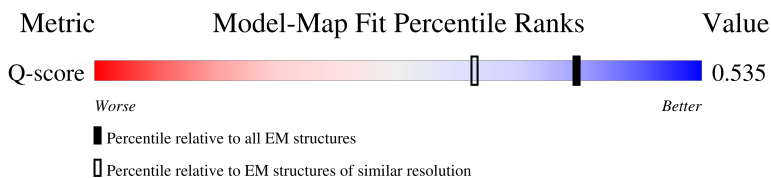
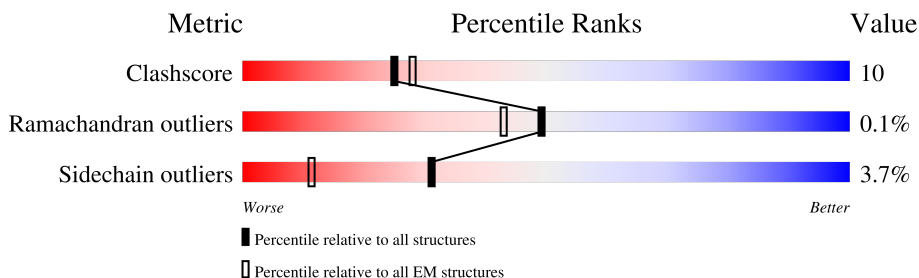
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.



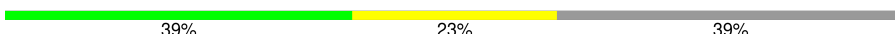
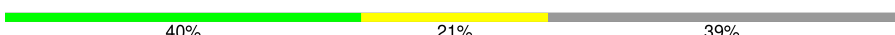
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	A	74	
2	t	137	
3	F	123	
4	K	145	

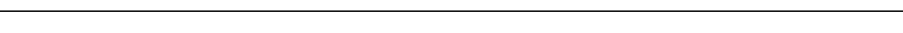
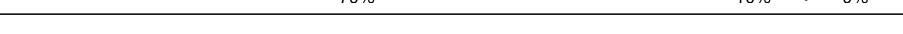
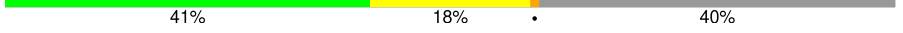
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Mol	Chain	Length	Quality of chain
5	U	357	
6	Z	114	
7	a	189	
8	i	347	
9	m	175	
10	p	221	
11	q	459	
12	Aa	82	
12	z	82	
13	0	91	
13	Ab	91	
14	1	64	
14	Ac	64	
15	3	56	
15	Ad	56	
16	Ag	70	
17	Ah	80	
18	Ai	80	
19	Aj	63	
20	Ak	514	
21	Al	228	
22	Am	261	
23	An	169	
24	Ao	152	
25	Ap	129	

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Mol	Chain	Length	Quality of chain
26	Aq	97	
27	Ar	86	
28	2	299	
28	4	299	
28	Ae	299	
28	Af	299	
29	5	480	
29	u	480	
30	6	453	
30	v	453	
31	7	379	
31	w	379	
32	8	326	
32	x	326	
33	9	111	
33	y	111	
34	B	464	
35	C	469	
36	D	264	
37	E	249	
38	G	727	
39	H	212	
40	I	258	
41	J	175	
42	L	372	

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Mol	Chain	Length	Quality of chain
43	M	113	
44	N	116	
45	O	156	
45	X	156	
46	P	99	
47	Q	154	
48	S	70	
49	T	169	
50	V	141	
51	W	144	
52	Y	105	
53	b	188	
54	c	186	
55	d	176	
56	e	154	
57	f	76	
58	g	122	
59	h	106	
60	j	115	
61	k	98	
62	l	606	
63	n	58	
64	o	129	
65	r	318	
66	s	249	

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Mol	Chain	Length	Quality of chain
67	R	110	

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
69	FES	2	301	-	-	X	-
71	HEC	8	401	X	-	-	-
71	HEC	x	401	X	-	-	-
73	SF4	B	502	-	-	X	-
73	SF4	G	802	-	-	X	-

2 Entry composition

There are 75 unique types of molecules in this entry. The entry contains 112807 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 c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	70	Total	C	N	O	S	0	0
			575	375	103	93	4		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	t	119	Total	C	N	O	S	0	0
			991	619	186	177	9		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	95	Total	C	N	O	S	0	0
			738	450	139	146	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	318	Total	C	N	O	S	0	0
			2562	1630	435	487	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	m	175	Total	C	N	O	S	0	0
			1338	897	190	238	13		

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

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

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 12 is a protein called Cytochrome b-c1 complex subunit 8.

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

- Molecule 13 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Ab	66	Total	C	N	O	S	0	0
			543	331	99	108	5		
13	0	68	Total	C	N	O	S	0	0
			561	341	101	114	5		

- Molecule 14 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Ac	59	Total	C	N	O	0	0
			485	318	85	82		
14	1	60	Total	C	N	O	0	0
			493	322	87	84		

- Molecule 15 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ad	51	Total	C	N	O	S	0	0
			421	281	74	65	1		
15	3	51	Total	C	N	O	S	0	0
			417	279	74	63	1		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Ag	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ah	56	Total	C	N	O	S	0	0
			437	281	73	80	3		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ai	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Aj	46	Total	C	N	O	S	0	0
			377	251	63	61	2		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ak	513	Total	C	N	O	S	0	0
			4014	2686	623	673	32		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Al	222	Total	C	N	O	S	0	0
			1785	1166	275	327	17		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Am	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	An	138	Total	C	N	O	S	0	0
			1154	752	189	209	4		

- Molecule 24 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ao	104	Total	C	N	O	S	0	0
			842	538	141	161	2		

- Molecule 25 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ap	91	Total	C	N	O	S	0	0
			697	433	123	135	6		

- Molecule 26 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Aq	73	Total	C	N	O	S	0	0
			606	392	116	97	1		

- Molecule 27 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ar	82	Total	C	N	O	S	0	0
			684	431	125	123	5		

- Molecule 28 is a protein called Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	195	Total	C	N	O	S	0	0
			1513	953	264	289	7		
28	4	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
28	Ae	39	Total	C	N	O	S	0	0
			275	172	53	47	3		
28	Af	33	Total	C	N	O	S	0	0
			223	141	39	41	2		

- Molecule 29 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5	435	Total	C	N	O	S	0	0
			3374	2105	594	656	19		
29	u	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		

- Molecule 30 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		
30	v	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		

- Molecule 31 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

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

- Molecule 32 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	239	Total	C	N	O	S	0	0
			1906	1217	328	345	16		
32	x	238	Total	C	N	O	S	0	0
			1896	1211	326	343	16		

- Molecule 33 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	9	101	Total	C	N	O	S	0	0
			893	572	157	162	2		
33	y	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C	430	Total	C	N	O	S	0	0
			3458	2210	594	630	24		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 38 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	J	118	Total	C	N	O	S	0	0
			962	608	173	178	3		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L	340	Total	C	N	O	S	0	0
			2735	1771	479	476	9		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5 isoform X1.

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

- Molecule 45 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	O	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
45	X	85	Total	C	N	O	S	0	0
			689	445	101	138	5		

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

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

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

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

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 1.

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

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 3.

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

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 51 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

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

- Molecule 52 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Y	62	Total	C	N	O	S	0	0
			536	355	89	91	1		

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	b	110	Total	C	N	O	S	0	0
			915	598	161	155	1		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	d	169	Total	C	N	O	S	0	0
			1420	892	256	264	8		

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	f	46	Total	C	N	O	0	0
			385	256	64	65		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 60 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	j	114	Total	C	N	O	S	0	0
			899	606	133	155	5		

- Molecule 61 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 62 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	l	602	Total	C	N	O	S	0	0
			4777	3169	740	818	50		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	o	128	Total	C	N	O		0	0
			1062	691	182	189			

- Molecule 65 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

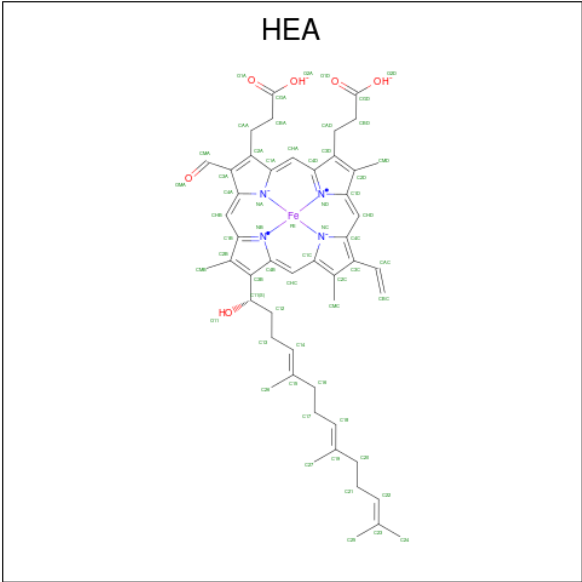
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

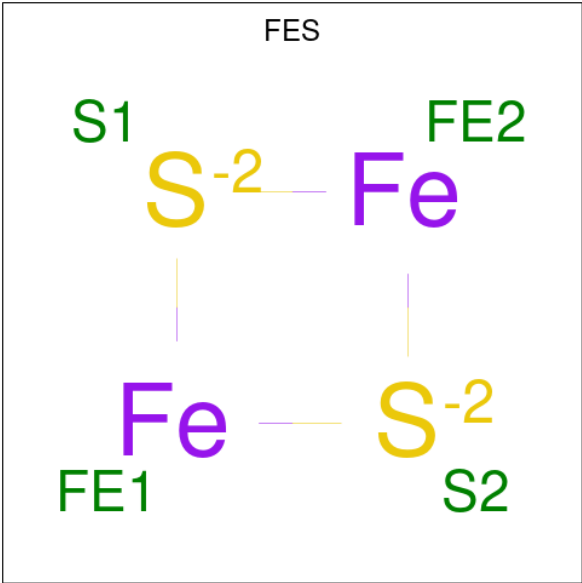
Mol	Chain	Residues	Atoms					AltConf	Trace
67	R	35	Total	C	N	O	S	0	0
			295	185	55	54	1		

- Molecule 68 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
68	Ak	1	Total 60	C 49	Fe 1	N 4	O 6	0
68	Ak	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 69 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



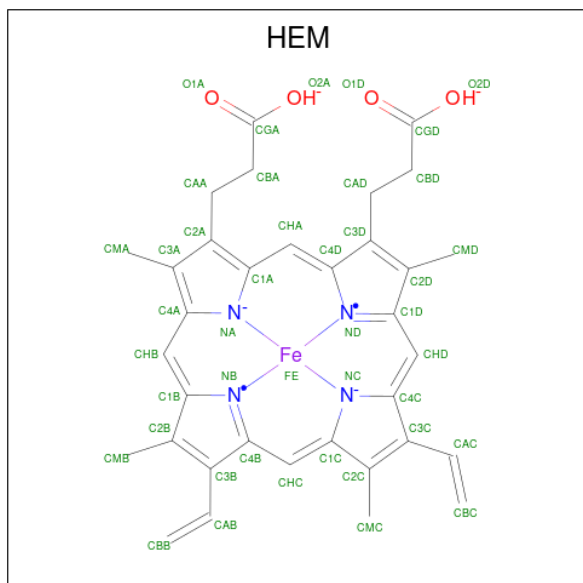
Mol	Chain	Residues	Atoms			AltConf
69	2	1	Total	Fe	S	0
			4	2	2	
69	4	1	Total	Fe	S	0
			4	2	2	

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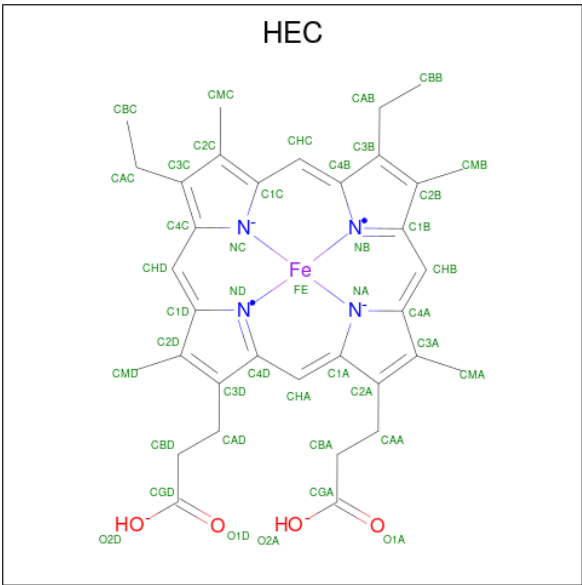
Mol	Chain	Residues	Atoms			AltConf
69	E	1	Total	Fe	S	0
			4	2	2	
69	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 70 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



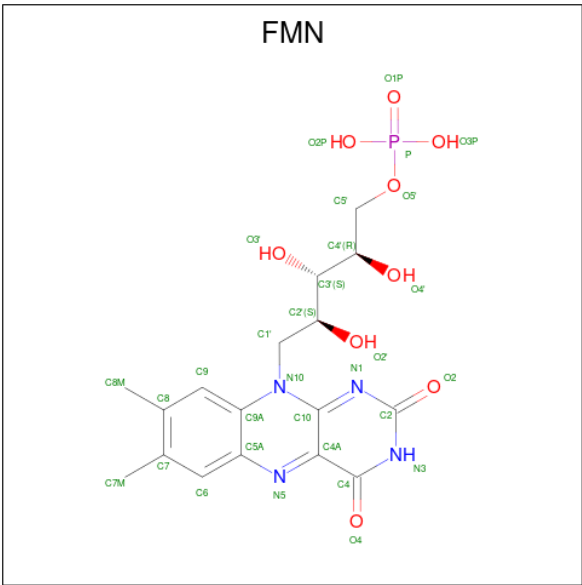
Mol	Chain	Residues	Atoms					AltConf
70	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 71 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



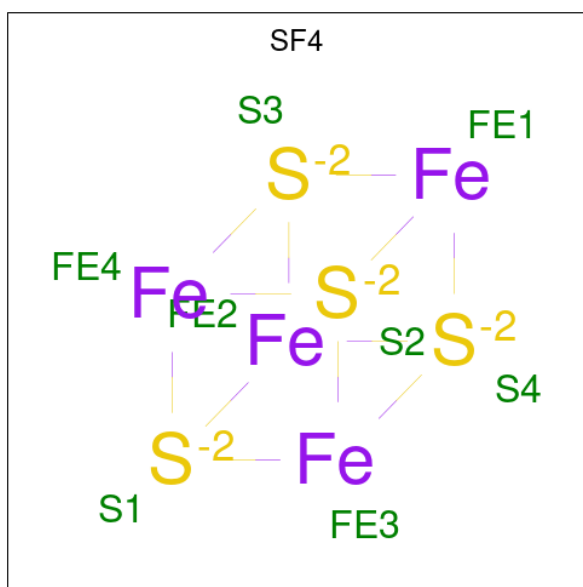
Mol	Chain	Residues	Atoms					AltConf
71	8	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
71	x	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 72 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



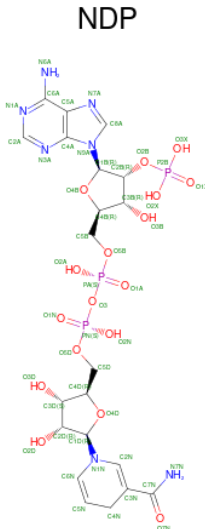
Mol	Chain	Residues	Atoms					AltConf
72	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 73 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



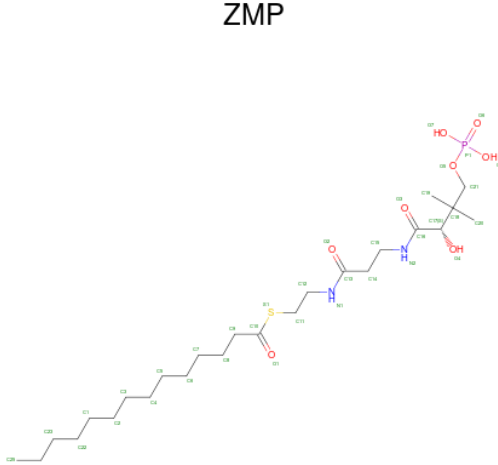
Mol	Chain	Residues	Atoms			AltConf
73	B	1	Total	Fe	S	0
			8	4	4	
73	G	1	Total	Fe	S	0
			8	4	4	
73	G	1	Total	Fe	S	0
			8	4	4	
73	H	1	Total	Fe	S	0
			8	4	4	
73	H	1	Total	Fe	S	0
			8	4	4	
73	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 74 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 75 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl}]\text{-beta-alaninyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



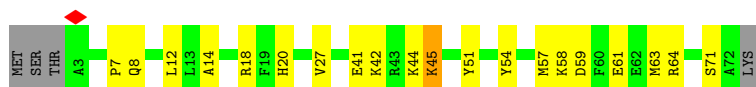
Mol	Chain	Residues	Atoms						AltConf
75	Q	1	Total 30	C 18	N 2	O 8	P 1	S 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

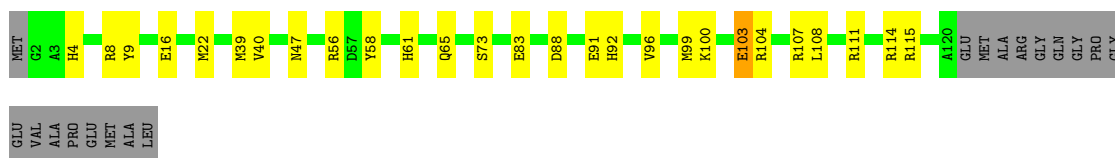
- Molecule 1: Cytochrome c oxidase subunit 6C

Chain A: 



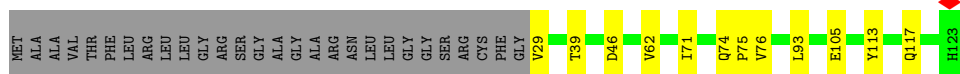
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain t: 



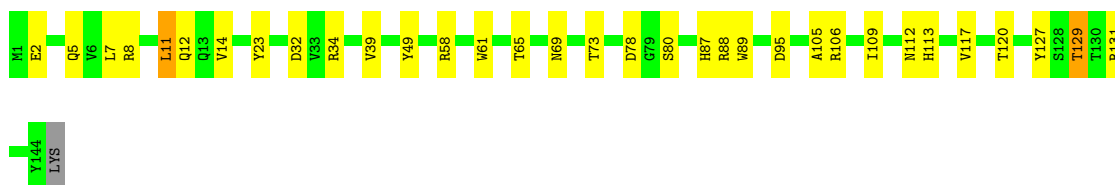
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain F: 



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain K: 



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

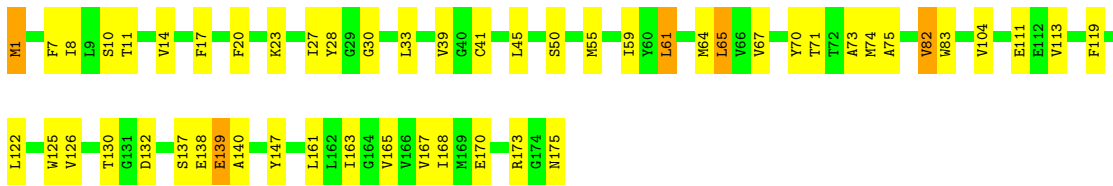
V271	D102	ALA	MET
V272	D107	LEU	ALA
L278	V108	ARG	LEU
D281	Q109	LEU	LEU
P284	L110	ARG	LEU
Q288	S115	LEU	ALA
L307	K118	PRO	PRO
N308	S130	ALA	ALA
Y309	L143	SER	ALA
T310	L148	ALA	ALA
T311	V159	VAL	PRO
I312	V160	ARG	PRO
P313	L161	GLY	ARG
V314	E162	LEU	GLY
P317	R163	ALA	GLY
H324	V170	VAL	ALA
V329	F171	ALA	ALA
L336	L172	GLN	ALA
D348	M175	ARG	VAL
V349	Q178	GLY	VAL
K352	Y189	GLY	GLY
W353	V205	THR	GLY
I354	N225	ALA	ALA
W355	E228	PRO	ALA
L356	M229	CYS	CYS
K357	D238	ARG	ARG
	D242	LEU	LEU
	K244	GLN	GLN
	L248	Y40	Y40
	P249	L43	L43
	E250	A44	A44
	C255	E49	E49
	E256	T56	T56
	V257	S59	S59
	L258	I62	I62
	Q259	K72	K72
	Y260	E78	E78
	R263	K82	K82
	E264	F88	F88

- | SER | GLN | ASN | LYS | ASP | LYS | LYS | HIS |
|-----|-----|-----|-----|-----|-----|------|------|
| MET | LEU | SER | VAL | LEU | ARG | GLY | GLN |
| | | | | | | ILE | ALA |
| | | | | | | ALA | VAL |
| | | | | | | SER | PHE |
| | | | | | | PRO | ILE |
| | | | | | | ASP | MET |
| | | | | | | ALA | GLN |
| | | | | | | HIS | GLY |
| | | | | | | HIS | GLY |
| | | | | | | LYS | GLU |
| | | | | | | HIS | GLY |
| | | | | | | HIS | |
| | | | | | | \$28 | X29 |
| | | | | | | X30 | E31 |
| | | | | | | | |
| | | | | | | Y35 | |
| | | | | | | T47 | V48 |
| | | | | | | Q49 | E50 |
| | | | | | | K51 | L52 |
| | | | | | | | |
| | | | | | | L57 | R63 |
| | | | | | | N64 | E65 |
| | | | | | | A66 | K67 |
| | | | | | | D68 | Y69 |
| | | | | | | | |
| | | | | | | K88 | V98 |
| | | | | | | | |
| | | | | | | E101 | Y103 |
| | | | | | | L104 | F105 |

- [illegible]

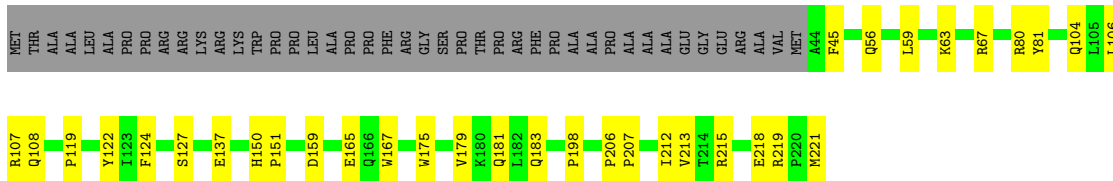
- | | | | |
|------|------|------|------|
| L337 | S222 | M104 | M1 |
| P338 | K105 | K105 | Y6 |
| M339 | L228 | L106 | L9 |
| T340 | | G107 | |
| P341 | | L108 | |
| A342 | S231 | | T12 |
| L343 | H232 | | V13 |
| S344 | T233 | H112 | M14 |
| S345 | W234 | | |
| L346 | M235 | V115 | T17 |
| N347 | K236 | P116 | M18 |
| | M237 | E117 | L19 |
| | M244 | | V20 |
| | M245 | I122 | |
| | | L128 | V26 |
| | L248 | | L27 |
| | L249 | K135 | L28 |
| | S250 | L136 | L29 |
| | M251 | A137 | W30 |
| | | P138 | I31 |
| | S258 | | |
| | G259 | V141 | E34 |
| | F260 | | M35 |
| | M261 | I145 | N36 |
| | | | L37 |
| | M265 | S148 | L38 |
| | I266 | I149 | A39 |
| | L267 | | M40 |
| | Q268 | M154 | I41 |
| | E269 | L155 | P42 |
| | M270 | | V43 |
| | | I164 | L44 |
| | M278 | | M45 |
| | | G168 | K46 |
| | M282 | | |
| | | Q172 | T57 |
| | N289 | | |
| | L290 | L175 | F60 |
| | Y291 | | L61 |
| | F292 | A180 | |
| | T293 | | T65 |
| | M294 | I184 | |
| | T295 | | M71 |
| | L296 | T191 | |
| | | A192 | I74 |
| | | V193 | |
| | N310 | | M77 |
| | M311 | | L78 |
| | K312 | M200 | L79 |
| | M313 | T201 | |
| | K314 | I202 | |
| | W315 | L203 | I86 |
| | Q316 | N204 | T87 |
| | F317 | | K88 |
| | | | M89 |
| | | I209 | |
| | L325 | | |
| | | L213 | N95 |
| | M329 | A214 | T96 |
| | | M215 | |
| | M336 | F218 | M100 |

- 



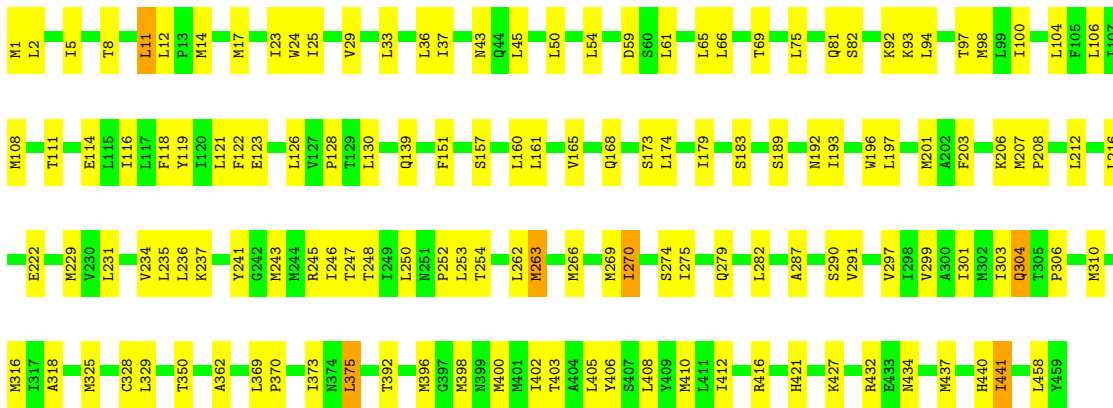
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p: 65% 15% 19%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4

Chain q: 70% 29% 1%



- Molecule 12: Cytochrome b-c1 complex subunit 8

Chain Aa: 74% 18% 5%



- Molecule 12: Cytochrome b-c1 complex subunit 8

Chain z: 79% 16% 5%



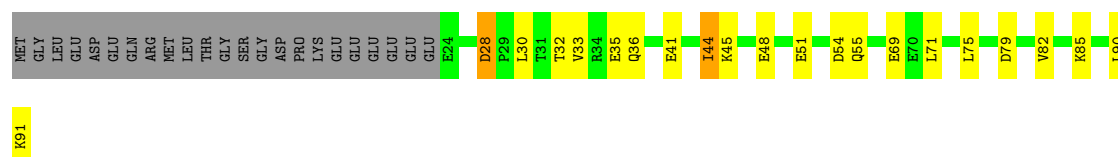
- Molecule 13: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ab: 



- Molecule 13: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 0: 



- Molecule 14: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain Ac: 



- Molecule 14: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 1: 



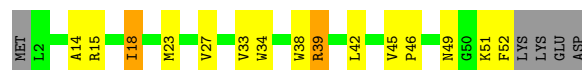
- Molecule 15: Cytochrome b-c1 complex subunit 10

Chain Ad: 

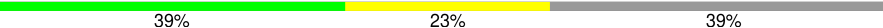


- Molecule 15: Cytochrome b-c1 complex subunit 10

Chain 3: 



- Molecule 16: Cytochrome c oxidase subunit 8

Chain Ag: 

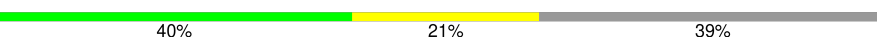


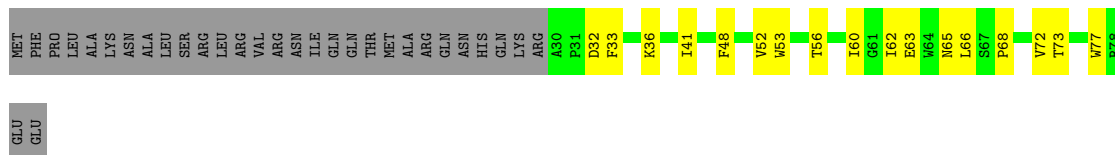
- Molecule 17: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain Ah: 



- Molecule 18: Cytochrome c oxidase subunit 7B

Chain Ai: 



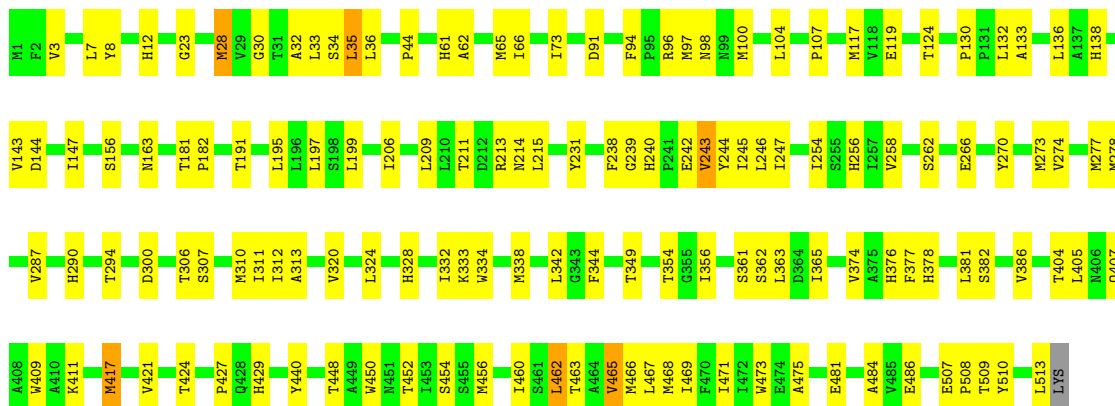
- Molecule 19: Cytochrome c oxidase subunit 7C, mitochondrial

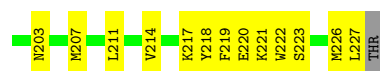
Chain Aj: 



- Molecule 20: Cytochrome c oxidase subunit 1

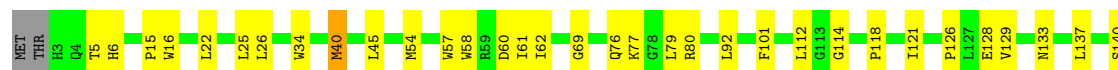
Chain Ak: 





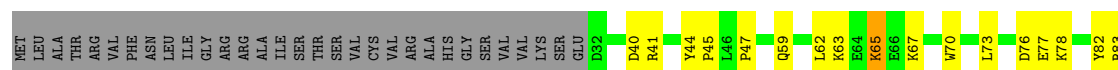
• Molecule 22: Cytochrome c oxidase subunit 3

Chain Am: 77% 21% ..



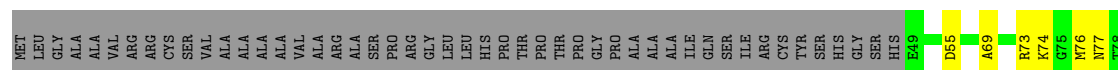
• Molecule 23: Cytochrome c oxidase subunit 4

Chain An: 56% 24% • 18%



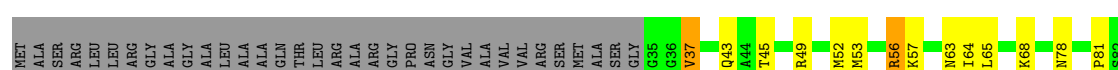
• Molecule 24: Cytochrome c oxidase subunit 5A, mitochondrial

Chain Ao: 50% 17% • 32%



• Molecule 25: Cytochrome c oxidase subunit 5B, mitochondrial

Chain Ap: 45% 24% • 29%



• Molecule 26: Cytochrome c oxidase subunit 6A2

Chain Aq: 57% 19% 25%



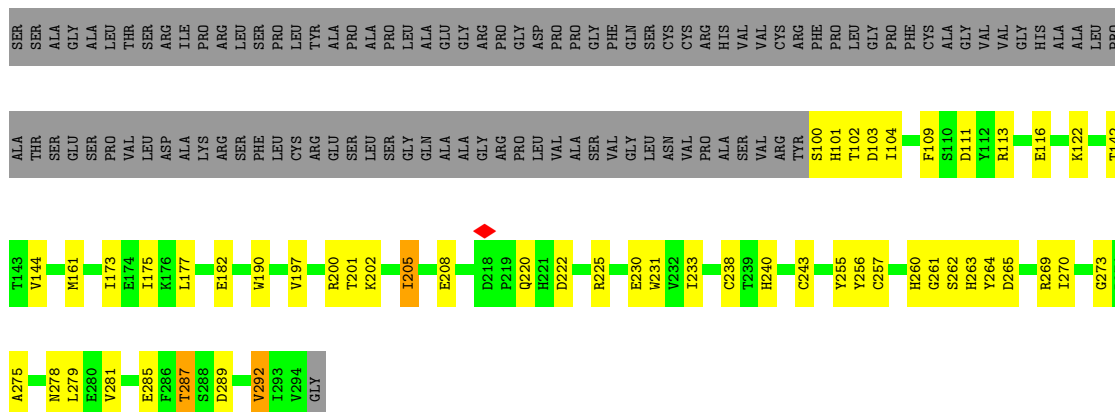
- Molecule 27: Cytochrome c oxidase subunit

Chain Ar: 55% 40% 5%



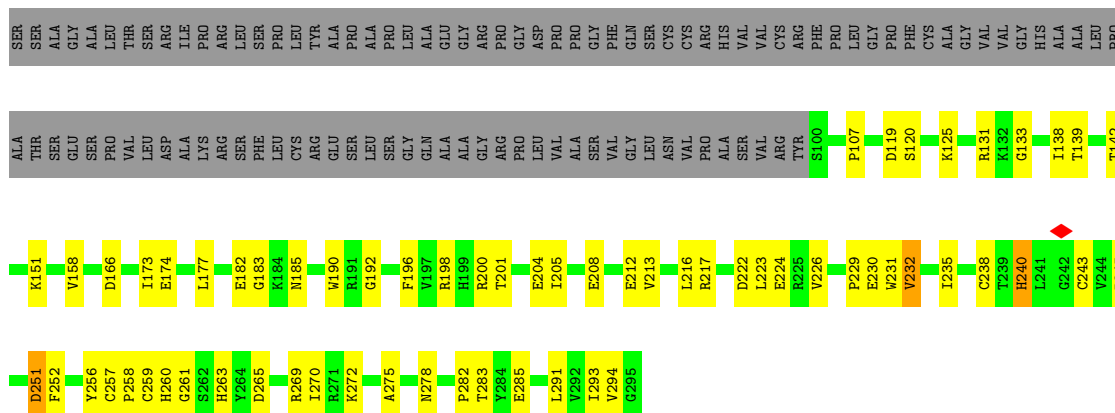
- Molecule 28: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain 2: 47% 17% 35%



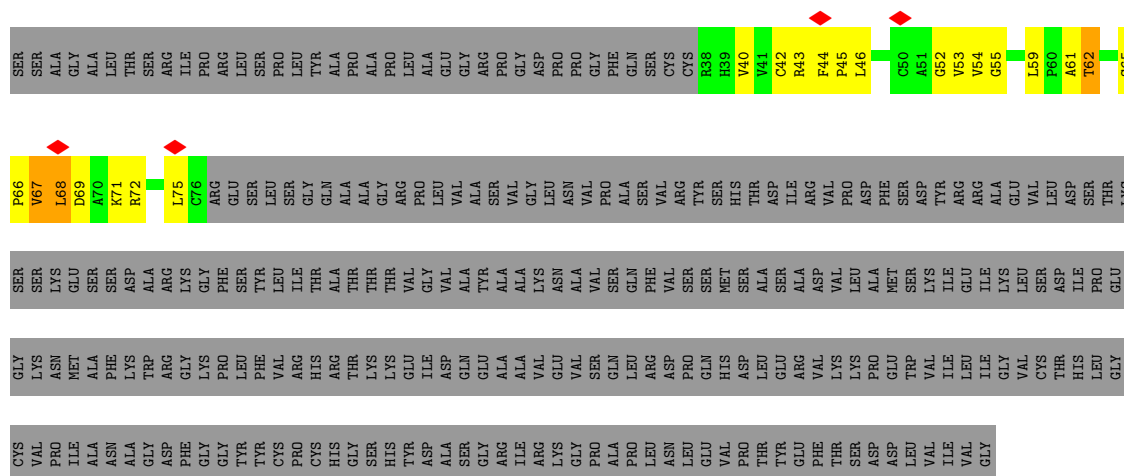
- Molecule 28: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain 4: 44% 21% 34%



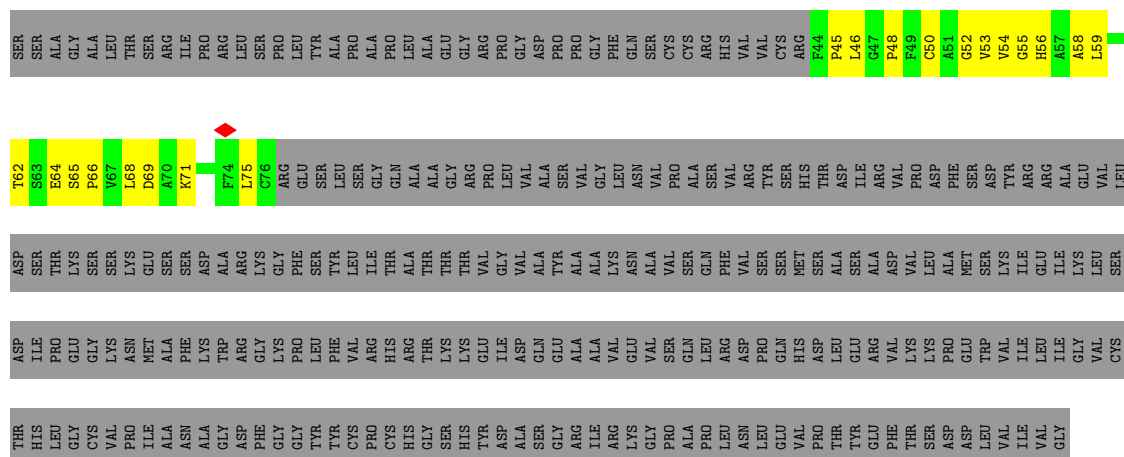
- Molecule 28: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain Ae: 6% 6% 87%



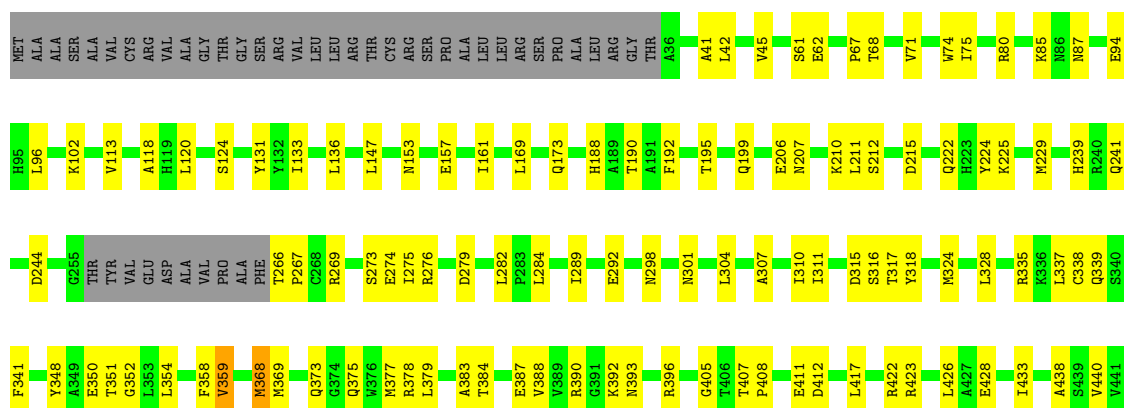
- Molecule 28: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

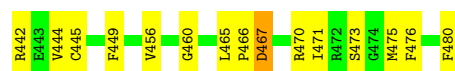
Chain Af: 5% 6% 89%



- Molecule 29: Cytochrome b-c1 complex subunit 1, mitochondrial

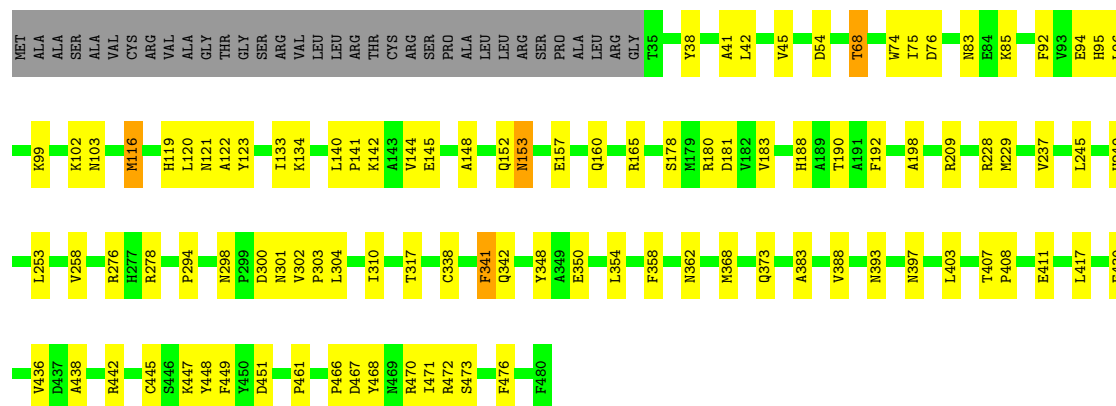
Chain 5: 64% 26% 9%





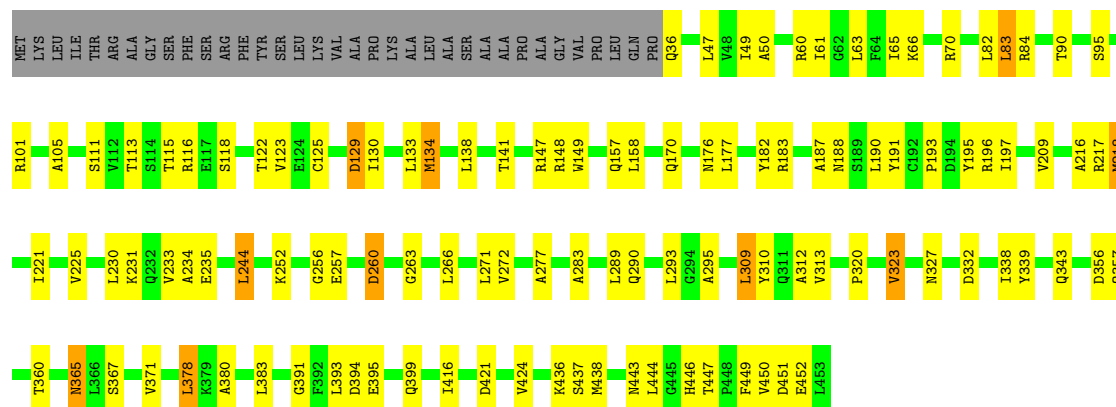
- Molecule 29: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain u: 72% 20% 7%



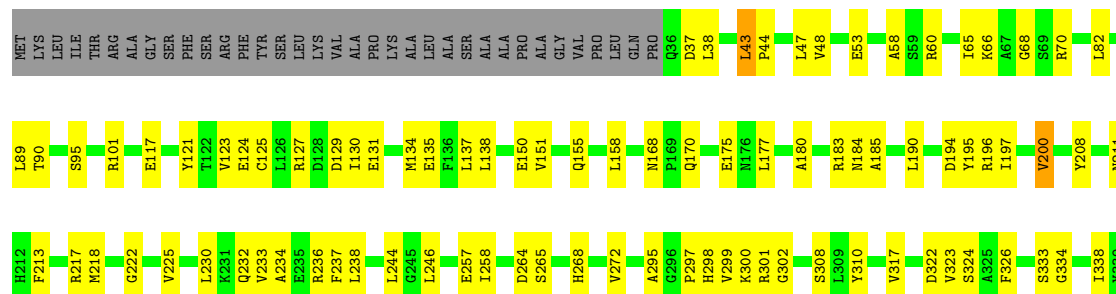
- Molecule 30: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 6: 67% 23% 8%



- Molecule 30: Cytochrome b-c1 complex subunit 2, mitochondrial

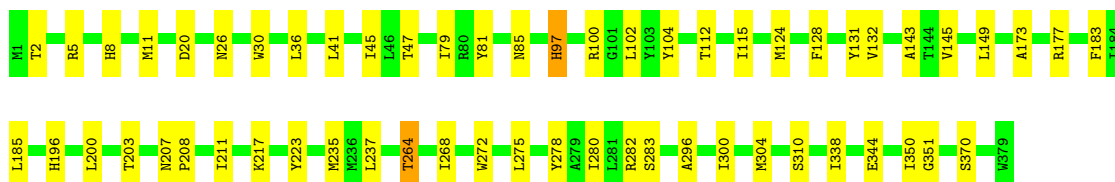
Chain v: 67% 24% 8%





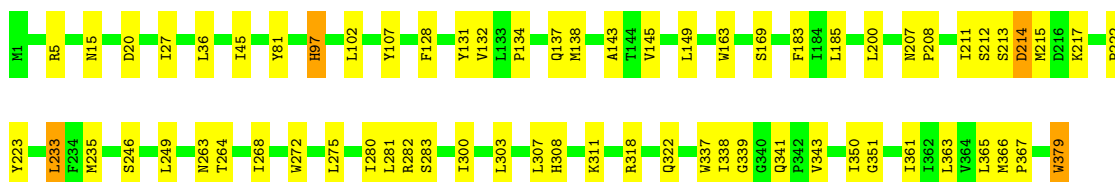
• Molecule 31: Cytochrome b

Chain 7: 85% 15%



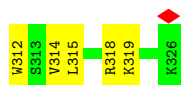
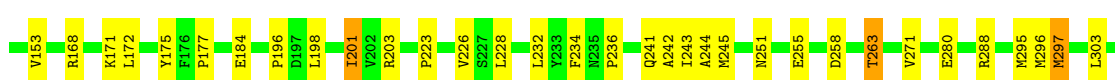
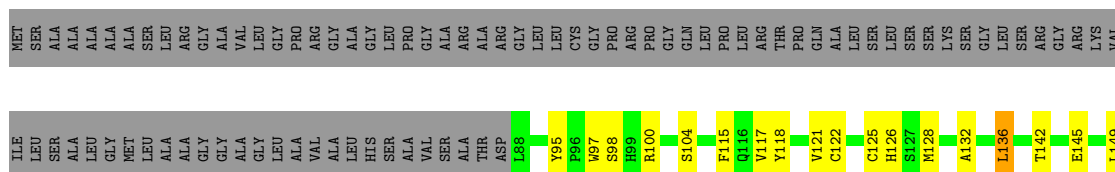
• Molecule 31: Cytochrome b

Chain w: 82% 17%



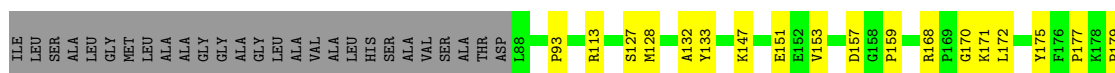
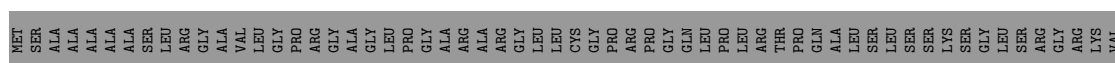
• Molecule 32: Cytochrome c1

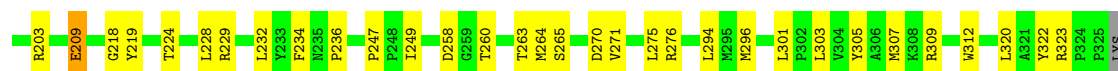
Chain 8: 56% 16% 27%



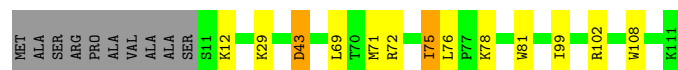
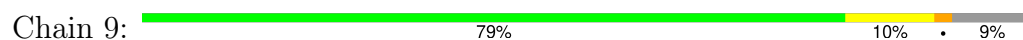
• Molecule 32: Cytochrome c1

Chain x: 58% 15% 27%

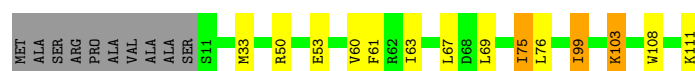
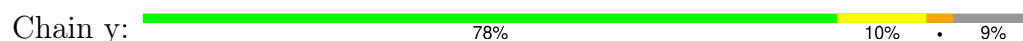




