



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 03:12 AM EDT

PDB ID : 9CE2 / pdb_00009ce2
EMDB ID : EMD-45490
Title : Respiratory supercomplex I+III₂+IV open state
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-06-25
Resolution : 3.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

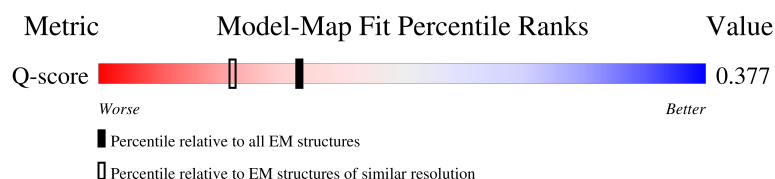
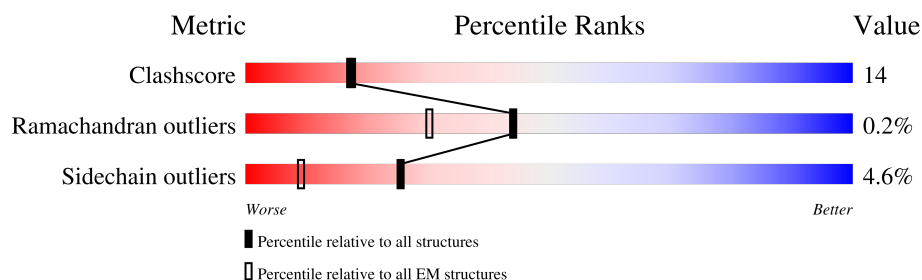
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 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.



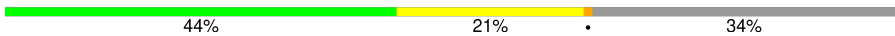
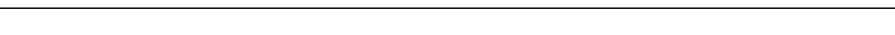
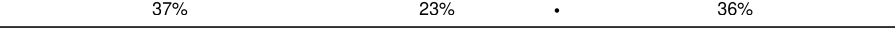
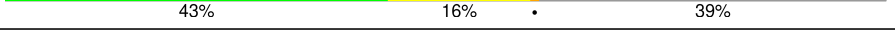
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13997 (2.91 - 3.91)

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

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

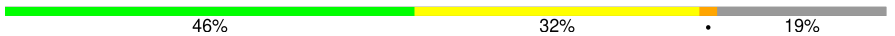
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Mol	Chain	Length	Quality of chain
3	2	299	
3	4	299	
3	Ae	299	
3	Af	299	
4	3	56	
4	Ad	56	
5	6	453	
5	v	453	
6	7	379	
6	w	379	
7	8	326	
7	x	326	
8	9	111	
8	y	111	
9	A	75	
10	a	189	
11	b	128	
12	c	186	
13	d	176	
14	e	154	
15	f	76	
16	g	122	
17	h	106	
18	i	347	
19	j	115	

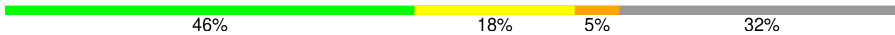
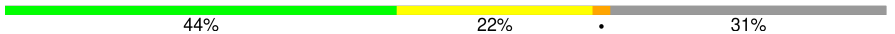
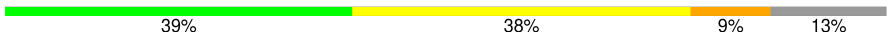
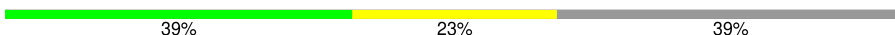
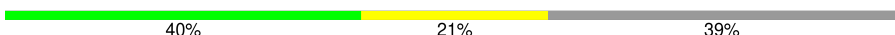
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Mol	Chain	Length	Quality of chain
20	k	98	
21	m	175	
22	n	58	
23	o	129	
24	p	221	
25	q	459	
26	r	318	
27	B	464	
28	C	469	
29	D	264	
30	E	249	
31	F	123	
32	H	212	
33	I	263	
34	J	175	
35	K	145	
36	N	116	
37	O	156	
37	X	156	
38	P	99	
39	Q	154	
40	R	110	
41	S	70	
42	T	169	
43	U	357	

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Mol	Chain	Length	Quality of chain
44	V	141	
45	W	144	
46	Y	105	
47	Z	114	
48	l	606	
49	s	249	
50	t	137	
51	5	480	
51	u	480	
52	Aa	82	
52	z	82	
53	Ag	70	
54	Ah	80	
55	Ai	80	
56	Aj	63	
57	Ak	514	
58	Al	228	
59	Am	261	
60	An	169	
61	Ao	152	
62	Ap	129	
63	Aq	97	
64	Ar	86	
65	G	727	
66	L	372	

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Mol	Chain	Length	Quality of chain
67	M	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
68	FES	2	301	-	-	X	-
68	FES	G	803	-	-	X	-
70	HEC	8	401	X	-	-	-
70	HEC	x	401	X	-	-	-
72	SF4	B	502	-	-	X	-
72	SF4	G	802	-	-	X	-
72	SF4	H	301	-	-	X	-
72	SF4	H	302	-	-	X	-
72	SF4	I	201	-	-	X	-

2 Entry composition

There are 75 unique types of molecules in this entry. The entry contains 111989 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	68	Total	C	N	O	S	0	0
			561	341	101	114	5		
1	Ab	66	Total	C	N	O	S	0	0
			543	331	99	108	5		

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called Cytochrome b.

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

- Molecule 7 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	239	Total	C	N	O	S	0	0
			1906	1217	328	345	16		
7	x	238	Total	C	N	O	S	0	0
			1896	1211	326	343	16		

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

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

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	63	Total	C	N	O	S	0	0
			510	335	88	85	2		

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

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

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	b	105	Total	C	N	O	S	0	0
			871	570	155	145	1		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	152	Total	C	N	O	S	0	0
			1278	829	205	236	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	99	Total	C	N	O	S	0	0
			822	527	136	155	4		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	j	91	Total	C	N	O	S	0	0
			721	492	106	120	3		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	161	Total	C	N	O	S	0	0
			1227	826	174	216	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	53	Total	C	N	O	S	0	0
			452	293	83	75	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	r	308	Total	C	N	O	S	0	0
			2435	1633	375	406	21		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

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

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

- Molecule 37 is a protein called Acyl carrier protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	60	Total	C	N	O	S	0	0
			524	347	87	89	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	l	602	Total	C	N	O	S	0	0
			4773	3166	739	818	50		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

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

7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	119	Total	C	N	O	S	0	0
			970	609	177	175	9		

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

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

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

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

- Molecule 53 is a protein called Cytochrome c oxidase subunit 8.

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

- Molecule 54 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

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

- Molecule 55 is a protein called Cytochrome c oxidase subunit 7B.

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

- Molecule 56 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

- Molecule 57 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ak	513	Total	C	N	O	S	0	0
			4002	2680	617	673	32		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 59 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 60 is a protein called Cytochrome c oxidase subunit 4.

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

- Molecule 61 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

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

- Molecule 62 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Ap	89	Total	C	N	O	S	0	0
			689	429	121	133	6		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6A2.

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

- Molecule 64 is a protein called Cytochrome c oxidase subunit.

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

- Molecule 65 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

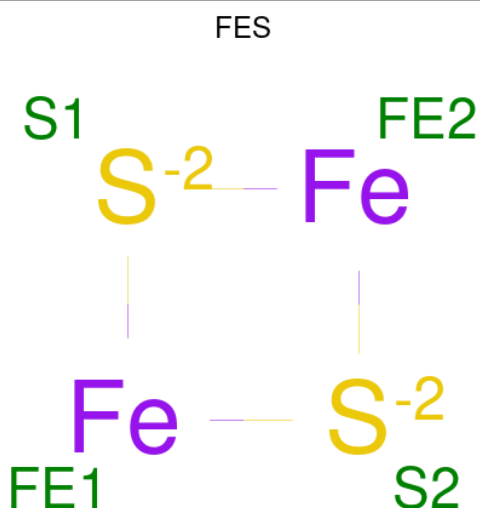
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	L	314	Total	C	N	O	S	0	0
			2493	1605	437	442	9		

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

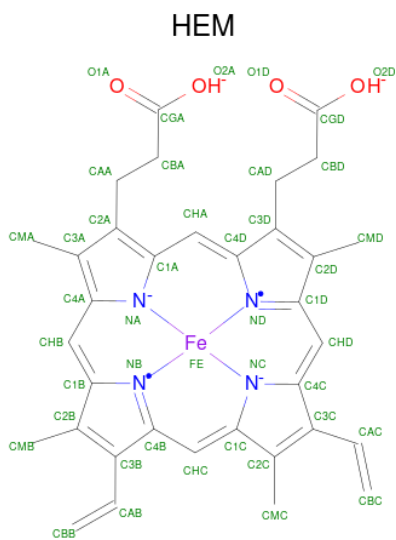
Mol	Chain	Residues	Atoms					AltConf	Trace
67	M	96	Total	C	N	O	S	0	0
			769	485	146	135	3		

- Molecule 68 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



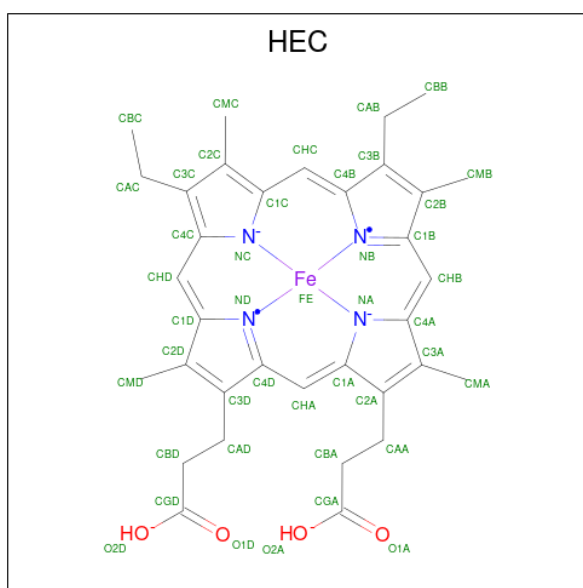
Mol	Chain	Residues	Atoms			AltConf
68	2	1	Total 4	Fe 2	S 2	0
68	4	1	Total 4	Fe 2	S 2	0
68	E	1	Total 4	Fe 2	S 2	0
68	G	1	Total 4	Fe 2	S 2	0

- Molecule 69 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



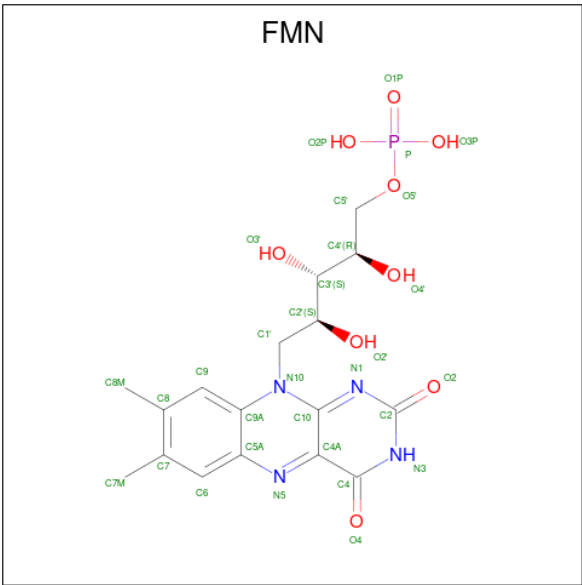
Mol	Chain	Residues	Atoms					AltConf
69	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
69	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
69	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
69	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 70 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



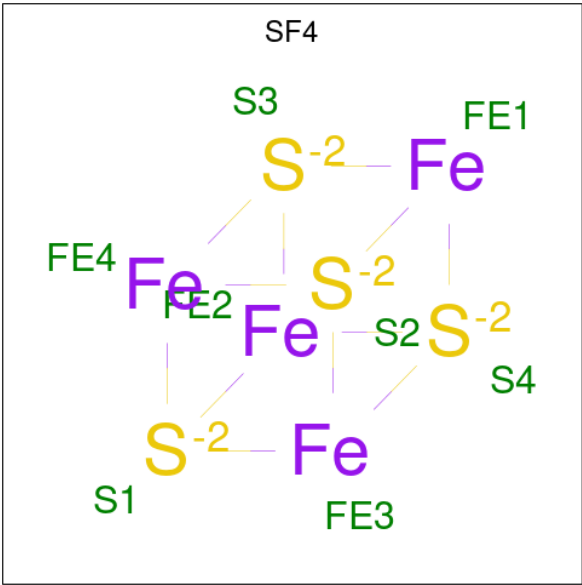
Mol	Chain	Residues	Atoms					AltConf
70	8	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	x	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 71 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 72 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



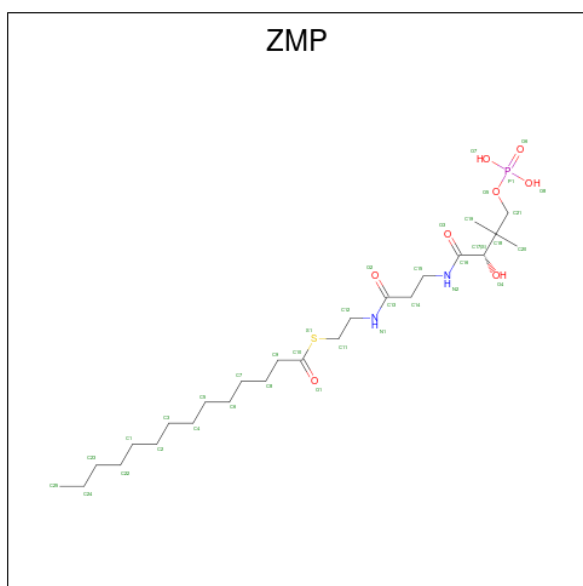
Mol	Chain	Residues	Atoms			AltConf
72	B	1	Total	Fe	S	0
			8	4	4	
72	H	1	Total	Fe	S	0
			8	4	4	
72	H	1	Total	Fe	S	0
			8	4	4	

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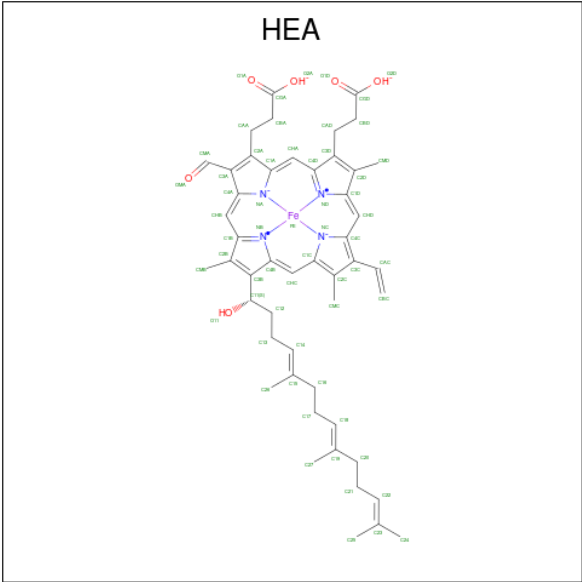
Mol	Chain	Residues	Atoms			AltConf
72	I	1	Total	Fe	S	0
			8	4	4	
72	G	1	Total	Fe	S	0
			8	4	4	
72	G	1	Total	Fe	S	0
			8	4	4	

- Molecule 73 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl} amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



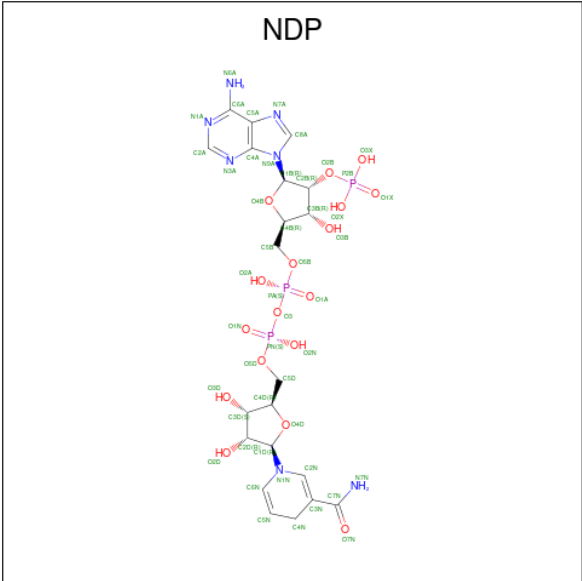
Mol	Chain	Residues	Atoms						AltConf
73	Q	1	Total	C	N	O	P	S	0
			30	18	2	8	1	1	

- Molecule 74 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 75 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

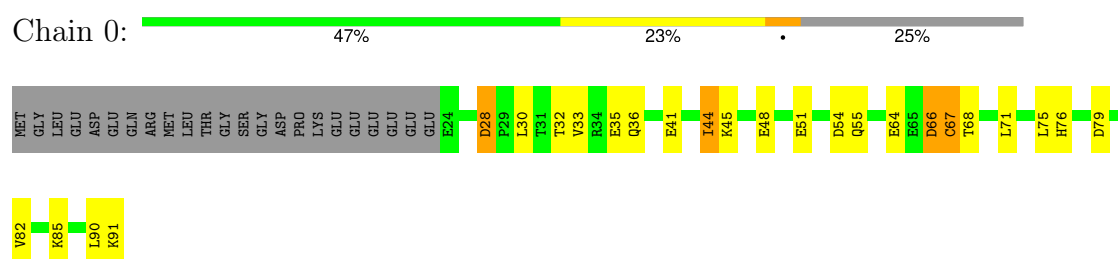


Mol	Chain	Residues	Atoms					AltConf
75	L	1	Total	C	N	O	P	0
			48	21	7	17	3	

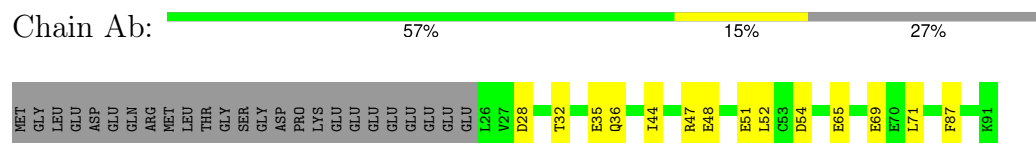
3 Residue-property plots

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

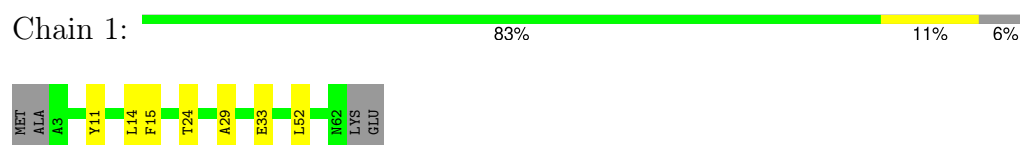
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



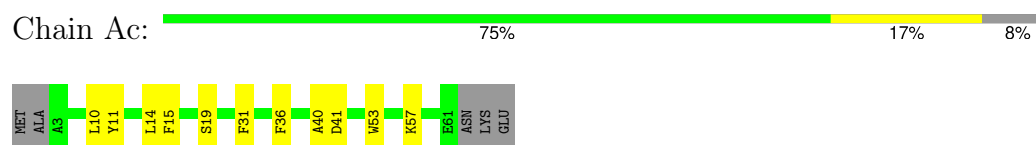
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



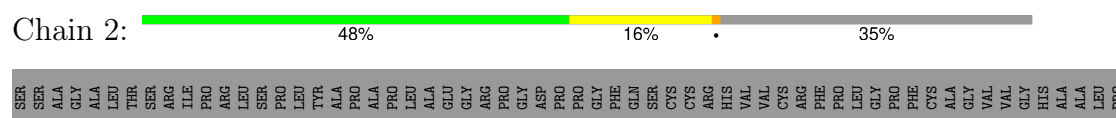
- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

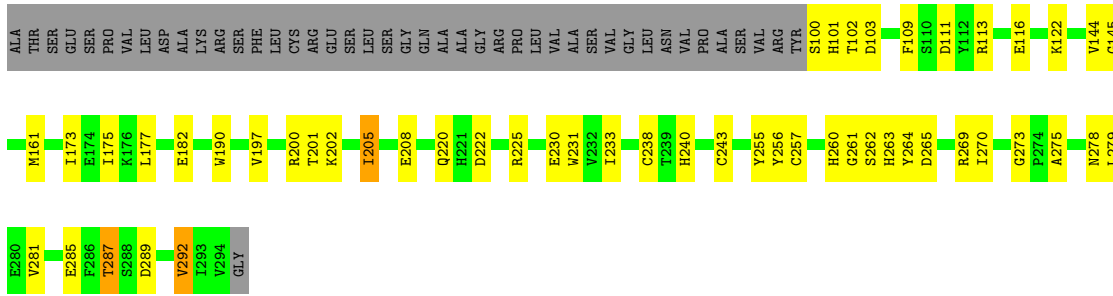


- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

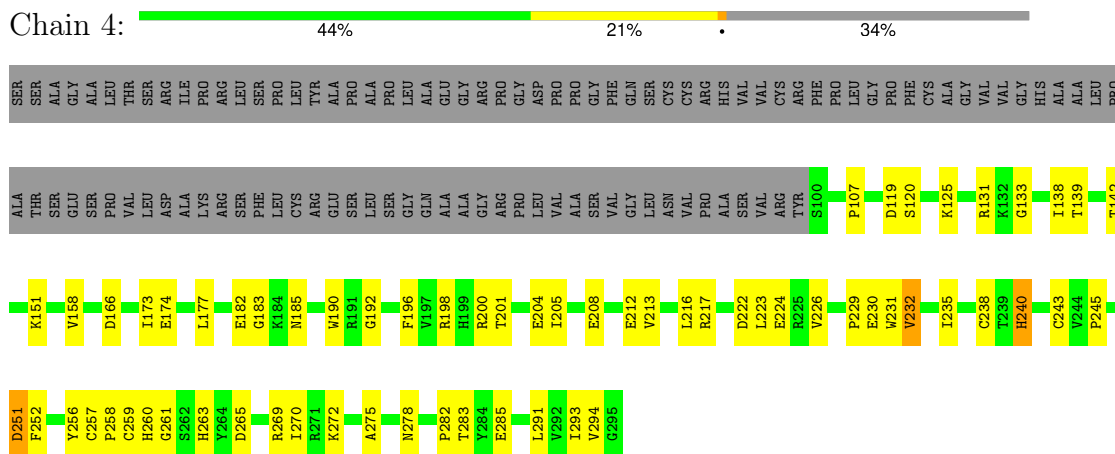


- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

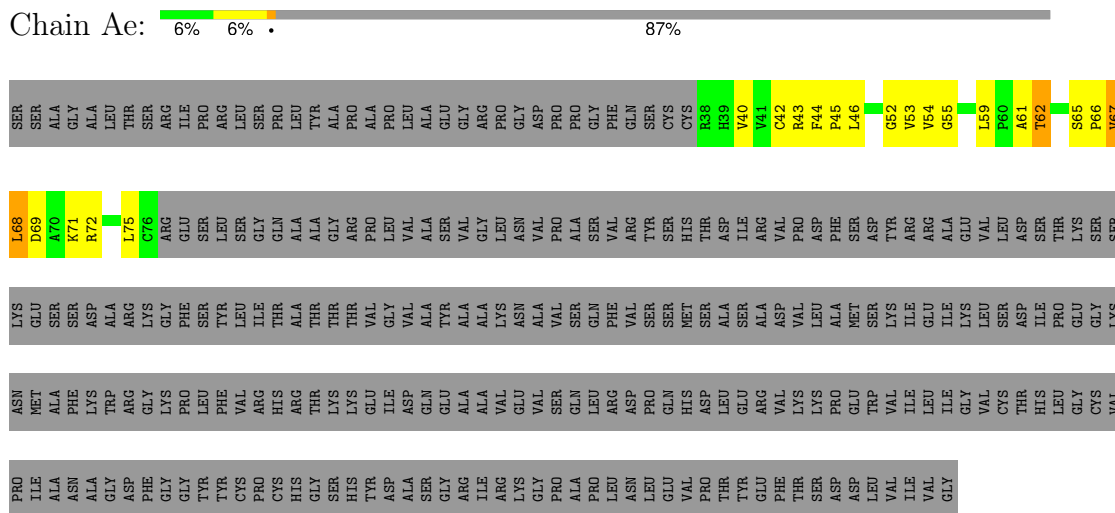




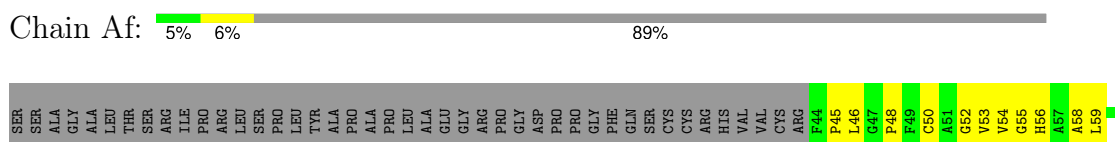
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1



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

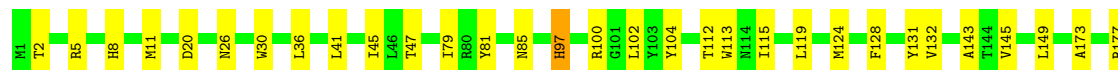
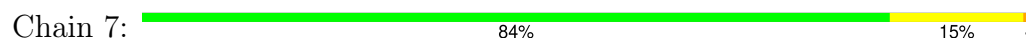


- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

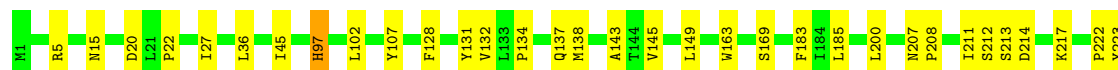
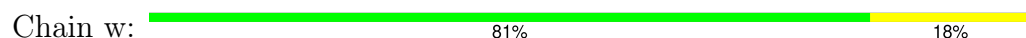




• Molecule 6: Cytochrome b



• Molecule 6: Cytochrome b

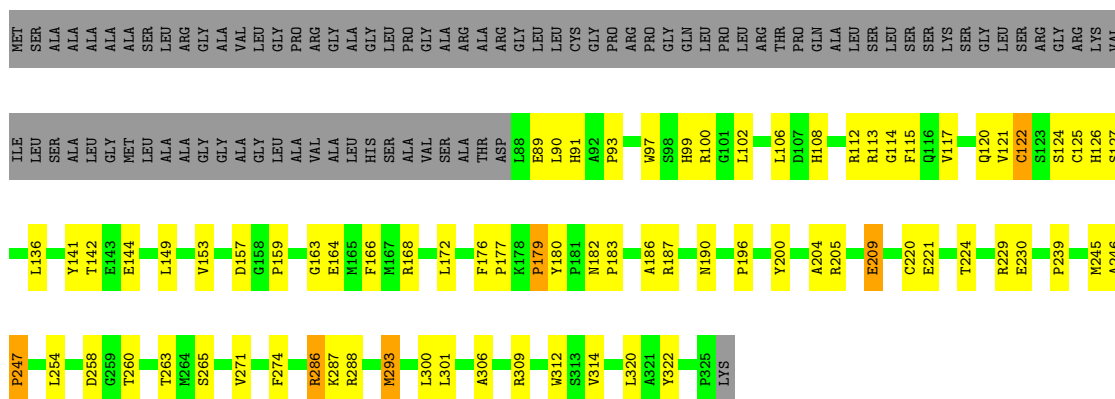


• Molecule 7: Cytochrome c1

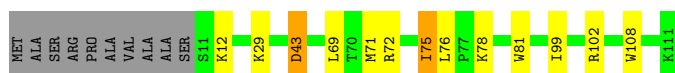


• Molecule 7: Cytochrome c1

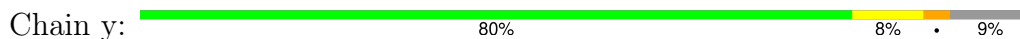




- Molecule 8: Cytochrome b-c1 complex subunit 7



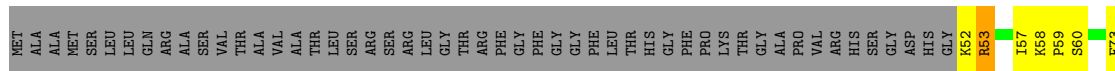
- Molecule 8: Cytochrome b-c1 complex subunit 7



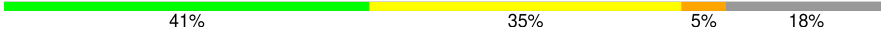
- Molecule 9: Cytochrome c oxidase subunit 6C

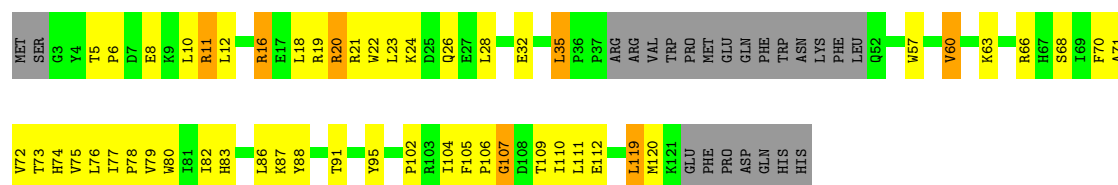


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



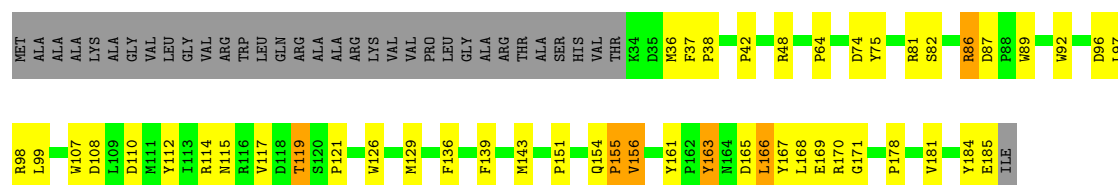
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b: 



- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 

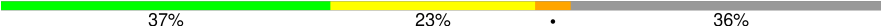


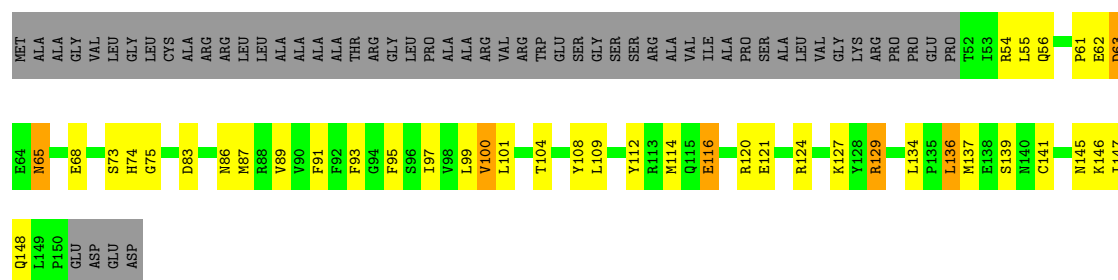
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 

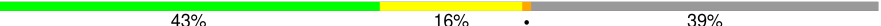


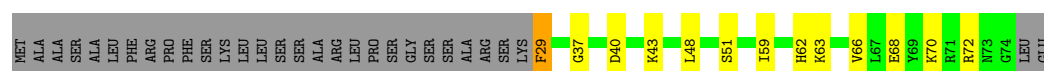
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 



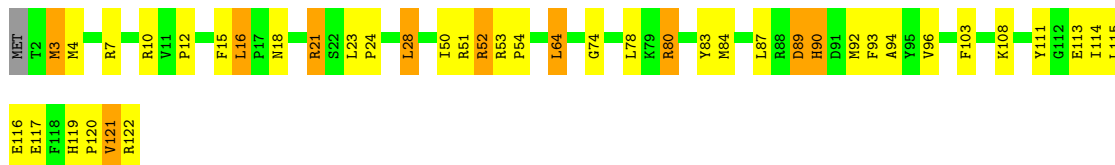
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 



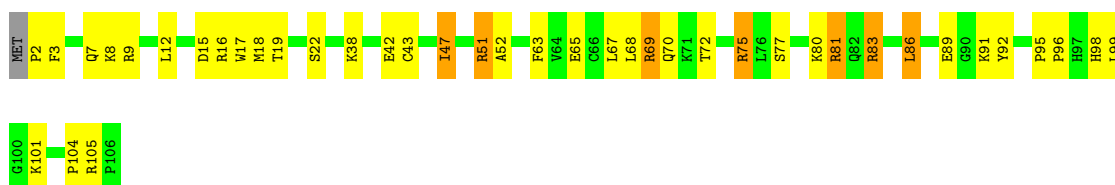
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 



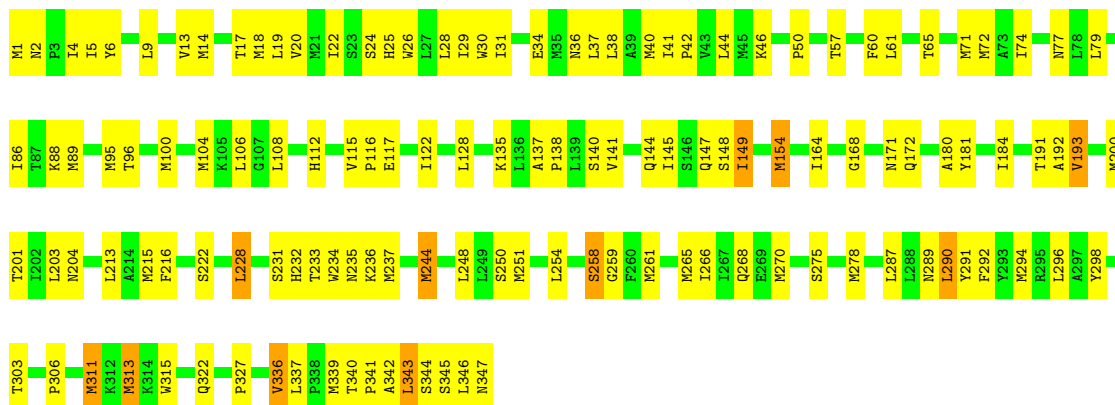
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 



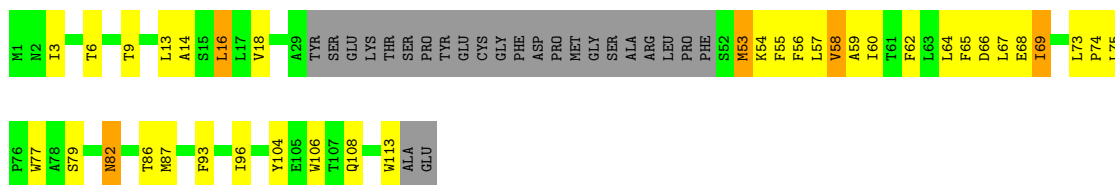
- Molecule 18: NADH-ubiquinone oxidoreductase chain 2

Chain i: 



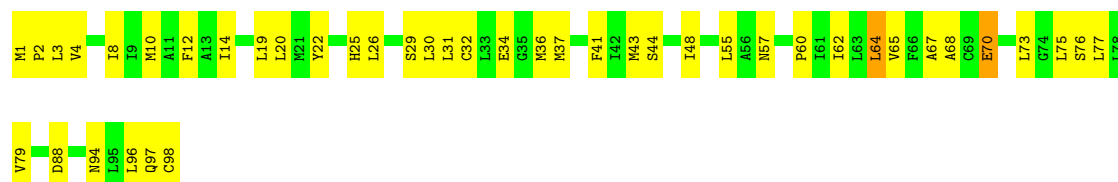
- Molecule 19: NADH-ubiquinone oxidoreductase chain 3

Chain j: 



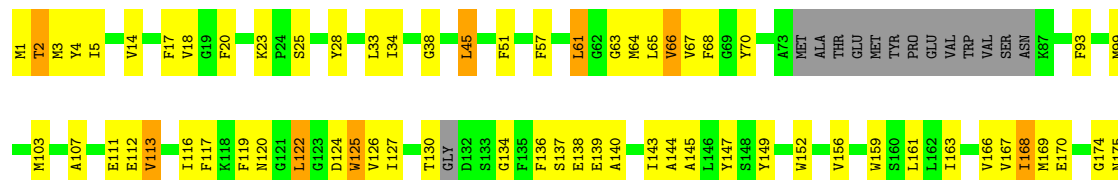
- Molecule 20: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 



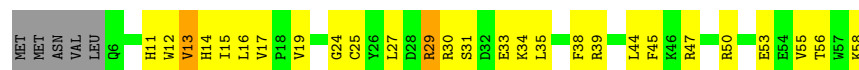
- Molecule 21: NADH-ubiquinone oxidoreductase chain 6

Chain m: 54% 33% 5% 8%



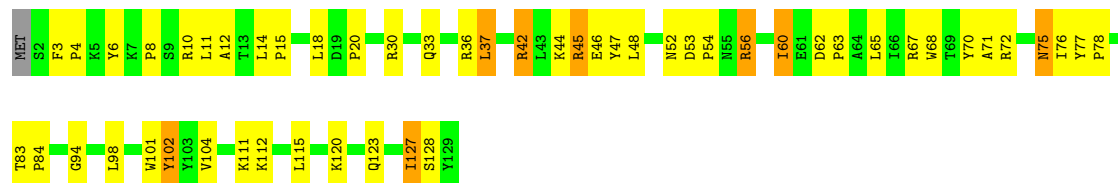
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n: 45% 43% 9%



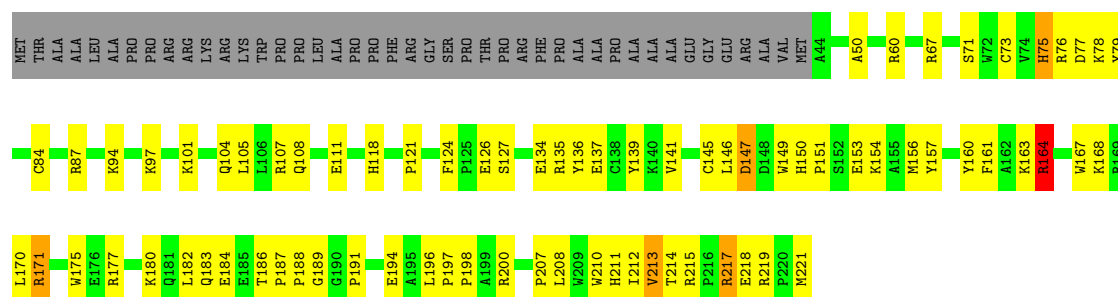
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o: 59% 34% 6%



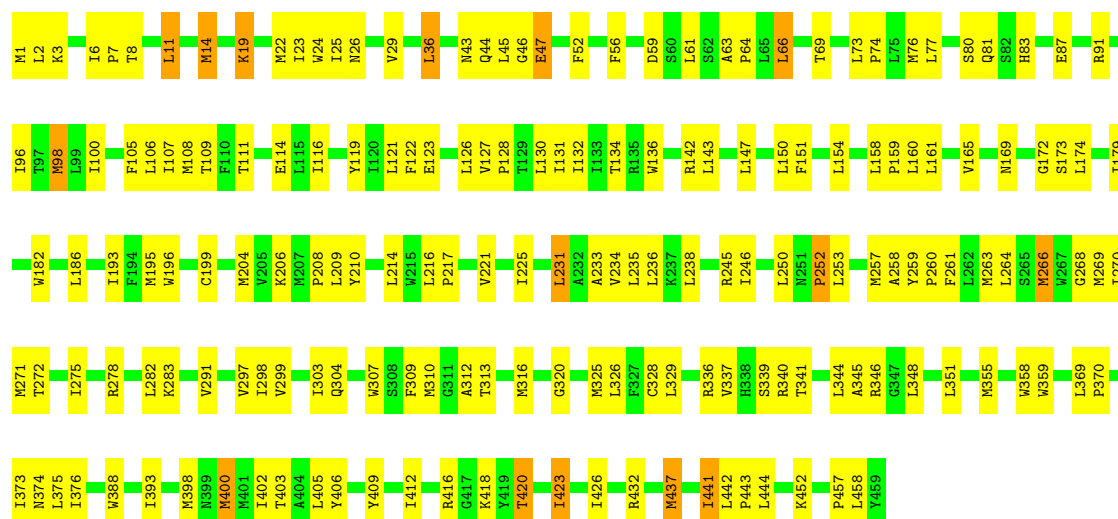
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p: 46% 32% 19%



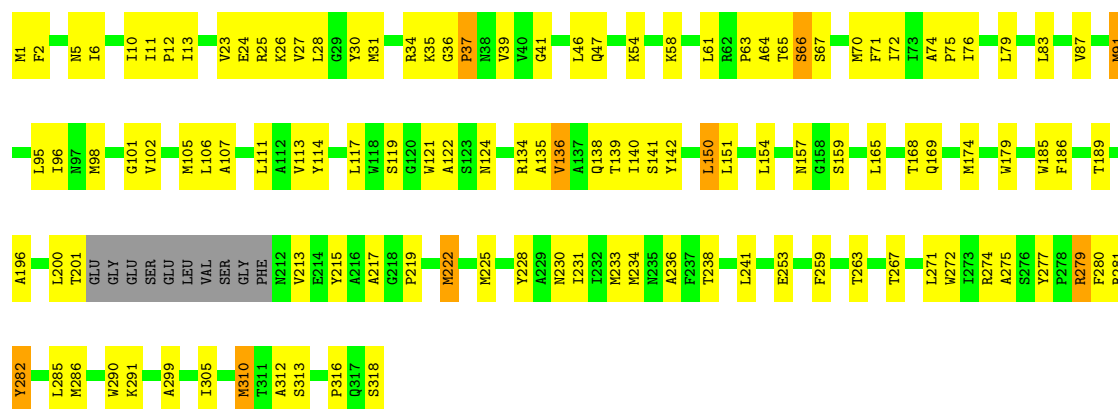
- Molecule 25: NADH-ubiquinone oxidoreductase chain 4

Chain q:  61% 36%



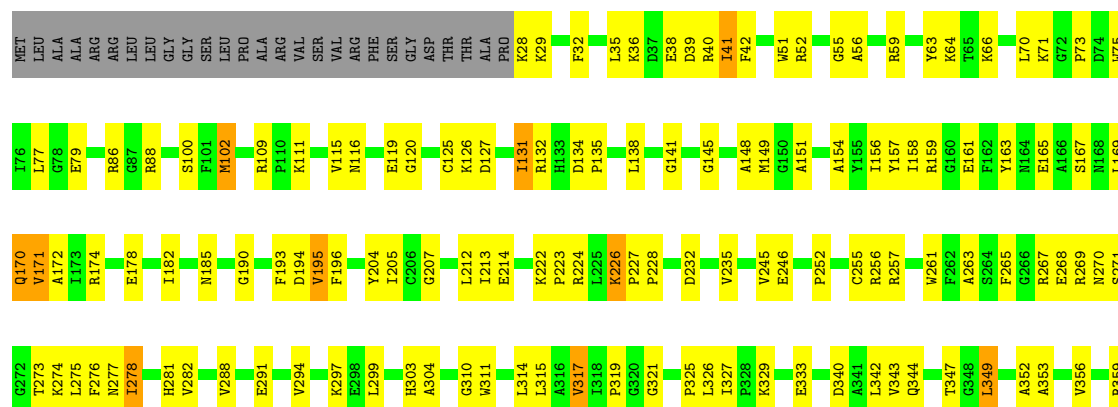
• Molecule 26: NADH-ubiquinone oxidoreductase chain 1

Chain r:  59% 35%



• Molecule 27: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain B:  58% 32% 7%



- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain C: 61% 27% 8%

- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

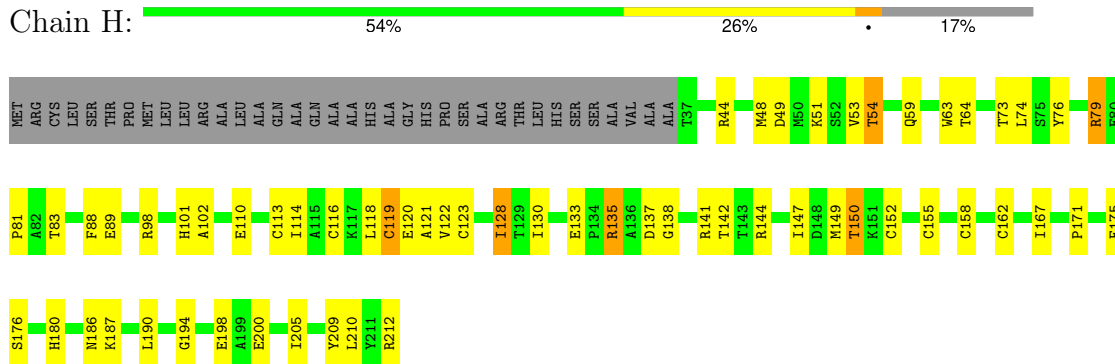
Chain D:  54% 24% . 21%

- Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

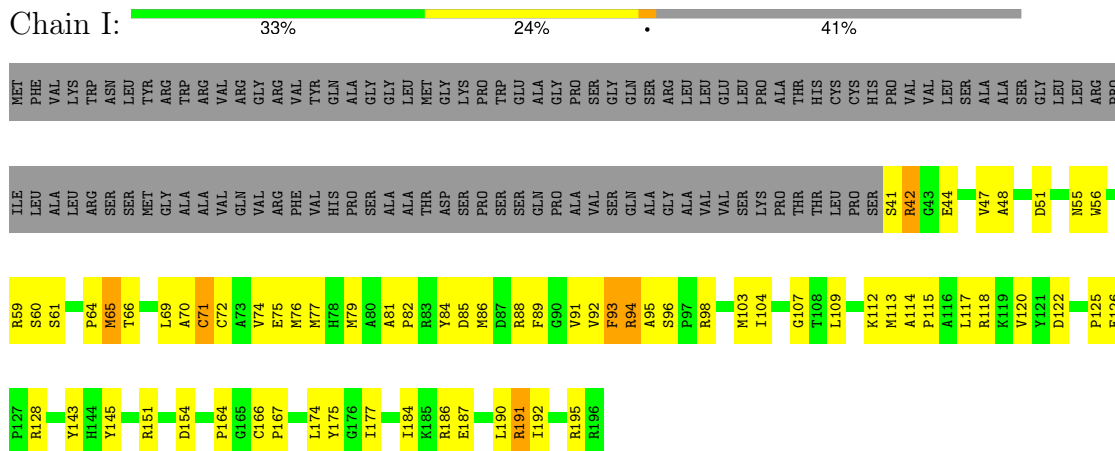
Chain E: 60% 24% • 14%

- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

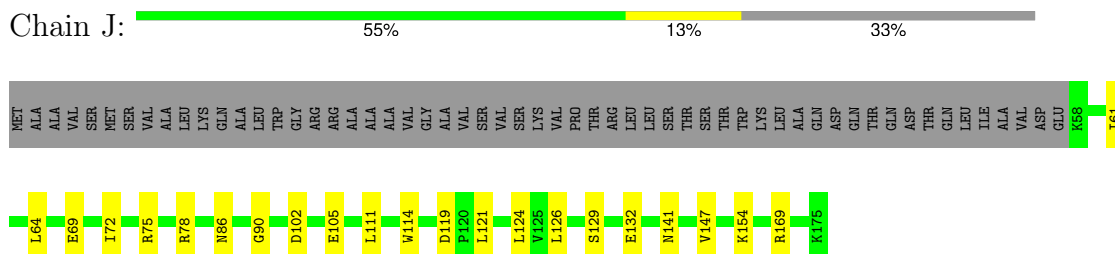
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



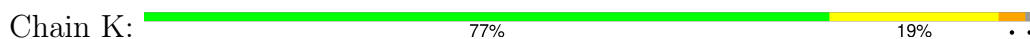
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12





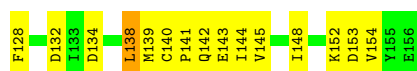
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain N: 72% 24% . .