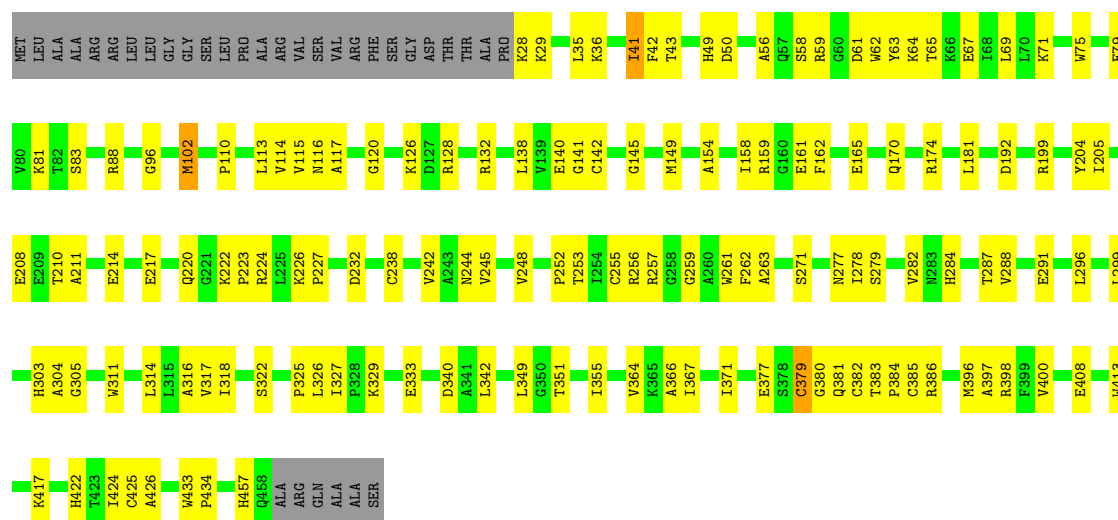
• Molecule 33: Cytochrome b-c1 complex subunit 7



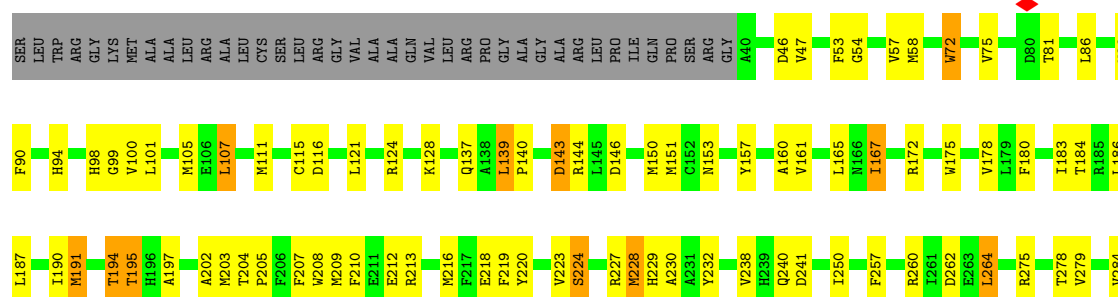
• Molecule 33: Cytochrome b-c1 complex subunit 7

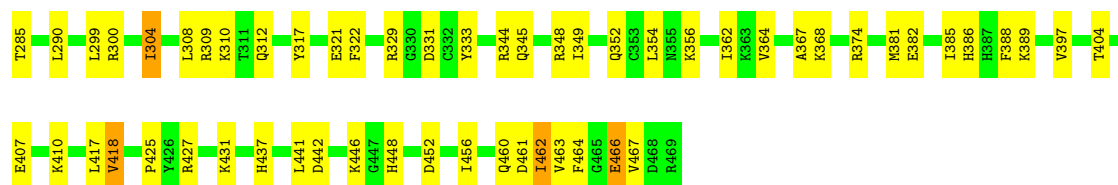


• Molecule 34: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



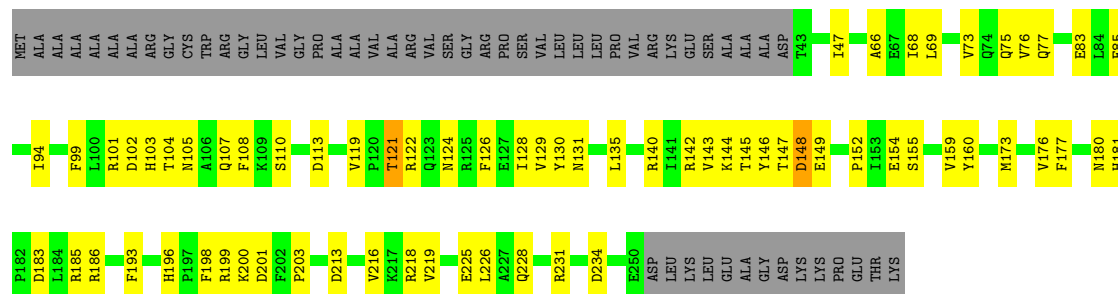
• Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





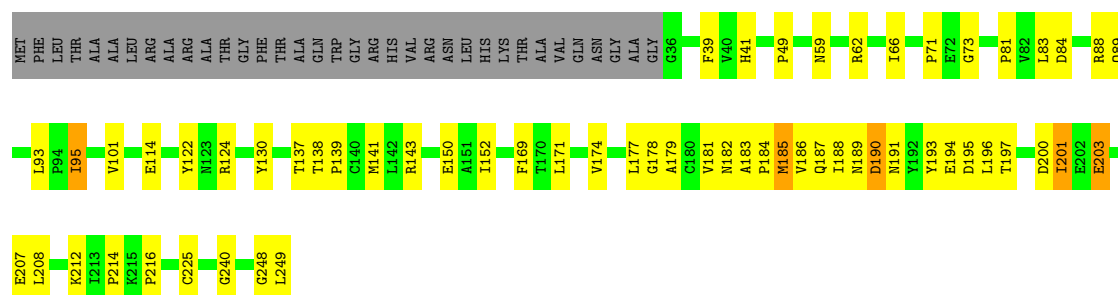
- Molecule 36: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain D: 53% 25% 21%



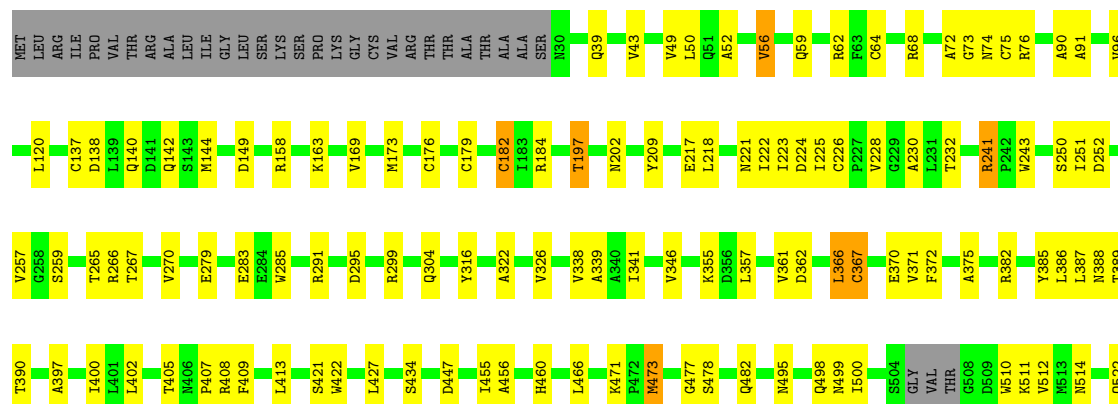
- Molecule 37: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 61% 22% 14%



- Molecule 38: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 70% 23% 6%





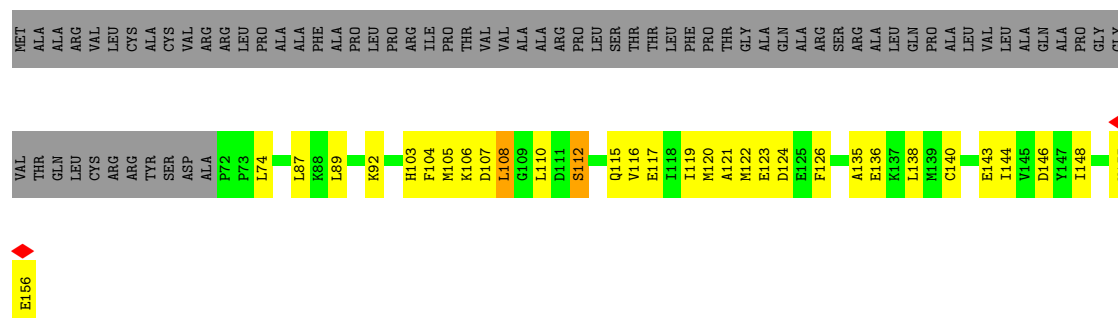
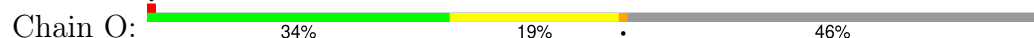
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



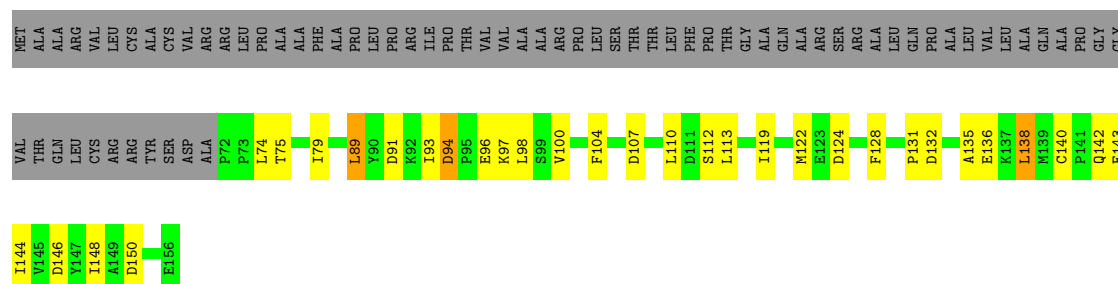
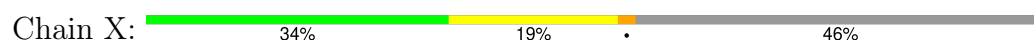
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



- Molecule 45: Acyl carrier protein

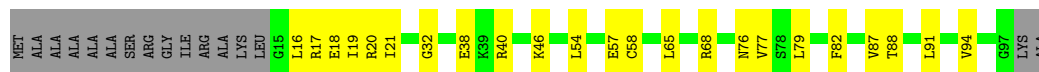


- Molecule 45: Acyl carrier protein



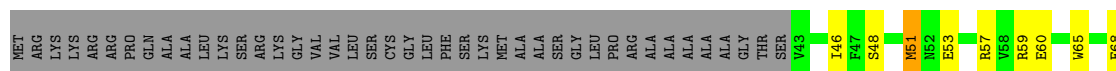
- Molecule 46: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P: 



- Molecule 47: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Q: 



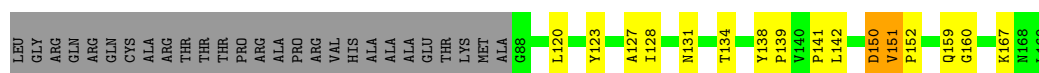
- Molecule 48: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 



- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain T: 



- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 



- Molecule 51: NADH:ubiquinone oxidoreductase subunit A13

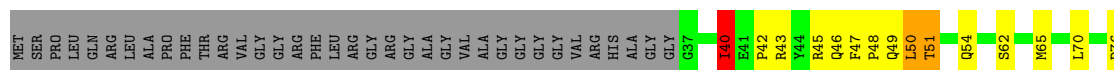
Chain W: 





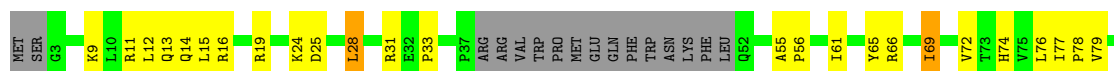
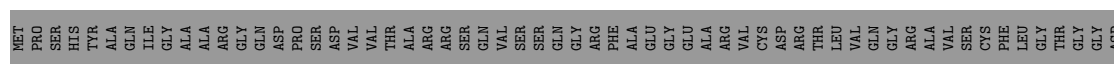
- Molecule 52: NADH:ubiquinone oxidoreductase subunit B2

Chain Y: 34% 21% 41%



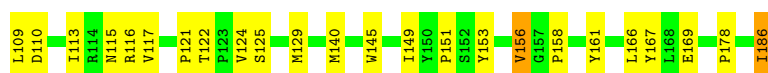
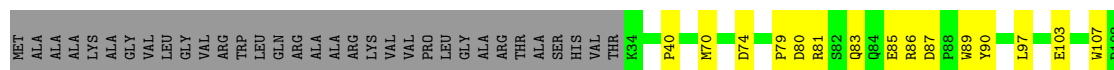
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b: 38% 19% 41%



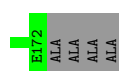
- Molecule 54: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 61% 20% 18%

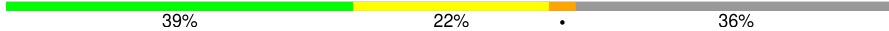


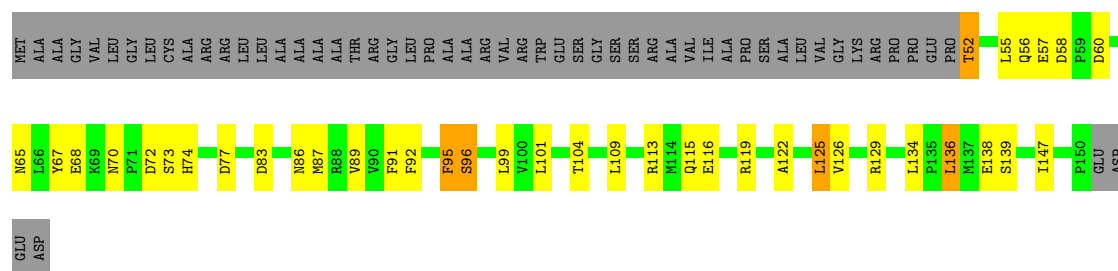
- Molecule 55: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 78% 18% 4%



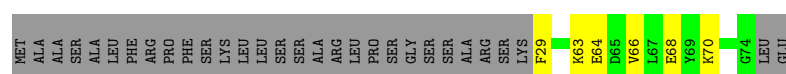
- Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 



- Molecule 57: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 



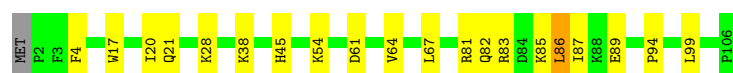
- Molecule 58: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 



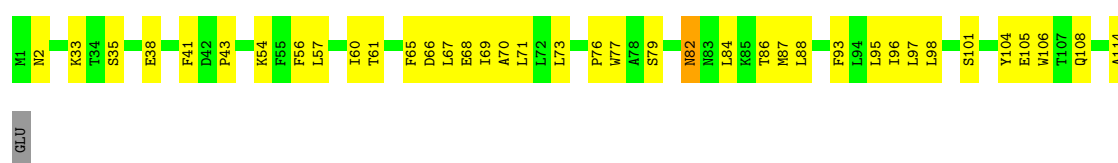
- Molecule 59: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 



- Molecule 60: NADH-ubiquinone oxidoreductase chain 3

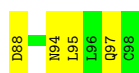
Chain j: 



- Molecule 61: NADH-ubiquinone oxidoreductase chain 4L

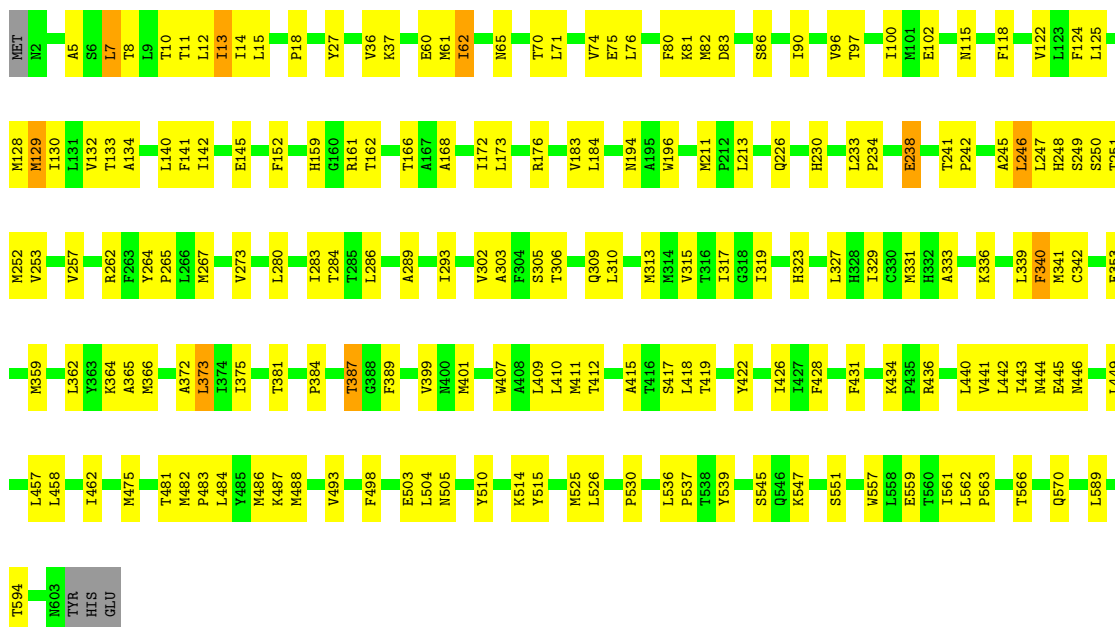
Chain k: 





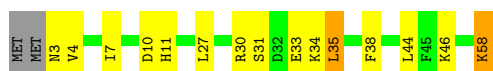
• Molecule 62: NADH-ubiquinone oxidoreductase chain 5

Chain l: 69% 29% ..



• Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n: 71% 22% . .



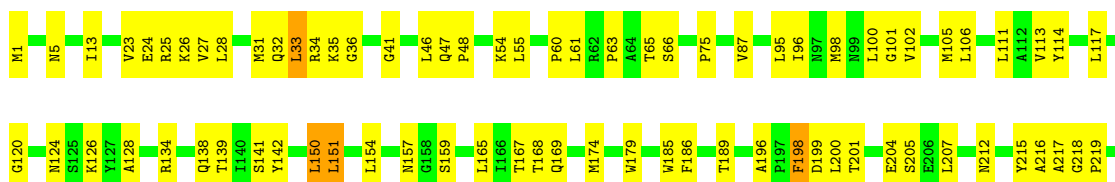
• Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o: 80% 19% .



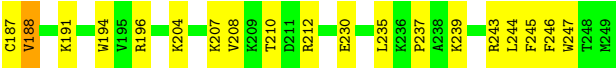
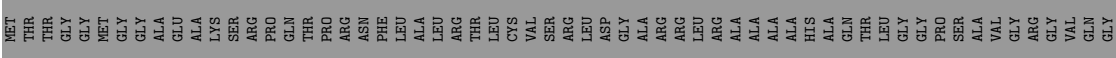
• Molecule 65: NADH-ubiquinone oxidoreductase chain 1

Chain r: 64% 34% .

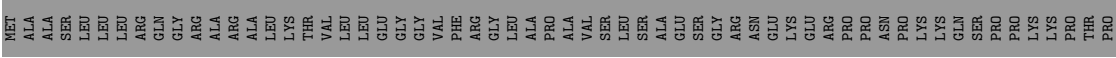




- Molecule 66: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 67: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54742	Depositor
Resolution determination method	OTHER	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	2.129	Depositor
Minimum map value	-0.160	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.039	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, HEC, HEA, HEM, FMN, FES, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/588	0.27	0/781
2	t	0.13	0/1015	0.28	0/1364
3	F	0.12	0/752	0.26	0/1013
4	K	0.11	0/1244	0.24	0/1693
5	U	0.11	0/2622	0.26	0/3552
6	Z	0.12	0/645	0.26	0/872
7	a	0.13	0/1184	0.27	0/1603
8	i	0.17	0/2774	0.32	0/3768
9	m	0.25	0/1373	0.42	0/1860
10	p	0.12	0/1590	0.27	0/2155
11	q	0.15	0/3721	0.30	0/5073
12	Aa	0.15	0/684	0.32	0/926
12	z	0.14	0/688	0.30	0/931
13	0	0.16	0/567	0.35	0/759
13	Ab	0.16	0/549	0.32	0/735
14	1	0.13	0/506	0.24	0/683
14	Ac	0.14	0/498	0.29	0/672
15	3	0.13	0/433	0.29	0/593
15	Ad	0.11	0/437	0.27	0/598
16	Ag	0.17	0/349	0.38	0/477
17	Ah	0.14	0/446	0.27	0/605
18	Ai	0.14	0/396	0.34	0/543
19	Aj	0.15	0/390	0.31	0/525
20	Ak	0.16	0/4154	0.32	0/5678
21	Al	0.22	0/1831	0.42	0/2496
22	Am	0.14	0/2179	0.27	0/2981
23	An	0.12	0/1188	0.27	0/1605
24	Ao	0.15	0/860	0.30	0/1167
25	Ap	0.14	0/712	0.33	0/966
26	Aq	0.14	0/633	0.27	0/866
27	Ar	0.15	0/704	0.32	0/951
28	2	0.15	0/1546	0.31	0/2093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	4	0.17	0/1551	0.34	1/2098 (0.0%)
28	Ae	0.23	0/281	0.60	0/383
28	Af	0.27	0/228	0.57	0/312
29	5	0.13	0/3442	0.28	0/4667
29	u	0.13	0/3531	0.29	0/4793
30	6	0.15	0/3192	0.30	0/4322
30	v	0.15	0/3192	0.31	0/4322
31	7	0.16	0/3123	0.31	0/4269
31	w	0.16	0/3123	0.29	0/4269
32	8	0.14	0/1964	0.32	0/2663
32	x	0.14	0/1954	0.28	0/2652
33	9	0.11	0/913	0.24	0/1223
33	y	0.12	0/913	0.23	0/1223
34	B	0.14	0/3393	0.31	0/4584
35	C	0.17	0/3551	0.34	0/4813
36	D	0.15	0/1783	0.35	0/2428
37	E	0.18	0/1698	0.38	0/2311
38	G	0.13	0/5347	0.28	0/7243
39	H	0.16	0/1443	0.32	0/1952
40	I	0.17	0/1279	0.32	0/1730
41	J	0.13	0/985	0.27	0/1329
42	L	0.13	0/2812	0.28	0/3812
43	M	0.11	0/791	0.28	0/1069
44	N	0.15	0/929	0.29	0/1258
45	O	0.13	0/701	0.34	0/946
45	X	0.15	0/701	0.34	0/946
46	P	0.15	0/680	0.36	0/916
47	Q	0.13	0/978	0.28	0/1317
48	S	0.15	0/577	0.30	0/777
49	T	0.12	0/659	0.28	0/905
50	V	0.12	0/1042	0.28	0/1411
51	W	0.23	1/1193 (0.1%)	0.31	1/1609 (0.1%)
52	Y	0.20	0/561	0.42	0/768
53	b	0.14	0/942	0.35	0/1282
54	c	0.13	0/1346	0.28	0/1840
55	d	0.13	0/1452	0.29	0/1958
56	e	0.42	2/849 (0.2%)	0.43	1/1153 (0.1%)
57	f	0.11	0/398	0.22	0/540
58	g	0.13	0/1031	0.30	0/1394
59	h	0.12	0/889	0.27	0/1190
60	j	0.17	0/923	0.34	0/1263
61	k	0.15	0/759	0.30	0/1029
62	l	0.15	0/4906	0.34	0/6673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	n	0.15	0/491	0.36	0/663
64	o	0.13	0/1092	0.28	0/1481
65	r	0.25	0/2581	0.42	0/3529
66	s	0.13	0/1436	0.32	0/1938
67	R	0.13	0/304	0.25	0/410
All	All	0.16	3/115167 (0.0%)	0.31	3/156247 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	e	95	PHE	C-N	9.73	1.47	1.34
51	W	11	PRO	CA-C	6.43	1.55	1.51
56	e	96	SER	C-N	-5.39	1.27	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	W	11	PRO	O-C-N	5.27	123.73	121.31
56	e	95	PHE	O-C-N	5.16	129.26	122.30
28	4	258	PRO	N-CA-C	-5.13	107.45	113.86

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	575	0	584	17	0
2	t	991	0	933	26	0
3	F	738	0	701	7	0
4	K	1203	0	1161	25	0
5	U	2562	0	2508	36	0
6	Z	626	0	607	11	0
7	a	1151	0	1164	24	0
8	i	2711	0	2874	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	m	1338	0	1338	49	0
10	p	1534	0	1470	29	0
11	q	3630	0	3837	97	0
12	Aa	662	0	660	12	0
12	z	666	0	663	13	0
13	0	561	0	542	15	0
13	Ab	543	0	530	7	0
14	1	493	0	491	5	0
14	Ac	485	0	485	9	0
15	3	417	0	414	10	0
15	Ad	421	0	418	9	0
16	Ag	338	0	342	11	0
17	Ah	437	0	436	7	0
18	Ai	383	0	366	13	0
19	Aj	377	0	372	9	0
20	Ak	4014	0	3993	111	0
21	Al	1785	0	1800	74	0
22	Am	2096	0	2027	46	0
23	An	1154	0	1137	36	0
24	Ao	842	0	838	17	0
25	Ap	697	0	682	25	0
26	Aq	606	0	575	12	0
27	Ar	684	0	647	23	0
28	2	1513	0	1497	42	0
28	4	1518	0	1498	47	0
28	Ae	275	0	276	29	0
28	Af	223	0	220	20	0
29	5	3374	0	3272	86	0
29	u	3459	0	3350	60	0
30	6	3140	0	3121	83	0
30	v	3140	0	3121	79	0
31	7	3025	0	3090	39	0
31	w	3025	0	3090	49	0
32	8	1906	0	1857	37	0
32	x	1896	0	1843	33	0
33	9	893	0	888	11	0
33	y	893	0	888	13	0
34	B	3318	0	3281	102	0
35	C	3458	0	3394	116	0
36	D	1732	0	1682	53	0
37	E	1658	0	1662	44	0
38	G	5260	0	5291	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	H	1412	0	1364	46	0
40	I	1248	0	1254	38	0
41	J	962	0	962	19	0
42	L	2735	0	2751	59	0
43	M	773	0	801	21	0
44	N	910	0	950	17	0
45	O	689	0	687	23	0
45	X	689	0	687	24	0
46	P	669	0	677	15	0
47	Q	954	0	960	18	0
48	S	562	0	557	21	0
49	T	638	0	637	15	0
50	V	1021	0	1027	7	0
51	W	1162	0	1156	30	0
52	Y	536	0	483	22	0
53	b	915	0	933	30	0
54	c	1291	0	1185	34	0
55	d	1420	0	1386	26	0
56	e	826	0	789	34	0
57	f	385	0	381	6	0
58	g	1000	0	994	29	0
59	h	867	0	871	17	0
60	j	899	0	931	35	0
61	k	748	0	799	38	0
62	l	4777	0	4923	126	0
63	n	479	0	486	12	0
64	o	1062	0	1072	20	0
65	r	2508	0	2607	91	0
66	s	1398	0	1378	35	0
67	R	295	0	279	11	0
68	Ak	120	0	108	13	0
69	2	4	0	0	6	0
69	4	4	0	0	1	0
69	E	4	0	0	0	0
69	G	4	0	0	1	0
70	7	86	0	60	12	0
70	w	86	0	60	8	0
71	8	43	0	31	3	0
71	x	43	0	30	2	0
72	B	31	0	19	1	0
73	B	8	0	0	2	0
73	G	16	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	H	16	0	0	1	0
73	I	8	0	0	1	0
74	L	48	0	26	3	0
75	Q	30	0	30	1	0
All	All	112807	0	112247	2364	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 (2364) 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)
38:G:179:CYS:SG	73:G:802:SF4:FE1	1.15	1.36
38:G:226:CYS:SG	73:G:802:SF4:FE3	1.17	1.35
38:G:182:CYS:SG	73:G:802:SF4:FE2	1.25	1.28
38:G:176:CYS:SG	73:G:802:SF4:FE4	1.30	1.22
35:C:275:ARG:O	35:C:279:VAL:HB	1.60	1.01
38:G:176:CYS:HG	73:G:802:SF4:FE4	0.75	0.96
20:Ak:65:MET:HB3	68:Ak:601:HEA:HBC1	1.51	0.90
28:4:174:GLU:HG3	28:4:291:LEU:HD11	1.54	0.90
8:i:65:THR:HG22	61:k:19:LEU:HD21	1.56	0.87
36:D:103:HIS:HB2	36:D:107:GLN:HG2	1.56	0.86
19:Aj:41:MET:HE1	20:Ak:473:TRP:HB2	1.58	0.86
20:Ak:35:LEU:HD21	20:Ak:462:LEU:HD12	1.57	0.86
28:2:257:CYS:HG	69:2:301:FES:FE2	0.58	0.85
37:E:183:ALA:HB3	37:E:195:ASP:HA	1.55	0.85
11:q:116:ILE:HG21	66:s:245:PHE:HB3	1.56	0.83
8:i:258:SER:HB2	8:i:336:VAL:HG12	1.57	0.83
42:L:71:MET:SD	42:L:249:LYS:NZ	2.51	0.82
62:l:319:ILE:HG13	62:l:399:VAL:HG22	1.63	0.81
38:G:179:CYS:SG	73:G:802:SF4:S4	2.78	0.80
39:H:77:LEU:HB2	65:r:31:MET:HG2	1.62	0.80
14:Ac:11:TYR:HA	14:Ac:15:PHE:HB2	1.63	0.80
28:2:257:CYS:SG	69:2:301:FES:FE2	1.72	0.80
35:C:183:ILE:HG23	35:C:216:MET:HE2	1.64	0.80
28:2:255:TYR:HB2	28:2:264:TYR:HB2	1.64	0.79
20:Ak:62:ALA:HB2	68:Ak:601:HEA:HBD1	1.65	0.79
70:7:401:HEM:HHD	70:7:401:HEM:HBC2	1.66	0.78
38:G:182:CYS:SG	73:G:802:SF4:S4	2.79	0.78
38:G:226:CYS:SG	73:G:802:SF4:S4	2.80	0.78
35:C:367:ALA:HB3	38:G:149:ASP:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Ae:55:GLY:HA3	28:Ae:59:LEU:HB3	1.65	0.76
65:r:28:LEU:HD22	65:r:275:ALA:HB2	1.66	0.76
63:n:7:ILE:O	63:n:11:HIS:HB2	1.86	0.75
42:L:121:VAL:HG23	42:L:156:VAL:HG11	1.69	0.75
11:q:114:GLU:HG2	66:s:246:PHE:HB3	1.68	0.75
5:U:324:HIS:HB2	56:e:56:GLN:HE22	1.52	0.75
20:Ak:274:VAL:HG12	20:Ak:278:MET:HE2	1.68	0.75
8:i:268:GLN:HA	11:q:165:VAL:HG11	1.67	0.74
20:Ak:28:MET:HE2	20:Ak:469:ILE:HD11	1.67	0.74
25:Ap:64:ILE:HG23	25:Ap:65:LEU:HD12	1.68	0.74
65:r:185:TRP:HE1	65:r:238:THR:HG22	1.52	0.74
38:G:338:VAL:HG12	38:G:544:VAL:HB	1.70	0.74
27:Ar:44:MET:SD	27:Ar:47:LYS:NZ	2.60	0.74
70:7:401:HEM:HHC	70:7:401:HEM:HBB2	1.70	0.73
8:i:128:LEU:HD11	8:i:213:LEU:HD23	1.70	0.73
48:S:38:VAL:O	48:S:44:GLN:NE2	2.20	0.73
30:v:324:SER:HB3	28:Af:68:LEU:HD13	1.69	0.73
28:4:142:THR:HG22	32:8:303:LEU:HB3	1.70	0.73
8:i:42:PRO:HG2	9:m:167:VAL:HG22	1.70	0.73
8:i:108:LEU:HD11	8:i:191:THR:HG21	1.70	0.73
35:C:160:ALA:HA	35:C:404:THR:HG21	1.71	0.72
45:X:119:ILE:HG21	45:X:135:ALA:HB1	1.70	0.72
40:I:86:MET:HB2	40:I:91:VAL:HB	1.70	0.72
7:a:91:VAL:HG23	55:d:52:ILE:HG12	1.71	0.72
22:Am:128:GLU:HG3	22:Am:129:VAL:H	1.55	0.72
9:m:126:VAL:HG13	51:W:122:GLY:HA3	1.71	0.72
38:G:367:CYS:HB3	38:G:531:LYS:HB3	1.72	0.72
30:6:170:GLN:HB3	28:Ae:67:VAL:HG22	1.69	0.72
37:E:183:ALA:HB1	37:E:184:PRO:HD2	1.71	0.72
2:t:73:SER:HB3	55:d:23:GLN:HE21	1.54	0.71
30:v:155:GLN:NE2	30:v:200:VAL:O	2.23	0.71
2:t:92:HIS:HD2	62:l:481:THR:HB	1.55	0.71
40:I:98:ARG:NH2	60:j:35:SER:O	2.24	0.71
60:j:67:LEU:HD11	61:k:68:ALA:HB3	1.73	0.71
30:6:123:VAL:HB	30:6:133:LEU:HD23	1.72	0.71
28:Ae:65:SER:HB3	28:Ae:66:PRO:HD2	1.72	0.71
35:C:143:ASP:OD1	35:C:143:ASP:N	2.22	0.70
9:m:67:VAL:HG11	61:k:31:LEU:HD21	1.74	0.70
28:4:185:ASN:HD21	28:4:196:PHE:HB3	1.55	0.70
39:H:37:THR:N	43:M:105:GLU:O	2.24	0.70
28:4:120:SER:HA	29:5:269:ARG:HE	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:E:39:PHE:HA	37:E:124:ARG:HH12	1.55	0.70
38:G:456:ALA:O	38:G:499:ASN:ND2	2.24	0.70
38:G:674:LEU:HD21	46:P:46:LYS:HZ1	1.56	0.70
38:G:326:VAL:HG23	38:G:626:LEU:HD13	1.73	0.70
34:B:222:LYS:HG2	34:B:379:CYS:HB3	1.74	0.70
8:i:232:HIS:HB3	8:i:311:MET:HE1	1.74	0.69
9:m:30:GLY:HA2	9:m:64:MET:HE2	1.74	0.69
45:O:116:VAL:HG12	45:O:120:MET:HE2	1.74	0.69
54:c:166:LEU:HB3	54:c:169:GLU:HB2	1.74	0.69
36:D:66:ALA:HA	36:D:73:VAL:HG21	1.74	0.69
67:R:100:GLN:HG3	67:R:101:PRO:HD2	1.74	0.69
35:C:385:ILE:HG23	38:G:140:GLN:HG2	1.75	0.69
42:L:119:ASN:HD22	42:L:120:VAL:HG23	1.56	0.69
2:t:8:ARG:HB2	2:t:16:GLU:HG2	1.74	0.69
60:j:54:LYS:HB3	60:j:114:ALA:H	1.56	0.69
18:Ai:68:PRO:HG2	23:An:156:PHE:HE1	1.58	0.69
20:Ak:381:LEU:HD23	68:Ak:601:HEA:HAC	1.74	0.69
55:d:163:MET:HE1	56:e:147:ILE:HG21	1.74	0.69
5:U:148:ALA:HB1	5:U:159:VAL:HG11	1.74	0.69
53:b:12:LEU:HB3	53:b:16:ARG:HH12	1.57	0.68
62:l:562:LEU:HB3	62:l:563:PRO:HD3	1.75	0.68
38:G:691:ILE:HG23	38:G:714:VAL:HG21	1.75	0.68
62:l:132:VAL:O	62:l:262:ARG:NH2	2.26	0.68
28:Ae:52:GLY:HA2	28:Ae:61:ALA:HA	1.74	0.68
20:Ak:107:PRO:HB3	22:Am:25:LEU:HB2	1.76	0.68
5:U:225:ASN:HB3	5:U:228:GLU:HB2	1.74	0.67
36:D:130:TYR:HB2	36:D:143:VAL:HG22	1.76	0.67
55:d:162:ARG:NH1	56:e:139:SER:O	2.27	0.67
15:3:39:ARG:HD3	15:3:39:ARG:H	1.59	0.67
35:C:310:LYS:HE2	39:H:37:THR:HB	1.74	0.67
29:u:120:LEU:HB3	30:v:299:VAL:HG12	1.76	0.67
29:u:388:VAL:HG21	29:u:438:ALA:HA	1.77	0.67
4:K:32:ASP:OD2	4:K:34:ARG:NH1	2.28	0.67
10:p:207:PRO:O	53:b:11:ARG:NH2	2.27	0.67
42:L:164:HIS:HB2	42:L:179:LYS:HD3	1.76	0.67
30:v:138:LEU:HD12	30:v:233:VAL:HG22	1.76	0.67
20:Ak:508:PRO:HG3	22:Am:6:HIS:HB3	1.77	0.67
38:G:179:CYS:SG	73:G:802:SF4:S2	2.88	0.67
30:6:82:LEU:HD13	30:6:158:LEU:HD11	1.75	0.67
11:q:208:PRO:HG3	11:q:216:LEU:HD13	1.76	0.66
35:C:180:PHE:O	35:C:184:THR:HG23	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Aq:26:ARG:HD3	26:Aq:26:ARG:H	1.59	0.66
21:Al:179:LEU:H	27:Ar:27:THR:HG23	1.58	0.66
15:3:45:VAL:O	15:3:49:ASN:ND2	2.28	0.66
7:a:82:VAL:HG11	56:e:104:THR:HG21	1.77	0.66
34:B:364:VAL:HG12	34:B:400:VAL:HG12	1.77	0.66
35:C:165:LEU:HD13	35:C:397:VAL:HG22	1.78	0.66
36:D:121:THR:HG21	41:J:129:SER:H	1.60	0.66
2:t:99:MET:HG3	54:c:156:VAL:HG23	1.78	0.66
29:5:267:PRO:HA	29:5:350:GLU:HG3	1.76	0.66
31:7:338:ILE:HD11	31:7:350:ILE:HG22	1.77	0.66
38:G:266:ARG:HG2	38:G:267:THR:HG23	1.78	0.66
21:Al:1:MET:HG2	23:An:150:VAL:HG21	1.75	0.66
34:B:425:CYS:SG	34:B:426:ALA:N	2.66	0.66
2:t:99:MET:HB3	52:Y:92:TRP:HH2	1.62	0.65
20:Ak:244:TYR:HA	20:Ak:247:ILE:HG22	1.77	0.65
28:4:270:ILE:HD13	28:4:275:ALA:HB3	1.76	0.65
35:C:441:LEU:HD13	35:C:460:GLN:HE22	1.61	0.65
29:u:134:LYS:HE3	30:v:384:MET:HE3	1.78	0.65
30:6:293:LEU:HD22	30:6:309:LEU:HD13	1.78	0.65
29:u:99:LYS:NZ	30:v:301:ARG:O	2.27	0.65
21:Al:83:ILE:HA	21:Al:86:MET:HE2	1.78	0.65
31:7:112:THR:O	31:7:196:HIS:NE2	2.29	0.65
65:r:236:ALA:HA	65:r:263:THR:HG22	1.77	0.65
28:4:216:LEU:HD13	28:4:269:ARG:HD2	1.77	0.65
30:6:84:ARG:NH2	30:6:190:LEU:O	2.27	0.65
35:C:285:THR:HG23	44:N:13:GLY:HA3	1.76	0.65
70:w:402:HEM:HBC2	70:w:402:HEM:HMC1	1.78	0.65
38:G:402:LEU:HD13	38:G:407:PRO:HG3	1.79	0.65
52:Y:65:MET:HE2	62:l:375:ILE:HG12	1.77	0.65
62:l:27:TYR:O	62:l:115:ASN:ND2	2.29	0.64
31:w:138:MET:HA	31:w:138:MET:HE3	1.80	0.64
8:i:100:MET:HE1	62:l:594:THR:HG22	1.79	0.64
34:B:140:GLU:HG3	34:B:252:PRO:HG3	1.79	0.64
52:Y:40:ILE:HD11	62:l:444:ASN:HB2	1.79	0.64
11:q:375:LEU:HD11	62:l:141:PHE:HE2	1.62	0.64
21:Al:134:ARG:HB2	23:An:132:THR:HG21	1.79	0.64
37:E:130:TYR:HA	37:E:189:ASN:HD21	1.62	0.64
56:e:126:VAL:HG23	56:e:136:LEU:HD11	1.77	0.64
62:l:341:MET:HE2	62:l:457:LEU:HD12	1.79	0.64
62:l:80:PHE:HB3	62:l:82:MET:HE3	1.79	0.64
1:A:20:HIS:HB3	21:Al:44:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:G:138:ASP:HB3	38:G:142:GLN:HE21	1.63	0.64
29:u:298:ASN:O	29:u:301:ASN:ND2	2.27	0.64
11:q:403:THR:HA	11:q:406:TYR:CE2	2.33	0.64
65:r:24:GLU:HA	65:r:271:LEU:HD13	1.80	0.64
9:m:59:ILE:HD11	60:j:70:ALA:HB2	1.80	0.64
9:m:125:TRP:HH2	51:W:126:GLY:HA2	1.62	0.64
34:B:222:LYS:HE3	41:J:175:LYS:HB2	1.79	0.64
38:G:397:ALA:HA	38:G:471:LYS:HB3	1.80	0.64
48:S:69:ILE:HD13	66:s:148:PHE:HB3	1.80	0.64
30:v:90:THR:HG23	30:v:95:SER:HA	1.79	0.64
35:C:431:LYS:HG3	36:D:113:ASP:HB3	1.80	0.64
50:V:69:ILE:HG13	50:V:100:THR:HG21	1.79	0.64
8:i:200:MET:HE1	8:i:343:LEU:HD11	1.80	0.64
8:i:88:LYS:HD3	8:i:148:SER:HB3	1.80	0.64
62:l:306:THR:HG22	62:l:336:LYS:HG2	1.80	0.64
8:i:57:THR:HG22	61:k:77:LEU:HB3	1.80	0.63
70:7:402:HEM:HBC2	70:7:402:HEM:HMC2	1.81	0.63
35:C:100:VAL:HG12	40:I:113:MET:HE3	1.80	0.63
35:C:304:ILE:HD11	36:D:135:LEU:HD22	1.80	0.63
53:b:119:LEU:HD21	53:b:121:LYS:HE2	1.79	0.63
65:r:102:VAL:HG13	65:r:150:LEU:HD11	1.80	0.63
51:W:88:ARG:NH1	51:W:92:GLU:OE2	2.31	0.63
30:6:66:LYS:O	30:6:217:ARG:NH2	2.30	0.63
23:An:155:GLY:H	23:An:158:ALA:HB3	1.63	0.63
28:2:257:CYS:SG	69:2:301:FES:S1	2.96	0.63
29:u:276:ARG:HB2	12:z:16:THR:HG23	1.79	0.63
1:A:61:GLU:OE1	1:A:64:ARG:NH1	2.31	0.63
30:6:395:GLU:OE2	30:6:399:GLN:NE2	2.32	0.63
35:C:187:LEU:HD21	35:C:216:MET:HB2	1.80	0.63
35:C:418:VAL:HG13	35:C:427:ARG:HB3	1.81	0.63
36:D:129:VAL:HG22	36:D:144:LYS:HG2	1.78	0.63
65:r:27:VAL:HG12	65:r:31:MET:HE2	1.81	0.63
6:Z:63:ARG:HH21	45:X:91:ASP:HA	1.64	0.63
11:q:328:CYS:HB2	11:q:437:MET:HE1	1.80	0.63
32:8:244:ALA:HB3	71:8:401:HEC:HBD2	1.81	0.63
40:I:81:ALA:HB1	40:I:82:PRO:HD2	1.81	0.63
12:z:61:THR:O	12:z:65:GLN:HG2	1.97	0.63
35:C:190:ILE:O	35:C:194:THR:HB	1.99	0.62
36:D:76:VAL:HG23	43:M:69:VAL:HB	1.81	0.62
11:q:1:MET:HE2	11:q:111:THR:HG21	1.82	0.62
29:5:422:ARG:NH2	29:5:428:GLU:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:E:49:PRO:HG3	37:E:95:ILE:HD13	1.81	0.62
5:U:178:GLN:NE2	5:U:238:ASP:OD2	2.32	0.62
30:6:444:LEU:O	30:6:446:HIS:N	2.33	0.62
29:u:75:ILE:HG12	29:u:229:MET:HG2	1.81	0.62
30:6:116:ARG:NH1	30:6:188:ASN:O	2.32	0.62
70:7:402:HEM:HMB1	70:7:402:HEM:HBB2	1.82	0.62
11:q:269:MET:HG3	11:q:270:ILE:HD12	1.81	0.62
29:5:318:TYR:HE1	28:Ae:54:VAL:HG23	1.65	0.62
29:u:76:ASP:O	29:u:228:ARG:NH2	2.30	0.62
8:i:289:ASN:HA	8:i:292:PHE:CE2	2.35	0.62
34:B:174:ARG:HA	67:R:93:LEU:HD21	1.80	0.62
23:An:78:LYS:HB3	24:Ao:104:PHE:CZ	2.33	0.62
28:4:213:VAL:HA	28:4:216:LEU:HD12	1.82	0.62
38:G:68:ARG:HE	38:G:283:GLU:HB3	1.64	0.62
38:G:388:ASN:HB3	38:G:511:LYS:HD2	1.82	0.62
70:w:401:HEM:HMC2	70:w:401:HEM:HBC2	1.80	0.62
65:r:31:MET:HE1	65:r:272:TRP:HA	1.81	0.62
30:6:176:ASN:ND2	30:6:260:ASP:OD2	2.32	0.62
36:D:126:PHE:HB2	36:D:147:THR:HG23	1.81	0.62
42:L:278:VAL:HG12	42:L:364:VAL:HG21	1.82	0.62
20:Ak:34:SER:HB3	20:Ak:61:HIS:CE1	2.34	0.61
28:4:204:GLU:O	28:4:208:GLU:HG2	2.00	0.61
64:o:121:LEU:HD23	64:o:123:GLN:HE21	1.63	0.61
29:u:276:ARG:NH2	29:u:466:PRO:O	2.33	0.61
29:u:445:CYS:O	29:u:449:PHE:HB2	2.00	0.61
8:i:337:LEU:O	8:i:340:THR:HG23	2.00	0.61
20:Ak:381:LEU:HD23	68:Ak:601:HEA:CAC	2.29	0.61
38:G:176:CYS:SG	73:G:802:SF4:S2	2.98	0.61
38:G:299:ARG:NH1	38:G:703:ALA:O	2.32	0.61
39:H:116:CYS:HB2	39:H:118:LEU:HD13	1.81	0.61
40:I:79:MET:HE1	40:I:177:ILE:HD12	1.80	0.61
45:O:104:PHE:HB3	45:O:110:LEU:HD11	1.81	0.61
45:O:104:PHE:HA	45:O:108:LEU:HB2	1.83	0.61
23:An:82:TYR:OH	24:Ao:109:ARG:NH2	2.33	0.61
43:M:46:SER:O	43:M:52:ASN:ND2	2.33	0.61
71:x:401:HEC:HBA1	71:x:401:HEC:HHA	1.83	0.61
9:m:45:LEU:HD22	9:m:50:SER:HA	1.81	0.61
20:Ak:354:THR:HG21	20:Ak:429:HIS:HE1	1.65	0.61
29:5:378:ARG:NH2	29:5:387:GLU:OE1	2.34	0.61
36:D:102:ASP:HB2	44:N:90:LEU:HD22	1.83	0.61
45:O:104:PHE:HE2	45:O:144:ILE:HD11	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:l:526:LEU:HD12	62:l:530:PRO:HG3	1.81	0.61
42:L:183:GLU:HG3	42:L:195:ILE:HD13	1.83	0.61
62:l:62:ILE:HD11	62:l:81:LYS:HG3	1.83	0.61
11:q:247:THR:HB	11:q:304:GLN:HE21	1.65	0.61
20:Ak:197:LEU:HA	22:Am:92:LEU:HD13	1.82	0.61
30:6:129:ASP:N	30:6:129:ASP:OD1	2.30	0.61
51:W:133:ILE:O	51:W:137:THR:HG22	2.00	0.61
30:v:43:LEU:HD22	30:v:44:PRO:HD2	1.83	0.61
65:r:157:ASN:HA	65:r:168:THR:HG21	1.82	0.61
33:y:75:ILE:HD12	12:z:40:ARG:HH21	1.64	0.61
11:q:252:PRO:HG3	58:g:119:HIS:CE1	2.35	0.60
29:5:222:GLN:O	29:5:225:LYS:NZ	2.34	0.60
30:6:61:ILE:HG13	30:6:130:ILE:HD11	1.82	0.60
32:8:228:LEU:HD11	32:8:234:PHE:HB2	1.82	0.60
35:C:101:LEU:HB2	35:C:464:PHE:CZ	2.36	0.60
46:P:79:LEU:HD22	46:P:87:VAL:HG22	1.82	0.60
1:A:7:PRO:HG2	24:Ao:124:ILE:HD13	1.84	0.60
10:p:213:VAL:O	53:b:19:ARG:NH1	2.33	0.60
30:6:320:PRO:HB3	28:Ae:75:LEU:HB3	1.82	0.60
62:l:401:MET:HE3	62:l:482:MET:HE3	1.83	0.60
8:i:128:LEU:HD13	8:i:216:PHE:HB2	1.84	0.60
11:q:119:TYR:CZ	11:q:161:LEU:HB2	2.36	0.60
38:G:279:GLU:OE1	41:J:154:LYS:NZ	2.33	0.60
51:W:98:MET:HG2	59:h:82:GLN:HG2	1.82	0.60
10:p:219:ARG:HD2	10:p:221:MET:HE1	1.84	0.60
21:Al:43:SER:O	21:Al:47:THR:HG22	2.00	0.60
30:6:61:ILE:HD11	30:6:225:VAL:HG21	1.82	0.60
34:B:311:TRP:HE1	34:B:333:GLU:HG2	1.65	0.60
36:D:183:ASP:OD2	36:D:185:ARG:NH1	2.34	0.60
47:Q:48:SER:HB2	47:Q:53:GLU:HB3	1.84	0.60
8:i:106:LEU:O	8:i:135:LYS:NZ	2.34	0.60
29:5:304:LEU:HD13	29:5:354:LEU:HD22	1.83	0.60
29:5:298:ASN:O	29:5:301:ASN:ND2	2.33	0.60
30:6:320:PRO:HG2	30:6:343:GLN:HE21	1.67	0.60
51:W:120:MET:HG3	51:W:123:GLU:H	1.67	0.60
11:q:243:MET:HB3	11:q:301:ILE:HG21	1.84	0.60
37:E:59:ASN:ND2	37:E:89:GLN:OE1	2.33	0.60
39:H:76:TYR:HA	39:H:79:ARG:HD3	1.83	0.60
9:m:65:LEU:HD12	65:r:117:LEU:HD21	1.83	0.60
21:Al:104:TRP:CG	21:Al:203:ASN:HB2	2.37	0.60
13:0:33:VAL:HG12	13:0:82:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B:36:LYS:HD3	34:B:36:LYS:H	1.66	0.60
35:C:205:PRO:HB3	35:C:264:LEU:HD12	1.84	0.60
10:p:107:ARG:HH22	64:o:20:PRO:HB3	1.66	0.59
11:q:266:MET:HE1	11:q:392:THR:HB	1.84	0.59
27:Ar:58:ARG:HH22	27:Ar:62:LYS:HD3	1.67	0.59
34:B:217:GLU:OE2	34:B:224:ARG:NH2	2.35	0.59
50:V:81:ARG:NH1	50:V:89:ASN:OD1	2.35	0.59
54:c:117:VAL:HG21	62:l:539:TYR:HB2	1.84	0.59
5:U:255:CYS:SG	5:U:256:GLU:N	2.73	0.59
11:q:196:TRP:CD1	11:q:250:LEU:HB3	2.37	0.59
38:G:339:ALA:HB3	38:G:542:PRO:HG3	1.83	0.59
10:p:218:GLU:HG2	10:p:219:ARG:HG2	1.84	0.59
11:q:274:SER:HB2	62:l:545:SER:HB2	1.85	0.59
28:2:100:SER:O	28:2:101:HIS:ND1	2.36	0.59
28:4:265:ASP:OD1	28:4:269:ARG:N	2.36	0.59
30:6:63:LEU:HD23	30:6:141:THR:HG21	1.84	0.59
39:H:205:ILE:O	39:H:209:TYR:HB3	2.03	0.59
62:l:76:LEU:HD21	62:l:196:TRP:HE3	1.67	0.59
30:v:70:ARG:HD2	30:v:117:GLU:HG2	1.83	0.59
13:Ab:71:LEU:HD22	32:8:223:PRO:HG3	1.84	0.59
21:Al:112:ASP:O	27:Ar:59:ARG:NH1	2.34	0.59
29:5:131:TYR:HH	29:5:224:TYR:HH	1.50	0.59
36:D:103:HIS:HB3	44:N:83:GLN:CD	2.27	0.59
37:E:191:ASN:HB3	37:E:216:PRO:HB3	1.84	0.59
38:G:498:GLN:NE2	38:G:499:ASN:OD1	2.36	0.59
35:C:260:ARG:HE	43:M:25:GLN:HB3	1.66	0.59
38:G:226:CYS:SG	73:G:802:SF4:S2	3.01	0.59
57:f:68:GLU:HG2	58:g:21:ARG:HB3	1.84	0.59
30:6:61:ILE:HD12	30:6:134:MET:HG3	1.85	0.59
31:w:338:ILE:HD11	31:w:350:ILE:HG22	1.84	0.59
11:q:24:TRP:HB3	11:q:81:GLN:HE21	1.68	0.59
11:q:98:MET:HE3	11:q:128:PRO:HA	1.84	0.59
28:2:100:SER:N	28:2:103:ASP:OD1	2.35	0.59
62:l:82:MET:HE1	62:l:133:THR:HB	1.85	0.59
62:l:86:SER:O	62:l:90:ILE:HG13	2.03	0.59
63:n:31:SER:HA	63:n:34:LYS:HE2	1.84	0.59
45:X:74:LEU:HB3	45:X:79:ILE:HD11	1.85	0.59
10:p:181:GLN:NE2	10:p:198:PRO:O	2.34	0.59
20:Ak:409:TRP:HB3	20:Ak:471:ILE:HG12	1.85	0.59
40:I:97:PRO:HA	40:I:100:SER:HB3	1.85	0.59
64:o:14:LEU:HD12	64:o:15:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:s:160:THR:HA	66:s:163:TRP:CD1	2.37	0.59
9:m:168:ILE:HG12	60:j:60:ILE:HG21	1.85	0.59
28:4:256:TYR:CE1	28:4:261:GLY:HA2	2.37	0.59
51:W:86:MET:HE3	51:W:124:LEU:HD22	1.85	0.59
29:u:393:ASN:O	29:u:397:ASN:ND2	2.32	0.59
12:z:37:ASN:OD1	12:z:40:ARG:NH1	2.36	0.59
5:U:260:TYR:HE2	5:U:271:VAL:HG13	1.67	0.58
28:4:240:HIS:HE1	28:4:260:HIS:CG	2.21	0.58
36:D:218:ARG:HD2	47:Q:127:THR:HA	1.84	0.58
37:E:197:THR:H	37:E:200:ASP:HB3	1.68	0.58
45:O:126:PHE:CE2	45:O:148:ILE:HD13	2.38	0.58
28:Ae:42:CYS:HA	28:Ae:45:PRO:HG3	1.84	0.58
2:t:108:LEU:HD23	52:Y:97:LEU:HD12	1.83	0.58
14:Ac:41:ASP:OD1	32:8:288:ARG:NH1	2.34	0.58
35:C:75:VAL:HG21	61:k:95:LEU:HD13	1.84	0.58
5:U:352:LYS:HD3	5:U:353:TRP:H	1.67	0.58
28:2:243:CYS:SG	69:2:301:FES:S2	3.01	0.58
30:6:309:LEU:HD21	30:6:338:ILE:HG22	1.84	0.58
32:8:118:TYR:HA	32:8:122:CYS:HB2	1.84	0.58
48:S:37:ARG:HD2	48:S:48:MET:HG2	1.84	0.58
62:l:249:SER:HB2	62:l:340:PHE:HD2	1.67	0.58
35:C:321:GLU:O	35:C:352:GLN:NE2	2.36	0.58
64:o:91:ALA:O	64:o:95:ILE:HG13	2.02	0.58
7:a:53:ARG:O	53:b:28:LEU:HB2	2.03	0.58
41:J:69:GLU:HA	41:J:72:ILE:HG22	1.84	0.58
65:r:185:TRP:NE1	65:r:238:THR:HG22	2.18	0.58
45:X:128:PHE:HZ	45:X:148:ILE:HG12	1.69	0.58
2:t:47:ASN:HD21	55:d:124:ASN:HD21	1.51	0.58
8:i:13:VAL:O	8:i:36:ASN:ND2	2.36	0.58
4:K:129:THR:HG23	39:H:186:ASN:HD21	1.68	0.58
17:Ah:46:GLY:N	17:Ah:49:ASP:OD2	2.36	0.58
42:L:203:GLY:H	42:L:206:ASP:HB2	1.68	0.58
33:y:60:VAL:HG11	12:z:11:MET:HG3	1.85	0.58
45:X:96:GLU:HG2	45:X:97:LYS:HD2	1.86	0.58
5:U:44:ALA:HB1	5:U:49:GLU:HG3	1.85	0.58
29:5:388:VAL:HG21	29:5:438:ALA:HA	1.85	0.58
37:E:188:ILE:HD13	37:E:208:LEU:HD11	1.85	0.58
40:I:79:MET:HE2	40:I:86:MET:HB3	1.86	0.58
62:l:313:MET:HE3	62:l:329:ILE:HG12	1.85	0.58
32:x:228:LEU:HD11	32:x:234:PHE:HB2	1.85	0.58
35:C:381:MET:HE2	35:C:385:ILE:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:x:153:VAL:HG21	32:x:177:PRO:HG2	1.86	0.58
4:K:113:HIS:CE1	39:H:196:LYS:HD3	2.39	0.58
21:Al:103:GLN:HE22	21:Al:159:VAL:HG11	1.68	0.58
14:1:14:LEU:HB3	14:1:24:THR:HG21	1.86	0.58
30:6:170:GLN:NE2	28:Ae:69:ASP:HB2	2.19	0.58
34:B:83:SER:HB2	34:B:262:PHE:HB3	1.85	0.58
43:M:33:LYS:O	43:M:36:GLN:NE2	2.36	0.58
58:g:87:LEU:HD23	66:s:235:LEU:HD21	1.86	0.58
31:w:5:ARG:NH1	31:w:20:ASP:OD2	2.34	0.58
35:C:437:HIS:HB2	35:C:462:ILE:HD11	1.86	0.57
45:X:104:PHE:HB3	45:X:110:LEU:HD11	1.86	0.57
25:Ap:81:PRO:O	25:Ap:87:ARG:NH1	2.34	0.57
29:5:315:ASP:OD1	29:5:316:SER:N	2.37	0.57
38:G:362:ASP:OD1	46:P:17:ARG:NH1	2.31	0.57
11:q:263:MET:HE2	64:o:101:TRP:HB3	1.85	0.57
23:An:152:PRO:HA	23:An:157:SER:HB2	1.85	0.57
66:s:188:VAL:HG13	66:s:194:TRP:HB2	1.87	0.57
67:R:80:GLU:OE1	67:R:80:GLU:N	2.37	0.57
7:a:186:THR:O	7:a:189:ASN:ND2	2.38	0.57
29:u:188:HIS:NE2	29:u:348:TYR:OH	2.30	0.57
4:K:88:ARG:HD2	39:H:200:GLU:HG3	1.87	0.57
11:q:11:LEU:HB3	11:q:100:ILE:HD13	1.87	0.57
31:7:338:ILE:HD13	31:7:351:GLY:HA2	1.86	0.57
58:g:2:THR:HG21	58:g:5:SER:HB3	1.87	0.57
28:Af:46:LEU:H	28:Af:66:PRO:HG3	1.70	0.57
20:Ak:378:HIS:CE1	68:Ak:601:HEA:NA	2.72	0.57
37:E:62:ARG:NH2	67:R:88:ASP:OD1	2.37	0.57
41:J:75:ARG:NH1	41:J:119:ASP:OD1	2.37	0.57
29:u:119:HIS:ND1	30:v:384:MET:HE1	2.19	0.57
28:Af:68:LEU:HG	28:Af:69:ASP:H	1.70	0.57
26:Aq:54:HIS:O	26:Aq:86:ARG:NH2	2.37	0.57
31:7:264:THR:HG22	31:7:268:ILE:HD11	1.87	0.57
49:T:152:PRO:HB3	49:T:159:GLN:HB2	1.87	0.57
62:l:359:MET:O	62:l:436:ARG:NH2	2.38	0.57
31:w:300:ILE:HD11	31:w:363:LEU:HD21	1.87	0.57
8:i:31:ILE:HD11	61:k:62:ILE:HG21	1.85	0.57
29:5:375:GLN:OE1	29:5:378:ARG:NH1	2.38	0.57
34:B:366:ALA:HA	37:E:141:MET:HE1	1.87	0.57
44:N:59:VAL:HG22	44:N:68:LEU:HD21	1.87	0.57
62:l:399:VAL:HG12	62:l:409:LEU:HD13	1.87	0.57
8:i:235:ASN:HB3	8:i:311:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:p:104:GLN:OE1	10:p:108:GLN:NE2	2.37	0.56
11:q:183:SER:O	55:d:153:ARG:NH2	2.37	0.56
21:Al:103:GLN:NE2	21:Al:159:VAL:HG11	2.20	0.56
21:Al:155:SER:HB2	21:Al:179:LEU:HD12	1.86	0.56
33:9:43:ASP:OD2	33:9:102:ARG:NH1	2.38	0.56
51:W:99:LYS:H	51:W:99:LYS:HD3	1.67	0.56
70:w:402:HEM:HBB2	70:w:402:HEM:HMB1	1.85	0.56
8:i:155:LEU:HD22	8:i:278:MET:HE2	1.87	0.56
11:q:306:PRO:HA	11:q:458:LEU:HD22	1.87	0.56
29:5:62:GLU:OE1	29:5:423:ARG:NH1	2.27	0.56
62:l:419:THR:HA	62:l:422:TYR:CE2	2.40	0.56
65:r:25:ARG:HH12	65:r:47:GLN:HE21	1.51	0.56
29:u:121:ASN:OD1	29:u:122:ALA:N	2.37	0.56
7:a:139:ILE:HG23	11:q:54:LEU:HD23	1.86	0.56
8:i:38:LEU:HD12	61:k:73:LEU:HD22	1.87	0.56
20:Ak:33:LEU:HB3	20:Ak:61:HIS:HB2	1.88	0.56
20:Ak:191:THR:HG23	20:Ak:245:ILE:HA	1.86	0.56
21:Al:145:PRO:HA	21:Al:214:VAL:O	2.06	0.56
22:Am:114:GLY:HA2	27:Ar:28:ARG:HH22	1.70	0.56
24:Ao:76:MET:O	24:Ao:80:VAL:HG13	2.05	0.56
35:C:207:PHE:HB3	40:I:82:PRO:HD3	1.86	0.56
44:N:38:ILE:O	44:N:45:ARG:NH1	2.38	0.56
62:l:257:VAL:HG21	62:l:313:MET:HE2	1.87	0.56
66:s:87:LEU:HA	66:s:90:LEU:HG	1.86	0.56
20:Ak:3:VAL:HG13	20:Ak:7:LEU:HD12	1.88	0.56
23:An:44:TYR:HE1	23:An:47:PRO:HA	1.70	0.56
28:4:243:CYS:HA	31:w:264:THR:HG21	1.86	0.56
32:8:125:CYS:SG	71:8:401:HEC:HBC2	2.45	0.56
56:e:116:GLU:OE1	56:e:116:GLU:N	2.38	0.56
30:v:53:GLU:OE1	30:v:127:ARG:NH2	2.36	0.56
15:Ad:46:PRO:O	15:Ad:49:ASN:ND2	2.38	0.56
19:Aj:51:ALA:O	19:Aj:55:ILE:HG12	2.05	0.56
28:4:240:HIS:HB2	28:4:275:ALA:HA	1.88	0.56
38:G:59:GLN:HE22	41:J:90:GLY:HA2	1.68	0.56
38:G:647:GLU:HB2	38:G:654:VAL:HG11	1.88	0.56
43:M:40:LYS:HB3	51:W:7:LYS:H	1.71	0.56
53:b:16:ARG:NE	45:X:150:ASP:OD2	2.38	0.56
29:5:310:ILE:HD11	29:5:388:VAL:HA	1.88	0.56
33:9:69:LEU:HD11	33:9:76:LEU:HD13	1.87	0.56
35:C:121:LEU:HB3	40:I:113:MET:HE2	1.88	0.56
51:W:144:THR:HB	65:r:96:ILE:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:145:GLU:HG2	29:u:249:HIS:CE1	2.41	0.56
22:Am:77:LYS:HD3	22:Am:80:ARG:HD3	1.88	0.56
24:Ao:98:CYS:SG	24:Ao:107:ALA:HB2	2.45	0.56
13:0:91:LYS:HD3	32:x:260:THR:HG23	1.88	0.56
35:C:312:GLN:OE1	36:D:140:ARG:NH1	2.38	0.56
51:W:95:ALA:HA	51:W:106:VAL:HG11	1.86	0.56
30:v:66:LYS:O	30:v:217:ARG:NH2	2.38	0.56
34:B:128:ARG:NH2	37:E:194:GLU:OE2	2.39	0.56
36:D:68:ILE:HG23	44:N:44:TYR:HB2	1.86	0.56
38:G:355:LYS:HA	38:G:366:LEU:HD22	1.87	0.56
62:l:372:ALA:HA	62:l:458:LEU:HD21	1.88	0.56
45:X:122:MET:HG2	45:X:144:ILE:HG21	1.87	0.56
8:i:26:TRP:CE2	8:i:86:ILE:HG13	2.40	0.56
23:An:67:LYS:HA	24:Ao:102:ASN:HD22	1.69	0.56
28:2:182:GLU:HG3	28:2:201:THR:HG22	1.87	0.56
34:B:56:ALA:HB1	34:B:61:ASP:HB2	1.87	0.56
58:g:122:ARG:C	64:o:109:ARG:HH12	2.14	0.56
8:i:1:MET:HE2	9:m:170:GLU:HG2	1.87	0.55
22:Am:62:ILE:HG12	22:Am:221:ARG:HH11	1.71	0.55
29:5:339:GLN:OE1	29:5:339:GLN:N	2.39	0.55
30:6:263:GLY:HA2	30:6:443:ASN:HB2	1.89	0.55
35:C:348:ARG:NH2	43:M:109:ASP:OD2	2.38	0.55
8:i:44:LEU:HD22	8:i:122:ILE:HG21	1.87	0.55
42:L:124:LEU:HD23	42:L:162:ILE:HG13	1.88	0.55
5:U:355:TRP:HE3	58:g:60:LEU:HD12	1.71	0.55
18:Ai:53:TRP:CE2	23:An:115:ALA:HB2	2.42	0.55
2:t:104:ARG:HD2	54:c:186:ILE:HD13	1.89	0.55
29:5:188:HIS:NE2	29:5:348:TYR:OH	2.33	0.55
34:B:424:ILE:HG22	38:G:76:ARG:CZ	2.37	0.55
37:E:188:ILE:HG22	37:E:189:ASN:H	1.71	0.55
54:c:115:ASN:HD21	62:l:162:THR:HB	1.72	0.55
30:6:216:ALA:HB3	30:6:244:LEU:H	1.71	0.55
34:B:211:ALA:HB2	34:B:223:PRO:HG3	1.87	0.55
35:C:389:LYS:HG3	38:G:144:MET:HG3	1.89	0.55
70:w:401:HEM:HBB2	70:w:401:HEM:HMB1	1.89	0.55
22:Am:16:TRP:NE1	22:Am:60:ASP:OD2	2.26	0.55
40:I:98:ARG:HA	40:I:125:PRO:HD3	1.87	0.55
55:d:79:GLU:HG2	58:g:109:LYS:O	2.07	0.55
62:l:306:THR:O	62:l:310:LEU:HG	2.07	0.55
8:i:193:VAL:HG23	8:i:201:THR:HG22	1.88	0.55
11:q:405:LEU:HD11	62:l:173:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B:355:ILE:HD13	37:E:139:PRO:HG3	1.87	0.55
47:Q:89:VAL:HG22	75:Q:201:ZMP:H7	1.88	0.55
62:l:303:ALA:O	62:l:306:THR:OG1	2.24	0.55
20:Ak:240:HIS:CD2	20:Ak:287:VAL:HG23	2.42	0.55
53:b:86:LEU:HA	53:b:90:VAL:HB	1.89	0.55
28:Af:45:PRO:HA	28:Af:66:PRO:HD3	1.87	0.55
8:i:95:MET:HE2	8:i:149:ILE:HA	1.89	0.55
27:Ar:29:ASN:OD1	27:Ar:33:ASN:ND2	2.40	0.55
38:G:226:CYS:SG	73:G:802:SF4:S1	3.04	0.55
42:L:342:LEU:HA	42:L:361:MET:HE1	1.88	0.55
29:u:102:LYS:HG2	29:u:153:ASN:HB3	1.87	0.55
30:v:295:ALA:HB1	28:Af:46:LEU:HD22	1.89	0.55
26:Aq:84:ASN:HB3	26:Aq:87:VAL:HG12	1.89	0.54
31:7:131:TYR:HA	70:7:401:HEM:HAA2	1.88	0.54
38:G:541:PRO:HB2	38:G:561:PRO:HD3	1.88	0.54
30:v:121:TYR:HB3	30:v:137:LEU:HD11	1.88	0.54
6:Z:69:TYR:HA	62:l:434:LYS:NZ	2.22	0.54
9:m:137:SER:HB3	9:m:140:ALA:HB3	1.90	0.54
11:q:43:ASN:HB2	56:e:109:LEU:HD22	1.88	0.54
20:Ak:510:TYR:HB3	25:Ap:89:VAL:HG22	1.88	0.54
25:Ap:94:GLU:H	25:Ap:97:ASN:HD21	1.54	0.54
31:7:115:ILE:HB	31:7:196:HIS:HD2	1.72	0.54
34:B:63:TYR:O	34:B:65:THR:N	2.35	0.54
34:B:220:GLN:HE21	37:E:114:GLU:HB3	1.72	0.54
45:O:119:ILE:HG21	45:O:135:ALA:HB1	1.89	0.54
62:l:249:SER:HB2	62:l:340:PHE:CD2	2.42	0.54
39:H:168:VAL:HG21	39:H:205:ILE:HD11	1.88	0.54
54:c:87:ASP:OD2	54:c:90:TYR:N	2.40	0.54
29:u:116:MET:HE1	29:u:142:LYS:HB3	1.88	0.54
30:v:297:PRO:HB3	28:Af:71:LYS:HG2	1.89	0.54
39:H:211:TYR:CZ	43:M:39:PRO:HG3	2.43	0.54
60:j:67:LEU:HD22	61:k:65:VAL:HA	1.89	0.54
65:r:230:ASN:HA	65:r:233:MET:HE3	1.88	0.54
28:Af:46:LEU:HG	28:Af:66:PRO:HB3	1.90	0.54
21:Al:13:THR:HB	21:Al:188:ARG:HH21	1.71	0.54
22:Am:151:LEU:HD22	22:Am:159:MET:HE3	1.89	0.54
28:2:142:THR:HG21	32:x:307:MET:SD	2.46	0.54
42:L:274:TYR:HB2	42:L:367:ALA:HB2	1.90	0.54
55:d:142:ARG:HD2	56:e:138:GLU:O	2.08	0.54
17:Ah:25:ARG:HH21	22:Am:224:LYS:HG2	1.72	0.54
21:Al:132:GLU:HB3	21:Al:137:GLU:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B:226:LYS:N	34:B:227:PRO:HD2	2.23	0.54
37:E:71:PRO:HA	67:R:100:GLN:HG2	1.89	0.54
62:l:184:LEU:HD21	62:l:211:MET:HG2	1.90	0.54
30:v:379:LYS:HG2	30:v:413:LEU:HD22	1.90	0.54
57:f:66:VAL:HG22	57:f:70:LYS:HE3	1.88	0.54
3:F:105:GLU:OE1	3:F:105:GLU:N	2.36	0.54
34:B:161:GLU:OE1	34:B:161:GLU:N	2.39	0.54
35:C:262:ASP:OD2	51:W:24:ASN:ND2	2.41	0.54
49:T:141:PRO:HG3	66:s:118:LYS:HD2	1.90	0.54
8:i:42:PRO:HG3	9:m:167:VAL:HG13	1.90	0.54
9:m:20:PHE:HZ	61:k:35:GLY:HA3	1.71	0.54
19:Aj:52:PRO:HG2	20:Ak:32:ALA:HB3	1.90	0.54
22:Am:128:GLU:HG3	22:Am:129:VAL:HG23	1.90	0.54
34:B:114:VAL:HB	34:B:242:VAL:HG22	1.90	0.54
36:D:186:ARG:NH2	36:D:193:PHE:O	2.40	0.54
40:I:82:PRO:HA	65:r:34:ARG:HG2	1.89	0.54
54:c:167:TYR:CG	54:c:178:PRO:HB3	2.42	0.54
65:r:61:LEU:H	65:r:216:ALA:HB3	1.73	0.54
28:Ae:43:ARG:HG3	28:Ae:44:PHE:H	1.72	0.54
20:Ak:28:MET:HE3	20:Ak:465:VAL:HG13	1.89	0.54
13:0:69:GLU:OE2	12:z:72:ARG:NE	2.39	0.54
29:u:304:LEU:HD13	29:u:354:LEU:HD22	1.89	0.54
30:v:131:GLU:O	30:v:135:GLU:HG2	2.08	0.54
10:p:104:GLN:O	10:p:108:GLN:HG2	2.07	0.53
11:q:208:PRO:HD3	11:q:236:LEU:HD22	1.88	0.53
11:q:325:MET:SD	11:q:441:ILE:HG12	2.48	0.53
22:Am:76:GLN:O	22:Am:80:ARG:HG3	2.09	0.53
28:4:238:CYS:HB3	28:4:245:PRO:HG3	1.90	0.53
62:l:97:THR:HG21	62:l:125:LEU:HD13	1.90	0.53
31:w:131:TYR:O	31:w:134:PRO:HD2	2.08	0.53
2:t:111:ARG:HA	2:t:114:ARG:HE	1.74	0.53
9:m:130:THR:HG21	51:W:124:LEU:HD12	1.91	0.53
20:Ak:486:GLU:OE1	20:Ak:486:GLU:N	2.35	0.53
28:2:230:GLU:HG2	28:2:231:TRP:CD1	2.43	0.53
35:C:212:GLU:O	35:C:216:MET:HG3	2.08	0.53
38:G:400:ILE:HD12	38:G:473:MET:HE3	1.90	0.53
53:b:79:VAL:HG23	62:l:10:THR:HG21	1.90	0.53
58:g:5:SER:HA	58:g:10:ARG:HH11	1.72	0.53
28:2:175:ILE:HB	28:2:292:VAL:HG13	1.90	0.53
34:B:204:TYR:HB3	34:B:377:GLU:HB3	1.90	0.53
35:C:172:ARG:NH1	35:C:241:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:D:181:HIS:HD2	36:D:183:ASP:H	1.56	0.53
5:U:309:TYR:HD1	5:U:312:ILE:HD11	1.74	0.53
28:4:201:THR:O	28:4:205:ILE:HG12	2.08	0.53
38:G:169:VAL:HG21	38:G:222:ILE:HD11	1.90	0.53
61:k:21:MET:HE3	62:l:589:LEU:HD21	1.91	0.53
62:l:289:ALA:HB1	62:l:418:LEU:HB2	1.90	0.53
42:L:238:VAL:HG12	42:L:242:LYS:HZ2	1.72	0.53
54:c:122:THR:OG1	54:c:124:VAL:O	2.27	0.53
62:l:130:ILE:O	62:l:134:ALA:HB2	2.08	0.53
31:w:138:MET:HE1	31:w:268:ILE:HA	1.90	0.53
8:i:341:PRO:HG3	66:s:247:TRP:CD1	2.44	0.53
9:m:173:ARG:HG3	9:m:175:ASN:H	1.73	0.53
11:q:400:MET:HE1	62:l:183:VAL:HG21	1.91	0.53
20:Ak:243:VAL:HB	68:Ak:602:HEA:HAC	1.89	0.53
28:4:198:ARG:HB3	28:4:232:VAL:HG13	1.90	0.53
29:5:120:LEU:HD13	29:5:133:ILE:HG12	1.89	0.53
39:H:79:ARG:HD2	43:M:20:LEU:HD13	1.91	0.53
54:c:85:GLU:OE2	64:o:13:THR:OG1	2.24	0.53
29:u:338:CYS:HB3	29:u:368:MET:HE3	1.89	0.53
32:x:322:TYR:HB2	33:y:61:PHE:CD1	2.43	0.53
35:C:90:PHE:HB2	35:C:105:MET:HE2	1.91	0.53
35:C:204:THR:OG1	65:r:275:ALA:O	2.27	0.53
39:H:208:ASP:OD2	39:H:212:ARG:NE	2.40	0.53
41:J:132:GLU:OE1	41:J:132:GLU:N	2.39	0.53
62:l:128:MET:HG2	62:l:251:THR:HG22	1.89	0.53
65:r:157:ASN:ND2	65:r:159:SER:O	2.42	0.53
28:Ae:40:VAL:HG22	28:Ae:42:CYS:H	1.74	0.53
5:U:110:LEU:HD13	5:U:336:LEU:HD11	1.90	0.53
20:Ak:243:VAL:HB	68:Ak:602:HEA:CAC	2.39	0.53
20:Ak:306:THR:HG22	20:Ak:310:MET:HE2	1.89	0.53
30:6:170:GLN:HG2	28:Ae:67:VAL:O	2.09	0.53
32:8:184:GLU:HG3	32:x:159:PRO:HB2	1.91	0.53
11:q:106:LEU:HD13	11:q:234:VAL:HG11	1.91	0.53
13:0:45:LYS:O	13:0:48:GLU:HG2	2.09	0.53
29:5:75:ILE:HG13	29:5:229:MET:HG2	1.90	0.53
29:5:190:THR:HB	29:5:275:ILE:HG13	1.89	0.53
29:5:351:THR:OG1	29:5:352:GLY:N	2.41	0.53
34:B:115:VAL:HG22	34:B:248:VAL:HG21	1.89	0.53
34:B:278:ILE:HG21	34:B:304:ALA:HB2	1.90	0.53
35:C:186:LEU:HB2	35:C:216:MET:HE1	1.91	0.53
42:L:59:PHE:HB3	74:L:401:NDP:O1N	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:X:94:ASP:HB2	45:X:97:LYS:HD3	1.90	0.53
28:Ae:46:LEU:HD13	28:Ae:68:LEU:HA	1.89	0.53
5:U:72:LYS:HE3	5:U:163:ARG:HG3	1.91	0.53
11:q:5:ILE:HG23	11:q:104:LEU:HD11	1.91	0.53
16:Ag:62:ASP:HA	16:Ag:65:LYS:HZ2	1.72	0.53
22:Am:151:LEU:HB2	22:Am:159:MET:HG3	1.90	0.53
27:Ar:40:CYS:O	27:Ar:44:MET:HG2	2.09	0.53
30:6:183:ARG:HD2	30:6:252:LYS:HE2	1.91	0.53
31:7:173:ALA:HB1	31:7:177:ARG:HH12	1.74	0.53
32:8:98:SER:O	32:8:104:SER:OG	2.24	0.53
36:D:154:GLU:OE2	36:D:180:ASN:ND2	2.42	0.53
42:L:298:ARG:HB2	42:L:311:ARG:HD2	1.90	0.53
62:l:559:GLU:O	62:l:563:PRO:HD2	2.08	0.53
31:w:81:TYR:OH	32:x:203:ARG:NH1	2.40	0.53
9:m:64:MET:HE1	61:k:31:LEU:HD22	1.90	0.52
20:Ak:405:LEU:HD22	20:Ak:471:ILE:HG22	1.89	0.52
20:Ak:463:THR:OG1	23:An:114:THR:OG1	2.25	0.52
34:B:50:ASP:O	34:B:59:ARG:NH2	2.34	0.52
34:B:159:ARG:HD3	34:B:161:GLU:HB2	1.91	0.52
34:B:314:LEU:HD11	34:B:317:VAL:HG23	1.90	0.52
45:O:105:MET:HE1	45:O:112:SER:HA	1.91	0.52
7:a:176:LYS:HD2	59:h:45:HIS:CD2	2.44	0.52
11:q:118:PHE:O	11:q:122:PHE:HB3	2.09	0.52
31:7:8:HIS:HB3	31:7:11:MET:HB2	1.89	0.52
35:C:184:THR:HG22	35:C:220:TYR:OH	2.08	0.52
39:H:209:TYR:HA	39:H:212:ARG:HD3	1.90	0.52
65:r:259:PHE:O	65:r:263:THR:HG23	2.10	0.52
30:v:375:LYS:NZ	30:v:419:VAL:O	2.41	0.52
67:R:106:GLN:HB2	67:R:110:HIS:CD2	2.43	0.52
9:m:161:LEU:HD13	60:j:68:GLU:HG3	1.91	0.52
27:Ar:59:ARG:HA	27:Ar:62:LYS:HE3	1.91	0.52
28:2:240:HIS:HB2	28:2:275:ALA:HA	1.91	0.52
31:7:36:LEU:HD22	31:7:235:MET:HE3	1.92	0.52
34:B:371:ILE:HD13	34:B:396:MET:HG3	1.92	0.52
37:E:143:ARG:HB3	37:E:184:PRO:HD3	1.91	0.52
38:G:64:CYS:HB3	38:G:75:CYS:HB3	1.92	0.52
60:j:66:ASP:O	60:j:69:ILE:HG13	2.10	0.52
62:l:145:GLU:OE1	62:l:176:ARG:NH1	2.43	0.52
65:r:205:SER:HB2	65:r:279:ARG:HH12	1.73	0.52
23:An:90:PHE:O	23:An:93:MET:HG2	2.10	0.52
28:4:230:GLU:HG2	28:4:231:TRP:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:9:12:LYS:HD3	33:9:12:LYS:H	1.74	0.52
36:D:68:ILE:HG21	36:D:99:PHE:CE1	2.43	0.52
63:n:4:VAL:O	63:n:7:ILE:HG13	2.09	0.52
2:t:96:VAL:HG22	52:Y:87:PRO:HG2	1.90	0.52
7:a:168:TRP:HB3	58:g:3:MET:HG2	1.91	0.52
8:i:96:THR:O	8:i:100:MET:HG2	2.08	0.52
23:An:90:PHE:HA	23:An:93:MET:SD	2.50	0.52
25:Ap:53:MET:O	25:Ap:57:LYS:HG2	2.08	0.52
38:G:176:CYS:SG	73:G:802:SF4:S3	3.07	0.52
29:u:451:ASP:O	29:u:472:ARG:NH2	2.43	0.52
45:X:138:LEU:HG	45:X:144:ILE:HG12	1.90	0.52
20:Ak:460:ILE:HG12	23:An:114:THR:HG21	1.91	0.52
24:Ao:55:ASP:HA	24:Ao:90:ILE:HD11	1.92	0.52
30:6:36:GLN:OE1	30:6:36:GLN:N	2.42	0.52
34:B:65:THR:O	34:B:69:LEU:HG	2.10	0.52
38:G:228:VAL:HG23	38:G:230:ALA:H	1.75	0.52
33:y:69:LEU:HD11	33:y:76:LEU:HD13	1.92	0.52
2:t:111:ARG:O	2:t:115:ARG:HG2	2.10	0.52
35:C:86:LEU:HD21	65:r:126:LYS:HD2	1.92	0.52
38:G:611:THR:OG1	41:J:105:GLU:HA	2.10	0.52
55:d:74:ILE:O	58:g:111:TYR:HB2	2.10	0.52
29:u:294:PRO:HG3	29:u:448:TYR:CZ	2.44	0.52
28:2:177:LEU:HB3	28:2:231:TRP:CZ2	2.44	0.52
59:h:17:TRP:HE3	61:k:55:LEU:HD13	1.74	0.52
31:w:5:ARG:NH1	31:w:15:ASN:OD1	2.43	0.52
2:t:92:HIS:O	2:t:96:VAL:HG23	2.09	0.52
5:U:352:LYS:HD3	5:U:353:TRP:N	2.24	0.52
22:Am:253:TYR:HA	22:Am:257:TYR:HD2	1.75	0.52
23:An:59:GLN:O	23:An:63:LYS:HG2	2.09	0.52
26:Aq:85:PRO:HB3	26:Aq:95:GLU:HG3	1.91	0.52
28:2:262:SER:HA	28:2:273:GLY:HA3	1.91	0.52
37:E:83:LEU:HD23	37:E:101:VAL:HG21	1.92	0.52
39:H:162:CYS:HB2	39:H:167:ILE:HG22	1.92	0.52
58:g:13:LEU:HD21	59:h:4:PHE:HB3	1.92	0.52
31:w:200:LEU:HD13	70:w:401:HEM:HAD2	1.92	0.52
6:Z:47:THR:O	6:Z:50:GLU:HG3	2.10	0.52
20:Ak:363:LEU:HD21	21:Al:24:HIS:HB2	1.92	0.52
29:5:311:ILE:HD12	29:5:375:GLN:HB3	1.92	0.52
35:C:46:ASP:OD1	35:C:47:VAL:N	2.33	0.52
46:P:18:GLU:HG3	46:P:68:ARG:HB3	1.92	0.52
56:e:91:PHE:HA	56:e:95:PHE:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:h:94:PRO:HG2	59:h:99:LEU:HD21	1.92	0.52
30:v:257:GLU:HA	30:v:438:MET:O	2.09	0.52
10:p:150:HIS:NE2	56:e:72:ASP:OD1	2.43	0.51
14:Ac:40:ALA:HB2	32:8:295:MET:HE1	1.93	0.51
38:G:304:GLN:HB2	38:G:316:TYR:HD1	1.74	0.51
38:G:371:VAL:N	38:G:482:GLN:OE1	2.42	0.51
55:d:107:GLN:OE1	62:l:194:ASN:ND2	2.43	0.51
30:v:323:VAL:HG23	30:v:340:THR:HG22	1.92	0.51
1:A:20:HIS:HB3	21:Al:44:LEU:HD11	1.91	0.51
4:K:131:ARG:NH2	39:H:133:GLU:OE1	2.43	0.51
6:Z:30:MET:HE1	52:Y:42:PRO:HG2	1.91	0.51
7:a:59:PRO:HG3	11:q:350:THR:O	2.10	0.51
7:a:130:GLU:HB2	63:n:58:LYS:HD2	1.93	0.51
29:5:318:TYR:HD2	29:5:324:MET:HE1	1.76	0.51
34:B:383:THR:HG21	38:G:120:LEU:HG	1.91	0.51
35:C:139:LEU:HD23	35:C:157:TYR:HD2	1.75	0.51
38:G:265:THR:HG22	38:G:270:VAL:HA	1.92	0.51
60:j:2:ASN:HB3	65:r:96:ILE:HD11	1.91	0.51
28:Af:48:PRO:HA	28:Af:65:SER:O	2.10	0.51
22:Am:204:HIS:NE2	22:Am:249:TRP:HB2	2.25	0.51
38:G:667:GLN:N	38:G:667:GLN:OE1	2.39	0.51
39:H:115:ALA:O	39:H:140:ARG:NH2	2.43	0.51
54:c:89:TRP:CE3	45:X:131:PRO:HG3	2.46	0.51
62:l:86:SER:HB3	62:l:133:THR:HG22	1.92	0.51
45:X:75:THR:O	45:X:79:ILE:HG12	2.10	0.51
14:1:11:TYR:HA	14:1:15:PHE:HB2	1.92	0.51
30:6:138:LEU:HD12	30:6:233:VAL:HG22	1.93	0.51
37:E:138:THR:HA	37:E:141:MET:HE2	1.92	0.51
38:G:182:CYS:SG	73:G:802:SF4:S1	3.08	0.51
39:H:196:LYS:HD2	39:H:197:TRP:NE1	2.25	0.51
42:L:169:ILE:HG23	42:L:170:LYS:HD3	1.92	0.51
50:V:51:GLU:OE1	50:V:51:GLU:N	2.39	0.51
65:r:63:PRO:HB2	65:r:66:SER:HB3	1.91	0.51
65:r:113:VAL:HG11	65:r:139:THR:HG21	1.91	0.51
31:w:137:GLN:NE2	31:w:263:ASN:O	2.43	0.51
20:Ak:287:VAL:HG21	20:Ak:312:ILE:HD11	1.92	0.51
27:Ar:85:LYS:HD3	27:Ar:85:LYS:H	1.73	0.51
13:0:51:GLU:O	13:0:55:GLN:HG2	2.11	0.51
30:6:90:THR:HG23	30:6:95:SER:HA	1.93	0.51
34:B:141:GLY:HA2	34:B:252:PRO:HD3	1.92	0.51
38:G:73:GLY:HA2	69:G:803:FES:S1	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:g:8:PRO:HG3	66:s:230:GLU:HG2	1.93	0.51
62:l:245:ALA:O	62:l:249:SER:HB3	2.11	0.51
1:A:14:ALA:O	1:A:18:ARG:HG3	2.10	0.51
8:i:61:LEU:O	8:i:65:THR:HG23	2.11	0.51
20:Ak:181:THR:O	20:Ak:270:TYR:OH	2.25	0.51
28:4:173:ILE:HG22	28:4:294:VAL:HB	1.92	0.51
38:G:176:CYS:SG	73:G:802:SF4:S1	3.08	0.51
40:I:85:ASP:OD2	65:r:34:ARG:HB3	2.11	0.51
47:Q:118:GLU:HB3	47:Q:124:LYS:HG3	1.93	0.51
30:v:317:VAL:HG21	30:v:350:VAL:HG22	1.91	0.51
28:Ae:46:LEU:HD13	28:Ae:68:LEU:HD23	1.92	0.51
9:m:168:ILE:HG13	61:k:76:SER:OG	2.09	0.51
21:Al:12:ALA:HB1	21:Al:17:MET:HB3	1.92	0.51
30:6:70:ARG:NH2	30:6:332:ASP:OD2	2.43	0.51
34:B:342:LEU:HD12	34:B:349:LEU:HA	1.91	0.51
51:W:88:ARG:NE	66:s:85:PRO:O	2.40	0.51
62:l:536:LEU:HB3	62:l:537:PRO:HD3	1.91	0.51
65:r:141:SER:HA	65:r:290:TRP:HE1	1.76	0.51
17:Ah:37:ASN:OD1	17:Ah:44:LYS:NZ	2.33	0.51
20:Ak:147:ILE:HG23	20:Ak:206:ILE:HB	1.93	0.51
20:Ak:239:GLY:O	20:Ak:242:GLU:HB3	2.11	0.51
26:Aq:62:TYR:HB2	26:Aq:65:LEU:HD12	1.93	0.51
28:2:265:ASP:OD1	28:2:269:ARG:N	2.43	0.51
29:5:113:VAL:HG13	29:5:118:ALA:HB3	1.92	0.51
29:5:276:ARG:NH2	29:5:466:PRO:O	2.44	0.51
9:m:1:MET:SD	9:m:1:MET:N	2.84	0.51
10:p:45:PHE:HE1	45:X:131:PRO:HG2	1.76	0.51
29:5:241:GLN:HA	29:5:244:ASP:OD2	2.11	0.51
34:B:263:ALA:HA	34:B:271:SER:HB2	1.93	0.51
36:D:213:ASP:OD1	42:L:70:ARG:NH2	2.44	0.51
65:r:26:LYS:HA	65:r:36:GLY:HA3	1.93	0.51
71:x:401:HEC:HBB3	71:x:401:HEC:HMB3	1.92	0.51
8:i:65:THR:OG1	8:i:104:MET:SD	2.68	0.51
8:i:231:SER:O	8:i:234:TRP:HD1	1.93	0.51
12:Aa:12:ARG:NH1	29:5:279:ASP:OD1	2.43	0.51
22:Am:101:PHE:HZ	22:Am:260:GLY:HA3	1.75	0.51
38:G:52:ALA:O	38:G:56:VAL:HG13	2.11	0.51
42:L:60:LEU:HA	42:L:237:ILE:HD11	1.93	0.51
45:O:143:GLU:HA	45:O:146:ASP:OD2	2.11	0.51
54:c:40:PRO:HA	64:o:79:ASN:HD21	1.74	0.51
58:g:19:GLU:OE1	58:g:19:GLU:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:g:122:ARG:HD2	64:o:116:ILE:HD13	1.92	0.51
31:w:45:ILE:HA	70:w:402:HEM:HMC2	1.93	0.51
23:An:44:TYR:CE1	23:An:47:PRO:HA	2.46	0.50
28:4:173:ILE:HB	28:4:190:TRP:CD1	2.46	0.50
30:6:327:ASN:H	28:Ae:66:PRO:HG3	1.76	0.50
34:B:192:ASP:HB3	67:R:98:MET:SD	2.51	0.50
35:C:368:LYS:HG2	35:C:386:HIS:CE1	2.47	0.50
62:l:162:THR:O	62:l:166:THR:HG23	2.12	0.50
62:l:566:THR:O	62:l:570:GLN:HG2	2.11	0.50
1:A:42:LYS:HA	1:A:45:LYS:HE2	1.92	0.50
5:U:82:LYS:HB2	5:U:272:VAL:HG21	1.93	0.50
8:i:342:ALA:O	8:i:344:SER:N	2.44	0.50
20:Ak:254:ILE:HG13	20:Ak:344:PHE:CD2	2.46	0.50
21:Al:133:MET:N	21:Al:133:MET:SD	2.85	0.50
27:Ar:58:ARG:HA	27:Ar:61:TYR:CD2	2.46	0.50
34:B:41:ILE:HG22	34:B:253:THR:HG21	1.93	0.50
32:x:305:TYR:O	32:x:309:ARG:HG2	2.11	0.50
24:Ao:110:ILE:O	24:Ao:114:VAL:HG13	2.11	0.50
25:Ap:105:VAL:HG12	25:Ap:122:LEU:HB2	1.92	0.50
30:6:312:ALA:HB2	30:6:357:GLN:HE21	1.76	0.50
34:B:381:GLN:O	38:G:74:ASN:HB2	2.10	0.50
38:G:586:GLY:O	38:G:616:ALA:HB1	2.11	0.50
49:T:127:ALA:HB2	65:r:312:ALA:HA	1.93	0.50
61:k:48:ILE:HG21	61:k:57:ASN:HA	1.93	0.50
28:Ae:45:PRO:HB3	28:Ae:66:PRO:HD3	1.94	0.50
10:p:167:TRP:NE1	53:b:25:ASP:OD2	2.34	0.50
11:q:94:LEU:O	11:q:98:MET:HG2	2.11	0.50
18:Ai:60:ILE:HG21	23:An:119:ILE:HG12	1.94	0.50
20:Ak:96:ARG:HG2	22:Am:57:TRP:HZ2	1.77	0.50
22:Am:22:LEU:O	22:Am:26:LEU:HG	2.11	0.50
30:6:148:ARG:NH2	33:y:50:ARG:O	2.45	0.50
36:D:219:VAL:HG21	40:I:115:PRO:HG3	1.93	0.50
39:H:91:GLY:N	40:I:171:GLU:OE2	2.29	0.50
4:K:95:ASP:OD1	43:M:35:THR:N	2.44	0.50
6:Z:67:TRP:CG	52:Y:45:ARG:HD3	2.45	0.50
31:7:173:ALA:HB1	31:7:177:ARG:NH1	2.27	0.50
34:B:220:GLN:NE2	38:G:197:THR:O	2.44	0.50
36:D:225:GLU:OE1	42:L:45:SER:OG	2.25	0.50
52:Y:50:LEU:HD21	62:l:364:LYS:O	2.12	0.50
56:e:65:ASN:OD1	56:e:68:GLU:N	2.45	0.50
62:l:484:LEU:HG	62:l:488:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:w:27:ILE:HA	31:w:208:PRO:HD3	1.94	0.50
10:p:150:HIS:CD2	10:p:151:PRO:HD2	2.47	0.50
10:p:212:ILE:O	10:p:215:ARG:NH1	2.44	0.50
20:Ak:307:SER:O	20:Ak:311:ILE:HG12	2.11	0.50
28:2:257:CYS:HB3	28:2:262:SER:HB2	1.92	0.50
32:8:232:LEU:HD13	32:8:242:ALA:HB1	1.94	0.50
34:B:165:GLU:OE1	34:B:165:GLU:N	2.44	0.50
35:C:285:THR:HA	44:N:12:VAL:HG23	1.93	0.50
54:c:81:ARG:NE	54:c:85:GLU:OE1	2.45	0.50
60:j:82:ASN:OD1	60:j:82:ASN:N	2.45	0.50
30:v:180:ALA:HB2	30:v:258:ILE:HG13	1.94	0.50
8:i:236:LYS:HG2	8:i:237:MET:HG3	1.94	0.50
16:Ag:26:TYR:HB2	20:Ak:484:ALA:HB3	1.94	0.50
18:Ai:32:ASP:O	18:Ai:36:LYS:HG2	2.10	0.50
28:4:252:PHE:HE2	28:4:272:LYS:HG2	1.76	0.50
29:5:279:ASP:HB3	29:5:282:LEU:HG	1.94	0.50
30:6:50:ALA:HB3	30:6:221:ILE:HG13	1.94	0.50
30:6:125:CYS:HB3	30:6:133:LEU:HD22	1.92	0.50
34:B:288:VAL:HG11	34:B:303:HIS:ND1	2.27	0.50
40:I:65:MET:HA	40:I:94:ARG:O	2.11	0.50
5:U:248:LEU:HD22	5:U:257:VAL:HG11	1.94	0.50
8:i:77:ASN:HB2	8:i:89:MET:HE2	1.93	0.50
14:Ac:10:LEU:HD22	14:Ac:14:LEU:HD11	1.94	0.50
19:Aj:38:LEU:HB2	20:Ak:473:TRP:NE1	2.25	0.50
20:Ak:94:PHE:HE1	22:Am:79:LEU:HD23	1.77	0.50
27:Ar:43:ALA:O	27:Ar:47:LYS:HG3	2.12	0.50
28:2:197:VAL:HG13	28:2:233:ILE:HG12	1.93	0.50
29:5:102:LYS:HB3	29:5:153:ASN:HB3	1.94	0.50
30:6:451:ASP:OD2	30:v:183:ARG:NH2	2.45	0.50
34:B:380:GLY:HA2	34:B:386:ARG:HB2	1.94	0.50
42:L:206:ASP:CG	42:L:208:PHE:H	2.20	0.50
45:O:140:CYS:O	45:O:144:ILE:HG13	2.12	0.50
65:r:218:GLY:O	65:r:222:MET:HG3	2.12	0.50
5:U:284:PRO:O	5:U:288:GLN:HG2	2.12	0.50
20:Ak:381:LEU:HB3	68:Ak:601:HEA:HAC	1.94	0.50
27:Ar:50:ASP:OD1	27:Ar:50:ASP:N	2.45	0.50
39:H:83:THR:HG21	65:r:35:LYS:H	1.76	0.50
30:v:129:ASP:N	30:v:129:ASP:OD1	2.45	0.50
32:x:229:ARG:HB3	32:x:232:LEU:HD12	1.93	0.50
7:a:101:ILE:HG12	55:d:64:TYR:HB3	1.94	0.49
13:Ab:44:ILE:HG12	13:Ab:47:ARG:HH21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:202:LYS:O	28:2:205:ILE:HG13	2.12	0.49
28:4:139:THR:O	28:4:142:THR:OG1	2.27	0.49
32:8:97:TRP:HD1	32:8:100:ARG:HH11	1.60	0.49
32:8:236:PRO:HA	32:8:241:GLN:HG3	1.93	0.49
34:B:205:ILE:HG12	34:B:379:CYS:SG	2.52	0.49
42:L:110:SER:O	42:L:114:VAL:HG12	2.11	0.49
54:c:169:GLU:OE1	54:c:169:GLU:N	2.42	0.49
62:l:342:CYS:HB2	62:l:373:LEU:HD23	1.94	0.49
8:i:228:LEU:HD22	35:C:54:GLY:HA3	1.94	0.49
28:2:220:GLN:OE1	28:2:278:ASN:ND2	2.39	0.49
28:2:260:HIS:HB2	69:2:301:FES:S1	2.51	0.49
30:6:339:TYR:HD1	28:Ae:68:LEU:HD12	1.77	0.49
30:6:451:ASP:N	30:6:451:ASP:OD1	2.44	0.49
34:B:67:GLU:N	34:B:67:GLU:OE1	2.45	0.49
38:G:50:LEU:HD11	38:G:62:ARG:HE	1.77	0.49
38:G:447:ASP:N	38:G:447:ASP:OD1	2.44	0.49
38:G:704:SER:HB3	38:G:707:MET:HG2	1.92	0.49
48:S:66:LEU:HA	48:S:69:ILE:HD12	1.94	0.49
62:l:246:LEU:HB3	62:l:247:LEU:HD12	1.94	0.49
65:r:196:ALA:HB3	65:r:274:ARG:HA	1.94	0.49
29:u:373:GLN:NE2	29:u:471:ILE:HG23	2.27	0.49
5:U:115:SER:HB3	5:U:118:LYS:HB3	1.94	0.49
11:q:427:LYS:HZ3	56:e:65:ASN:HB3	1.77	0.49
38:G:138:ASP:HB3	38:G:142:GLN:NE2	2.27	0.49
56:e:125:LEU:O	56:e:129:ARG:HG2	2.11	0.49
62:l:71:LEU:N	62:l:74:VAL:O	2.45	0.49
66:s:160:THR:HA	66:s:163:TRP:NE1	2.28	0.49
27:Ar:34:TYR:OH	27:Ar:74:ASP:OD1	2.24	0.49
31:7:5:ARG:NH1	31:7:20:ASP:OD2	2.46	0.49
31:7:26:ASN:HD21	31:7:207:ASN:HB2	1.78	0.49
34:B:132:ARG:HB2	34:B:165:GLU:HG3	1.95	0.49
52:Y:51:THR:O	52:Y:54:GLN:HG2	2.13	0.49
30:v:82:LEU:HD22	30:v:200:VAL:HB	1.93	0.49
8:i:30:TRP:O	8:i:34:GLU:HG2	2.12	0.49
10:p:206:PRO:HG3	53:b:14:GLN:OE1	2.13	0.49
11:q:23:ILE:HD11	11:q:92:LYS:HE2	1.94	0.49
35:C:190:ILE:HD11	35:C:257:PHE:CZ	2.47	0.49
40:I:133:MET:SD	40:I:173:LEU:HD22	2.53	0.49
62:l:8:THR:HB	62:l:82:MET:SD	2.53	0.49
65:r:96:ILE:HG22	65:r:98:MET:HG3	1.94	0.49
31:w:128:PHE:O	31:w:132:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:263:ARG:HD3	5:U:264:GLU:HG3	1.93	0.49
11:q:168:GLN:HB2	11:q:174:LEU:HG	1.94	0.49
11:q:231:LEU:HD23	11:q:235:LEU:HD12	1.95	0.49
20:Ak:124:THR:HG22	20:Ak:132:LEU:HG	1.93	0.49
21:Al:134:ARG:HG2	21:Al:135:LEU:HG	1.93	0.49
22:Am:112:LEU:HB3	22:Am:118:PRO:HB3	1.94	0.49
34:B:257:ARG:HG2	34:B:261:TRP:CD2	2.47	0.49
35:C:308:LEU:HB2	35:C:407:GLU:HB2	1.93	0.49
65:r:273:ILE:HG23	65:r:277:TYR:CD2	2.48	0.49
29:u:103:ASN:OD1	29:u:153:ASN:ND2	2.44	0.49
31:w:282:ARG:NH1	31:w:339:GLY:HA2	2.27	0.49
31:w:282:ARG:HH12	31:w:339:GLY:HA2	1.77	0.49
11:q:247:THR:HB	11:q:304:GLN:NE2	2.26	0.49
14:Ac:31:PHE:HA	15:Ad:48:ILE:HD11	1.94	0.49
14:l:29:ALA:HA	28:2:144:VAL:HG13	1.93	0.49
30:6:193:PRO:O	30:6:197:ILE:HG12	2.13	0.49
31:7:278:TYR:CE2	31:7:282:ARG:HD3	2.48	0.49
38:G:512:VAL:O	38:G:514:ASN:ND2	2.45	0.49
38:G:639:LEU:HD21	38:G:643:ARG:HH21	1.77	0.49
38:G:667:GLN:HE21	46:P:38:GLU:HA	1.77	0.49
46:P:32:GLY:HA3	46:P:82:PHE:O	2.13	0.49
49:T:123:TYR:HB2	65:r:310:MET:O	2.13	0.49
51:W:90:ASN:HA	51:W:93:GLU:HG2	1.94	0.49
52:Y:51:THR:HG22	52:Y:54:GLN:HE21	1.78	0.49
56:e:113:ARG:HD2	56:e:115:GLN:HE22	1.77	0.49
29:u:119:HIS:CD2	30:v:298:HIS:HA	2.47	0.49
11:q:275:ILE:O	11:q:279:GLN:HG2	2.12	0.49
20:Ak:509:THR:HG21	25:Ap:102:TRP:HZ3	1.78	0.49
21:Al:162:SER:HB3	21:Al:197:SER:HB2	1.95	0.49
28:2:161:MET:C	31:7:177:ARG:HH21	2.20	0.49
70:7:402:HEM:HBA1	70:7:402:HEM:HHA	1.95	0.49
36:D:203:PRO:HD3	41:J:124:LEU:HD12	1.95	0.49
37:E:66:ILE:HD13	37:E:81:PRO:HB2	1.95	0.49
56:e:60:ASP:OD1	56:e:60:ASP:N	2.43	0.49
62:l:7:LEU:O	62:l:11:THR:HG23	2.13	0.49
3:F:39:THR:HG22	3:F:62:VAL:HG22	1.95	0.49
9:m:73:ALA:HB3	9:m:74:MET:HE2	1.94	0.49
20:Ak:509:THR:HG21	25:Ap:102:TRP:CZ3	2.48	0.49
25:Ap:49:ARG:O	25:Ap:53:MET:HG2	2.13	0.49
29:5:61:SER:OG	29:5:239:HIS:ND1	2.41	0.49
30:6:177:LEU:HD11	30:6:272:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B:110:PRO:O	34:B:238:CYS:HB3	2.13	0.49
34:B:217:GLU:OE1	41:J:171:ARG:NH1	2.35	0.49
35:C:144:ARG:HH21	39:H:153:ILE:HB	1.78	0.49
35:C:382:GLU:OE1	35:C:382:GLU:N	2.41	0.49
49:T:142:LEU:HD21	49:T:151:VAL:HG11	1.95	0.49
30:v:299:VAL:HG23	30:v:302:GLY:HA3	1.94	0.49
17:Ah:39:LEU:HD11	62:l:510:TYR:HB3	1.95	0.49
28:2:116:GLU:OE1	28:2:116:GLU:N	2.39	0.49
28:2:263:HIS:O	28:2:270:ILE:HD12	2.13	0.49
30:6:183:ARG:NH2	30:v:451:ASP:OD1	2.45	0.49
32:8:118:TYR:CZ	32:8:128:MET:HG3	2.48	0.49
34:B:279:SER:HB3	37:E:181:VAL:HA	1.95	0.49
38:G:250:SER:OG	38:G:251:ILE:N	2.46	0.49
53:b:12:LEU:HB3	53:b:16:ARG:NH1	2.25	0.49
54:c:145:TRP:CE2	54:c:149:ILE:HD11	2.48	0.49
29:5:341:PHE:HB2	29:5:358:PHE:HB3	1.94	0.48
30:6:378:LEU:HD13	30:6:416:ILE:HD12	1.93	0.48
31:7:128:PHE:O	31:7:132:VAL:HG23	2.13	0.48
35:C:151:MET:HB2	35:C:184:THR:HG21	1.95	0.48
35:C:456:ILE:HG22	35:C:460:GLN:NE2	2.28	0.48
36:D:149:GLU:OE1	36:D:149:GLU:N	2.43	0.48
38:G:400:ILE:HG13	38:G:427:LEU:HD21	1.94	0.48
52:Y:40:ILE:HB	52:Y:49:GLN:HG3	1.94	0.48
65:r:138:GLN:HG3	65:r:285:LEU:HD21	1.95	0.48
1:A:57:MET:O	1:A:61:GLU:HG2	2.14	0.48
8:i:20:VAL:HG11	8:i:137:ALA:HB1	1.95	0.48
36:D:124:ASN:ND2	36:D:148:ASP:OD1	2.46	0.48
38:G:179:CYS:SG	73:G:802:SF4:S3	3.11	0.48
41:J:72:ILE:HD11	41:J:141:ASN:O	2.13	0.48
42:L:301:GLU:HG2	42:L:310:THR:HG23	1.95	0.48
51:W:116:TRP:HE3	66:s:131:ARG:HH11	1.59	0.48
60:j:79:SER:HA	60:j:87:MET:HE2	1.93	0.48
4:K:69:ASN:ND2	4:K:112:ASN:HD21	2.11	0.48
4:K:117:VAL:O	4:K:120:THR:OG1	2.26	0.48
8:i:261:MET:SD	8:i:340:THR:HG22	2.53	0.48
11:q:299:VAL:O	11:q:303:ILE:HG12	2.13	0.48
11:q:318:ALA:HB2	11:q:373:ILE:HG13	1.95	0.48
22:Am:197:PHE:HD2	22:Am:256:ILE:HG21	1.77	0.48
28:4:251:ASP:OD1	28:4:251:ASP:N	2.38	0.48
29:5:67:PRO:HB2	30:6:383:LEU:HD13	1.95	0.48
29:5:335:ARG:HB2	29:5:337:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:6:271:LEU:HD11	30:6:436:LYS:HB3	1.95	0.48
34:B:35:LEU:HB2	34:B:291:GLU:HG3	1.95	0.48
46:P:21:ILE:HD11	46:P:91:LEU:HD21	1.95	0.48
46:P:91:LEU:HA	46:P:94:VAL:HG12	1.95	0.48
11:q:82:SER:HB3	11:q:432:ARG:NH2	2.27	0.48
11:q:93:LYS:O	11:q:97:THR:HG23	2.14	0.48
22:Am:133:ASN:HB3	22:Am:173:PHE:CE2	2.48	0.48
27:Ar:47:LYS:HZ2	27:Ar:49:GLY:HA3	1.78	0.48
31:7:102:LEU:HD22	31:7:304:MET:HE2	1.94	0.48
34:B:384:PRO:HD2	38:G:76:ARG:HG3	1.95	0.48
38:G:257:VAL:HG11	38:G:413:LEU:HB2	1.95	0.48
48:S:23:THR:HA	65:r:5:ASN:HD21	1.78	0.48
53:b:110:ILE:HB	55:d:17:THR:HG23	1.95	0.48
62:l:102:GLU:HG2	62:l:449:LEU:HB3	1.95	0.48
63:n:30:ARG:O	63:n:33:GLU:HG2	2.13	0.48
65:r:75:PRO:HG2	65:r:219:PRO:HB3	1.96	0.48
30:v:300:LYS:HD2	30:v:301:ARG:HG2	1.95	0.48
31:w:272:TRP:HA	31:w:275:LEU:HG	1.95	0.48
9:m:20:PHE:CZ	61:k:35:GLY:HA3	2.47	0.48
21:Al:217:LYS:O	21:Al:220:GLU:HG2	2.13	0.48
29:5:328:LEU:HB2	29:5:375:GLN:HG3	1.95	0.48
34:B:49:HIS:HB2	34:B:59:ARG:HH21	1.79	0.48
35:C:368:LYS:HE2	35:C:386:HIS:HE1	1.79	0.48
35:C:410:LYS:NZ	35:C:461:ASP:OD1	2.46	0.48
41:J:61:ILE:HG22	41:J:64:LEU:HB2	1.95	0.48
65:r:113:VAL:CG1	65:r:139:THR:HG21	2.43	0.48
8:i:203:LEU:HD22	8:i:343:LEU:HD23	1.96	0.48
20:Ak:507:GLU:HA	22:Am:5:THR:HB	1.96	0.48
23:An:62:LEU:HD11	23:An:77:GLU:HB3	1.96	0.48
28:4:125:LYS:HD3	29:5:292:GLU:HG2	1.96	0.48
28:4:223:LEU:HD11	28:4:229:PRO:HG3	1.95	0.48
35:C:139:LEU:HB3	35:C:140:PRO:HD3	1.95	0.48
53:b:31:ARG:HG2	53:b:33:PRO:HD3	1.94	0.48
2:t:111:ARG:HH21	2:t:115:ARG:HH21	1.62	0.48
11:q:325:MET:HB2	11:q:440:HIS:HB3	1.96	0.48
28:4:270:ILE:HG22	28:4:278:ASN:OD1	2.14	0.48
38:G:357:LEU:O	38:G:361:VAL:HG23	2.13	0.48
38:G:696:MET:SD	38:G:702:ARG:HA	2.53	0.48
60:j:106:TRP:CE2	65:r:291:LYS:HD2	2.48	0.48
31:w:132:VAL:HG22	31:w:143:ALA:HB2	1.96	0.48
31:w:217:LYS:HG3	12:z:8:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:134:GLU:HB3	63:n:38:PHE:O	2.13	0.48
12:Aa:67:PHE:HE1	31:7:344:GLU:HG3	1.78	0.48
17:Ah:51:ILE:HD11	62:l:504:LEU:HG	1.96	0.48
28:2:109:PHE:O	28:2:113:ARG:HG3	2.14	0.48
35:C:178:VAL:HG23	35:C:317:TYR:CZ	2.48	0.48
42:L:206:ASP:OD1	42:L:207:ARG:N	2.47	0.48
42:L:267:LEU:HG	42:L:370:VAL:HG21	1.96	0.48
57:f:64:GLU:OE1	58:g:21:ARG:NH2	2.46	0.48
45:X:100:VAL:HG12	45:X:142:GLN:HB2	1.95	0.48
5:U:307:LEU:HD13	8:i:313:MET:HG2	1.96	0.48
9:m:7:PHE:HZ	9:m:104:VAL:HG13	1.78	0.48
20:Ak:507:GLU:OE2	25:Ap:83:ILE:N	2.45	0.48
68:Ak:601:HEA:HBD2	68:Ak:601:HEA:HHA	1.96	0.48
21:Al:223:SER:O	21:Al:227:LEU:HG	2.13	0.48
22:Am:126:PRO:O	22:Am:253:TYR:OH	2.26	0.48
29:5:136:LEU:HD21	30:6:380:ALA:HA	1.95	0.48
30:6:147:ARG:HD3	30:6:149:TRP:CZ2	2.49	0.48
37:E:84:ASP:O	37:E:88:ARG:HG3	2.13	0.48
42:L:288:LEU:HD12	42:L:289:PRO:HD2	1.95	0.48
2:t:107:ARG:NH1	52:Y:93:THR:O	2.46	0.48
8:i:112:HIS:HB2	8:i:184:ILE:HD13	1.95	0.48
18:Ai:52:VAL:O	18:Ai:56:THR:HG23	2.13	0.48
24:Ao:69:ALA:O	24:Ao:73:ARG:HG3	2.14	0.48
27:Ar:66:PRO:HG2	27:Ar:69:TRP:CG	2.49	0.48
34:B:62:TRP:CD2	34:B:181:LEU:HD13	2.48	0.48
48:S:68:ASN:HD22	66:s:96:LYS:HB3	1.79	0.48
56:e:115:GLN:OE1	56:e:115:GLN:N	2.45	0.48
8:i:115:VAL:HG12	8:i:180:ALA:HB1	1.96	0.47
68:Ak:602:HEA:H211	21:Al:34:ILE:HG21	1.94	0.47
25:Ap:113:CYS:SG	25:Ap:115:SER:OG	2.70	0.47
29:5:195:THR:HG21	29:5:269:ARG:H	1.79	0.47
34:B:145:GLY:O	34:B:149:MET:HG2	2.14	0.47
35:C:322:PHE:HA	35:C:348:ARG:HH11	1.79	0.47
38:G:295:ASP:OD2	38:G:705:GLN:N	2.46	0.47
40:I:62:LEU:O	40:I:91:VAL:HA	2.13	0.47
53:b:82:ILE:HD11	62:l:13:ILE:HD13	1.96	0.47
55:d:68:PHE:HB3	63:n:44:LEU:HD11	1.96	0.47
62:l:373:LEU:HG	62:l:431:PHE:HZ	1.78	0.47
29:u:407:THR:HB	29:u:408:PRO:HD3	1.96	0.47
30:v:371:VAL:HG12	30:v:375:LYS:HD2	1.95	0.47
30:v:421:ASP:OD1	30:v:421:ASP:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Ai:63:GLU:OE2	18:Ai:65:ASN:HB2	2.14	0.47
28:4:257:CYS:SG	28:4:259:CYS:HB3	2.54	0.47
34:B:326:LEU:HD23	34:B:367:ILE:HD11	1.96	0.47
34:B:380:GLY:O	34:B:386:ARG:HD3	2.13	0.47
35:C:140:PRO:O	35:C:144:ARG:HG2	2.14	0.47
36:D:199:ARG:C	36:D:201:ASP:H	2.22	0.47
39:H:135:ARG:CZ	39:H:141:ARG:HG3	2.44	0.47
49:T:151:VAL:O	66:s:207:LYS:NZ	2.45	0.47
61:k:25:HIS:ND1	61:k:88:ASP:OD1	2.37	0.47
31:w:183:PHE:CZ	70:w:402:HEM:HBC1	2.50	0.47
33:y:99:ILE:O	33:y:103:LYS:HG2	2.14	0.47
21:Al:152:MET:HE3	21:Al:152:MET:HB3	1.82	0.47
28:4:138:ILE:O	28:4:142:THR:HG23	2.14	0.47
30:6:452:GLU:OE2	30:v:183:ARG:NH1	2.47	0.47
34:B:288:VAL:HG11	34:B:303:HIS:CE1	2.50	0.47
35:C:167:ILE:HG23	35:C:364:VAL:HG21	1.96	0.47
36:D:113:ASP:OD1	36:D:131:ASN:ND2	2.47	0.47
40:I:184:ILE:HA	40:I:187:GLU:HG3	1.95	0.47
56:e:113:ARG:HB2	56:e:115:GLN:OE1	2.14	0.47
32:x:133:TYR:HB2	32:x:172:LEU:HA	1.97	0.47
4:K:113:HIS:HE1	39:H:196:LYS:HD3	1.78	0.47
9:m:17:PHE:HA	9:m:20:PHE:CE2	2.48	0.47
11:q:139:GLN:HB2	11:q:222:GLU:OE1	2.14	0.47
26:Aq:34:GLY:O	26:Aq:38:PRO:HG2	2.13	0.47
28:2:225:ARG:NH2	28:2:279:LEU:O	2.48	0.47
28:4:166:ASP:N	28:4:166:ASP:OD1	2.47	0.47
30:6:449:PHE:CZ	30:v:183:ARG:HB2	2.50	0.47
56:e:73:SER:O	56:e:74:HIS:HB2	2.14	0.47
66:s:97:VAL:HG13	66:s:101:VAL:HB	1.96	0.47
30:v:409:PRO:O	30:v:413:LEU:HG	2.14	0.47
9:m:165:VAL:HG21	60:j:101:SER:HB2	1.97	0.47
11:q:248:THR:HG22	55:d:149:HIS:CE1	2.49	0.47
20:Ak:96:ARG:NH1	20:Ak:97:MET:HB2	2.29	0.47
20:Ak:182:PRO:HB3	20:Ak:256:HIS:CE1	2.50	0.47
30:6:134:MET:SD	30:6:233:VAL:HG11	2.55	0.47
35:C:260:ARG:NH2	43:M:23:LYS:O	2.47	0.47
38:G:372:PHE:H	38:G:532:PRO:HB2	1.80	0.47
38:G:495:ASN:O	38:G:498:GLN:HG3	2.14	0.47
42:L:56:ALA:HB3	42:L:77:VAL:HG13	1.96	0.47
53:b:9:LYS:O	53:b:13:GLN:HG3	2.14	0.47
56:e:67:TYR:HA	56:e:70:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:v:360:THR:HG22	30:v:365:ASN:HB2	1.97	0.47
32:x:147:LYS:NZ	32:x:151:GLU:OE2	2.40	0.47
3:F:76:VAL:HG22	3:F:117:GLN:HB2	1.97	0.47
10:p:119:PRO:HB3	62:l:525:MET:HE2	1.96	0.47
20:Ak:240:HIS:NE2	20:Ak:290:HIS:HE1	2.12	0.47
20:Ak:320:VAL:O	20:Ak:324:LEU:HG	2.15	0.47
23:An:142:THR:HG23	23:An:156:PHE:HZ	1.79	0.47
35:C:53:PHE:HD1	35:C:58:MET:HE1	1.80	0.47
38:G:182:CYS:SG	73:G:802:SF4:S3	3.12	0.47
62:l:161:ARG:HH12	62:l:238:GLU:HG3	1.79	0.47
62:l:428:PHE:CD2	62:l:505:ASN:HB3	2.50	0.47
65:r:24:GLU:O	65:r:28:LEU:HG	2.15	0.47
65:r:134:ARG:HD3	65:r:200:LEU:HD22	1.96	0.47
29:u:362:ASN:HB3	29:u:461:PRO:HB2	1.97	0.47
7:a:184:LYS:HA	59:h:28:LYS:HB3	1.96	0.47
20:Ak:66:ILE:HG23	20:Ak:246:LEU:HD11	1.97	0.47
20:Ak:240:HIS:HD2	20:Ak:287:VAL:HG23	1.80	0.47
21:Al:100:MET:HE3	21:Al:157:GLU:HG2	1.97	0.47
23:An:70:TRP:CH2	24:Ao:99:ARG:HA	2.49	0.47
34:B:41:ILE:HG12	34:B:42:PHE:N	2.28	0.47
34:B:113:LEU:HB2	34:B:149:MET:HE3	1.97	0.47
34:B:381:GLN:NE2	73:B:502:SF4:S2	2.87	0.47
35:C:374:ARG:HG3	39:H:212:ARG:HB3	1.97	0.47
38:G:223:ILE:HG23	38:G:232:THR:HA	1.97	0.47
40:I:108:THR:OG1	40:I:136:CYS:SG	2.69	0.47
42:L:126:GLY:O	74:L:401:NDP:H52A	2.15	0.47
48:S:12:MET:HE3	65:r:264:LEU:HD22	1.96	0.47
53:b:55:ALA:HB3	53:b:56:PRO:HD3	1.97	0.47
55:d:127:LYS:HG3	55:d:128:GLU:N	2.30	0.47
56:e:122:ALA:O	56:e:126:VAL:HG12	2.15	0.47
60:j:73:LEU:O	60:j:76:PRO:HD2	2.15	0.47
61:k:4:VAL:O	61:k:8:ILE:HG12	2.14	0.47
65:r:169:GLN:HG2	65:r:174:MET:HG3	1.97	0.47
29:u:317:THR:HG21	28:Af:53:VAL:HG21	1.97	0.47
2:t:107:ARG:HB3	52:Y:97:LEU:HD13	1.96	0.47
6:Z:35:TYR:HB2	45:X:89:LEU:HD13	1.96	0.47
7:a:147:ALA:HB2	11:q:173:SER:HB2	1.97	0.47
14:Ac:19:SER:OG	29:5:480:PHE:O	2.27	0.47
21:Al:90:ILE:HD12	27:Ar:17:PHE:CZ	2.49	0.47
22:Am:137:LEU:HB3	22:Am:246:ASP:OD1	2.15	0.47
26:Aq:37:LEU:HB3	26:Aq:38:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:0:30:LEU:HB2	32:x:265:SER:OG	2.15	0.47
28:4:235:ILE:HG13	28:4:282:PRO:HD3	1.97	0.47
30:6:290:GLN:HG2	30:6:295:ALA:HB2	1.96	0.47
31:7:81:TYR:OH	32:8:203:ARG:NH1	2.48	0.47
34:B:116:ASN:O	34:B:245:VAL:HG23	2.15	0.47
37:E:130:TYR:HB2	37:E:169:PHE:CD1	2.50	0.47
38:G:434:SER:HB3	38:G:686:PRO:HD2	1.96	0.47
48:S:26:ILE:HG13	65:r:1:MET:HE3	1.97	0.47
58:g:110:THR:O	58:g:114:ILE:HG22	2.15	0.47
62:l:15:LEU:O	62:l:18:PRO:HD2	2.14	0.47
2:t:56:ARG:HH22	55:d:120:SER:HB3	1.79	0.47
9:m:17:PHE:HA	9:m:20:PHE:CD2	2.50	0.47
9:m:111:GLU:HG3	59:h:81:ARG:HH11	1.80	0.47
20:Ak:374:VAL:HA	20:Ak:377:PHE:CE2	2.50	0.47
22:Am:62:ILE:HG12	22:Am:221:ARG:NH1	2.29	0.47
29:5:42:LEU:HD22	29:5:426:LEU:HB3	1.97	0.47
29:5:282:LEU:HD12	29:5:460:GLY:HA2	1.97	0.47
35:C:329:ARG:HB2	35:C:331:ASP:OD1	2.15	0.47
38:G:140:GLN:HG3	73:G:801:SF4:S2	2.55	0.47
38:G:421:SER:HB3	38:G:427:LEU:HD22	1.96	0.47
38:G:478:SER:O	38:G:482:GLN:HG2	2.14	0.47
40:I:169:THR:HG22	40:I:171:GLU:H	1.80	0.47
51:W:96:ILE:O	51:W:99:LYS:HD2	2.15	0.47
30:v:65:ILE:HG12	30:v:218:MET:HG2	1.97	0.47
1:A:8:GLN:O	24:Ao:124:ILE:HD11	2.15	0.47
1:A:58:LYS:HE3	1:A:58:LYS:HB3	1.70	0.47
11:q:193:ILE:HA	11:q:253:LEU:HD21	1.97	0.47
11:q:250:LEU:O	11:q:254:THR:OG1	2.31	0.47
13:Ab:32:THR:O	13:Ab:36:GLN:HG2	2.14	0.47
68:Ak:601:HEA:HHC	68:Ak:601:HEA:H122	1.96	0.47
21:Al:100:MET:HA	21:Al:155:SER:O	2.15	0.47
24:Ao:91:ILE:O	24:Ao:95:LEU:HG	2.14	0.47
24:Ao:111:LEU:O	24:Ao:114:VAL:HG22	2.15	0.47
30:6:65:ILE:HG23	30:6:218:MET:HG3	1.97	0.47
34:B:126:LYS:HG2	34:B:277:ASN:HD21	1.80	0.47
35:C:344:ARG:HB3	51:W:21:TYR:O	2.15	0.47
38:G:619:ASP:O	38:G:623:ILE:HG12	2.15	0.47
51:W:108:GLU:HA	66:s:81:ILE:HD13	1.96	0.47
60:j:98:LEU:HD22	65:r:298:LEU:HD11	1.96	0.47
30:v:47:LEU:HD23	30:v:234:ALA:HB1	1.96	0.47
5:U:170:VAL:HG13	5:U:242:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:p:124:PHE:O	10:p:127:SER:OG	2.24	0.46
11:q:8:THR:O	11:q:11:LEU:HB2	2.15	0.46
11:q:263:MET:HA	11:q:263:MET:HE3	1.96	0.46
21:Al:43:SER:HA	21:Al:46:LEU:HG	1.97	0.46
21:Al:191:LEU:HB2	23:An:148:MET:HE2	1.97	0.46
23:An:83:ARG:NH2	23:An:92:GLU:OE2	2.47	0.46
13:0:79:ASP:HB3	32:x:93:PRO:HG2	1.97	0.46
28:2:200:ARG:HG2	28:2:205:ILE:HG23	1.97	0.46
31:7:81:TYR:O	31:7:85:ASN:ND2	2.40	0.46
32:8:243:ILE:HG12	32:8:245:MET:H	1.79	0.46
34:B:115:VAL:HG21	34:B:142:CYS:SG	2.56	0.46
34:B:120:GLY:HA3	34:B:204:TYR:HD1	1.80	0.46
35:C:99:GLY:HA3	40:I:68:GLY:O	2.16	0.46
35:C:224:SER:CB	35:C:230:ALA:HB1	2.45	0.46
35:C:448:HIS:HB3	35:C:452:ASP:HB2	1.97	0.46
37:E:186:VAL:HG22	37:E:196:LEU:HD11	1.95	0.46
38:G:76:ARG:NH2	38:G:90:ALA:HB2	2.31	0.46
38:G:422:TRP:HA	38:G:427:LEU:HB3	1.97	0.46
42:L:251:PRO:O	42:L:254:LYS:HD2	2.14	0.46
46:P:18:GLU:HG2	46:P:68:ARG:NH1	2.30	0.46
59:h:87:ILE:HD11	59:h:94:PRO:HD3	1.96	0.46
65:r:189:THR:HG22	65:r:234:MET:HE3	1.96	0.46