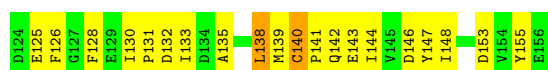
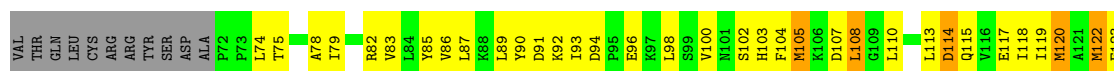
- Molecule 37: Acyl carrier protein

Chain O: 24% 27% . 46%



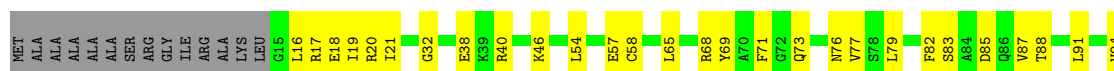
- Molecule 37: Acyl carrier protein

Chain X: 20% 30% . 46%



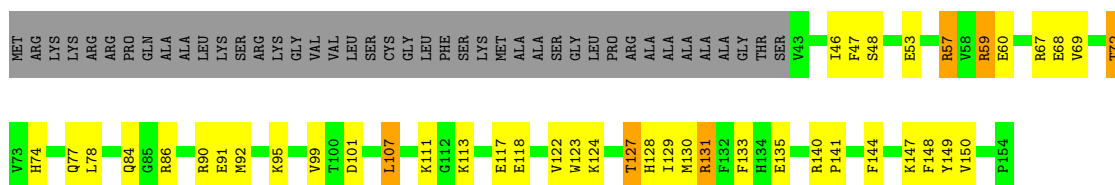
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P: 56% 28% 16%



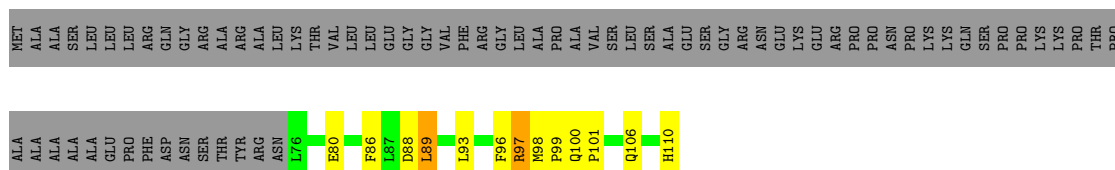
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Q: 44% 25% . 27%



- Molecule 40: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain R: 20% 10% 68%



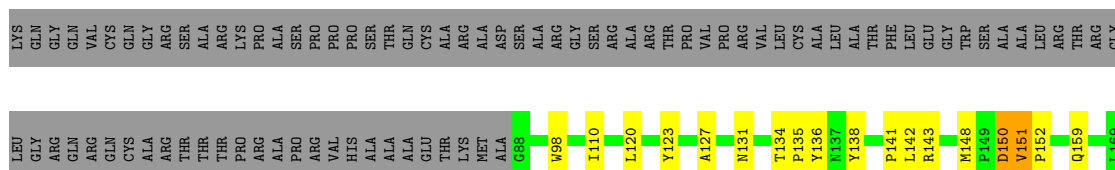
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 60% 36%



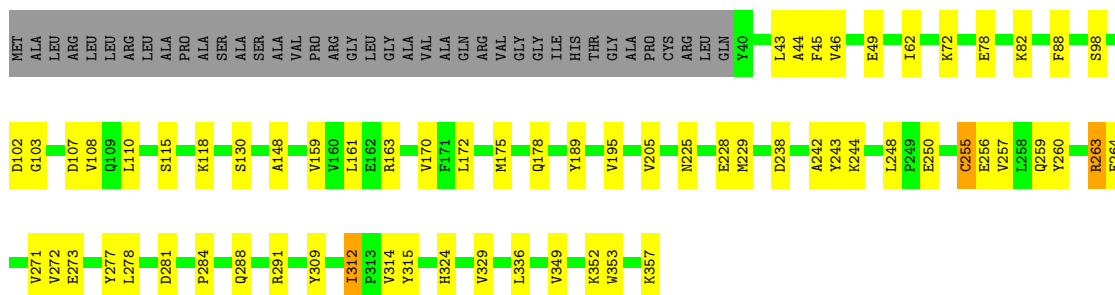
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain T: 38% 9% 51%



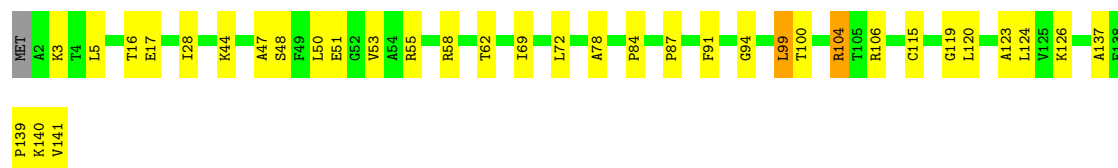
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain U: 71% 18% 11%



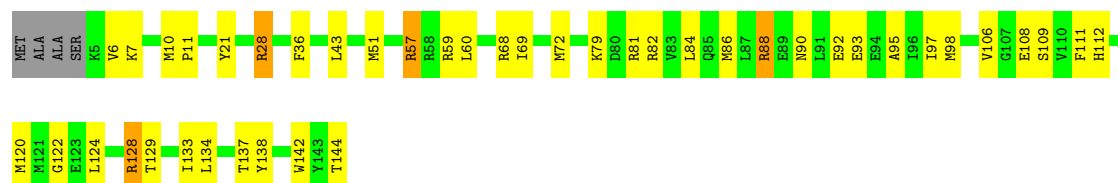
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 74% 23%



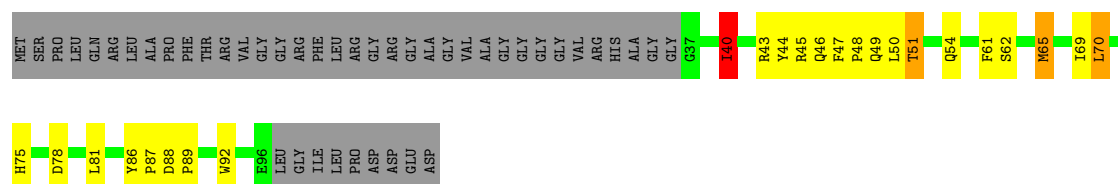
- Molecule 45: NADH:ubiquinone oxidoreductase subunit A13

Chain W: 67% 27%



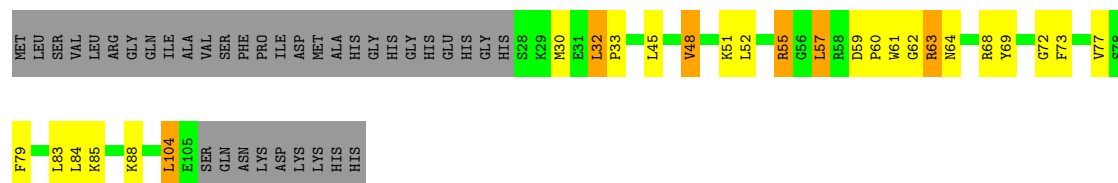
- Molecule 46: NADH:ubiquinone oxidoreductase subunit B2

Chain Y: 34% 19% 43%



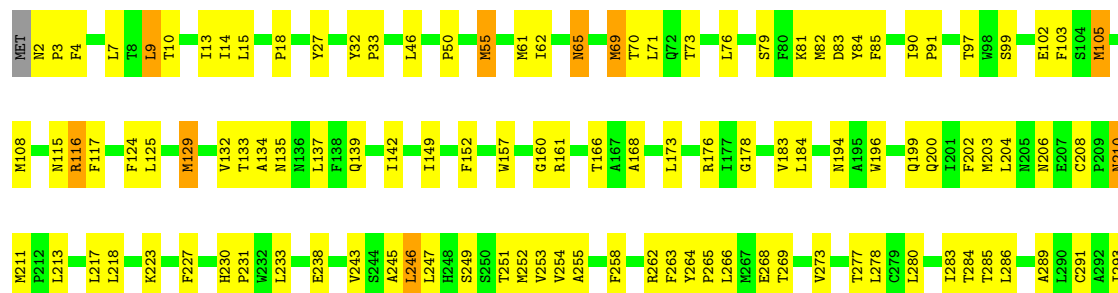
- Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

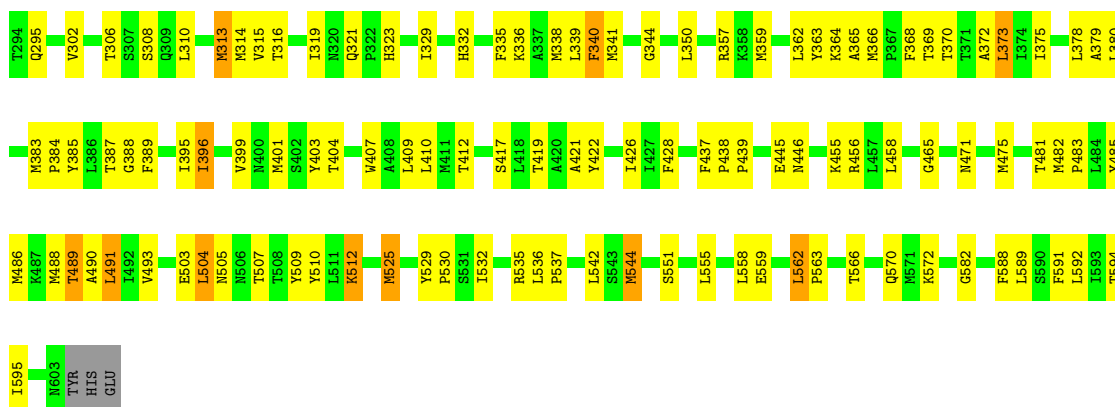
Chain Z: 46% 18% 5% 32%



- Molecule 48: NADH-ubiquinone oxidoreductase chain 5

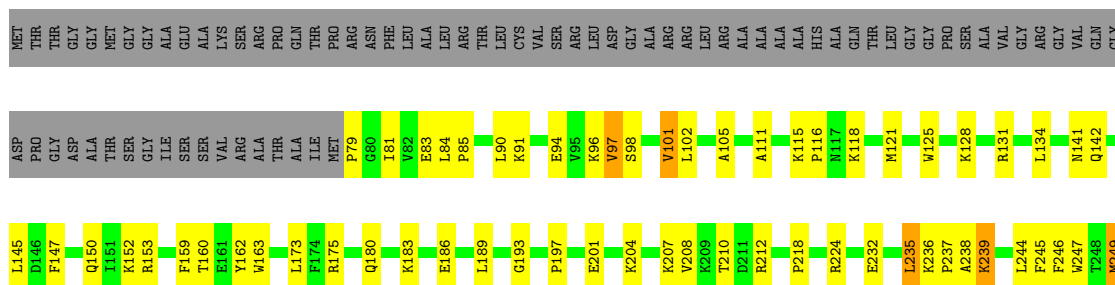
Chain I: 62% 34%





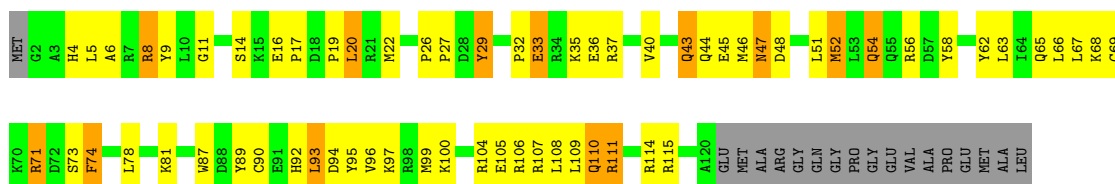
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain s: 44% 22% 31%



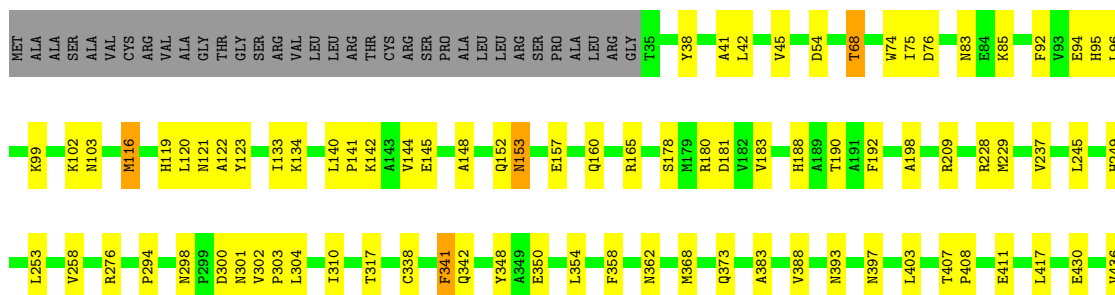
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain t: 39% 38% 9% 13%



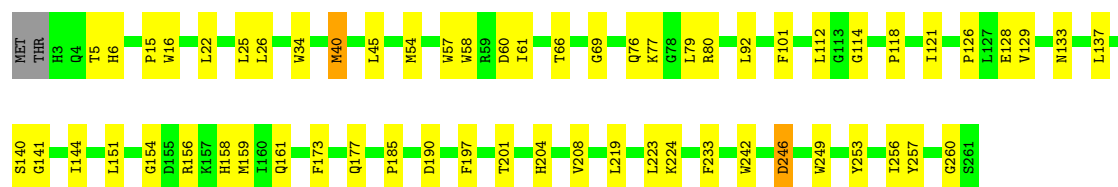
- Molecule 51: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain u: 72% 20% 7%



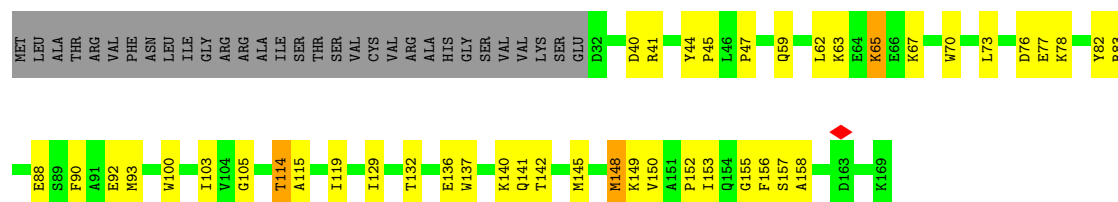


Chain Am:  76% 22% ..



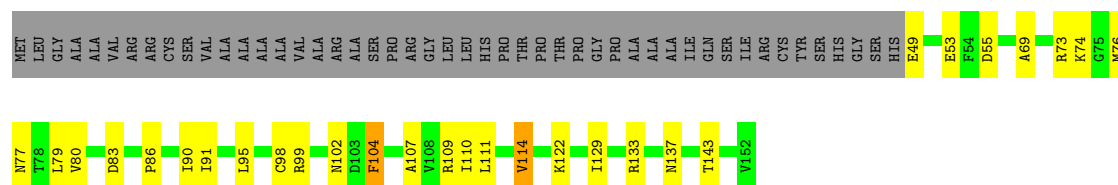
- Molecule 60: Cytochrome c oxidase subunit 4

Chain An:  56% 24% 18%

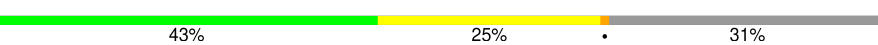


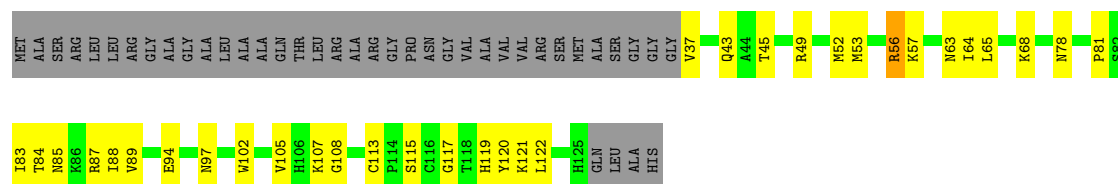
- Molecule 61: Cytochrome c oxidase subunit 5A, mitochondrial

Chain Ao:  49% 18% 32%



- Molecule 62: Cytochrome c oxidase subunit 5B, mitochondrial

Chain Ap:  43% 25% 31%



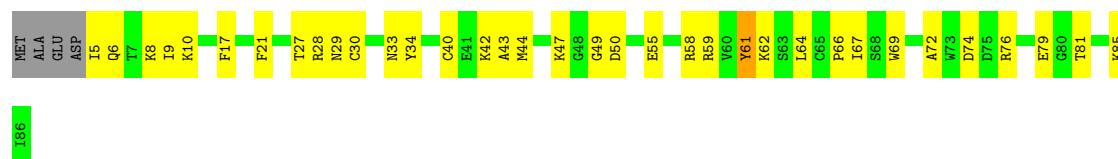
- Molecule 63: Cytochrome c oxidase subunit 6A2

Chain Aq:  56% 20% 25%



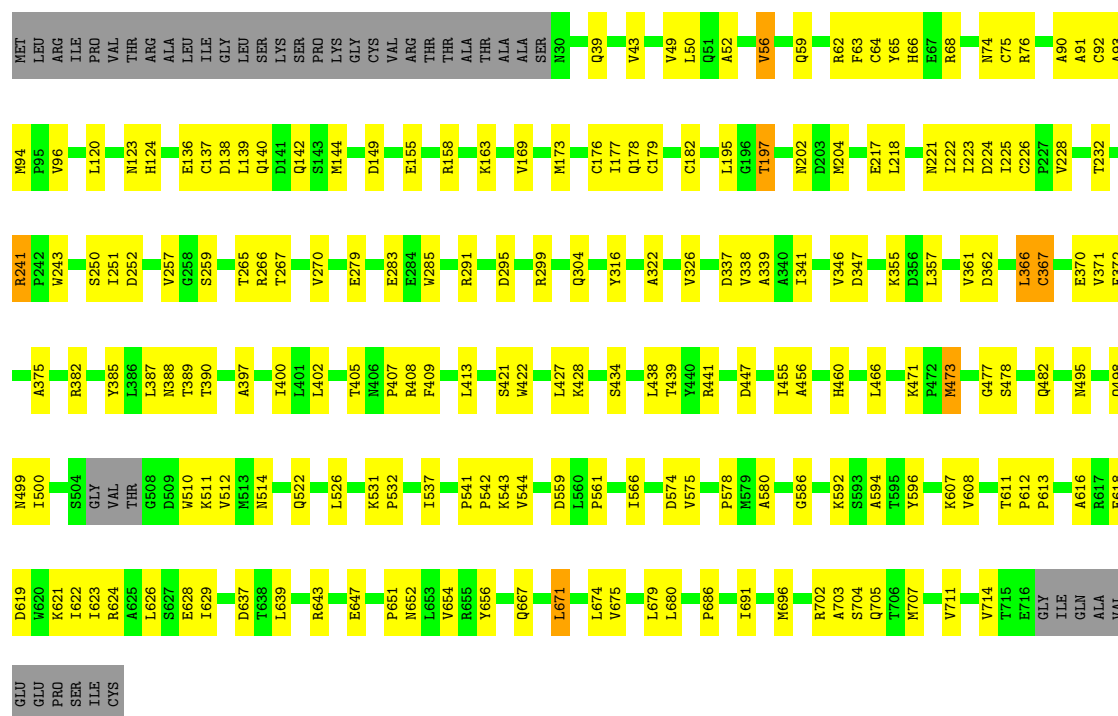
- Molecule 64: Cytochrome c oxidase subunit

Chain Ar:  55% 40% 5%



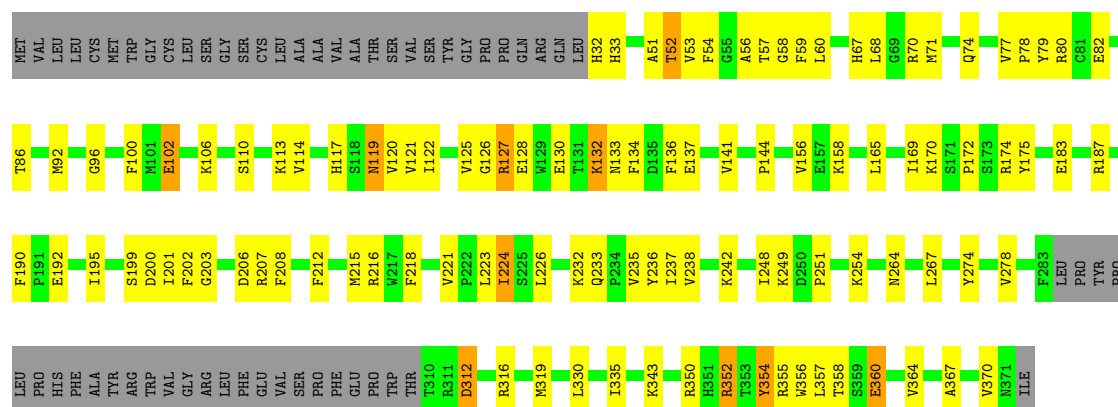
- Molecule 65: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 68% 26% • 6%



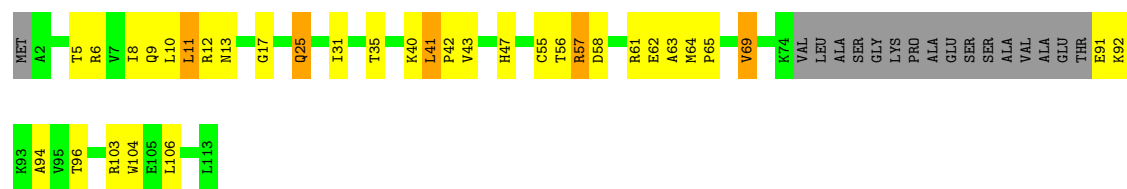
- Molecule 66: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain L: 55% 26% • 16%



- Molecule 67: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Response	Percentage
Best for the country	55%
Not the best for the country	26%
Don't know	1%
Refuse to answer	15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.151	Depositor
Minimum map value	-0.164	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.1	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: FES, NDP, FMN, SF4, HEC, HEM, ZMP, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.36	0/567	0.51	0/759
1	Ab	0.16	0/549	0.32	0/735
2	1	0.13	0/506	0.24	0/683
2	Ac	0.14	0/498	0.29	0/672
3	2	0.15	0/1546	0.31	0/2093
3	4	0.17	0/1551	0.34	1/2098 (0.0%)
3	Ae	0.23	0/281	0.60	0/383
3	Af	0.27	0/228	0.57	0/312
4	3	0.13	0/433	0.29	0/593
4	Ad	0.11	0/437	0.27	0/598
5	6	0.15	0/3192	0.30	0/4322
5	v	0.15	0/3192	0.31	0/4322
6	7	0.16	0/3123	0.31	0/4269
6	w	0.16	0/3123	0.29	0/4269
7	8	0.14	0/1964	0.32	0/2663
7	x	0.92	0/1954	1.12	0/2652
8	9	0.11	0/913	0.24	0/1223
8	y	0.12	0/913	0.23	0/1223
9	A	0.65	0/522	0.85	0/697
10	a	0.88	0/1184	1.16	0/1603
11	b	0.90	0/896	1.08	0/1219
12	c	0.86	0/1332	1.09	0/1821
13	d	0.89	0/1452	1.16	0/1958
14	e	0.88	0/845	1.14	0/1149
15	f	0.86	0/398	1.15	0/540
16	g	0.89	0/1031	1.14	0/1394
17	h	0.89	0/889	1.18	1/1190 (0.1%)
18	i	0.21	0/2774	0.35	0/3768
19	j	0.61	0/737	0.79	0/1009
20	k	0.22	0/759	0.37	0/1029
21	m	0.90	0/1256	1.20	1/1696 (0.1%)
22	n	0.88	0/464	1.12	0/627

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	o	0.87	0/1092	1.15	0/1481
24	p	0.79	0/1590	0.99	0/2155
25	q	0.91	0/3721	1.16	0/5073
26	r	0.61	0/2506	0.82	1/3427 (0.0%)
27	B	0.93	0/3393	1.17	1/4584 (0.0%)
28	C	0.37	0/3551	0.53	0/4813
29	D	0.19	0/1783	0.38	0/2428
30	E	0.24	0/1698	0.44	0/2311
31	F	0.36	0/752	0.48	0/1013
32	H	0.89	0/1443	1.15	0/1952
33	I	0.88	0/1279	1.12	0/1730
34	J	0.13	0/985	0.27	0/1329
35	K	0.46	0/1244	0.55	0/1693
36	N	0.28	0/929	0.39	0/1258
37	O	0.91	0/701	1.19	0/946
37	X	0.90	0/701	1.21	0/946
38	P	0.15	0/680	0.36	0/916
39	Q	0.52	0/978	0.74	0/1317
40	R	0.35	0/304	0.43	0/410
41	S	0.89	0/577	1.14	1/777 (0.1%)
42	T	0.13	0/659	0.28	0/905
43	U	0.23	0/2622	0.38	0/3552
44	V	0.90	0/1042	1.25	0/1411
45	W	0.88	0/1193	1.16	0/1609
46	Y	0.73	0/549	0.95	0/752
47	Z	0.88	0/645	1.12	0/872
48	l	0.91	0/4902	1.17	0/6669
49	s	0.90	0/1436	1.11	0/1938
50	t	0.89	0/994	1.16	0/1339
51	5	0.13	0/3442	0.28	0/4667
51	u	0.13	0/3531	0.29	0/4793
52	Aa	0.15	0/684	0.32	0/926
52	z	0.89	0/688	1.14	0/931
53	Ag	0.17	0/349	0.38	0/477
54	Ah	0.44	0/446	0.59	0/605
55	Ai	0.14	0/396	0.34	0/543
56	Aj	0.15	0/390	0.31	0/525
57	Ak	0.27	0/4142	0.43	1/5664 (0.0%)
58	Al	0.38	0/1831	0.55	0/2496
59	Am	0.30	0/2179	0.43	0/2981
60	An	0.12	0/1188	0.27	0/1605
61	Ao	0.33	0/860	0.48	0/1167
62	Ap	0.28	0/704	0.44	0/956

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	Aq	0.22	0/633	0.37	0/866
64	Ar	0.15	0/704	0.32	0/951
65	G	0.29	0/5347	0.41	0/7243
66	L	0.51	0/2554	0.66	0/3455
67	M	0.97	0/787	1.10	0/1064
All	All	0.57	0/114313	0.75	7/155090 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	x	0	5
9	A	0	2
10	a	0	5
11	b	0	4
12	c	0	3
13	d	0	5
14	e	0	2
16	g	0	4
17	h	0	6
22	n	0	2
23	o	0	1
24	p	0	3
25	q	0	4
26	r	0	3
27	B	0	7
31	F	0	1
32	H	0	4
33	I	0	5
35	K	0	2
39	Q	0	3
40	R	0	1
41	S	0	2
44	V	0	1
45	W	0	4
47	Z	0	2
48	l	0	3
49	s	0	1
50	t	0	4
52	z	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	Ah	0	1
66	L	0	4
67	M	0	4
All	All	0	99

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	280	PHE	CB-CA-C	-6.87	105.82	114.40
27	B	310	GLY	CA-C-O	-5.75	118.26	122.23
41	S	57	VAL	N-CA-C	-5.47	107.15	112.29
17	h	47	ILE	N-CA-C	-5.37	107.74	112.90
21	m	116	ILE	N-CA-C	-5.14	106.90	113.22
3	4	258	PRO	N-CA-C	-5.13	107.45	113.86
57	Ak	125	GLY	CA-C-O	-5.08	118.17	122.29

There are no chirality outliers.

All (99) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	A	10	ARG	Sidechain
9	A	18	ARG	Sidechain
54	Ah	25	ARG	Sidechain
27	B	109	ARG	Sidechain
27	B	132	ARG	Sidechain
27	B	159	ARG	Sidechain
27	B	267	ARG	Sidechain
27	B	269	ARG	Sidechain
27	B	405	ARG	Sidechain
27	B	86	ARG	Sidechain
31	F	97	ARG	Sidechain
32	H	212	ARG	Sidechain
32	H	44	ARG	Sidechain
32	H	79	ARG	Sidechain
32	H	98	ARG	Sidechain
33	I	151	ARG	Sidechain
33	I	186	ARG	Sidechain
33	I	191	ARG	Sidechain
33	I	94	ARG	Sidechain
33	I	98	ARG	Sidechain

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Mol	Chain	Res	Type	Group
35	K	34	ARG	Sidechain
35	K	58	ARG	Sidechain
66	L	127	ARG	Sidechain
66	L	216	ARG	Sidechain
66	L	350	ARG	Sidechain
66	L	352	ARG	Sidechain
67	M	103	ARG	Sidechain
67	M	57	ARG	Sidechain
67	M	6	ARG	Sidechain
67	M	61	ARG	Sidechain
39	Q	131	ARG	Sidechain
39	Q	57	ARG	Sidechain
39	Q	59	ARG	Sidechain
40	R	97	ARG	Sidechain
41	S	50	ARG	Sidechain
41	S	59	ARG	Sidechain
44	V	104	ARG	Sidechain
45	W	128	ARG	Sidechain
45	W	28	ARG	Sidechain
45	W	57	ARG	Sidechain
45	W	59	ARG	Sidechain
47	Z	63	ARG	Sidechain
47	Z	68	ARG	Sidechain
10	a	119	ARG	Sidechain
10	a	150	ARG	Sidechain
10	a	158	ARG	Sidechain
10	a	161	ARG	Sidechain
10	a	53	ARG	Sidechain
11	b	11	ARG	Sidechain
11	b	16	ARG	Sidechain
11	b	20	ARG	Sidechain
11	b	66	ARG	Sidechain
12	c	170	ARG	Sidechain
12	c	48	ARG	Sidechain
12	c	86	ARG	Sidechain
13	d	116	ARG	Sidechain
13	d	153	ARG	Sidechain
13	d	162	ARG	Sidechain
13	d	60	ARG	Sidechain
13	d	93	ARG	Sidechain
14	e	129	ARG	Sidechain
14	e	54	ARG	Sidechain

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Mol	Chain	Res	Type	Group
16	g	10	ARG	Sidechain
16	g	21	ARG	Sidechain
16	g	52	ARG	Sidechain
16	g	80	ARG	Sidechain
17	h	51	ARG	Sidechain
17	h	69	ARG	Sidechain
17	h	75	ARG	Sidechain
17	h	81	ARG	Sidechain
17	h	83	ARG	Sidechain
17	h	9	ARG	Sidechain
48	l	116	ARG	Sidechain
48	l	262	ARG	Sidechain
48	l	357	ARG	Sidechain
22	n	29	ARG	Sidechain
22	n	47	ARG	Sidechain
23	o	42	ARG	Sidechain
24	p	164	ARG	Sidechain
24	p	200	ARG	Sidechain
24	p	217	ARG	Sidechain
25	q	278	ARG	Sidechain
25	q	336	ARG	Sidechain
25	q	340	ARG	Sidechain
25	q	432	ARG	Sidechain
26	r	134	ARG	Sidechain
26	r	279	ARG	Sidechain
26	r	91	MET	Peptide
49	s	131	ARG	Sidechain
50	t	111	ARG	Sidechain
50	t	71	ARG	Sidechain
50	t	74	PHE	Peptide
50	t	8	ARG	Sidechain
7	x	168	ARG	Sidechain
7	x	187	ARG	Sidechain
7	x	205	ARG	Sidechain
7	x	286	ARG	Sidechain
7	x	288	ARG	Sidechain
52	z	72	ARG	Sidechain

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	0	561	0	542	19	0
1	Ab	543	0	530	7	0
2	1	493	0	491	5	0
2	Ac	485	0	485	9	0
3	2	1513	0	1497	41	0
3	4	1518	0	1498	47	0
3	Ae	275	0	276	29	0
3	Af	223	0	220	20	0
4	3	417	0	414	10	0
4	Ad	421	0	418	9	0
5	6	3140	0	3121	83	0
5	v	3140	0	3121	79	0
6	7	3025	0	3090	41	0
6	w	3025	0	3090	62	0
7	8	1906	0	1857	38	0
7	x	1896	0	1843	70	0
8	9	893	0	888	11	0
8	y	893	0	888	11	0
9	A	510	0	511	16	0
10	a	1151	0	1164	57	0
11	b	871	0	899	50	0
12	c	1278	0	1169	67	0
13	d	1420	0	1384	70	0
14	e	822	0	778	41	0
15	f	385	0	381	14	0
16	g	1000	0	994	46	0
17	h	867	0	871	36	0
18	i	2711	0	2874	118	0
19	j	721	0	768	62	0
20	k	748	0	799	56	0
21	m	1227	0	1236	75	0
22	n	452	0	449	27	0
23	o	1062	0	1072	58	0
24	p	1534	0	1470	79	0
25	q	3630	0	3837	151	0
26	r	2435	0	2543	121	0
27	B	3318	0	3283	121	0
28	C	3458	0	3394	126	0
29	D	1732	0	1682	54	0
30	E	1658	0	1664	46	0
31	F	738	0	701	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	H	1412	0	1369	62	0
33	I	1248	0	1257	69	0
34	J	962	0	962	20	0
35	K	1203	0	1161	26	0
36	N	910	0	950	21	0
37	O	689	0	687	42	0
37	X	689	0	687	70	0
38	P	669	0	677	17	0
39	Q	954	0	960	33	0
40	R	295	0	279	26	0
41	S	562	0	557	29	0
42	T	638	0	637	16	0
43	U	2562	0	2508	47	0
44	V	1021	0	1027	23	0
45	W	1162	0	1156	48	0
46	Y	524	0	469	25	0
47	Z	626	0	607	41	0
48	l	4773	0	4912	174	0
49	s	1398	0	1378	56	0
50	t	970	0	898	55	0
51	5	3374	0	3272	86	0
51	u	3459	0	3350	59	0
52	Aa	662	0	660	12	0
52	z	666	0	663	27	0
53	Ag	338	0	342	11	0
54	Ah	437	0	436	17	0
55	Ai	383	0	366	13	0
56	Aj	377	0	372	9	0
57	Ak	4002	0	3971	122	0
58	Al	1785	0	1800	79	0
59	Am	2096	0	2027	46	0
60	An	1154	0	1137	36	0
61	Ao	842	0	838	17	0
62	Ap	689	0	676	26	0
63	Aq	606	0	575	13	0
64	Ar	684	0	647	23	0
65	G	5260	0	5296	139	0
66	L	2493	0	2512	69	0
67	M	769	0	797	24	0
68	2	4	0	0	6	0
68	4	4	0	0	1	0
68	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	G	4	0	0	8	0
69	7	86	0	60	12	0
69	w	86	0	60	8	0
70	8	43	0	31	3	0
70	x	43	0	31	13	0
71	B	31	0	19	0	0
72	B	8	0	0	6	0
72	G	16	0	0	11	0
72	H	16	0	0	12	0
72	I	8	0	0	11	0
73	Q	30	0	30	1	0
74	Ak	120	0	108	20	0
75	L	48	0	26	6	0
All	All	111989	0	111432	3056	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 14.