29:u:144:VAL:HG11	29:u:245:LEU:HB3	1.96	0.46
5:U:311:THR:HG22	8:i:310:ASN:HB2	1.96	0.46
8:i:14:MET:O	8:i:18:MET:HG2	2.15	0.46
9:m:20:PHE:HE1	61:k:32:CYS:HA	1.80	0.46
21:Al:163:TRP:HZ2	21:Al:211:LEU:HD21	1.80	0.46
28:4:200:ARG:HH12	28:4:226:VAL:HG11	1.79	0.46
35:C:309:ARG:HG3	35:C:407:GLU:HB3	1.96	0.46
38:G:389:THR:O	38:G:390:THR:OG1	2.25	0.46
38:G:592:LYS:HA	38:G:608:VAL:HG22	1.97	0.46
42:L:132:LYS:HG2	42:L:133:ASN:N	2.30	0.46
45:O:92:LYS:HE3	45:O:92:LYS:HB2	1.77	0.46
54:c:79:PRO:HB2	54:c:81:ARG:HG2	1.96	0.46
58:g:4:MET:HG2	58:g:84:MET:HE1	1.96	0.46
62:l:302:VAL:O	62:l:306:THR:HG23	2.14	0.46
62:l:482:MET:HE2	62:l:487:LYS:HD3	1.95	0.46
9:m:71:THR:HA	9:m:75:ALA:HB3	1.98	0.46
11:q:287:ALA:O	11:q:290:SER:OG	2.24	0.46
13:0:28:ASP:HB2	32:x:263:THR:HB	1.98	0.46
29:5:318:TYR:CE1	28:Ae:55:GLY:HA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:383:ALA:HB3	29:5:442:ARG:HG3	1.97	0.46
32:8:153:VAL:HG21	32:8:177:PRO:HG2	1.98	0.46
40:I:95:ALA:O	40:I:96:SER:OG	2.30	0.46
62:l:118:PHE:O	62:l:122:VAL:HG23	2.15	0.46
62:l:483:PRO:HG2	62:l:486:MET:HE3	1.95	0.46
65:r:234:MET:O	65:r:238:THR:HG23	2.14	0.46
29:u:383:ALA:HB3	29:u:442:ARG:HG3	1.97	0.46
30:v:70:ARG:O	30:v:185:ALA:HB1	2.15	0.46
30:v:135:GLU:OE2	30:v:236:ARG:NH2	2.48	0.46
8:i:20:VAL:HG13	8:i:29:ILE:HG23	1.98	0.46
8:i:193:VAL:HG21	8:i:266:ILE:HG12	1.96	0.46
16:Ag:44:SER:O	16:Ag:48:LEU:HG	2.16	0.46
21:Al:218:TYR:HA	21:Al:221:LYS:HG2	1.97	0.46
29:5:373:GLN:O	29:5:377:MET:HG2	2.16	0.46
34:B:102:MET:HG2	34:B:149:MET:HB2	1.96	0.46
34:B:199:ARG:NH1	37:E:84:ASP:OD2	2.48	0.46
38:G:405:THR:HB	38:G:477:GLY:HA3	1.97	0.46
38:G:647:GLU:O	38:G:651:PRO:HG3	2.16	0.46
46:P:40:ARG:NH1	46:P:88:THR:OG1	2.47	0.46
62:l:5:ALA:HB2	62:l:61:MET:SD	2.55	0.46
1:A:41:GLU:HA	1:A:44:LYS:HZ2	1.80	0.46
8:i:340:THR:N	8:i:341:PRO:HD2	2.31	0.46
21:Al:161:HIS:HB2	21:Al:174:ALA:HB3	1.96	0.46
23:An:65:LYS:HB3	23:An:73:LEU:HD21	1.97	0.46
71:8:401:HEC:HHD	71:8:401:HEC:HBC3	1.97	0.46
33:9:71:MET:HE3	33:9:72:ARG:HG3	1.98	0.46
34:B:284:HIS:HD2	34:B:305:GLY:HA3	1.81	0.46
34:B:396:MET:O	34:B:400:VAL:HG13	2.16	0.46
35:C:219:PHE:O	35:C:223:VAL:HG22	2.15	0.46
45:O:103:HIS:H	45:O:107:ASP:CG	2.22	0.46
53:b:105:PHE:O	53:b:107:GLY:N	2.45	0.46
54:c:70:MET:SD	64:o:86:THR:HG22	2.56	0.46
62:l:547:LYS:O	62:l:551:SER:OG	2.34	0.46
7:a:179:ILE:HG21	59:h:38:LYS:HG3	1.97	0.46
13:Ab:28:ASP:HB2	32:8:251:ASN:HD21	1.79	0.46
20:Ak:334:TRP:CZ2	21:Al:46:LEU:HB2	2.51	0.46
21:Al:10:GLN:NE2	21:Al:167:SER:OG	2.49	0.46
32:8:223:PRO:HD2	32:8:226:VAL:HG21	1.97	0.46
35:C:90:PHE:O	35:C:94:HIS:HB2	2.14	0.46
38:G:455:ILE:HD13	38:G:460:HIS:HB3	1.97	0.46
44:N:36:GLY:HA2	44:N:45:ARG:NH2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:l:280:LEU:O	62:l:283:ILE:HG22	2.16	0.46
7:a:131:LYS:HA	63:n:58:LYS:HA	1.96	0.46
9:m:41:CYS:O	9:m:45:LEU:HD23	2.15	0.46
9:m:137:SER:O	9:m:139:GLU:N	2.49	0.46
20:Ak:23:GLY:HA3	20:Ak:73:ILE:HG13	1.97	0.46
20:Ak:463:THR:HA	20:Ak:466:MET:HE2	1.97	0.46
35:C:417:LEU:HD11	35:C:425:PRO:HB3	1.97	0.46
37:E:93:LEU:HD12	37:E:122:TYR:HB3	1.98	0.46
43:M:31:ILE:H	43:M:31:ILE:HG13	1.55	0.46
43:M:109:ASP:OD1	43:M:109:ASP:N	2.36	0.46
44:N:19:THR:OG1	44:N:22:GLU:HB2	2.16	0.46
45:O:126:PHE:HE2	45:O:148:ILE:HD13	1.80	0.46
46:P:79:LEU:HD23	46:P:82:PHE:HD2	1.81	0.46
48:S:69:ILE:HD11	66:s:97:VAL:HG21	1.98	0.46
62:l:96:VAL:O	62:l:100:ILE:HG12	2.16	0.46
65:r:165:LEU:HD23	65:r:241:LEU:HA	1.97	0.46
1:A:41:GLU:OE2	1:A:44:LYS:NZ	2.38	0.46
11:q:416:ARG:HG2	62:l:159:HIS:HB3	1.96	0.46
13:Ab:28:ASP:OD1	32:8:263:THR:OG1	2.34	0.46
20:Ak:30:GLY:C	20:Ak:65:MET:HE2	2.40	0.46
20:Ak:104:LEU:HB2	20:Ak:156:SER:HB2	1.98	0.46
20:Ak:132:LEU:HA	21:Al:159:VAL:HG22	1.98	0.46
22:Am:154:GLY:HA2	25:Ap:37:VAL:HG22	1.96	0.46
38:G:217:GLU:OE2	38:G:409:PHE:HA	2.16	0.46
54:c:109:LEU:O	54:c:113:ILE:HG23	2.16	0.46
8:i:12:THR:HG21	9:m:163:ILE:HG21	1.97	0.46
27:Ar:21:PHE:CE1	27:Ar:28:ARG:HB3	2.51	0.46
28:4:269:ARG:HA	28:4:278:ASN:CG	2.40	0.46
29:5:465:LEU:HD12	29:5:466:PRO:HD2	1.97	0.46
30:6:83:LEU:HD11	30:6:209:VAL:HG22	1.98	0.46
34:B:79:GLU:OE2	34:B:259:GLY:N	2.42	0.46
35:C:111:MET:HE3	35:C:111:MET:HB3	1.89	0.46
37:E:73:GLY:HA2	67:R:106:GLN:O	2.15	0.46
38:G:671:LEU:HD13	38:G:671:LEU:HA	1.78	0.46
40:I:76:MET:HG2	40:I:93:PHE:HZ	1.81	0.46
55:d:69:ARG:NH2	63:n:46:LYS:O	2.49	0.46
32:x:168:ARG:HG2	32:x:170:GLY:H	1.80	0.46
1:A:12:LEU:H	1:A:12:LEU:HD12	1.81	0.46
10:p:59:LEU:HD11	45:X:112:SER:HB2	1.97	0.46
21:Al:188:ARG:HH12	23:An:153:ILE:HG13	1.81	0.46
23:An:137:TRP:HE1	23:An:141:GLN:HE21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Ap:108:GLY:O	25:Ap:121:LYS:NZ	2.47	0.46
28:2:111:ASP:OD1	28:2:111:ASP:N	2.41	0.46
29:5:284:LEU:HB3	29:5:359:VAL:HG12	1.98	0.46
30:6:111:SER:HB3	28:Ae:59:LEU:HG	1.97	0.46
30:6:257:GLU:HA	30:6:438:MET:O	2.16	0.46
34:B:71:LYS:NZ	37:E:248:GLY:O	2.49	0.46
35:C:300:ARG:NH2	35:C:407:GLU:OE2	2.45	0.46
36:D:128:ILE:HB	36:D:145:THR:HG23	1.98	0.46
38:G:618:GLU:O	38:G:622:ILE:HG13	2.16	0.46
43:M:42:PRO:HD3	51:W:6:VAL:HG13	1.97	0.46
54:c:83:GLN:NE2	54:c:97:LEU:O	2.45	0.46
56:e:91:PHE:O	56:e:95:PHE:HB2	2.15	0.46
62:l:415:ALA:O	62:l:419:THR:HG23	2.16	0.46
65:r:139:THR:HA	65:r:142:TYR:CE2	2.51	0.46
29:u:92:PHE:O	29:u:96:LEU:HG	2.16	0.46
4:K:14:VAL:HA	4:K:23:TYR:CD1	2.51	0.45
5:U:56:THR:O	5:U:59:SER:OG	2.33	0.45
5:U:62:ILE:HG12	5:U:205:VAL:HB	1.98	0.45
11:q:157:SER:O	11:q:160:LEU:HB3	2.16	0.45
11:q:203:PHE:HB2	11:q:243:MET:HG3	1.97	0.45
11:q:328:CYS:CB	11:q:437:MET:HE1	2.45	0.45
13:0:41:GLU:HA	13:0:44:ILE:HG22	1.97	0.45
15:3:14:ALA:O	15:3:18:ILE:HG12	2.16	0.45
58:g:89:ASP:OD1	66:s:243:ARG:NH2	2.42	0.45
65:r:264:LEU:O	65:r:268:ILE:HG12	2.16	0.45
30:v:190:LEU:HD13	28:Af:62:THR:HB	1.98	0.45
31:w:300:ILE:HD12	31:w:303:LEU:HD13	1.97	0.45
32:x:322:TYR:HB2	33:y:61:PHE:CG	2.51	0.45
3:F:113:TYR:O	39:H:141:ARG:NH2	2.44	0.45
4:K:5:GLN:HA	4:K:8:ARG:HB2	1.99	0.45
7:a:170:GLN:O	58:g:6:GLY:HA3	2.16	0.45
22:Am:79:LEU:HB3	22:Am:233:PHE:CE2	2.51	0.45
25:Ap:94:GLU:H	25:Ap:97:ASN:ND2	2.14	0.45
29:5:407:THR:HB	29:5:408:PRO:HD3	1.97	0.45
30:6:256:GLY:O	30:6:437:SER:HA	2.17	0.45
31:7:183:PHE:CE2	70:7:401:HEM:HBC1	2.50	0.45
35:C:210:PHE:HA	35:C:213:ARG:HB2	1.98	0.45
35:C:250:ILE:HG22	35:C:354:LEU:HD11	1.98	0.45
35:C:464:PHE:HA	35:C:467:VAL:HB	1.97	0.45
37:E:196:LEU:HD13	37:E:201:ILE:HG12	1.98	0.45
65:r:169:GLN:NE2	65:r:241:LEU:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:120:LEU:HD13	29:u:133:ILE:HG12	1.98	0.45
29:u:123:TYR:OH	29:u:411:GLU:OE1	2.26	0.45
30:v:58:ALA:HB1	30:v:124:GLU:OE2	2.16	0.45
31:w:307:LEU:HD11	31:w:363:LEU:HD23	1.98	0.45
32:x:132:ALA:HA	32:x:175:TYR:HA	1.98	0.45
32:x:168:ARG:HH11	32:x:171:LYS:HE3	1.82	0.45
7:a:80:ILE:O	7:a:84:ILE:HG12	2.16	0.45
28:4:173:ILE:HD12	28:4:190:TRP:HB2	1.97	0.45
35:C:150:MET:SD	35:C:150:MET:N	2.85	0.45
37:E:152:ILE:HG21	37:E:171:LEU:HD13	1.97	0.45
38:G:158:ARG:HG2	38:G:202:ASN:HD21	1.82	0.45
45:O:117:GLU:HA	45:O:120:MET:HE3	1.98	0.45
47:Q:51:MET:HE1	47:Q:105:VAL:HG21	1.97	0.45
64:o:42:ARG:O	64:o:46:GLU:HG2	2.17	0.45
66:s:85:PRO:HD3	66:s:131:ARG:HG2	1.98	0.45
29:u:148:ALA:O	29:u:152:GLN:HG3	2.16	0.45
30:v:222:GLY:HA3	30:v:230:LEU:HD21	1.98	0.45
18:Ai:77:TRP:HA	23:An:140:LYS:HD2	1.97	0.45
31:7:272:TRP:HA	31:7:275:LEU:HG	1.97	0.45
34:B:115:VAL:HG11	34:B:138:LEU:HD11	1.98	0.45
35:C:89:ASN:HB2	60:j:38:GLU:HG3	1.97	0.45
35:C:460:GLN:HB3	35:C:462:ILE:HD13	1.98	0.45
45:O:115:GLN:O	45:O:119:ILE:HG12	2.16	0.45
45:O:122:MET:HG2	45:O:144:ILE:HG21	1.99	0.45
56:e:56:GLN:NE2	56:e:57:GLU:HG2	2.31	0.45
56:e:119:ARG:NH2	62:l:75:GLU:OE2	2.49	0.45
62:l:100:ILE:HG21	62:l:246:LEU:HB2	1.98	0.45
66:s:181:GLN:OE1	66:s:196:ARG:NH1	2.50	0.45
29:u:74:TRP:CZ2	29:u:411:GLU:HA	2.52	0.45
30:v:89:LEU:HD22	30:v:150:GLU:HB3	1.99	0.45
28:Af:56:HIS:C	28:Af:58:ALA:H	2.25	0.45
2:t:100:LYS:HB3	54:c:186:ILE:HG13	1.98	0.45
8:i:141:VAL:O	8:i:145:ILE:HG13	2.16	0.45
10:p:221:MET:SD	10:p:221:MET:N	2.90	0.45
16:Ag:37:THR:O	16:Ag:41:ILE:HG13	2.16	0.45
21:Al:91:ASN:OD1	21:Al:91:ASN:N	2.49	0.45
28:4:107:PRO:HB2	32:8:319:LYS:HD2	1.99	0.45
31:7:45:ILE:HA	70:7:401:HEM:HMC2	1.98	0.45
32:8:132:ALA:HA	32:8:175:TYR:HA	1.98	0.45
35:C:137:GLN:O	35:C:140:PRO:HD2	2.17	0.45
38:G:49:VAL:HB	38:G:91:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:H:180:HIS:CE1	42:L:95:LEU:HD21	2.52	0.45
60:j:93:PHE:O	60:j:96:ILE:HG13	2.17	0.45
65:r:65:THR:O	65:r:124:ASN:ND2	2.43	0.45
30:v:333:SER:OG	30:v:334:GLY:N	2.49	0.45
2:t:4:HIS:NE2	54:c:153:TYR:O	2.49	0.45
9:m:70:TYR:OH	60:j:56:PHE:HB2	2.16	0.45
10:p:56:GLN:NE2	45:X:136:GLU:OE2	2.49	0.45
18:Ai:33:PHE:HA	18:Ai:36:LYS:HE2	1.98	0.45
20:Ak:509:THR:HG23	25:Ap:88:ILE:HG22	1.98	0.45
28:2:122:LYS:HE2	28:2:122:LYS:HB3	1.83	0.45
29:5:74:TRP:CZ2	29:5:411:GLU:HA	2.52	0.45
29:5:94:GLU:OE1	29:5:124:SER:OG	2.33	0.45
31:7:41:LEU:HD12	70:7:401:HEM:HBB1	1.99	0.45
35:C:190:ILE:HG21	35:C:213:ARG:HG3	1.99	0.45
36:D:101:ARG:NH1	36:D:159:VAL:O	2.50	0.45
37:E:174:VAL:HG21	37:E:177:LEU:HD21	1.99	0.45
54:c:161:TYR:HB3	54:c:166:LEU:HD12	1.99	0.45
62:l:152:PHE:CD1	62:l:168:ALA:HB1	2.51	0.45
29:u:302:VAL:HB	29:u:303:PRO:HD3	1.98	0.45
29:u:310:ILE:HD11	29:u:388:VAL:HA	1.99	0.45
29:u:470:ARG:HD3	31:w:222:PRO:HD3	1.98	0.45
32:x:157:ASP:OD1	32:x:168:ARG:NE	2.47	0.45
32:x:209:GLU:OE1	32:x:276:ARG:NE	2.35	0.45
28:Ae:72:ARG:O	28:Ae:72:ARG:HD3	2.15	0.45
8:i:106:LEU:HG	8:i:138:PRO:HB2	1.99	0.45
8:i:278:MET:HE3	8:i:278:MET:HB3	1.85	0.45
21:Al:27:THR:HG23	21:Al:76:ILE:HD12	1.98	0.45
22:Am:54:MET:HB3	22:Am:58:TRP:CZ3	2.52	0.45
29:5:316:SER:N	29:5:339:GLN:O	2.49	0.45
31:7:47:THR:HG23	31:7:79:ILE:HG23	1.99	0.45
33:9:29:LYS:HD3	33:9:75:ILE:HD13	1.98	0.45
42:L:212:PHE:HD1	42:L:215:MET:HE2	1.82	0.45
42:L:342:LEU:HD23	42:L:361:MET:HE1	1.98	0.45
46:P:65:LEU:HB3	46:P:77:VAL:HG22	1.98	0.45
47:Q:78:LEU:HD11	47:Q:129:ILE:HG21	1.99	0.45
60:j:38:GLU:HB3	60:j:41:PHE:O	2.17	0.45
2:t:61:HIS:O	2:t:65:GLN:HG2	2.17	0.45
2:t:103:GLU:HG3	52:Y:89:PRO:HB3	1.98	0.45
8:i:57:THR:HA	61:k:77:LEU:HD13	1.98	0.45
8:i:193:VAL:HG13	8:i:266:ILE:HG23	1.99	0.45
9:m:55:MET:SD	60:j:73:LEU:HD12	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:q:81:GLN:NE2	56:e:86:ASN:HD21	2.15	0.45
21:Al:128:LEU:HD11	21:Al:134:ARG:HA	1.99	0.45
22:Am:34:TRP:CD1	22:Am:40:MET:HG3	2.52	0.45
25:Ap:119:HIS:H	25:Ap:119:HIS:CD2	2.35	0.45
35:C:124:ARG:HG2	40:I:108:THR:HG21	1.98	0.45
36:D:75:GLN:HE21	43:M:68:ILE:HD12	1.82	0.45
43:M:94:ALA:HB3	44:N:51:ILE:HD11	1.99	0.45
45:O:121:ALA:HA	45:O:124:ASP:OD2	2.17	0.45
56:e:74:HIS:CE1	56:e:87:MET:HE2	2.52	0.45
65:r:267:THR:O	65:r:271:LEU:HG	2.16	0.45
66:s:187:CYS:O	66:s:191:LYS:HE2	2.17	0.45
29:u:140:LEU:HD22	29:u:237:VAL:HG12	1.99	0.45
29:u:192:PHE:O	29:u:198:ALA:HB2	2.16	0.45
31:w:207:ASN:ND2	31:w:211:ILE:O	2.47	0.45
7:a:130:GLU:O	7:a:134:GLU:HG2	2.16	0.45
27:Ar:9:ILE:HD13	27:Ar:55:GLU:HB3	1.98	0.45
29:5:206:GLU:O	29:5:210:LYS:HG2	2.17	0.45
29:5:467:ASP:OD2	29:5:470:ARG:HG2	2.17	0.45
35:C:352:GLN:O	35:C:356:LYS:HG2	2.16	0.45
30:v:151:VAL:O	30:v:155:GLN:HG3	2.17	0.45
31:w:145:VAL:O	31:w:149:LEU:HG	2.17	0.45
11:q:25:ILE:O	11:q:29:VAL:HG23	2.17	0.45
24:Ao:122:LYS:HD2	24:Ao:122:LYS:HA	1.75	0.45
25:Ap:68:LYS:HE2	25:Ap:68:LYS:HB3	1.79	0.45
28:2:285:GLU:OE2	28:2:287:THR:HG23	2.17	0.45
30:6:310:TYR:CE1	28:Ae:71:LYS:HD2	2.52	0.45
35:C:232:TYR:OH	35:C:240:GLN:O	2.27	0.45
36:D:83:GLU:OE1	36:D:142:ARG:NH2	2.30	0.45
48:S:4:GLU:O	48:S:7:PRO:HD2	2.17	0.45
49:T:128:ILE:HG12	60:j:84:LEU:HB2	1.99	0.45
54:c:86:ARG:NH2	54:c:103:GLU:OE2	2.42	0.45
62:l:241:THR:OG1	62:l:242:PRO:HD3	2.17	0.45
66:s:126:GLU:OE1	66:s:212:ARG:NH1	2.49	0.45
32:x:294:LEU:HD23	32:x:294:LEU:HA	1.87	0.45
20:Ak:12:HIS:CD2	20:Ak:91:ASP:HA	2.53	0.44
20:Ak:258:VAL:HA	20:Ak:338:MET:HE1	1.99	0.44
28:2:269:ARG:HA	28:2:278:ASN:CG	2.41	0.44
31:7:30:TRP:HB3	31:7:100:ARG:HG3	1.99	0.44
34:B:120:GLY:HA2	34:B:159:ARG:NH2	2.32	0.44
34:B:385:CYS:HB3	73:B:502:SF4:S3	2.56	0.44
42:L:127:ARG:HD2	42:L:129:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:j:38:GLU:HB2	60:j:43:PRO:HG3	1.98	0.44
31:w:107:TYR:OH	31:w:308:HIS:ND1	2.38	0.44
8:i:291:TYR:HA	11:q:151:PHE:HZ	1.81	0.44
9:m:28:TYR:HB3	9:m:83:TRP:CH2	2.53	0.44
11:q:369:LEU:HD12	11:q:370:PRO:HD2	1.98	0.44
14:Ac:36:PHE:CZ	32:8:296:MET:HG2	2.51	0.44
15:Ad:14:ALA:O	15:Ad:18:ILE:HG12	2.16	0.44
21:Al:153:LEU:HD11	27:Ar:64:LEU:HD23	1.98	0.44
28:2:240:HIS:HB3	69:2:301:FES:S1	2.57	0.44
29:5:85:LYS:C	29:5:207:ASN:HD21	2.26	0.44
70:7:402:HEM:HHa	70:7:402:HEM:HBD1	1.99	0.44
34:B:162:PHE:HB3	34:B:165:GLU:HB2	1.99	0.44
35:C:204:THR:HG22	35:C:208:TRP:CE2	2.52	0.44
36:D:152:PRO:HB3	36:D:177:PHE:HD2	1.83	0.44
38:G:522:GLN:O	38:G:526:LEU:HG	2.16	0.44
42:L:67:HIS:HA	42:L:70:ARG:HG2	1.99	0.44
53:b:69:ILE:HA	53:b:72:VAL:HG12	1.98	0.44
4:K:78:ASP:OD2	4:K:80:SER:OG	2.34	0.44
6:Z:52:LEU:HD12	6:Z:52:LEU:HA	1.88	0.44
8:i:61:LEU:HD11	61:k:26:LEU:HD11	1.99	0.44
8:i:250:SER:O	8:i:259:GLY:HA3	2.16	0.44
25:Ap:84:THR:OG1	25:Ap:85:ASN:N	2.47	0.44
13:0:90:LEU:HD23	13:0:90:LEU:HA	1.76	0.44
28:4:174:GLU:OE1	28:4:293:ILE:HG13	2.17	0.44
30:6:101:ARG:HB3	33:y:108:TRP:CZ2	2.53	0.44
32:8:168:ARG:HH12	32:8:171:LYS:HG2	1.82	0.44
36:D:200:LYS:O	41:J:126:LEU:HD21	2.17	0.44
38:G:218:LEU:HB3	38:G:221:ASN:ND2	2.32	0.44
38:G:667:GLN:NE2	46:P:38:GLU:HA	2.32	0.44
39:H:149:MET:HA	39:H:152:CYS:SG	2.58	0.44
47:Q:124:LYS:HB3	47:Q:128:HIS:HB2	1.99	0.44
53:b:61:ILE:O	53:b:65:TYR:HB3	2.17	0.44
62:l:65:ASN:HD21	62:l:80:PHE:HE1	1.66	0.44
62:l:97:THR:HG22	62:l:246:LEU:HD21	1.98	0.44
62:l:514:LYS:HG2	62:l:515:TYR:H	1.83	0.44
65:r:215:TYR:CD1	65:r:219:PRO:HB2	2.53	0.44
29:u:141:PRO:O	29:u:145:GLU:HG3	2.17	0.44
30:v:322:ASP:C	28:Af:68:LEU:HD21	2.42	0.44
30:v:415:GLN:O	30:v:419:VAL:HG23	2.17	0.44
7:a:67:PHE:CE2	11:q:434:ASN:HB3	2.53	0.44
8:i:89:MET:HB2	8:i:95:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:115:VAL:HB	8:i:116:PRO:HD3	1.99	0.44
8:i:344:SER:HA	8:i:347:ASN:HB2	1.99	0.44
9:m:23:LYS:NZ	61:k:21:MET:O	2.51	0.44
9:m:170:GLU:OE2	9:m:173:ARG:NH1	2.51	0.44
29:5:317:THR:HA	30:6:157:GLN:NE2	2.32	0.44
30:6:277:ALA:O	30:6:283:ALA:HB2	2.18	0.44
38:G:471:LYS:HG3	38:G:510:TRP:CD2	2.53	0.44
61:k:44:SER:O	61:k:48:ILE:HG12	2.16	0.44
65:r:60:PRO:HA	65:r:216:ALA:HB3	1.98	0.44
8:i:71:MET:HE3	8:i:74:ILE:HB	1.98	0.44
11:q:17:MET:HE1	58:g:56:VAL:HG21	1.99	0.44
11:q:274:SER:O	62:l:545:SER:OG	2.32	0.44
20:Ak:328:HIS:ND1	21:Al:45:MET:SD	2.84	0.44
20:Ak:333:LYS:HE2	20:Ak:333:LYS:HB2	1.64	0.44
21:Al:23:PHE:CZ	21:Al:80:SER:HB2	2.53	0.44
29:5:87:ASN:HD21	29:5:199:GLN:HB3	1.83	0.44
31:7:97:HIS:HE1	70:7:402:HEM:NA	2.15	0.44
34:B:287:THR:HB	37:E:225:CYS:SG	2.57	0.44
37:E:193:TYR:OH	37:E:214:PRO:HG2	2.18	0.44
37:E:203:GLU:O	37:E:207:GLU:HG3	2.18	0.44
37:E:212:LYS:HE3	37:E:212:LYS:HB2	1.82	0.44
40:I:161:ILE:HG13	40:I:180:LEU:HB2	2.00	0.44
42:L:140:PHE:O	42:L:182:GLY:HA3	2.17	0.44
45:O:108:LEU:HD13	45:O:108:LEU:HA	1.85	0.44
52:Y:43:ARG:HD2	52:Y:47:PHE:O	2.18	0.44
58:g:8:PRO:CG	66:s:230:GLU:HG2	2.47	0.44
31:w:280:ILE:O	31:w:283:SER:OG	2.35	0.44
1:A:71:SER:HB2	21:Al:222:TRP:CD1	2.53	0.44
8:i:341:PRO:HD3	66:s:247:TRP:CE2	2.53	0.44
10:p:63:LYS:HD3	45:X:132:ASP:OD1	2.17	0.44
11:q:216:LEU:HD22	11:q:291:VAL:HG23	1.99	0.44
16:Ag:38:GLU:HG2	19:Aj:35:TRP:CZ2	2.52	0.44
19:Aj:29:PHE:HB2	19:Aj:40:MET:HE1	1.98	0.44
20:Ak:362:SER:HB2	21:Al:20:LEU:HD21	2.00	0.44
22:Am:58:TRP:HD1	22:Am:61:ILE:HD12	1.82	0.44
34:B:296:LEU:HD21	34:B:317:VAL:HG11	1.98	0.44
38:G:224:ASP:OD1	38:G:291:ARG:NH1	2.47	0.44
38:G:252:ASP:OD1	38:G:259:SER:N	2.50	0.44
38:G:574:ASP:OD2	38:G:702:ARG:HD2	2.17	0.44
40:I:126:GLU:HG3	60:j:33:LYS:NZ	2.33	0.44
31:w:36:LEU:HD22	31:w:235:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:w:214:ASP:HB3	12:z:9:THR:HB	1.99	0.44
31:w:223:TYR:HB3	32:x:312:TRP:CE2	2.53	0.44
6:Z:48:VAL:HG13	10:p:81:TYR:HB2	2.00	0.44
8:i:340:THR:O	8:i:343:LEU:HB2	2.18	0.44
10:p:175:TRP:O	10:p:179:VAL:HG23	2.18	0.44
11:q:189:SER:OG	11:q:192:ASN:OD1	2.33	0.44
18:Ai:48:PHE:O	18:Ai:52:VAL:HG22	2.17	0.44
18:Ai:66:LEU:HA	21:Al:5:PHE:HE2	1.83	0.44
20:Ak:440:TYR:OH	21:Al:195:GLN:HB3	2.18	0.44
27:Ar:6:GLN:O	27:Ar:10:LYS:HG2	2.18	0.44
29:5:207:ASN:O	29:5:211:LEU:HG	2.18	0.44
30:6:313:VAL:HG21	30:6:323:VAL:HG11	2.00	0.44
33:9:99:ILE:HG12	33:9:102:ARG:HH12	1.83	0.44
42:L:206:ASP:OD2	42:L:208:PHE:HB3	2.17	0.44
48:S:13:ALA:HB2	65:r:264:LEU:HD11	1.99	0.44
55:d:68:PHE:HD2	63:n:44:LEU:HD21	1.82	0.44
64:o:25:ILE:HG21	64:o:30:ARG:CZ	2.48	0.44
30:v:123:VAL:HG13	30:v:137:LEU:HD13	1.99	0.44
30:v:233:VAL:HG23	30:v:236:ARG:NH2	2.32	0.44
30:v:264:ASP:OD1	30:v:265:SER:N	2.50	0.44
10:p:213:VAL:HG13	53:b:19:ARG:HA	1.98	0.44
11:q:370:PRO:HB2	62:l:142:ILE:HA	2.00	0.44
16:Ag:58:LEU:HA	16:Ag:61:LEU:HG	2.00	0.44
21:Al:73:LEU:HD13	21:Al:73:LEU:HA	1.77	0.44
13:0:75:LEU:O	13:0:79:ASP:HB2	2.17	0.44
28:2:104:ILE:HG22	32:x:323:ARG:HE	1.83	0.44
28:4:185:ASN:HD22	28:4:198:ARG:HB2	1.82	0.44
34:B:325:PRO:HG3	34:B:433:TRP:HB3	2.00	0.44
36:D:94:ILE:HD11	36:D:155:SER:O	2.17	0.44
36:D:152:PRO:HD3	47:Q:46:ILE:HG12	2.00	0.44
42:L:51:ALA:HA	42:L:120:VAL:O	2.17	0.44
42:L:122:ILE:HD11	42:L:248:ILE:HD11	2.00	0.44
42:L:172:PRO:HD2	42:L:319:MET:HE2	2.00	0.44
50:V:124:LEU:HA	50:V:127:MET:HE3	2.00	0.44
51:W:127:LEU:HD22	59:h:83:ARG:HE	1.83	0.44
54:c:40:PRO:HA	64:o:79:ASN:ND2	2.33	0.44
58:g:122:ARG:O	64:o:109:ARG:NH1	2.48	0.44
62:l:83:ASP:OD2	62:l:262:ARG:NH1	2.51	0.44
62:l:407:TRP:O	62:l:411:MET:HG2	2.18	0.44
29:u:350:GLU:OE1	29:u:350:GLU:N	2.44	0.44
31:w:207:ASN:HD22	31:w:213:SER:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:36:ASN:O	8:i:40:MET:HB2	2.18	0.44
8:i:154:MET:SD	8:i:191:THR:HB	2.58	0.44
9:m:23:LYS:HE2	61:k:22:TYR:HA	1.99	0.44
20:Ak:28:MET:N	20:Ak:28:MET:SD	2.90	0.44
20:Ak:334:TRP:O	20:Ak:411:LYS:NZ	2.39	0.44
22:Am:140:SER:HB2	22:Am:242:TRP:HE1	1.83	0.44
29:5:422:ARG:HH22	29:5:428:GLU:CD	2.25	0.44
30:6:195:TYR:CE2	30:6:196:ARG:HG2	2.53	0.44
35:C:229:HIS:NE2	40:I:71:CYS:SG	2.77	0.44
36:D:173:MET:O	36:D:196:HIS:HB3	2.18	0.44
37:E:177:LEU:HD13	37:E:187:GLN:HB2	1.99	0.44
40:I:61:SER:O	65:r:54:LYS:HD3	2.18	0.44
50:V:25:SER:HB3	50:V:67:GLY:O	2.18	0.44
58:g:33:LEU:HD12	58:g:33:LEU:HA	1.89	0.44
63:n:35:LEU:HD12	63:n:35:LEU:HA	1.84	0.44
65:r:228:TYR:HA	65:r:231:ILE:HD12	1.99	0.44
30:v:348:GLY:HA2	30:v:448:PRO:HD3	2.00	0.44
32:x:271:VAL:O	32:x:275:LEU:HG	2.17	0.44
8:i:79:LEU:HD12	61:k:47:ILE:HG12	2.00	0.43
10:p:122:TYR:OH	62:l:353:GLU:OE2	2.28	0.43
11:q:421:HIS:HB3	64:o:51:TYR:OH	2.18	0.43
29:5:350:GLU:OE1	29:5:350:GLU:N	2.50	0.43
31:7:280:ILE:O	31:7:283:SER:OG	2.31	0.43
35:C:115:CYS:SG	35:C:442:ASP:HA	2.58	0.43
35:C:128:LYS:HB2	36:D:198:PHE:CE1	2.53	0.43
37:E:182:ASN:HB3	37:E:194:GLU:HB3	2.00	0.43
42:L:233:GLN:HG3	42:L:264:ASN:O	2.18	0.43
48:S:69:ILE:O	66:s:152:LYS:NZ	2.45	0.43
54:c:125:SER:O	54:c:129:MET:HG3	2.18	0.43
61:k:94:ASN:O	61:k:94:ASN:ND2	2.45	0.43
45:X:89:LEU:HD12	45:X:89:LEU:HA	1.82	0.43
28:Af:46:LEU:N	28:Af:66:PRO:HG3	2.32	0.43
2:t:96:VAL:HG12	2:t:100:LYS:HD3	2.00	0.43
7:a:134:GLU:HG3	63:n:58:LYS:HB2	2.00	0.43
10:p:137:GLU:OE1	10:p:137:GLU:N	2.51	0.43
11:q:65:LEU:O	11:q:69:THR:HG23	2.18	0.43
34:B:28:LYS:HG2	34:B:29:LYS:H	1.83	0.43
35:C:72:TRP:CD1	35:C:72:TRP:H	2.36	0.43
35:C:204:THR:HG23	65:r:32:GLN:HG2	2.00	0.43
35:C:278:THR:O	35:C:333:TYR:HB2	2.18	0.43
38:G:217:GLU:OE1	38:G:408:ARG:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:G:241:ARG:HG2	38:G:243:TRP:CH2	2.54	0.43
62:l:280:LEU:O	62:l:284:THR:HG23	2.18	0.43
62:l:366:MET:HA	62:l:445:GLU:OE2	2.18	0.43
62:l:375:ILE:HD13	62:l:462:ILE:HD11	2.01	0.43
8:i:294:MET:SD	11:q:130:LEU:HD21	2.58	0.43
9:m:64:MET:HA	9:m:67:VAL:HB	2.00	0.43
12:Aa:22:PHE:O	28:4:131:ARG:HD2	2.18	0.43
29:5:338:CYS:HB3	29:5:368:MET:SD	2.59	0.43
35:C:204:THR:HB	35:C:205:PRO:HD3	1.98	0.43
35:C:224:SER:HB2	35:C:230:ALA:HB1	2.01	0.43
35:C:290:LEU:HD22	36:D:110:SER:HB3	2.00	0.43
38:G:39:GLN:HE22	38:G:56:VAL:HG12	1.83	0.43
38:G:575:VAL:O	38:G:578:PRO:HD2	2.18	0.43
47:Q:106:ASP:O	47:Q:110:ILE:HG12	2.18	0.43
52:Y:87:PRO:HB2	52:Y:92:TRP:HZ2	1.83	0.43
53:b:88:TYR:CE1	55:d:49:ARG:HG2	2.53	0.43
66:s:150:GLN:HG2	66:s:153:ARG:NH2	2.33	0.43
31:w:361:ILE:HG12	31:w:365:LEU:HD12	2.00	0.43
45:X:93:ILE:HD11	45:X:98:LEU:HD13	2.00	0.43
11:q:123:GLU:O	11:q:126:LEU:HB2	2.17	0.43
11:q:207:MET:HG2	11:q:236:LEU:O	2.19	0.43
20:Ak:349:THR:HG23	68:Ak:602:HEA:H272	1.99	0.43
20:Ak:452:THR:HG22	20:Ak:456:MET:HE3	1.99	0.43
21:Al:78:LEU:HB2	21:Al:79:PRO:HD3	2.00	0.43
30:6:266:LEU:HD22	28:Ae:72:ARG:HH21	1.84	0.43
35:C:388:PHE:CE2	39:H:118:LEU:HD11	2.53	0.43
36:D:226:LEU:HD21	40:I:145:TYR:CD1	2.54	0.43
42:L:330:LEU:HB3	42:L:335:ILE:HG23	2.00	0.43
49:T:131:ASN:O	49:T:134:THR:OG1	2.36	0.43
31:w:97:HIS:HE1	70:w:401:HEM:NA	2.15	0.43
31:w:138:MET:CE	31:w:268:ILE:HA	2.48	0.43
31:w:311:LYS:HG3	31:w:379:TRP:HB3	2.01	0.43
5:U:172:LEU:HD22	5:U:189:TYR:CD1	2.53	0.43
8:i:248:LEU:HD11	8:i:296:LEU:HD22	2.00	0.43
11:q:59:ASP:CG	11:q:245:ARG:HH22	2.25	0.43
12:Aa:20:SER:O	12:Aa:24:GLN:HG2	2.17	0.43
22:Am:118:PRO:HG2	22:Am:121:ILE:HG13	2.00	0.43
13:0:85:LYS:HA	13:0:85:LYS:HD3	1.90	0.43
28:4:217:ARG:NH1	28:4:275:ALA:O	2.51	0.43
30:6:191:TYR:CE1	28:Ae:62:THR:HG21	2.54	0.43
42:L:78:PRO:HB2	42:L:103:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:l:213:LEU:HB3	62:l:273:VAL:HG11	2.01	0.43
62:l:257:VAL:HG13	62:l:317:ILE:HD11	2.00	0.43
66:s:208:VAL:HG12	66:s:210:THR:HG23	2.00	0.43
5:U:102:ASP:HB3	57:f:29:PHE:CE1	2.53	0.43
15:Ad:34:TRP:CE2	28:4:151:LYS:HD2	2.54	0.43
25:Ap:78:ASN:HB2	25:Ap:120:TYR:CD1	2.53	0.43
15:3:15:ARG:HD3	15:3:15:ARG:N	2.34	0.43
34:B:88:ARG:HB2	34:B:244:ASN:HD22	1.82	0.43
34:B:208:GLU:OE1	34:B:210:THR:N	2.51	0.43
34:B:322:SER:O	34:B:434:PRO:HG3	2.18	0.43
38:G:466:LEU:HD13	38:G:500:ILE:HD11	2.00	0.43
40:I:64:PRO:HA	40:I:102:VAL:O	2.19	0.43
41:J:111:LEU:HD13	42:L:96:GLY:HA3	2.00	0.43
49:T:138:TYR:HB2	51:W:72:MET:HE3	2.00	0.43
62:l:124:PHE:CE1	62:l:252:MET:HB2	2.54	0.43
65:r:41:GLY:HA3	65:r:46:LEU:HD13	2.00	0.43
29:u:341:PHE:HB2	29:u:358:PHE:HB3	2.00	0.43
31:w:233:LEU:HD13	32:x:301:LEU:HD23	2.01	0.43
4:K:11:LEU:HD13	4:K:11:LEU:HA	1.89	0.43
6:Z:103:TYR:HD1	6:Z:104:LEU:HD22	1.84	0.43
7:a:132:ASN:HD22	11:q:45:LEU:HD12	1.84	0.43
11:q:282:LEU:HD21	11:q:410:MET:HG3	2.00	0.43
11:q:412:ILE:HG13	11:q:416:ARG:HD3	2.01	0.43
20:Ak:270:TYR:O	20:Ak:274:VAL:HG23	2.18	0.43
20:Ak:338:MET:O	20:Ak:342:LEU:HG	2.19	0.43
20:Ak:361:SER:O	20:Ak:365:ILE:HG12	2.19	0.43
20:Ak:424:THR:HG23	20:Ak:454:SER:O	2.19	0.43
21:Al:17:MET:HE1	21:Al:21:LEU:HD21	2.00	0.43
29:5:71:VAL:HG13	29:5:147:LEU:HD11	2.00	0.43
29:5:471:ILE:O	29:5:475:MET:HG2	2.19	0.43
30:6:391:GLY:HA2	30:6:394:ASP:OD2	2.19	0.43
31:7:207:ASN:ND2	31:7:211:ILE:O	2.49	0.43
31:7:237:LEU:HD13	32:8:297:MET:HG2	2.00	0.43
32:8:315:LEU:O	32:8:318:ARG:HG2	2.18	0.43
34:B:382:CYS:SG	34:B:424:ILE:HG23	2.58	0.43
38:G:387:LEU:HD12	38:G:514:ASN:HB3	2.01	0.43
42:L:53:VAL:O	42:L:78:PRO:HD2	2.19	0.43
59:h:85:LYS:O	59:h:89:GLU:HG2	2.19	0.43
62:l:61:MET:O	62:l:62:ILE:HD12	2.19	0.43
29:u:165:ARG:HD3	29:u:209:ARG:HA	2.01	0.43
29:u:467:ASP:OD1	29:u:468:TYR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:v:412:VAL:O	30:v:416:ILE:HG12	2.19	0.43
5:U:88:PHE:HB2	5:U:161:LEU:HD23	2.01	0.43
10:p:179:VAL:HG12	10:p:183:GLN:OE1	2.19	0.43
11:q:262:LEU:O	11:q:266:MET:HG3	2.19	0.43
11:q:325:MET:HE3	11:q:362:ALA:HB2	2.01	0.43
20:Ak:144:ASP:OD1	20:Ak:213:ARG:NH1	2.50	0.43
20:Ak:508:PRO:HG2	25:Ap:63:ASN:HB2	2.00	0.43
23:An:136:GLU:O	23:An:140:LYS:HG2	2.18	0.43
27:Ar:72:ALA:O	27:Ar:76:ARG:HD3	2.18	0.43
30:6:60:ARG:HG2	30:6:393:LEU:HD22	2.01	0.43
30:6:293:LEU:HB3	30:6:309:LEU:HD22	2.00	0.43
48:S:12:MET:HE2	65:r:23:VAL:HG21	1.99	0.43
50:V:61:PHE:HD2	50:V:104:ARG:NH1	2.15	0.43
53:b:76:LEU:HD23	53:b:76:LEU:HA	1.81	0.43
54:c:86:ARG:HH22	54:c:103:GLU:CD	2.24	0.43
54:c:145:TRP:CZ2	54:c:149:ILE:HD11	2.53	0.43
29:u:38:TYR:CE2	29:u:430:GLU:HG3	2.54	0.43
31:w:337:TRP:O	31:w:341:GLN:HG2	2.18	0.43
45:X:138:LEU:HD13	45:X:138:LEU:HA	1.84	0.43
5:U:257:VAL:HG12	5:U:259:GLN:HG3	2.01	0.43
8:i:222:SER:HB2	8:i:233:THR:HG21	2.01	0.43
11:q:33:LEU:O	11:q:37:ILE:HG12	2.17	0.43
11:q:122:PHE:CE1	11:q:206:LYS:HG3	2.54	0.43
11:q:237:LYS:HE2	11:q:316:MET:O	2.18	0.43
12:Aa:19:LEU:HD22	29:5:273:SER:HB3	2.00	0.43
12:Aa:21:PRO:HG3	32:8:314:VAL:HG23	2.01	0.43
20:Ak:262:SER:HA	20:Ak:332:ILE:HD13	2.00	0.43
23:An:45:PRO:O	23:An:47:PRO:HD3	2.19	0.43
25:Ap:49:ARG:HA	25:Ap:52:MET:HG2	1.99	0.43
29:5:41:ALA:O	29:5:45:VAL:HG23	2.19	0.43
29:5:289:ILE:HG21	29:5:369:MET:HE1	2.01	0.43
32:8:126:HIS:HE1	32:8:196:PRO:HD2	1.82	0.43
35:C:197:ALA:HB1	35:C:202:ALA:HB3	2.00	0.43
36:D:76:VAL:HG22	43:M:70:MET:HB3	2.01	0.43
40:I:63:TRP:HB2	40:I:101:ASP:OD1	2.18	0.43
44:N:58:MET:HE1	44:N:72:LEU:HA	2.01	0.43
53:b:72:VAL:HG23	53:b:76:LEU:HD12	2.01	0.43
54:c:140:MET:HE3	62:l:283:ILE:HD12	2.00	0.43
60:j:76:PRO:HD3	65:r:151:LEU:HD21	1.99	0.43
62:l:248:HIS:HA	62:l:253:VAL:HG13	2.01	0.43
65:r:198:PHE:CD2	65:r:285:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:278:ARG:NH2	12:z:9:THR:O	2.52	0.43
29:u:373:GLN:HE22	29:u:471:ILE:HG23	1.82	0.43
1:A:63:MET:HE2	23:An:149:LYS:HB2	2.01	0.43
9:m:61:LEU:HD12	9:m:61:LEU:HA	1.72	0.43
20:Ak:96:ARG:HG2	22:Am:57:TRP:CZ2	2.54	0.43
20:Ak:98:ASN:HB2	20:Ak:163:ASN:ND2	2.34	0.43
20:Ak:130:PRO:HD3	20:Ak:231:TYR:CD1	2.54	0.43
20:Ak:273:MET:O	20:Ak:277:MET:HG3	2.19	0.43
14:l:33:GLU:OE1	15:3:34:TRP:NE1	2.52	0.43
29:5:373:GLN:NE2	29:5:471:ILE:HG23	2.33	0.43
36:D:145:THR:OG1	36:D:146:TYR:N	2.52	0.43
38:G:371:VAL:H	38:G:482:GLN:CD	2.26	0.43
61:k:32:CYS:O	61:k:36:MET:HG3	2.18	0.43
62:l:315:VAL:O	62:l:319:ILE:HG12	2.19	0.43
29:u:303:PRO:HG3	29:u:436:VAL:HG22	2.01	0.43
30:v:82:LEU:HD13	30:v:158:LEU:HD11	2.00	0.43
28:Af:50:CYS:C	28:Af:52:GLY:H	2.27	0.43
6:Z:101:GLU:O	6:Z:105:GLU:HG2	2.19	0.42
11:q:408:LEU:HD12	62:l:172:ILE:HG21	2.00	0.42
30:6:357:GLN:O	30:6:360:THR:OG1	2.34	0.42
35:C:191:MET:O	35:C:195:THR:OG1	2.32	0.42
35:C:228:MET:SD	40:I:167:PRO:HG3	2.58	0.42
48:S:66:LEU:H	48:S:66:LEU:HD22	1.84	0.42
56:e:77:ASP:HB3	56:e:83:ASP:OD1	2.19	0.42
61:k:41:PHE:CE2	61:k:60:PRO:HB2	2.54	0.42
62:l:90:ILE:HG12	62:l:129:MET:CE	2.49	0.42
62:l:323:HIS:CE1	62:l:475:MET:HE3	2.54	0.42
65:r:204:GLU:N	65:r:207:LEU:O	2.52	0.42
29:u:180:ARG:O	29:u:183:VAL:HG12	2.19	0.42
4:K:87:HIS:HB3	39:H:200:GLU:OE1	2.19	0.42
8:i:30:TRP:CZ2	61:k:37:MET:HE1	2.54	0.42
9:m:10:SER:O	9:m:14:VAL:HG23	2.20	0.42
11:q:216:LEU:HD23	11:q:287:ALA:HB1	2.01	0.42
20:Ak:242:GLU:HA	20:Ak:245:ILE:HD12	2.01	0.42
29:5:328:LEU:HD11	29:5:368:MET:HE2	2.01	0.42
31:7:296:ALA:O	31:7:300:ILE:HB	2.17	0.42
33:9:12:LYS:HD3	33:9:12:LYS:N	2.34	0.42
35:C:368:LYS:HE2	35:C:386:HIS:CE1	2.55	0.42
42:L:231:VAL:HG22	42:L:267:LEU:HD23	2.01	0.42
52:Y:78:ASP:HA	52:Y:82:GLY:H	1.84	0.42
65:r:185:TRP:O	65:r:189:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:r:186:PHE:O	65:r:189:THR:OG1	2.28	0.42
29:u:83:ASN:OD1	29:u:85:LYS:HG2	2.19	0.42
31:w:338:ILE:HD13	31:w:351:GLY:HA2	2.01	0.42
4:K:69:ASN:HD21	4:K:112:ASN:HD21	1.68	0.42
8:i:60:PHE:HE1	61:k:70:GLU:HG3	1.84	0.42
11:q:306:PRO:O	11:q:310:MET:HG3	2.19	0.42
21:Al:163:TRP:CZ2	21:Al:211:LEU:HD21	2.54	0.42
29:5:317:THR:HB	28:Ae:53:VAL:HG21	2.01	0.42
30:6:115:THR:HG23	30:6:118:SER:H	1.84	0.42
32:8:172:LEU:H	32:8:172:LEU:HD12	1.84	0.42
34:B:113:LEU:O	34:B:154:ALA:HA	2.19	0.42
36:D:69:LEU:O	36:D:73:VAL:HG22	2.20	0.42
47:Q:65:TRP:O	47:Q:69:VAL:HG23	2.19	0.42
47:Q:69:VAL:HG11	47:Q:86:ARG:HG3	2.00	0.42
49:T:160:GLY:HA3	66:s:204:LYS:HE3	2.02	0.42
53:b:74:HIS:O	62:l:14:ILE:HG13	2.19	0.42
59:h:21:GLN:NE2	61:k:51:THR:O	2.52	0.42
33:y:53:GLU:OE2	12:z:12:ARG:HD3	2.19	0.42
2:t:111:ARG:HH11	52:Y:97:LEU:HG	1.84	0.42
8:i:26:TRP:CD2	8:i:86:ILE:HG13	2.54	0.42
8:i:261:MET:O	8:i:265:MET:HG2	2.19	0.42
9:m:74:MET:SD	61:k:79:VAL:HG23	2.59	0.42
15:Ad:3:SER:HA	15:Ad:6:LEU:HD23	2.02	0.42
20:Ak:209:LEU:O	20:Ak:213:ARG:HG3	2.19	0.42
22:Am:69:GLY:HA3	25:Ap:45:THR:O	2.18	0.42
27:Ar:79:GLU:HG3	27:Ar:81:THR:HG23	2.02	0.42
13:O:90:LEU:HD11	32:x:265:SER:HB3	2.00	0.42
28:2:173:ILE:HG23	28:2:190:TRP:HD1	1.85	0.42
34:B:208:GLU:HG3	34:B:425:CYS:SG	2.58	0.42
38:G:382:ARG:HA	38:G:385:TYR:CE2	2.55	0.42
39:H:103:LEU:O	39:H:194:GLY:HA3	2.20	0.42
44:N:19:THR:OG1	44:N:19:THR:O	2.33	0.42
46:P:65:LEU:O	46:P:76:ASN:HA	2.19	0.42
48:S:59:ARG:HG2	48:S:61:HIS:CE1	2.55	0.42
51:W:43:LEU:HG	65:r:179:TRP:HE1	1.83	0.42
62:l:60:GLU:HG2	62:l:83:ASP:HA	2.01	0.42
62:l:315:VAL:HG11	62:l:412:THR:HG21	2.01	0.42
29:u:304:LEU:HD23	29:u:304:LEU:HA	1.82	0.42
30:v:232:GLN:HE22	30:v:236:ARG:NH1	2.17	0.42
30:v:338:ILE:HG21	30:v:354:ALA:HB1	2.01	0.42
2:t:99:MET:HE1	52:Y:87:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Ai:41:ILE:HG22	23:An:105:GLY:HA3	2.01	0.42
21:Al:62:GLU:HA	21:Al:65:TRP:NE1	2.33	0.42
21:Al:171:LYS:HE2	21:Al:171:LYS:HB2	1.84	0.42
22:Am:185:PRO:O	26:Aq:88:ASN:ND2	2.53	0.42
24:Ao:133:ARG:NE	24:Ao:137:ASN:OD1	2.47	0.42
25:Ap:53:MET:HA	25:Ap:56:ARG:HH11	1.84	0.42
28:4:257:CYS:HB3	69:4:301:FES:S2	2.59	0.42
30:6:356:ASP:O	30:6:360:THR:HG23	2.19	0.42
31:7:223:TYR:HB3	32:8:312:TRP:CZ2	2.54	0.42
32:8:198:LEU:HA	32:8:201:ILE:HB	2.01	0.42
34:B:398:ARG:HH22	34:B:408:GLU:CD	2.27	0.42
35:C:227:ARG:HH11	40:I:169:THR:HG23	1.84	0.42
42:L:283:PHE:CE2	42:L:285:PRO:HG3	2.54	0.42
55:d:78:GLU:HA	58:g:110:THR:HA	2.00	0.42
58:g:33:LEU:HG	58:g:71:VAL:HG13	2.00	0.42
60:j:38:GLU:OE2	65:r:126:LYS:NZ	2.53	0.42
62:l:233:LEU:HB3	62:l:234:PRO:HD3	2.01	0.42
62:l:562:LEU:HB3	62:l:563:PRO:CD	2.47	0.42
65:r:238:THR:OG1	65:r:266:LEU:HD13	2.18	0.42
66:s:239:LYS:HB3	66:s:239:LYS:HE3	1.84	0.42
31:w:282:ARG:HE	31:w:343:VAL:HG22	1.85	0.42
32:x:218:GLY:O	32:x:236:PRO:HD2	2.19	0.42
5:U:312:ILE:HG22	5:U:314:VAL:HG23	2.01	0.42
11:q:12:LEU:HD23	11:q:97:THR:HG22	2.01	0.42
11:q:282:LEU:HD23	11:q:282:LEU:HA	1.89	0.42
11:q:329:LEU:HG	11:q:437:MET:HE2	2.02	0.42
17:Ah:67:SER:O	17:Ah:71:LEU:HG	2.19	0.42
20:Ak:417:MET:O	20:Ak:421:VAL:HG22	2.20	0.42
21:Al:100:MET:HB2	21:Al:107:SER:OG	2.19	0.42
22:Am:141:GLY:O	22:Am:144:ILE:HG22	2.19	0.42
26:Aq:60:ILE:HB	26:Aq:62:TYR:CE2	2.55	0.42
38:G:386:LEU:HD23	38:G:386:LEU:HA	1.90	0.42
39:H:83:THR:HG21	65:r:35:LYS:N	2.35	0.42
42:L:78:PRO:HB2	42:L:103:TRP:CG	2.55	0.42
44:N:26:ILE:O	44:N:30:LYS:HG3	2.19	0.42
44:N:89:SER:OG	44:N:93:LYS:NZ	2.51	0.42
47:Q:130:MET:HE3	47:Q:135:GLU:OE2	2.19	0.42
47:Q:140:ARG:HD3	47:Q:141:PRO:O	2.19	0.42
54:c:80:ASP:OD1	54:c:80:ASP:N	2.53	0.42
56:e:125:LEU:HD23	56:e:129:ARG:HH12	1.84	0.42
62:l:12:LEU:HD22	62:l:129:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:o:5:LYS:HA	64:o:5:LYS:HD3	1.88	0.42
29:u:99:LYS:HB3	29:u:160:GLN:HG2	2.01	0.42
30:v:195:TYR:CE2	30:v:196:ARG:HG2	2.54	0.42
33:y:103:LYS:HA	33:y:103:LYS:HD2	1.72	0.42
3:F:74:GLN:HG3	3:F:75:PRO:HD2	2.02	0.42
4:K:39:VAL:HG21	4:K:89:TRP:CZ2	2.55	0.42
4:K:65:THR:O	4:K:73:THR:OG1	2.32	0.42
8:i:168:GLY:O	8:i:172:GLN:HG2	2.20	0.42
11:q:61:LEU:HD22	11:q:241:TYR:HD1	1.84	0.42
20:Ak:132:LEU:HA	21:Al:159:VAL:CG2	2.49	0.42
20:Ak:405:LEU:HD23	20:Ak:475:ALA:HB2	2.01	0.42
21:Al:136:LEU:HD22	21:Al:193:TYR:HB3	2.01	0.42
21:Al:188:ARG:NH1	23:An:152:PRO:HG2	2.34	0.42
13:0:32:THR:O	13:0:36:GLN:HG2	2.20	0.42
30:6:365:ASN:OD1	30:6:365:ASN:N	2.51	0.42
30:6:421:ASP:N	30:6:421:ASP:OD1	2.52	0.42
34:B:64:LYS:HB3	34:B:67:GLU:OE1	2.20	0.42
34:B:117:ALA:HB3	34:B:158:ILE:HA	2.02	0.42
38:G:221:ASN:ND2	38:G:285:TRP:HB3	2.35	0.42
38:G:375:ALA:HB1	38:G:675:VAL:HG11	2.01	0.42
38:G:711:VAL:HA	38:G:714:VAL:HG12	2.01	0.42
39:H:162:CYS:HA	73:H:302:SF4:S2	2.59	0.42
42:L:236:TYR:CE2	42:L:343:LYS:HE2	2.55	0.42
47:Q:147:LYS:HA	47:Q:150:VAL:HG12	2.02	0.42
51:W:88:ARG:O	51:W:92:GLU:HG2	2.19	0.42
60:j:106:TRP:CZ2	65:r:291:LYS:HD2	2.55	0.42
33:y:76:LEU:HD12	33:y:76:LEU:HA	1.95	0.42
1:A:71:SER:OG	21:Al:222:TRP:HB2	2.19	0.42
7:a:146:LYS:O	7:a:150:ARG:HG3	2.19	0.42
8:i:31:ILE:HG23	61:k:66:PHE:CZ	2.55	0.42
8:i:192:ALA:HB1	8:i:270:MET:HE1	2.00	0.42
10:p:67:ARG:HA	10:p:67:ARG:HD3	1.91	0.42
11:q:231:LEU:O	11:q:236:LEU:HG	2.19	0.42
20:Ak:195:LEU:HD22	20:Ak:199:LEU:HD11	2.02	0.42
20:Ak:294:THR:HG22	20:Ak:365:ILE:HD13	2.02	0.42
21:Al:41:ILE:O	21:Al:45:MET:HG2	2.20	0.42
21:Al:91:ASN:ND2	21:Al:183:THR:OG1	2.53	0.42
21:Al:104:TRP:CD1	21:Al:203:ASN:HB2	2.55	0.42
22:Am:137:LEU:HA	22:Am:137:LEU:HD23	1.70	0.42
30:6:125:CYS:SG	30:6:133:LEU:HD22	2.60	0.42
30:6:170:GLN:HG3	30:6:339:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:6:289:LEU:HB2	30:6:424:VAL:HG13	2.02	0.42
30:6:290:GLN:NE2	28:Ae:44:PHE:O	2.48	0.42
38:G:566:ILE:HB	38:G:580:ALA:HA	2.01	0.42
40:I:193:TRP:O	40:I:196:ARG:HG2	2.20	0.42
41:J:121:LEU:HD23	41:J:124:LEU:HD13	2.01	0.42
47:Q:140:ARG:HG2	47:Q:141:PRO:HD2	2.02	0.42
55:d:106:ILE:HG13	55:d:135:VAL:HG21	2.01	0.42
56:e:92:PHE:O	56:e:96:SER:HB2	2.19	0.42
62:l:264:TYR:CD2	62:l:265:PRO:HD3	2.54	0.42
65:r:288:LEU:O	65:r:292:SER:OG	2.33	0.42
4:K:78:ASP:HB2	40:I:175:TYR:HE1	1.85	0.42
11:q:11:LEU:HA	11:q:14:MET:HE3	2.00	0.42
16:Ag:27:ALA:HB2	20:Ak:404:THR:HG21	2.00	0.42
20:Ak:195:LEU:HD23	20:Ak:245:ILE:HD13	2.01	0.42
28:2:142:THR:HB	32:x:303:LEU:HB3	2.02	0.42
15:3:23:MET:O	15:3:27:VAL:HG23	2.20	0.42
72:B:501:FMN:HM81	72:B:501:FMN:HM73	1.80	0.42
38:G:643:ARG:NH1	38:G:656:TYR:OH	2.52	0.42
43:M:43:VAL:HB	43:M:47:HIS:CG	2.55	0.42
48:S:67:GLU:HG2	48:S:68:ASN:N	2.35	0.42
49:T:167:LYS:HE3	49:T:167:LYS:HB2	1.89	0.42
51:W:53:TRP:NE1	65:r:167:THR:O	2.46	0.42
58:g:96:VAL:HG23	58:g:103:PHE:CB	2.50	0.42
65:r:199:ASP:O	65:r:201:THR:N	2.51	0.42
29:u:38:TYR:CZ	29:u:42:LEU:HD11	2.55	0.42
1:A:54:TYR:OH	1:A:59:ASP:OD2	2.38	0.42
9:m:8:ILE:O	9:m:11:THR:OG1	2.31	0.42
12:Aa:19:LEU:HD22	12:Aa:19:LEU:HA	1.86	0.42
15:Ad:18:ILE:HD13	15:Ad:18:ILE:HA	1.83	0.42
20:Ak:240:HIS:O	20:Ak:243:VAL:HG22	2.20	0.42
20:Ak:382:SER:O	20:Ak:386:VAL:HB	2.20	0.42
21:Al:103:GLN:N	21:Al:158:ASP:OD2	2.53	0.42
25:Ap:113:CYS:N	25:Ap:117:GLY:O	2.53	0.42
29:5:192:PHE:HB3	29:5:195:THR:OG1	2.20	0.42
34:B:58:SER:O	37:E:240:GLY:HA2	2.20	0.42
34:B:422:HIS:O	38:G:76:ARG:HD3	2.19	0.42
39:H:76:TYR:CE2	65:r:33:LEU:HG	2.54	0.42
42:L:352:ARG:HD3	42:L:356:TRP:O	2.19	0.42
51:W:97:ILE:HG23	59:h:86:LEU:HD13	2.02	0.42
28:Ae:45:PRO:HA	28:Ae:66:PRO:HB3	2.01	0.42
28:Af:53:VAL:HG22	28:Af:54:VAL:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:58:ARG:HH21	39:H:85:ASN:HB2	1.84	0.41
8:i:37:LEU:O	8:i:41:ILE:HG12	2.19	0.41
20:Ak:334:TRP:HH2	21:Al:46:LEU:HD22	1.85	0.41
22:Am:177:GLN:HE22	22:Am:201:THR:HB	1.85	0.41
26:Aq:66:ARG:HB3	26:Aq:91:PRO:HG3	2.01	0.41
29:5:157:GLU:O	29:5:161:ILE:HG13	2.20	0.41
29:5:307:ALA:HB1	29:5:379:LEU:HD13	2.01	0.41
29:5:412:ASP:OD2	29:5:423:ARG:NE	2.53	0.41
32:8:136:LEU:H	32:8:136:LEU:HG	1.74	0.41
33:9:108:TRP:CZ2	30:v:101:ARG:HB3	2.55	0.41
34:B:397:ALA:O	34:B:400:VAL:HG22	2.20	0.41
36:D:103:HIS:CE1	36:D:105:ASN:HA	2.55	0.41
39:H:184:LEU:HD23	41:J:112:MET:HG3	2.02	0.41
49:T:138:TYR:CZ	66:s:121:MET:HG3	2.54	0.41
51:W:99:LYS:NZ	59:h:86:LEU:HD21	2.35	0.41
54:c:115:ASN:C	54:c:116:ARG:HG2	2.44	0.41
55:d:115:GLN:CD	62:l:62:ILE:HD13	2.45	0.41
59:h:61:ASP:HA	59:h:64:VAL:HG12	2.02	0.41
62:l:250:SER:HB2	62:l:333:ALA:HA	2.01	0.41
62:l:362:LEU:HA	62:l:365:ALA:HB3	2.02	0.41
62:l:381:THR:HG21	62:l:498:PHE:CZ	2.55	0.41
65:r:55:LEU:HB3	65:r:217:ALA:O	2.20	0.41
30:v:310:TYR:OH	28:Af:75:LEU:HD11	2.20	0.41
5:U:329:VAL:HG12	8:i:315:TRP:HZ3	1.85	0.41
10:p:159:ASP:OD1	53:b:31:ARG:NH2	2.53	0.41
20:Ak:266:GLU:OE2	20:Ak:270:TYR:HB2	2.20	0.41
24:Ao:79:LEU:HD21	24:Ao:86:PRO:HB3	2.01	0.41
15:3:46:PRO:O	15:3:49:ASN:ND2	2.53	0.41
34:B:214:GLU:CD	34:B:224:ARG:HE	2.28	0.41
35:C:98:HIS:HB2	35:C:464:PHE:CE2	2.55	0.41
42:L:33:HIS:HE2	42:L:117:HIS:HD2	1.66	0.41
47:Q:57:ARG:O	47:Q:60:GLU:HG2	2.20	0.41
49:T:139:PRO:HD3	51:W:69:ILE:HD13	2.00	0.41
52:Y:89:PRO:HA	52:Y:92:TRP:CD2	2.55	0.41
55:d:9:VAL:HG22	56:e:126:VAL:HG13	2.03	0.41
65:r:87:VAL:HG13	65:r:95:LEU:HD23	2.02	0.41
30:v:170:GLN:HE21	30:v:268:HIS:CE1	2.37	0.41
31:w:246:SER:HB2	31:w:249:LEU:HB2	2.02	0.41
32:x:127:SER:HB2	32:x:179:PRO:HD2	2.02	0.41
33:y:63:ILE:O	33:y:67:LEU:HG	2.20	0.41
28:Af:64:GLU:O	28:Af:65:SER:OG	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:22:MET:HE3	54:c:158:PRO:HD3	2.03	0.41
5:U:107:ASP:OD1	5:U:108:VAL:N	2.54	0.41
5:U:244:LYS:HA	5:U:248:LEU:HD12	2.01	0.41
6:Z:64:ASN:HA	45:X:89:LEU:HD23	2.02	0.41
11:q:392:THR:O	11:q:396:MET:HG2	2.21	0.41
12:Aa:3:ARG:NH1	31:7:203:THR:O	2.54	0.41
12:Aa:15:ILE:HA	29:5:276:ARG:O	2.20	0.41
19:Aj:38:LEU:HD22	20:Ak:473:TRP:CZ2	2.55	0.41
20:Ak:211:THR:HG22	20:Ak:215:LEU:HD12	2.02	0.41
21:Al:9:PHE:HE2	21:Al:24:HIS:CG	2.37	0.41
15:3:18:ILE:HD13	15:3:18:ILE:HA	1.83	0.41
28:4:182:GLU:OE2	28:4:183:GLY:N	2.53	0.41
29:5:417:LEU:HD23	29:5:417:LEU:HA	1.86	0.41
30:6:170:GLN:HG2	28:Ae:67:VAL:HG13	2.02	0.41
30:6:295:ALA:O	28:Ae:46:LEU:HD12	2.20	0.41
32:8:142:THR:HG23	32:8:145:GLU:H	1.85	0.41
36:D:231:ARG:NH2	39:H:128:ILE:O	2.53	0.41
42:L:238:VAL:HG12	42:L:242:LYS:NZ	2.34	0.41
48:S:66:LEU:HD21	66:s:159:PHE:HD2	1.83	0.41
53:b:77:ILE:HB	53:b:78:PRO:HD3	2.01	0.41
54:c:121:PRO:HB3	64:o:13:THR:O	2.20	0.41
55:d:144:SER:O	55:d:158:LYS:NZ	2.42	0.41
57:f:68:GLU:HG2	58:g:21:ARG:HE	1.85	0.41
62:l:226:GLN:O	62:l:230:HIS:N	2.53	0.41
30:v:60:ARG:CZ	30:v:390:GLU:HG3	2.50	0.41
30:v:217:ARG:HD2	30:v:244:LEU:O	2.21	0.41
31:w:128:PHE:CZ	31:w:143:ALA:HA	2.55	0.41
31:w:215:MET:HB2	12:z:11:MET:HE2	2.03	0.41
12:z:4:GLU:O	12:z:8:LEU:HG	2.20	0.41
5:U:329:VAL:HG12	8:i:315:TRP:CZ3	2.55	0.41
8:i:9:LEU:HD13	8:i:42:PRO:HB2	2.01	0.41
9:m:113:VAL:HG13	9:m:119:PHE:HB2	2.02	0.41
10:p:80:ARG:HD3	10:p:80:ARG:HA	1.77	0.41
12:Aa:68:GLU:O	12:Aa:72:ARG:HG2	2.21	0.41
15:Ad:23:MET:O	15:Ad:27:VAL:HG23	2.21	0.41
16:Ag:28:LYS:HD2	20:Ak:481:GLU:HB2	2.02	0.41
20:Ak:465:VAL:HG22	68:Ak:601:HEA:H273	2.02	0.41
22:Am:156:ARG:HG3	22:Am:222:GLN:NE2	2.35	0.41
29:5:473:SER:HA	29:5:476:PHE:CE2	2.55	0.41
32:8:203:ARG:CZ	32:8:280:GLU:HG2	2.50	0.41
33:9:43:ASP:N	33:9:43:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:9:78:LYS:HB2	33:9:78:LYS:HE3	1.76	0.41
34:B:256:ARG:HA	37:E:249:LEU:HD11	2.02	0.41
35:C:345:GLN:O	35:C:349:ILE:HG13	2.20	0.41
36:D:77:GLN:HG3	36:D:85:GLU:HG3	2.01	0.41
36:D:103:HIS:O	36:D:103:HIS:CG	2.74	0.41
38:G:341:ILE:HG12	38:G:537:ILE:HD12	2.01	0.41
38:G:370:GLU:OE1	38:G:478:SER:OG	2.35	0.41
40:I:174:LEU:O	40:I:178:LEU:HG	2.20	0.41
42:L:165:LEU:HA	42:L:197:LYS:HB3	2.03	0.41
53:b:66:ARG:HA	53:b:69:ILE:HG22	2.02	0.41
56:e:87:MET:HE3	56:e:87:MET:HB3	1.96	0.41
58:g:24:PRO:HD2	66:s:237:PRO:HG3	2.03	0.41
60:j:65:PHE:O	60:j:69:ILE:HG23	2.21	0.41
60:j:104:TYR:O	60:j:108:GLN:HG2	2.20	0.41
30:v:354:ALA:O	30:v:358:VAL:HG23	2.20	0.41
31:w:318:ARG:O	31:w:322:GLN:HG3	2.21	0.41
32:x:113:ARG:HD2	32:x:270:ASP:OD2	2.20	0.41
3:F:93:LEU:HD21	39:H:209:TYR:CG	2.55	0.41
4:K:8:ARG:O	4:K:12:GLN:HG2	2.20	0.41
9:m:82:VAL:HG12	9:m:83:TRP:H	1.85	0.41
12:Aa:78:TYR:CD2	13:Ab:65:GLU:HG3	2.56	0.41
16:Ag:47:PHE:O	16:Ag:51:LEU:HG	2.21	0.41
19:Aj:56:VAL:HG21	20:Ak:36:LEU:HD13	2.02	0.41
20:Ak:8:TYR:CZ	22:Am:15:PRO:HB3	2.55	0.41
20:Ak:214:ASN:HA	26:Aq:70:LYS:HD3	2.01	0.41
20:Ak:240:HIS:CD2	20:Ak:244:TYR:HE2	2.38	0.41
33:9:76:LEU:O	33:9:81:TRP:NE1	2.44	0.41
35:C:146:ASP:HB2	35:C:466:GLU:CD	2.46	0.41
35:C:191:MET:HE2	35:C:195:THR:HG23	2.03	0.41
37:E:88:ARG:NH2	37:E:190:ASP:OD2	2.53	0.41
38:G:72:ALA:HB2	38:G:184:ARG:NE	2.35	0.41
38:G:322:ALA:O	38:G:326:VAL:HG22	2.20	0.41
38:G:618:GLU:HB3	38:G:621:LYS:HG3	2.01	0.41
39:H:74:LEU:HD12	39:H:77:LEU:HD23	2.02	0.41
43:M:30:GLU:OE1	43:M:30:GLU:N	2.28	0.41
45:O:155:TYR:CD2	45:O:156:GLU:HG3	2.55	0.41
48:S:16:LEU:O	48:S:19:PRO:HD2	2.21	0.41
48:S:57:VAL:HG13	48:S:59:ARG:HB2	2.01	0.41
50:V:107:SER:HB3	50:V:110:ILE:HB	2.02	0.41
55:d:103:VAL:HG22	55:d:135:VAL:HG12	2.03	0.41
55:d:146:LEU:HD23	55:d:150:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:e:99:LEU:HD23	56:e:99:LEU:HA	1.80	0.41
60:j:77:TRP:HH2	65:r:100:LEU:HD21	1.83	0.41
62:l:331:MET:HB3	62:l:387:THR:HB	2.03	0.41
65:r:138:GLN:O	65:r:141:SER:OG	2.26	0.41
29:u:447:LYS:HE3	29:u:448:TYR:CE2	2.56	0.41
29:u:473:SER:HA	29:u:476:PHE:CE1	2.56	0.41
8:i:112:HIS:CE1	8:i:164:ILE:HD13	2.56	0.41
11:q:2:LEU:HD23	11:q:2:LEU:HA	1.92	0.41
16:Ag:61:LEU:HA	16:Ag:64:TYR:CD2	2.56	0.41
21:Al:16:ILE:HA	21:Al:19:GLU:OE1	2.21	0.41
23:An:100:TRP:HA	23:An:103:ILE:HG12	2.01	0.41
24:Ao:77:ASN:O	24:Ao:80:VAL:HG22	2.20	0.41
28:2:265:ASP:OD2	28:2:269:ARG:HB2	2.21	0.41
29:5:212:SER:N	29:5:215:ASP:OD2	2.43	0.41
34:B:43:THR:OG1	34:B:59:ARG:HD3	2.19	0.41
34:B:126:LYS:HE2	34:B:351:THR:HB	2.02	0.41
35:C:161:VAL:O	35:C:165:LEU:HB2	2.21	0.41
35:C:290:LEU:HD23	35:C:290:LEU:HA	1.92	0.41
38:G:59:GLN:NE2	41:J:90:GLY:HA2	2.34	0.41
38:G:371:VAL:HG23	38:G:482:GLN:HE22	1.86	0.41
38:G:389:THR:OG1	38:G:514:ASN:ND2	2.49	0.41
42:L:57:THR:HG21	42:L:86:THR:HG22	2.03	0.41
42:L:68:LEU:HA	42:L:71:MET:HE2	2.03	0.41
42:L:199:SER:OG	42:L:200:ASP:N	2.53	0.41
45:O:89:LEU:HD12	45:O:89:LEU:HA	1.93	0.41
45:O:104:PHE:CE2	45:O:144:ILE:HD11	2.50	0.41
46:P:20:ARG:HG3	46:P:54:LEU:HB2	2.03	0.41
53:b:109:THR:OG1	53:b:113:THR:N	2.53	0.41
56:e:138:GLU:H	56:e:138:GLU:CD	2.29	0.41
60:j:97:LEU:HD23	60:j:97:LEU:HA	1.86	0.41
65:r:47:GLN:HB3	65:r:48:PRO:HD3	2.03	0.41
29:u:178:SER:HB3	29:u:181:ASP:OD2	2.20	0.41
28:Af:55:GLY:HA3	28:Af:59:LEU:HD13	2.02	0.41
4:K:127:TYR:OH	39:H:188:GLU:HG3	2.20	0.41
8:i:112:HIS:CE1	8:i:164:ILE:HG21	2.55	0.41
8:i:215:MET:HG3	8:i:251:MET:SD	2.61	0.41
13:Ab:87:PHE:CE2	32:8:95:TYR:HB3	2.56	0.41
17:Ah:42:HIS:HB2	22:Am:16:TRP:HZ2	1.86	0.41
28:2:100:SER:C	28:2:102:THR:H	2.28	0.41
15:3:33:VAL:HG13	15:3:38:TRP:HB3	2.02	0.41
29:5:68:THR:HG22	29:5:136:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:169:LEU:O	29:5:173:GLN:HG2	2.20	0.41
31:7:200:LEU:HD13	70:7:402:HEM:HAD2	2.03	0.41
35:C:86:LEU:HB3	35:C:107:LEU:HD12	2.01	0.41
35:C:218:GLU:CD	40:I:83:ARG:HH12	2.29	0.41
36:D:228:GLN:HB2	41:J:114:TRP:CE3	2.55	0.41
49:T:134:THR:HG21	51:W:58:ARG:HH21	1.86	0.41
54:c:107:TRP:CZ2	64:o:76:ILE:HD11	2.56	0.41
54:c:110:ASP:OD1	54:c:110:ASP:N	2.53	0.41
58:g:109:LYS:HE3	58:g:109:LYS:HB3	1.92	0.41
60:j:61:THR:HG21	60:j:105:GLU:CD	2.46	0.41
62:l:557:TRP:O	62:l:561:ILE:HG12	2.21	0.41
30:v:177:LEU:HD21	30:v:272:VAL:HG11	2.02	0.41
30:v:268:HIS:CE1	30:v:341:ILE:HG12	2.55	0.41
30:v:401:LEU:HD12	30:v:401:LEU:HA	1.93	0.41
1:A:51:TYR:HE2	23:An:153:ILE:HD11	1.85	0.41
4:K:105:ALA:O	4:K:106:ARG:HD2	2.20	0.41
5:U:143:LEU:HD21	8:i:317:PHE:HZ	1.85	0.41
7:a:188:ASP:CG	66:s:124:ARG:HH22	2.28	0.41
8:i:215:MET:HE2	8:i:215:MET:HA	2.03	0.41
8:i:278:MET:O	8:i:282:MET:HG3	2.20	0.41
9:m:147:TYR:OH	60:j:71:LEU:O	2.33	0.41
12:Aa:8:LEU:HD13	31:7:217:LYS:HG3	2.03	0.41
15:Ad:33:VAL:HG13	15:Ad:38:TRP:HB3	2.02	0.41
16:Ag:49:SER:HB3	19:Aj:42:THR:HG23	2.02	0.41
21:Al:1:MET:HE1	21:Al:133:MET:HG3	2.02	0.41
22:Am:204:HIS:O	22:Am:208:VAL:HG23	2.20	0.41
28:2:256:TYR:CE1	28:2:261:GLY:HA2	2.55	0.41
15:3:51:LYS:HG2	15:3:52:PHE:CD2	2.56	0.41
28:4:185:ASN:HA	28:4:198:ARG:HA	2.03	0.41
29:5:405:GLY:C	29:5:408:PRO:HD2	2.45	0.41
34:B:299:LEU:HD12	34:B:303:HIS:CD2	2.55	0.41
34:B:413:TRP:O	34:B:417:LYS:HG2	2.20	0.41
35:C:299:LEU:HB3	35:C:304:ILE:HG23	2.02	0.41
41:J:102:ASP:N	41:J:102:ASP:OD1	2.54	0.41
42:L:275:ILE:HG23	42:L:348:LEU:HD13	2.03	0.41
57:f:63:LYS:O	57:f:66:VAL:HG12	2.20	0.41
62:l:417:SER:HB3	62:l:493:VAL:HG13	2.01	0.41
65:r:101:GLY:O	65:r:105:MET:HG3	2.21	0.41
65:r:102:VAL:HG21	65:r:154:LEU:HD11	2.03	0.41
66:s:244:LEU:HG	66:s:245:PHE:H	1.86	0.41
30:v:65:ILE:HG21	30:v:213:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:39:MET:SD	2:t:58:TYR:HA	2.61	0.41
4:K:109:ILE:HG12	39:H:198:GLU:HB3	2.03	0.41
5:U:348:ASP:OD1	5:U:349:VAL:HG13	2.21	0.41
8:i:175:LEU:HD22	8:i:296:LEU:HD11	2.03	0.41
8:i:339:MET:HE2	8:i:339:MET:HA	2.03	0.41
9:m:23:LYS:HB2	61:k:23:ARG:HD3	2.03	0.41
11:q:75:LEU:HB3	11:q:229:MET:HE1	2.03	0.41
11:q:197:LEU:O	11:q:201:MET:HG2	2.20	0.41
11:q:207:MET:HE1	11:q:297:VAL:HG12	2.02	0.41
11:q:243:MET:HA	11:q:246:ILE:HG22	2.03	0.41
15:Ad:8:PRO:HD2	33:y:111:LYS:HB3	2.02	0.41
20:Ak:44:PRO:HD3	20:Ak:448:THR:HG23	2.03	0.41
20:Ak:407:GLN:H	20:Ak:407:GLN:CD	2.28	0.41
21:Al:145:PRO:HD3	21:Al:219:PHE:CG	2.56	0.41
21:Al:196:CYS:HB2	21:Al:207:MET:HB2	2.03	0.41
22:Am:253:TYR:HA	22:Am:257:TYR:CD2	2.55	0.41
23:An:40:ASP:OD2	23:An:88:GLU:HG2	2.20	0.41
28:2:200:ARG:HH11	28:2:208:GLU:HG3	1.85	0.41
28:2:289:ASP:OD1	28:2:289:ASP:N	2.54	0.41
28:4:222:ASP:O	28:4:226:VAL:HG22	2.20	0.41
29:5:377:MET:HE2	29:5:476:PHE:HA	2.02	0.41
29:5:445:CYS:O	29:5:449:PHE:HB2	2.21	0.41
30:6:115:THR:OG1	30:6:116:ARG:N	2.54	0.41
31:7:104:TYR:CD1	31:7:208:PRO:HA	2.56	0.41
31:7:145:VAL:O	31:7:149:LEU:HG	2.21	0.41
34:B:75:TRP:HZ3	34:B:255:CYS:HG	1.69	0.41
34:B:113:LEU:HD13	34:B:149:MET:HE1	2.02	0.41
34:B:314:LEU:HB3	34:B:329:LYS:HG3	2.03	0.41
35:C:101:LEU:HD22	35:C:464:PHE:HZ	1.86	0.41
35:C:144:ARG:HD2	73:I:201:SF4:S4	2.61	0.41
35:C:146:ASP:HB3	35:C:153:ASN:OD1	2.21	0.41
35:C:207:PHE:CD1	65:r:34:ARG:HD3	2.56	0.41
36:D:85:GLU:HA	36:D:142:ARG:O	2.21	0.41
36:D:103:HIS:HB3	44:N:83:GLN:OE1	2.21	0.41
36:D:128:ILE:HD11	36:D:176:VAL:HG21	2.01	0.41
37:E:141:MET:HE2	37:E:141:MET:HB3	1.95	0.41
38:G:43:VAL:HG21	38:G:96:VAL:HG21	2.03	0.41
38:G:74:ASN:OD1	38:G:74:ASN:N	2.54	0.41
39:H:86:TYR:CD1	39:H:87:PRO:HA	2.56	0.41
39:H:86:TYR:CG	39:H:87:PRO:HA	2.56	0.41
39:H:148:ASP:CG	39:H:150:THR:HG22	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:N:56:LEU:HG	44:N:60:LYS:HE2	2.02	0.41
48:S:48:MET:HE2	48:S:48:MET:HB3	1.95	0.41
60:j:60:ILE:HG23	61:k:72:ALA:HB1	2.03	0.41
60:j:88:LEU:HD13	65:r:309:ILE:HD12	2.03	0.41
61:k:37:MET:HE3	61:k:67:ALA:HB2	2.01	0.41
62:l:440:LEU:HG	62:l:442:LEU:HD11	2.03	0.41
64:o:113:GLU:O	64:o:117:GLN:HG2	2.20	0.41
29:u:94:GLU:OE2	30:v:300:LYS:NZ	2.52	0.41
29:u:300:ASP:C	29:u:303:PRO:HD2	2.46	0.41
30:v:68:GLY:O	30:v:208:TYR:OH	2.39	0.41
30:v:124:GLU:OE2	30:v:125:CYS:N	2.53	0.41
30:v:326:PHE:HD2	28:Af:66:PRO:O	2.04	0.41
30:v:400:ALA:HA	30:v:404:GLY:O	2.21	0.41
45:X:113:LEU:H	45:X:113:LEU:HD12	1.86	0.41
67:R:95:LYS:HG3	67:R:96:PHE:N	2.35	0.41
8:i:6:TYR:CE1	8:i:46:LYS:HD2	2.56	0.41
9:m:61:LEU:O	65:r:114:TYR:OH	2.32	0.41
11:q:108:MET:HB3	11:q:121:LEU:HD13	2.03	0.41
20:Ak:143:VAL:HB	20:Ak:213:ARG:CZ	2.51	0.41
20:Ak:427:PRO:HB3	20:Ak:450:TRP:CE3	2.55	0.41
21:Al:86:MET:HE2	21:Al:86:MET:HB3	1.75	0.41
21:Al:116:LEU:HD11	21:Al:226:MET:HE3	2.02	0.41
21:Al:158:ASP:OD1	21:Al:158:ASP:N	2.55	0.41
22:Am:204:HIS:CE1	22:Am:249:TRP:HB2	2.55	0.41
28:2:200:ARG:NH1	28:2:208:GLU:HG3	2.36	0.41
28:2:225:ARG:HE	28:2:281:VAL:CG2	2.34	0.41
29:5:80:ARG:NH2	29:5:350:GLU:OE2	2.41	0.41
30:6:47:LEU:HD21	30:6:234:ALA:HB1	2.03	0.41
30:6:182:TYR:O	30:6:187:ALA:HB2	2.21	0.41
30:6:244:LEU:HA	30:6:244:LEU:HD13	1.90	0.41
31:7:310:SER:HB2	31:7:370:SER:HB3	2.03	0.41
35:C:86:LEU:HD22	35:C:107:LEU:HD11	2.03	0.41
35:C:175:TRP:HA	35:C:178:VAL:HG12	2.02	0.41
39:H:80:GLU:HB2	48:S:1:MET:HE1	2.03	0.41
42:L:103:TRP:CZ3	42:L:105:GLY:HA2	2.56	0.41
42:L:163:SER:O	74:L:401:NDP:H6N	2.21	0.41
45:O:144:ILE:O	45:O:148:ILE:HD12	2.21	0.41
47:Q:69:VAL:O	47:Q:72:THR:HG22	2.20	0.41
62:l:97:THR:HG22	62:l:246:LEU:HD11	2.03	0.41
62:l:289:ALA:O	62:l:293:ILE:HG12	2.21	0.41
8:i:215:MET:HE1	8:i:244:MET:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Ac:11:TYR:HB2	28:4:133:GLY:CA	2.51	0.40
20:Ak:133:ALA:O	20:Ak:213:ARG:NE	2.50	0.40
20:Ak:486:GLU:HG3	23:An:41:ARG:NH1	2.37	0.40
22:Am:190:ASP:HB3	26:Aq:65:LEU:HD23	2.03	0.40
27:Ar:5:ILE:O	27:Ar:9:ILE:HG13	2.21	0.40
28:4:192:GLY:HA3	31:w:169:SER:OG	2.21	0.40
29:5:392:LYS:O	29:5:396:ARG:HG3	2.21	0.40
29:5:440:VAL:O	29:5:444:VAL:HG23	2.21	0.40
30:6:49:ILE:HD13	30:6:231:LYS:HA	2.03	0.40
30:6:113:THR:HA	28:Ae:61:ALA:O	2.21	0.40
31:7:185:LEU:HD23	31:7:185:LEU:HA	1.78	0.40
35:C:202:ALA:O	35:C:203:MET:HG2	2.21	0.40
35:C:322:PHE:CG	35:C:349:ILE:HD11	2.55	0.40
37:E:179:ALA:HB3	37:E:185:MET:SD	2.61	0.40
40:I:134:GLY:HA2	40:I:165:GLY:O	2.21	0.40
45:O:136:GLU:OE1	47:Q:59:ARG:NH2	2.54	0.40
59:h:67:LEU:HD23	59:h:67:LEU:HA	1.91	0.40
62:l:245:ALA:HB2	62:l:340:PHE:HB3	2.03	0.40
62:l:305:SER:O	62:l:309:GLN:HG2	2.21	0.40
65:r:212:ASN:HA	65:r:215:TYR:HD2	1.86	0.40
65:r:266:LEU:O	65:r:269:THR:OG1	2.31	0.40
29:u:68:THR:HG21	30:v:384:MET:CG	2.51	0.40
30:v:101:ARG:HA	30:v:101:ARG:HD3	1.89	0.40
12:z:73:LYS:HG2	12:z:74:ASN:N	2.36	0.40
3:F:71:ILE:HD12	3:F:71:ILE:HA	1.96	0.40
8:i:28:LEU:HD23	8:i:31:ILE:HD12	2.02	0.40
8:i:325:LEU:O	8:i:329:MET:HG2	2.21	0.40
11:q:398:MET:O	11:q:402:ILE:HG13	2.21	0.40
14:Ac:53:TRP:O	14:Ac:57:LYS:HG3	2.21	0.40
18:Ai:53:TRP:NE1	23:An:115:ALA:HB2	2.37	0.40
18:Ai:60:ILE:HD11	18:Ai:62:ILE:HD11	2.03	0.40
25:Ap:107:LYS:HE3	25:Ap:107:LYS:HB2	1.91	0.40
13:0:45:LYS:HB2	13:0:45:LYS:HE2	1.79	0.40
29:5:274:GLU:HA	29:5:456:VAL:O	2.21	0.40
32:8:115:PHE:CE2	32:8:149:LEU:HD13	2.56	0.40
34:B:81:LYS:HG2	34:B:96:GLY:HA3	2.03	0.40
34:B:113:LEU:HD12	34:B:114:VAL:H	1.86	0.40
34:B:162:PHE:CZ	37:E:178:GLY:HA3	2.57	0.40
35:C:260:ARG:NE	43:M:25:GLN:HB3	2.34	0.40
36:D:108:PHE:O	36:D:160:TYR:OH	2.30	0.40
37:E:41:HIS:HB2	38:G:209:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:l:327:LEU:O	62:l:331:MET:HG2	2.21	0.40
65:r:253:GLU:H	65:r:253:GLU:HG2	1.70	0.40
29:u:41:ALA:O	29:u:45:VAL:HG23	2.21	0.40
67:R:93:LEU:O	67:R:97:ARG:HD3	2.21	0.40
2:t:9:TYR:OH	54:c:151:PRO:O	2.30	0.40
4:K:49:TYR:HB2	4:K:61:TRP:CE2	2.56	0.40
5:U:130:SER:HB3	5:U:175:MET:HE3	2.03	0.40
5:U:317:PRO:HB3	56:e:52:THR:O	2.22	0.40
8:i:117:GLU:HG2	61:k:97:GLN:O	2.22	0.40
9:m:7:PHE:CE1	61:k:3:LEU:HD23	2.56	0.40
9:m:122:LEU:HD23	9:m:122:LEU:HA	1.87	0.40
21:Al:13:THR:HG23	21:Al:168:LEU:HD23	2.03	0.40
28:4:263:HIS:O	28:4:270:ILE:HD12	2.22	0.40
29:5:379:LEU:HD23	29:5:379:LEU:HA	1.91	0.40
31:7:132:VAL:HG22	31:7:143:ALA:HB2	2.03	0.40
34:B:128:ARG:HG2	34:B:132:ARG:NH1	2.36	0.40
35:C:463:VAL:HG13	35:C:466:GLU:HB2	2.02	0.40
38:G:163:LYS:HD3	38:G:173:MET:HG3	2.02	0.40
39:H:75:SER:HB3	43:M:15:ALA:HB3	2.04	0.40
42:L:59:PHE:HZ	42:L:203:GLY:HA3	1.85	0.40
49:T:150:ASP:O	49:T:159:GLN:HB3	2.20	0.40
52:Y:54:GLN:NE2	62:l:446:ASN:HD21	2.19	0.40
52:Y:70:LEU:HD13	52:Y:70:LEU:HA	1.97	0.40
56:e:136:LEU:HD13	56:e:136:LEU:HA	1.77	0.40
62:l:310:LEU:HD23	62:l:313:MET:HE1	2.03	0.40
65:r:120:GLY:HA2	65:r:128:ALA:HB1	2.03	0.40
30:v:194:ASP:HA	30:v:197:ILE:HG12	2.03	0.40
30:v:211:ASN:HB3	30:v:246:LEU:HG	2.03	0.40
31:w:223:TYR:HB3	32:x:312:TRP:CZ2	2.56	0.40
31:w:300:ILE:HD12	31:w:300:ILE:HA	1.93	0.40
31:w:366:MET:HB2	31:w:367:PRO:HD3	2.03	0.40
32:x:219:TYR:CD2	32:x:247:PRO:HG3	2.57	0.40
67:R:106:GLN:OE1	67:R:106:GLN:N	2.43	0.40
28:Ae:52:GLY:CA	28:Ae:61:ALA:HA	2.47	0.40
4:K:2:GLU:HA	4:K:5:GLN:NE2	2.36	0.40
7:a:174:ILE:HG21	59:h:20:ILE:HG21	2.04	0.40
8:i:136:LEU:HD21	8:i:209:ILE:HD11	2.03	0.40
8:i:245:MET:HE3	8:i:245:MET:HB3	1.95	0.40
20:Ak:313:ALA:HB2	20:Ak:356:ILE:HD11	2.03	0.40
20:Ak:467:LEU:O	20:Ak:471:ILE:HG13	2.22	0.40
21:Al:12:ALA:CB	21:Al:17:MET:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Al:146:MET:HG2	21:Al:214:VAL:C	2.46	0.40
14:l:36:PHE:CZ	32:x:296:MET:HG2	2.56	0.40
29:5:384:THR:O	29:5:387:GLU:HG2	2.22	0.40
32:8:117:VAL:HG11	32:8:271:VAL:HB	2.03	0.40
36:D:69:LEU:HD11	36:D:99:PHE:CD2	2.56	0.40
39:H:135:ARG:NH2	39:H:141:ARG:HG3	2.36	0.40
42:L:190:PHE:CE1	42:L:192:GLU:HG2	2.57	0.40
44:N:66:LYS:HA	44:N:66:LYS:HD2	1.91	0.40
45:O:120:MET:HA	45:O:123:GLU:HG2	2.03	0.40
53:b:119:LEU:HG	53:b:121:LYS:HG3	2.03	0.40
61:k:73:LEU:HD12	61:k:73:LEU:HA	1.88	0.40
62:l:339:LEU:HD22	62:l:373:LEU:HD22	2.04	0.40
62:l:441:VAL:HG13	62:l:443:ILE:HD13	2.03	0.40
65:r:310:MET:HE3	65:r:310:MET:HB3	1.81	0.40
30:v:37:ASP:OD1	30:v:38:LEU:N	2.55	0.40
30:v:48:VAL:HG11	30:v:400:ALA:HB1	2.03	0.40
30:v:138:LEU:HD13	30:v:237:PHE:HB2	2.03	0.40
30:v:213:PHE:HB3	30:v:218:MET:HE3	2.04	0.40
45:X:143:GLU:HA	45:X:146:ASP:OD2	2.21	0.40
28:Af:75:LEU:H	28:Af:75:LEU:HD12	1.87	0.40
8:i:244:MET:HB2	8:i:244:MET:HE2	1.66	0.40
21:Al:17:MET:HG2	21:Al:169:GLY:HA3	2.02	0.40
28:4:158:VAL:HG13	31:w:163:TRP:NE1	2.36	0.40
28:4:251:ASP:OD1	28:4:263:HIS:ND1	2.54	0.40
29:5:390:ARG:HG3	30:6:105:ALA:HA	2.03	0.40
29:5:393:ASN:OD1	29:5:396:ARG:NH1	2.55	0.40
30:6:367:SER:O	30:6:371:VAL:HG23	2.22	0.40
30:6:444:LEU:HB3	30:6:447:THR:HB	2.03	0.40
34:B:102:MET:HB3	34:B:149:MET:HB2	2.03	0.40
35:C:116:ASP:OD2	36:D:185:ARG:NH2	2.55	0.40
38:G:612:PRO:HA	38:G:613:PRO:HD3	1.90	0.40
38:G:624:ARG:HH12	38:G:628:GLU:CD	2.29	0.40
42:L:297:GLY:O	42:L:301:GLU:HG3	2.22	0.40
51:W:12:PRO:HD3	51:W:16:TYR:CZ	2.56	0.40
53:b:99:GLU:H	53:b:99:GLU:HG3	1.71	0.40
60:j:95:LEU:HB3	65:r:302:MET:HE2	2.03	0.40
62:l:384:PRO:HA	62:l:389:PHE:CD1	2.57	0.40
64:o:48:LEU:HD23	64:o:48:LEU:HA	1.92	0.40
31:w:185:LEU:HD23	31:w:185:LEU:HA	1.87	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	A	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
2	t	117/137 (85%)	114 (97%)	3 (3%)	0	100	100
3	F	93/123 (76%)	89 (96%)	4 (4%)	0	100	100
4	K	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
5	U	316/357 (88%)	308 (98%)	7 (2%)	1 (0%)	36	66
6	Z	76/114 (67%)	75 (99%)	1 (1%)	0	100	100
7	a	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
8	i	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
9	m	173/175 (99%)	165 (95%)	7 (4%)	1 (1%)	21	51
10	p	176/221 (80%)	173 (98%)	3 (2%)	0	100	100
11	q	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
12	Aa	76/82 (93%)	75 (99%)	1 (1%)	0	100	100
12	z	77/82 (94%)	77 (100%)	0	0	100	100
13	0	66/91 (72%)	64 (97%)	2 (3%)	0	100	100
13	Ab	64/91 (70%)	62 (97%)	2 (3%)	0	100	100
14	1	58/64 (91%)	58 (100%)	0	0	100	100
14	Ac	57/64 (89%)	57 (100%)	0	0	100	100
15	3	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
15	Ad	49/56 (88%)	46 (94%)	3 (6%)	0	100	100
16	Ag	41/70 (59%)	41 (100%)	0	0	100	100
17	Ah	54/80 (68%)	54 (100%)	0	0	100	100
18	Ai	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
19	Aj	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
20	Ak	511/514 (99%)	498 (98%)	13 (2%)	0	100	100
21	Al	218/228 (96%)	211 (97%)	6 (3%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	Am	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
23	An	136/169 (80%)	132 (97%)	4 (3%)	0	100	100
24	Ao	102/152 (67%)	100 (98%)	2 (2%)	0	100	100
25	Ap	89/129 (69%)	86 (97%)	3 (3%)	0	100	100
26	Aq	71/97 (73%)	66 (93%)	5 (7%)	0	100	100
27	Ar	80/86 (93%)	80 (100%)	0	0	100	100
28	2	193/299 (64%)	186 (96%)	7 (4%)	0	100	100
28	4	194/299 (65%)	189 (97%)	5 (3%)	0	100	100
28	Ae	37/299 (12%)	26 (70%)	11 (30%)	0	100	100
28	Af	31/299 (10%)	20 (64%)	11 (36%)	0	100	100
29	5	431/480 (90%)	415 (96%)	16 (4%)	0	100	100
29	u	444/480 (92%)	432 (97%)	12 (3%)	0	100	100
30	6	416/453 (92%)	402 (97%)	14 (3%)	0	100	100
30	v	416/453 (92%)	407 (98%)	9 (2%)	0	100	100
31	7	377/379 (100%)	373 (99%)	4 (1%)	0	100	100
31	w	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
32	8	237/326 (73%)	231 (98%)	6 (2%)	0	100	100
32	x	236/326 (72%)	229 (97%)	7 (3%)	0	100	100
33	9	99/111 (89%)	99 (100%)	0	0	100	100
33	y	99/111 (89%)	99 (100%)	0	0	100	100
34	B	429/464 (92%)	414 (96%)	14 (3%)	1 (0%)	43	72
35	C	428/469 (91%)	407 (95%)	21 (5%)	0	100	100
36	D	206/264 (78%)	180 (87%)	25 (12%)	1 (0%)	24	55
37	E	212/249 (85%)	202 (95%)	10 (5%)	0	100	100
38	G	680/727 (94%)	662 (97%)	18 (3%)	0	100	100
39	H	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
40	I	154/258 (60%)	146 (95%)	8 (5%)	0	100	100
41	J	116/175 (66%)	116 (100%)	0	0	100	100
42	L	338/372 (91%)	326 (96%)	12 (4%)	0	100	100
43	M	92/113 (81%)	86 (94%)	6 (6%)	0	100	100
44	N	110/116 (95%)	108 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	O	83/156 (53%)	79 (95%)	4 (5%)	0	100	100
45	X	83/156 (53%)	82 (99%)	1 (1%)	0	100	100
46	P	81/99 (82%)	73 (90%)	8 (10%)	0	100	100
47	Q	110/154 (71%)	107 (97%)	2 (2%)	1 (1%)	14	41
48	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
49	T	80/169 (47%)	76 (95%)	4 (5%)	0	100	100
50	V	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
51	W	138/144 (96%)	136 (99%)	2 (1%)	0	100	100
52	Y	60/105 (57%)	54 (90%)	4 (7%)	2 (3%)	3	11
53	b	106/188 (56%)	99 (93%)	7 (7%)	0	100	100
54	c	151/186 (81%)	147 (97%)	4 (3%)	0	100	100
55	d	167/176 (95%)	166 (99%)	1 (1%)	0	100	100
56	e	97/154 (63%)	91 (94%)	6 (6%)	0	100	100
57	f	44/76 (58%)	43 (98%)	1 (2%)	0	100	100
58	g	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
59	h	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
60	j	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
61	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
62	l	600/606 (99%)	576 (96%)	24 (4%)	0	100	100
63	n	54/58 (93%)	48 (89%)	6 (11%)	0	100	100
64	o	126/129 (98%)	124 (98%)	2 (2%)	0	100	100
65	r	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
66	s	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
67	R	33/110 (30%)	33 (100%)	0	0	100	100
All	All	13905/16854 (82%)	13458 (97%)	439 (3%)	8 (0%)	49	77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	Y	40	ILE
9	m	138	GLU
34	B	316	ALA
5	U	255	CYS
21	Al	158	ASP

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Mol	Chain	Res	Type
36	D	122	ARG
52	Y	48	PRO
47	Q	122	VAL

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	A	55/59 (93%)	53 (96%)	2 (4%)	31	66
2	t	101/120 (84%)	96 (95%)	5 (5%)	22	54
3	F	79/97 (81%)	77 (98%)	2 (2%)	42	76
4	K	130/131 (99%)	127 (98%)	3 (2%)	44	78
5	U	278/307 (91%)	269 (97%)	9 (3%)	34	70
6	Z	60/90 (67%)	53 (88%)	7 (12%)	5	18
7	a	121/158 (77%)	120 (99%)	1 (1%)	73	90
8	i	311/311 (100%)	297 (96%)	14 (4%)	24	58
9	m	141/141 (100%)	132 (94%)	9 (6%)	16	44
10	p	159/190 (84%)	157 (99%)	2 (1%)	61	86
11	q	409/409 (100%)	398 (97%)	11 (3%)	39	74
12	Aa	70/73 (96%)	64 (91%)	6 (9%)	10	31
12	z	70/73 (96%)	68 (97%)	2 (3%)	37	73
13	0	65/85 (76%)	60 (92%)	5 (8%)	12	36
13	Ab	63/85 (74%)	57 (90%)	6 (10%)	8	26
14	1	49/52 (94%)	49 (100%)	0	100	100
14	Ac	48/52 (92%)	48 (100%)	0	100	100
15	3	40/46 (87%)	37 (92%)	3 (8%)	12	37
15	Ad	41/46 (89%)	39 (95%)	2 (5%)	22	55
16	Ag	37/57 (65%)	37 (100%)	0	100	100
17	Ah	47/68 (69%)	44 (94%)	3 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Ai	38/66 (58%)	36 (95%)	2 (5%)	20	52
19	Aj	39/55 (71%)	38 (97%)	1 (3%)	40	75
20	Ak	424/425 (100%)	408 (96%)	16 (4%)	29	64
21	Al	206/212 (97%)	201 (98%)	5 (2%)	43	77
22	Am	223/225 (99%)	220 (99%)	3 (1%)	61	86
23	An	123/149 (83%)	117 (95%)	6 (5%)	22	55
24	Ao	91/124 (73%)	85 (93%)	6 (7%)	15	43
25	Ap	77/101 (76%)	74 (96%)	3 (4%)	28	64
26	Aq	64/80 (80%)	63 (98%)	1 (2%)	55	83
27	Ar	73/76 (96%)	68 (93%)	5 (7%)	14	42
28	2	166/245 (68%)	161 (97%)	5 (3%)	36	72
28	4	166/245 (68%)	157 (95%)	9 (5%)	20	51
28	Ae	29/245 (12%)	26 (90%)	3 (10%)	7	23
28	Af	23/245 (9%)	23 (100%)	0	100	100
29	5	363/397 (91%)	357 (98%)	6 (2%)	53	83
29	u	372/397 (94%)	359 (96%)	13 (4%)	32	67
30	6	329/355 (93%)	315 (96%)	14 (4%)	26	60
30	v	329/355 (93%)	317 (96%)	12 (4%)	31	66
31	7	332/332 (100%)	328 (99%)	4 (1%)	63	87
31	w	332/332 (100%)	325 (98%)	7 (2%)	47	79
32	8	204/259 (79%)	197 (97%)	7 (3%)	32	68
32	x	203/259 (78%)	196 (97%)	7 (3%)	32	68
33	9	93/99 (94%)	91 (98%)	2 (2%)	45	78
33	y	93/99 (94%)	89 (96%)	4 (4%)	26	60
34	B	345/368 (94%)	335 (97%)	10 (3%)	37	73
35	C	371/398 (93%)	349 (94%)	22 (6%)	18	48
36	D	188/228 (82%)	181 (96%)	7 (4%)	30	65
37	E	183/207 (88%)	176 (96%)	7 (4%)	29	64
38	G	576/610 (94%)	559 (97%)	17 (3%)	36	72
39	H	151/176 (86%)	142 (94%)	9 (6%)	17	47
40	I	132/212 (62%)	129 (98%)	3 (2%)	44	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	J	107/152 (70%)	105 (98%)	2 (2%)	50	81
42	L	294/320 (92%)	279 (95%)	15 (5%)	21	54
43	M	86/98 (88%)	79 (92%)	7 (8%)	11	33
44	N	99/101 (98%)	93 (94%)	6 (6%)	17	46
45	O	79/132 (60%)	73 (92%)	6 (8%)	12	36
45	X	79/132 (60%)	73 (92%)	6 (8%)	12	36
46	P	74/82 (90%)	70 (95%)	4 (5%)	20	51
47	Q	105/134 (78%)	99 (94%)	6 (6%)	18	49
48	S	58/58 (100%)	57 (98%)	1 (2%)	53	83
49	T	69/134 (52%)	66 (96%)	3 (4%)	26	60
50	V	101/102 (99%)	100 (99%)	1 (1%)	68	88
51	W	122/124 (98%)	120 (98%)	2 (2%)	55	83
52	Y	55/84 (66%)	44 (80%)	11 (20%)	1	4
53	b	100/166 (60%)	93 (93%)	7 (7%)	14	40
54	c	138/160 (86%)	135 (98%)	3 (2%)	45	78
55	d	152/156 (97%)	148 (97%)	4 (3%)	40	75
56	e	91/129 (70%)	83 (91%)	8 (9%)	9	29
57	f	41/66 (62%)	41 (100%)	0	100	100
58	g	108/109 (99%)	104 (96%)	4 (4%)	30	65
59	h	93/94 (99%)	91 (98%)	2 (2%)	45	78
60	j	97/100 (97%)	94 (97%)	3 (3%)	35	70
61	k	85/85 (100%)	80 (94%)	5 (6%)	18	48
62	l	536/540 (99%)	518 (97%)	18 (3%)	32	68
63	n	53/55 (96%)	48 (91%)	5 (9%)	8	27
64	o	113/114 (99%)	111 (98%)	2 (2%)	51	82
65	r	275/275 (100%)	265 (96%)	10 (4%)	31	66
66	s	153/206 (74%)	149 (97%)	4 (3%)	40	75
67	R	34/92 (37%)	33 (97%)	1 (3%)	37	73
All	All	12109/14226 (85%)	11655 (96%)	454 (4%)	31	65