All (3056) 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)
65:G:75:CYS:SG	68:G:803:FES:FE2	1.25	1.29
30:E:176:CYS:SG	30:E:180:CYS:SG	2.37	1.22
33:I:71:CYS:SG	72:I:201:SF4:FE1	1.32	1.20
67:M:43:VAL:HB	67:M:47:HIS:ND1	1.65	1.12
65:G:179:CYS:SG	72:G:802:SF4:FE1	1.42	1.08
18:i:42:PRO:CG	21:m:167:VAL:HG13	1.84	1.06
27:B:171:VAL:HG23	40:R:89:LEU:HD21	1.31	1.04
28:C:275:ARG:O	28:C:279:VAL:HB	1.60	1.01
7:x:122:CYS:H	70:x:401:HEC:HMC2	1.23	1.01
19:j:106:TRP:CE2	26:r:291:LYS:HD2	1.96	1.00
24:p:154:LYS:HA	24:p:161:PHE:HE2	1.24	0.99
32:H:116:CYS:SG	72:H:302:SF4:FE4	1.53	0.98
22:n:30:ARG:O	22:n:33:GLU:HG2	1.62	0.98
65:G:179:CYS:HG	72:G:802:SF4:FE1	0.69	0.98
65:G:226:CYS:HG	72:G:802:SF4:FE3	0.82	0.97
7:x:127:SER:HB2	7:x:179:PRO:HD3	1.43	0.96
37:X:92:LYS:H	47:Z:60:PRO:HB3	1.27	0.95
32:H:113:CYS:HG	72:H:302:SF4:FE2	0.68	0.94
65:G:176:CYS:SG	72:G:802:SF4:FE4	1.57	0.94
33:I:166:CYS:HG	72:I:201:SF4:FE3	0.64	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:72:CYS:SG	72:I:201:SF4:FE4	1.62	0.92
19:j:18:VAL:HG11	26:r:76:ILE:HG12	1.52	0.91
19:j:56:PHE:CE2	20:k:79:VAL:HG21	2.06	0.90
3:4:174:GLU:HG3	3:4:291:LEU:HD11	1.54	0.90
18:i:1:MET:HE2	21:m:170:GLU:HG2	1.52	0.90
48:l:503:GLU:HG3	54:Ah:54:ARG:HE	1.36	0.90
32:H:155:CYS:SG	72:H:301:SF4:FE3	1.64	0.89
24:p:60:ARG:HG2	37:X:132:ASP:HB3	1.53	0.89
18:i:42:PRO:HG3	21:m:167:VAL:HG13	1.53	0.88
18:i:65:THR:HG22	20:k:19:LEU:HD21	1.51	0.88
27:B:311:TRP:HE1	27:B:333:GLU:HG2	1.37	0.87
21:m:113:VAL:HG13	21:m:119:PHE:HB2	1.56	0.87
27:B:171:VAL:HG23	40:R:89:LEU:CD2	2.04	0.87
48:l:562:LEU:HB3	48:l:563:PRO:HD3	1.57	0.87
19:j:106:TRP:CZ2	26:r:291:LYS:HD2	2.09	0.86
23:o:37:LEU:HD22	24:p:50:ALA:HB2	1.57	0.86
56:Aj:41:MET:HE1	57:Ak:473:TRP:HB2	1.58	0.86
57:Ak:35:LEU:HD21	57:Ak:462:LEU:HD12	1.57	0.86
3:2:257:CYS:HG	68:2:301:FES:FE2	0.58	0.85
30:E:183:ALA:HB3	30:E:195:ASP:HA	1.55	0.85
12:c:166:LEU:HG	12:c:169:GLU:HB3	1.56	0.85
18:i:258:SER:HB2	18:i:336:VAL:HG12	1.57	0.85
28:C:367:ALA:HB3	65:G:149:ASP:HB2	1.56	0.85
29:D:103:HIS:HB2	29:D:107:GLN:HG2	1.56	0.85
22:n:25:CYS:CB	22:n:29:ARG:NH2	2.40	0.84
27:B:170:GLN:HE22	40:R:93:LEU:HD12	1.40	0.84
12:c:184:TYR:HA	50:t:36:GLU:HB2	1.59	0.84
32:H:155:CYS:HG	72:H:301:SF4:FE3	0.93	0.84
32:H:162:CYS:SG	72:H:302:SF4:FE1	1.69	0.83
66:L:71:MET:SD	66:L:249:LYS:NZ	2.51	0.83
24:p:154:LYS:HA	24:p:161:PHE:CE2	2.11	0.83
65:G:92:CYS:HG	68:G:803:FES:FE1	0.94	0.82
18:i:42:PRO:HG2	21:m:167:VAL:HG13	1.60	0.82
22:n:25:CYS:O	22:n:29:ARG:HG3	1.80	0.81
36:N:51:ILE:HD11	67:M:94:ALA:CB	2.10	0.81
14:e:56:GLN:HE22	43:U:324:HIS:HB2	1.45	0.81
25:q:328:CYS:HB2	25:q:437:MET:HE1	1.62	0.81
57:Ak:381:LEU:HB3	74:Ak:601:HEA:HAC	1.63	0.81
22:n:25:CYS:HB3	22:n:29:ARG:NH2	1.97	0.80
65:G:176:CYS:HG	72:G:802:SF4:FE4	0.51	0.80
57:Ak:243:VAL:HB	74:Ak:602:HEA:HAC	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:j:56:PHE:CE2	20:k:79:VAL:HG11	2.17	0.80
27:B:163:TYR:CE1	40:R:86:PHE:HB2	2.17	0.80
2:Ac:11:TYR:HA	2:Ac:15:PHE:HB2	1.63	0.80
3:2:257:CYS:SG	68:2:301:FES:FE2	1.72	0.80
22:n:31:SER:HA	22:n:34:LYS:HE2	1.62	0.80
28:C:183:ILE:HG23	28:C:216:MET:HE2	1.64	0.80
37:X:102:SER:HB3	37:X:108:LEU:HD21	1.62	0.79
3:2:255:TYR:HB2	3:2:264:TYR:HB2	1.64	0.79
33:I:166:CYS:SG	72:I:201:SF4:FE3	1.74	0.79
20:k:2:PRO:HG3	21:m:127:ILE:HG21	1.65	0.79
21:m:134:GLY:HA2	41:S:43:TYR:HB2	1.65	0.79
27:B:425:CYS:SG	72:B:502:SF4:FE3	1.74	0.79
11:b:95:TYR:HE2	13:d:109:ARG:HA	1.48	0.79
17:h:43:CYS:HA	49:s:224:ARG:HD2	1.65	0.78
27:B:423:THR:HB	72:B:502:SF4:S1	2.22	0.78
50:t:17:PRO:HA	50:t:105:GLU:OE2	1.83	0.78
69:7:401:HEM:HHD	69:7:401:HEM:HBC2	1.66	0.78
48:l:437:PHE:HB2	48:l:438:PRO:HD2	1.64	0.78
57:Ak:65:MET:HB3	74:Ak:601:HEA:HBC1	1.65	0.78
65:G:182:CYS:HG	72:G:802:SF4:FE2	1.00	0.78
22:n:25:CYS:HB3	22:n:29:ARG:HH21	1.49	0.78
19:j:59:ALA:HB1	21:m:67:VAL:HG12	1.66	0.78
48:l:227:PHE:H	48:l:284:THR:HG22	1.49	0.78
7:x:122:CYS:N	70:x:401:HEC:HMC2	1.99	0.77
57:Ak:359:ALA:HB2	74:Ak:602:HEA:HMB1	1.66	0.77
10:a:73:PHE:CD2	10:a:74:TYR:CE1	2.72	0.77
18:i:268:GLN:HA	25:q:165:VAL:HG11	1.66	0.77
22:n:25:CYS:HB2	22:n:29:ARG:NH2	2.00	0.77
26:r:28:LEU:HD22	26:r:275:ALA:HB2	1.66	0.77
65:G:226:CYS:SG	72:G:802:SF4:FE3	1.75	0.77
37:X:125:GLU:HG2	48:l:439:PRO:HG2	1.64	0.77
12:c:119:THR:HB	23:o:11:LEU:HA	1.67	0.77
17:h:65:GLU:HB3	45:W:111:PHE:HE1	1.50	0.77
14:e:148:GLN:HB2	16:g:113:GLU:HA	1.66	0.76
33:I:74:VAL:HA	33:I:77:MET:HE2	1.67	0.76
57:Ak:62:ALA:HB2	74:Ak:601:HEA:HBD1	1.65	0.76
3:Ae:55:GLY:HA3	3:Ae:59:LEU:HB3	1.65	0.76
7:8:184:GLU:HG3	7:x:159:PRO:HB2	1.67	0.76
13:d:147:GLY:HA3	16:g:121:VAL:HG21	1.66	0.76
27:B:174:ARG:HA	40:R:93:LEU:HD21	1.67	0.76
74:Ak:601:HEA:HHC	74:Ak:601:HEA:H122	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:j:3:ILE:HD13	26:r:96:ILE:HG21	1.68	0.76
19:j:56:PHE:HE2	20:k:79:VAL:HG11	1.51	0.76
65:G:75:CYS:HG	68:G:803:FES:FE2	0.46	0.76
13:d:139:PHE:HB2	14:e:137:MET:HE1	1.68	0.76
16:g:90:HIS:CE1	16:g:94:ALA:HB2	2.20	0.76
46:Y:87:PRO:HD2	50:t:99:MET:HE1	1.66	0.76
6:w:319:PRO:HB3	52:z:48:ARG:CZ	2.15	0.75
7:x:121:VAL:HG11	70:x:401:HEC:HAB	1.69	0.75
16:g:23:LEU:HD21	49:s:235:LEU:HB3	1.68	0.75
33:I:64:PRO:HG3	33:I:91:VAL:HG13	1.67	0.75
33:I:71:CYS:HG	72:I:201:SF4:FE1	0.46	0.75
27:B:79:GLU:HG2	27:B:255:CYS:HA	1.68	0.75
57:Ak:274:VAL:HG12	57:Ak:278:MET:HE2	1.68	0.75
66:L:121:VAL:HG23	66:L:156:VAL:HG11	1.69	0.75
57:Ak:28:MET:HE2	57:Ak:469:ILE:HD11	1.67	0.74
27:B:170:GLN:NE2	40:R:93:LEU:HD12	2.02	0.74
1:O:79:ASP:HB3	7:x:93:PRO:HG2	1.69	0.74
26:r:185:TRP:HE1	26:r:238:THR:HG22	1.52	0.74
37:O:104:PHE:HA	37:O:108:LEU:HB2	1.68	0.74
18:i:57:THR:HG22	20:k:77:LEU:HB3	1.68	0.74
43:U:98:SER:HA	43:U:103:GLY:HA2	1.69	0.74
62:Ap:64:ILE:HG23	62:Ap:65:LEU:HD12	1.68	0.74
18:i:128:LEU:HD11	18:i:213:LEU:HD23	1.70	0.74
25:q:116:ILE:HG21	49:s:245:PHE:HB3	1.70	0.74
33:I:72:CYS:HG	72:I:201:SF4:FE4	1.00	0.74
65:G:124:HIS:NE2	72:G:801:SF4:FE3	1.55	0.74
67:M:58:ASP:O	67:M:62:GLU:HG3	1.87	0.74
18:i:108:LEU:HD11	18:i:191:THR:HG21	1.70	0.74
64:Ar:44:MET:SD	64:Ar:47:LYS:NZ	2.60	0.74
69:7:401:HEM:HHC	69:7:401:HEM:HBB2	1.70	0.73
37:O:95:PRO:HA	37:O:98:LEU:HB3	1.69	0.73
5:v:324:SER:HB3	3:Af:68:LEU:HD13	1.69	0.73
11:b:26:GLN:HB3	24:p:217:ARG:HH12	1.52	0.73
12:c:126:TRP:HA	12:c:129:MET:HE2	1.71	0.73
3:4:142:THR:HG22	7:8:303:LEU:HB3	1.70	0.73
10:a:73:PHE:HD2	10:a:74:TYR:CE1	2.03	0.73
28:C:385:ILE:HG23	65:G:140:GLN:HG2	1.69	0.73
33:I:79:MET:HE1	33:I:177:ILE:HD12	1.69	0.73
23:o:45:ARG:HG2	24:p:191:PRO:HG3	1.69	0.73
65:G:338:VAL:HG12	65:G:544:VAL:HB	1.70	0.73
36:N:51:ILE:HD11	67:M:94:ALA:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:183:ALA:HB1	30:E:184:PRO:HD2	1.71	0.72
13:d:139:PHE:HD2	23:o:127:ILE:CG2	2.02	0.72
28:C:160:ALA:HA	28:C:404:THR:HG21	1.71	0.72
21:m:122:LEU:HD13	21:m:126:VAL:HG21	1.70	0.72
26:r:34:ARG:HG2	33:I:82:PRO:HA	1.72	0.72
27:B:364:VAL:HG12	27:B:400:VAL:HG12	1.70	0.72
59:Am:128:GLU:HG3	59:Am:129:VAL:H	1.55	0.72
65:G:92:CYS:SG	68:G:803:FES:FE1	1.80	0.72
22:n:30:ARG:O	22:n:33:GLU:CG	2.36	0.72
22:n:13:VAL:HG23	25:q:14:MET:HG2	1.72	0.72
27:B:35:LEU:HB2	27:B:291:GLU:HG3	1.69	0.72
1:0:28:ASP:HB2	7:x:263:THR:HB	1.70	0.72
27:B:131:ILE:HG13	27:B:165:GLU:HB3	1.69	0.72
5:6:170:GLN:HB3	3:Ae:67:VAL:HG22	1.69	0.72
12:c:156:VAL:HG21	50:t:95:TYR:CE1	2.25	0.72
19:j:67:LEU:HD21	20:k:68:ALA:HB3	1.70	0.71
28:C:143:ASP:OD1	28:C:143:ASP:N	2.22	0.71
48:l:510:TYR:HB3	48:l:512:LYS:HE3	1.72	0.71
22:n:15:ILE:O	22:n:19:VAL:HG23	1.89	0.71
65:G:367:CYS:HB3	65:G:531:LYS:HB3	1.72	0.71
48:l:507:THR:HA	48:l:510:TYR:HD2	1.54	0.71
7:x:286:ARG:HH22	7:x:287:LYS:HE3	1.54	0.71
5:v:155:GLN:NE2	5:v:200:VAL:O	2.23	0.71
34:J:90:GLY:HA2	65:G:59:GLN:HE22	1.56	0.71
26:r:310:MET:O	42:T:123:TYR:HB2	1.91	0.71
33:I:79:MET:HE2	33:I:86:MET:HG2	1.72	0.71
5:6:123:VAL:HB	5:6:133:LEU:HD23	1.72	0.71
3:Ae:65:SER:HB3	3:Ae:66:PRO:HD2	1.72	0.71
30:E:39:PHE:HA	30:E:124:ARG:HH12	1.55	0.71
25:q:199:CYS:HB2	25:q:250:LEU:HD11	1.72	0.70
36:N:23:ARG:NH2	43:U:277:TYR:OH	2.24	0.70
45:W:88:ARG:HD2	49:s:85:PRO:O	1.90	0.70
48:l:97:THR:HG21	48:l:125:LEU:HD13	1.72	0.70
65:G:456:ALA:O	65:G:499:ASN:ND2	2.24	0.70
3:4:185:ASN:HD21	3:4:196:PHE:HB3	1.55	0.70
29:D:103:HIS:HB3	36:N:83:GLN:CD	2.17	0.70
3:4:120:SER:HA	51:5:269:ARG:HE	1.56	0.70
48:l:481:THR:HG23	50:t:95:TYR:HD2	1.56	0.70
66:L:119:ASN:HD22	66:L:120:VAL:HG23	1.56	0.70
12:c:161:TYR:HB3	12:c:166:LEU:HD13	1.72	0.70
46:Y:45:ARG:HH12	47:Z:64:ASN:HD21	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:312:GLN:OE1	29:D:140:ARG:NH1	2.24	0.70
10:a:147:ALA:HB2	25:q:173:SER:HB2	1.74	0.70
11:b:95:TYR:CE2	13:d:109:ARG:HA	2.26	0.70
24:p:137:GLU:HG3	25:q:418:LYS:HD3	1.73	0.70
48:l:313:MET:HE3	48:l:329:ILE:HG12	1.73	0.70
44:V:47:ALA:HB3	44:V:51:GLU:HG3	1.73	0.69
24:p:160:TYR:HA	24:p:163:LYS:HD2	1.73	0.69
25:q:370:PRO:HB2	48:l:142:ILE:HA	1.74	0.69
40:R:100:GLN:HG3	40:R:101:PRO:HD2	1.75	0.69
18:i:232:HIS:HB3	18:i:311:MET:HE1	1.74	0.69
27:B:314:LEU:HD11	27:B:317:VAL:HG23	1.75	0.69
40:R:98:MET:HE3	40:R:99:PRO:HD2	1.73	0.69
43:U:225:ASN:HB3	43:U:228:GLU:HB2	1.74	0.69
48:l:243:VAL:HG13	48:l:247:LEU:HD13	1.74	0.69
55:Ai:68:PRO:HG2	60:An:156:PHE:HE1	1.58	0.69
27:B:317:VAL:HG22	27:B:356:VAL:HA	1.73	0.69
17:h:7:GLN:HB2	17:h:16:ARG:HH21	1.57	0.69
37:X:86:VAL:HG12	47:Z:61:TRP:CZ3	2.28	0.69
26:r:61:LEU:HD21	33:I:125:PRO:HB3	1.75	0.68
65:G:326:VAL:HG23	65:G:626:LEU:HD13	1.74	0.68
26:r:275:ALA:HA	28:C:203:MET:HE2	1.76	0.68
33:I:81:ALA:HB1	33:I:82:PRO:HD2	1.75	0.68
41:S:68:ASN:HD22	49:s:96:LYS:HB3	1.58	0.68
43:U:148:ALA:HB1	43:U:159:VAL:HG11	1.74	0.68
3:Ae:52:GLY:HA2	3:Ae:61:ALA:HA	1.74	0.68
23:o:115:LEU:HD22	23:o:120:LYS:HD2	1.75	0.68
30:E:185:MET:HB3	30:E:194:GLU:HA	1.75	0.68
37:X:89:LEU:HB3	47:Z:64:ASN:HB2	1.74	0.68
49:s:180:GLN:HA	49:s:183:LYS:HD3	1.74	0.68
13:d:23:GLN:HE21	50:t:73:SER:HB3	1.58	0.68
13:d:155:CYS:HG	14:e:141:CYS:HG	1.39	0.68
24:p:187:PRO:C	24:p:189:GLY:H	2.00	0.68
27:B:170:GLN:HE22	40:R:93:LEU:CD1	2.06	0.68
32:H:155:CYS:SG	72:H:301:SF4:S2	2.92	0.68
7:x:309:ARG:HH21	52:z:27:PHE:HA	1.59	0.68
57:Ak:107:PRO:HB3	59:Am:25:LEU:HB2	1.76	0.68
26:r:66:SER:HB2	26:r:124:ASN:HB2	1.75	0.67
27:B:315:LEU:HB2	27:B:359:ARG:HA	1.76	0.67
4:3:39:ARG:HD3	4:3:39:ARG:H	1.59	0.67
16:g:90:HIS:HE1	16:g:94:ALA:HB2	1.58	0.67
28:C:122:LEU:HD11	33:I:70:ALA:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:j:9:THR:HG21	26:r:6:ILE:HG21	1.76	0.67
26:r:24:GLU:HA	26:r:271:LEU:HD13	1.76	0.67
51:u:120:LEU:HB3	5:v:299:VAL:HG12	1.76	0.67
13:d:142:ARG:HD2	14:e:139:SER:HA	1.75	0.67
23:o:65:LEU:HD11	25:q:341:THR:HG21	1.77	0.67
37:X:86:VAL:HG12	47:Z:61:TRP:HZ3	1.57	0.67
51:u:388:VAL:HG21	51:u:438:ALA:HA	1.77	0.67
19:j:58:VAL:HG11	26:r:286:MET:SD	2.33	0.67
26:r:25:ARG:HH12	26:r:47:GLN:HE21	1.40	0.67
21:m:34:ILE:HA	21:m:61:LEU:HD11	1.77	0.67
28:C:180:PHE:O	28:C:184:THR:HG23	1.94	0.67
29:D:130:TYR:HB2	29:D:143:VAL:HG22	1.76	0.67
32:H:81:PRO:HD2	41:S:1:MET:HG2	1.76	0.67
48:l:536:LEU:HB3	48:l:537:PRO:HD3	1.76	0.67
5:v:138:LEU:HD12	5:v:233:VAL:HG22	1.76	0.67
6:w:319:PRO:HB3	52:z:48:ARG:NH2	2.08	0.67
57:Ak:508:PRO:HG3	59:Am:6:HIS:HB3	1.77	0.67
10:a:179:ILE:HG21	17:h:38:LYS:HG3	1.77	0.67
14:e:93:PHE:HA	14:e:97:ILE:HB	1.77	0.67
25:q:108:MET:HB3	25:q:121:LEU:HD13	1.77	0.67
5:6:82:LEU:HD13	5:6:158:LEU:HD11	1.75	0.67
66:L:203:GLY:H	66:L:206:ASP:HB2	1.60	0.67
66:L:212:PHE:HA	66:L:215:MET:HE2	1.77	0.67
19:j:59:ALA:HA	26:r:140:ILE:CD1	2.25	0.66
29:D:121:THR:HG21	34:J:129:SER:H	1.58	0.66
47:Z:55:ARG:HH22	54:Ah:36:ASP:HB3	1.60	0.66
65:G:691:ILE:HG23	65:G:714:VAL:HG21	1.75	0.66
4:3:45:VAL:O	4:3:49:ASN:ND2	2.28	0.66
10:a:129:PRO:HB3	14:e:112:TYR:CE1	2.30	0.66
24:p:187:PRO:C	24:p:189:GLY:N	2.53	0.66
58:Al:179:LEU:H	64:Ar:27:THR:HG23	1.58	0.66
42:T:141:PRO:HG3	49:s:118:LYS:HD2	1.78	0.66
37:X:114:ASP:O	37:X:118:ILE:HG12	1.95	0.66
6:7:338:ILE:HD11	6:7:350:ILE:HG22	1.77	0.66
21:m:136:PHE:CE1	42:T:136:TYR:HB3	2.30	0.66
51:5:267:PRO:HA	51:5:350:GLU:HG3	1.76	0.66
33:I:41:SER:N	33:I:44:GLU:OE2	2.28	0.66
57:Ak:465:VAL:HG22	74:Ak:601:HEA:H273	1.78	0.66
65:G:266:ARG:HG2	65:G:267:THR:HG23	1.78	0.66
12:c:169:GLU:HA	13:d:123:GLN:HE22	1.61	0.66
18:i:50:PRO:HG2	28:C:75:VAL:HG12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Al:1:MET:HG2	60:An:150:VAL:HG21	1.75	0.66
24:p:183:GLN:HA	24:p:186:THR:HB	1.77	0.66
25:q:269:MET:HG3	25:q:270:ILE:HD12	1.77	0.66
28:C:165:LEU:HD13	28:C:397:VAL:HG22	1.78	0.66
61:Ao:55:ASP:HA	61:Ao:90:ILE:HD11	1.77	0.66
10:a:73:PHE:CD2	10:a:74:TYR:CD1	2.84	0.66
12:c:37:PHE:HB3	23:o:70:TYR:CE2	2.31	0.66
19:j:62:PHE:HB2	26:r:140:ILE:HG23	1.77	0.66
28:C:305:GLN:HB3	67:M:104:TRP:CE3	2.31	0.66
25:q:403:THR:HA	25:q:406:TYR:CE2	2.31	0.65
41:S:66:LEU:HB3	49:s:152:LYS:HE2	1.78	0.65
7:x:102:LEU:O	7:x:287:LYS:HD2	1.95	0.65
57:Ak:244:TYR:HA	57:Ak:247:ILE:HG22	1.77	0.65
66:L:201:ILE:HD12	75:L:401:NDP:H42N	1.77	0.65
3:4:270:ILE:HD13	3:4:275:ALA:HB3	1.76	0.65
10:a:52:LYS:HE2	10:a:53:ARG:HD3	1.78	0.65
37:X:90:TYR:HD2	37:X:93:ILE:HG22	1.61	0.65
51:u:134:LYS:HE3	5:v:384:MET:HE3	1.78	0.65
5:6:293:LEU:HD22	5:6:309:LEU:HD13	1.78	0.65
19:j:59:ALA:HA	26:r:140:ILE:HD13	1.76	0.65
50:t:51:LEU:HD13	50:t:63:LEU:HD23	1.77	0.65
59:Am:156:ARG:HG2	62:Ap:37:VAL:HG12	1.78	0.65
65:G:402:LEU:HD13	65:G:407:PRO:HG3	1.79	0.65
12:c:38:PRO:HD2	23:o:70:TYR:HD2	1.60	0.65
30:E:177:LEU:HB2	30:E:185:MET:HE1	1.77	0.65
51:u:99:LYS:NZ	5:v:301:ARG:O	2.27	0.65
6:7:112:THR:O	6:7:196:HIS:NE2	2.29	0.65
28:C:441:LEU:HD13	28:C:460:GLN:HE22	1.61	0.65
58:Al:83:ILE:HA	58:Al:86:MET:HE2	1.78	0.65
3:4:216:LEU:HD13	3:4:269:ARG:HD2	1.77	0.65
5:6:84:ARG:NH2	5:6:190:LEU:O	2.27	0.65
29:D:129:VAL:HG22	29:D:144:LYS:HG2	1.78	0.65
43:U:110:LEU:HD13	43:U:336:LEU:HD11	1.77	0.65
7:x:122:CYS:HB2	70:x:401:HEC:HMC2	1.78	0.65
32:H:54:THR:HG23	45:W:36:PHE:HE2	1.62	0.65
41:S:37:ARG:HD2	41:S:48:MET:HG3	1.78	0.65
69:w:402:HEM:HBC2	69:w:402:HEM:HMC1	1.78	0.65
37:O:87:LEU:HD12	37:O:118:ILE:HD12	1.79	0.65
44:V:94:GLY:HA3	44:V:119:GLY:HA2	1.79	0.65
23:o:101:TRP:HB2	25:q:263:MET:HE1	1.80	0.64
6:w:138:MET:HA	6:w:138:MET:HE3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:x:122:CYS:H	70:x:401:HEC:CMC	2.06	0.64
7:x:122:CYS:HB3	7:x:125:CYS:H	1.62	0.64
65:G:138:ASP:HB3	65:G:142:GLN:HE21	1.63	0.64
14:e:86:ASN:ND2	25:q:25:ILE:HG13	2.11	0.64
12:c:167:TYR:CE2	12:c:181:VAL:HG21	2.33	0.64
24:p:150:HIS:CD2	24:p:151:PRO:HD2	2.32	0.64
58:Al:134:ARG:HB2	60:An:132:THR:HG21	1.79	0.64
16:g:90:HIS:ND1	16:g:90:HIS:C	2.55	0.64
25:q:216:LEU:HB3	25:q:217:PRO:HD3	1.78	0.64
37:X:119:ILE:HD12	37:X:138:LEU:HD23	1.79	0.64
12:c:167:TYR:HE2	12:c:181:VAL:HG21	1.61	0.64
13:d:71:VAL:HG22	13:d:72:PRO:HD2	1.80	0.64
20:k:2:PRO:HG3	21:m:127:ILE:HD13	1.79	0.64
48:l:551:SER:HA	48:l:555:LEU:HB2	1.78	0.64
51:u:298:ASN:O	51:u:301:ASN:ND2	2.27	0.64
3:2:145:GLY:HA3	7:x:300:LEU:HD21	1.78	0.64
16:g:90:HIS:C	16:g:90:HIS:HD1	2.06	0.64
22:n:24:GLY:HA2	25:q:6:ILE:HD12	1.79	0.64
5:v:90:THR:HG23	5:v:95:SER:HA	1.79	0.64
7:x:114:GLY:HA3	7:x:274:PHE:HB2	1.80	0.64
10:a:131:LYS:HG3	22:n:58:LYS:HA	1.79	0.64
17:h:47:ILE:HB	17:h:51:ARG:HH21	1.63	0.64
27:B:425:CYS:SG	72:B:502:SF4:S1	2.87	0.64
46:Y:44:TYR:HD2	47:Z:33:PRO:HD2	1.62	0.64
26:r:102:VAL:HG13	26:r:150:LEU:HD11	1.80	0.63
26:r:219:PRO:HA	26:r:222:MET:HE2	1.79	0.63
37:O:138:LEU:HG	37:O:144:ILE:HG12	1.80	0.63
37:X:83:VAL:HG22	37:X:122:MET:HG3	1.80	0.63
37:X:131:PRO:HB2	37:X:133:ILE:HG12	1.80	0.63
12:c:169:GLU:CA	13:d:123:GLN:HE22	2.11	0.63
33:I:71:CYS:SG	72:I:201:SF4:S3	2.96	0.63
48:l:90:ILE:HA	48:l:129:MET:HE2	1.80	0.63
5:6:66:LYS:O	5:6:217:ARG:NH2	2.30	0.63
30:E:130:TYR:HA	30:E:189:ASN:HD21	1.62	0.63
41:S:69:ILE:O	41:S:70:ASP:C	2.42	0.63
3:2:257:CYS:SG	68:2:301:FES:S1	2.96	0.63
28:C:272:ARG:HH22	32:H:63:TRP:HA	1.64	0.63
33:I:175:TYR:HE1	35:K:78:ASP:HB2	1.63	0.63
37:O:152:LYS:O	37:O:153:ASP:HB2	1.98	0.63
60:An:155:GLY:H	60:An:158:ALA:HB3	1.63	0.63
9:A:61:GLU:OE1	9:A:64:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:G:68:ARG:HE	65:G:283:GLU:HB3	1.64	0.63
65:G:397:ALA:HA	65:G:471:LYS:HB3	1.80	0.63
5:6:395:GLU:OE2	5:6:399:GLN:NE2	2.32	0.63
10:a:179:ILE:HG23	17:h:22:SER:HB3	1.79	0.63
12:c:129:MET:HB3	48:l:532:ILE:HD11	1.79	0.63
18:i:88:LYS:HD3	18:i:148:SER:HB3	1.80	0.63
23:o:112:LYS:NZ	25:q:388:TRP:O	2.32	0.63
7:8:244:ALA:HB3	70:8:401:HEC:HBD2	1.81	0.63
10:a:106:VAL:HB	22:n:50:ARG:HH21	1.62	0.63
37:X:118:ILE:HD13	47:Z:61:TRP:HZ2	1.62	0.63
24:p:104:GLN:O	24:p:108:GLN:HG2	1.99	0.63
17:h:89:GLU:HB3	17:h:91:LYS:HE2	1.81	0.62
23:o:52:ASN:HA	24:p:211:HIS:NE2	2.14	0.62
50:t:8:ARG:HB2	50:t:16:GLU:HG2	1.80	0.62
14:e:56:GLN:NE2	43:U:324:HIS:HB2	2.14	0.62
30:E:49:PRO:HG3	30:E:95:ILE:HD13	1.81	0.62
32:H:116:CYS:HB2	32:H:118:LEU:HD13	1.79	0.62
51:5:422:ARG:NH2	51:5:428:GLU:OE1	2.32	0.62
65:G:179:CYS:SG	72:G:802:SF4:S4	2.97	0.62
5:6:444:LEU:O	5:6:446:HIS:N	2.33	0.62
17:h:65:GLU:CG	45:W:111:PHE:CE1	2.82	0.62
18:i:200:MET:HE1	18:i:343:LEU:HD11	1.80	0.62
25:q:127:VAL:HB	25:q:128:PRO:HD3	1.80	0.62
25:q:313:THR:HA	25:q:316:MET:HE2	1.79	0.62
48:l:55:MET:HG2	48:l:471:ASN:HB3	1.81	0.62
48:l:481:THR:HG23	50:t:95:TYR:CD2	2.34	0.62
51:u:75:ILE:HG12	51:u:229:MET:HG2	1.81	0.62
65:G:75:CYS:SG	68:G:803:FES:S2	2.96	0.62
5:6:116:ARG:NH1	5:6:188:ASN:O	2.32	0.62
28:C:190:ILE:O	28:C:194:THR:HB	1.99	0.62
30:E:179:ALA:HB3	30:E:185:MET:HE3	1.79	0.62
63:Aq:26:ARG:HD3	63:Aq:26:ARG:H	1.63	0.62
13:d:140:GLN:HE22	23:o:123:GLN:HB3	1.64	0.62
28:C:418:VAL:HG13	28:C:427:ARG:HB3	1.81	0.62
51:u:76:ASP:O	51:u:228:ARG:NH2	2.30	0.62
51:5:318:TYR:HE1	3:Ae:54:VAL:HG23	1.65	0.62
10:a:153:GLU:HA	16:g:92:MET:HE2	1.82	0.62
26:r:30:TYR:HE1	32:H:81:PRO:HG3	1.65	0.62
58:Al:104:TRP:CG	58:Al:203:ASN:HB2	2.35	0.62
3:4:213:VAL:HA	3:4:216:LEU:HD12	1.82	0.62
10:a:157:ARG:HG2	10:a:168:TRP:CZ3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:q:329:LEU:HG	25:q:437:MET:HE2	1.81	0.62
69:w:401:HEM:HMC2	69:w:401:HEM:HBC2	1.80	0.62
60:An:78:LYS:HB3	61:Ao:104:PHE:CZ	2.33	0.62
10:a:169:TYR:H	16:g:3:MET:HA	1.62	0.62
18:i:289:ASN:HA	18:i:292:PHE:CE2	2.35	0.62
48:l:99:SER:HA	48:l:456:ARG:HH21	1.65	0.62
43:U:178:GLN:NE2	43:U:238:ASP:OD2	2.32	0.62
44:V:69:ILE:HG13	44:V:100:THR:HG21	1.81	0.62
5:6:176:ASN:ND2	5:6:260:ASP:OD2	2.32	0.62
10:a:73:PHE:HD2	10:a:74:TYR:CD1	2.18	0.62
10:a:106:VAL:HB	22:n:50:ARG:NH2	2.15	0.62
3:4:204:GLU:O	3:4:208:GLU:HG2	2.00	0.61
20:k:75:LEU:HD11	21:m:68:PHE:CE1	2.34	0.61
49:s:201:GLU:HA	49:s:204:LYS:HD3	1.82	0.61
51:u:276:ARG:NH2	51:u:466:PRO:O	2.33	0.61
51:u:445:CYS:O	51:u:449:PHE:HB2	2.00	0.61
57:Ak:34:SER:HB3	57:Ak:61:HIS:CE1	2.34	0.61
49:s:97:VAL:HG12	49:s:102:LEU:HG	1.83	0.61
25:q:123:GLU:HA	25:q:126:LEU:HD13	1.81	0.61
27:B:257:ARG:HG2	27:B:261:TRP:CG	2.35	0.61
28:C:187:LEU:HD21	28:C:216:MET:HB2	1.80	0.61
32:H:162:CYS:HG	72:H:302:SF4:FE1	0.49	0.61
48:l:85:PHE:HB3	48:l:258:PHE:HE1	1.64	0.61
48:l:387:THR:HG22	48:l:465:GLY:H	1.64	0.61
70:x:401:HEC:HBA1	70:x:401:HEC:HHA	1.83	0.61
60:An:82:TYR:OH	61:Ao:109:ARG:NH2	2.33	0.61
17:h:65:GLU:HB3	45:W:111:PHE:CE1	2.34	0.61
30:E:59:ASN:ND2	30:E:89:GLN:OE1	2.33	0.61
41:S:63:THR:HG23	49:s:98:SER:HB3	1.82	0.61
43:U:255:CYS:SG	43:U:256:GLU:N	2.73	0.61
51:5:378:ARG:NH2	51:5:387:GLU:OE1	2.34	0.61
26:r:157:ASN:HA	26:r:168:THR:HG21	1.82	0.61
32:H:186:ASN:HD21	35:K:129:THR:HG23	1.65	0.61
6:w:245:PHE:CD1	7:x:102:LEU:HD11	2.35	0.61
18:i:106:LEU:O	18:i:135:LYS:NZ	2.34	0.61
18:i:337:LEU:O	18:i:340:THR:HG23	2.00	0.61
25:q:345:ALA:HB1	25:q:348:LEU:HD21	1.83	0.61
41:S:18:ILE:HA	41:S:21:MET:HE2	1.83	0.61
5:6:129:ASP:N	5:6:129:ASP:OD1	2.30	0.61
28:C:389:LYS:HG3	65:G:144:MET:HG3	1.83	0.61
37:X:118:ILE:HD13	47:Z:61:TRP:CZ2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Ak:197:LEU:HA	59:Am:92:LEU:HD13	1.82	0.61
19:j:106:TRP:CE2	26:r:291:LYS:CD	2.81	0.61
5:v:43:LEU:HD22	5:v:44:PRO:HD2	1.83	0.61
66:L:183:GLU:HG3	66:L:195:ILE:HD13	1.83	0.61
13:d:92:TRP:HE3	13:d:93:ARG:HG2	1.65	0.61
26:r:117:LEU:HD11	26:r:136:VAL:HG22	1.81	0.61
28:C:101:LEU:HB2	28:C:464:PHE:CZ	2.36	0.61
65:G:388:ASN:HB3	65:G:511:LYS:HD2	1.82	0.61
29:D:126:PHE:HB2	29:D:147:THR:HG23	1.81	0.61
48:l:280:LEU:O	48:l:284:THR:HG23	2.01	0.61
48:l:316:THR:HG22	48:l:321:GLN:HB2	1.81	0.61
5:6:61:ILE:HG13	5:6:130:ILE:HD11	1.82	0.60
7:8:228:LEU:HD11	7:8:234:PHE:HB2	1.82	0.60
17:h:65:GLU:CB	45:W:111:PHE:HE1	2.14	0.60
27:B:38:GLU:HA	30:E:239:LYS:HD2	1.83	0.60
51:5:222:GLN:O	51:5:225:LYS:NZ	2.34	0.60
12:c:36:MET:HB3	23:o:67:ARG:HH21	1.67	0.60
26:r:215:TYR:HB3	26:r:219:PRO:HB2	1.83	0.60
48:l:227:PHE:N	48:l:284:THR:HG22	2.16	0.60
5:6:320:PRO:HB3	3:Ae:75:LEU:HB3	1.82	0.60
41:S:66:LEU:H	41:S:66:LEU:HD22	1.66	0.60
48:l:483:PRO:HB2	48:l:486:MET:HB2	1.83	0.60
65:G:339:ALA:HB3	65:G:542:PRO:HG3	1.83	0.60
11:b:22:TRP:HB2	24:p:213:VAL:CG1	2.32	0.60
19:j:113:TRP:HZ3	26:r:282:TYR:CZ	2.18	0.60
32:H:116:CYS:HG	72:H:302:SF4:FE4	1.15	0.60
48:l:2:ASN:HB3	48:l:3:PRO:HD3	1.83	0.60
57:Ak:334:TRP:HZ2	58:Al:46:LEU:HB2	1.67	0.60
5:6:61:ILE:HD11	5:6:225:VAL:HG21	1.82	0.60
6:7:119:LEU:HD22	69:7:402:HEM:HBB2	1.83	0.60
23:o:47:TYR:CE1	23:o:60:ILE:HD12	2.37	0.60
24:p:219:ARG:HD2	24:p:221:MET:HE1	1.84	0.60
27:B:299:LEU:HD12	27:B:303:HIS:HD2	1.65	0.60
31:F:97:ARG:HH11	31:F:97:ARG:HG3	1.67	0.60
33:I:66:THR:HG23	33:I:76:MET:HE3	1.82	0.60
66:L:352:ARG:HB3	66:L:356:TRP:HB3	1.84	0.60
37:O:132:ASP:HB3	39:Q:59:ARG:HH21	1.65	0.60
51:5:304:LEU:HD13	51:5:354:LEU:HD22	1.83	0.60
5:6:320:PRO:HG2	5:6:343:GLN:HE21	1.67	0.60
14:e:95:PHE:HA	14:e:99:LEU:HB2	1.84	0.60
51:5:298:ASN:O	51:5:301:ASN:ND2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:r:26:LYS:HA	26:r:36:GLY:HA3	1.84	0.60
38:P:79:LEU:HD22	38:P:87:VAL:HG22	1.83	0.60
67:M:43:VAL:HB	67:M:47:HIS:CG	2.35	0.60
18:i:128:LEU:HD13	18:i:216:PHE:HB2	1.84	0.60
1:0:33:VAL:HG12	1:0:82:VAL:HG22	1.83	0.60
14:e:112:TYR:HD2	25:q:43:ASN:HD21	1.50	0.60
25:q:14:MET:SD	25:q:26:ASN:HB3	2.42	0.60
25:q:98:MET:HE2	25:q:131:ILE:HD12	1.84	0.60
29:D:183:ASP:OD2	29:D:185:ARG:NH1	2.34	0.60
12:c:38:PRO:HG2	23:o:71:ALA:HB2	1.84	0.59
18:i:2:ASN:ND2	43:U:45:PHE:HE2	2.00	0.59
18:i:4:ILE:HD11	43:U:46:VAL:HG13	1.84	0.59
27:B:163:TYR:CE1	40:R:86:PHE:CB	2.84	0.59
29:D:63:GLN:HE21	67:M:69:VAL:HG12	1.67	0.59
64:Ar:58:ARG:HH22	64:Ar:62:LYS:HD3	1.67	0.59
43:U:260:TYR:HE2	43:U:271:VAL:HG13	1.67	0.59
3:2:100:SER:O	3:2:101:HIS:ND1	2.36	0.59
3:4:265:ASP:OD1	3:4:269:ARG:N	2.36	0.59
5:6:63:LEU:HD23	5:6:141:THR:HG21	1.84	0.59
24:p:218:GLU:HG2	24:p:219:ARG:HG2	1.84	0.59
25:q:339:SER:HB3	25:q:344:LEU:HD22	1.84	0.59
39:Q:48:SER:HB2	39:Q:53:GLU:HB3	1.84	0.59
5:v:70:ARG:HD2	5:v:117:GLU:HG2	1.83	0.59
65:G:49:VAL:HB	65:G:91:ALA:HA	1.83	0.59
7:8:223:PRO:HG3	1:Ab:71:LEU:HD22	1.84	0.59
27:B:141:GLY:HA2	27:B:252:PRO:HD3	1.84	0.59
27:B:170:GLN:NE2	40:R:93:LEU:CD1	2.65	0.59
32:H:54:THR:HA	42:T:98:TRP:HE1	1.66	0.59
58:Al:112:ASP:O	64:Ar:59:ARG:NH1	2.34	0.59
18:i:13:VAL:O	18:i:36:ASN:ND2	2.36	0.59
20:k:22:TYR:HA	21:m:23:LYS:HE2	1.82	0.59
24:p:153:GLU:HA	24:p:156:MET:HE2	1.83	0.59
27:B:88:ARG:HD2	27:B:274:LYS:HD3	1.83	0.59
38:P:46:LYS:HZ1	65:G:674:LEU:HD21	1.67	0.59
52:z:51:PRO:HB2	52:z:52:PRO:HD3	1.83	0.59
5:6:61:ILE:HD12	5:6:134:MET:HG3	1.85	0.59
19:j:67:LEU:HD22	20:k:65:VAL:HA	1.85	0.59
41:S:66:LEU:HD21	49:s:159:PHE:CD2	2.37	0.59
6:w:338:ILE:HD11	6:w:350:ILE:HG22	1.84	0.59
54:Ah:22:LEU:HB3	54:Ah:25:ARG:HH12	1.66	0.59
3:2:100:SER:N	3:2:103:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:q:132:ILE:HA	25:q:136:TRP:HE3	1.65	0.59
25:q:221:VAL:HA	25:q:283:LYS:HD3	1.83	0.59
25:q:272:THR:HA	25:q:275:ILE:HD12	1.84	0.59
47:Z:88:LYS:H	47:Z:88:LYS:HD3	1.68	0.59
57:Ak:381:LEU:HD23	74:Ak:601:HEA:HAC	1.84	0.59
43:U:352:LYS:HD3	43:U:353:TRP:H	1.67	0.59
57:Ak:381:LEU:HD23	74:Ak:601:HEA:CAC	2.32	0.59
57:Ak:409:TRP:HB3	57:Ak:471:ILE:HG12	1.85	0.59
11:b:22:TRP:CD1	24:p:214:THR:HA	2.37	0.59
11:b:28:LEU:HD21	11:b:32:GLU:HB2	1.84	0.59
16:g:90:HIS:ND1	16:g:90:HIS:O	2.30	0.59
25:q:299:VAL:O	25:q:303:ILE:HG12	2.03	0.59
37:O:119:ILE:HD12	37:O:138:LEU:HD23	1.85	0.59
3:4:256:TYR:CE1	3:4:261:GLY:HA2	2.37	0.59
13:d:79:GLU:HB2	16:g:108:LYS:HE2	1.85	0.59
19:j:18:VAL:HA	26:r:222:MET:SD	2.43	0.59
30:E:197:THR:H	30:E:200:ASP:HB3	1.68	0.59
51:u:393:ASN:O	51:u:397:ASN:ND2	2.32	0.59
3:4:240:HIS:HE1	3:4:260:HIS:CG	2.21	0.58
27:B:288:VAL:HG21	27:B:303:HIS:HB3	1.85	0.58
48:l:384:PRO:HA	48:l:389:PHE:HB2	1.85	0.58
65:G:498:GLN:NE2	65:G:499:ASN:OD1	2.36	0.58
3:Ae:42:CYS:HA	3:Ae:45:PRO:HG3	1.84	0.58
7:8:288:ARG:NH1	2:Ac:41:ASP:OD1	2.34	0.58
17:h:17:TRP:HE3	20:k:55:LEU:HD13	1.69	0.58
20:k:14:ILE:HD13	21:m:18:VAL:HG22	1.85	0.58
24:p:71:SER:HB2	24:p:118:HIS:HD2	1.67	0.58
28:C:431:LYS:HG3	29:D:113:ASP:HB3	1.85	0.58
30:E:191:ASN:HB3	30:E:216:PRO:HB3	1.84	0.58
48:l:507:THR:HA	48:l:510:TYR:CD2	2.37	0.58
67:M:43:VAL:HB	67:M:47:HIS:CE1	2.38	0.58
3:2:243:CYS:SG	68:2:301:FES:S2	3.01	0.58
5:6:309:LEU:HD21	5:6:338:ILE:HG22	1.84	0.58
7:8:118:TYR:HA	7:8:122:CYS:HB2	1.84	0.58
17:h:65:GLU:HG3	45:W:111:PHE:CE1	2.38	0.58
27:B:342:LEU:HD12	27:B:349:LEU:HA	1.85	0.58
34:J:69:GLU:HA	34:J:72:ILE:HG22	1.84	0.58
44:V:106:ARG:HA	44:V:106:ARG:HE	1.68	0.58
12:c:168:LEU:HD21	12:c:178:PRO:HB3	1.84	0.58
23:o:20:PRO:HB3	24:p:107:ARG:HH22	1.68	0.58
27:B:102:MET:HG2	27:B:149:MET:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:R:80:GLU:OE1	40:R:80:GLU:N	2.37	0.58
51:5:131:TYR:HH	51:5:224:TYR:HH	1.51	0.58
11:b:95:TYR:HE2	13:d:109:ARG:CA	2.16	0.58
12:c:97:LEU:HB3	12:c:99:LEU:HG	1.86	0.58
25:q:208:PRO:HB2	25:q:291:VAL:HG13	1.86	0.58
28:C:272:ARG:NH2	32:H:63:TRP:HA	2.18	0.58
7:x:314:VAL:HG13	52:z:18:SER:HB3	1.84	0.58
21:m:2:THR:HA	21:m:5:ILE:HG12	1.86	0.58
48:l:491:LEU:H	48:l:491:LEU:HD22	1.68	0.58
7:x:153:VAL:HG21	7:x:177:PRO:HG2	1.85	0.58
65:G:299:ARG:NH1	65:G:703:ALA:O	2.32	0.58
10:a:129:PRO:HB3	14:e:112:TYR:HE1	1.68	0.58
13:d:93:ARG:HB2	25:q:47:GLU:OE1	2.03	0.58
26:r:185:TRP:NE1	26:r:238:THR:HG22	2.18	0.58
6:w:326:TRP:NE1	52:z:49:VAL:HG22	2.19	0.58
54:Ah:46:GLY:N	54:Ah:49:ASP:OD2	2.36	0.58
13:d:146:LEU:HD12	13:d:154:LYS:HB3	1.86	0.58
37:X:91:ASP:HB3	47:Z:60:PRO:HA	1.84	0.58
51:5:388:VAL:HG21	51:5:438:ALA:HA	1.85	0.58
13:d:8:ASP:HB3	14:e:127:LYS:HZ1	1.67	0.58
16:g:119:HIS:CE1	25:q:252:PRO:HG3	2.38	0.58
18:i:5:ILE:HG23	21:m:166:VAL:CG1	2.34	0.58
32:H:122:VAL:O	32:H:123:CYS:C	2.46	0.58
66:L:60:LEU:HA	66:L:237:ILE:HD11	1.86	0.58
2:1:14:LEU:HB3	2:1:24:THR:HG21	1.86	0.58
5:6:170:GLN:NE2	3:Ae:69:ASP:HB2	2.19	0.58
11:b:95:TYR:HD2	13:d:108:GLU:HB3	1.69	0.58
17:h:47:ILE:HD11	17:h:52:ALA:HA	1.86	0.58
18:i:4:ILE:CD1	43:U:46:VAL:HG13	2.34	0.58
25:q:73:LEU:HA	25:q:76:MET:HE2	1.86	0.58
28:C:72:TRP:CE3	43:U:312:ILE:HD12	2.39	0.58
34:J:75:ARG:NH1	34:J:119:ASP:OD1	2.37	0.58
6:w:5:ARG:NH1	6:w:20:ASP:OD2	2.34	0.58
58:Al:103:GLN:HE22	58:Al:159:VAL:HG11	1.68	0.58
44:V:44:LYS:HB2	44:V:55:ARG:HH12	1.68	0.57
48:l:152:PHE:HD1	48:l:168:ALA:HB1	1.68	0.57
50:t:104:ARG:O	50:t:108:LEU:HG	2.03	0.57
52:z:76:ALA:HA	52:z:79:GLU:HB2	1.85	0.57
25:q:400:MET:HE1	48:l:183:VAL:HG21	1.85	0.57
26:r:35:LYS:H	32:H:83:THR:HG21	1.69	0.57
26:r:74:ALA:HB3	26:r:75:PRO:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:69:MET:HE3	48:l:76:LEU:HD12	1.86	0.57
48:l:82:MET:HE1	48:l:133:THR:HB	1.84	0.57
62:Ap:81:PRO:O	62:Ap:87:ARG:NH1	2.34	0.57
51:5:315:ASP:OD1	51:5:316:SER:N	2.37	0.57
11:b:21:ARG:HB3	24:p:167:TRP:HH2	1.69	0.57
28:C:321:GLU:O	28:C:352:GLN:NE2	2.36	0.57
28:C:437:HIS:HB2	28:C:462:ILE:HD11	1.86	0.57
50:t:68:LYS:HG3	50:t:71:ARG:HH21	1.68	0.57
60:An:152:PRO:HA	60:An:157:SER:HB2	1.85	0.57
66:L:54:PHE:HB3	66:L:125:VAL:HG23	1.86	0.57
17:h:95:PRO:HG2	17:h:98:HIS:HD2	1.69	0.57
21:m:51:PHE:HD2	21:m:143:ILE:HD13	1.69	0.57
24:p:182:LEU:O	24:p:186:THR:N	2.37	0.57
33:I:76:MET:HE1	33:I:104:ILE:HB	1.86	0.57
50:t:29:TYR:HE2	50:t:108:LEU:HD13	1.70	0.57
51:u:188:HIS:NE2	51:u:348:TYR:OH	2.30	0.57
25:q:122:PHE:CZ	25:q:206:LYS:HG3	2.39	0.57
7:x:97:TRP:HB2	7:x:100:ARG:HD3	1.86	0.57
6:7:338:ILE:HD13	6:7:351:GLY:HA2	1.86	0.57
13:d:101:GLU:HA	13:d:104:ASN:HB2	1.85	0.57
13:d:135:VAL:HG13	14:e:137:MET:HE3	1.87	0.57
14:e:112:TYR:C	14:e:114:MET:H	2.12	0.57
18:i:26:TRP:CE2	18:i:86:ILE:HG13	2.40	0.57
26:r:72:ILE:O	26:r:76:ILE:HG13	2.04	0.57
42:T:152:PRO:HB3	42:T:159:GLN:HB2	1.87	0.57
3:Af:46:LEU:H	3:Af:66:PRO:HG3	1.70	0.57
27:B:75:TRP:HH2	30:E:249:LEU:HD22	1.70	0.57
36:N:38:ILE:O	36:N:45:ARG:NH1	2.38	0.57
46:Y:54:GLN:HB3	48:l:446:ASN:HD21	1.70	0.57
51:u:119:HIS:ND1	5:v:384:MET:HE1	2.19	0.57
3:Af:68:LEU:HG	3:Af:69:ASP:H	1.70	0.57
6:7:264:THR:HG22	6:7:268:ILE:HD11	1.87	0.57
27:B:371:ILE:CD1	27:B:396:MET:HG3	2.35	0.57
34:J:111:LEU:HD13	66:L:96:GLY:HA3	1.85	0.57
6:w:300:ILE:HD11	6:w:363:LEU:HD21	1.87	0.57
63:Aq:54:HIS:O	63:Aq:86:ARG:NH2	2.37	0.57
11:b:22:TRP:HB2	24:p:213:VAL:HG13	1.87	0.57
18:i:235:ASN:HB3	18:i:311:MET:HE3	1.87	0.57
27:B:51:TRP:HH2	27:B:171:VAL:HG12	1.69	0.57
28:C:228:MET:HG3	33:I:167:PRO:HG3	1.86	0.57
28:C:304:ILE:HD11	29:D:135:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:71:PRO:HA	40:R:100:GLN:HG2	1.86	0.57
48:l:46:LEU:O	48:l:50:PRO:HD2	2.04	0.57
51:5:375:GLN:OE1	51:5:378:ARG:NH1	2.38	0.57
66:L:127:ARG:HH21	75:L:401:NDP:H52A	1.70	0.57
8:9:43:ASP:OD2	8:9:102:ARG:NH1	2.38	0.56
29:D:68:ILE:HG23	36:N:44:TYR:HB2	1.85	0.56
69:w:402:HEM:HBB2	69:w:402:HEM:HMB1	1.85	0.56
58:Al:103:GLN:NE2	58:Al:159:VAL:HG11	2.20	0.56
58:Al:155:SER:HB2	58:Al:179:LEU:HD12	1.86	0.56
66:L:59:PHE:HZ	66:L:203:GLY:HA3	1.69	0.56
25:q:266:MET:HA	25:q:269:MET:HE3	1.87	0.56
27:B:278:ILE:HG21	27:B:304:ALA:HB2	1.85	0.56
29:D:152:PRO:HD3	39:Q:46:ILE:HG12	1.86	0.56
30:E:188:ILE:HD13	30:E:208:LEU:HD11	1.85	0.56
51:u:121:ASN:OD1	51:u:122:ALA:N	2.37	0.56
57:Ak:313:ALA:HB2	57:Ak:356:ILE:HD11	1.87	0.56
51:5:62:GLU:OE1	51:5:423:ARG:NH1	2.27	0.56
10:a:89:VAL:HG13	10:a:93:ILE:HD12	1.87	0.56
12:c:168:LEU:HD21	12:c:178:PRO:CB	2.36	0.56
17:h:15:ASP:HB2	18:i:25:HIS:HB2	1.88	0.56
27:B:182:ILE:HD12	27:B:195:VAL:CG2	2.36	0.56
36:N:59:VAL:HG22	36:N:68:LEU:HD21	1.87	0.56
43:U:44:ALA:HB1	43:U:49:GLU:HG3	1.85	0.56
48:l:419:THR:HA	48:l:422:TYR:CZ	2.39	0.56
49:s:94:GLU:HA	49:s:141:ASN:HD21	1.70	0.56
49:s:97:VAL:HG13	49:s:101:VAL:HB	1.86	0.56
57:Ak:33:LEU:HB3	57:Ak:61:HIS:HB2	1.88	0.56
57:Ak:191:THR:HG23	57:Ak:245:ILE:HA	1.86	0.56
58:Al:145:PRO:HA	58:Al:214:VAL:O	2.06	0.56
59:Am:114:GLY:HA2	64:Ar:28:ARG:HH22	1.70	0.56
61:Ao:76:MET:O	61:Ao:80:VAL:HG13	2.05	0.56
3:4:243:CYS:HA	6:w:264:THR:HG21	1.86	0.56
7:8:125:CYS:SG	70:8:401:HEC:HBC2	2.45	0.56
33:I:48:ALA:HA	33:I:191:ARG:HD2	1.88	0.56
5:v:53:GLU:OE1	5:v:127:ARG:NH2	2.36	0.56
57:Ak:3:VAL:HG13	57:Ak:7:LEU:HD12	1.88	0.56
57:Ak:243:VAL:HB	74:Ak:602:HEA:CAC	2.32	0.56
60:An:44:TYR:HE1	60:An:47:PRO:HA	1.70	0.56
3:4:240:HIS:HB2	3:4:275:ALA:HA	1.88	0.56
48:l:264:TYR:N	48:l:265:PRO:HD2	2.21	0.56
48:l:481:THR:HB	50:t:92:HIS:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:96:VAL:HA	50:t:99:MET:HE2	1.86	0.56
52:z:20:SER:HB3	52:z:23:GLU:HG3	1.86	0.56
4:Ad:46:PRO:O	4:Ad:49:ASN:ND2	2.38	0.56
56:Aj:51:ALA:O	56:Aj:55:ILE:HG12	2.05	0.56
8:9:69:LEU:HD11	8:9:76:LEU:HD13	1.87	0.56
27:B:326:LEU:HD22	27:B:363:ILE:HD11	1.87	0.56
37:O:128:PHE:CZ	37:O:148:ILE:HG12	2.41	0.56
51:u:145:GLU:HG2	51:u:249:HIS:CE1	2.41	0.56
51:5:310:ILE:HD11	51:5:388:VAL:HA	1.88	0.56
65:G:541:PRO:HB2	65:G:561:PRO:HD3	1.88	0.56
13:d:159:GLN:HG3	13:d:163:MET:HE2	1.86	0.56
26:r:196:ALA:HB3	26:r:274:ARG:HA	1.88	0.56
37:O:104:PHE:HB3	37:O:110:LEU:HD21	1.88	0.56
5:v:66:LYS:O	5:v:217:ARG:NH2	2.38	0.56
59:Am:77:LYS:HD3	59:Am:80:ARG:HD3	1.88	0.56
61:Ao:98:CYS:SG	61:Ao:107:ALA:HB2	2.45	0.56
65:G:355:LYS:HA	65:G:366:LEU:HD22	1.87	0.56
19:j:62:PHE:CE2	21:m:66:VAL:HG11	2.40	0.56
21:m:117:PHE:HB2	21:m:119:PHE:CE1	2.41	0.56
32:H:116:CYS:SG	72:H:302:SF4:S2	3.04	0.56
33:I:71:CYS:SG	72:I:201:SF4:S2	3.04	0.56
45:W:60:LEU:HD13	49:s:175:ARG:HD2	1.86	0.56
45:W:79:LYS:HG3	45:W:82:ARG:NH2	2.21	0.56
67:M:64:MET:HB2	67:M:65:PRO:HD2	1.88	0.56
3:2:182:GLU:HG3	3:2:201:THR:HG22	1.87	0.56
11:b:57:TRP:HA	11:b:60:VAL:HB	1.87	0.56
18:i:44:LEU:HD22	18:i:122:ILE:HG21	1.87	0.56
18:i:57:THR:HA	20:k:77:LEU:HD13	1.88	0.56
18:i:100:MET:HE1	48:l:594:THR:HG22	1.86	0.56
25:q:77:LEU:O	25:q:81:GLN:HG3	2.05	0.56
25:q:114:GLU:OE2	25:q:174:LEU:HB2	2.05	0.56
26:r:37:PRO:HA	33:I:88:ARG:HA	1.87	0.56
60:An:67:LYS:HA	61:Ao:102:ASN:HD22	1.69	0.56
66:L:278:VAL:HA	66:L:364:VAL:HG11	1.88	0.56
25:q:304:GLN:HA	25:q:309:PHE:CE1	2.41	0.56
27:B:182:ILE:HD12	27:B:195:VAL:HG21	1.88	0.56
37:X:90:TYR:CE2	37:X:92:LYS:HB2	2.40	0.56
7:x:99:HIS:HB3	7:x:106:LEU:HD23	1.87	0.56
19:j:9:THR:CG2	26:r:6:ILE:HG21	2.36	0.55
26:r:65:THR:C	26:r:67:SER:H	2.13	0.55
45:W:84:LEU:HD13	49:s:85:PRO:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:5:339:GLN:OE1	51:5:339:GLN:N	2.39	0.55
65:G:647:GLU:HB2	65:G:654:VAL:HG11	1.88	0.55
5:6:263:GLY:HA2	5:6:443:ASN:HB2	1.89	0.55
12:c:165:ASP:HB3	12:c:167:TYR:CE1	2.41	0.55
12:c:171:GLY:N	13:d:123:GLN:HE21	2.02	0.55
17:h:105:ARG:HH12	49:s:91:LYS:HD3	1.72	0.55
19:j:6:THR:HB	26:r:2:PHE:CE2	2.41	0.55
25:q:186:LEU:O	25:q:252:PRO:HD2	2.06	0.55
25:q:271:MET:HE1	48:l:544:MET:HE2	1.88	0.55
28:C:426:TYR:CZ	29:D:200:LYS:HE3	2.41	0.55
13:d:78:GLU:HB3	13:d:81:ASP:HB2	1.89	0.55
17:h:2:PRO:HD2	18:i:140:SER:HA	1.87	0.55
7:x:127:SER:HB2	7:x:179:PRO:CD	2.28	0.55
55:Ai:53:TRP:CE2	60:An:115:ALA:HB2	2.42	0.55
57:Ak:424:THR:HG21	74:Ak:601:HEA:HMB1	1.89	0.55
11:b:83:HIS:HD2	13:d:41:VAL:HG12	1.72	0.55
25:q:420:THR:HB	25:q:423:ILE:HG13	1.89	0.55
26:r:41:GLY:HA3	26:r:46:LEU:HD13	1.89	0.55
26:r:230:ASN:HA	26:r:233:MET:HE3	1.88	0.55
7:x:246:ALA:O	7:x:247:PRO:C	2.49	0.55
51:5:188:HIS:NE2	51:5:348:TYR:OH	2.33	0.55
5:6:216:ALA:HB3	5:6:244:LEU:H	1.71	0.55
7:8:184:GLU:HB2	7:x:163:GLY:HA2	1.87	0.55
12:c:163:TYR:HB2	50:t:43:GLN:CD	2.31	0.55
30:E:188:ILE:HG22	30:E:189:ASN:H	1.72	0.55
69:w:401:HEM:HBB2	69:w:401:HEM:HMB1	1.89	0.55
1:0:66:ASP:C	1:0:68:THR:H	2.15	0.55
24:p:154:LYS:CA	24:p:161:PHE:HE2	2.07	0.55
26:r:138:GLN:HG3	26:r:285:LEU:HD21	1.87	0.55
41:S:66:LEU:HD11	49:s:159:PHE:HE2	1.71	0.55
59:Am:16:TRP:NE1	59:Am:60:ASP:OD2	2.26	0.55
16:g:89:ASP:HB3	16:g:93:PHE:CE2	2.42	0.55
17:h:95:PRO:HG2	17:h:98:HIS:CD2	2.42	0.55
25:q:309:PHE:HB3	25:q:458:LEU:HD13	1.89	0.55
28:C:47:VAL:HG13	43:U:315:TYR:CB	2.37	0.55
28:C:201:GLY:O	28:C:202:ALA:C	2.50	0.55
48:l:419:THR:HA	48:l:422:TYR:CE2	2.42	0.55
48:l:503:GLU:OE2	54:Ah:50:ASN:HB3	2.06	0.55
6:w:223:TYR:HB3	7:x:312:TRP:CE2	2.41	0.55
10:a:171:TYR:CD2	18:i:147:GLN:NE2	2.75	0.55
26:r:1:MET:HE3	41:S:26:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:213:ILE:HG23	27:B:235:VAL:HA	1.88	0.55
27:B:222:LYS:HA	27:B:379:CYS:SG	2.46	0.55
27:B:321:GLY:H	27:B:353:ALA:HB3	1.72	0.55
39:Q:84:GLN:HG2	39:Q:133:PHE:HE2	1.70	0.55
50:t:66:LEU:O	50:t:69:CYS:SG	2.65	0.55
6:w:245:PHE:CG	7:x:102:LEU:HD11	2.42	0.55
57:Ak:240:HIS:CD2	57:Ak:287:VAL:HG23	2.42	0.55
3:Af:45:PRO:HA	3:Af:66:PRO:HD3	1.87	0.55
22:n:27:LEU:HD23	25:q:2:LEU:HD13	1.89	0.55
23:o:44:LYS:HE3	23:o:48:LEU:HD21	1.89	0.55
39:Q:69:VAL:HG11	39:Q:86:ARG:HG3	1.89	0.55
44:V:62:THR:HG23	44:V:104:ARG:HH21	1.72	0.55
51:u:102:LYS:HG2	51:u:153:ASN:HB3	1.87	0.55
5:v:295:ALA:HB1	3:Af:46:LEU:HD22	1.89	0.55
64:Ar:29:ASN:OD1	64:Ar:33:ASN:ND2	2.40	0.55
6:7:131:TYR:HA	69:7:401:HEM:HAA2	1.88	0.54
13:d:103:VAL:O	13:d:107:GLN:HB2	2.06	0.54
19:j:56:PHE:CE2	20:k:79:VAL:CG2	2.87	0.54
25:q:158:LEU:HB2	25:q:159:PRO:HD3	1.88	0.54
26:r:272:TRP:CZ2	32:H:74:LEU:HB2	2.41	0.54
30:E:62:ARG:NH2	40:R:88:ASP:OD1	2.40	0.54
37:O:128:PHE:HZ	37:O:148:ILE:HG12	1.71	0.54
5:v:121:TYR:HB3	5:v:137:LEU:HD11	1.88	0.54
63:Aq:84:ASN:HB3	63:Aq:87:VAL:HG12	1.89	0.54
6:7:115:ILE:HB	6:7:196:HIS:HD2	1.72	0.54
26:r:119:SER:HB2	26:r:215:TYR:CE1	2.42	0.54
27:B:157:TYR:HB2	27:B:212:LEU:HD21	1.88	0.54
37:X:102:SER:H	37:X:141:PRO:HD2	1.72	0.54
57:Ak:510:TYR:HB3	62:Ap:89:VAL:HG22	1.88	0.54
62:Ap:94:GLU:H	62:Ap:97:ASN:HD21	1.54	0.54
18:i:193:VAL:HG23	18:i:201:THR:HG22	1.88	0.54
19:j:53:MET:HA	19:j:56:PHE:HB3	1.88	0.54
24:p:94:LYS:HE3	37:X:113:LEU:HD11	1.89	0.54
25:q:25:ILE:O	25:q:29:VAL:HG23	2.08	0.54
27:B:163:TYR:HE1	40:R:86:PHE:CB	2.20	0.54
29:D:190:ASP:HA	33:I:112:LYS:HD3	1.90	0.54
37:X:100:VAL:HG12	37:X:142:GLN:HB2	1.88	0.54
37:X:115:GLN:O	37:X:119:ILE:HG12	2.07	0.54
51:u:116:MET:HE1	51:u:142:LYS:HB3	1.88	0.54
5:v:297:PRO:HB3	3:Af:71:LYS:HG2	1.89	0.54
20:k:34:GLU:OE2	21:m:68:PHE:CE1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:r:54:LYS:HE2	33:l:61:SER:O	2.08	0.54
26:r:113:VAL:HG11	26:r:139:THR:HG21	1.89	0.54
28:C:184:THR:HG22	28:C:220:TYR:OH	2.08	0.54
29:D:103:HIS:HB3	36:N:83:GLN:OE1	2.07	0.54
37:X:92:LYS:N	47:Z:60:PRO:HB3	2.11	0.54
3:Af:46:LEU:HG	3:Af:66:PRO:HB3	1.90	0.54
12:c:82:SER:HB2	12:c:119:THR:H	1.73	0.54
18:i:95:MET:HE2	18:i:149:ILE:HA	1.89	0.54
18:i:228:LEU:HD22	28:C:54:GLY:HA3	1.88	0.54
21:m:125:TRP:HB2	45:W:137:THR:HG21	1.90	0.54
24:p:212:ILE:O	24:p:215:ARG:NH1	2.35	0.54
25:q:87:GLU:HG3	25:q:91:ARG:HB2	1.89	0.54
37:X:90:TYR:HA	47:Z:60:PRO:O	2.08	0.54
48:l:396:ILE:HG21	48:l:490:ALA:HB2	1.88	0.54
58:Al:13:THR:HB	58:Al:188:ARG:HH21	1.71	0.54
11:b:22:TRP:NE1	24:p:214:THR:HA	2.22	0.54
12:c:126:TRP:HZ3	48:l:535:ARG:HD2	1.71	0.54
13:d:92:TRP:CE3	13:d:93:ARG:HG2	2.42	0.54
19:j:66:ASP:O	19:j:69:ILE:HG13	2.08	0.54
25:q:196:TRP:HB2	25:q:253:LEU:HD23	1.90	0.54
26:r:96:ILE:HG23	45:W:144:THR:HB	1.90	0.54
29:D:186:ARG:NH2	29:D:193:PHE:O	2.40	0.54
32:H:101:HIS:H	32:H:149:MET:HE1	1.71	0.54
34:J:132:GLU:OE1	34:J:132:GLU:N	2.39	0.54
48:l:380:LEU:HD21	48:l:422:TYR:HE1	1.73	0.54
5:v:379:LYS:HG2	5:v:413:LEU:HD22	1.90	0.54
58:Al:132:GLU:HB3	58:Al:137:GLU:HG3	1.88	0.54
12:c:121:PRO:HA	23:o:6:TYR:OH	2.08	0.54
19:j:60:ILE:HG21	21:m:168:ILE:HG12	1.89	0.54
20:k:3:LEU:HD21	21:m:107:ALA:HB1	1.90	0.54
37:X:126:PHE:CE2	37:X:148:ILE:HD13	2.42	0.54
49:s:128:LYS:HD2	49:s:218:PRO:HB2	1.90	0.54
13:d:139:PHE:HD2	23:o:127:ILE:HG22	1.71	0.54
25:q:63:ALA:HB3	25:q:64:PRO:HD3	1.89	0.54
26:r:236:ALA:HA	26:r:263:THR:HG22	1.90	0.54
44:V:87:PRO:HA	44:V:126:LYS:HG2	1.88	0.54
48:l:378:LEU:HD13	48:l:383:MET:HE3	1.90	0.54
16:g:4:MET:HA	16:g:7:ARG:HG3	1.90	0.54
21:m:66:VAL:O	21:m:70:TYR:HB3	2.08	0.54
23:o:15:PRO:HG2	23:o:18:LEU:HG	1.90	0.54
25:q:193:ILE:HA	25:q:253:LEU:HD21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:181:HIS:HD2	29:D:183:ASP:H	1.56	0.54
32:H:76:TYR:HA	32:H:79:ARG:HD3	1.90	0.54
37:X:78:ALA:O	37:X:82:ARG:HG3	2.08	0.54
56:Aj:52:PRO:HG2	57:Ak:32:ALA:HB3	1.90	0.54
57:Ak:334:TRP:CZ2	58:Al:46:LEU:HB2	2.43	0.54
59:Am:128:GLU:HG3	59:Am:129:VAL:HG23	1.90	0.54
65:G:75:CYS:SG	68:G:803:FES:S1	3.06	0.54
3:Ae:43:ARG:HG3	3:Ae:44:PHE:H	1.72	0.54
12:c:163:TYR:CD2	50:t:43:GLN:HG2	2.43	0.54
28:C:88:LEU:N	28:C:105:MET:O	2.39	0.54
46:Y:86:TYR:CZ	48:l:483:PRO:HD3	2.42	0.54
51:u:304:LEU:HD13	51:u:354:LEU:HD22	1.89	0.54
5:v:131:GLU:O	5:v:135:GLU:HG2	2.08	0.54
57:Ak:28:MET:HE3	57:Ak:465:VAL:HG13	1.89	0.54
3:4:238:CYS:HB3	3:4:245:PRO:HG3	1.90	0.53
11:b:19:ARG:HG2	24:p:215:ARG:NH2	2.21	0.53
21:m:163:ILE:O	21:m:167:VAL:HG23	2.09	0.53
23:o:33:GLN:HA	23:o:36:ARG:HD2	1.89	0.53
24:p:75:HIS:CE1	48:l:509:TYR:HA	2.43	0.53
24:p:187:PRO:O	24:p:189:GLY:N	2.41	0.53
25:q:105:PHE:O	25:q:109:THR:HG23	2.08	0.53
26:r:65:THR:C	26:r:67:SER:N	2.65	0.53
28:C:172:ARG:NH1	28:C:241:ASP:OD1	2.41	0.53
29:D:68:ILE:HG21	29:D:99:PHE:CE1	2.43	0.53
45:W:88:ARG:NH2	49:s:84:LEU:O	2.41	0.53
6:w:131:TYR:O	6:w:134:PRO:HD2	2.08	0.53
59:Am:76:GLN:O	59:Am:80:ARG:HG3	2.09	0.53
3:2:230:GLU:HG2	3:2:231:TRP:CD1	2.43	0.53
17:h:68:LEU:HB3	17:h:70:GLN:HG3	1.89	0.53
20:k:41:PHE:CD2	20:k:64:LEU:HD13	2.43	0.53
24:p:60:ARG:HH22	37:X:133:ILE:HA	1.73	0.53
27:B:28:LYS:HG2	27:B:29:LYS:H	1.73	0.53
27:B:171:VAL:CG2	40:R:89:LEU:HD21	2.22	0.53
28:C:137:GLN:HE21	32:H:122:VAL:HA	1.72	0.53
48:l:338:MET:HA	48:l:341:MET:HE2	1.90	0.53
57:Ak:486:GLU:OE1	57:Ak:486:GLU:N	2.35	0.53
65:G:400:ILE:HD12	65:G:473:MET:HE3	1.91	0.53
3:2:175:ILE:HB	3:2:292:VAL:HG13	1.90	0.53
12:c:107:TRP:CZ2	23:o:76:ILE:HD11	2.43	0.53
25:q:119:TYR:CZ	25:q:161:LEU:HB2	2.44	0.53
33:I:79:MET:HE3	33:I:174:LEU:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:5:LEU:HD22	50:t:9:TYR:HE2	1.73	0.53
51:u:276:ARG:HB2	52:z:16:THR:HG23	1.89	0.53
6:w:326:TRP:CE2	52:z:49:VAL:HG22	2.43	0.53
66:L:126:GLY:O	75:L:401:NDP:H8A	2.09	0.53
3:4:201:THR:O	3:4:205:ILE:HG12	2.08	0.53
13:d:114:GLN:HG2	13:d:121:TYR:CD2	2.43	0.53
18:i:1:MET:HG3	21:m:170:GLU:OE1	2.08	0.53
18:i:61:LEU:HD11	20:k:26:LEU:HD11	1.90	0.53
19:j:106:TRP:CH2	26:r:291:LYS:HB3	2.44	0.53
21:m:38:GLY:HA2	21:m:57:PHE:CE1	2.44	0.53
27:B:156:ILE:HD12	27:B:169:LEU:HD21	1.90	0.53
6:w:138:MET:HE1	6:w:268:ILE:HA	1.90	0.53
3:4:198:ARG:HB3	3:4:232:VAL:HG13	1.90	0.53
10:a:111:GLU:HG2	13:d:64:TYR:HE2	1.73	0.53
11:b:11:ARG:HD2	24:p:197:PRO:O	2.09	0.53
12:c:185:GLU:N	50:t:36:GLU:HA	2.23	0.53
18:i:254:LEU:HD21	25:q:154:LEU:HD11	1.89	0.53
20:k:20:LEU:HD13	48:l:592:LEU:HB2	1.91	0.53
20:k:65:VAL:HG13	21:m:161:LEU:HD21	1.91	0.53
43:U:309:TYR:HD1	43:U:312:ILE:HD11	1.74	0.53
48:l:362:LEU:HA	48:l:365:ALA:HB3	1.89	0.53
48:l:512:LYS:NZ	54:Ah:43:LEU:O	2.42	0.53
51:u:338:CYS:HB3	51:u:368:MET:HE3	1.89	0.53
51:5:120:LEU:HD13	51:5:133:ILE:HG12	1.89	0.53
41:S:57:VAL:HG11	41:S:62:VAL:HG21	1.91	0.53
48:l:247:LEU:HD12	48:l:247:LEU:H	1.74	0.53
3:Ae:40:VAL:HG22	3:Ae:42:CYS:H	1.74	0.53
5:6:170:GLN:HG2	3:Ae:67:VAL:O	2.09	0.53
14:e:112:TYR:C	14:e:114:MET:N	2.64	0.53
16:g:120:PRO:HB2	16:g:122:ARG:HG3	1.90	0.53
18:i:42:PRO:HG3	21:m:167:VAL:CG1	2.34	0.53
26:r:277:TYR:HB3	28:C:273:ILE:HD12	1.91	0.53
28:C:381:MET:HE2	28:C:385:ILE:HG13	1.89	0.53
32:H:130:ILE:HA	32:H:144:ARG:O	2.08	0.53
33:I:85:ASP:O	33:I:88:ARG:HG2	2.08	0.53
57:Ak:306:THR:HG22	57:Ak:310:MET:HE2	1.89	0.53
1:0:45:LYS:O	1:0:48:GLU:HG2	2.09	0.53
2:1:52:LEU:HA	7:x:108:HIS:HD2	1.73	0.53
11:b:19:ARG:HG2	24:p:215:ARG:HH22	1.74	0.53
28:C:186:LEU:HB2	28:C:216:MET:HE1	1.91	0.53
42:T:138:TYR:CZ	49:s:121:MET:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:108:MET:HG3	48:l:117:PHE:CE2	2.44	0.53
51:5:75:ILE:HG13	51:5:229:MET:HG2	1.90	0.53
51:5:190:THR:HB	51:5:275:ILE:HG13	1.89	0.53
51:5:351:THR:OG1	51:5:352:GLY:N	2.41	0.53
3:Ae:46:LEU:HD13	3:Ae:68:LEU:HA	1.89	0.53
5:6:183:ARG:HD2	5:6:252:LYS:HE2	1.91	0.53
6:7:173:ALA:HB1	6:7:177:ARG:HH12	1.74	0.53
7:8:98:SER:O	7:8:104:SER:OG	2.24	0.53
12:c:107:TRP:CH2	23:o:76:ILE:HD11	2.44	0.53
25:q:231:LEU:O	25:q:236:LEU:HG	2.09	0.53
25:q:337:VAL:HG11	25:q:345:ALA:HB2	1.90	0.53
26:r:157:ASN:ND2	26:r:159:SER:O	2.42	0.53
27:B:163:TYR:OH	40:R:86:PHE:N	2.28	0.53
28:C:212:GLU:O	28:C:216:MET:HG3	2.08	0.53
30:E:143:ARG:HB3	30:E:184:PRO:HD3	1.91	0.53
48:l:428:PHE:CD2	48:l:505:ASN:HB3	2.44	0.53
53:Ag:62:ASP:HA	53:Ag:65:LYS:HZ2	1.72	0.53
64:Ar:40:CYS:O	64:Ar:44:MET:HG2	2.09	0.53
1:0:64:GLU:HB2	52:z:78:TYR:HE1	1.74	0.52
1:0:76:HIS:HB2	7:x:90:LEU:HD11	1.90	0.52
13:d:139:PHE:HD2	23:o:127:ILE:HG21	1.74	0.52
21:m:152:TRP:O	21:m:156:VAL:HG23	2.08	0.52
26:r:139:THR:HA	26:r:142:TYR:CE2	2.44	0.52
34:J:169:ARG:HH12	65:G:428:LYS:NZ	2.07	0.52
41:S:66:LEU:HD21	49:s:159:PHE:HD2	1.74	0.52
43:U:72:LYS:HE3	43:U:163:ARG:HG3	1.91	0.52
57:Ak:405:LEU:HD22	57:Ak:471:ILE:HG22	1.89	0.52
57:Ak:463:THR:OG1	60:An:114:THR:OG1	2.25	0.52
59:Am:151:LEU:HB2	59:Am:159:MET:HG3	1.91	0.52
66:L:274:TYR:HB2	66:L:367:ALA:HB2	1.91	0.52
6:7:8:HIS:HB3	6:7:11:MET:HB2	1.89	0.52
25:q:25:ILE:H	25:q:25:ILE:HD12	1.74	0.52
26:r:312:ALA:HA	42:T:127:ALA:HB2	1.91	0.52
40:R:106:GLN:HB2	40:R:110:HIS:CD2	2.43	0.52
37:X:115:GLN:HG3	37:X:139:MET:HA	1.89	0.52
50:t:5:LEU:HD22	50:t:9:TYR:CE2	2.44	0.52
50:t:32:PRO:O	50:t:33:GLU:C	2.52	0.52
5:v:375:LYS:NZ	5:v:419:VAL:O	2.41	0.52
7:x:122:CYS:CB	70:x:401:HEC:HMC2	2.38	0.52
57:Ak:31:THR:OG1	74:Ak:601:HEA:H14	2.10	0.52
66:L:206:ASP:OD2	66:L:208:PHE:HB3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:240:HIS:HB2	3:2:275:ALA:HA	1.91	0.52
6:7:36:LEU:HD22	6:7:235:MET:HE3	1.92	0.52
69:7:402:HEM:HBA1	69:7:402:HEM:HHA	1.90	0.52
10:a:52:LYS:HG2	10:a:53:ARG:HG3	1.91	0.52
18:i:294:MET:SD	25:q:130:LEU:HD21	2.50	0.52
27:B:329:LYS:O	27:B:333:GLU:HG3	2.09	0.52
27:B:383:THR:HG21	65:G:120:LEU:HG	1.92	0.52
38:P:18:GLU:HG3	38:P:68:ARG:HB3	1.92	0.52
43:U:352:LYS:HD3	43:U:353:TRP:N	2.24	0.52
48:l:483:PRO:HB3	48:l:485:TYR:CE1	2.44	0.52
49:s:111:ALA:HB2	49:s:197:PRO:HD3	1.91	0.52
7:x:306:ALA:HA	52:z:27:PHE:HE1	1.74	0.52
64:Ar:59:ARG:HA	64:Ar:62:LYS:HE3	1.91	0.52
3:4:230:GLU:HG2	3:4:231:TRP:CD1	2.45	0.52
8:9:12:LYS:HD3	8:9:12:LYS:H	1.74	0.52
16:g:117:GLU:C	16:g:117:GLU:OE1	2.53	0.52
18:i:96:THR:O	18:i:100:MET:HG2	2.08	0.52
27:B:154:ALA:HB3	27:B:195:VAL:HG12	1.91	0.52
27:B:227:PRO:HB2	27:B:228:PRO:HD3	1.91	0.52
27:B:263:ALA:HA	27:B:271:SER:HB2	1.91	0.52
28:C:46:ASP:OD1	28:C:47:VAL:N	2.34	0.52
28:C:139:LEU:HD23	28:C:157:TYR:HD2	1.75	0.52
37:X:123:GLU:HG3	37:X:128:PHE:O	2.09	0.52
60:An:90:PHE:O	60:An:93:MET:HG2	2.10	0.52
65:G:64:CYS:HB3	65:G:75:CYS:HB3	1.92	0.52
65:G:169:VAL:HG21	65:G:222:ILE:HD11	1.89	0.52
66:L:127:ARG:NH2	75:L:401:NDP:H2B	2.24	0.52
11:b:63:LYS:H	11:b:63:LYS:HD3	1.74	0.52
19:j:56:PHE:HA	21:m:70:TYR:OH	2.10	0.52
21:m:57:PHE:HB3	26:r:107:ALA:HB1	1.91	0.52
32:H:101:HIS:HB3	32:H:167:ILE:HD11	1.90	0.52
37:X:82:ARG:HH21	48:l:439:PRO:HB2	1.74	0.52
51:u:451:ASP:O	51:u:472:ARG:NH2	2.43	0.52
60:An:90:PHE:HA	60:An:93:MET:SD	2.50	0.52
62:Ap:53:MET:O	62:Ap:57:LYS:HG2	2.08	0.52
5:6:36:GLN:OE1	5:6:36:GLN:N	2.42	0.52
37:O:90:TYR:HD2	37:O:93:ILE:HG13	1.75	0.52
37:X:117:GLU:HB3	47:Z:61:TRP:HE1	1.74	0.52
8:y:69:LEU:HD11	8:y:76:LEU:HD13	1.92	0.52
57:Ak:460:ILE:HG12	60:An:114:THR:HG21	1.91	0.52
11:b:74:HIS:O	48:l:14:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:c:154:GLN:HG2	48:l:401:MET:SD	2.50	0.52
24:p:76:ARG:N	47:Z:69:TYR:OH	2.43	0.52
25:q:8:THR:O	25:q:11:LEU:HB2	2.09	0.52
27:B:138:LEU:HD13	27:B:245:VAL:HG13	1.92	0.52
28:C:144:ARG:HD2	72:I:201:SF4:S4	2.49	0.52
33:I:114:ALA:HB3	33:I:115:PRO:HD3	1.92	0.52
43:U:98:SER:HA	43:U:103:GLY:CA	2.39	0.52
48:l:512:LYS:HG3	54:Ah:46:GLY:HA2	1.91	0.52
51:u:294:PRO:HG3	51:u:448:TYR:CZ	2.44	0.52
3:2:177:LEU:HB3	3:2:231:TRP:CZ2	2.44	0.52
16:g:119:HIS:CG	25:q:252:PRO:HB3	2.45	0.52
28:C:285:THR:HG23	36:N:13:GLY:HA3	1.92	0.52
29:D:154:GLU:OE2	29:D:180:ASN:ND2	2.42	0.52
29:D:203:PRO:HD3	34:J:124:LEU:HD12	1.92	0.52
37:X:89:LEU:HB3	47:Z:64:ASN:CB	2.38	0.52
6:w:5:ARG:NH1	6:w:15:ASN:OD1	2.43	0.52
65:G:304:GLN:HB2	65:G:316:TYR:HD1	1.74	0.52
3:2:262:SER:HA	3:2:273:GLY:HA3	1.91	0.52
10:a:80:ILE:HB	10:a:81:PRO:HD3	1.92	0.52
30:E:83:LEU:HD23	30:E:101:VAL:HG21	1.92	0.52
48:l:97:THR:HG22	48:l:246:LEU:HD11	1.91	0.52
48:l:366:MET:HE2	48:l:369:THR:HG21	1.91	0.52
6:w:200:LEU:HD13	69:w:401:HEM:HAD2	1.92	0.52
59:Am:253:TYR:HA	59:Am:257:TYR:HD2	1.75	0.52
60:An:59:GLN:O	60:An:63:LYS:HG2	2.09	0.52
63:Aq:85:PRO:HB3	63:Aq:95:GLU:HG3	1.91	0.52
65:G:667:GLN:OE1	65:G:667:GLN:N	2.39	0.52
18:i:275:SER:HB3	44:V:137:ALA:HB3	1.91	0.52
23:o:54:PRO:HA	24:p:171:ARG:NH2	2.25	0.52
27:B:394:LYS:HB3	65:G:155:GLU:HG2	1.92	0.52
37:O:110:LEU:HB2	37:O:114:ASP:CB	2.39	0.52
45:W:84:LEU:HD12	49:s:134:LEU:HD21	1.92	0.52
45:W:88:ARG:O	45:W:92:GLU:HG2	2.10	0.52
5:v:257:GLU:HA	5:v:438:MET:O	2.09	0.52
57:Ak:363:LEU:HD21	58:Al:24:HIS:HB2	1.92	0.52
51:5:311:ILE:HD12	51:5:375:GLN:HB3	1.92	0.52
7:8:295:MET:HE1	2:Ac:40:ALA:HB2	1.93	0.51
21:m:126:VAL:HG13	45:W:122:GLY:HA3	1.92	0.51
41:S:43:TYR:CZ	45:W:68:ARG:HG3	2.45	0.51
48:l:399:VAL:HG12	48:l:409:LEU:HD13	1.93	0.51