All (454) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	45	LYS
2	t	40	VAL
2	t	83	GLU
2	t	88	ASP
2	t	91	GLU
2	t	103	GLU
3	F	29	VAL
3	F	46	ASP
4	K	7	LEU
4	K	11	LEU
4	K	129	THR
5	U	43	LEU
5	U	78	GLU
5	U	229	MET
5	U	243	TYR
5	U	250	GLU
5	U	263	ARG
5	U	278	LEU
5	U	281	ASP
5	U	312	ILE
6	Z	29	LYS
6	Z	31	GLU
6	Z	52	LEU
6	Z	57	LEU
6	Z	65	GLU
6	Z	88	LYS
6	Z	98	VAL
7	a	130	GLU
8	i	17	THR
8	i	149	ILE
8	i	154	MET
8	i	193	VAL
8	i	204	ASN
8	i	228	LEU
8	i	244	MET
8	i	258	SER
8	i	290	LEU
8	i	311	MET
8	i	313	MET
8	i	336	VAL
8	i	343	LEU
8	i	346	LEU

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Mol	Chain	Res	Type
9	m	1	MET
9	m	27	ILE
9	m	33	LEU
9	m	39	VAL
9	m	61	LEU
9	m	65	LEU
9	m	82	VAL
9	m	132	ASP
9	m	139	GLU
10	p	106	LEU
10	p	165	GLU
11	q	11	LEU
11	q	36	LEU
11	q	50	LEU
11	q	66	LEU
11	q	179	ILE
11	q	212	LEU
11	q	263	MET
11	q	270	ILE
11	q	304	GLN
11	q	375	LEU
11	q	441	ILE
12	Aa	5	PHE
12	Aa	12	ARG
12	Aa	19	LEU
12	Aa	32	THR
12	Aa	35	ILE
12	Aa	71	LYS
13	Ab	35	GLU
13	Ab	48	GLU
13	Ab	51	GLU
13	Ab	52	LEU
13	Ab	54	ASP
13	Ab	69	GLU
15	Ad	6	LEU
15	Ad	18	ILE
17	Ah	25	ARG
17	Ah	32	ILE
17	Ah	49	ASP
18	Ai	72	VAL
18	Ai	73	THR
19	Aj	43	LEU

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Mol	Chain	Res	Type
20	Ak	28	MET
20	Ak	35	LEU
20	Ak	100	MET
20	Ak	117	MET
20	Ak	119	GLU
20	Ak	136	LEU
20	Ak	138	HIS
20	Ak	238	PHE
20	Ak	243	VAL
20	Ak	300	ASP
20	Ak	376	HIS
20	Ak	417	MET
20	Ak	462	LEU
20	Ak	465	VAL
20	Ak	468	MET
20	Ak	513	LEU
21	Al	29	MET
21	Al	73	LEU
21	Al	89	GLU
21	Al	133	MET
21	Al	160	LEU
22	Am	40	MET
22	Am	45	LEU
22	Am	246	ASP
23	An	65	LYS
23	An	76	ASP
23	An	114	THR
23	An	129	ILE
23	An	145	MET
23	An	148	MET
24	Ao	74	LYS
24	Ao	84	LEU
24	Ao	104	PHE
24	Ao	114	VAL
24	Ao	129	ILE
24	Ao	143	THR
25	Ap	37	VAL
25	Ap	43	GLN
25	Ap	56	ARG
26	Aq	81	LEU
27	Ar	8	LYS
27	Ar	30	CYS

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Mol	Chain	Res	Type
27	Ar	42	LYS
27	Ar	61	TYR
27	Ar	67	ILE
13	0	28	ASP
13	0	35	GLU
13	0	44	ILE
13	0	54	ASP
13	0	71	LEU
28	2	205	ILE
28	2	222	ASP
28	2	238	CYS
28	2	287	THR
28	2	292	VAL
15	3	18	ILE
15	3	39	ARG
15	3	42	LEU
28	4	119	ASP
28	4	177	LEU
28	4	212	GLU
28	4	224	GLU
28	4	232	VAL
28	4	240	HIS
28	4	251	ASP
28	4	283	THR
28	4	285	GLU
29	5	96	LEU
29	5	266	THR
29	5	359	VAL
29	5	368	MET
29	5	433	ILE
29	5	467	ASP
30	6	83	LEU
30	6	122	THR
30	6	129	ASP
30	6	134	MET
30	6	218	MET
30	6	230	LEU
30	6	235	GLU
30	6	244	LEU
30	6	260	ASP
30	6	309	LEU
30	6	323	VAL

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Mol	Chain	Res	Type
30	6	365	ASN
30	6	378	LEU
30	6	450	VAL
31	7	2	THR
31	7	97	HIS
31	7	124	MET
31	7	264	THR
32	8	121	VAL
32	8	136	LEU
32	8	201	ILE
32	8	255	GLU
32	8	258	ASP
32	8	263	THR
32	8	297	MET
33	9	43	ASP
33	9	75	ILE
34	B	41	ILE
34	B	102	MET
34	B	170	GLN
34	B	232	ASP
34	B	282	VAL
34	B	318	ILE
34	B	327	ILE
34	B	340	ASP
34	B	379	CYS
34	B	457	HIS
35	C	57	VAL
35	C	72	TRP
35	C	81	THR
35	C	107	LEU
35	C	139	LEU
35	C	143	ASP
35	C	167	ILE
35	C	191	MET
35	C	194	THR
35	C	195	THR
35	C	209	MET
35	C	224	SER
35	C	228	MET
35	C	238	VAL
35	C	264	LEU
35	C	284	VAL

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Mol	Chain	Res	Type
35	C	304	ILE
35	C	362	ILE
35	C	418	VAL
35	C	446	LYS
35	C	462	ILE
35	C	466	GLU
36	D	47	ILE
36	D	104	THR
36	D	119	VAL
36	D	121	THR
36	D	148	ASP
36	D	216	VAL
36	D	234	ASP
37	E	95	ILE
37	E	137	THR
37	E	150	GLU
37	E	185	MET
37	E	190	ASP
37	E	201	ILE
37	E	203	GLU
38	G	56	VAL
38	G	137	CYS
38	G	182	CYS
38	G	197	THR
38	G	225	ILE
38	G	241	ARG
38	G	346	VAL
38	G	366	LEU
38	G	367	CYS
38	G	473	MET
38	G	534	VAL
38	G	559	ASP
38	G	637	ASP
38	G	652	ASN
38	G	671	LEU
38	G	679	LEU
38	G	680	LEU
39	H	39	LYS
39	H	49	ASP
39	H	83	THR
39	H	114	ILE
39	H	116	CYS