5:v:323:VAL:HG23	5:v:340:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:67:CYS:HG	7:x:224:THR:HG1	1.57	0.51
20:k:30:LEU:CB	21:m:68:PHE:HE2	2.23	0.51
25:q:122:PHE:CE1	25:q:238:LEU:HB3	2.45	0.51
51:5:318:TYR:HD2	51:5:324:MET:HE1	1.76	0.51
3:Af:48:PRO:HA	3:Af:65:SER:O	2.10	0.51
32:H:54:THR:HG23	45:W:36:PHE:CE2	2.44	0.51
49:s:238:ALA:O	49:s:239:LYS:C	2.53	0.51
7:x:322:TYR:HB2	8:y:61:PHE:CG	2.44	0.51
59:Am:204:HIS:NE2	59:Am:249:TRP:HB2	2.25	0.51
2:1:11:TYR:HA	2:1:15:PHE:HB2	1.92	0.51
5:6:138:LEU:HD12	5:6:233:VAL:HG22	1.93	0.51
10:a:153:GLU:HB2	16:g:92:MET:HE1	1.91	0.51
12:c:82:SER:HB2	12:c:119:THR:HG23	1.91	0.51
13:d:99:ASP:HA	13:d:102:ILE:HD12	1.92	0.51
18:i:231:SER:O	18:i:234:TRP:HD1	1.92	0.51
30:E:177:LEU:HB3	30:E:192:TYR:HE1	1.75	0.51
37:O:97:LYS:HE3	37:O:107:ASP:HB2	1.93	0.51
6:w:137:GLN:NE2	6:w:263:ASN:O	2.43	0.51
1:0:51:GLU:O	1:0:55:GLN:HG2	2.11	0.51
5:6:90:THR:HG23	5:6:95:SER:HA	1.93	0.51
10:a:74:TYR:CG	14:e:91:PHE:HB3	2.46	0.51
23:o:42:ARG:O	23:o:46:GLU:HG2	2.11	0.51
26:r:10:ILE:HG23	26:r:83:LEU:HD13	1.91	0.51
57:Ak:287:VAL:HG21	57:Ak:312:ILE:HD11	1.92	0.51
64:Ar:85:LYS:HD3	64:Ar:85:LYS:H	1.73	0.51
3:4:173:ILE:HG22	3:4:294:VAL:HB	1.92	0.51
12:c:166:LEU:HG	12:c:169:GLU:CB	2.36	0.51
13:d:150:TYR:OH	25:q:458:LEU:HA	2.09	0.51
18:i:5:ILE:CD1	19:j:104:TYR:OH	2.59	0.51
18:i:61:LEU:O	18:i:65:THR:HG23	2.11	0.51
25:q:351:LEU:HD12	25:q:426:ILE:HD12	1.93	0.51
25:q:393:ILE:HG21	48:l:184:LEU:HD12	1.91	0.51
32:H:171:PRO:HG3	32:H:200:GLU:CD	2.36	0.51
48:l:81:LYS:HB2	48:l:135:ASN:HB2	1.92	0.51
48:l:152:PHE:CD1	48:l:168:ALA:HB1	2.46	0.51
5:v:317:VAL:HG21	5:v:350:VAL:HG22	1.91	0.51
57:Ak:181:THR:O	57:Ak:270:TYR:OH	2.25	0.51
3:Ae:46:LEU:HD13	3:Ae:68:LEU:HD23	1.92	0.51
5:6:70:ARG:NH2	5:6:332:ASP:OD2	2.43	0.51
17:h:17:TRP:CE3	20:k:55:LEU:HD13	2.46	0.51
18:i:65:THR:OG1	18:i:104:MET:SD	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:r:179:TRP:HE1	45:W:43:LEU:HG	1.76	0.51
44:V:140:LYS:O	44:V:141:VAL:C	2.53	0.51
7:x:124:SER:HB2	7:x:180:TYR:CE2	2.46	0.51
58:Al:12:ALA:HB1	58:Al:17:MET:HB3	1.92	0.51
65:G:704:SER:HB3	65:G:707:MET:HG2	1.92	0.51
66:L:169:ILE:HG23	66:L:170:LYS:HD3	1.92	0.51
3:2:265:ASP:OD1	3:2:269:ARG:N	2.43	0.51
26:r:141:SER:HA	26:r:290:TRP:HE1	1.76	0.51
32:H:53:VAL:HG12	42:T:98:TRP:CD1	2.45	0.51
39:Q:118:GLU:HB3	39:Q:124:LYS:HG3	1.93	0.51
48:l:306:THR:HG22	48:l:336:LYS:HG2	1.91	0.51
48:l:319:ILE:HG13	48:l:399:VAL:HG22	1.92	0.51
8:y:75:ILE:HD12	52:z:40:ARG:HH21	1.75	0.51
57:Ak:147:ILE:HG23	57:Ak:206:ILE:HB	1.93	0.51
57:Ak:239:GLY:O	57:Ak:242:GLU:HB3	2.11	0.51
63:Aq:62:TYR:HB2	63:Aq:65:LEU:HD12	1.93	0.51
51:5:113:VAL:HG13	51:5:118:ALA:HB3	1.92	0.51
51:5:276:ARG:NH2	51:5:466:PRO:O	2.44	0.51
65:G:179:CYS:SG	72:G:802:SF4:S2	3.08	0.51
65:G:265:THR:HG22	65:G:270:VAL:HA	1.92	0.51
66:L:312:ASP:HB3	66:L:316:ARG:HH21	1.75	0.51
10:a:73:PHE:CE2	10:a:74:TYR:CE1	2.99	0.51
13:d:138:ALA:HB3	14:e:137:MET:SD	2.51	0.51
14:e:129:ARG:HD2	14:e:134:LEU:HB2	1.93	0.51
27:B:145:GLY:O	27:B:149:MET:HG2	2.10	0.51
28:C:88:LEU:HD22	28:C:107:LEU:HD21	1.92	0.51
70:x:401:HEC:HBB3	70:x:401:HEC:HMB3	1.92	0.51
51:5:241:GLN:HA	51:5:244:ASP:OD2	2.11	0.51
11:b:21:ARG:HB3	24:p:167:TRP:CH2	2.45	0.51
12:c:169:GLU:C	13:d:123:GLN:HE22	2.19	0.51
25:q:24:TRP:CD2	25:q:81:GLN:HG2	2.46	0.51
27:B:131:ILE:HD12	27:B:158:ILE:HD13	1.93	0.51
45:W:108:GLU:HA	49:s:81:ILE:HD13	1.92	0.51
37:X:104:PHE:HA	37:X:108:LEU:HD23	1.93	0.51
6:w:45:ILE:HA	69:w:402:HEM:HMC2	1.93	0.51
52:Aa:12:ARG:NH1	51:5:279:ASP:OD1	2.43	0.51
57:Ak:440:TYR:OH	58:Al:195:GLN:HB3	2.11	0.51
59:Am:101:PHE:HZ	59:Am:260:GLY:HA3	1.75	0.51
3:4:173:ILE:HB	3:4:190:TRP:CD1	2.46	0.50
5:6:327:ASN:H	3:Ae:66:PRO:HG3	1.76	0.50
25:q:73:LEU:HB3	25:q:74:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:36:LYS:HD3	27:B:36:LYS:H	1.76	0.50
32:H:205:ILE:O	32:H:209:TYR:N	2.44	0.50
43:U:82:LYS:HB2	43:U:272:VAL:HG21	1.93	0.50
46:Y:44:TYR:CD2	47:Z:32:LEU:HB3	2.46	0.50
60:An:44:TYR:CE1	60:An:47:PRO:HA	2.46	0.50
20:k:68:ALA:HB2	21:m:64:MET:HE2	1.92	0.50
23:o:128:SER:HB2	48:l:194:ASN:OD1	2.11	0.50
24:p:84:CYS:SG	47:Z:57:LEU:HB3	2.51	0.50
28:C:368:LYS:HG2	28:C:386:HIS:CE1	2.46	0.50
37:O:134:ASP:O	37:O:138:LEU:HD22	2.11	0.50
43:U:115:SER:HB3	43:U:118:LYS:HB3	1.94	0.50
50:t:29:TYR:CE2	50:t:108:LEU:HD13	2.45	0.50
57:Ak:254:ILE:HG13	57:Ak:344:PHE:CD2	2.46	0.50
58:Al:133:MET:N	58:Al:133:MET:SD	2.85	0.50
64:Ar:58:ARG:HA	64:Ar:61:TYR:CD2	2.46	0.50
65:G:52:ALA:O	65:G:56:VAL:HG13	2.11	0.50
5:6:312:ALA:HB2	5:6:357:GLN:HE21	1.76	0.50
10:a:130:GLU:O	10:a:134:GLU:HG2	2.12	0.50
13:d:110:LEU:HD22	48:l:203:MET:HG2	1.92	0.50
25:q:328:CYS:CB	25:q:437:MET:HE1	2.37	0.50
26:r:139:THR:HA	26:r:142:TYR:CD2	2.46	0.50
37:O:104:PHE:HB3	37:O:110:LEU:HD11	1.93	0.50
37:X:86:VAL:HA	47:Z:64:ASN:OD1	2.10	0.50
48:l:315:VAL:O	48:l:319:ILE:HG12	2.10	0.50
48:l:395:ILE:O	48:l:399:VAL:HG23	2.11	0.50
61:Ao:110:ILE:O	61:Ao:114:VAL:HG13	2.11	0.50
62:Ap:105:VAL:HG12	62:Ap:122:LEU:HB2	1.92	0.50
3:Ae:45:PRO:HB3	3:Ae:66:PRO:HD3	1.94	0.50
5:6:148:ARG:NH2	8:y:50:ARG:O	2.45	0.50
11:b:5:THR:H	11:b:8:GLU:HB2	1.76	0.50
18:i:77:ASN:HB2	18:i:89:MET:HE2	1.93	0.50
18:i:342:ALA:O	18:i:344:SER:N	2.44	0.50
48:l:62:ILE:HG12	48:l:199:GLN:NE2	2.27	0.50
48:l:559:GLU:O	48:l:563:PRO:HD2	2.10	0.50
7:x:112:ARG:HG3	7:x:141:TYR:CE1	2.46	0.50
55:Ai:60:ILE:HG21	60:An:119:ILE:HG12	1.94	0.50
57:Ak:96:ARG:HG2	59:Am:57:TRP:HZ2	1.77	0.50
59:Am:22:LEU:O	59:Am:26:LEU:HG	2.11	0.50
6:7:173:ALA:HB1	6:7:177:ARG:NH1	2.27	0.50
11:b:82:ILE:HD11	48:l:13:ILE:HG12	1.94	0.50
20:k:48:ILE:HG21	20:k:57:ASN:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S:69:ILE:O	49:s:152:LYS:NZ	2.44	0.50
43:U:248:LEU:HD22	43:U:257:VAL:HG11	1.94	0.50
37:X:74:LEU:HB3	37:X:79:ILE:HD11	1.94	0.50
48:l:253:VAL:HB	48:l:310:LEU:HD11	1.92	0.50
6:w:27:ILE:HA	6:w:208:PRO:HD3	1.94	0.50
65:G:50:LEU:HD21	65:G:62:ARG:HH21	1.76	0.50
66:L:110:SER:O	66:L:114:VAL:HG12	2.11	0.50
3:2:257:CYS:HB3	3:2:262:SER:HB2	1.92	0.50
7:8:232:LEU:HD13	7:8:242:ALA:HB1	1.94	0.50
24:p:147:ASP:N	24:p:147:ASP:OD1	2.43	0.50
28:C:382:GLU:OE1	28:C:382:GLU:N	2.41	0.50
50:t:20:LEU:HD22	50:t:20:LEU:H	1.76	0.50
5:v:180:ALA:HB2	5:v:258:ILE:HG13	1.94	0.50
57:Ak:307:SER:O	57:Ak:311:ILE:HG12	2.11	0.50
3:4:252:PHE:HE2	3:4:272:LYS:HG2	1.76	0.50
5:6:50:ALA:HB3	5:6:221:ILE:HG13	1.94	0.50
5:6:125:CYS:HB3	5:6:133:LEU:HD22	1.92	0.50
10:a:134:GLU:HG3	22:n:58:LYS:HB3	1.94	0.50
11:b:20:ARG:HG2	37:X:155:TYR:HA	1.94	0.50
18:i:236:LYS:HG2	18:i:237:MET:HG3	1.94	0.50
21:m:174:GLY:O	21:m:175:ASN:C	2.55	0.50
41:S:18:ILE:HB	41:S:19:PRO:HD3	1.93	0.50
43:U:263:ARG:HD3	43:U:264:GLU:HG3	1.93	0.50
48:l:264:TYR:CD1	48:l:265:PRO:HD3	2.46	0.50
50:t:47:ASN:HA	50:t:56:ARG:CZ	2.42	0.50
53:Ag:26:TYR:HB2	57:Ak:484:ALA:HB3	1.94	0.50
55:Ai:32:ASP:O	55:Ai:36:LYS:HG2	2.10	0.50
51:5:279:ASP:HB3	51:5:282:LEU:HG	1.94	0.50
65:G:586:GLY:O	65:G:616:ALA:HB1	2.11	0.50
3:2:197:VAL:HG13	3:2:233:ILE:HG12	1.93	0.50
5:6:451:ASP:OD2	5:v:183:ARG:NH2	2.45	0.50
26:r:36:GLY:O	26:r:37:PRO:C	2.54	0.50
30:E:138:THR:HA	30:E:141:MET:HE2	1.92	0.50
43:U:284:PRO:O	43:U:288:GLN:HG2	2.12	0.50
44:V:5:LEU:HD23	44:V:28:ILE:HA	1.94	0.50
2:Ac:10:LEU:HD22	2:Ac:14:LEU:HD11	1.94	0.50
56:Aj:38:LEU:HB2	57:Ak:473:TRP:NE1	2.25	0.50
57:Ak:94:PHE:HE1	59:Am:79:LEU:HD23	1.77	0.50
64:Ar:43:ALA:O	64:Ar:47:LYS:HG3	2.12	0.50
51:5:102:LYS:HB3	51:5:153:ASN:HB3	1.94	0.50
66:L:223:LEU:O	66:L:226:LEU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:i:30:TRP:O	18:i:34:GLU:HG2	2.12	0.50
19:j:77:TRP:HB2	21:m:144:ALA:HB2	1.94	0.50
19:j:82:ASN:OD1	19:j:82:ASN:N	2.45	0.50
23:o:68:TRP:O	23:o:72:ARG:HG2	2.11	0.50
24:p:118:HIS:O	24:p:121:PRO:HD3	2.11	0.50
25:q:307:TRP:HA	25:q:310:MET:HE2	1.94	0.50
46:Y:45:ARG:HB2	47:Z:33:PRO:HG3	1.93	0.50
48:l:339:LEU:HD22	48:l:373:LEU:HD22	1.94	0.50
50:t:111:ARG:O	50:t:115:ARG:HG2	2.11	0.50
5:v:129:ASP:N	5:v:129:ASP:OD1	2.45	0.50
7:x:142:THR:HG23	7:x:144:GLU:HG2	1.94	0.50
59:Am:158:HIS:HA	59:Am:161:GLN:HE21	1.76	0.50
64:Ar:50:ASP:OD1	64:Ar:50:ASP:N	2.45	0.50
3:2:202:LYS:O	3:2:205:ILE:HG13	2.12	0.49
3:4:139:THR:O	3:4:142:THR:OG1	2.27	0.49
7:8:97:TRP:HD1	7:8:100:ARG:HH11	1.60	0.49
7:8:236:PRO:HA	7:8:241:GLN:HG3	1.93	0.49
18:i:38:LEU:HD12	20:k:73:LEU:HD22	1.93	0.49
26:r:138:GLN:O	26:r:141:SER:OG	2.25	0.49
27:B:115:VAL:HG11	27:B:138:LEU:HD11	1.94	0.49
28:C:190:ILE:HD11	28:C:257:PHE:CZ	2.47	0.49
29:D:102:ASP:HB2	36:N:90:LEU:HD22	1.93	0.49
1:Ab:44:ILE:HG12	1:Ab:47:ARG:HH21	1.76	0.49
3:2:220:GLN:OE1	3:2:278:ASN:ND2	2.39	0.49
3:2:260:HIS:HB2	68:2:301:FES:S1	2.51	0.49
5:6:339:TYR:HD1	3:Ae:68:LEU:HD12	1.77	0.49
5:6:451:ASP:N	5:6:451:ASP:OD1	2.44	0.49
11:b:19:ARG:NH1	11:b:22:TRP:HD1	2.10	0.49
19:j:6:THR:HA	26:r:6:ILE:CD1	2.41	0.49
21:m:66:VAL:HA	26:r:114:TYR:OH	2.12	0.49
24:p:163:LYS:O	24:p:167:TRP:HD1	1.95	0.49
26:r:318:SER:HB3	41:S:41:PHE:HE2	1.76	0.49
32:H:135:ARG:HD2	32:H:137:ASP:HB2	1.94	0.49
48:l:291:CYS:O	48:l:295:GLN:HG2	2.12	0.49
51:u:373:GLN:NE2	51:u:471:ILE:HG23	2.27	0.49
65:G:400:ILE:HG13	65:G:427:LEU:HD21	1.94	0.49
10:a:78:THR:HG22	10:a:82:VAL:HG23	1.94	0.49
23:o:83:THR:HB	23:o:84:PRO:HD2	1.93	0.49
24:p:136:TYR:HA	24:p:139:TYR:HD2	1.77	0.49
27:B:77:LEU:HD13	27:B:100:SER:HA	1.94	0.49
27:B:223:PRO:HD2	72:B:502:SF4:S2	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Y:69:ILE:HG23	48:l:385:TYR:HD2	1.77	0.49
66:L:202:PHE:HA	66:L:206:ASP:OD2	2.12	0.49
6:7:5:ARG:NH1	6:7:20:ASP:OD2	2.46	0.49
6:7:26:ASN:HD21	6:7:207:ASN:HB2	1.78	0.49
10:a:160:MET:SD	10:a:168:TRP:HB2	2.52	0.49
12:c:151:PRO:HB3	48:l:403:TYR:CE1	2.48	0.49
19:j:79:SER:HA	19:j:87:MET:HE2	1.93	0.49
27:B:276:PHE:HD1	27:B:352:ALA:HB1	1.77	0.49
27:B:383:THR:N	27:B:384:PRO:HD2	2.27	0.49
46:Y:51:THR:O	46:Y:54:GLN:HG2	2.13	0.49
5:v:82:LEU:HD22	5:v:200:VAL:HB	1.93	0.49
64:Ar:34:TYR:OH	64:Ar:74:ASP:OD1	2.24	0.49
14:e:89:VAL:CG1	25:q:29:VAL:HG22	2.43	0.49
17:h:80:LYS:HB3	17:h:83:ARG:HH21	1.77	0.49
25:q:233:ALA:HA	25:q:320:GLY:HA2	1.93	0.49
25:q:304:GLN:HA	25:q:309:PHE:HE1	1.78	0.49
25:q:442:LEU:HB2	25:q:443:PRO:HD3	1.94	0.49
26:r:96:ILE:HG22	26:r:98:MET:HG3	1.94	0.49
28:C:308:LEU:HB2	28:C:407:GLU:HB2	1.93	0.49
6:w:128:PHE:O	6:w:132:VAL:HG23	2.12	0.49
65:G:371:VAL:N	65:G:482:GLN:OE1	2.41	0.49
65:G:639:LEU:HD21	65:G:643:ARG:HH21	1.77	0.49
6:7:113:TRP:HE3	69:7:402:HEM:HMD1	1.76	0.49
19:j:18:VAL:HG11	26:r:76:ILE:CG1	2.35	0.49
19:j:56:PHE:CZ	20:k:79:VAL:HG11	2.47	0.49
19:j:62:PHE:HE2	21:m:66:VAL:HG11	1.78	0.49
26:r:275:ALA:O	28:C:204:THR:OG1	2.31	0.49
27:B:382:CYS:HA	65:G:74:ASN:O	2.13	0.49
32:H:113:CYS:SG	72:H:302:SF4:S1	3.10	0.49
38:P:32:GLY:HA3	38:P:82:PHE:O	2.13	0.49
48:l:62:ILE:HG13	48:l:81:LYS:HA	1.95	0.49
51:u:103:ASN:OD1	51:u:153:ASN:ND2	2.44	0.49
6:w:282:ARG:NH1	6:w:339:GLY:HA2	2.27	0.49
6:w:282:ARG:HH12	6:w:339:GLY:HA2	1.77	0.49
58:Al:134:ARG:HG2	58:Al:135:LEU:HG	1.93	0.49
59:Am:112:LEU:HB3	59:Am:118:PRO:HB3	1.94	0.49
67:M:12:ARG:HG3	67:M:13:ASN:N	2.27	0.49
2:1:29:ALA:HA	3:2:144:VAL:HG13	1.93	0.49
5:6:193:PRO:O	5:6:197:ILE:HG12	2.13	0.49
6:7:278:TYR:CE2	6:7:282:ARG:HD3	2.48	0.49
14:e:148:GLN:HG2	16:g:113:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:q:204:MET:HE1	25:q:298:ILE:HG23	1.95	0.49
32:H:89:GLU:HG2	35:K:61:TRP:HB3	1.95	0.49
37:O:82:ARG:HB2	37:O:126:PHE:CZ	2.48	0.49
46:Y:51:THR:HG22	46:Y:54:GLN:HE21	1.78	0.49
51:u:119:HIS:CD2	5:v:298:HIS:HA	2.47	0.49
2:Ac:31:PHE:HA	4:Ad:48:ILE:HD11	1.94	0.49
3:2:161:MET:C	6:7:177:ARG:HH21	2.20	0.49
11:b:77:ILE:HB	11:b:78:PRO:HD3	1.93	0.49
14:e:61:PRO:O	14:e:62:GLU:C	2.56	0.49
15:f:59:ILE:O	15:f:63:LYS:HG2	2.12	0.49
21:m:25:SER:HB3	21:m:28:TYR:HD2	1.77	0.49
30:E:66:ILE:HD13	30:E:81:PRO:HB2	1.95	0.49
33:I:65:MET:HG3	33:I:103:MET:HA	1.95	0.49
48:l:293:ILE:HD12	48:l:421:ALA:HB3	1.94	0.49
57:Ak:509:THR:HG21	62:Ap:102:TRP:HZ3	1.78	0.49
58:Al:162:SER:HB3	58:Al:197:SER:HB2	1.95	0.49
65:G:512:VAL:O	65:G:514:ASN:ND2	2.45	0.49
66:L:137:GLU:H	66:L:174:ARG:HH22	1.61	0.49
5:6:177:LEU:HD11	5:6:272:VAL:HG22	1.95	0.49
11:b:12:LEU:O	11:b:16:ARG:HD2	2.13	0.49
15:f:66:VAL:HG22	15:f:70:LYS:HE3	1.95	0.49
16:g:53:ARG:O	16:g:54:PRO:C	2.54	0.49
27:B:226:LYS:O	27:B:227:PRO:C	2.56	0.49
28:C:137:GLN:NE2	32:H:121:ALA:O	2.46	0.49
32:H:88:PHE:CE2	35:K:30:ALA:HA	2.48	0.49
34:J:90:GLY:HA2	65:G:59:GLN:NE2	2.26	0.49
37:O:144:ILE:O	37:O:148:ILE:HG13	2.12	0.49
5:v:299:VAL:HG23	5:v:302:GLY:HA3	1.94	0.49
57:Ak:509:THR:HG21	62:Ap:102:TRP:CZ3	2.48	0.49
62:Ap:49:ARG:O	62:Ap:53:MET:HG2	2.13	0.49
51:5:61:SER:OG	51:5:239:HIS:ND1	2.41	0.49
65:G:447:ASP:N	65:G:447:ASP:OD1	2.44	0.49
3:2:116:GLU:OE1	3:2:116:GLU:N	2.39	0.49
3:2:263:HIS:O	3:2:270:ILE:HD12	2.13	0.49
5:6:183:ARG:NH2	5:v:451:ASP:OD1	2.45	0.49
7:8:118:TYR:CZ	7:8:128:MET:HG3	2.48	0.49
12:c:86:ARG:HB3	12:c:92:TRP:CZ2	2.48	0.49
12:c:115:ASN:HA	48:l:166:THR:HG22	1.95	0.49
15:f:29:PHE:CD2	43:U:102:ASP:HB3	2.47	0.49
18:i:261:MET:SD	18:i:340:THR:HG22	2.53	0.49
20:k:32:CYS:HA	21:m:20:PHE:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:44:LEU:HD23	22:n:45:PHE:CE2	2.48	0.49
30:E:84:ASP:O	30:E:88:ARG:HG3	2.13	0.49
34:J:72:ILE:HD11	34:J:141:ASN:O	2.13	0.49
39:Q:57:ARG:O	39:Q:60:GLU:HG2	2.13	0.49
40:R:110:HIS:CD2	65:G:441:ARG:HH12	2.31	0.49
6:w:245:PHE:CD1	7:x:102:LEU:CD1	2.96	0.49
5:6:378:LEU:HD13	5:6:416:ILE:HD12	1.93	0.48
6:7:128:PHE:O	6:7:132:VAL:HG23	2.13	0.48
13:d:80:LYS:HA	25:q:182:TRP:NE1	2.28	0.48
25:q:297:VAL:HG13	25:q:312:ALA:HB1	1.94	0.48
28:C:456:ILE:HG22	28:C:460:GLN:NE2	2.28	0.48
31:F:39:THR:HG22	31:F:62:VAL:HG22	1.95	0.48
37:X:90:TYR:C	47:Z:63:ARG:HH21	2.21	0.48
37:X:138:LEU:HG	37:X:144:ILE:HA	1.95	0.48
46:Y:40:ILE:HB	46:Y:49:GLN:HG3	1.94	0.48
57:Ak:359:ALA:HA	74:Ak:602:HEA:OMA	2.13	0.48
51:5:341:PHE:HB2	51:5:358:PHE:HB3	1.94	0.48
9:A:57:MET:O	9:A:61:GLU:HG2	2.14	0.48
11:b:75:VAL:HG13	48:l:46:LEU:HD11	1.95	0.48
16:g:111:TYR:HA	16:g:114:ILE:HG22	1.95	0.48
25:q:114:GLU:HG2	49:s:246:PHE:HB3	1.95	0.48
27:B:73:PRO:HB3	27:B:148:ALA:HA	1.95	0.48
28:C:151:MET:HB2	28:C:184:THR:HG21	1.95	0.48
28:C:178:VAL:HG23	28:C:317:TYR:CZ	2.48	0.48
29:D:149:GLU:OE1	29:D:149:GLU:N	2.43	0.48
32:H:119:CYS:O	32:H:123:CYS:N	2.45	0.48
33:I:184:ILE:O	33:I:187:GLU:HB2	2.13	0.48
42:T:142:LEU:HD21	42:T:151:VAL:HG11	1.95	0.48
45:W:79:LYS:HG3	45:W:82:ARG:HH21	1.78	0.48
59:Am:154:GLY:HA2	62:Ap:37:VAL:HG22	1.93	0.48
66:L:267:LEU:HG	66:L:370:VAL:HG21	1.96	0.48
67:M:9:GLN:HA	67:M:12:ARG:HG2	1.94	0.48
3:4:251:ASP:OD1	3:4:251:ASP:N	2.38	0.48
5:6:271:LEU:HD11	5:6:436:LYS:HB3	1.95	0.48
5:6:383:LEU:HD13	51:5:67:PRO:HB2	1.95	0.48
18:i:203:LEU:HD22	18:i:343:LEU:HD23	1.96	0.48
25:q:59:ASP:CG	25:q:245:ARG:HH22	2.21	0.48
49:s:162:TYR:HA	49:s:180:GLN:HB3	1.96	0.48
7:x:122:CYS:HB2	70:x:401:HEC:CMC	2.42	0.48
59:Am:197:PHE:HD2	59:Am:256:ILE:HG21	1.77	0.48
51:5:335:ARG:HB2	51:5:337:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:G:138:ASP:HB3	65:G:142:GLN:NE2	2.27	0.48
65:G:295:ASP:OD2	65:G:705:GLN:N	2.46	0.48
6:7:102:LEU:HD22	6:7:304:MET:HE2	1.94	0.48
10:a:110:TRP:HE3	10:a:119:ARG:HB3	1.78	0.48
13:d:80:LYS:HG2	16:g:108:LYS:HZ1	1.78	0.48
17:h:3:PHE:HB2	18:i:144:GLN:CD	2.39	0.48
20:k:94:ASN:O	20:k:94:ASN:ND2	2.45	0.48
25:q:132:ILE:HA	25:q:136:TRP:CE3	2.48	0.48
28:C:410:LYS:NZ	28:C:461:ASP:OD1	2.46	0.48
39:Q:144:PHE:HZ	65:G:621:LYS:HA	1.78	0.48
44:V:58:ARG:O	44:V:62:THR:HG23	2.13	0.48
46:Y:89:PRO:HA	46:Y:92:TRP:HB2	1.95	0.48
48:l:102:GLU:HA	48:l:105:MET:HE2	1.96	0.48
5:v:300:LYS:HD2	5:v:301:ARG:HG2	1.95	0.48
6:w:272:TRP:HA	6:w:275:LEU:HG	1.95	0.48
57:Ak:65:MET:HE3	74:Ak:601:HEA:HHC	1.95	0.48
59:Am:133:ASN:HB3	59:Am:173:PHE:CE2	2.48	0.48
64:Ar:47:LYS:HZ2	64:Ar:49:GLY:HA3	1.78	0.48
25:q:457:PRO:HG2	25:q:458:LEU:HD12	1.95	0.48
27:B:35:LEU:HD22	27:B:273:THR:HG21	1.96	0.48
30:E:186:VAL:HG22	30:E:196:LEU:HD11	1.95	0.48
33:I:47:VAL:HG12	33:I:191:ARG:HD3	1.95	0.48
36:N:30:LYS:NZ	43:U:273:GLU:OE2	2.22	0.48
38:P:21:ILE:HD11	38:P:91:LEU:HD21	1.96	0.48
48:l:90:ILE:HB	48:l:91:PRO:HD3	1.95	0.48
50:t:54:GLN:HE21	50:t:54:GLN:HB2	1.47	0.48
70:x:401:HEC:HMC3	70:x:401:HEC:HBC3	1.95	0.48
58:Al:217:LYS:O	58:Al:220:GLU:HG2	2.13	0.48
51:5:328:LEU:HB2	51:5:375:GLN:HG3	1.95	0.48
65:G:357:LEU:O	65:G:361:VAL:HG23	2.13	0.48
65:G:696:MET:SD	65:G:702:ARG:HA	2.53	0.48
3:4:125:LYS:HD3	51:5:292:GLU:HG2	1.96	0.48
3:4:223:LEU:HD11	3:4:229:PRO:HG3	1.95	0.48
10:a:171:TYR:HD1	10:a:171:TYR:H	1.60	0.48
12:c:168:LEU:O	13:d:123:GLN:NE2	2.47	0.48
19:j:65:PHE:O	19:j:69:ILE:HG23	2.13	0.48
27:B:167:SER:HA	27:B:170:GLN:HB2	1.96	0.48
28:C:139:LEU:HB3	28:C:140:PRO:HD3	1.95	0.48
29:D:124:ASN:ND2	29:D:148:ASP:OD1	2.46	0.48
37:X:115:GLN:HE21	37:X:139:MET:H	1.60	0.48
47:Z:77:VAL:HG11	48:l:363:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Ak:507:GLU:HA	59:Am:5:THR:HB	1.96	0.48
60:An:62:LEU:HD11	60:An:77:GLU:HB3	1.96	0.48
3:4:270:ILE:HG22	3:4:278:ASN:OD1	2.14	0.48
14:e:121:GLU:HG2	14:e:124:ARG:HH21	1.79	0.48
18:i:112:HIS:HB2	18:i:184:ILE:HD13	1.95	0.48
18:i:117:GLU:O	20:k:96:LEU:HD13	2.14	0.48
25:q:43:ASN:C	25:q:44:GLN:HE21	2.22	0.48
30:E:114:GLU:HG2	65:G:197:THR:O	2.13	0.48
33:I:126:GLU:HG2	33:I:128:ARG:HG2	1.94	0.48
38:P:91:LEU:HA	38:P:94:VAL:HG12	1.95	0.48
44:V:16:THR:HG22	44:V:17:GLU:HG3	1.96	0.48
37:X:123:GLU:HB2	37:X:130:ILE:HG13	1.96	0.48
6:w:132:VAL:HG22	6:w:143:ALA:HB2	1.96	0.48
52:z:29:HIS:HB3	52:z:32:THR:OG1	2.14	0.48
65:G:66:HIS:CE1	65:G:68:ARG:HB2	2.49	0.48
65:G:257:VAL:HG11	65:G:413:LEU:HB2	1.95	0.48
66:L:221:VAL:HG12	66:L:223:LEU:HG	1.94	0.48
3:2:109:PHE:O	3:2:113:ARG:HG3	2.14	0.48
6:7:344:GLU:HG3	52:Aa:67:PHE:HE1	1.78	0.48
13:d:139:PHE:N	14:e:137:MET:SD	2.87	0.48
18:i:72:MET:HE3	20:k:12:PHE:CG	2.49	0.48
32:H:147:ILE:HG13	32:H:190:LEU:HD11	1.96	0.48
37:X:94:ASP:OD1	37:X:96:GLU:HG2	2.13	0.48
48:l:332:HIS:HA	48:l:335:PHE:CZ	2.48	0.48
5:6:147:ARG:HD3	5:6:149:TRP:CZ2	2.49	0.48
5:6:380:ALA:HA	51:5:136:LEU:HD21	1.95	0.48
6:7:200:LEU:CD2	69:7:402:HEM:HAA1	2.44	0.48
10:a:171:TYR:N	10:a:171:TYR:CD1	2.82	0.48
10:a:176:LYS:HE3	17:h:42:GLU:HA	1.95	0.48
12:c:163:TYR:HB2	50:t:43:GLN:OE1	2.14	0.48
16:g:80:ARG:HG2	18:i:345:SER:HA	1.96	0.48
16:g:119:HIS:NE2	25:q:252:PRO:HG3	2.29	0.48
18:i:20:VAL:HG11	18:i:137:ALA:HB1	1.95	0.48
19:j:6:THR:HB	26:r:2:PHE:HE2	1.79	0.48
26:r:67:SER:HB2	26:r:121:TRP:HZ3	1.77	0.48
27:B:185:ASN:OD1	27:B:190:GLY:N	2.46	0.48
34:J:61:ILE:HG22	34:J:64:LEU:HB2	1.95	0.48
48:l:566:THR:O	48:l:570:GLN:HG2	2.14	0.48
50:t:97:LYS:HA	50:t:100:LYS:HD3	1.95	0.48
7:x:309:ARG:HG3	52:z:27:PHE:CE1	2.48	0.48
57:Ak:507:GLU:OE2	62:Ap:83:ILE:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Al:223:SER:O	58:Al:227:LEU:HG	2.13	0.48
59:Am:126:PRO:O	59:Am:253:TYR:OH	2.26	0.48
11:b:26:GLN:CB	24:p:217:ARG:HH12	2.22	0.48
12:c:161:TYR:O	12:c:165:ASP:HA	2.13	0.48
19:j:14:ALA:HA	26:r:79:LEU:HD23	1.95	0.48
20:k:4:VAL:O	20:k:8:ILE:HG12	2.14	0.48
31:F:105:GLU:OE1	31:F:105:GLU:N	2.36	0.48
35:K:69:ASN:ND2	35:K:112:ASN:HD21	2.11	0.48
37:O:140:CYS:HB3	37:O:143:GLU:HG3	1.96	0.48
37:X:105:MET:N	37:X:105:MET:SD	2.85	0.48
49:s:244:LEU:HD23	49:s:247:TRP:CE3	2.49	0.48
55:Ai:52:VAL:O	55:Ai:56:THR:HG23	2.13	0.48
61:Ao:69:ALA:O	61:Ao:73:ARG:HG3	2.14	0.48
64:Ar:66:PRO:HG2	64:Ar:69:TRP:CG	2.49	0.48
18:i:115:VAL:HG12	18:i:180:ALA:HB1	1.96	0.47
22:n:39:ARG:O	22:n:58:LYS:HE3	2.14	0.47
23:o:6:TYR:HD2	23:o:14:LEU:HD12	1.79	0.47
26:r:117:LEU:HD21	26:r:136:VAL:HG13	1.95	0.47
28:C:267:MET:HE3	28:C:267:MET:HB3	1.78	0.47
42:T:148:MET:HE3	49:s:207:LYS:HD2	1.95	0.47
37:X:82:ARG:O	37:X:86:VAL:HG23	2.14	0.47
51:u:407:THR:HB	51:u:408:PRO:HD3	1.96	0.47
5:v:371:VAL:HG12	5:v:375:LYS:HD2	1.95	0.47
5:v:421:ASP:OD1	5:v:421:ASP:N	2.43	0.47
6:w:233:LEU:HD13	7:x:301:LEU:HD23	1.95	0.47
62:Ap:113:CYS:SG	62:Ap:115:SER:OG	2.70	0.47
51:5:195:THR:HG21	51:5:269:ARG:H	1.79	0.47
65:G:478:SER:O	65:G:482:GLN:HG2	2.14	0.47
3:4:257:CYS:SG	3:4:259:CYS:HB3	2.54	0.47
21:m:4:TYR:O	21:m:5:ILE:C	2.57	0.47
24:p:84:CYS:HB3	47:Z:52:LEU:HD11	1.96	0.47
24:p:137:GLU:HB3	48:l:160:GLY:HA3	1.95	0.47
26:r:236:ALA:HB1	26:r:259:PHE:CZ	2.49	0.47
28:C:368:LYS:HE2	28:C:386:HIS:HE1	1.79	0.47
44:V:48:SER:H	44:V:51:GLU:HB2	1.77	0.47
45:W:97:ILE:HG22	45:W:98:MET:HG3	1.94	0.47
48:l:137:LEU:HD21	48:l:263:PHE:HZ	1.79	0.47
48:l:202:PHE:HA	48:l:266:LEU:HD21	1.96	0.47
6:w:183:PHE:CZ	69:w:402:HEM:HBC1	2.50	0.47
8:y:99:ILE:O	8:y:103:LYS:HG2	2.14	0.47
55:Ai:63:GLU:OE2	55:Ai:65:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:138:ILE:O	3:4:142:THR:HG23	2.14	0.47
5:6:452:GLU:OE2	5:v:183:ARG:NH1	2.47	0.47
14:e:73:SER:C	14:e:75:GLY:H	2.23	0.47
20:k:97:GLN:HA	48:l:582:GLY:HA3	1.96	0.47
23:o:63:PRO:O	23:o:67:ARG:HG3	2.14	0.47
29:D:226:LEU:HD21	33:I:145:TYR:CD1	2.49	0.47
31:F:50:TYR:CE2	66:L:74:GLN:HG2	2.50	0.47
32:H:176:SER:HA	33:I:164:PRO:HD3	1.96	0.47
37:X:90:TYR:CD1	47:Z:61:TRP:CE2	3.02	0.47
58:Al:152:MET:HE3	58:Al:152:MET:HB3	1.82	0.47
3:2:225:ARG:NH2	3:2:279:LEU:O	2.48	0.47
3:4:166:ASP:N	3:4:166:ASP:OD1	2.47	0.47
5:6:449:PHE:CZ	5:v:183:ARG:HB2	2.50	0.47
13:d:98:VAL:O	13:d:102:ILE:HG13	2.14	0.47
24:p:196:LEU:HD11	24:p:208:LEU:HD12	1.96	0.47
27:B:111:LYS:HB2	27:B:151:ALA:HA	1.96	0.47
27:B:174:ARG:O	27:B:178:GLU:HG2	2.15	0.47
28:C:204:THR:HG22	28:C:208:TRP:CE2	2.48	0.47
28:C:322:PHE:HA	28:C:348:ARG:HH11	1.79	0.47
29:D:66:ALA:HA	29:D:73:VAL:HG21	1.96	0.47
30:E:177:LEU:HD13	30:E:187:GLN:HB2	1.96	0.47
33:I:64:PRO:HG3	33:I:91:VAL:CG1	2.40	0.47
33:I:79:MET:O	33:I:86:MET:HG3	2.14	0.47
44:V:50:LEU:HA	44:V:53:VAL:HG12	1.96	0.47
45:W:86:MET:HE3	45:W:124:LEU:HD22	1.96	0.47
46:Y:62:SER:HB3	47:Z:85:LYS:O	2.14	0.47
5:v:409:PRO:O	5:v:413:LEU:HG	2.14	0.47
57:Ak:354:THR:HG21	57:Ak:429:HIS:HE1	1.80	0.47
63:Aq:34:GLY:O	63:Aq:38:PRO:HG2	2.13	0.47
5:6:134:MET:SD	5:6:233:VAL:HG11	2.55	0.47
11:b:86:LEU:O	11:b:91:THR:HG23	2.14	0.47
17:h:65:GLU:CB	45:W:111:PHE:CE1	2.96	0.47
17:h:86:LEU:HB3	17:h:92:TYR:HB3	1.95	0.47
25:q:11:LEU:HD13	25:q:14:MET:HE2	1.95	0.47
27:B:163:TYR:CZ	40:R:86:PHE:HB2	2.50	0.47
27:B:265:PHE:CD2	27:B:273:THR:HG23	2.49	0.47
29:D:199:ARG:C	29:D:201:ASP:H	2.22	0.47
30:E:130:TYR:HB2	30:E:169:PHE:CD1	2.50	0.47
48:l:32:TYR:N	48:l:33:PRO:HD2	2.29	0.47
5:v:360:THR:HG22	5:v:365:ASN:HB2	1.97	0.47
57:Ak:96:ARG:NH1	57:Ak:97:MET:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Ak:182:PRO:HB3	57:Ak:256:HIS:CE1	2.50	0.47
65:G:389:THR:O	65:G:390:THR:OG1	2.25	0.47
66:L:251:PRO:O	66:L:254:LYS:HD2	2.14	0.47
12:c:119:THR:O	12:c:119:THR:OG1	2.31	0.47
13:d:147:GLY:HA3	16:g:121:VAL:CG2	2.42	0.47
20:k:75:LEU:HD21	21:m:68:PHE:CZ	2.50	0.47
28:C:150:MET:SD	28:C:150:MET:N	2.85	0.47
33:I:42:ARG:HD3	33:I:42:ARG:HA	1.78	0.47
33:I:92:VAL:HG12	33:I:94:ARG:H	1.78	0.47
33:I:187:GLU:HB3	66:L:82:GLU:OE2	2.13	0.47
48:l:230:HIS:CG	48:l:231:PRO:HD3	2.50	0.47
50:t:63:LEU:HD22	50:t:87:TRP:CZ2	2.50	0.47
51:u:362:ASN:HB3	51:u:461:PRO:HB2	1.97	0.47
57:Ak:240:HIS:NE2	57:Ak:290:HIS:HE1	2.12	0.47
57:Ak:320:VAL:O	57:Ak:324:LEU:HG	2.15	0.47
60:An:142:THR:HG23	60:An:156:PHE:HZ	1.79	0.47
65:G:495:ASN:O	65:G:498:GLN:HG3	2.14	0.47
66:L:56:ALA:HB3	66:L:77:VAL:HG13	1.96	0.47
15:f:51:SER:HB3	16:g:64:LEU:HD13	1.96	0.47
15:f:62:HIS:CG	16:g:28:LEU:HD21	2.50	0.47
18:i:14:MET:O	18:i:18:MET:HG2	2.15	0.47
19:j:106:TRP:CZ2	26:r:291:LYS:HB3	2.50	0.47
21:m:38:GLY:HA2	21:m:57:PHE:HE1	1.78	0.47
23:o:8:PRO:HB3	23:o:14:LEU:HB2	1.97	0.47
25:q:147:LEU:HD22	25:q:151:PHE:CE2	2.50	0.47
25:q:259:TYR:HB2	25:q:260:PRO:HD3	1.95	0.47
26:r:27:VAL:HG12	26:r:31:MET:HE2	1.95	0.47
26:r:169:GLN:HG2	26:r:174:MET:HG3	1.97	0.47
26:r:189:THR:HG22	26:r:234:MET:HE3	1.96	0.47
27:B:273:THR:HG22	27:B:291:GLU:HA	1.97	0.47
27:B:389:VAL:HA	27:B:392:MET:HE2	1.97	0.47
28:C:53:PHE:HD1	28:C:58:MET:HE1	1.80	0.47
28:C:167:ILE:HG23	28:C:364:VAL:HG21	1.96	0.47
28:C:302:SER:O	36:N:12:VAL:HG22	2.14	0.47
28:C:309:ARG:HG3	28:C:407:GLU:HB3	1.95	0.47
32:H:119:CYS:SG	32:H:128:ILE:HD12	2.55	0.47
33:I:175:TYR:CE1	35:K:78:ASP:HB2	2.47	0.47
37:X:125:GLU:HG2	48:l:439:PRO:CG	2.38	0.47
48:l:289:ALA:O	48:l:293:ILE:HG12	2.14	0.47
48:l:302:VAL:O	48:l:306:THR:HG23	2.14	0.47
51:u:317:THR:HG21	3:Af:53:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:x:136:LEU:HD11	7:x:176:PHE:CZ	2.49	0.47
7:x:209:GLU:CD	7:x:209:GLU:H	2.23	0.47
57:Ak:66:ILE:HG23	57:Ak:246:LEU:HD11	1.97	0.47
57:Ak:240:HIS:HD2	57:Ak:287:VAL:HG23	1.80	0.47
58:Al:100:MET:HE3	58:Al:157:GLU:HG2	1.97	0.47
60:An:70:TRP:CH2	61:Ao:99:ARG:HA	2.49	0.47
65:G:372:PHE:H	65:G:532:PRO:HB2	1.80	0.47
66:L:79:TYR:HE2	66:L:100:PHE:HB3	1.79	0.47
3:4:235:ILE:HG13	3:4:282:PRO:HD3	1.97	0.47
5:6:290:GLN:HG2	5:6:295:ALA:HB2	1.96	0.47
6:7:81:TYR:OH	7:8:203:ARG:NH1	2.48	0.47
16:g:83:TYR:CZ	16:g:87:LEU:HD11	2.49	0.47
17:h:104:PRO:O	41:S:53:CYS:SG	2.62	0.47
28:C:448:HIS:HB3	28:C:452:ASP:HB2	1.97	0.47
38:P:18:GLU:HG2	38:P:68:ARG:NH1	2.30	0.47
2:Ac:19:SER:OG	51:5:480:PHE:O	2.27	0.47
58:Al:90:ILE:HD12	64:Ar:17:PHE:CZ	2.49	0.47
59:Am:137:LEU:HB3	59:Am:246:ASP:OD1	2.15	0.47
63:Aq:37:LEU:HB3	63:Aq:38:PRO:HD3	1.96	0.47
65:G:76:ARG:NH2	65:G:90:ALA:HB2	2.29	0.47
65:G:421:SER:HB3	65:G:427:LEU:HD22	1.96	0.47
65:G:422:TRP:HA	65:G:427:LEU:HB3	1.97	0.47
65:G:592:LYS:HA	65:G:608:VAL:HG22	1.97	0.47
26:r:23:VAL:HG21	41:S:12:MET:HE2	1.95	0.47
26:r:234:MET:O	26:r:238:THR:HG23	2.14	0.47
28:C:209:MET:HE1	28:C:260:ARG:HB3	1.97	0.47
37:O:110:LEU:HB2	37:O:114:ASP:HB2	1.97	0.47
49:s:160:THR:HA	49:s:163:TRP:CD1	2.50	0.47
5:v:65:ILE:HG12	5:v:218:MET:HG2	1.97	0.47
57:Ak:374:VAL:HA	57:Ak:377:PHE:CE2	2.50	0.47
51:5:42:LEU:HD22	51:5:426:LEU:HB3	1.97	0.47
51:5:282:LEU:HD12	51:5:460:GLY:HA2	1.97	0.47
65:G:250:SER:OG	65:G:251:ILE:N	2.46	0.47
65:G:434:SER:HB3	65:G:686:PRO:HD2	1.96	0.47
5:6:65:ILE:HG23	5:6:218:MET:HG3	1.97	0.47
9:A:58:LYS:HE3	9:A:58:LYS:HB3	1.70	0.47
26:r:318:SER:HB3	41:S:41:PHE:CE2	2.50	0.47
28:C:224:SER:CB	28:C:230:ALA:HB1	2.45	0.47
29:D:113:ASP:OD1	29:D:131:ASN:ND2	2.47	0.47
31:F:76:VAL:HG22	31:F:117:GLN:HB2	1.97	0.47
36:N:36:GLY:HA2	36:N:45:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S:50:ARG:O	41:S:54:ILE:HG12	2.15	0.47
37:X:90:TYR:HD1	47:Z:61:TRP:CE2	2.32	0.47
46:Y:78:ASP:HA	46:Y:81:LEU:HB3	1.97	0.47
47:Z:59:ASP:OD1	47:Z:62:GLY:HA3	2.15	0.47
49:s:142:GLN:HA	49:s:145:LEU:HD12	1.97	0.47
5:v:47:LEU:HD23	5:v:234:ALA:HB1	1.96	0.47
1:Ab:32:THR:O	1:Ab:36:GLN:HG2	2.14	0.47
58:Al:52:HIS:CG	61:Ao:83:ASP:HB2	2.50	0.47
58:Al:100:MET:HA	58:Al:155:SER:O	2.15	0.47
61:Ao:91:ILE:O	61:Ao:95:LEU:HG	2.14	0.47
61:Ao:111:LEU:O	61:Ao:114:VAL:HG22	2.15	0.47
75:L:401:NDP:H2N	75:L:401:NDP:H2D	1.72	0.47
3:2:200:ARG:HG2	3:2:205:ILE:HG23	1.97	0.46
6:7:81:TYR:O	6:7:85:ASN:ND2	2.40	0.46
7:8:243:ILE:HG12	7:8:245:MET:H	1.79	0.46
22:n:17:VAL:HG21	25:q:11:LEU:HD22	1.97	0.46
25:q:235:LEU:O	25:q:238:LEU:HB2	2.15	0.46
25:q:258:ALA:O	25:q:259:TYR:C	2.58	0.46
27:B:64:LYS:HE2	30:E:249:LEU:C	2.40	0.46
32:H:200:GLU:OE1	35:K:87:HIS:HB3	2.14	0.46
45:W:10:MET:HE3	45:W:11:PRO:HD2	1.97	0.46
37:X:92:LYS:H	47:Z:60:PRO:CB	2.15	0.46
50:t:89:TYR:O	50:t:93:LEU:HD22	2.15	0.46
51:u:144:VAL:HG11	51:u:245:LEU:HB3	1.96	0.46
7:x:245:MET:HB2	70:x:401:HEC:C1D	2.44	0.46
54:Ah:23:GLU:H	54:Ah:25:ARG:HH12	1.62	0.46
58:Al:191:LEU:HB2	60:An:148:MET:HE2	1.97	0.46
60:An:83:ARG:NH2	60:An:92:GLU:OE2	2.47	0.46
3:4:200:ARG:HH12	3:4:226:VAL:HG11	1.79	0.46
12:c:184:TYR:HE1	50:t:27:PRO:HB3	1.80	0.46
27:B:397:ALA:O	27:B:400:VAL:HG22	2.15	0.46
28:C:329:ARG:HB2	28:C:331:ASP:OD1	2.15	0.46
28:C:417:LEU:HD11	28:C:425:PRO:HB3	1.97	0.46
32:H:135:ARG:HG3	32:H:138:GLY:H	1.80	0.46
37:O:138:LEU:O	37:O:139:MET:HB2	2.15	0.46
45:W:128:ARG:HG2	45:W:128:ARG:HH11	1.79	0.46
49:s:97:VAL:CG1	49:s:102:LEU:HG	2.44	0.46
49:s:235:LEU:HD23	49:s:235:LEU:HA	1.71	0.46
58:Al:163:TRP:HZ2	58:Al:211:LEU:HD21	1.80	0.46
7:8:153:VAL:HG21	7:8:177:PRO:HG2	1.98	0.46
18:i:141:VAL:O	18:i:145:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:j:56:PHE:CE2	20:k:79:VAL:CG1	2.95	0.46
21:m:137:SER:HB3	21:m:140:ALA:HB3	1.97	0.46
25:q:165:VAL:HG12	25:q:169:ASN:HD21	1.81	0.46
28:C:89:ASN:HD21	28:C:102:ARG:HG3	1.80	0.46
30:E:152:ILE:HG21	30:E:171:LEU:HD13	1.97	0.46
48:l:525:MET:HE3	48:l:525:MET:HB2	1.79	0.46
51:u:383:ALA:HB3	51:u:442:ARG:HG3	1.97	0.46
5:v:70:ARG:O	5:v:185:ALA:HB1	2.15	0.46
5:v:135:GLU:OE2	5:v:236:ARG:NH2	2.48	0.46
7:x:121:VAL:O	7:x:122:CYS:C	2.58	0.46
51:5:318:TYR:CE1	3:Ae:55:GLY:HA2	2.50	0.46
51:5:383:ALA:HB3	51:5:442:ARG:HG3	1.97	0.46
18:i:193:VAL:HG21	18:i:266:ILE:HG12	1.96	0.46
19:j:59:ALA:CB	21:m:70:TYR:HE2	2.29	0.46
20:k:25:HIS:ND1	20:k:88:ASP:OD1	2.37	0.46
30:E:93:LEU:HD12	30:E:122:TYR:HB3	1.98	0.46
37:O:116:VAL:HG12	37:O:120:MET:HE2	1.96	0.46
50:t:17:PRO:HG3	50:t:105:GLU:HG2	1.97	0.46
7:x:229:ARG:HD2	7:x:230:GLU:HG3	1.98	0.46
53:Ag:44:SER:O	53:Ag:48:LEU:HG	2.16	0.46
58:Al:218:TYR:HA	58:Al:221:LYS:HG2	1.97	0.46
51:5:373:GLN:O	51:5:377:MET:HG2	2.16	0.46
70:8:401:HEC:HHD	70:8:401:HEC:HBC3	1.97	0.46
8:9:71:MET:HE3	8:9:72:ARG:HG3	1.98	0.46
12:c:185:GLU:HB2	50:t:36:GLU:HA	1.97	0.46
13:d:100:GLN:HA	48:l:73:THR:HG22	1.96	0.46
14:e:65:ASN:HD22	14:e:65:ASN:H	1.62	0.46
14:e:97:ILE:O	14:e:101:LEU:HB3	2.15	0.46
14:e:136:LEU:H	14:e:136:LEU:HD22	1.80	0.46
23:o:45:ARG:HG2	24:p:191:PRO:CG	2.43	0.46
25:q:6:ILE:HB	25:q:7:PRO:HD3	1.96	0.46
26:r:64:ALA:HB3	26:r:124:ASN:HB3	1.97	0.46
28:C:306:TRP:CD2	29:D:135:LEU:HD23	2.50	0.46
29:D:191:TYR:CE1	39:Q:123:TRP:HB3	2.50	0.46
32:H:209:TYR:CE1	32:H:210:LEU:HG	2.51	0.46
37:O:83:VAL:O	37:O:87:LEU:HD22	2.16	0.46
38:P:17:ARG:NH1	65:G:362:ASP:OD1	2.42	0.46
38:P:40:ARG:NH1	38:P:88:THR:OG1	2.47	0.46
48:l:230:HIS:ND1	48:l:231:PRO:HD3	2.30	0.46
58:Al:161:HIS:HB2	58:Al:174:ALA:HB3	1.96	0.46
60:An:65:LYS:HB3	60:An:73:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:G:455:ILE:HD13	65:G:460:HIS:HB3	1.97	0.46
66:L:80:ARG:HE	75:L:401:NDP:P2B	2.39	0.46
7:8:223:PRO:HD2	7:8:226:VAL:HG21	1.97	0.46
7:8:251:ASN:HD21	1:Ab:28:ASP:HB2	1.79	0.46
20:k:30:LEU:HB3	21:m:68:PHE:HE2	1.81	0.46
20:k:44:SER:O	20:k:48:ILE:HG12	2.16	0.46
22:n:13:VAL:HA	22:n:16:LEU:HG	1.97	0.46
25:q:193:ILE:HG23	25:q:257:MET:SD	2.56	0.46
26:r:259:PHE:O	26:r:263:THR:HG23	2.16	0.46
26:r:299:ALA:HB1	42:T:110:ILE:HG22	1.98	0.46
36:N:19:THR:OG1	36:N:22:GLU:HB2	2.16	0.46
45:W:138:TYR:HB3	45:W:142:TRP:CD2	2.51	0.46
47:Z:51:LYS:O	47:Z:55:ARG:NE	2.49	0.46
48:l:27:TYR:O	48:l:115:ASN:ND2	2.47	0.46
6:w:237:LEU:HD22	7:x:301:LEU:HD11	1.98	0.46
7:x:127:SER:CB	7:x:179:PRO:HD3	2.31	0.46
58:Al:10:GLN:NE2	58:Al:167:SER:OG	2.49	0.46
65:G:619:ASP:O	65:G:623:ILE:HG12	2.15	0.46
67:M:25:GLN:H	67:M:25:GLN:HG2	1.60	0.46
9:A:17:LEU:HD13	57:Ak:328:HIS:CE1	2.51	0.46
12:c:112:TYR:OH	23:o:10:ARG:NH2	2.49	0.46
13:d:140:GLN:HE22	23:o:123:GLN:CB	2.29	0.46
17:h:96:PRO:HA	17:h:99:LEU:HB3	1.98	0.46
21:m:124:ASP:C	21:m:126:VAL:N	2.73	0.46
33:I:66:THR:HG23	33:I:76:MET:HG2	1.97	0.46
37:X:120:MET:HE3	37:X:120:MET:HB3	1.68	0.46
48:l:210:ASN:O	48:l:211:MET:C	2.58	0.46
48:l:399:VAL:CG1	48:l:409:LEU:HD13	2.46	0.46
57:Ak:23:GLY:HA3	57:Ak:73:ILE:HG13	1.97	0.46
57:Ak:463:THR:HA	57:Ak:466:MET:HE2	1.97	0.46
58:Al:160:LEU:HD22	58:Al:198:GLU:HG2	1.98	0.46
65:G:217:GLU:OE2	65:G:409:PHE:HA	2.16	0.46
7:8:263:THR:OG1	1:Ab:28:ASP:OD1	2.34	0.46
11:b:83:HIS:CD2	13:d:41:VAL:HG12	2.49	0.46
18:i:19:LEU:HD11	21:m:156:VAL:HG11	1.97	0.46
18:i:290:LEU:HD22	25:q:150:LEU:HD21	1.97	0.46
24:p:73:CYS:HB2	24:p:79:TYR:HB2	1.98	0.46
25:q:66:LEU:CD1	25:q:107:ILE:HA	2.46	0.46
27:B:205:ILE:HG12	27:B:379:CYS:SG	2.56	0.46
27:B:423:THR:HG21	27:B:428:GLY:HA3	1.98	0.46
28:C:47:VAL:HG13	43:U:315:TYR:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:464:PHE:HA	28:C:467:VAL:HB	1.97	0.46
33:I:69:LEU:HB2	33:I:107:GLY:HA3	1.98	0.46
33:I:126:GLU:HA	33:I:128:ARG:N	2.31	0.46
37:X:82:ARG:HD3	37:X:126:PHE:HE1	1.81	0.46
50:t:62:TYR:HB3	50:t:87:TRP:HB2	1.98	0.46
57:Ak:30:GLY:C	57:Ak:65:MET:HE2	2.40	0.46
57:Ak:104:LEU:HB2	57:Ak:156:SER:HB2	1.98	0.46
57:Ak:132:LEU:HA	58:Al:159:VAL:HG22	1.98	0.46
74:Ak:601:HEA:H122	74:Ak:601:HEA:CHC	2.40	0.46
65:G:223:ILE:HG23	65:G:232:THR:HA	1.97	0.46
3:4:269:ARG:HA	3:4:278:ASN:CG	2.40	0.46
5:6:83:LEU:HD11	5:6:209:VAL:HG22	1.98	0.46
17:h:105:ARG:HH12	49:s:91:LYS:HA	1.81	0.46
19:j:18:VAL:HG23	26:r:222:MET:HE1	1.98	0.46
26:r:236:ALA:HB1	26:r:259:PHE:HZ	1.80	0.46
27:B:256:ARG:HA	30:E:249:LEU:HD11	1.97	0.46
32:H:198:GLU:HB3	35:K:109:ILE:HG12	1.98	0.46
45:W:133:ILE:O	45:W:137:THR:HG22	2.15	0.46
37:X:110:LEU:HB3	37:X:114:ASP:CB	2.45	0.46
48:l:213:LEU:HB3	48:l:273:VAL:HG11	1.98	0.46
57:Ak:424:THR:HG21	74:Ak:601:HEA:CMB	2.45	0.46
64:Ar:21:PHE:CE1	64:Ar:28:ARG:HB3	2.51	0.46
51:5:465:LEU:HD12	51:5:466:PRO:HD2	1.97	0.46
1:0:30:LEU:HB2	7:x:265:SER:OG	2.16	0.46
1:0:64:GLU:HB2	52:z:78:TYR:CE1	2.51	0.46
3:2:111:ASP:OD1	3:2:111:ASP:N	2.41	0.46
5:6:111:SER:HB3	3:Ae:59:LEU:HG	1.97	0.46
5:6:257:GLU:HA	5:6:438:MET:O	2.16	0.46
11:b:72:VAL:HA	11:b:76:LEU:HB2	1.98	0.46
12:c:143:MET:HB3	48:l:407:TRP:CD2	2.51	0.46
12:c:155:PRO:HD3	50:t:4:HIS:CG	2.51	0.46
18:i:340:THR:N	18:i:341:PRO:HD2	2.31	0.46
24:p:60:ARG:HG2	37:X:132:ASP:CB	2.36	0.46
26:r:165:LEU:HD23	26:r:241:LEU:HA	1.97	0.46
26:r:169:GLN:NE2	26:r:241:LEU:O	2.48	0.46
32:H:186:ASN:ND2	35:K:129:THR:HG23	2.30	0.46
34:J:154:LYS:NZ	65:G:279:GLU:OE1	2.43	0.46
39:Q:47:PHE:HB3	39:Q:57:ARG:CZ	2.46	0.46
39:Q:107:LEU:HD12	39:Q:107:LEU:HA	1.83	0.46
48:l:372:ALA:HA	48:l:458:LEU:HD21	1.98	0.46
48:l:417:SER:HB3	48:l:493:VAL:CG1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:26:PRO:HG2	50:t:29:TYR:HB2	1.98	0.46
51:u:92:PHE:O	51:u:96:LEU:HG	2.16	0.46
58:Al:188:ARG:HH12	60:An:153:ILE:HG13	1.81	0.46
60:An:137:TRP:HE1	60:An:141:GLN:HE21	1.64	0.46
62:Ap:108:GLY:O	62:Ap:121:LYS:NZ	2.47	0.46
51:5:284:LEU:HB3	51:5:359:VAL:HG12	1.98	0.46
65:G:405:THR:HB	65:G:477:GLY:HA3	1.97	0.46
65:G:522:GLN:O	65:G:526:LEU:HG	2.16	0.46
65:G:618:GLU:O	65:G:622:ILE:HG13	2.16	0.46
1:0:41:GLU:HA	1:0:44:ILE:HG22	1.97	0.45
4:3:14:ALA:O	4:3:18:ILE:HG12	2.16	0.45
13:d:99:ASP:HA	13:d:102:ILE:CD1	2.46	0.45
16:g:3:MET:HB3	16:g:4:MET:H	1.54	0.45
18:i:20:VAL:HG13	18:i:29:ILE:HG23	1.98	0.45
18:i:291:TYR:HA	25:q:151:PHE:HZ	1.81	0.45
27:B:29:LYS:HE3	27:B:32:PHE:CE1	2.51	0.45
34:J:64:LEU:HD22	39:Q:111:LYS:NZ	2.31	0.45
35:K:5:GLN:HA	35:K:8:ARG:HB2	1.99	0.45
48:l:83:ASP:O	48:l:84:TYR:C	2.60	0.45
48:l:278:LEU:HD21	48:l:404:THR:HG23	1.98	0.45
5:v:190:LEU:HD13	3:Af:62:THR:HB	1.98	0.45
6:w:300:ILE:HD12	6:w:303:LEU:HD13	1.97	0.45
5:6:256:GLY:O	5:6:437:SER:HA	2.17	0.45
6:7:183:PHE:CE2	69:7:401:HEM:HBC1	2.50	0.45
12:c:161:TYR:CB	12:c:166:LEU:HB2	2.47	0.45
17:h:65:GLU:O	17:h:69:ARG:N	2.44	0.45
25:q:196:TRP:HZ3	25:q:261:PHE:CE2	2.34	0.45
28:C:137:GLN:O	28:C:140:PRO:HD2	2.17	0.45
34:J:105:GLU:HA	65:G:611:THR:OG1	2.16	0.45
35:K:14:VAL:HA	35:K:23:TYR:CD1	2.51	0.45
43:U:170:VAL:HG13	43:U:242:ALA:HB3	1.97	0.45
51:u:120:LEU:HD13	51:u:133:ILE:HG12	1.98	0.45
51:u:123:TYR:OH	51:u:411:GLU:OE1	2.26	0.45
5:v:58:ALA:HB1	5:v:124:GLU:OE2	2.16	0.45
6:w:307:LEU:HD11	6:w:363:LEU:HD23	1.98	0.45
57:Ak:62:ALA:HB2	74:Ak:601:HEA:CB	2.40	0.45
58:Al:44:LEU:HA	58:Al:47:THR:HG22	1.97	0.45
59:Am:79:LEU:HB3	59:Am:233:PHE:CE2	2.51	0.45
62:Ap:94:GLU:H	62:Ap:97:ASN:ND2	2.14	0.45
51:5:407:THR:HB	51:5:408:PRO:HD3	1.97	0.45
65:G:671:LEU:HD13	65:G:671:LEU:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:173:ILE:HD12	3:4:190:TRP:HB2	1.97	0.45
11:b:73:THR:HA	11:b:77:ILE:HD12	1.98	0.45
18:i:106:LEU:HG	18:i:138:PRO:HB2	1.99	0.45
26:r:35:LYS:N	32:H:83:THR:HG21	2.31	0.45
28:C:352:GLN:O	28:C:356:LYS:HG2	2.16	0.45
29:D:83:GLU:OE1	29:D:142:ARG:NH2	2.30	0.45
29:D:190:ASP:OD1	39:Q:128:HIS:NE2	2.42	0.45
30:E:196:LEU:HD13	30:E:201:ILE:HG12	1.98	0.45
37:X:85:TYR:OH	47:Z:33:PRO:HG2	2.15	0.45
46:Y:70:LEU:HD13	46:Y:70:LEU:HA	1.81	0.45
49:s:249:MET:HE3	49:s:249:MET:HB3	1.75	0.45
51:u:148:ALA:O	51:u:152:GLN:HG3	2.16	0.45
5:v:222:GLY:HA3	5:v:230:LEU:HD21	1.98	0.45
52:z:19:LEU:HD23	52:z:24:GLN:HB3	1.98	0.45
67:M:55:CYS:SG	67:M:56:THR:HG23	2.55	0.45
6:7:272:TRP:HA	6:7:275:LEU:HG	1.97	0.45
16:g:16:LEU:HD13	16:g:16:LEU:HA	1.80	0.45
28:C:460:GLN:HB3	28:C:462:ILE:HD13	1.98	0.45
33:I:75:GLU:HG3	33:I:167:PRO:HB2	1.98	0.45
38:P:79:LEU:HD23	38:P:82:PHE:HD2	1.81	0.45
38:P:83:SER:OG	38:P:85:ASP:OD1	2.33	0.45
47:Z:72:GLY:O	48:l:364:LYS:NZ	2.49	0.45
48:l:15:LEU:O	48:l:18:PRO:HD2	2.17	0.45
48:l:251:THR:O	48:l:254:VAL:HG22	2.17	0.45
51:u:74:TRP:CZ2	51:u:411:GLU:HA	2.52	0.45
5:v:89:LEU:HD22	5:v:150:GLU:HB3	1.99	0.45
7:x:136:LEU:H	7:x:136:LEU:HD12	1.81	0.45
55:Ai:77:TRP:HA	60:An:140:LYS:HD2	1.97	0.45
3:Af:56:HIS:C	3:Af:58:ALA:H	2.25	0.45
3:4:107:PRO:HB2	7:8:319:LYS:HD2	1.99	0.45
6:7:45:ILE:HA	69:7:401:HEM:HMC2	1.98	0.45
7:8:132:ALA:HA	7:8:175:TYR:HA	1.98	0.45
13:d:139:PHE:CD2	23:o:127:ILE:HG22	2.50	0.45
14:e:62:GLU:O	14:e:63:ASP:C	2.60	0.45
14:e:73:SER:O	14:e:74:HIS:HB2	2.16	0.45
20:k:34:GLU:OE2	21:m:68:PHE:CZ	2.68	0.45
24:p:221:MET:SD	24:p:221:MET:N	2.90	0.45
25:q:209:LEU:O	25:q:210:TYR:C	2.60	0.45
27:B:29:LYS:HE3	27:B:32:PHE:HE1	1.82	0.45
27:B:120:GLY:HA3	27:B:204:TYR:HD1	1.82	0.45
29:D:101:ARG:NH1	29:D:159:VAL:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:228:GLN:HB2	34:J:114:TRP:CE3	2.52	0.45
39:Q:78:LEU:HD11	39:Q:129:ILE:HG21	1.99	0.45
48:l:62:ILE:HG12	48:l:199:GLN:HE22	1.80	0.45
5:v:333:SER:OG	5:v:334:GLY:N	2.49	0.45
52:z:49:VAL:O	52:z:52:PRO:HD2	2.17	0.45
53:Ag:37:THR:O	53:Ag:41:ILE:HG13	2.16	0.45
58:Al:91:ASN:OD1	58:Al:91:ASN:N	2.49	0.45
65:G:158:ARG:HG2	65:G:202:ASN:HD21	1.82	0.45
3:2:122:LYS:HE2	3:2:122:LYS:HB3	1.83	0.45
6:7:41:LEU:HD12	69:7:401:HEM:HBB1	1.99	0.45
17:h:77:SER:O	17:h:81:ARG:HG2	2.17	0.45
18:i:89:MET:HB2	18:i:95:MET:HG2	1.99	0.45
22:n:38:PHE:O	22:n:39:ARG:C	2.59	0.45
24:p:135:ARG:HA	48:l:161:ARG:HG3	1.99	0.45
25:q:122:PHE:HE1	25:q:238:LEU:HB3	1.81	0.45
27:B:41:ILE:HG23	27:B:261:TRP:HH2	1.80	0.45
27:B:116:ASN:ND2	27:B:212:LEU:HD12	2.32	0.45
28:C:190:ILE:HG21	28:C:213:ARG:HG3	1.99	0.45
32:H:158:CYS:N	72:H:301:SF4:S2	2.90	0.45
45:W:68:ARG:HG2	45:W:72:MET:SD	2.57	0.45
51:u:302:VAL:HB	51:u:303:PRO:HD3	1.98	0.45
51:u:310:ILE:HD11	51:u:388:VAL:HA	1.99	0.45
51:u:470:ARG:HD3	6:w:222:PRO:HD3	1.98	0.45
55:Ai:33:PHE:HA	55:Ai:36:LYS:HE2	1.98	0.45
57:Ak:509:THR:HG23	62:Ap:88:ILE:HG22	1.98	0.45
51:5:74:TRP:CZ2	51:5:411:GLU:HA	2.52	0.45
51:5:94:GLU:OE1	51:5:124:SER:OG	2.33	0.45
65:G:370:GLU:OE1	65:G:478:SER:OG	2.35	0.45
65:G:647:GLU:O	65:G:651:PRO:HG3	2.16	0.45
3:Ae:72:ARG:O	3:Ae:72:ARG:HD3	2.15	0.45
6:7:47:THR:HG23	6:7:79:ILE:HG23	1.99	0.45
8:9:29:LYS:HD3	8:9:75:ILE:HD13	1.98	0.45
11:b:75:VAL:O	11:b:79:VAL:HG23	2.17	0.45
11:b:109:THR:HB	11:b:112:GLU:HB3	1.98	0.45
15:f:29:PHE:CE1	43:U:349:VAL:HG11	2.51	0.45
18:i:344:SER:HA	18:i:347:ASN:HB2	1.99	0.45
20:k:30:LEU:HB3	21:m:68:PHE:CE2	2.52	0.45
20:k:75:LEU:HD11	21:m:68:PHE:CD1	2.52	0.45
21:m:117:PHE:HB2	21:m:119:PHE:CZ	2.52	0.45
27:B:367:ILE:HG13	27:B:438:LEU:HB2	1.98	0.45
33:I:47:VAL:HG13	33:I:190:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:55:ASN:O	33:I:59:ARG:HG2	2.17	0.45
39:Q:77:GLN:HE21	66:L:358:THR:HB	1.81	0.45
42:T:135:PRO:HB2	45:W:69:ILE:HD11	1.99	0.45
37:X:91:ASP:HB2	47:Z:63:ARG:HD3	1.99	0.45
47:Z:30:MET:HG3	47:Z:32:LEU:HG	1.99	0.45
48:l:503:GLU:CB	54:Ah:54:ARG:HG2	2.47	0.45
58:Al:27:THR:HG23	58:Al:76:ILE:HD12	1.98	0.45
58:Al:41:ILE:O	58:Al:45:MET:HG2	2.17	0.45
59:Am:54:MET:HB3	59:Am:58:TRP:CZ3	2.52	0.45
51:5:316:SER:N	51:5:339:GLN:O	2.49	0.45
66:L:79:TYR:CE1	66:L:102:GLU:HG3	2.52	0.45
10:a:161:ARG:HH12	44:V:139:PRO:HB3	1.81	0.45
18:i:1:MET:N	43:U:291:ARG:HH21	2.14	0.45
18:i:171:ASN:O	28:C:57:VAL:HG22	2.17	0.45
18:i:250:SER:O	18:i:259:GLY:HA3	2.16	0.45
19:j:56:PHE:CD2	20:k:79:VAL:HG21	2.49	0.45
19:j:108:GLN:HB2	21:m:169:MET:HE1	1.98	0.45
27:B:214:GLU:CD	27:B:224:ARG:HE	2.25	0.45
28:C:72:TRP:HD1	43:U:195:VAL:HG21	1.82	0.45
28:C:210:PHE:HA	28:C:213:ARG:HB2	1.98	0.45
51:u:140:LEU:HD22	51:u:237:VAL:HG12	1.99	0.45
51:u:192:PHE:O	51:u:198:ALA:HB2	2.16	0.45
6:w:207:ASN:ND2	6:w:211:ILE:O	2.47	0.45
58:Al:128:LEU:HD11	58:Al:134:ARG:HA	1.99	0.45
59:Am:34:TRP:CD1	59:Am:40:MET:HG3	2.52	0.45
62:Ap:119:HIS:H	62:Ap:119:HIS:CD2	2.35	0.45
18:i:79:LEU:HD21	20:k:1:MET:SD	2.57	0.45
22:n:39:ARG:HD3	22:n:55:VAL:HB	1.99	0.45
23:o:56:ARG:HD2	23:o:60:ILE:HG12	1.98	0.45
25:q:257:MET:O	25:q:260:PRO:HD2	2.17	0.45
26:r:58:LYS:HB3	26:r:217:ALA:HB2	1.99	0.45
26:r:113:VAL:CG1	26:r:139:THR:HG21	2.46	0.45
28:C:290:LEU:HD22	29:D:110:SER:HB3	1.99	0.45
29:D:128:ILE:HB	29:D:145:THR:HG23	1.98	0.45
32:H:102:ALA:HB1	32:H:194:GLY:HA2	1.98	0.45
39:Q:149:TYR:OH	65:G:629:ILE:HD11	2.17	0.45
40:R:110:HIS:CD2	65:G:441:ARG:NH1	2.85	0.45
41:S:66:LEU:HD11	49:s:159:PHE:CE2	2.51	0.45
44:V:99:LEU:HD13	44:V:99:LEU:HA	1.79	0.45
5:v:151:VAL:O	5:v:155:GLN:HG3	2.17	0.45
6:w:145:VAL:O	6:w:149:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:x:220:CYS:SG	7:x:221:GLU:N	2.90	0.45
57:Ak:440:TYR:CZ	58:Al:205:SER:HA	2.52	0.45
64:Ar:9:ILE:HD13	64:Ar:55:GLU:HB3	1.98	0.45
51:5:206:GLU:O	51:5:210:LYS:HG2	2.17	0.45
51:5:467:ASP:OD2	51:5:470:ARG:HG2	2.17	0.45
3:2:285:GLU:OE2	3:2:287:THR:HG23	2.17	0.45
5:6:310:TYR:CE1	3:Ae:71:LYS:HD2	2.52	0.45
12:c:89:TRP:CD2	37:X:131:PRO:HB3	2.52	0.45
14:e:116:GLU:O	14:e:120:ARG:HD3	2.17	0.45
15:f:37:GLY:O	43:U:357:LYS:HG3	2.17	0.45
18:i:193:VAL:HG13	18:i:266:ILE:HG23	1.99	0.45
19:j:93:PHE:O	19:j:96:ILE:HG13	2.17	0.45
24:p:134:GLU:HB2	48:l:161:ARG:HA	1.99	0.45
25:q:412:ILE:HG13	25:q:416:ARG:HD2	1.98	0.45
27:B:196:PHE:HA	40:R:97:ARG:HH21	1.81	0.45
37:O:88:LYS:HG2	37:O:95:PRO:HB3	1.98	0.45
38:P:38:GLU:HA	65:G:667:GLN:HE21	1.82	0.45
38:P:65:LEU:HB3	38:P:77:VAL:HG22	1.98	0.45
44:V:78:ALA:HB1	44:V:84:PRO:HA	1.99	0.45
48:l:323:HIS:CD2	48:l:475:MET:HB3	2.51	0.45
50:t:62:TYR:CD2	50:t:90:CYS:HB2	2.51	0.45
61:Ao:122:LYS:HD2	61:Ao:122:LYS:HA	1.75	0.45
62:Ap:68:LYS:HE2	62:Ap:68:LYS:HB3	1.79	0.45
66:L:51:ALA:HA	66:L:120:VAL:O	2.17	0.45
3:2:269:ARG:HA	3:2:278:ASN:CG	2.41	0.44
6:7:30:TRP:HB3	6:7:100:ARG:HG3	1.99	0.44
10:a:98:LEU:H	10:a:98:LEU:HD12	1.81	0.44
10:a:186:THR:OG1	10:a:189:ASN:ND2	2.50	0.44
12:c:82:SER:HB2	12:c:119:THR:N	2.32	0.44
15:f:63:LYS:O	15:f:66:VAL:HG12	2.17	0.44
18:i:71:MET:HE3	18:i:74:ILE:HB	1.98	0.44
37:O:90:TYR:CE2	37:O:92:LYS:HB2	2.52	0.44
37:O:94:ASP:OD2	37:O:97:LYS:HG2	2.17	0.44
48:l:200:GLN:HE21	48:l:204:LEU:HD11	1.81	0.44
48:l:206:ASN:O	48:l:269:THR:HG21	2.17	0.44
48:l:314:MET:HE3	48:l:314:MET:HB3	1.83	0.44
48:l:363:TYR:HA	48:l:370:THR:HG21	1.98	0.44
6:w:107:TYR:OH	6:w:308:HIS:ND1	2.38	0.44
54:Ah:25:ARG:HD3	59:Am:224:LYS:HB3	1.99	0.44
57:Ak:12:HIS:CD2	57:Ak:91:ASP:HA	2.53	0.44
57:Ak:258:VAL:HA	57:Ak:338:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Ak:357:VAL:HG13	57:Ak:363:LEU:HD13	1.99	0.44
3:2:240:HIS:HB3	68:2:301:FES:S1	2.57	0.44
7:8:296:MET:HG2	2:Ac:36:PHE:CZ	2.51	0.44
12:c:154:GLN:O	12:c:156:VAL:N	2.50	0.44
12:c:155:PRO:HD3	50:t:4:HIS:ND1	2.32	0.44
18:i:4:ILE:HD13	43:U:46:VAL:HG22	1.98	0.44
27:B:319:PRO:HB2	27:B:342:LEU:HD13	1.98	0.44
29:D:94:ILE:HD11	29:D:155:SER:O	2.17	0.44
31:F:59:GLN:HG2	35:K:122:GLN:HA	1.99	0.44
41:S:63:THR:HG23	49:s:98:SER:CB	2.45	0.44
45:W:109:SER:O	49:s:79:PRO:CD	2.65	0.44
37:X:143:GLU:HA	37:X:146:ASP:OD2	2.18	0.44
49:s:189:LEU:O	49:s:193:GLY:HA2	2.17	0.44
4:Ad:14:ALA:O	4:Ad:18:ILE:HG12	2.16	0.44
58:Al:153:LEU:HD11	64:Ar:64:LEU:HD23	1.98	0.44
51:5:85:LYS:C	51:5:207:ASN:HD21	2.26	0.44
66:L:132:LYS:HG2	66:L:133:ASN:N	2.31	0.44
1:0:90:LEU:HD23	1:0:90:LEU:HA	1.76	0.44
3:4:174:GLU:OE1	3:4:293:ILE:HG13	2.17	0.44
5:6:101:ARG:HB3	8:y:108:TRP:CZ2	2.53	0.44
7:8:168:ARG:HH12	7:8:171:LYS:HG2	1.82	0.44
13:d:103:VAL:HG13	13:d:132:PHE:HE1	1.81	0.44
21:m:99:MET:O	21:m:103:MET:HG2	2.17	0.44
25:q:154:LEU:O	25:q:158:LEU:HG	2.18	0.44
43:U:62:ILE:HG12	43:U:205:VAL:HB	1.98	0.44
45:W:88:ARG:HH21	49:s:84:LEU:HB2	1.82	0.44
37:X:96:GLU:H	37:X:96:GLU:CD	2.25	0.44
37:X:117:GLU:HB3	47:Z:61:TRP:NE1	2.31	0.44
47:Z:84:LEU:O	47:Z:85:LYS:C	2.60	0.44
51:u:141:PRO:O	51:u:145:GLU:HG3	2.17	0.44
5:v:322:ASP:C	3:Af:68:LEU:HD21	2.42	0.44
5:v:415:GLN:O	5:v:419:VAL:HG23	2.17	0.44
62:Ap:84:THR:OG1	62:Ap:85:ASN:N	2.47	0.44
65:G:252:ASP:OD1	65:G:259:SER:N	2.50	0.44
66:L:223:LEU:O	66:L:224:ILE:C	2.60	0.44
5:6:157:GLN:NE2	51:5:317:THR:HA	2.32	0.44
5:6:277:ALA:O	5:6:283:ALA:HB2	2.18	0.44
12:c:96:ASP:N	12:c:96:ASP:OD1	2.50	0.44
13:d:8:ASP:HB3	14:e:127:LYS:NZ	2.31	0.44
21:m:3:MET:HA	45:W:134:LEU:HD21	1.99	0.44
28:C:204:THR:HB	28:C:205:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:232:TYR:OH	28:C:240:GLN:O	2.27	0.44
28:C:247:LEU:HD22	28:C:354:LEU:CD2	2.47	0.44
42:T:138:TYR:CE2	49:s:121:MET:HG3	2.52	0.44
45:W:95:ALA:HA	45:W:106:VAL:HG11	2.00	0.44
37:X:105:MET:HA	37:X:110:LEU:O	2.17	0.44
48:l:529:TYR:N	48:l:530:PRO:HD2	2.33	0.44
65:G:471:LYS:HG3	65:G:510:TRP:CD2	2.53	0.44
11:b:70:PHE:O	11:b:74:HIS:HB2	2.18	0.44
11:b:83:HIS:CE1	11:b:87:LYS:HD2	2.53	0.44
12:c:136:PHE:CE2	48:l:283:ILE:HD11	2.53	0.44
18:i:5:ILE:HD11	19:j:104:TYR:OH	2.18	0.44
25:q:374:ASN:HD22	25:q:374:ASN:H	1.66	0.44
27:B:119:GLU:OE2	27:B:127:ASP:N	2.49	0.44
37:O:126:PHE:CD2	37:O:148:ILE:HG21	2.52	0.44
46:Y:43:ARG:HD2	46:Y:47:PHE:O	2.18	0.44
46:Y:45:ARG:NH1	47:Z:64:ASN:HD21	2.12	0.44
48:l:486:MET:HA	48:l:489:THR:OG1	2.18	0.44
50:t:6:ALA:O	50:t:11:GLY:N	2.47	0.44
50:t:45:GLU:HA	50:t:48:ASP:HB2	1.99	0.44
6:w:280:ILE:O	6:w:283:SER:OG	2.35	0.44
6:w:326:TRP:CD1	52:z:48:ARG:O	2.71	0.44
57:Ak:333:LYS:HE2	57:Ak:333:LYS:HB2	1.64	0.44
58:Al:23:PHE:CZ	58:Al:80:SER:HB2	2.53	0.44
51:5:87:ASN:HD21	51:5:199:GLN:HB3	1.83	0.44
65:G:217:GLU:OE1	65:G:408:ARG:HG2	2.17	0.44
66:L:67:HIS:HA	66:L:70:ARG:HG2	1.99	0.44
9:A:71:SER:HB2	58:Al:222:TRP:CD1	2.53	0.44
19:j:75:LEU:HD13	26:r:305:ILE:HD11	2.00	0.44
25:q:1:MET:HG2	25:q:52:PHE:CD2	2.53	0.44
27:B:451:GLN:O	27:B:455:LEU:HG	2.17	0.44
33:I:71:CYS:SG	72:I:201:SF4:S4	3.16	0.44
35:K:32:ASP:OD2	35:K:34:ARG:HG3	2.17	0.44
35:K:95:ASP:OD1	67:M:35:THR:N	2.42	0.44
37:O:100:VAL:HG12	37:O:142:GLN:HB2	1.99	0.44
37:O:126:PHE:HB3	37:O:152:LYS:NZ	2.33	0.44
39:Q:148:PHE:HZ	65:G:622:ILE:HG12	1.82	0.44
48:l:62:ILE:HD11	48:l:81:LYS:HG3	1.99	0.44
6:w:36:LEU:HD22	6:w:235:MET:HE3	1.99	0.44
53:Ag:38:GLU:HG2	56:Aj:35:TRP:CZ2	2.52	0.44
56:Aj:29:PHE:HB2	56:Aj:40:MET:HE1	1.98	0.44
57:Ak:362:SER:HB2	58:Al:20:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Am:58:TRP:HD1	59:Am:61:ILE:HD12	1.82	0.44
65:G:218:LEU:HB3	65:G:221:ASN:ND2	2.32	0.44
1:0:91:LYS:HD3	7:x:260:THR:HG23	1.99	0.44
5:6:313:VAL:HG21	5:6:323:VAL:HG11	2.00	0.44
8:9:99:ILE:HG12	8:9:102:ARG:HH12	1.83	0.44
12:c:36:MET:HB3	23:o:67:ARG:HE	1.83	0.44
12:c:37:PHE:HB3	23:o:70:TYR:CD2	2.53	0.44
12:c:155:PRO:HB3	50:t:4:HIS:HB3	2.00	0.44
25:q:119:TYR:CE2	25:q:161:LEU:HB2	2.53	0.44
25:q:208:PRO:HD3	25:q:236:LEU:HD22	1.99	0.44
27:B:71:LYS:HG2	27:B:75:TRP:CE3	2.53	0.44
28:C:291:ASN:O	29:D:162:ALA:HB2	2.18	0.44
28:C:300:ARG:NH2	28:C:407:GLU:OE2	2.45	0.44
29:D:105:ASN:HB3	67:M:96:THR:HG22	1.99	0.44
30:E:193:TYR:OH	30:E:214:PRO:HG2	2.18	0.44
41:S:64:LYS:HD3	41:S:68:ASN:CG	2.42	0.44
45:W:28:ARG:HD2	67:M:17:GLY:HA3	1.99	0.44
5:v:123:VAL:HG13	5:v:137:LEU:HD13	1.99	0.44
5:v:233:VAL:HG23	5:v:236:ARG:NH2	2.32	0.44
5:v:264:ASP:OD1	5:v:265:SER:N	2.50	0.44
6:w:244:LEU:O	7:x:286:ARG:HG2	2.17	0.44
55:Ai:48:PHE:O	55:Ai:52:VAL:HG22	2.17	0.44
55:Ai:66:LEU:HA	58:Al:5:PHE:HE2	1.83	0.44
64:Ar:6:GLN:O	64:Ar:10:LYS:HG2	2.18	0.44
51:5:207:ASN:O	51:5:211:LEU:HG	2.18	0.44
65:G:39:GLN:HE22	65:G:56:VAL:HG12	1.83	0.44
65:G:574:ASP:OD2	65:G:702:ARG:HD2	2.17	0.44