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Mol	Chain	Res	Type
39	H	133	GLU
39	H	143	THR
39	H	150	THR
39	H	158	CYS
40	I	71	CYS
40	I	166	CYS
40	I	177	ILE
41	J	86	ASN
41	J	147	VAL
42	L	32	HIS
42	L	52	THR
42	L	92	MET
42	L	102	GLU
42	L	113	LYS
42	L	119	ASN
42	L	124	LEU
42	L	158	LYS
42	L	207	ARG
42	L	232	LYS
42	L	235	VAL
42	L	305	PHE
42	L	312	ASP
42	L	363	ASP
42	L	364	VAL
43	M	8	ILE
43	M	10	LEU
43	M	16	SER
43	M	31	ILE
43	M	41	LEU
43	M	106	LEU
43	M	109	ASP
44	N	5	LEU
44	N	11	LEU
44	N	19	THR
44	N	70	GLU
44	N	88	LEU
44	N	95	LEU
45	O	74	LEU
45	O	87	LEU
45	O	106	LYS
45	O	108	LEU
45	O	112	SER

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Mol	Chain	Res	Type
45	O	138	LEU
46	P	16	LEU
46	P	19	ILE
46	P	57	GLU
46	P	58	CYS
47	Q	51	MET
47	Q	68	GLU
47	Q	72	THR
47	Q	107	LEU
47	Q	117	GLU
47	Q	127	THR
48	S	59	ARG
49	T	120	LEU
49	T	150	ASP
49	T	151	VAL
50	V	48	SER
51	W	110	VAL
51	W	120	MET
52	Y	40	ILE
52	Y	46	GLN
52	Y	50	LEU
52	Y	51	THR
52	Y	62	SER
52	Y	76	ASP
52	Y	78	ASP
52	Y	80	VAL
52	Y	88	ASP
52	Y	95	GLU
52	Y	96	GLU
53	b	15	LEU
53	b	24	LYS
53	b	28	LEU
53	b	69	ILE
53	b	117	ILE
53	b	119	LEU
53	b	120	MET
54	c	74	ASP
54	c	156	VAL
54	c	186	ILE
55	d	8	ASP
55	d	17	THR
55	d	50	GLU

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Mol	Chain	Res	Type
55	d	84	CYS
56	e	52	THR
56	e	55	LEU
56	e	58	ASP
56	e	89	VAL
56	e	101	LEU
56	e	125	LEU
56	e	134	LEU
56	e	136	LEU
58	g	2	THR
58	g	16	LEU
58	g	27	LYS
58	g	114	ILE
59	h	54	LYS
59	h	86	LEU
60	j	57	LEU
60	j	82	ASN
60	j	86	THR
61	k	10	MET
61	k	29	SER
61	k	43	MET
61	k	70	GLU
61	k	76	SER
62	l	7	LEU
62	l	13	ILE
62	l	36	VAL
62	l	37	LYS
62	l	62	ILE
62	l	70	THR
62	l	129	MET
62	l	140	LEU
62	l	238	GLU
62	l	246	LEU
62	l	267	MET
62	l	286	LEU
62	l	340	PHE
62	l	373	LEU
62	l	387	THR
62	l	410	LEU
62	l	426	ILE
62	l	503	GLU
63	n	3	ASN

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Mol	Chain	Res	Type
63	n	10	ASP
63	n	27	LEU
63	n	35	LEU
63	n	58	LYS
64	o	50	GLN
64	o	57	LEU
65	r	13	ILE
65	r	33	LEU
65	r	106	LEU
65	r	111	LEU
65	r	150	LEU
65	r	151	LEU
65	r	198	PHE
65	r	227	GLU
65	r	282	TYR
65	r	310	MET
66	s	97	VAL
66	s	177	CYS
66	s	186	GLU
66	s	188	VAL
29	u	54	ASP
29	u	68	THR
29	u	95	HIS
29	u	116	MET
29	u	153	ASN
29	u	157	GLU
29	u	190	THR
29	u	253	LEU
29	u	258	VAL
29	u	341	PHE
29	u	342	GLN
29	u	403	LEU
29	u	417	LEU
30	v	43	LEU
30	v	130	ILE
30	v	134	MET
30	v	168	ASN
30	v	175	GLU
30	v	184	ASN
30	v	200	VAL
30	v	225	VAL
30	v	238	LEU

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Mol	Chain	Res	Type
30	v	308	SER
30	v	421	ASP
30	v	451	ASP
31	w	97	HIS
31	w	102	LEU
31	w	212	SER
31	w	214	ASP
31	w	233	LEU
31	w	281	LEU
31	w	379	TRP
32	x	128	MET
32	x	209	GLU
32	x	224	THR
32	x	249	ILE
32	x	258	ASP
32	x	264	MET
32	x	320	LEU
33	y	33	MET
33	y	75	ILE
33	y	99	ILE
33	y	103	LYS
12	z	5	PHE
12	z	16	THR
45	X	89	LEU
45	X	94	ASP
45	X	107	ASP
45	X	124	ASP
45	X	138	LEU
45	X	140	CYS
67	R	89	LEU
28	Ae	62	THR
28	Ae	67	VAL
28	Ae	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

Mol	Chain	Res	Type
2	t	44	GLN
2	t	47	ASN
2	t	54	GLN
2	t	92	HIS
3	F	74	GLN

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Mol	Chain	Res	Type
4	K	59	HIS
4	K	69	ASN
4	K	112	ASN
4	K	113	HIS
4	K	123	GLN
4	K	135	GLN
5	U	144	GLN
5	U	204	HIS
7	a	141	GLN
7	a	170	GLN
7	a	181	HIS
7	a	189	ASN
8	i	134	GLN
8	i	171	ASN
8	i	221	HIS
8	i	232	HIS
8	i	289	ASN
10	p	56	GLN
11	q	30	HIS
11	q	44	GLN
11	q	144	ASN
11	q	184	HIS
11	q	374	ASN
12	Aa	65	GLN
13	Ab	36	GLN
13	Ab	76	HIS
17	Ah	34	GLN
20	Ak	55	ASN
20	Ak	138	HIS
20	Ak	151	HIS
20	Ak	178	GLN
20	Ak	214	ASN
20	Ak	422	ASN
20	Ak	491	ASN
21	Al	10	GLN
21	Al	22	HIS
22	Am	56	GLN
22	Am	68	GLN
22	Am	149	HIS
23	An	54	ASN
23	An	165	ASN
24	Ao	130	GLN

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Mol	Chain	Res	Type
25	Ap	63	ASN
25	Ap	97	ASN
25	Ap	119	HIS
27	Ar	26	GLN
27	Ar	33	ASN
27	Ar	38	HIS
13	0	88	ASN
28	2	240	HIS
15	3	16	ASN
28	4	185	ASN
28	4	220	GLN
28	4	221	HIS
29	5	152	GLN
29	5	207	ASN
29	5	247	GLN
29	5	469	ASN
30	6	36	GLN
30	6	75	ASN
30	6	155	GLN
30	6	168	ASN
30	6	170	GLN
30	6	311	GLN
30	6	318	HIS
30	6	319	GLN
30	6	343	GLN
30	6	357	GLN
30	6	443	ASN
31	7	97	HIS
32	8	91	HIS
32	8	116	GLN
32	8	241	GLN
32	8	251	ASN
32	8	310	HIS
33	9	23	ASN
34	B	244	ASN
34	B	270	ASN
34	B	277	ASN
34	B	303	HIS
34	B	452	GLN
35	C	196	HIS
35	C	239	HIS
35	C	240	GLN

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Mol	Chain	Res	Type
35	C	271	ASN
35	C	305	GLN
35	C	460	GLN
36	D	57	GLN
36	D	75	GLN
36	D	124	ASN
36	D	181	HIS
36	D	236	ASN
37	E	41	HIS
37	E	99	ASN
37	E	144	ASN
37	E	153	GLN
37	E	189	ASN
38	G	202	ASN
38	G	304	GLN
38	G	498	GLN
38	G	652	ASN
38	G	666	GLN
38	G	688	GLN
39	H	159	GLN
40	I	123	GLN
40	I	179	GLN
41	J	85	ASN
42	L	74	GLN
42	L	117	HIS
42	L	145	HIS
42	L	149	GLN
43	M	25	GLN
43	M	51	ASN
44	N	41	ASN
44	N	50	GLN
45	O	142	GLN
46	P	31	GLN
46	P	81	ASN
47	Q	77	GLN
48	S	44	GLN
48	S	46	ASN
48	S	61	HIS
48	S	68	ASN
49	T	156	GLN
51	W	61	GLN
51	W	76	GLN

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Mol	Chain	Res	Type
52	Y	54	GLN
52	Y	57	GLN
52	Y	83	HIS
53	b	59	ASN
53	b	126	GLN
54	c	115	ASN
55	d	23	GLN
55	d	107	GLN
55	d	123	GLN
56	e	74	HIS
56	e	86	ASN
56	e	148	GLN
59	h	7	GLN
59	h	82	GLN
60	j	28	ASN
62	l	56	HIS
62	l	194	ASN
62	l	309	GLN
62	l	323	HIS
62	l	446	ASN
62	l	506	ASN
62	l	546	GLN
62	l	580	GLN
62	l	603	ASN
63	n	3	ASN
63	n	14	HIS
64	o	55	ASN
64	o	123	GLN
65	r	5	ASN
65	r	47	GLN
65	r	138	GLN
65	r	169	GLN
65	r	194	ASN
65	r	304	HIS
66	s	112	GLN
66	s	150	GLN
66	s	154	HIS
66	s	228	ASN
29	u	49	GLN
29	u	160	GLN
29	u	222	GLN
29	u	247	GLN

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Mol	Chain	Res	Type
29	u	469	ASN
30	v	75	ASN
30	v	170	GLN
30	v	184	ASN
30	v	188	ASN
30	v	239	ASN
30	v	372	GLN
30	v	443	ASN
31	w	255	ASN
33	y	23	ASN
67	R	78	HIS
67	R	79	HIS
67	R	90	ASN
28	Ae	39	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 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
73	SF4	B	502	34	0,12,12	-	-	-		
73	SF4	G	801	38	0,12,12	-	-	-		
72	FMN	B	501	-	33,33,33	1.11	2 (6%)	48,50,50	1.28	8 (16%)
71	HEC	8	401	32	50,50,50	1.73	5 (10%)	68,82,82	1.50	8 (11%)
73	SF4	I	201	40	0,12,12	-	-	-		
74	NDP	L	401	-	51,52,52	0.49	0	71,80,80	0.77	1 (1%)
70	HEM	w	402	31	50,50,50	1.45	6 (12%)	67,82,82	0.96	1 (1%)
70	HEM	7	402	-	50,50,50	1.34	6 (12%)	67,82,82	1.09	5 (7%)
69	FES	2	301	28	0,4,4	-	-	-		
70	HEM	w	401	-	50,50,50	1.33	6 (12%)	67,82,82	1.10	3 (4%)
73	SF4	H	301	39	0,12,12	-	-	-		
68	HEA	Ak	602	20	67,67,67	1.20	6 (8%)	81,103,103	1.55	19 (23%)
69	FES	G	803	38	0,4,4	-	-	-		
73	SF4	G	802	-	0,12,12	-	-	-		
69	FES	4	301	28	0,4,4	-	-	-		
73	SF4	H	302	39	0,12,12	-	-	-		
68	HEA	Ak	601	20	67,67,67	1.22	7 (10%)	81,103,103	1.57	18 (22%)
75	ZMP	Q	201	-	27,29,36	1.80	6 (22%)	34,38,45	1.77	7 (20%)
70	HEM	7	401	31	50,50,50	1.46	6 (12%)	67,82,82	1.19	3 (4%)
69	FES	E	301	37	0,4,4	-	-	-		
71	HEC	x	401	32	50,50,50	1.72	5 (10%)	68,82,82	1.33	7 (10%)

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
73	SF4	B	502	34	-	-	0/6/5/5
73	SF4	G	801	38	-	-	0/6/5/5
72	FMN	B	501	-	-	6/18/18/18	0/3/3/3
71	HEC	8	401	32	1/1/3/7	2/14/54/54	-
74	NDP	L	401	-	-	8/34/77/77	0/5/5/5
73	SF4	I	201	40	-	-	0/6/5/5
70	HEM	w	402	31	-	3/14/54/54	-
70	HEM	7	402	-	-	4/14/54/54	-
69	FES	2	301	28	-	-	0/1/1/1
70	HEM	w	401	-	-	3/14/54/54	-
73	SF4	H	301	39	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	HEA	Ak	602	20	-	8/36/76/76	-
69	FES	G	803	38	-	-	0/1/1/1
73	SF4	G	802	-	-	-	0/6/5/5
69	FES	4	301	28	-	-	0/1/1/1
73	SF4	H	302	39	-	-	0/6/5/5
68	HEA	Ak	601	20	-	14/36/76/76	-
75	ZMP	Q	201	-	-	13/36/36/43	-
70	HEM	7	401	31	-	8/14/54/54	-
69	FES	E	301	37	-	-	0/1/1/1
71	HEC	x	401	32	1/1/3/7	9/14/54/54	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	8	401	HEC	C3D-C2D	7.98	1.54	1.36
71	x	401	HEC	C3D-C2D	7.69	1.53	1.36
75	Q	201	ZMP	C16-N2	5.31	1.46	1.33
75	Q	201	ZMP	C13-N1	5.24	1.45	1.33
71	8	401	HEC	FE-ND	4.45	2.08	1.94
68	Ak	602	HEA	CMA-C3A	-4.00	1.36	1.45
71	x	401	HEC	FE-ND	3.83	2.06	1.94
71	8	401	HEC	FE-NB	3.83	2.06	1.94
68	Ak	601	HEA	CMA-C3A	-3.78	1.36	1.45
70	7	401	HEM	FE-ND	3.71	2.06	1.94
70	7	401	HEM	FE-NB	3.65	2.06	1.94
70	7	401	HEM	FE-NC	3.64	2.07	1.95
70	w	402	HEM	FE-NB	3.63	2.06	1.94
71	x	401	HEC	FE-NA	3.63	2.07	1.95
70	w	402	HEM	FE-ND	3.58	2.05	1.94
68	Ak	601	HEA	C1D-C2D	3.44	1.51	1.44
70	w	402	HEM	FE-NC	3.44	2.06	1.95
71	x	401	HEC	FE-NB	3.43	2.05	1.94
72	B	501	FMN	C4A-N5	3.42	1.38	1.30
70	w	401	HEM	FE-ND	3.28	2.05	1.94
71	x	401	HEC	FE-NC	3.27	2.05	1.95
70	7	402	HEM	FE-ND	3.20	2.04	1.94
70	w	401	HEM	CAC-C3C	3.06	1.55	1.47
70	7	402	HEM	CAC-C3C	3.01	1.55	1.47
70	7	402	HEM	CAB-C3B	2.99	1.55	1.47
70	w	402	HEM	CAB-C3B	2.99	1.55	1.47
70	w	401	HEM	CAB-C3B	2.98	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	w	402	HEM	CAC-C3C	2.98	1.55	1.47
70	7	401	HEM	FE-NA	2.96	2.04	1.95
70	w	402	HEM	FE-NA	2.89	2.04	1.95
70	7	401	HEM	CAC-C3C	2.89	1.55	1.47
70	7	401	HEM	CAB-C3B	2.81	1.54	1.47
71	8	401	HEC	FE-NC	2.79	2.04	1.95
70	7	402	HEM	FE-NC	2.78	2.04	1.95
68	Ak	602	HEA	C1D-C2D	2.78	1.50	1.44
70	w	401	HEM	FE-NA	2.61	2.03	1.95
70	w	401	HEM	FE-NB	2.60	2.02	1.94
70	7	402	HEM	FE-NB	2.57	2.02	1.94
71	8	401	HEC	FE-NA	2.56	2.03	1.95
68	Ak	601	HEA	CHC-C1C	-2.51	1.33	1.39
75	Q	201	ZMP	C10-S1	2.50	1.82	1.76
68	Ak	602	HEA	FE-NC	2.48	2.03	1.95
68	Ak	602	HEA	CMD-C2D	2.41	1.55	1.50
72	B	501	FMN	C10-N1	2.40	1.38	1.33
70	w	401	HEM	FE-NC	2.38	2.03	1.95
75	Q	201	ZMP	O3-C16	-2.33	1.18	1.23
70	7	402	HEM	FE-NA	2.33	2.02	1.95
68	Ak	601	HEA	FE-NC	2.32	2.02	1.95
68	Ak	602	HEA	CHC-C1C	-2.30	1.34	1.39
75	Q	201	ZMP	O2-C13	-2.28	1.18	1.23
68	Ak	601	HEA	CMD-C2D	2.21	1.55	1.50
75	Q	201	ZMP	C9-C10	2.19	1.53	1.50
68	Ak	601	HEA	C4C-NC	-2.16	1.35	1.39
68	Ak	601	HEA	O2A-CGA	-2.13	1.23	1.30
68	Ak	602	HEA	C4C-NC	-2.00	1.35	1.39

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	Q	201	ZMP	C9-C10-S1	5.52	119.98	113.40
71	8	401	HEC	C1D-ND-C4D	5.50	111.72	105.21
71	x	401	HEC	C1D-ND-C4D	5.06	111.20	105.21
74	L	401	NDP	P2B-O2B-C2B	-5.05	109.96	123.43
71	8	401	HEC	CAC-C3C-C4C	4.49	131.09	124.91
68	Ak	601	HEA	CAA-C2A-C1A	-4.07	116.58	124.85
68	Ak	601	HEA	CHB-C4A-NA	-3.99	120.11	124.45
68	Ak	602	HEA	CHB-C4A-NA	-3.66	120.46	124.45
68	Ak	602	HEA	OMA-CMA-C3A	-3.61	117.48	125.62
75	Q	201	ZMP	O1-C10-C9	-3.58	119.85	123.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	Ak	601	HEA	CMD-C2D-C1D	3.56	130.59	125.03
68	Ak	601	HEA	C3D-C4D-ND	3.45	113.68	110.35
72	B	501	FMN	C4-N3-C2	-3.39	119.63	125.64
68	Ak	601	HEA	C3C-C4C-NC	3.16	112.46	109.80
68	Ak	601	HEA	CMB-C2B-C3B	-3.10	124.28	130.28
75	Q	201	ZMP	O3-C16-N2	-2.99	116.66	122.98
68	Ak	602	HEA	C1D-C2D-C3D	-2.95	103.88	106.98
71	8	401	HEC	CAC-C3C-C2C	-2.88	122.34	126.89
75	Q	201	ZMP	C11-S1-C10	2.86	110.29	101.84
70	w	401	HEM	C4D-ND-C1D	2.77	108.49	105.21
72	B	501	FMN	C4A-C4-N3	2.73	120.21	113.25
75	Q	201	ZMP	C17-C16-N2	2.70	121.60	116.48
72	B	501	FMN	O4-C4-C4A	-2.69	119.43	126.53
72	B	501	FMN	C4A-C10-N10	2.67	120.30	116.48
68	Ak	602	HEA	CBD-CAD-C3D	2.65	119.86	112.53
68	Ak	601	HEA	C4A-C3A-C2A	-2.61	104.55	106.81
70	7	402	HEM	C4D-ND-C1D	2.57	108.25	105.21
68	Ak	601	HEA	CHD-C1D-ND	-2.51	121.26	124.37
68	Ak	602	HEA	C3D-C4D-ND	2.50	112.77	110.35
70	7	401	HEM	C3B-C2B-C1B	2.46	108.25	106.41
70	w	401	HEM	C3D-C4D-ND	-2.43	107.50	110.17
68	Ak	602	HEA	C13-C12-C11	-2.40	110.56	114.39
68	Ak	601	HEA	CHC-C4B-NB	2.40	127.33	124.37
68	Ak	601	HEA	C20-C19-C18	-2.39	115.80	121.17
68	Ak	602	HEA	C3C-C4C-NC	2.39	111.81	109.80
68	Ak	601	HEA	CBA-CAA-C2A	2.38	119.12	112.53
68	Ak	601	HEA	C1D-C2D-C3D	-2.37	104.48	106.98
68	Ak	602	HEA	CMC-C2C-C3C	2.36	132.11	126.55
71	x	401	HEC	C2A-C1A-NA	-2.35	108.06	110.32
72	B	501	FMN	C5A-C9A-N10	2.34	120.09	117.97
71	x	401	HEC	CHA-C4D-ND	2.31	126.91	124.42
71	8	401	HEC	C2A-C1A-NA	-2.31	108.09	110.32
68	Ak	601	HEA	C26-C15-C14	-2.31	117.70	123.63
72	B	501	FMN	C10-C4A-N5	-2.26	120.20	124.81
68	Ak	602	HEA	CAD-C3D-C4D	-2.26	120.77	124.70
68	Ak	602	HEA	CAD-C3D-C2D	2.25	132.09	127.87
70	w	401	HEM	C2A-C1A-NA	-2.24	107.67	110.15
68	Ak	601	HEA	O1D-CGD-CBD	-2.21	116.09	123.09
68	Ak	602	HEA	CMD-C2D-C1D	2.20	128.47	125.03
71	8	401	HEC	C3B-C4B-NB	-2.20	107.76	110.17
71	8	401	HEC	C2C-C1C-NC	-2.20	106.62	110.14
68	Ak	602	HEA	CBA-CAA-C2A	2.19	118.58	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	Ak	602	HEA	C2B-C1B-NB	2.18	112.43	109.90
71	x	401	HEC	CAB-C3B-C4B	-2.17	121.96	124.79
68	Ak	602	HEA	CMB-C2B-C3B	-2.17	126.08	130.28
70	7	402	HEM	C3D-C4D-ND	-2.16	107.80	110.17
70	7	401	HEM	C4D-ND-C1D	2.16	107.76	105.21
71	x	401	HEC	CAA-C2A-C3A	-2.16	123.83	127.87
70	7	402	HEM	C2A-C1A-NA	-2.14	107.78	110.15
68	Ak	601	HEA	CHB-C1B-NB	2.13	126.71	124.42
71	x	401	HEC	CMB-C2B-C1B	-2.12	121.72	125.03
70	7	402	HEM	CAA-C2A-C1A	2.11	129.06	124.94
68	Ak	601	HEA	C12-C11-C3B	2.10	115.41	112.12
75	Q	201	ZMP	C14-C15-N2	-2.10	107.53	112.00
68	Ak	601	HEA	OMA-CMA-C3A	-2.09	120.90	125.62
70	7	402	HEM	C1B-NB-C4B	2.07	107.66	105.21
68	Ak	602	HEA	CHA-C4D-C3D	-2.06	121.77	124.77
71	x	401	HEC	CAD-CBD-CGD	-2.06	108.21	113.67
71	8	401	HEC	CAA-CBA-CGA	-2.06	108.21	113.67
71	8	401	HEC	CHA-C1A-NA	2.05	126.69	124.45
70	w	402	HEM	C4D-ND-C1D	2.05	107.63	105.21
68	Ak	601	HEA	C13-C14-C15	-2.05	122.94	127.62
72	B	501	FMN	C9A-C5A-N5	-2.05	120.28	122.45
70	7	401	HEM	C1B-NB-C4B	2.04	107.63	105.21
68	Ak	602	HEA	C2C-C1C-NC	2.04	113.41	110.14
68	Ak	602	HEA	CHA-C1A-NA	-2.03	122.24	124.45
72	B	501	FMN	C4A-C10-N1	-2.02	119.65	124.59
68	Ak	602	HEA	C13-C14-C15	-2.01	123.03	127.62
75	Q	201	ZMP	C14-C13-N1	2.01	120.00	116.34
68	Ak	602	HEA	C2D-C1D-ND	2.01	112.14	109.84

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
71	8	401	HEC	NA
71	x	401	HEC	NA

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	Ak	601	HEA	C1A-C2A-CAA-CBA
68	Ak	601	HEA	C2A-C3A-CMA-OMA
68	Ak	601	HEA	C2C-C3C-CAC-CBC
68	Ak	601	HEA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
68	Ak	602	HEA	C2A-C3A-CMA-OMA
68	Ak	602	HEA	C4A-C3A-CMA-OMA
68	Ak	602	HEA	C2D-C3D-CAD-CBD
68	Ak	602	HEA	C4D-C3D-CAD-CBD
70	7	402	HEM	C1A-C2A-CAA-CBA
72	B	501	FMN	C1'-C2'-C3'-O3'
72	B	501	FMN	C1'-C2'-C3'-C4'
72	B	501	FMN	O2'-C2'-C3'-O3'
72	B	501	FMN	O2'-C2'-C3'-C4'
72	B	501	FMN	C3'-C4'-C5'-O5'
72	B	501	FMN	O4'-C4'-C5'-O5'
75	Q	201	ZMP	O3-C16-C17-C18
75	Q	201	ZMP	N2-C16-C17-O4
75	Q	201	ZMP	C17-C16-N2-C15
75	Q	201	ZMP	S1-C11-C12-N1
75	Q	201	ZMP	C12-C11-S1-C10
71	x	401	HEC	C4B-C3B-CAB-CBB
71	x	401	HEC	C2B-C3B-CAB-CBB
71	8	401	HEC	C2C-C3C-CAC-CBC
71	8	401	HEC	C4C-C3C-CAC-CBC
68	Ak	601	HEA	C14-C15-C16-C17
75	Q	201	ZMP	O3-C16-N2-C15
68	Ak	601	HEA	C3A-C2A-CAA-CBA
70	7	402	HEM	C3A-C2A-CAA-CBA
68	Ak	601	HEA	C17-C18-C19-C27
74	L	401	NDP	C2D-C1D-N1N-C6N
68	Ak	601	HEA	O11-C11-C12-C13
74	L	401	NDP	C2D-C1D-N1N-C2N
74	L	401	NDP	O4B-C4B-C5B-O5B
74	L	401	NDP	O4D-C4D-C5D-O5D
68	Ak	601	HEA	C26-C15-C16-C17
70	7	401	HEM	C3D-CAD-CBD-CGD
71	x	401	HEC	C1A-C2A-CAA-CBA
74	L	401	NDP	C3B-C4B-C5B-O5B
70	7	401	HEM	C4C-C3C-CAC-CBC
75	Q	201	ZMP	O3-C16-C17-O4
71	x	401	HEC	C3A-C2A-CAA-CBA
68	Ak	601	HEA	C3B-C11-C12-C13
75	Q	201	ZMP	N2-C16-C17-C18
75	Q	201	ZMP	O1-C10-S1-C11
75	Q	201	ZMP	C9-C10-S1-C11
70	7	401	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
70	7	401	HEM	C4B-C3B-CAB-CBB
70	w	402	HEM	C2A-CAA-CBA-CGA
74	L	401	NDP	O4D-C1D-N1N-C2N
70	7	402	HEM	C4D-C3D-CAD-CBD
68	Ak	601	HEA	C4A-C3A-CMA-OMA
74	L	401	NDP	O4D-C1D-N1N-C6N
70	7	402	HEM	C2D-C3D-CAD-CBD
75	Q	201	ZMP	C11-C12-N1-C13
75	Q	201	ZMP	C4-C5-C6-C7
70	7	401	HEM	CAA-CBA-CGA-O1A
70	7	401	HEM	CAA-CBA-CGA-O2A
70	w	401	HEM	CAA-CBA-CGA-O1A
70	w	402	HEM	CAA-CBA-CGA-O1A
70	w	402	HEM	CAA-CBA-CGA-O2A
68	Ak	601	HEA	CAA-CBA-CGA-O2A
68	Ak	602	HEA	CAD-CBD-CGD-O2D
68	Ak	601	HEA	C11-C12-C13-C14
71	x	401	HEC	C4C-C3C-CAC-CBC
68	Ak	602	HEA	CAD-CBD-CGD-O1D
70	w	401	HEM	CAA-CBA-CGA-O2A
71	x	401	HEC	CAD-CBD-CGD-O2D
75	Q	201	ZMP	C6-C7-C8-C9
70	w	401	HEM	C4D-C3D-CAD-CBD
68	Ak	601	HEA	CAA-CBA-CGA-O1A
71	x	401	HEC	C2C-C3C-CAC-CBC
71	x	401	HEC	CAD-CBD-CGD-O1D
70	7	401	HEM	CAD-CBD-CGD-O1D
70	7	401	HEM	CAD-CBD-CGD-O2D
68	Ak	602	HEA	C26-C15-C16-C17
68	Ak	602	HEA	C21-C22-C23-C24
71	x	401	HEC	CAA-CBA-CGA-O2A
74	L	401	NDP	PN-O3-PA-O2A

There are no ring outliers.

19 monomers are involved in 73 short contacts:

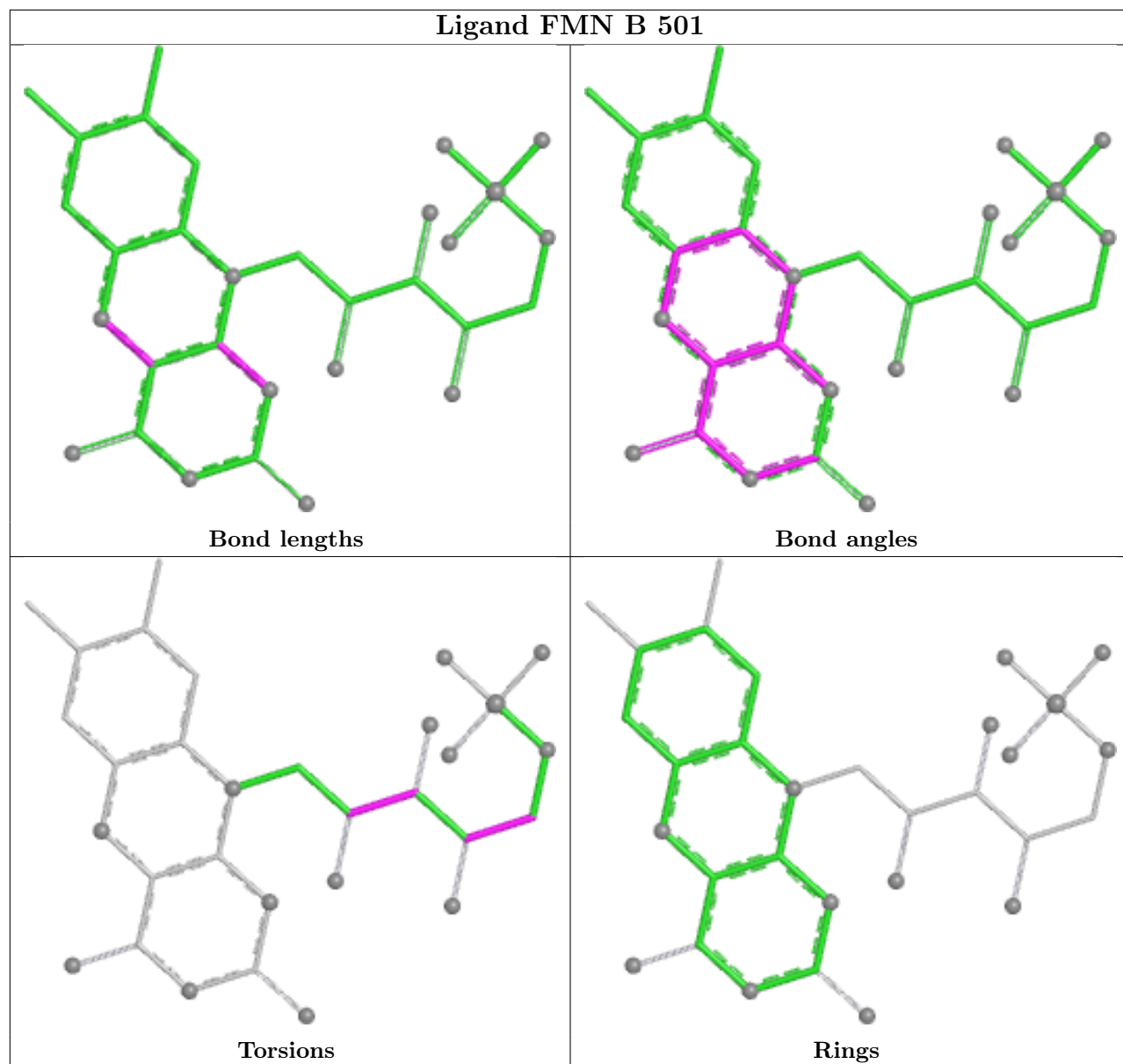
Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	B	502	SF4	2	0
73	G	801	SF4	1	0
72	B	501	FMN	1	0
71	8	401	HEC	3	0
73	I	201	SF4	1	0

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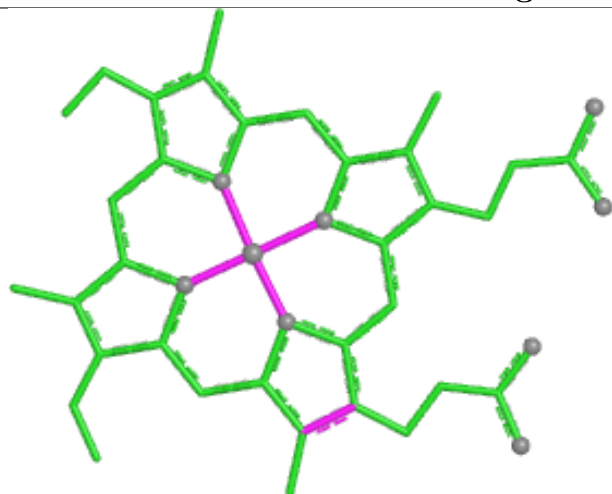
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	L	401	NDP	3	0
70	w	402	HEM	4	0
70	7	402	HEM	6	0
69	2	301	FES	6	0
70	w	401	HEM	4	0
68	Ak	602	HEA	4	0
69	G	803	FES	1	0
73	G	802	SF4	17	0
69	4	301	FES	1	0
73	H	302	SF4	1	0
68	Ak	601	HEA	9	0
75	Q	201	ZMP	1	0
70	7	401	HEM	6	0
71	x	401	HEC	2	0

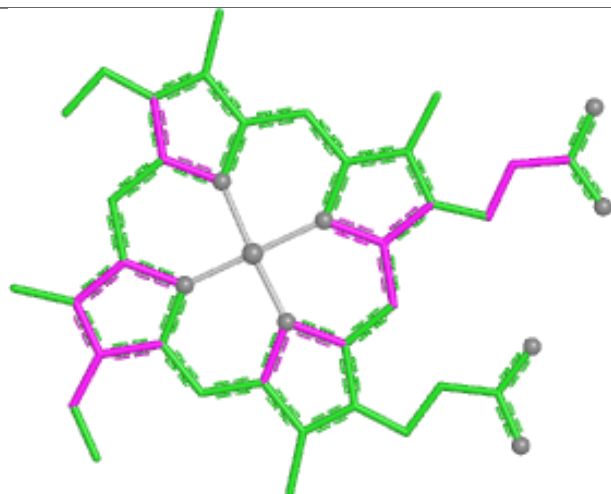
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



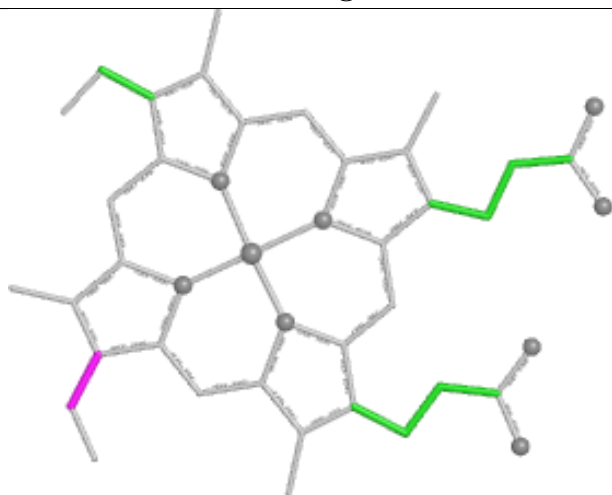
Ligand HEC 8 401



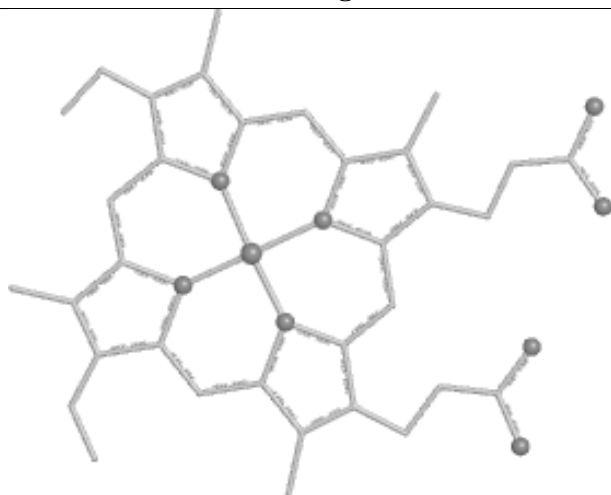
Bond lengths



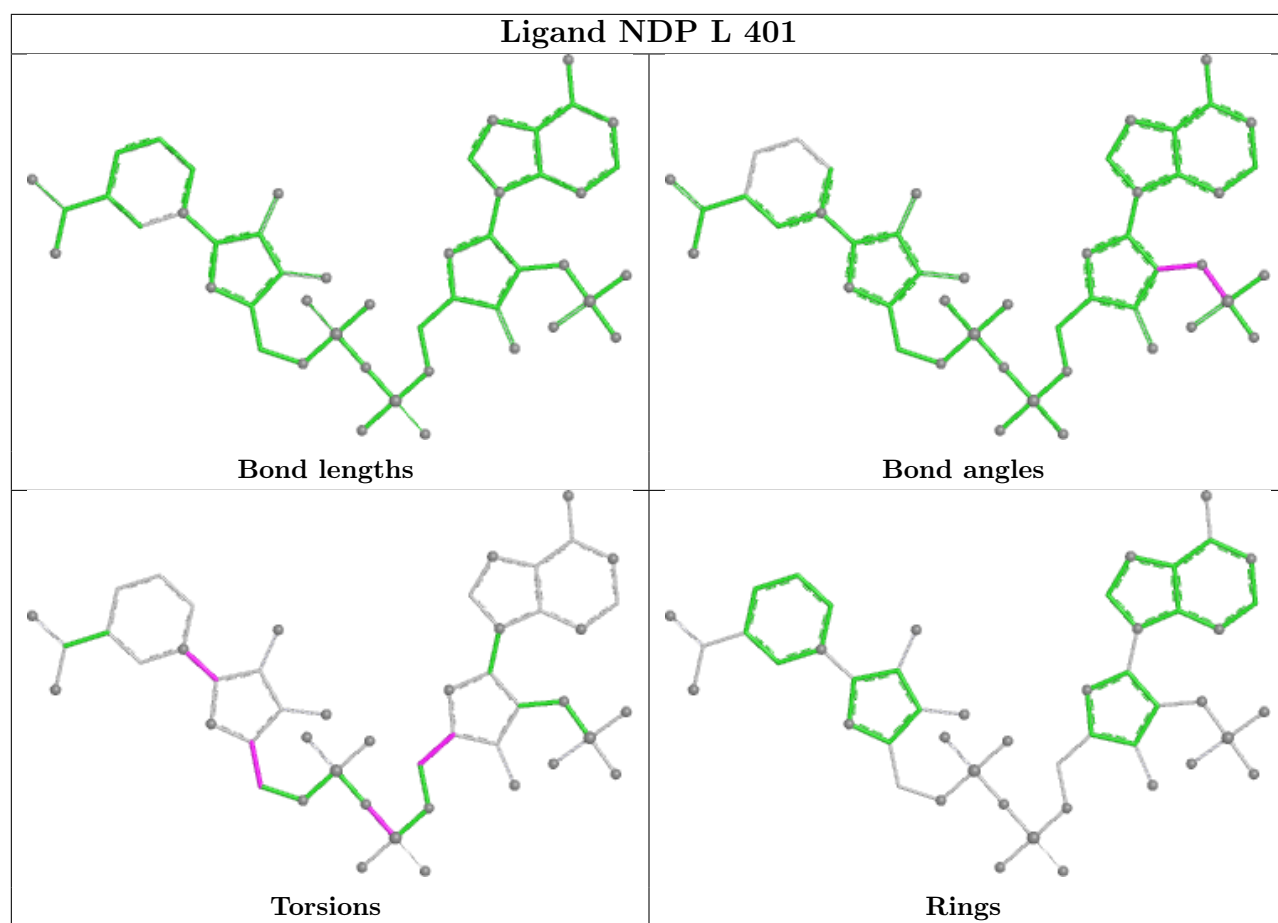
Bond angles

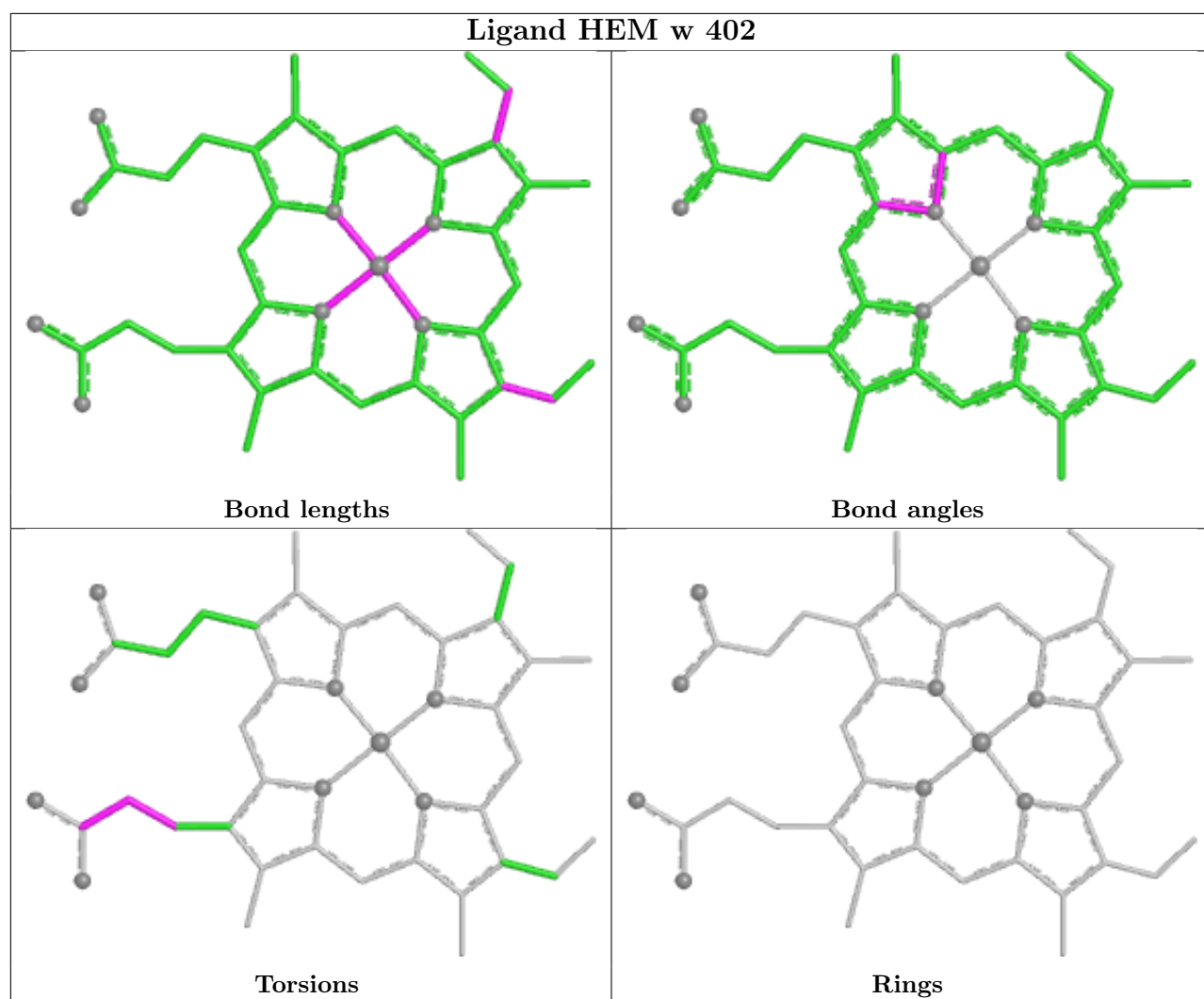


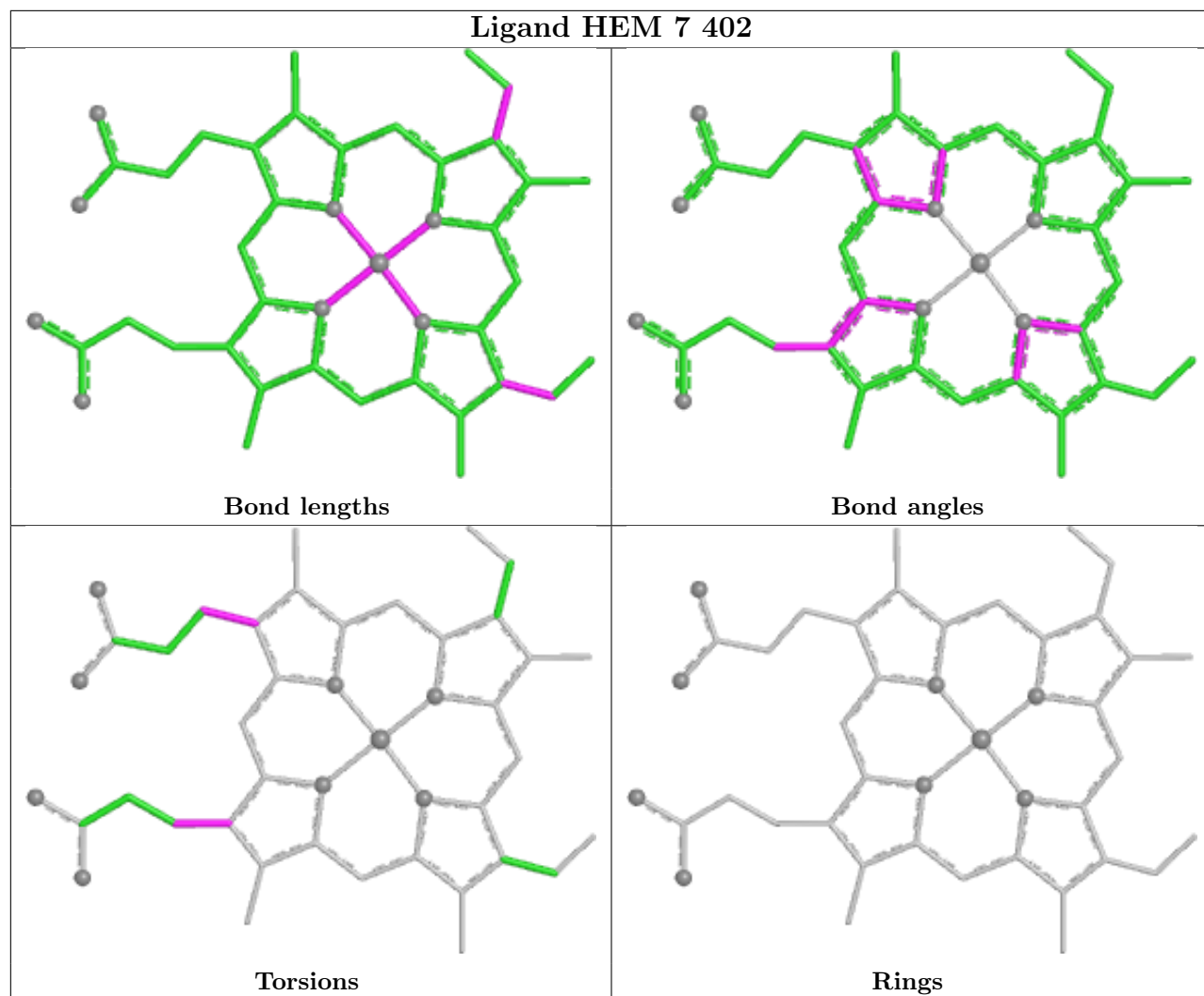
Torsions

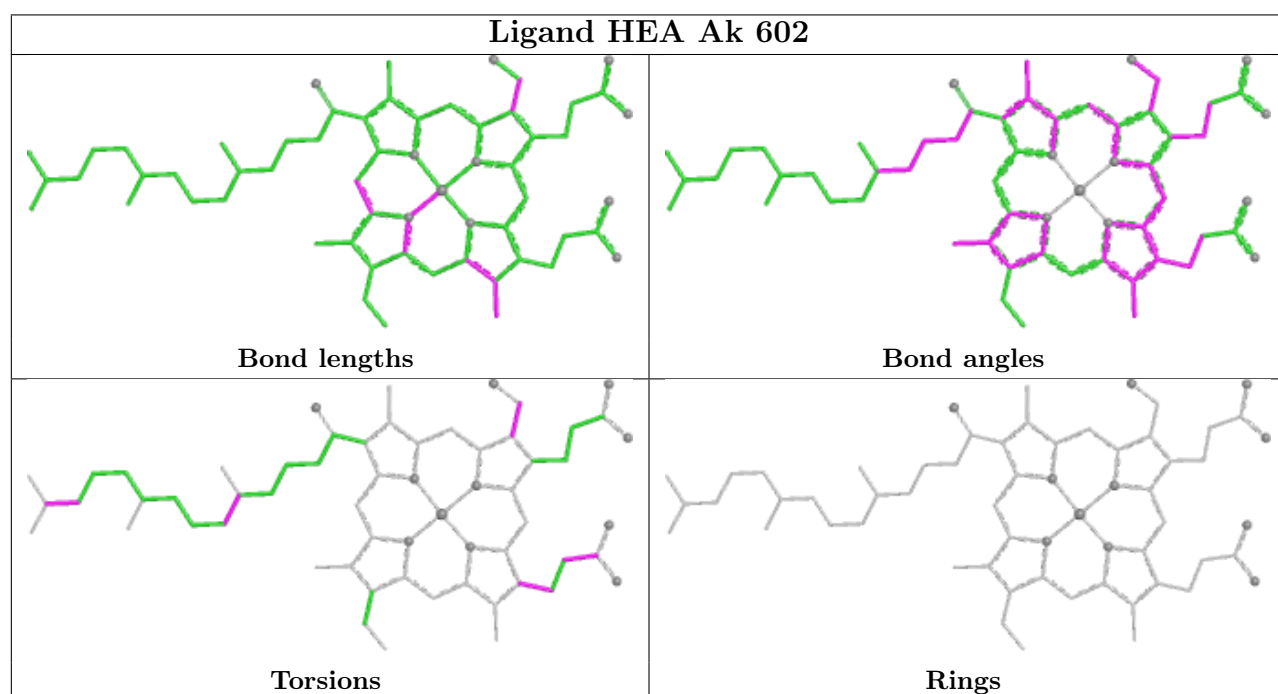
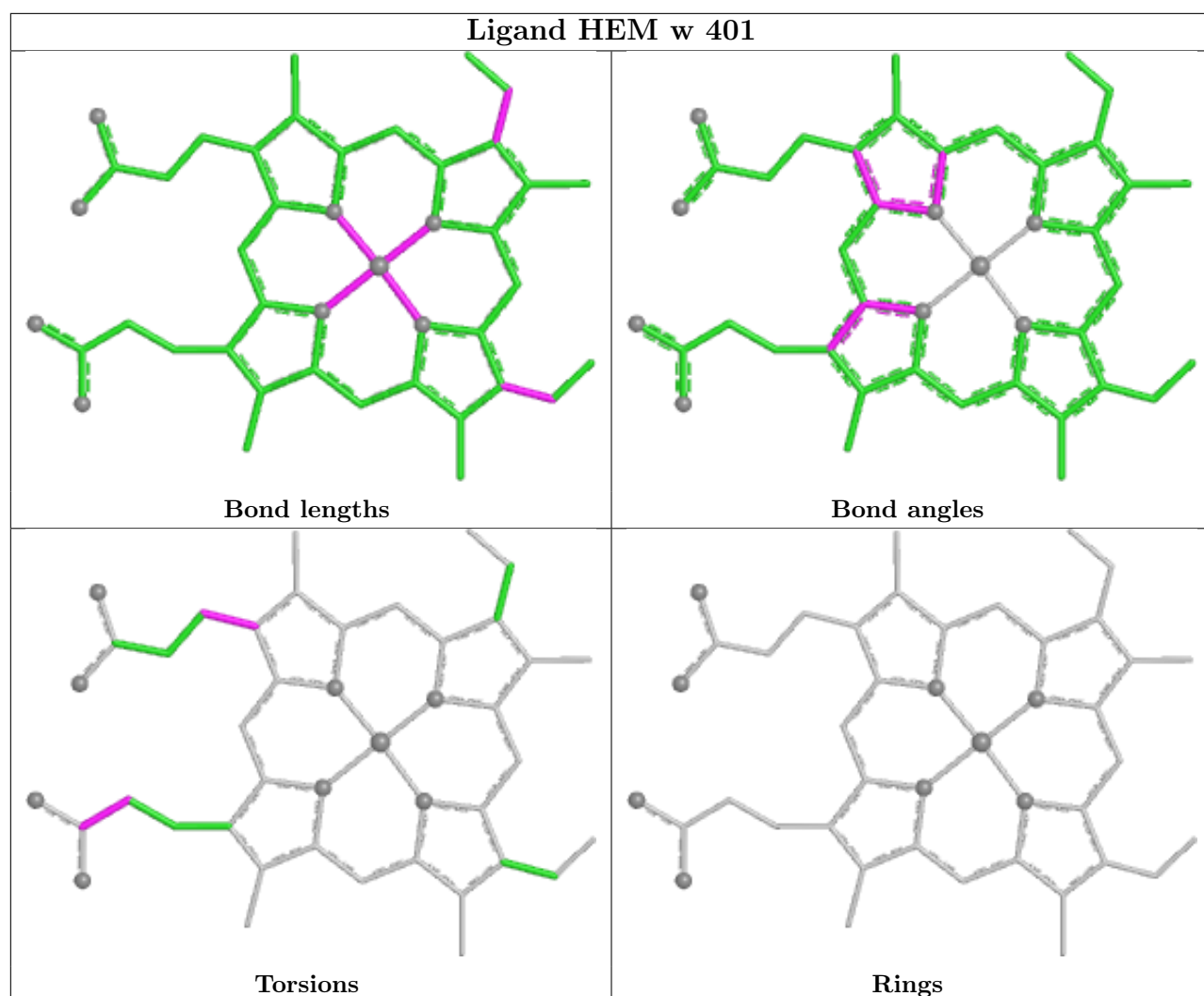