65:G:575:VAL:O	65:G:578:PRO:HD2	2.18	0.44
66:L:172:PRO:HD2	66:L:319:MET:HE2	2.00	0.44
1:0:75:LEU:O	1:0:79:ASP:HB2	2.17	0.44
3:4:185:ASN:HD22	3:4:198:ARG:HB2	1.82	0.44
18:i:115:VAL:HB	18:i:116:PRO:HD3	1.99	0.44
19:j:59:ALA:CA	26:r:140:ILE:HD13	2.44	0.44
23:o:75:ASN:C	23:o:78:PRO:HD2	2.43	0.44
23:o:94:GLY:O	23:o:98:LEU:HG	2.18	0.44
24:p:135:ARG:HA	48:l:161:ARG:CG	2.47	0.44
25:q:405:LEU:HD11	48:l:173:LEU:HD13	1.98	0.44
28:C:115:CYS:SG	28:C:442:ASP:HA	2.58	0.44
29:D:152:PRO:HB3	29:D:177:PHE:HD2	1.83	0.44
39:Q:124:LYS:HB3	39:Q:128:HIS:HB2	2.00	0.44
48:l:79:SER:OG	48:l:135:ASN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:315:VAL:HG11	48:l:412:THR:HG21	1.98	0.44
51:u:350:GLU:OE1	51:u:350:GLU:N	2.44	0.44
6:w:207:ASN:HD22	6:w:213:SER:HB3	1.82	0.44
52:z:35:ILE:HB	52:z:36:PRO:HD3	1.99	0.44
53:Ag:58:LEU:HA	53:Ag:61:LEU:HG	2.00	0.44
58:Al:73:LEU:HD13	58:Al:73:LEU:HA	1.77	0.44
66:L:233:GLN:HG3	66:L:264:ASN:O	2.18	0.44
5:6:195:TYR:CE2	5:6:196:ARG:HG2	2.53	0.44
11:b:80:TRP:HE1	13:d:41:VAL:HA	1.83	0.44
13:d:107:GLN:OE1	48:l:194:ASN:ND2	2.51	0.44
18:i:154:MET:SD	18:i:191:THR:HB	2.58	0.44
20:k:32:CYS:O	20:k:36:MET:HG3	2.18	0.44
25:q:199:CYS:HB3	25:q:246:ILE:HG12	2.00	0.44
25:q:337:VAL:HG12	25:q:423:ILE:HG21	2.00	0.44
26:r:11:ILE:HB	26:r:12:PRO:HD3	1.98	0.44
27:B:174:ARG:CA	40:R:93:LEU:HD21	2.43	0.44
27:B:194:ASP:OD2	40:R:98:MET:N	2.51	0.44
36:N:19:THR:OG1	36:N:19:THR:O	2.33	0.44
43:U:172:LEU:HD22	43:U:189:TYR:CD1	2.53	0.44
45:W:81:ARG:NH2	49:s:141:ASN:HD22	2.16	0.44
48:l:124:PHE:HZ	48:l:251:THR:HG1	1.64	0.44
48:l:273:VAL:O	48:l:277:THR:HG23	2.18	0.44
5:v:348:GLY:HA2	5:v:448:PRO:HD3	2.00	0.44
57:Ak:28:MET:N	57:Ak:28:MET:SD	2.90	0.44
57:Ak:334:TRP:O	57:Ak:411:LYS:NZ	2.39	0.44
58:Al:104:TRP:CD1	58:Al:203:ASN:HB2	2.53	0.44
59:Am:140:SER:HB2	59:Am:242:TRP:HE1	1.83	0.44
51:5:422:ARG:HH22	51:5:428:GLU:CD	2.25	0.44
66:L:122:ILE:HD11	66:L:248:ILE:HD11	2.00	0.44
1:0:90:LEU:HD11	7:x:265:SER:HB3	1.99	0.43
6:7:280:ILE:O	6:7:283:SER:OG	2.31	0.43
10:a:75:ILE:O	10:a:75:ILE:CG2	2.65	0.43
11:b:102:PRO:HB2	13:d:18:PRO:HD3	2.00	0.43
13:d:80:LYS:O	25:q:182:TRP:HZ2	2.01	0.43
14:e:108:TYR:O	14:e:109:LEU:C	2.61	0.43
16:g:15:PHE:O	16:g:80:ARG:HD2	2.18	0.43
20:k:22:TYR:HE1	48:l:588:PHE:CG	2.36	0.43
25:q:196:TRP:CD1	25:q:250:LEU:HB3	2.52	0.43
26:r:281:ARG:NH1	28:C:452:ASP:OD1	2.51	0.43
30:E:203:GLU:O	30:E:207:GLU:HG3	2.18	0.43
33:I:118:ARG:HA	33:I:118:ARG:HD2	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:O:104:PHE:HE2	37:O:144:ILE:HD11	1.82	0.43
37:O:115:GLN:O	37:O:119:ILE:HG12	2.18	0.43
42:T:143:ARG:HH22	49:s:212:ARG:HG3	1.83	0.43
44:V:72:LEU:HD23	44:V:72:LEU:HA	1.82	0.43
37:X:119:ILE:HG13	37:X:135:ALA:O	2.17	0.43
46:Y:61:PHE:CZ	48:l:455:LYS:HG2	2.53	0.43
48:l:116:ARG:HB3	48:l:157:TRP:HH2	1.83	0.43
48:l:366:MET:HA	48:l:445:GLU:OE2	2.18	0.43
51:5:350:GLU:OE1	51:5:350:GLU:N	2.50	0.43
65:G:182:CYS:HB2	65:G:195:LEU:HD13	2.00	0.43
3:Af:46:LEU:N	3:Af:66:PRO:HG3	2.32	0.43
10:a:161:ARG:HH12	44:V:139:PRO:CB	2.31	0.43
13:d:110:LEU:HD21	13:d:129:LEU:HA	2.00	0.43
16:g:24:PRO:CD	49:s:237:PRO:HG3	2.48	0.43
18:i:315:TRP:HZ3	43:U:329:VAL:HG12	1.84	0.43
18:i:340:THR:O	18:i:343:LEU:HB2	2.18	0.43
21:m:112:GLU:OE1	21:m:120:ASN:ND2	2.51	0.43
23:o:77:TYR:O	23:o:78:PRO:C	2.61	0.43
24:p:118:HIS:HB3	24:p:121:PRO:HB3	2.00	0.43
24:p:164:ARG:HH21	24:p:168:LYS:HD2	1.82	0.43
25:q:160:LEU:HD13	25:q:199:CYS:HA	1.99	0.43
26:r:61:LEU:HD21	33:I:125:PRO:CB	2.47	0.43
33:I:79:MET:O	33:I:79:MET:HG2	2.18	0.43
35:K:59:HIS:CD2	35:K:60:ARG:HG3	2.53	0.43
37:O:108:LEU:HD13	37:O:108:LEU:HA	1.78	0.43
39:Q:77:GLN:NE2	66:L:358:THR:HB	2.32	0.43
42:T:131:ASN:O	42:T:134:THR:OG1	2.36	0.43
48:l:503:GLU:HG3	54:Ah:54:ARG:NE	2.17	0.43
48:l:591:PHE:O	48:l:595:ILE:HG13	2.19	0.43
65:G:224:ASP:OD1	65:G:291:ARG:NH1	2.47	0.43
65:G:241:ARG:HG2	65:G:243:TRP:CH2	2.53	0.43
67:M:91:GLU:O	67:M:92:LYS:C	2.61	0.43
3:4:131:ARG:HD2	52:Aa:22:PHE:O	2.18	0.43
69:7:402:HEM:HBA1	69:7:402:HEM:CHA	2.48	0.43
10:a:150:ARG:HD2	25:q:172:GLY:O	2.18	0.43
15:f:68:GLU:HG2	16:g:21:ARG:HB3	1.99	0.43
18:i:248:LEU:HD11	18:i:296:LEU:HD22	2.00	0.43
20:k:41:PHE:CE2	20:k:60:PRO:HB2	2.54	0.43
23:o:37:LEU:HB2	24:p:50:ALA:HA	2.00	0.43
24:p:213:VAL:O	24:p:215:ARG:N	2.46	0.43
26:r:39:VAL:HG21	33:I:89:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:319:PRO:HG3	27:B:347:THR:HB	1.99	0.43
30:E:182:ASN:HB3	30:E:194:GLU:HB3	2.01	0.43
35:K:60:ARG:HH22	35:K:95:ASP:HA	1.82	0.43
37:O:141:PRO:O	37:O:145:VAL:HG23	2.18	0.43
47:Z:104:LEU:HD13	47:Z:104:LEU:HA	1.86	0.43
6:w:361:ILE:HG12	6:w:365:LEU:HD12	2.00	0.43
63:Aq:26:ARG:HG2	63:Aq:27:THR:N	2.33	0.43
51:5:338:CYS:HB3	51:5:368:MET:SD	2.59	0.43
65:G:371:VAL:H	65:G:482:GLN:CD	2.26	0.43
5:6:266:LEU:HD22	3:Ae:72:ARG:HH21	1.84	0.43
11:b:77:ILE:HA	11:b:80:TRP:CE3	2.52	0.43
15:f:40:ASP:HB3	15:f:43:LYS:HB3	2.01	0.43
16:g:50:ILE:HD12	18:i:327:PRO:HG3	2.01	0.43
25:q:325:MET:HE1	25:q:441:ILE:HG12	1.99	0.43
45:W:109:SER:O	49:s:79:PRO:HD2	2.18	0.43
6:w:97:HIS:HE1	69:w:401:HEM:NA	2.15	0.43
6:w:138:MET:CE	6:w:268:ILE:HA	2.48	0.43
6:w:311:LYS:HG3	6:w:379:TRP:HB3	2.01	0.43
7:x:120:GLN:OE1	7:x:254:LEU:HB2	2.19	0.43
57:Ak:452:THR:HG22	57:Ak:456:MET:HE3	1.99	0.43
58:Al:78:LEU:HB2	58:Al:79:PRO:HD3	2.00	0.43
1:0:85:LYS:HA	1:0:85:LYS:HD3	1.90	0.43
3:4:217:ARG:NH1	3:4:275:ALA:O	2.51	0.43
5:6:191:TYR:CE1	3:Ae:62:THR:HG21	2.54	0.43
9:A:35:TYR:HE2	58:Al:25:ASP:O	2.02	0.43
21:m:14:VAL:O	21:m:18:VAL:HG23	2.19	0.43
21:m:159:TRP:CZ2	21:m:163:ILE:HD11	2.53	0.43
44:V:91:PHE:HB2	44:V:123:ALA:HB2	2.00	0.43
37:X:87:LEU:O	37:X:90:TYR:HB3	2.18	0.43
6:w:224:TYR:CE1	7:x:312:TRP:HH2	2.37	0.43
52:Aa:20:SER:O	52:Aa:24:GLN:HG2	2.17	0.43
57:Ak:291:HIS:HA	74:Ak:602:HEA:HAA1	2.01	0.43
59:Am:118:PRO:HG2	59:Am:121:ILE:HG13	2.00	0.43
67:M:5:THR:H	67:M:8:ILE:HD12	1.82	0.43
4:3:15:ARG:HD3	4:3:15:ARG:N	2.34	0.43
3:4:151:LYS:HD2	4:Ad:34:TRP:CE2	2.54	0.43
10:a:59:PRO:HA	24:p:145:CYS:SG	2.59	0.43
12:c:97:LEU:HD11	25:q:346:ARG:HD3	2.00	0.43
13:d:159:GLN:HA	13:d:162:ARG:NE	2.34	0.43
16:g:51:ARG:HD3	18:i:322:GLN:HG3	2.00	0.43
16:g:74:GLY:O	16:g:78:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:64:MET:HE3	21:m:64:MET:HB2	1.84	0.43
25:q:96:ILE:O	25:q:100:ILE:HG13	2.19	0.43
26:r:5:ASN:HD21	41:S:23:THR:HA	1.83	0.43
27:B:35:LEU:HD21	27:B:40:ARG:HG2	2.00	0.43
27:B:154:ALA:HB2	27:B:193:PHE:CE2	2.53	0.43
28:C:90:PHE:HB2	28:C:105:MET:HE2	1.99	0.43
29:D:173:MET:O	29:D:196:HIS:HB3	2.18	0.43
33:I:79:MET:HE3	33:I:174:LEU:HD13	2.00	0.43
33:I:122:ASP:HA	33:I:128:ARG:HH12	1.83	0.43
45:W:112:HIS:HA	49:s:79:PRO:HG2	2.00	0.43
46:Y:61:PHE:CE2	48:l:455:LYS:HG2	2.53	0.43
49:s:150:GLN:HG2	49:s:153:ARG:HH21	1.83	0.43
50:t:94:ASP:O	50:t:97:LYS:HB3	2.18	0.43
51:u:341:PHE:HB2	51:u:358:PHE:HB3	2.00	0.43
74:Ak:601:HEA:H172	74:Ak:601:HEA:H261	1.86	0.43
62:Ap:78:ASN:HB2	62:Ap:120:TYR:CD1	2.53	0.43
5:6:391:GLY:HA2	5:6:394:ASP:OD2	2.19	0.43
6:7:207:ASN:ND2	6:7:211:ILE:O	2.49	0.43
6:7:237:LEU:HD13	7:8:297:MET:HG2	2.00	0.43
7:8:315:LEU:O	7:8:318:ARG:HG2	2.18	0.43
9:A:43:ARG:HH11	58:Al:21:LEU:HB3	1.83	0.43
14:e:87:MET:HE3	14:e:87:MET:HB3	1.80	0.43
18:i:4:ILE:CD1	43:U:46:VAL:HG22	2.48	0.43
21:m:18:VAL:HG12	21:m:93:PHE:HA	2.00	0.43
25:q:264:LEU:O	25:q:268:GLY:N	2.50	0.43
26:r:96:ILE:HD13	26:r:96:ILE:HA	1.79	0.43
26:r:228:TYR:HA	26:r:231:ILE:HD12	1.99	0.43
28:C:344:ARG:HB3	45:W:21:TYR:O	2.18	0.43
31:F:71:ILE:HD13	32:H:110:GLU:HB2	1.99	0.43
35:K:65:THR:O	35:K:73:THR:OG1	2.32	0.43
37:O:104:PHE:HA	37:O:108:LEU:CB	2.46	0.43
51:u:165:ARG:HD3	51:u:209:ARG:HA	2.01	0.43
51:u:467:ASP:OD1	51:u:468:TYR:N	2.52	0.43
5:v:412:VAL:O	5:v:416:ILE:HG12	2.19	0.43
6:w:223:TYR:HB3	7:x:312:TRP:CZ2	2.53	0.43
57:Ak:270:TYR:O	57:Ak:274:VAL:HG23	2.18	0.43
57:Ak:338:MET:O	57:Ak:342:LEU:HG	2.19	0.43
57:Ak:361:SER:O	57:Ak:365:ILE:HG12	2.19	0.43
57:Ak:424:THR:HG23	57:Ak:454:SER:O	2.19	0.43
58:Al:17:MET:HE1	58:Al:21:LEU:HD21	2.00	0.43
51:5:71:VAL:HG13	51:5:147:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:5:471:ILE:O	51:5:475:MET:HG2	2.19	0.43
66:L:79:TYR:CE2	66:L:100:PHE:HB3	2.54	0.43
5:6:60:ARG:HG2	5:6:393:LEU:HD22	2.01	0.43
5:6:293:LEU:HB3	5:6:309:LEU:HD22	2.00	0.43
10:a:152:LYS:HD3	16:g:96:VAL:HG21	2.01	0.43
17:h:3:PHE:HZ	18:i:24:SER:HB3	1.83	0.43
18:i:72:MET:HE3	20:k:12:PHE:CD2	2.54	0.43
18:i:306:PRO:HG2	43:U:315:TYR:CE1	2.54	0.43
25:q:214:LEU:HD11	48:l:558:LEU:HB3	2.00	0.43
27:B:63:TYR:CE2	30:E:245:VAL:HG21	2.54	0.43
28:C:247:LEU:HD22	28:C:354:LEU:HD23	2.00	0.43
29:D:145:THR:OG1	29:D:146:TYR:N	2.52	0.43
32:H:89:GLU:OE1	35:K:58:ARG:HG2	2.18	0.43
36:N:26:ILE:O	36:N:30:LYS:HG3	2.19	0.43
43:U:257:VAL:HG12	43:U:259:GLN:HG3	2.01	0.43
47:Z:55:ARG:NH2	54:Ah:36:ASP:HB3	2.31	0.43
48:l:65:ASN:ND2	48:l:65:ASN:H	2.16	0.43
48:l:285:THR:HG22	48:l:308:SER:O	2.18	0.43
51:u:38:TYR:CE2	51:u:430:GLU:HG3	2.54	0.43
6:w:337:TRP:O	6:w:341:GLN:HG2	2.18	0.43
57:Ak:144:ASP:OD1	57:Ak:213:ARG:NH1	2.50	0.43
57:Ak:508:PRO:HG2	62:Ap:63:ASN:HB2	2.00	0.43
60:An:136:GLU:O	60:An:140:LYS:HG2	2.18	0.43
61:Ao:49:GLU:HB2	61:Ao:53:GLU:CD	2.44	0.43
64:Ar:72:ALA:O	64:Ar:76:ARG:HD3	2.18	0.43
66:L:238:VAL:HG12	66:L:242:LYS:HZ2	1.84	0.43
7:8:126:HIS:HE1	7:8:196:PRO:HD2	1.82	0.43
7:8:314:VAL:HG23	52:Aa:21:PRO:HG3	2.01	0.43
10:a:111:GLU:HG3	10:a:119:ARG:NH2	2.34	0.43
10:a:133:TYR:HE1	13:d:90:MET:HG3	1.83	0.43
11:b:71:ALA:O	11:b:75:VAL:HB	2.19	0.43
12:c:98:ARG:HG3	12:c:114:ARG:HD2	1.99	0.43
18:i:26:TRP:CD2	18:i:86:ILE:HG13	2.54	0.43
23:o:53:ASP:HA	24:p:175:TRP:CZ2	2.53	0.43
26:r:313:SER:CB	45:W:51:MET:HA	2.49	0.43
28:C:72:TRP:CD1	28:C:72:TRP:H	2.36	0.43
28:C:191:MET:O	28:C:195:THR:OG1	2.32	0.43
33:I:109:LEU:HD11	33:I:114:ALA:HA	2.01	0.43
37:X:82:ARG:HD3	37:X:126:PHE:CE1	2.54	0.43
37:X:87:LEU:HD21	37:X:118:ILE:HG23	2.01	0.43
48:l:134:ALA:HA	48:l:139:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:245:ALA:HB2	48:l:340:PHE:HB3	1.99	0.43
49:s:160:THR:HA	49:s:163:TRP:NE1	2.34	0.43
51:u:373:GLN:HE22	51:u:471:ILE:HG23	1.82	0.43
52:Aa:19:LEU:HD22	51:5:273:SER:HB3	2.00	0.43
57:Ak:262:SER:HA	57:Ak:332:ILE:HD13	2.00	0.43
60:An:45:PRO:O	60:An:47:PRO:HD3	2.19	0.43
62:Ap:49:ARG:HA	62:Ap:52:MET:HG2	1.99	0.43
51:5:41:ALA:O	51:5:45:VAL:HG23	2.19	0.43
51:5:289:ILE:HG21	51:5:369:MET:HE1	2.01	0.43
2:l:33:GLU:OE1	4:3:34:TRP:NE1	2.52	0.43
9:A:63:MET:HE2	60:An:149:LYS:HB2	2.01	0.43
10:a:58:LYS:C	24:p:141:VAL:HG11	2.44	0.43
10:a:88:LEU:O	10:a:91:VAL:HG12	2.19	0.43
10:a:165:ASP:OD1	10:a:165:ASP:N	2.52	0.43
14:e:95:PHE:HD1	14:e:99:LEU:HD12	1.83	0.43
15:f:72:ARG:NH2	16:g:18:ASN:OD1	2.44	0.43
19:j:67:LEU:HD11	20:k:68:ALA:HB3	2.00	0.43
23:o:111:LYS:O	23:o:115:LEU:HG	2.18	0.43
25:q:369:LEU:HD13	48:l:149:ILE:HG13	2.01	0.43
27:B:51:TRP:HA	27:B:59:ARG:HH12	1.83	0.43
28:C:166:ASN:HB2	67:M:63:ALA:HB2	2.01	0.43
28:C:228:MET:SD	33:I:167:PRO:HG3	2.59	0.43
36:N:89:SER:OG	36:N:93:LYS:NZ	2.51	0.43
37:X:125:GLU:CG	48:l:439:PRO:HG2	2.42	0.43
48:l:9:LEU:HD13	48:l:9:LEU:HA	1.87	0.43
51:u:303:PRO:HG3	51:u:436:VAL:HG22	2.01	0.43
5:v:82:LEU:HD13	5:v:158:LEU:HD11	2.00	0.43
6:w:217:LYS:HG3	52:z:8:LEU:HD13	2.01	0.43
57:Ak:96:ARG:HG2	59:Am:57:TRP:CZ2	2.54	0.43
57:Ak:98:ASN:HB2	57:Ak:163:ASN:ND2	2.34	0.43
57:Ak:130:PRO:HD3	57:Ak:231:TYR:CD1	2.54	0.43
57:Ak:273:MET:O	57:Ak:277:MET:HG3	2.19	0.43
51:5:373:GLN:NE2	51:5:471:ILE:HG23	2.33	0.43
65:G:711:VAL:HA	65:G:714:VAL:HG12	2.01	0.43
66:L:238:VAL:HG12	66:L:242:LYS:NZ	2.34	0.43
3:Af:50:CYS:C	3:Af:52:GLY:H	2.27	0.43
5:6:357:GLN:O	5:6:360:THR:OG1	2.34	0.42
18:i:9:LEU:HD13	18:i:42:PRO:HB2	2.01	0.42
18:i:36:ASN:O	18:i:40:MET:HB2	2.18	0.42
18:i:222:SER:HB2	18:i:233:THR:HG21	2.01	0.42
19:j:53:MET:O	19:j:54:LYS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:33:LEU:HD23	21:m:33:LEU:HA	1.84	0.42
25:q:114:GLU:CG	25:q:116:ILE:HG22	2.49	0.42
25:q:355:MET:HA	25:q:358:TRP:HD1	1.84	0.42
26:r:185:TRP:O	26:r:189:THR:HG23	2.19	0.42
27:B:268:GLU:C	27:B:270:ASN:H	2.27	0.42
28:C:388:PHE:CE2	32:H:118:LEU:HD11	2.54	0.42
30:E:140:CYS:HB3	30:E:145:SER:HB2	2.01	0.42
34:J:169:ARG:HH12	65:G:428:LYS:HZ2	1.67	0.42
39:Q:144:PHE:CE1	65:G:624:ARG:HG3	2.54	0.42
48:l:137:LEU:HD21	48:l:263:PHE:CZ	2.54	0.42
50:t:44:GLN:HG3	50:t:48:ASP:OD2	2.19	0.42
51:u:180:ARG:O	51:u:183:VAL:HG12	2.19	0.42
7:x:293:MET:HE3	7:x:293:MET:HB3	1.73	0.42
65:G:65:TYR:HB2	68:G:803:FES:S2	2.59	0.42
65:G:466:LEU:HD13	65:G:500:ILE:HD11	2.00	0.42
66:L:330:LEU:HB3	66:L:335:ILE:HG23	2.00	0.42
6:7:296:ALA:O	6:7:300:ILE:HB	2.17	0.42
8:9:12:LYS:HD3	8:9:12:LYS:N	2.34	0.42
13:d:80:LYS:HA	25:q:182:TRP:HE1	1.83	0.42
17:h:16:ARG:HA	17:h:19:THR:HG23	1.99	0.42
18:i:31:ILE:HD11	20:k:62:ILE:HG21	2.00	0.42
39:Q:130:MET:HE3	39:Q:135:GLU:OE2	2.19	0.42
37:X:87:LEU:HD13	37:X:98:LEU:HD11	2.01	0.42
37:X:103:HIS:O	37:X:107:ASP:N	2.52	0.42
37:X:140:CYS:HB3	37:X:143:GLU:HG2	2.01	0.42
48:l:350:LEU:HD12	48:l:359:MET:HG2	2.01	0.42
51:u:83:ASN:OD1	51:u:85:LYS:HG2	2.19	0.42
6:w:338:ILE:HD13	6:w:351:GLY:HA2	2.01	0.42
57:Ak:242:GLU:HA	57:Ak:245:ILE:HD12	2.01	0.42
51:5:328:LEU:HD11	51:5:368:MET:HE2	2.01	0.42
65:G:177:ILE:HG23	65:G:228:VAL:HG11	2.01	0.42
66:L:53:VAL:O	66:L:78:PRO:HD2	2.19	0.42
5:6:115:THR:HG23	5:6:118:SER:H	1.84	0.42
7:8:172:LEU:H	7:8:172:LEU:HD12	1.84	0.42
15:f:51:SER:CB	16:g:64:LEU:HD13	2.49	0.42
15:f:72:ARG:NH2	16:g:21:ARG:HD3	2.34	0.42
19:j:6:THR:HA	26:r:6:ILE:HD13	2.01	0.42
24:p:101:LYS:O	24:p:105:LEU:HG	2.18	0.42
24:p:118:HIS:CD2	24:p:121:PRO:HA	2.53	0.42
25:q:398:MET:O	25:q:402:ILE:HG13	2.19	0.42
27:B:51:TRP:CZ3	27:B:172:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:85:SER:OG	31:F:97:ARG:NH1	2.52	0.42
32:H:149:MET:HA	32:H:152:CYS:SG	2.59	0.42
43:U:88:PHE:HB2	43:U:161:LEU:HD23	2.01	0.42
7:x:126:HIS:HE1	7:x:196:PRO:HD2	1.84	0.42
58:Al:163:TRP:CZ2	58:Al:211:LEU:HD21	2.54	0.42
51:5:317:THR:HB	3:Ae:53:VAL:HG21	2.01	0.42
3:2:173:ILE:HG23	3:2:190:TRP:HD1	1.85	0.42
12:c:169:GLU:OE1	50:t:43:GLN:NE2	2.52	0.42
13:d:33:LEU:HD13	13:d:33:LEU:HA	1.82	0.42
13:d:159:GLN:O	13:d:162:ARG:HG2	2.20	0.42
13:d:163:MET:CE	14:e:147:ILE:HG21	2.49	0.42
25:q:69:THR:HG22	25:q:234:VAL:HG11	2.00	0.42
26:r:186:PHE:O	26:r:189:THR:OG1	2.28	0.42
27:B:56:ALA:O	27:B:59:ARG:HG2	2.19	0.42
28:C:368:LYS:HE2	28:C:386:HIS:CE1	2.55	0.42
29:D:77:GLN:HG3	29:D:85:GLU:HG3	2.01	0.42
29:D:200:LYS:O	34:J:126:LEU:HD21	2.19	0.42
37:O:79:ILE:HD13	37:O:148:ILE:HG22	2.00	0.42
50:t:35:LYS:C	50:t:37:ARG:N	2.77	0.42
50:t:109:LEU:HD23	50:t:109:LEU:HA	1.92	0.42
51:u:304:LEU:HD23	51:u:304:LEU:HA	1.82	0.42
5:v:232:GLN:HE22	5:v:236:ARG:NH1	2.17	0.42
5:v:338:ILE:HG21	5:v:354:ALA:HB1	2.01	0.42
4:Ad:3:SER:HA	4:Ad:6:LEU:HD23	2.02	0.42
57:Ak:209:LEU:O	57:Ak:213:ARG:HG3	2.19	0.42
59:Am:69:GLY:HA3	62:Ap:45:THR:O	2.18	0.42
64:Ar:79:GLU:HG3	64:Ar:81:THR:HG23	2.02	0.42
65:G:93:ALA:O	65:G:94:MET:C	2.62	0.42
66:L:130:GLU:HG2	66:L:136:PHE:H	1.84	0.42
66:L:357:LEU:O	66:L:358:THR:C	2.62	0.42
3:4:257:CYS:HB3	68:4:301:FES:S2	2.59	0.42
5:6:356:ASP:O	5:6:360:THR:HG23	2.19	0.42
6:7:223:TYR:HB3	7:8:312:TRP:CZ2	2.54	0.42
7:8:198:LEU:HA	7:8:201:ILE:HB	2.01	0.42
11:b:10:LEU:HD23	24:p:198:PRO:HG3	2.02	0.42
12:c:108:ASP:HB2	12:c:112:TYR:CE2	2.54	0.42
18:i:192:ALA:HB1	18:i:270:MET:HE1	2.00	0.42
19:j:113:TRP:HZ3	26:r:282:TYR:CE2	2.37	0.42
25:q:3:LYS:O	25:q:7:PRO:HG2	2.20	0.42
26:r:316:PRO:HD2	45:W:57:ARG:HE	1.83	0.42
30:E:174:VAL:HG21	30:E:177:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:78:ARG:HD2	65:G:607:LYS:NZ	2.33	0.42
39:Q:127:THR:O	39:Q:131:ARG:HG3	2.19	0.42
39:Q:140:ARG:HD3	39:Q:141:PRO:O	2.20	0.42
41:S:55:SER:O	41:S:64:LYS:HE2	2.19	0.42
37:X:90:TYR:CZ	37:X:92:LYS:HB2	2.54	0.42
6:w:282:ARG:HE	6:w:343:VAL:HG22	1.85	0.42
55:Ai:41:ILE:HG22	60:An:105:GLY:HA3	2.01	0.42
58:Al:62:GLU:HA	58:Al:65:TRP:NE1	2.33	0.42
58:Al:171:LYS:HE2	58:Al:171:LYS:HB2	1.84	0.42
59:Am:185:PRO:O	63:Aq:88:ASN:ND2	2.53	0.42
61:Ao:133:ARG:NE	61:Ao:137:ASN:OD1	2.47	0.42
62:Ap:53:MET:HA	62:Ap:56:ARG:HH11	1.84	0.42
65:G:382:ARG:HA	65:G:385:TYR:CE2	2.55	0.42
10:a:144:ALA:CB	13:d:82:ILE:HG21	2.49	0.42
11:b:5:THR:HB	11:b:6:PRO:HD2	2.01	0.42
12:c:86:ARG:O	12:c:87:ASP:C	2.62	0.42
23:o:3:PHE:O	23:o:4:PRO:C	2.62	0.42
25:q:329:LEU:HB3	25:q:359:TRP:CZ2	2.54	0.42
26:r:179:TRP:NE1	45:W:43:LEU:HG	2.34	0.42
27:B:311:TRP:NE1	27:B:333:GLU:HG2	2.19	0.42
31:F:74:GLN:HG3	31:F:75:PRO:HD2	2.02	0.42
32:H:116:CYS:SG	72:H:302:SF4:S3	3.03	0.42
37:O:122:MET:HG2	37:O:144:ILE:HG21	2.01	0.42
43:U:244:LYS:HA	43:U:248:LEU:HD12	2.01	0.42
37:X:100:VAL:CG1	37:X:142:GLN:HB2	2.49	0.42
37:X:130:ILE:HG23	37:X:147:TYR:HE1	1.83	0.42
46:Y:45:ARG:HH12	47:Z:64:ASN:ND2	2.11	0.42
48:l:562:LEU:HB3	48:l:563:PRO:CD	2.40	0.42
51:u:99:LYS:HB3	51:u:160:GLN:HG2	2.01	0.42
5:v:195:TYR:CE2	5:v:196:ARG:HG2	2.54	0.42
7:x:182:ASN:HB2	7:x:183:PRO:HD2	2.01	0.42
8:y:103:LYS:HA	8:y:103:LYS:HD2	1.72	0.42
54:Ah:67:SER:O	54:Ah:71:LEU:HG	2.19	0.42
57:Ak:417:MET:O	57:Ak:421:VAL:HG22	2.20	0.42
58:Al:100:MET:HB2	58:Al:107:SER:OG	2.19	0.42
59:Am:141:GLY:O	59:Am:144:ILE:HG22	2.19	0.42
63:Aq:60:ILE:HB	63:Aq:62:TYR:CE2	2.55	0.42
66:L:199:SER:OG	66:L:200:ASP:N	2.53	0.42
1:0:32:THR:O	1:0:36:GLN:HG2	2.20	0.42
5:6:365:ASN:OD1	5:6:365:ASN:N	2.51	0.42
5:6:421:ASP:N	5:6:421:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:i:28:LEU:HD23	18:i:31:ILE:HD12	2.02	0.42
23:o:44:LYS:HG2	24:p:194:GLU:OE2	2.20	0.42
25:q:45:LEU:O	25:q:46:GLY:C	2.63	0.42
25:q:56:PHE:HZ	25:q:108:MET:HE3	1.85	0.42
26:r:72:ILE:HG22	26:r:76:ILE:HD11	2.02	0.42
27:B:39:ASP:CG	27:B:261:TRP:HE1	2.28	0.42
28:C:111:MET:HE3	28:C:111:MET:HB3	1.89	0.42
33:I:65:MET:HE1	33:I:120:VAL:HG11	2.00	0.42
44:V:120:LEU:O	44:V:124:LEU:HG	2.20	0.42
49:s:105:ALA:HB1	49:s:147:PHE:CZ	2.55	0.42
49:s:208:VAL:HG12	49:s:210:THR:HG23	2.00	0.42
7:x:144:GLU:H	7:x:144:GLU:CD	2.28	0.42
8:y:76:LEU:HD12	8:y:76:LEU:HA	1.95	0.42
57:Ak:132:LEU:HA	58:Al:159:VAL:CG2	2.49	0.42
57:Ak:405:LEU:HD23	57:Ak:475:ALA:HB2	2.01	0.42
58:Al:136:LEU:HD22	58:Al:193:TYR:HB3	2.01	0.42
58:Al:188:ARG:NH1	60:An:152:PRO:HG2	2.34	0.42
65:G:176:CYS:SG	72:G:802:SF4:S3	3.18	0.42
65:G:375:ALA:HB1	65:G:675:VAL:HG11	2.01	0.42
66:L:128:GLU:HG3	66:L:207:ARG:HH21	1.85	0.42
5:6:125:CYS:SG	5:6:133:LEU:HD22	2.60	0.42
5:6:170:GLN:HG3	5:6:339:TYR:OH	2.19	0.42
5:6:289:LEU:HB2	5:6:424:VAL:HG13	2.02	0.42
5:6:290:GLN:NE2	3:Ae:44:PHE:O	2.48	0.42
9:A:71:SER:OG	58:Al:222:TRP:HB2	2.19	0.42
13:d:163:MET:HE1	14:e:147:ILE:HG21	2.02	0.42
16:g:23:LEU:CD1	16:g:83:TYR:HA	2.50	0.42
18:i:37:LEU:O	18:i:41:ILE:HG12	2.19	0.42
18:i:60:PHE:HE1	20:k:70:GLU:HG3	1.85	0.42
18:i:298:TYR:HE1	25:q:134:THR:HG21	1.85	0.42
18:i:313:MET:HE2	18:i:313:MET:HB2	1.82	0.42
26:r:91:MET:HG2	26:r:259:PHE:CE2	2.54	0.42
27:B:438:LEU:HD21	27:B:446:LEU:HD21	2.01	0.42
30:E:201:ILE:HD13	30:E:201:ILE:HA	1.91	0.42
33:I:56:TRP:CD1	33:I:60:SER:HG	2.37	0.42
35:K:39:VAL:HG21	35:K:89:TRP:CZ2	2.55	0.42
46:Y:65:MET:HE3	46:Y:65:MET:HB3	1.75	0.42
48:l:132:VAL:HA	48:l:258:PHE:CE2	2.54	0.42
49:s:173:LEU:HB3	49:s:175:ARG:HG3	2.01	0.42
52:z:64:THR:O	52:z:68:GLU:HG2	2.19	0.42
54:Ah:26:VAL:HG13	59:Am:66:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Ak:195:LEU:HD22	57:Ak:199:LEU:HD11	2.02	0.42
57:Ak:294:THR:HG22	57:Ak:365:ILE:HD13	2.02	0.42
58:Al:91:ASN:ND2	58:Al:183:THR:OG1	2.53	0.42
59:Am:137:LEU:HA	59:Am:137:LEU:HD23	1.70	0.42
65:G:387:LEU:HD12	65:G:514:ASN:HB3	2.01	0.42
66:L:187:ARG:HD3	66:L:187:ARG:HA	1.85	0.42
4:3:23:MET:O	4:3:27:VAL:HG23	2.20	0.42
10:a:156:VAL:HG21	16:g:92:MET:HG3	2.02	0.42
11:b:88:TYR:CD2	13:d:49:ARG:HD2	2.55	0.42
18:i:341:PRO:HA	49:s:244:LEU:HD22	2.02	0.42
19:j:59:ALA:HB2	21:m:70:TYR:HE2	1.85	0.42
21:m:45:LEU:HD13	21:m:45:LEU:HA	1.89	0.42
21:m:124:ASP:O	21:m:125:TRP:C	2.63	0.42
23:o:47:TYR:O	23:o:48:LEU:C	2.62	0.42
23:o:98:LEU:HA	25:q:263:MET:HE2	2.02	0.42
24:p:146:LEU:CD1	24:p:160:TYR:HE2	2.32	0.42
28:C:140:PRO:O	28:C:144:ARG:HG2	2.20	0.42
28:C:202:ALA:C	28:C:204:THR:H	2.28	0.42
29:D:87:PHE:HB3	36:N:112:TRP:CZ2	2.55	0.42
29:D:103:HIS:CE1	29:D:105:ASN:HA	2.55	0.42
29:D:128:ILE:HD11	29:D:176:VAL:HG21	2.02	0.42
32:H:150:THR:HG21	32:H:180:HIS:NE2	2.35	0.42
36:N:58:MET:HE1	36:N:72:LEU:HA	2.01	0.42
39:Q:147:LYS:HA	39:Q:150:VAL:HG12	2.02	0.42
51:u:38:TYR:CZ	51:u:42:LEU:HD11	2.55	0.42
6:w:244:LEU:HD12	7:x:293:MET:HE2	2.02	0.42
7:x:115:PHE:CE2	7:x:149:LEU:HD13	2.54	0.42
53:Ag:27:ALA:HB2	57:Ak:404:THR:HG21	2.00	0.42
57:Ak:195:LEU:HD23	57:Ak:245:ILE:HD13	2.01	0.42
65:G:221:ASN:ND2	65:G:285:TRP:HB3	2.35	0.42
65:G:612:PRO:HA	65:G:613:PRO:HD3	1.90	0.42
66:L:33:HIS:HE2	66:L:117:HIS:HD2	1.66	0.42
9:A:54:TYR:OH	9:A:59:ASP:OD2	2.38	0.42
10:a:78:THR:C	10:a:81:PRO:HD2	2.45	0.42
12:c:107:TRP:CH2	23:o:72:ARG:HA	2.55	0.42
14:e:89:VAL:HG11	25:q:29:VAL:HG22	2.02	0.42
18:i:261:MET:O	18:i:265:MET:HG2	2.19	0.42
24:p:180:LYS:O	24:p:184:GLU:HG3	2.20	0.42
26:r:30:TYR:CE1	32:H:81:PRO:HG3	2.50	0.42
26:r:87:VAL:HG13	26:r:95:LEU:HD23	2.02	0.42
27:B:125:CYS:SG	30:E:180:CYS:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:161:GLU:HB3	30:E:192:TYR:OH	2.20	0.42
28:C:306:TRP:CZ2	29:D:133:LEU:HD21	2.55	0.42
28:C:450:LEU:HA	28:C:450:LEU:HD12	1.84	0.42
32:H:142:THR:O	32:H:187:LYS:NZ	2.52	0.42
32:H:158:CYS:SG	32:H:167:ILE:HG21	2.59	0.42
32:H:186:ASN:ND2	35:K:127:TYR:O	2.53	0.42
37:O:103:HIS:H	37:O:107:ASP:CG	2.27	0.42
37:O:120:MET:HG2	39:Q:67:ARG:HH12	1.85	0.42
39:Q:92:MET:HB2	73:Q:201:ZMP:H9A	2.02	0.42
41:S:1:MET:HB3	41:S:2:TRP:H	1.63	0.42
37:X:144:ILE:H	37:X:144:ILE:HG13	1.69	0.42
47:Z:79:PHE:O	47:Z:83:LEU:HG	2.20	0.42
48:l:368:PHE:HZ	48:l:455:LYS:HG3	1.85	0.42
50:t:106:ARG:HG2	50:t:110:GLN:NE2	2.35	0.42
6:w:22:PRO:HB3	52:z:8:LEU:HD11	2.02	0.42
52:Aa:19:LEU:HD22	52:Aa:19:LEU:HA	1.86	0.42
4:Ad:18:ILE:HD13	4:Ad:18:ILE:HA	1.83	0.42
57:Ak:240:HIS:O	57:Ak:243:VAL:HG22	2.20	0.42
57:Ak:382:SER:O	57:Ak:386:VAL:HB	2.20	0.42
57:Ak:442:ASP:OD2	58:Al:134:ARG:NH2	2.52	0.42
58:Al:103:GLN:N	58:Al:158:ASP:OD2	2.53	0.42
62:Ap:113:CYS:N	62:Ap:117:GLY:O	2.53	0.42
51:5:192:PHE:HB3	51:5:195:THR:OG1	2.20	0.42
65:G:63:PHE:CZ	65:G:139:LEU:HA	2.54	0.42
66:L:57:THR:HG21	66:L:86:THR:HG22	2.01	0.42
67:M:11:LEU:HD13	67:M:11:LEU:HA	1.80	0.42
3:Ae:45:PRO:HA	3:Ae:66:PRO:HB3	2.01	0.42
3:Af:53:VAL:HG22	3:Af:54:VAL:H	1.85	0.42
7:8:136:LEU:H	7:8:136:LEU:HG	1.74	0.41
8:9:108:TRP:CZ2	5:v:101:ARG:HB3	2.55	0.41
11:b:119:LEU:H	11:b:119:LEU:HG	1.67	0.41
12:c:42:PRO:CG	12:c:64:PRO:HG3	2.50	0.41
13:d:159:GLN:HE21	13:d:163:MET:HE2	1.85	0.41
16:g:96:VAL:HA	16:g:103:PHE:CD2	2.54	0.41
19:j:53:MET:HE3	19:j:53:MET:HB2	1.84	0.41
23:o:71:ALA:HA	23:o:75:ASN:HB2	2.01	0.41
23:o:102:TYR:HB2	25:q:263:MET:HG3	2.02	0.41
24:p:67:ARG:HD3	24:p:67:ARG:HA	1.82	0.41
24:p:87:ARG:HH12	37:X:114:ASP:HA	1.85	0.41
24:p:167:TRP:HB3	24:p:210:TRP:HZ3	1.85	0.41
25:q:11:LEU:HB3	25:q:100:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:q:326:LEU:HD23	25:q:326:LEU:HA	1.91	0.41
27:B:66:LYS:O	27:B:70:LEU:HG	2.20	0.41
45:W:6:VAL:HG21	67:M:42:PRO:HB3	2.02	0.41
45:W:112:HIS:H	45:W:112:HIS:CD2	2.38	0.41
5:v:310:TYR:OH	3:Af:75:LEU:HD11	2.20	0.41
7:x:271:VAL:HG21	70:x:401:HEC:HBB3	2.01	0.41
59:Am:177:GLN:HE22	59:Am:201:THR:HB	1.85	0.41
63:Aq:66:ARG:HB3	63:Aq:91:PRO:HG3	2.01	0.41
51:5:157:GLU:O	51:5:161:ILE:HG13	2.20	0.41
51:5:307:ALA:HB1	51:5:379:LEU:HD13	2.01	0.41
51:5:412:ASP:OD2	51:5:423:ARG:NE	2.53	0.41
65:G:92:CYS:SG	68:G:803:FES:S1	3.17	0.41
65:G:592:LYS:NZ	65:G:596:TYR:OH	2.50	0.41
66:L:106:LYS:HE3	66:L:134:PHE:CZ	2.55	0.41
66:L:137:GLU:H	66:L:174:ARG:NH2	2.18	0.41
66:L:215:MET:HA	66:L:218:PHE:CD2	2.55	0.41
4:3:46:PRO:O	4:3:49:ASN:ND2	2.53	0.41
11:b:5:THR:N	11:b:8:GLU:HB2	2.35	0.41
16:g:80:ARG:O	16:g:84:MET:HG2	2.20	0.41
18:i:336:VAL:HG22	18:i:339:MET:HB2	2.02	0.41
20:k:30:LEU:HB2	21:m:68:PHE:HE2	1.84	0.41