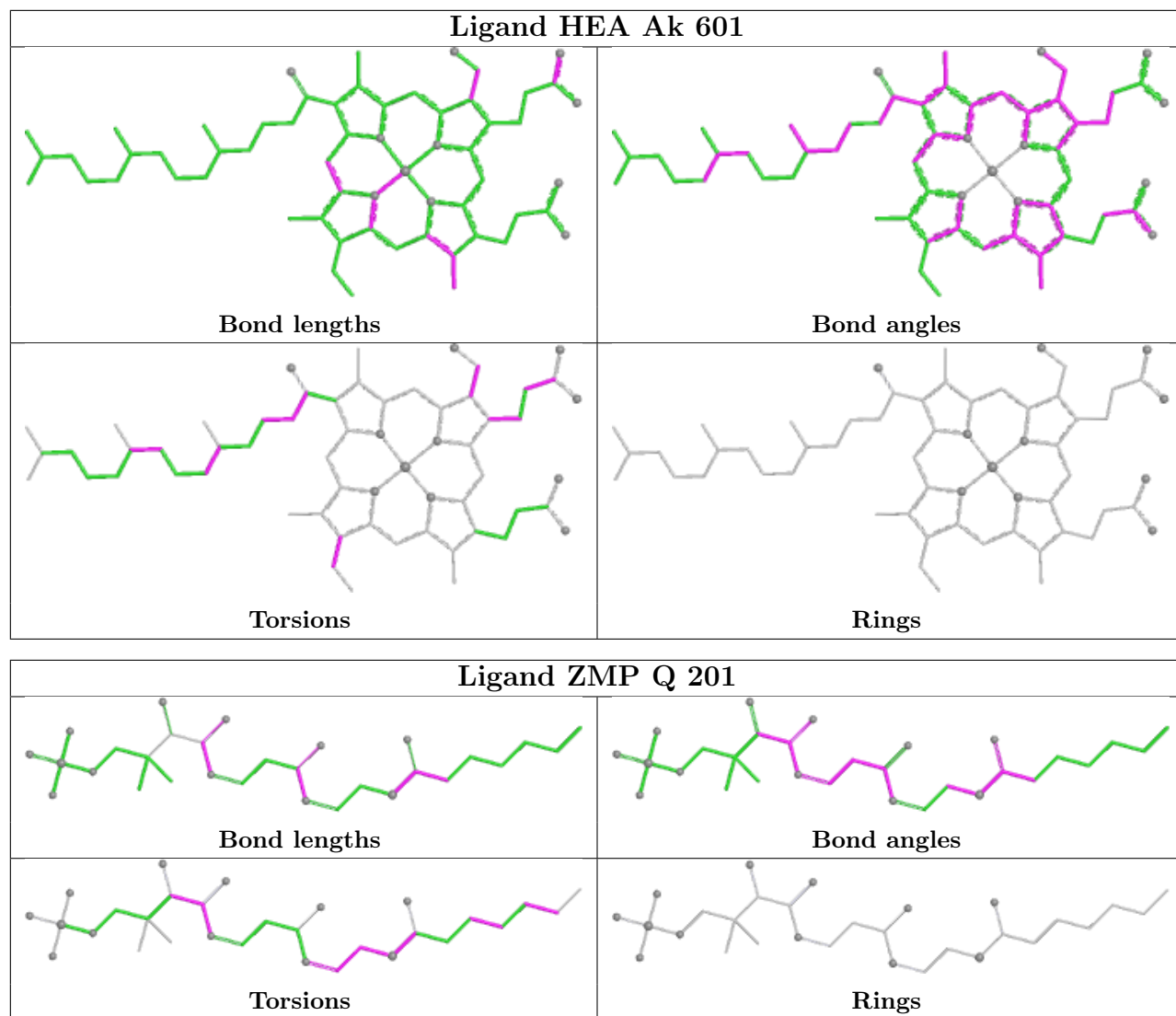
Rings

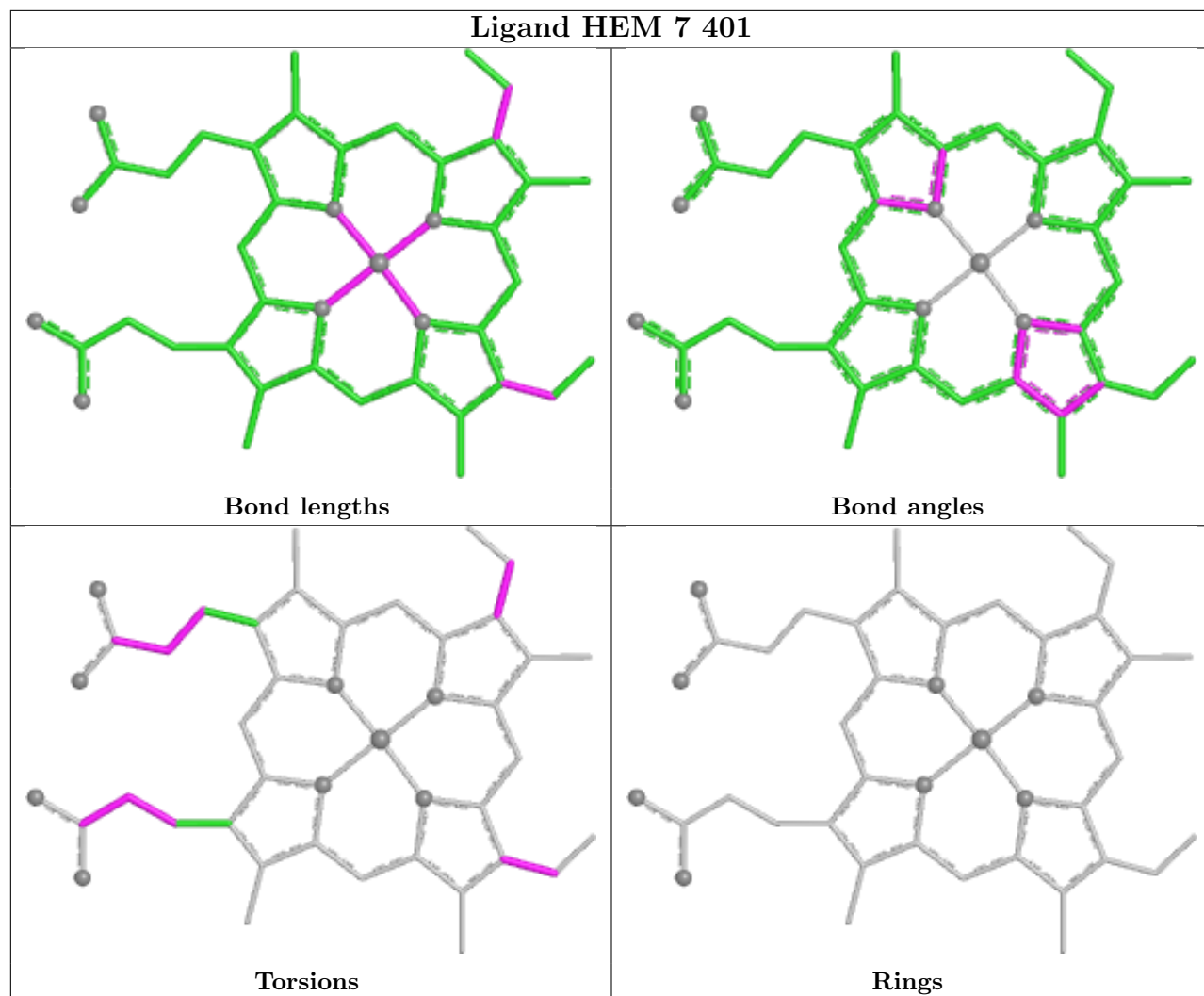


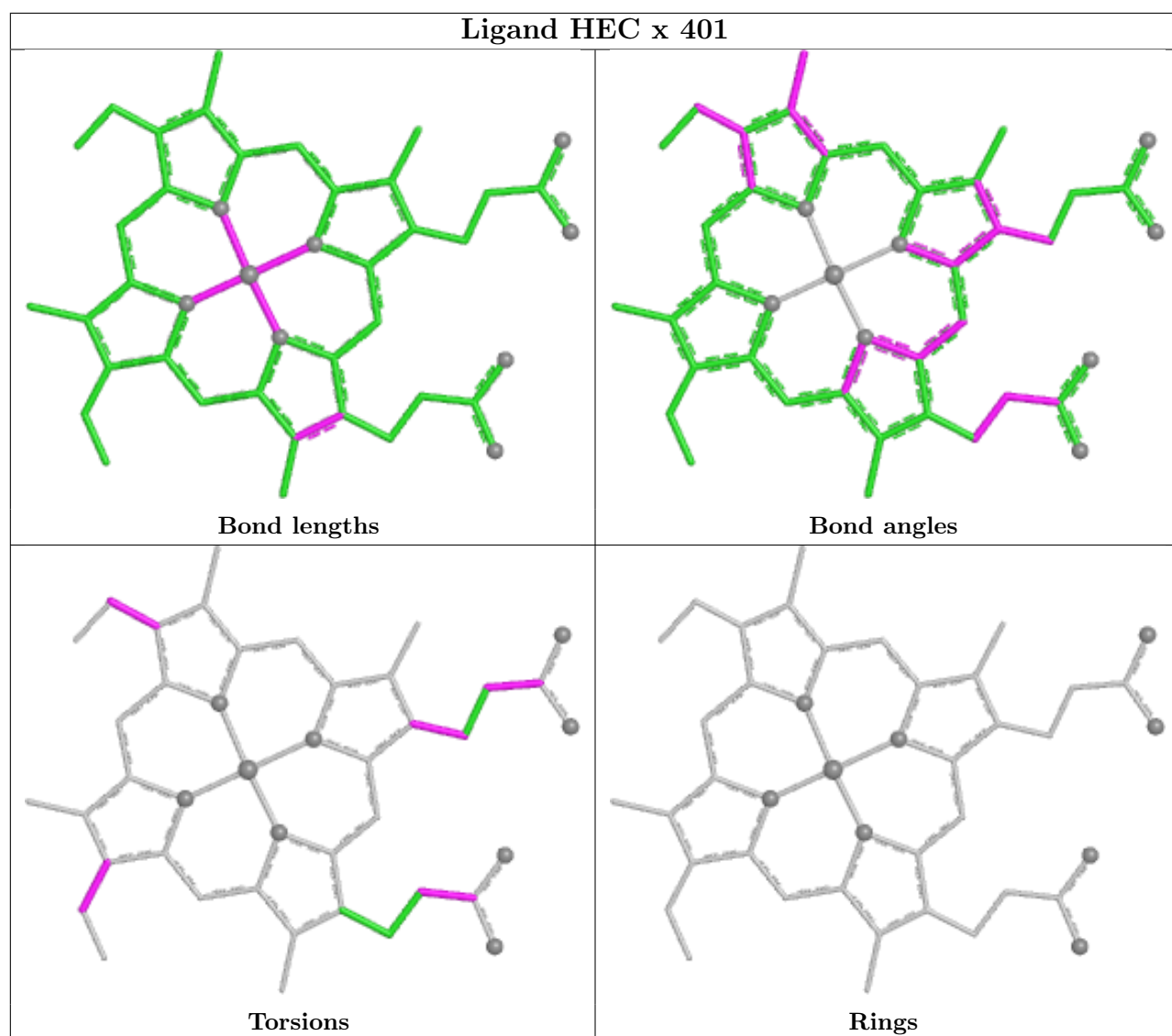












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

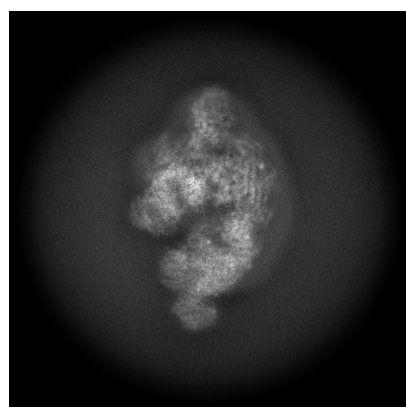
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44908. These allow visual inspection of the internal detail of the map and identification of artifacts.

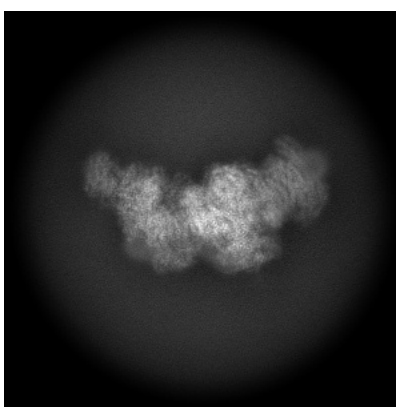
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

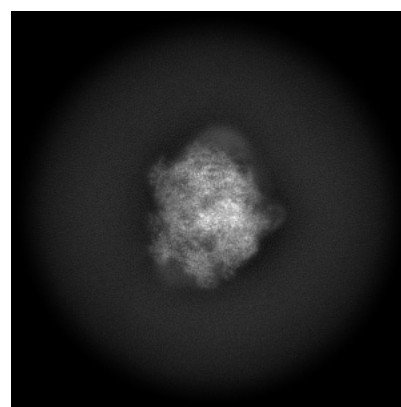
6.1.1 Primary map



X



Y

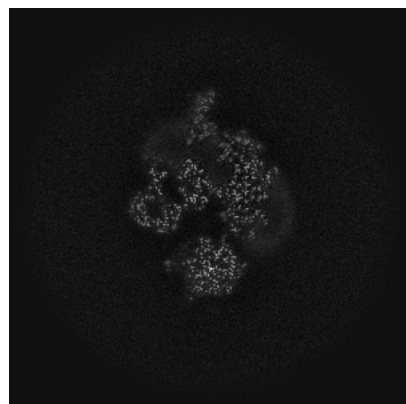


Z

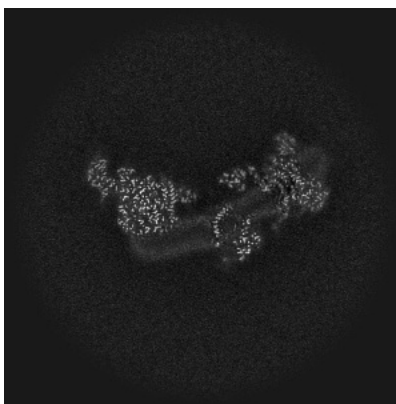
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

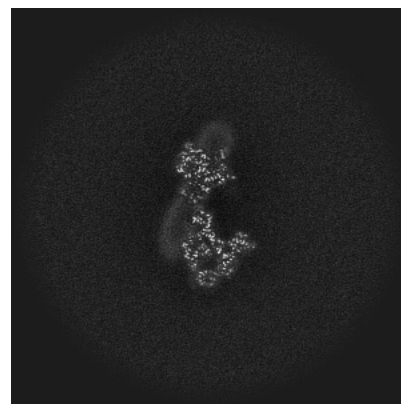
6.2.1 Primary map



X Index: 256



Y Index: 256

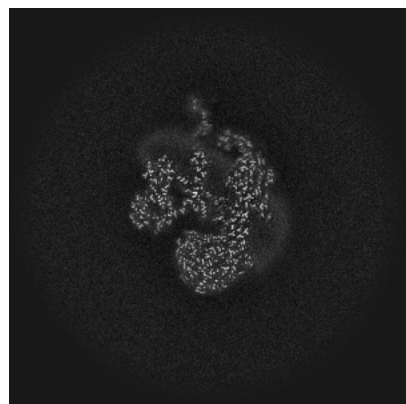


Z Index: 256

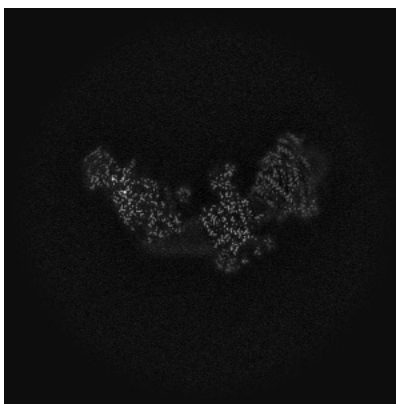
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

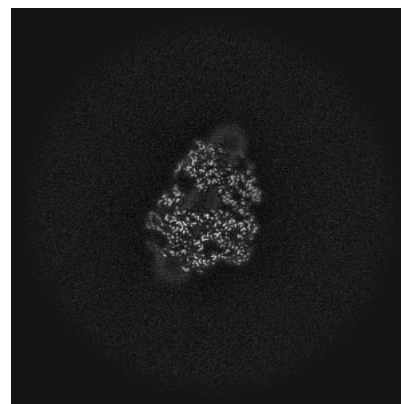
6.3.1 Primary map



X Index: 244



Y Index: 242

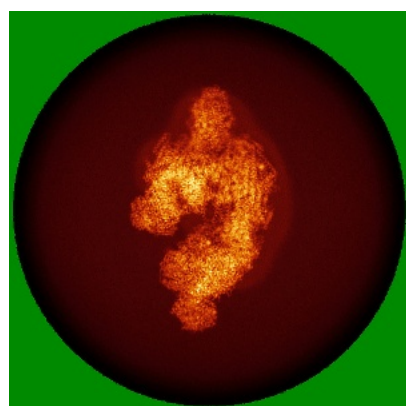


Z Index: 294

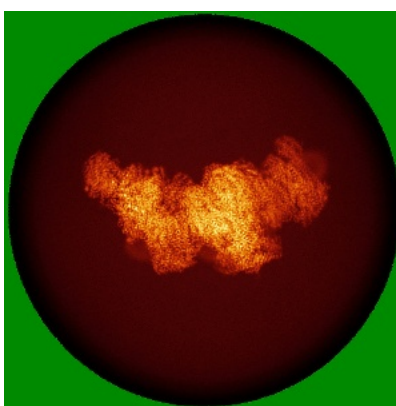
The images above show the largest variance slices of the map in three orthogonal directions.

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

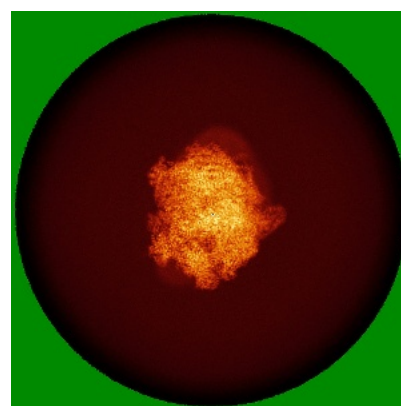
6.4.1 Primary map



X



Y

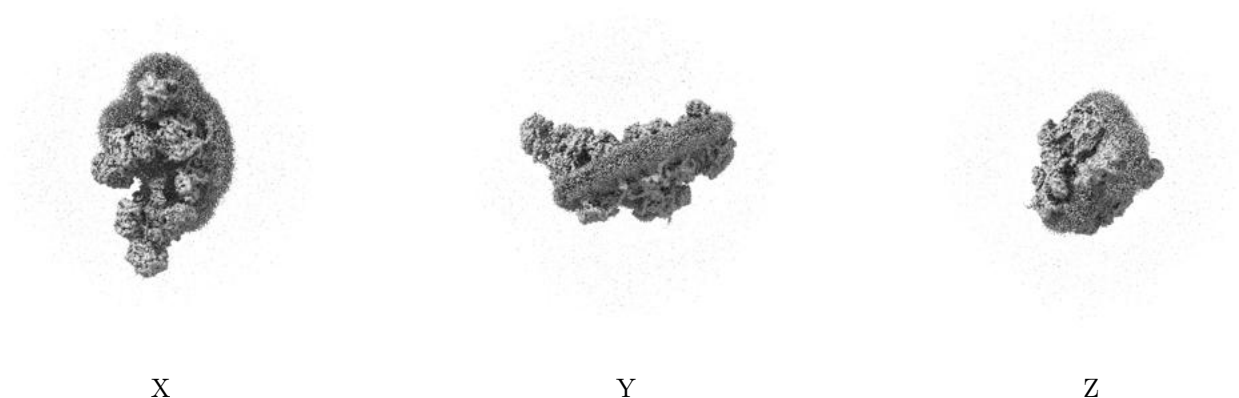


Z

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



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.

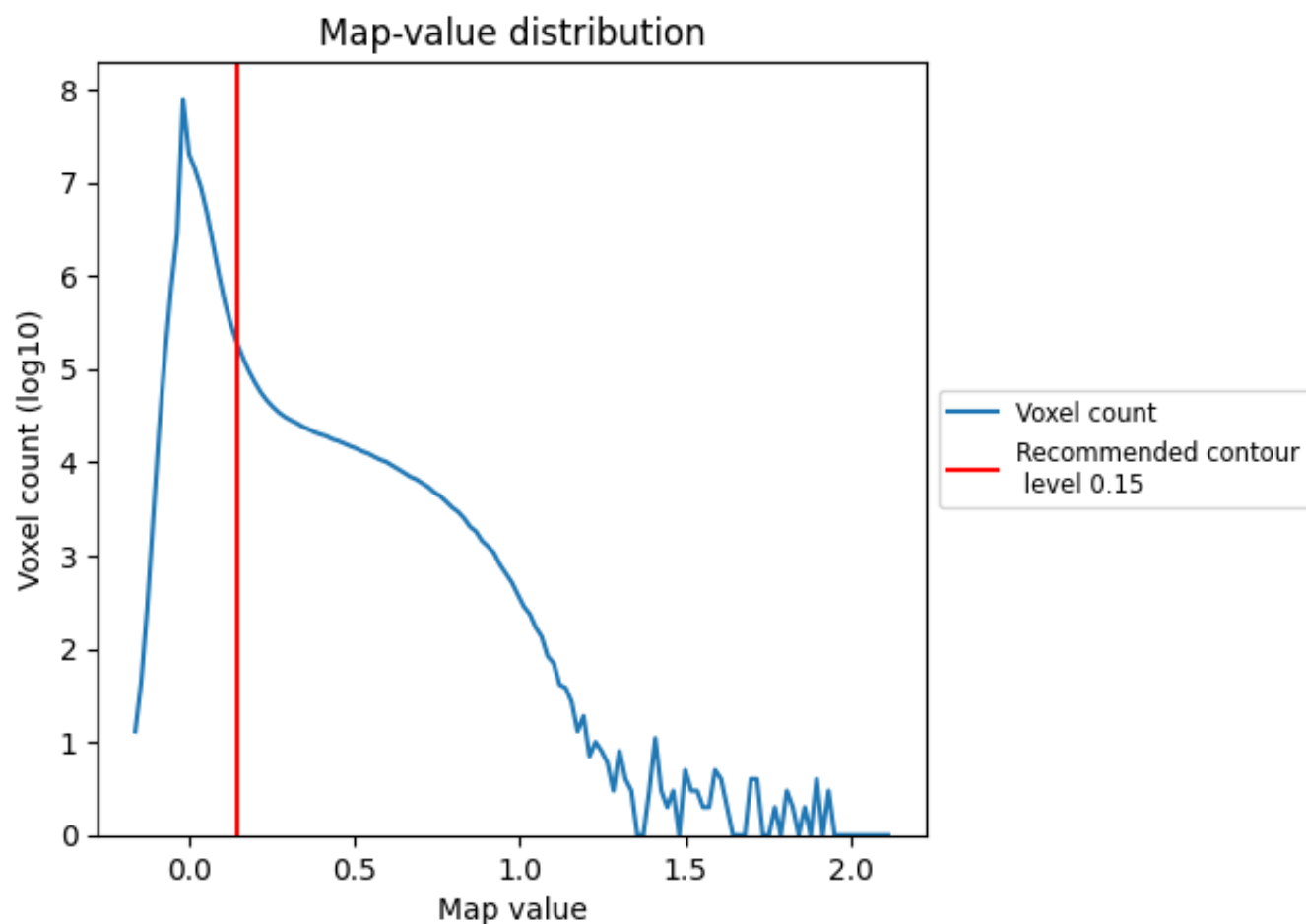
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

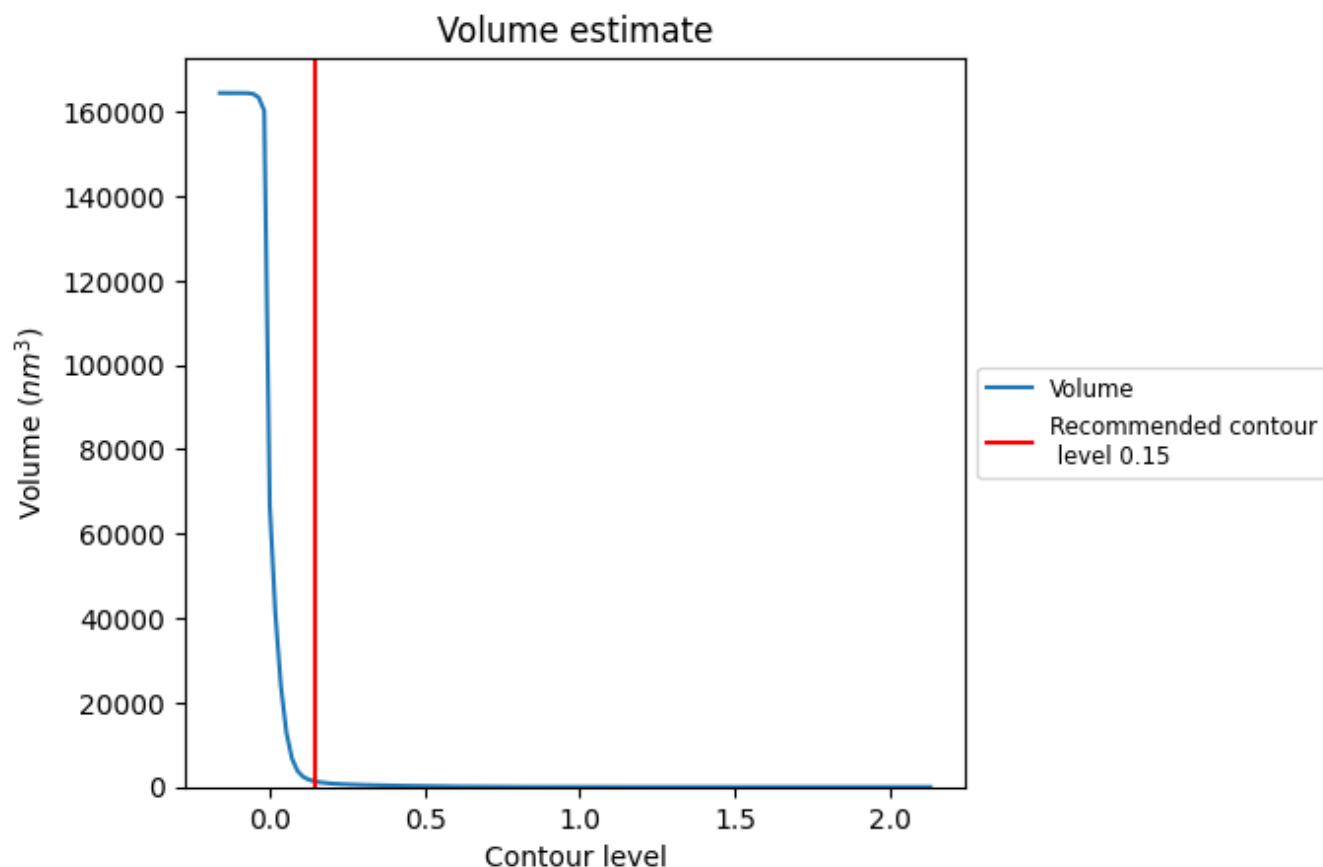
This section contains the results of statistical analysis of the map.

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.

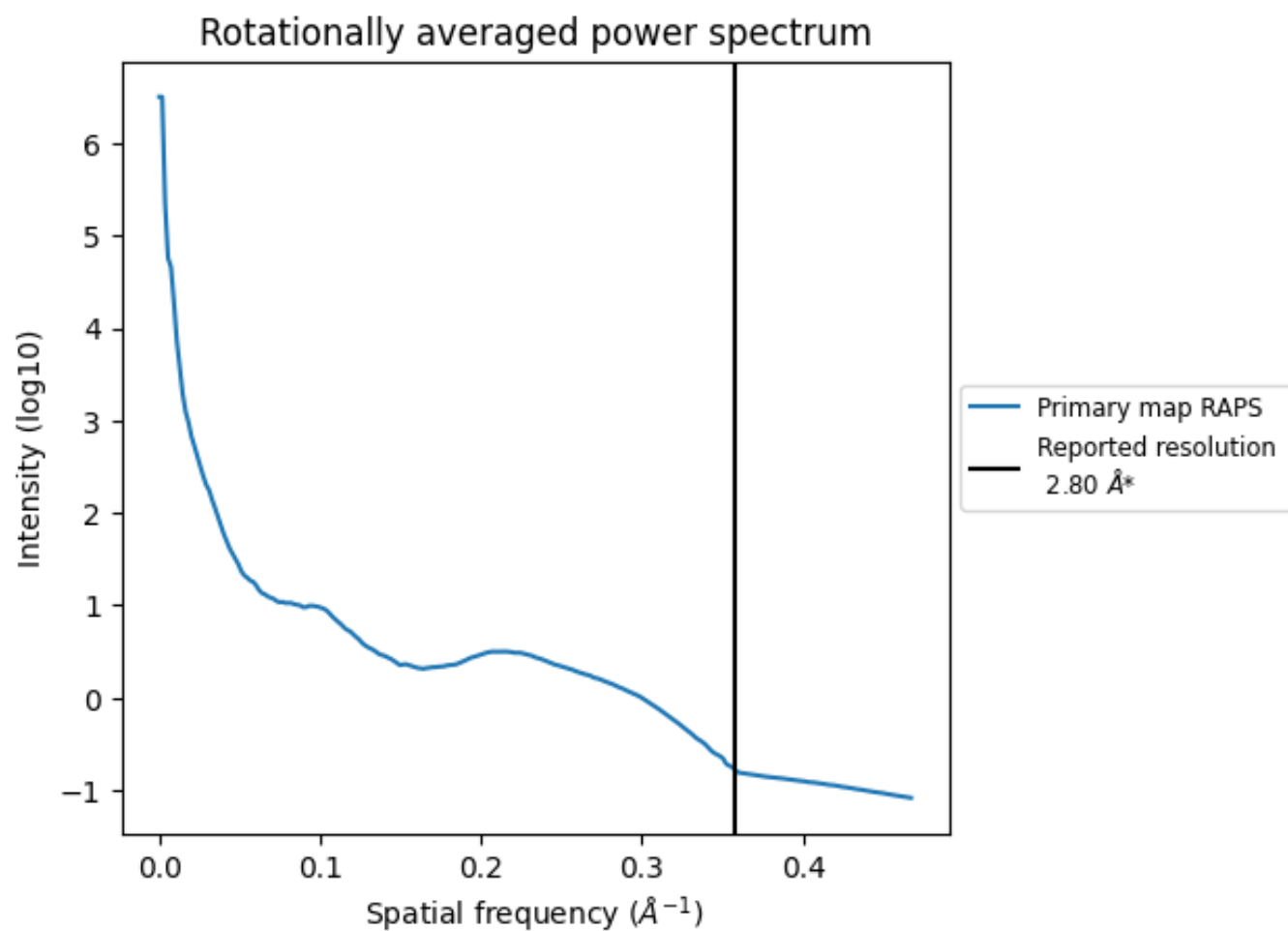
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1279 nm^3 ; this corresponds to an approximate mass of 1155 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 0.357 Å⁻¹

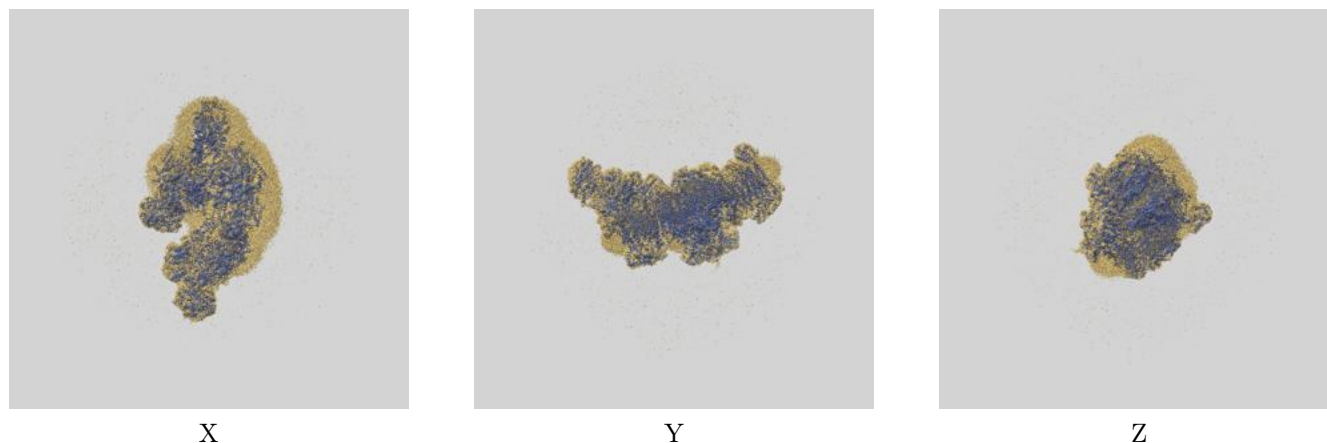
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

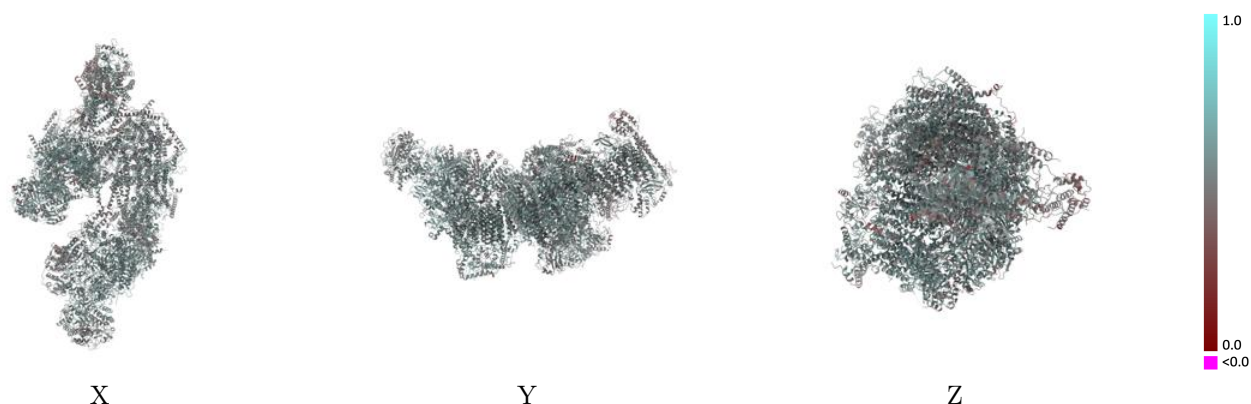
This section contains information regarding the fit between EMDB map EMD-44908 and PDB model 9BUH. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



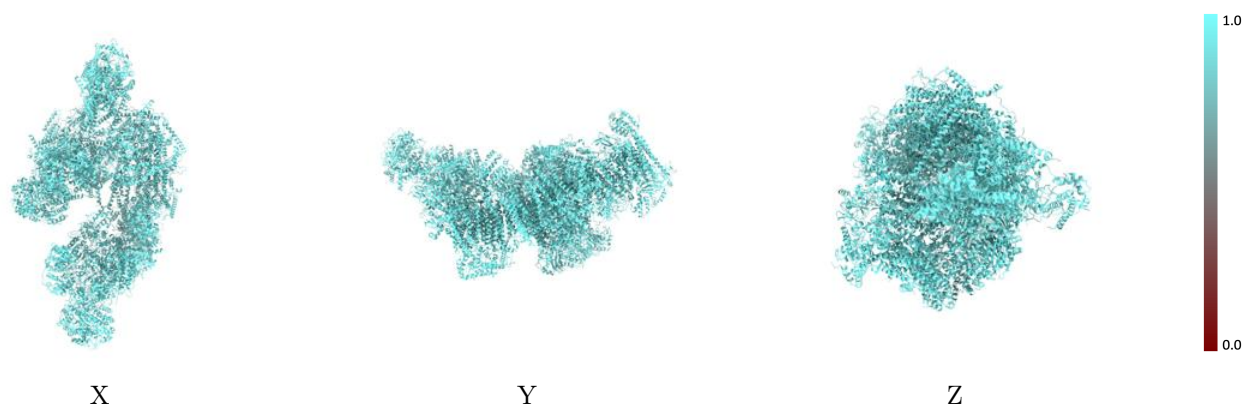
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



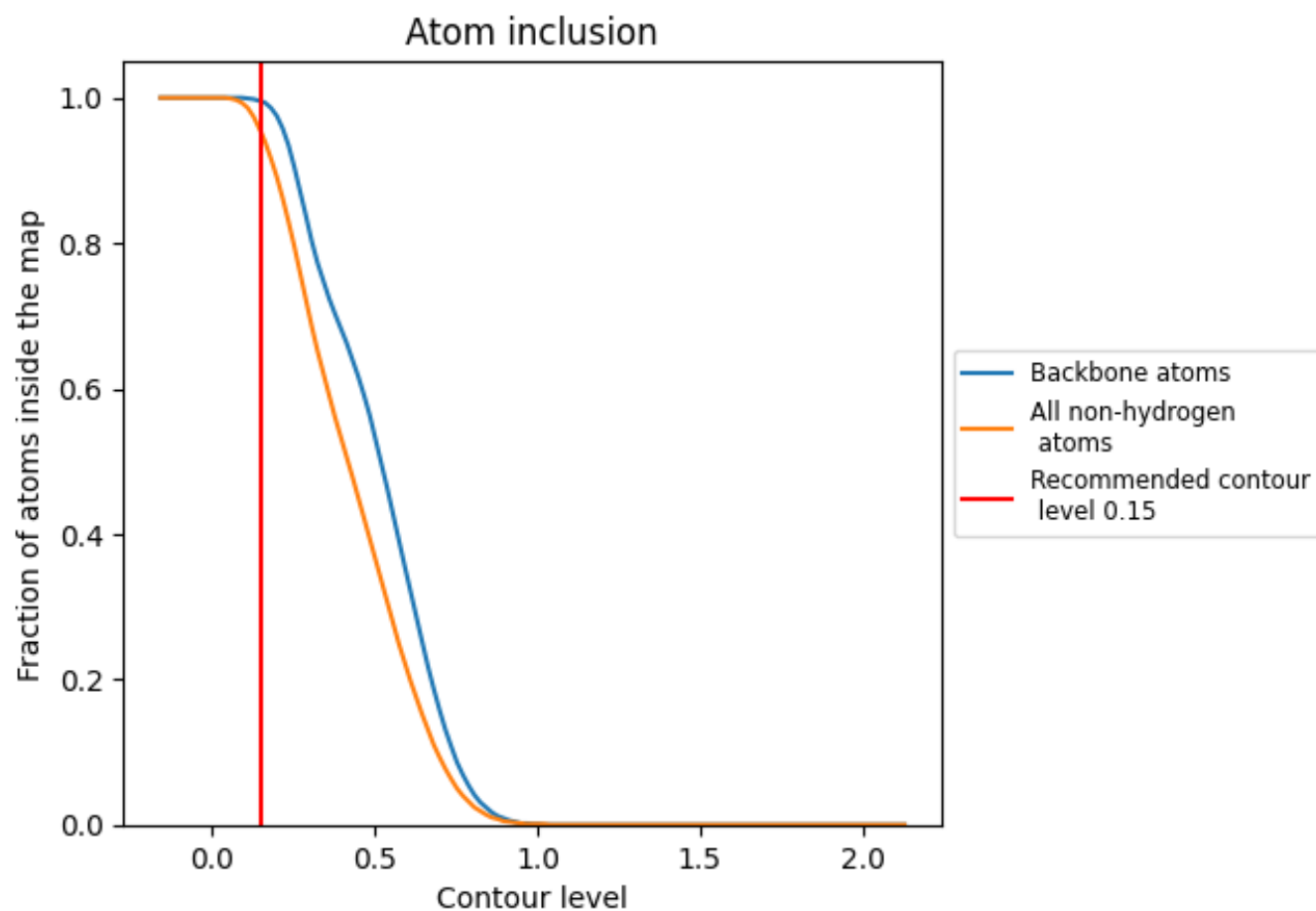
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



At the recommended contour level, 100% of all backbone atoms, 95% 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	 0.9520	 0.5350
0	 0.9050	 0.4930
1	 0.9650	 0.5750
2	 0.9080	 0.5020
3	 0.9780	 0.5580
4	 0.9180	 0.5050
5	 0.9630	 0.5490
6	 0.9590	 0.5460
7	 0.9760	 0.5700
8	 0.9670	 0.5530
9	 0.9560	 0.5590
A	 0.9050	 0.4660
Aa	 0.9730	 0.5540
Ab	 0.9190	 0.4880
Ac	 0.9730	 0.5590
Ad	 0.9830	 0.5520
Ae	 0.7100	 0.3260
Af	 0.7830	 0.3660
Ag	 0.9150	 0.4820
Ah	 0.8900	 0.4840
Ai	 0.9390	 0.4870
Aj	 0.9600	 0.5290
Ak	 0.9700	 0.5390
Al	 0.9400	 0.5120
Am	 0.9500	 0.5190
An	 0.9120	 0.4770
Ao	 0.9100	 0.4400
Ap	 0.8920	 0.4840
Aq	 0.9060	 0.4700
Ar	 0.9490	 0.4840
B	 0.9530	 0.5140
C	 0.9680	 0.5630
D	 0.9730	 0.5600
E	 0.9340	 0.5110
F	 0.9390	 0.5560



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Chain	Atom inclusion	Q-score
G	 0.9520	 0.5360
H	 0.9810	 0.5700
I	 0.9860	 0.5720
J	 0.9560	 0.5620
K	 0.9670	 0.5670
L	 0.9540	 0.5430
M	 0.9750	 0.5630
N	 0.9500	 0.5430
O	 0.8520	 0.4460
P	 0.9310	 0.4760
Q	 0.9420	 0.5520
R	 0.9340	 0.5100
S	 0.9780	 0.5550
T	 0.9570	 0.5290
U	 0.9330	 0.5160
V	 0.9530	 0.5250
W	 0.9520	 0.5340
X	 0.9190	 0.4910
Y	 0.9080	 0.4650
Z	 0.9180	 0.4880
a	 0.9580	 0.5520
b	 0.9490	 0.4760
c	 0.9360	 0.5310
d	 0.9420	 0.5190
e	 0.9340	 0.5100
f	 0.9360	 0.5100
g	 0.9650	 0.5430
h	 0.9430	 0.5370
i	 0.9750	 0.5590
j	 0.9640	 0.5550
k	 0.9720	 0.5600
l	 0.9480	 0.5320
m	 0.9320	 0.5240
n	 0.9270	 0.5020
o	 0.9250	 0.5250
p	 0.9490	 0.5300
q	 0.9750	 0.5560
r	 0.9710	 0.5550
s	 0.9440	 0.5290
t	 0.9320	 0.4760
u	 0.9630	 0.5590
v	 0.9640	 0.5500

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Chain	Atom inclusion	Q-score
w	 0.9810	 0.5730
x	 0.9720	 0.5650
y	 0.9380	 0.5590
z	 0.9720	 0.5640