22:n:25:CYS:HB2	22:n:29:ARG:HH22	1.81	0.41
24:p:124:PHE:HB2	24:p:127:SER:HB3	2.02	0.41
25:q:36:LEU:HD23	25:q:36:LEU:HA	1.84	0.41
25:q:66:LEU:HD21	25:q:111:THR:HG23	2.01	0.41
27:B:433:TRP:HB2	27:B:434:PRO:HD3	2.02	0.41
37:O:123:GLU:HB2	37:O:128:PHE:O	2.20	0.41
38:P:65:LEU:O	38:P:76:ASN:HA	2.19	0.41
46:Y:54:GLN:HB3	48:l:446:ASN:ND2	2.33	0.41
48:l:375:ILE:HD12	48:l:458:LEU:HD22	2.02	0.41
50:t:110:GLN:O	50:t:114:ARG:HG2	2.20	0.41
5:v:170:GLN:HE21	5:v:268:HIS:CE1	2.37	0.41
6:w:246:SER:HB2	6:w:249:LEU:HB2	2.02	0.41
7:x:180:TYR:CD2	7:x:186:ALA:HA	2.55	0.41
8:y:63:ILE:O	8:y:67:LEU:HG	2.20	0.41
54:Ah:23:GLU:O	54:Ah:25:ARG:NH1	2.54	0.41
57:Ak:266:GLU:OE2	57:Ak:270:TYR:HB2	2.20	0.41
61:Ao:79:LEU:HD21	61:Ao:86:PRO:HB3	2.01	0.41
66:L:68:LEU:HA	66:L:71:MET:HE2	2.03	0.41
3:Af:64:GLU:O	3:Af:65:SER:OG	2.24	0.41
4:3:18:ILE:HD13	4:3:18:ILE:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:182:GLU:OE2	3:4:183:GLY:N	2.53	0.41
5:6:170:GLN:HG2	3:Ae:67:VAL:HG13	2.02	0.41
5:6:295:ALA:O	3:Ae:46:LEU:HD12	2.20	0.41
6:7:203:THR:O	52:Aa:3:ARG:NH1	2.54	0.41
7:8:142:THR:HG23	7:8:145:GLU:H	1.85	0.41
10:a:110:TRP:CD1	10:a:110:TRP:H	2.38	0.41
11:b:79:VAL:HA	48:l:10:THR:HG21	2.02	0.41
19:j:59:ALA:HA	26:r:140:ILE:HD11	2.01	0.41
20:k:37:MET:HE3	20:k:67:ALA:HB2	2.01	0.41
25:q:109:THR:HG22	25:q:121:LEU:CB	2.50	0.41
27:B:326:LEU:HD23	27:B:367:ILE:HD11	2.02	0.41
28:C:72:TRP:CD1	43:U:195:VAL:HG21	2.56	0.41
28:C:345:GLN:O	28:C:349:ILE:HG13	2.20	0.41
32:H:59:GLN:HA	32:H:64:THR:HG23	2.02	0.41
38:P:20:ARG:HG3	38:P:54:LEU:HB2	2.03	0.41
37:X:86:VAL:CG2	37:X:125:GLU:HG3	2.49	0.41
46:Y:47:PHE:CZ	48:l:364:LYS:HE2	2.54	0.41
48:l:562:LEU:CB	48:l:563:PRO:HD3	2.39	0.41
5:v:60:ARG:CZ	5:v:390:GLU:HG3	2.50	0.41
5:v:217:ARG:HD2	5:v:244:LEU:O	2.21	0.41
6:w:128:PHE:CZ	6:w:143:ALA:HA	2.55	0.41
52:Aa:15:ILE:HA	51:5:276:ARG:O	2.20	0.41
56:Aj:38:LEU:HD22	57:Ak:473:TRP:CZ2	2.55	0.41
57:Ak:211:THR:HG22	57:Ak:215:LEU:HD12	2.02	0.41
57:Ak:440:TYR:CE2	58:Al:205:SER:HA	2.56	0.41
58:Al:9:PHE:HE2	58:Al:24:HIS:CG	2.37	0.41
51:5:417:LEU:HD23	51:5:417:LEU:HA	1.86	0.41
65:G:341:ILE:HG12	65:G:537:ILE:HD12	2.01	0.41
7:8:203:ARG:CZ	7:8:280:GLU:HG2	2.50	0.41
8:9:43:ASP:N	8:9:43:ASP:OD1	2.53	0.41
8:9:78:LYS:HB2	8:9:78:LYS:HE3	1.76	0.41
12:c:74:ASP:O	12:c:75:TYR:C	2.62	0.41
14:e:65:ASN:HD21	14:e:68:GLU:HB2	1.85	0.41
24:p:164:ARG:O	24:p:168:LYS:HG3	2.21	0.41
27:B:51:TRP:HB2	27:B:135:PRO:HD2	2.03	0.41
27:B:297:LYS:HA	27:B:311:TRP:CH2	2.55	0.41
28:C:124:ARG:HD2	33:I:143:TYR:CE2	2.55	0.41
28:C:175:TRP:HA	28:C:178:VAL:HG12	2.02	0.41
31:F:71:ILE:HD12	31:F:71:ILE:HA	1.96	0.41
37:O:90:TYR:CD2	37:O:118:ILE:HD11	2.56	0.41
39:Q:74:HIS:CE1	66:L:360:GLU:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:U:312:ILE:HG22	43:U:314:VAL:HG23	2.01	0.41
48:l:76:LEU:HD21	48:l:196:TRP:HE3	1.84	0.41
5:v:354:ALA:O	5:v:358:VAL:HG23	2.20	0.41
6:w:318:ARG:O	6:w:322:GLN:HG3	2.21	0.41
7:x:125:CYS:HA	7:x:190:ASN:HD21	1.86	0.41
7:x:322:TYR:HB2	8:y:61:PHE:CD1	2.54	0.41
52:Aa:68:GLU:O	52:Aa:72:ARG:HG2	2.21	0.41
4:Ad:23:MET:O	4:Ad:27:VAL:HG23	2.21	0.41
53:Ag:28:LYS:HD2	57:Ak:481:GLU:HB2	2.02	0.41
51:5:473:SER:HA	51:5:476:PHE:CE2	2.55	0.41
66:L:354:TYR:HD1	66:L:355:ARG:H	1.68	0.41
8:9:76:LEU:O	8:9:81:TRP:NE1	2.44	0.41
12:c:117:VAL:HG23	48:l:542:LEU:HD12	2.01	0.41
12:c:126:TRP:CZ2	48:l:532:ILE:HG23	2.56	0.41
12:c:151:PRO:HB3	48:l:403:TYR:CZ	2.55	0.41
14:e:95:PHE:O	14:e:100:VAL:HG23	2.21	0.41
18:i:112:HIS:CE1	18:i:164:ILE:HG21	2.55	0.41
18:i:168:GLY:O	18:i:172:GLN:HG2	2.20	0.41
19:j:16:LEU:HD13	19:j:16:LEU:HA	1.78	0.41
19:j:54:LYS:HG3	19:j:55:PHE:HD1	1.84	0.41
21:m:159:TRP:O	21:m:163:ILE:HG12	2.20	0.41
26:r:61:LEU:HD11	33:I:125:PRO:HB3	2.02	0.41
26:r:66:SER:N	26:r:122:ALA:O	2.53	0.41
26:r:200:LEU:O	26:r:201:THR:C	2.63	0.41
27:B:325:PRO:HD2	27:B:347:THR:HA	2.02	0.41
32:H:119:CYS:O	32:H:122:VAL:N	2.53	0.41
32:H:128:ILE:HD13	32:H:147:ILE:HG12	2.02	0.41
33:I:113:MET:O	33:I:114:ALA:C	2.63	0.41
34:J:102:ASP:N	34:J:102:ASP:OD1	2.54	0.41
43:U:107:ASP:OD1	43:U:108:VAL:N	2.54	0.41
44:V:3:LYS:HE3	44:V:3:LYS:HB3	1.96	0.41
48:l:504:LEU:HD23	48:l:504:LEU:HA	1.86	0.41
51:u:447:LYS:HE3	51:u:448:TYR:CE2	2.56	0.41
51:u:473:SER:HA	51:u:476:PHE:CE1	2.56	0.41
6:w:22:PRO:HA	52:z:5:PHE:CZ	2.55	0.41
52:Aa:78:TYR:CD2	1:Ab:65:GLU:HG3	2.56	0.41
53:Ag:47:PHE:O	53:Ag:51:LEU:HG	2.21	0.41
56:Aj:56:VAL:HG21	57:Ak:36:LEU:HD13	2.02	0.41
57:Ak:8:TYR:CZ	59:Am:15:PRO:HB3	2.55	0.41
57:Ak:214:ASN:HA	63:Aq:70:LYS:HD3	2.01	0.41
57:Ak:240:HIS:CD2	57:Ak:244:TYR:HE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:G:643:ARG:NH1	65:G:656:TYR:OH	2.52	0.41
66:L:236:TYR:CE2	66:L:343:LYS:HE2	2.55	0.41
3:2:265:ASP:OD2	3:2:269:ARG:HB2	2.21	0.41
11:b:110:ILE:O	11:b:111:LEU:HB3	2.20	0.41
19:j:104:TYR:O	19:j:108:GLN:HG2	2.20	0.41
23:o:101:TRP:HB2	25:q:263:MET:CE	2.49	0.41
25:q:208:PRO:HG3	25:q:216:LEU:CD1	2.50	0.41
26:r:71:PHE:O	26:r:215:TYR:HE2	2.03	0.41
26:r:101:GLY:O	26:r:105:MET:HG3	2.21	0.41
27:B:281:HIS:CE1	30:E:142:LEU:HD22	2.56	0.41
28:C:98:HIS:HB2	28:C:464:PHE:CE2	2.55	0.41
28:C:146:ASP:HB2	28:C:466:GLU:CD	2.46	0.41
30:E:88:ARG:NH2	30:E:190:ASP:OD2	2.53	0.41
35:K:105:ALA:O	35:K:106:ARG:HD2	2.20	0.41
48:l:176:ARG:HA	48:l:176:ARG:HD3	1.91	0.41
50:t:78:LEU:HA	50:t:81:LYS:HZ3	1.86	0.41
51:u:178:SER:HB3	51:u:181:ASP:OD2	2.20	0.41
53:Ag:61:LEU:HA	53:Ag:64:TYR:CD2	2.56	0.41
57:Ak:349:THR:HG23	74:Ak:602:HEA:H272	2.02	0.41
58:Al:16:ILE:HA	58:Al:19:GLU:OE1	2.21	0.41
60:An:100:TRP:HA	60:An:103:ILE:HG12	2.01	0.41
61:Ao:77:ASN:O	61:Ao:80:VAL:HG22	2.20	0.41
51:5:212:SER:N	51:5:215:ASP:OD2	2.43	0.41
65:G:566:ILE:HB	65:G:580:ALA:HA	2.01	0.41
3:Af:55:GLY:HA3	3:Af:59:LEU:HD13	2.02	0.41
3:2:100:SER:C	3:2:102:THR:H	2.28	0.41
3:2:111:ASP:O	52:z:25:ARG:NH2	2.54	0.41
4:3:33:VAL:HG13	4:3:38:TRP:HB3	2.02	0.41
6:7:97:HIS:HE1	69:7:402:HEM:NA	2.18	0.41
7:8:95:TYR:HB3	1:Ab:87:PHE:CE2	2.56	0.41
9:A:20:HIS:HB3	58:Al:44:LEU:HD21	2.03	0.41
10:a:60:SER:HA	24:p:149:TRP:NE1	2.36	0.41
11:b:35:LEU:H	11:b:35:LEU:HD22	1.86	0.41
17:h:86:LEU:HB3	17:h:92:TYR:CB	2.51	0.41
18:i:339:MET:HA	18:i:339:MET:HE2	2.03	0.41
20:k:73:LEU:HD12	20:k:73:LEU:HA	1.88	0.41
25:q:225:ILE:HD11	25:q:328:CYS:HA	2.02	0.41
25:q:373:ILE:HA	25:q:376:ILE:HD12	2.02	0.41
26:r:102:VAL:HG21	26:r:154:LEU:HD11	2.03	0.41
26:r:263:THR:O	26:r:267:THR:HG23	2.21	0.41
27:B:387:GLU:OE1	65:G:123:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:161:VAL:O	28:C:165:LEU:HB2	2.21	0.41
28:C:322:PHE:CG	28:C:349:ILE:HD11	2.55	0.41
28:C:362:ILE:H	28:C:362:ILE:HG13	1.75	0.41
33:I:48:ALA:HA	33:I:191:ARG:NH1	2.36	0.41
35:K:34:ARG:HD2	35:K:54:GLN:NE2	2.35	0.41
45:W:7:LYS:H	67:M:40:LYS:HB3	1.84	0.41
45:W:124:LEU:HD23	45:W:124:LEU:HA	1.86	0.41
48:l:4:PHE:HE1	48:l:82:MET:HB3	1.86	0.41
49:s:83:GLU:OE1	49:s:83:GLU:HA	2.19	0.41
5:v:177:LEU:HD21	5:v:272:VAL:HG11	2.02	0.41
5:v:268:HIS:CE1	5:v:341:ILE:HG12	2.55	0.41
5:v:401:LEU:HD12	5:v:401:LEU:HA	1.93	0.41
54:Ah:42:HIS:HB2	59:Am:16:TRP:HZ2	1.86	0.41
51:5:68:THR:HG22	51:5:136:LEU:HD23	2.02	0.41
51:5:169:LEU:O	51:5:173:GLN:HG2	2.20	0.41
66:L:52:THR:CG2	66:L:121:VAL:HG22	2.51	0.41
3:2:256:TYR:CE1	3:2:261:GLY:HA2	2.55	0.41
4:3:51:LYS:HG2	4:3:52:PHE:CD2	2.56	0.41
3:4:185:ASN:HA	3:4:198:ARG:HA	2.03	0.41
6:7:217:LYS:HG3	52:Aa:8:LEU:HD13	2.03	0.41
9:A:12:LEU:H	9:A:12:LEU:HD12	1.85	0.41
9:A:51:TYR:HE2	60:An:153:ILE:HD11	1.85	0.41
14:e:100:VAL:O	14:e:104:THR:HG23	2.21	0.41
18:i:100:MET:HE2	48:l:595:ILE:HA	2.03	0.41
23:o:6:TYR:OH	23:o:12:ALA:HB1	2.20	0.41
25:q:412:ILE:O	25:q:416:ARG:HB2	2.21	0.41
28:C:191:MET:HE2	28:C:195:THR:HG23	2.03	0.41
28:C:463:VAL:HG13	28:C:466:GLU:HB2	2.02	0.41
29:D:124:ASN:OD1	36:N:108:PRO:HG2	2.20	0.41
37:O:117:GLU:OE2	39:Q:90:ARG:NH2	2.54	0.41
39:Q:91:GLU:HG2	39:Q:95:LYS:NZ	2.36	0.41
39:Q:140:ARG:HG2	39:Q:141:PRO:HD2	2.02	0.41
40:R:106:GLN:OE1	40:R:106:GLN:N	2.43	0.41
48:l:124:PHE:CE2	48:l:247:LEU:HG	2.55	0.41
48:l:368:PHE:CZ	48:l:455:LYS:HG3	2.56	0.41
50:t:52:MET:H	50:t:52:MET:HG2	1.54	0.41
5:v:65:ILE:HG21	5:v:213:PHE:CD1	2.55	0.41
6:w:217:LYS:HE3	52:z:3:ARG:HH22	1.84	0.41
7:x:200:TYR:O	7:x:204:ALA:N	2.54	0.41
4:Ad:33:VAL:HG13	4:Ad:38:TRP:HB3	2.02	0.41
53:Ag:49:SER:HB3	56:Aj:42:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Al:1:MET:HE1	58:Al:133:MET:HG3	2.02	0.41
59:Am:204:HIS:O	59:Am:208:VAL:HG23	2.20	0.41
51:5:405:GLY:C	51:5:408:PRO:HD2	2.45	0.41
65:G:43:VAL:HG21	65:G:96:VAL:HG21	2.03	0.41
65:G:322:ALA:O	65:G:326:VAL:HG22	2.20	0.41
3:2:200:ARG:HH11	3:2:208:GLU:HG3	1.85	0.41
3:2:289:ASP:OD1	3:2:289:ASP:N	2.54	0.41
3:4:222:ASP:O	3:4:226:VAL:HG22	2.20	0.41
5:6:115:THR:OG1	5:6:116:ARG:N	2.54	0.41
6:7:104:TYR:CD1	6:7:208:PRO:HA	2.56	0.41
6:7:145:VAL:O	6:7:149:LEU:HG	2.21	0.41
9:A:36:LYS:HG3	9:A:40:ALA:HB3	2.03	0.41
9:A:41:GLU:HG3	9:A:45:LYS:HZ1	1.86	0.41
12:c:38:PRO:CG	23:o:71:ALA:HB2	2.49	0.41
13:d:146:LEU:HD13	13:d:146:LEU:HA	1.86	0.41
15:f:72:ARG:CZ	16:g:21:ARG:HB2	2.50	0.41
16:g:12:PRO:HG2	17:h:8:LYS:HG2	2.03	0.41
18:i:215:MET:HE1	18:i:244:MET:HG3	2.02	0.41
18:i:298:TYR:O	18:i:303:THR:OG1	2.26	0.41
18:i:303:THR:HG21	25:q:143:LEU:HD11	2.03	0.41
20:k:75:LEU:HD21	21:m:68:PHE:CE1	2.55	0.41
24:p:77:ASP:OD1	24:p:78:LYS:N	2.53	0.41
25:q:106:LEU:HD13	25:q:234:VAL:HG11	2.01	0.41
25:q:339:SER:HB3	25:q:344:LEU:CD2	2.49	0.41
28:C:101:LEU:HD22	28:C:464:PHE:HZ	1.86	0.41
28:C:105:MET:HE3	28:C:105:MET:HB2	1.89	0.41
28:C:146:ASP:HB3	28:C:153:ASN:OD1	2.21	0.41
29:D:80:CYS:SG	67:M:64:MET:HG3	2.60	0.41
29:D:85:GLU:HA	29:D:142:ARG:O	2.21	0.41
30:E:108:PRO:HA	30:E:109:PRO:HD3	1.97	0.41
32:H:119:CYS:O	32:H:120:GLU:C	2.63	0.41
33:I:51:ASP:HB2	33:I:190:LEU:HB2	2.03	0.41
33:I:72:CYS:SG	72:I:201:SF4:S3	3.06	0.41
33:I:76:MET:HE1	33:I:104:ILE:HD12	2.02	0.41
33:I:195:ARG:O	66:L:133:ASN:ND2	2.54	0.41
34:J:121:LEU:HD23	34:J:124:LEU:HD13	2.02	0.41
35:K:8:ARG:O	35:K:12:GLN:HG2	2.20	0.41
35:K:11:LEU:HD13	35:K:11:LEU:HA	1.89	0.41
37:O:74:LEU:HD23	37:O:74:LEU:HA	1.83	0.41
38:P:71:PHE:CE1	65:G:362:ASP:HB2	2.55	0.41
39:Q:69:VAL:O	39:Q:72:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:T:150:ASP:O	42:T:159:GLN:HB3	2.20	0.41
44:V:104:ARG:HD2	44:V:104:ARG:HA	1.95	0.41
45:W:90:ASN:O	45:W:93:GLU:HG2	2.21	0.41
46:Y:89:PRO:HA	46:Y:92:TRP:CG	2.56	0.41
47:Z:45:LEU:O	47:Z:48:VAL:HG12	2.21	0.41
48:l:223:LYS:HG2	48:l:255:ALA:HB3	2.02	0.41
51:u:94:GLU:OE2	5:v:300:LYS:NZ	2.52	0.41
51:u:300:ASP:C	51:u:303:PRO:HD2	2.46	0.41
5:v:68:GLY:O	5:v:208:TYR:OH	2.39	0.41
5:v:124:GLU:OE2	5:v:125:CYS:N	2.53	0.41
5:v:326:PHE:HD2	3:Af:66:PRO:O	2.04	0.41
5:v:400:ALA:HA	5:v:404:GLY:O	2.21	0.41
7:x:89:GLU:HG2	7:x:239:PRO:HA	2.02	0.41
8:y:111:LYS:HB3	4:Ad:8:PRO:HD2	2.02	0.41
54:Ah:30:GLN:O	54:Ah:34:GLN:HB2	2.21	0.41
57:Ak:44:PRO:HD3	57:Ak:448:THR:HG23	2.03	0.41
57:Ak:407:GLN:H	57:Ak:407:GLN:CD	2.28	0.41
58:Al:145:PRO:HD3	58:Al:219:PHE:CG	2.56	0.41
58:Al:196:CYS:HB2	58:Al:207:MET:HB2	2.03	0.41
59:Am:253:TYR:HA	59:Am:257:TYR:CD2	2.55	0.41
60:An:40:ASP:OD2	60:An:88:GLU:HG2	2.20	0.41
51:5:377:MET:HE2	51:5:476:PHE:HA	2.02	0.41
51:5:445:CYS:O	51:5:449:PHE:HB2	2.21	0.41
65:G:371:VAL:HG23	65:G:482:GLN:HE22	1.86	0.41
65:G:618:GLU:HB3	65:G:621:LYS:HG3	2.01	0.41
65:G:624:ARG:HH12	65:G:628:GLU:CD	2.29	0.41
3:2:200:ARG:NH1	3:2:208:GLU:HG3	2.36	0.41
3:2:225:ARG:HE	3:2:281:VAL:CG2	2.34	0.41
5:6:47:LEU:HD21	5:6:234:ALA:HB1	2.03	0.41
5:6:182:TYR:O	5:6:187:ALA:HB2	2.21	0.41
5:6:244:LEU:HA	5:6:244:LEU:HD13	1.90	0.41
6:7:310:SER:HB2	6:7:370:SER:HB3	2.03	0.41
10:a:111:GLU:HG3	10:a:119:ARG:HH22	1.86	0.41
10:a:113:PHE:O	13:d:63:TYR:HB2	2.21	0.41
10:a:142:ILE:O	10:a:146:LYS:HG3	2.20	0.41
18:i:112:HIS:CE1	18:i:164:ILE:HD13	2.56	0.41
18:i:215:MET:HE2	18:i:215:MET:HA	2.03	0.41
18:i:215:MET:HG3	18:i:251:MET:SD	2.61	0.41
19:j:6:THR:HA	26:r:6:ILE:HD11	2.02	0.41
25:q:196:TRP:HZ3	25:q:261:PHE:HE2	1.68	0.41
26:r:222:MET:HA	26:r:225:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:126:LYS:HB2	27:B:275:LEU:HD23	2.03	0.41
27:B:379:CYS:HB2	72:B:502:SF4:FE1	1.55	0.41
28:C:197:ALA:HB1	28:C:202:ALA:HB3	2.02	0.41
28:C:200:ILE:HD12	28:C:274:TRP:CZ3	2.56	0.41
28:C:246:LEU:O	28:C:250:ILE:HG13	2.21	0.41
28:C:272:ARG:HG2	28:C:276:ASN:HD21	1.86	0.41
33:I:65:MET:HA	33:I:95:ALA:HB1	2.03	0.41
35:K:2:GLU:HA	35:K:5:GLN:NE2	2.36	0.41
37:O:84:LEU:HB3	37:O:88:LYS:HE2	2.03	0.41
40:R:93:LEU:HD23	40:R:96:PHE:HD2	1.85	0.41
48:l:103:PHE:HZ	48:l:344:GLY:HA3	1.84	0.41
50:t:14:SER:O	50:t:109:LEU:HD22	2.20	0.41
50:t:111:ARG:HG3	50:t:115:ARG:HH11	1.85	0.41
7:x:117:VAL:HG12	70:x:401:HEC:HBB1	2.03	0.41
57:Ak:143:VAL:HB	57:Ak:213:ARG:CZ	2.51	0.41
57:Ak:427:PRO:HB3	57:Ak:450:TRP:CE3	2.55	0.41
58:Al:86:MET:HE2	58:Al:86:MET:HB3	1.75	0.41
58:Al:116:LEU:HD11	58:Al:226:MET:HE3	2.02	0.41
58:Al:158:ASP:OD1	58:Al:158:ASP:N	2.55	0.41
59:Am:204:HIS:CE1	59:Am:249:TRP:HB2	2.55	0.41
51:5:80:ARG:NH2	51:5:350:GLU:OE2	2.41	0.41
66:L:354:TYR:N	66:L:354:TYR:CD1	2.90	0.41
3:4:133:GLY:CA	2:Ac:11:TYR:HB2	2.51	0.40
3:4:192:GLY:HA3	6:w:169:SER:OG	2.21	0.40
5:6:49:ILE:HD13	5:6:231:LYS:HA	2.03	0.40
5:6:113:THR:HA	3:Ae:61:ALA:O	2.21	0.40
6:7:185:LEU:HD23	6:7:185:LEU:HA	1.78	0.40
12:c:38:PRO:HD2	23:o:70:TYR:CD2	2.49	0.40
13:d:71:VAL:HB	22:n:44:LEU:HD13	2.02	0.40
19:j:74:PRO:O	19:j:75:LEU:C	2.64	0.40
21:m:130:THR:HG21	45:W:124:LEU:HD12	2.03	0.40
23:o:62:ASP:O	23:o:63:PRO:C	2.64	0.40
24:p:126:GLU:H	24:p:126:GLU:CD	2.29	0.40
24:p:156:MET:HE3	24:p:157:TYR:CE2	2.56	0.40
25:q:19:LYS:H	25:q:19:LYS:HG2	1.46	0.40
25:q:22:MET:HA	25:q:25:ILE:HD13	2.02	0.40
25:q:142:ARG:CZ	28:C:42:GLN:HE21	2.33	0.40
27:B:42:PHE:HZ	27:B:246:GLU:HG3	1.85	0.40
27:B:380:GLY:N	72:B:502:SF4:S3	2.93	0.40
29:D:69:LEU:HD11	29:D:99:PHE:CD2	2.56	0.40
36:N:56:LEU:HG	36:N:60:LYS:HE2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:8:ARG:HH22	50:t:19:PRO:HD3	1.86	0.40
51:u:68:THR:HG21	5:v:384:MET:CG	2.51	0.40
5:v:101:ARG:HA	5:v:101:ARG:HD3	1.89	0.40
7:x:157:ASP:HB3	7:x:166:PHE:CE1	2.56	0.40
57:Ak:133:ALA:O	57:Ak:213:ARG:NE	2.50	0.40
57:Ak:486:GLU:HG3	60:An:41:ARG:NH1	2.37	0.40
58:Al:200:CYS:SG	58:Al:207:MET:SD	3.14	0.40
59:Am:190:ASP:HB3	63:Aq:65:LEU:HD23	2.03	0.40
64:Ar:5:ILE:O	64:Ar:9:ILE:HG13	2.21	0.40
51:5:392:LYS:O	51:5:396:ARG:HG3	2.21	0.40
51:5:440:VAL:O	51:5:444:VAL:HG23	2.21	0.40
65:G:337:ASP:O	65:G:543:LYS:N	2.53	0.40
65:G:438:LEU:O	65:G:439:THR:OG1	2.30	0.40
1:0:45:LYS:HB2	1:0:45:LYS:HE2	1.79	0.40
7:8:115:PHE:CE2	7:8:149:LEU:HD13	2.56	0.40
9:A:20:HIS:HB3	58:Al:44:LEU:CD2	2.50	0.40
18:i:287:LEU:HD21	25:q:158:LEU:HD11	2.03	0.40
19:j:87:MET:HG2	21:m:147:TYR:HB3	2.03	0.40
21:m:17:PHE:HA	21:m:20:PHE:CD2	2.57	0.40
21:m:145:ALA:O	21:m:149:TYR:N	2.54	0.40
22:n:11:HIS:O	22:n:12:TRP:C	2.64	0.40
22:n:50:ARG:HG2	22:n:53:GLU:CD	2.46	0.40
25:q:23:ILE:HG13	25:q:24:TRP:H	1.86	0.40
25:q:238:LEU:HD23	25:q:238:LEU:HA	1.91	0.40
27:B:52:ARG:O	27:B:55:GLY:N	2.54	0.40
27:B:77:LEU:HD23	27:B:77:LEU:HA	1.90	0.40
27:B:116:ASN:ND2	27:B:207:GLY:O	2.53	0.40
27:B:340:ASP:O	27:B:344:GLN:HG2	2.21	0.40
32:H:49:ASP:OD2	32:H:51:LYS:HB3	2.21	0.40
35:K:69:ASN:HD21	35:K:112:ASN:HD21	1.68	0.40
38:P:69:TYR:HB2	38:P:73:GLN:NE2	2.36	0.40
51:u:41:ALA:O	51:u:45:VAL:HG23	2.21	0.40
6:w:224:TYR:CE1	7:x:312:TRP:CH2	3.08	0.40
7:x:113:ARG:O	7:x:117:VAL:HG23	2.21	0.40
2:Ac:53:TRP:O	2:Ac:57:LYS:HG3	2.21	0.40
55:Ai:53:TRP:NE1	60:An:115:ALA:HB2	2.37	0.40
55:Ai:60:ILE:HD11	55:Ai:62:ILE:HD11	2.03	0.40
57:Ak:371:TYR:CD1	57:Ak:436:MET:HG2	2.57	0.40
59:Am:219:LEU:O	59:Am:223:LEU:HG	2.21	0.40
62:Ap:107:LYS:HE3	62:Ap:107:LYS:HB2	1.91	0.40
51:5:274:GLU:HA	51:5:456:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:L:58:GLY:O	66:L:59:PHE:C	2.64	0.40
3:4:263:HIS:O	3:4:270:ILE:HD12	2.22	0.40
6:7:132:VAL:HG22	6:7:143:ALA:HB2	2.03	0.40
10:a:60:SER:HA	24:p:149:TRP:CD1	2.56	0.40
17:h:7:GLN:HB3	17:h:12:LEU:O	2.21	0.40
18:i:181:TYR:OH	20:k:98:CYS:HB3	2.21	0.40
19:j:60:ILE:O	19:j:64:LEU:HG	2.21	0.40
24:p:149:TRP:HZ3	24:p:157:TYR:CD2	2.40	0.40
26:r:58:LYS:HB3	26:r:217:ALA:CB	2.52	0.40
26:r:63:PRO:HG2	26:r:71:PHE:CE2	2.56	0.40
26:r:135:ALA:O	26:r:139:THR:HG23	2.22	0.40
28:C:299:LEU:HB3	28:C:304:ILE:HG23	2.02	0.40
43:U:130:SER:HB3	43:U:175:MET:HE3	2.03	0.40
46:Y:92:TRP:O	50:t:107:ARG:NH2	2.55	0.40
48:l:366:MET:HB3	48:l:369:THR:OG1	2.20	0.40
5:v:194:ASP:HA	5:v:197:ILE:HG12	2.03	0.40
5:v:211:ASN:HB3	5:v:246:LEU:HG	2.03	0.40
6:w:300:ILE:HD12	6:w:300:ILE:HA	1.93	0.40
6:w:366:MET:HB2	6:w:367:PRO:HD3	2.03	0.40
52:z:33:LYS:C	52:z:36:PRO:HD2	2.46	0.40
58:Al:13:THR:HG23	58:Al:168:LEU:HD23	2.03	0.40
51:5:379:LEU:HD23	51:5:379:LEU:HA	1.91	0.40
65:G:178:GLN:HG2	65:G:204:MET:HE2	2.02	0.40
65:G:347:ASP:CB	65:G:594:ALA:HB1	2.51	0.40
66:L:137:GLU:HB2	66:L:174:ARG:HH12	1.86	0.40
3:Ae:52:GLY:CA	3:Ae:61:ALA:HA	2.47	0.40
7:8:117:VAL:HG11	7:8:271:VAL:HB	2.03	0.40
10:a:101:ILE:HG23	10:a:107:PRO:HD3	2.03	0.40
10:a:139:ILE:HG13	22:n:35:LEU:HD22	2.04	0.40
10:a:186:THR:O	10:a:189:ASN:ND2	2.54	0.40
11:b:11:ARG:NH2	24:p:207:PRO:O	2.55	0.40
11:b:68:SER:O	11:b:72:VAL:HG12	2.21	0.40
13:d:28:ASN:ND2	50:t:74:PHE:HD2	2.19	0.40
13:d:171:LYS:O	13:d:172:GLU:C	2.64	0.40
20:k:31:LEU:HD23	21:m:68:PHE:CD2	2.56	0.40
24:p:107:ARG:O	24:p:111:GLU:HG3	2.21	0.40
27:B:35:LEU:CD2	27:B:40:ARG:HG2	2.51	0.40
28:C:382:GLU:O	28:C:386:HIS:HD2	2.04	0.40
28:C:438:LEU:HD12	28:C:438:LEU:HA	1.97	0.40
28:C:450:LEU:O	28:C:454:VAL:HG23	2.22	0.40
29:D:47:ILE:HD11	67:M:57:ARG:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:65:MET:HE3	33:I:65:MET:HB2	1.73	0.40
39:Q:99:VAL:HG12	39:Q:101:ASP:H	1.86	0.40
39:Q:113:LYS:HD2	39:Q:113:LYS:HA	1.94	0.40
41:S:6:LEU:O	41:S:7:PRO:C	2.61	0.40
48:l:178:GLY:HA2	48:l:218:LEU:HG	2.04	0.40
5:v:37:ASP:OD1	5:v:38:LEU:N	2.55	0.40
5:v:48:VAL:HG11	5:v:400:ALA:HB1	2.03	0.40
5:v:138:LEU:HD13	5:v:237:PHE:HB2	2.03	0.40
5:v:213:PHE:HB3	5:v:218:MET:HE3	2.04	0.40
57:Ak:467:LEU:O	57:Ak:471:ILE:HG13	2.22	0.40
58:Al:12:ALA:CB	58:Al:17:MET:HB3	2.51	0.40
58:Al:146:MET:HG2	58:Al:214:VAL:C	2.46	0.40
51:5:384:THR:O	51:5:387:GLU:HG2	2.22	0.40
65:G:163:LYS:HD3	65:G:173:MET:HG3	2.02	0.40
66:L:141:VAL:C	66:L:144:PRO:HD2	2.47	0.40
3:Af:75:LEU:H	3:Af:75:LEU:HD12	1.87	0.40
3:4:158:VAL:HG13	6:w:163:TRP:NE1	2.36	0.40
3:4:251:ASP:OD1	3:4:263:HIS:ND1	2.54	0.40
5:6:105:ALA:HA	51:5:390:ARG:HG3	2.03	0.40
5:6:367:SER:O	5:6:371:VAL:HG23	2.22	0.40
5:6:444:LEU:HB3	5:6:447:THR:HB	2.03	0.40
11:b:105:PHE:O	11:b:107:GLY:N	2.55	0.40
13:d:110:LEU:HD23	13:d:110:LEU:HA	1.80	0.40
17:h:63:PHE:CZ	17:h:67:LEU:HD11	2.57	0.40
18:i:5:ILE:HG23	21:m:166:VAL:HG11	2.01	0.40
18:i:6:TYR:CE1	18:i:46:LYS:HD2	2.57	0.40
18:i:18:MET:O	18:i:22:ILE:HG12	2.22	0.40
23:o:10:ARG:HG3	23:o:11:LEU:N	2.36	0.40
25:q:80:SER:HA	25:q:83:HIS:CE1	2.56	0.40
25:q:109:THR:HG22	25:q:121:LEU:HB2	2.03	0.40
27:B:343:VAL:HA	27:B:347:THR:O	2.20	0.40
28:C:147:TYR:HB3	33:I:71:CYS:HB3	2.03	0.40
29:D:103:HIS:O	29:D:103:HIS:CG	2.74	0.40
30:E:133:GLN:HG3	30:E:172:ILE:HG23	2.04	0.40
32:H:113:CYS:O	32:H:141:ARG:NH1	2.54	0.40
33:I:77:MET:HG2	33:I:93:PHE:HZ	1.85	0.40
48:l:379:ALA:O	48:l:388:GLY:HA3	2.21	0.40
49:s:115:LYS:N	49:s:116:PRO:HD2	2.36	0.40
6:w:185:LEU:HD23	6:w:185:LEU:HA	1.87	0.40
58:Al:17:MET:HG2	58:Al:169:GLY:HA3	2.02	0.40
51:5:393:ASN:OD1	51:5:396:ARG:NH1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:L:165:LEU:HD12	66:L:199:SER:HB2	2.03	0.40
66:L:190:PHE:CE1	66:L:192:GLU:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	66/91 (72%)	63 (96%)	2 (3%)	1 (2%)	8	30
1	Ab	64/91 (70%)	62 (97%)	2 (3%)	0	100	100
2	1	58/64 (91%)	58 (100%)	0	0	100	100
2	Ac	57/64 (89%)	57 (100%)	0	0	100	100
3	2	193/299 (64%)	186 (96%)	7 (4%)	0	100	100
3	4	194/299 (65%)	189 (97%)	5 (3%)	0	100	100
3	Ae	37/299 (12%)	26 (70%)	11 (30%)	0	100	100
3	Af	31/299 (10%)	20 (64%)	11 (36%)	0	100	100
4	3	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
4	Ad	49/56 (88%)	46 (94%)	3 (6%)	0	100	100
5	6	416/453 (92%)	402 (97%)	14 (3%)	0	100	100
5	v	416/453 (92%)	407 (98%)	9 (2%)	0	100	100
6	7	377/379 (100%)	373 (99%)	4 (1%)	0	100	100
6	w	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
7	8	237/326 (73%)	231 (98%)	6 (2%)	0	100	100
7	x	236/326 (72%)	223 (94%)	11 (5%)	2 (1%)	16	44
8	9	99/111 (89%)	99 (100%)	0	0	100	100
8	y	99/111 (89%)	99 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	A	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
10	a	136/189 (72%)	128 (94%)	8 (6%)	0	100	100
11	b	101/128 (79%)	87 (86%)	12 (12%)	2 (2%)	6	24
12	c	150/186 (81%)	139 (93%)	9 (6%)	2 (1%)	9	33
13	d	167/176 (95%)	160 (96%)	7 (4%)	0	100	100
14	e	97/154 (63%)	88 (91%)	9 (9%)	0	100	100
15	f	44/76 (58%)	41 (93%)	3 (7%)	0	100	100
16	g	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
17	h	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
18	i	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
19	j	87/115 (76%)	85 (98%)	2 (2%)	0	100	100
20	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
21	m	155/175 (89%)	142 (92%)	10 (6%)	3 (2%)	6	26
22	n	51/58 (88%)	43 (84%)	8 (16%)	0	100	100
23	o	126/129 (98%)	120 (95%)	5 (4%)	1 (1%)	16	44
24	p	176/221 (80%)	168 (96%)	6 (3%)	2 (1%)	11	37
25	q	457/459 (100%)	445 (97%)	12 (3%)	0	100	100
26	r	304/318 (96%)	290 (95%)	12 (4%)	2 (1%)	18	47
27	B	429/464 (92%)	405 (94%)	24 (6%)	0	100	100
28	C	428/469 (91%)	403 (94%)	24 (6%)	1 (0%)	43	71
29	D	206/264 (78%)	180 (87%)	25 (12%)	1 (0%)	24	54
30	E	212/249 (85%)	201 (95%)	11 (5%)	0	100	100
31	F	93/123 (76%)	88 (95%)	5 (5%)	0	100	100
32	H	174/212 (82%)	168 (97%)	6 (3%)	0	100	100
33	I	154/263 (59%)	144 (94%)	9 (6%)	1 (1%)	21	49
34	J	116/175 (66%)	116 (100%)	0	0	100	100
35	K	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
36	N	110/116 (95%)	108 (98%)	2 (2%)	0	100	100
37	O	83/156 (53%)	79 (95%)	4 (5%)	0	100	100
37	X	83/156 (53%)	79 (95%)	4 (5%)	0	100	100
38	P	81/99 (82%)	73 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	Q	110/154 (71%)	106 (96%)	3 (3%)	1 (1%)	14	41
40	R	33/110 (30%)	33 (100%)	0	0	100	100
41	S	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
42	T	80/169 (47%)	76 (95%)	4 (5%)	0	100	100
43	U	316/357 (88%)	308 (98%)	7 (2%)	1 (0%)	36	65
44	V	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
45	W	138/144 (96%)	134 (97%)	4 (3%)	0	100	100
46	Y	58/105 (55%)	52 (90%)	4 (7%)	2 (3%)	3	17
47	Z	76/114 (67%)	72 (95%)	4 (5%)	0	100	100
48	l	600/606 (99%)	567 (94%)	29 (5%)	4 (1%)	18	47
49	s	169/249 (68%)	153 (90%)	14 (8%)	2 (1%)	10	35
50	t	117/137 (85%)	107 (92%)	9 (8%)	1 (1%)	14	41
51	5	431/480 (90%)	415 (96%)	16 (4%)	0	100	100
51	u	444/480 (92%)	432 (97%)	12 (3%)	0	100	100
52	Aa	76/82 (93%)	75 (99%)	1 (1%)	0	100	100
52	z	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
53	Ag	41/70 (59%)	41 (100%)	0	0	100	100
54	Ah	54/80 (68%)	53 (98%)	1 (2%)	0	100	100
55	Ai	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
56	Aj	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
57	Ak	511/514 (99%)	498 (98%)	13 (2%)	0	100	100
58	Al	218/228 (96%)	212 (97%)	4 (2%)	2 (1%)	14	41
59	Am	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
60	An	136/169 (80%)	132 (97%)	4 (3%)	0	100	100
61	Ao	102/152 (67%)	100 (98%)	2 (2%)	0	100	100
62	Ap	87/129 (67%)	85 (98%)	2 (2%)	0	100	100
63	Aq	71/97 (73%)	66 (93%)	5 (7%)	0	100	100
64	Ar	80/86 (93%)	80 (100%)	0	0	100	100
65	G	680/727 (94%)	658 (97%)	21 (3%)	1 (0%)	48	78
66	L	310/372 (83%)	291 (94%)	18 (6%)	1 (0%)	36	65
67	M	92/113 (81%)	85 (92%)	6 (6%)	1 (1%)	11	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	13802/16800 (82%)	13230 (96%)	538 (4%)	34 (0%)	44	71

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	Y	40	ILE
7	x	179	PRO
66	L	224	ILE
1	0	67	CYS
48	l	562	LEU
49	s	239	LYS
11	b	106	PRO
21	m	138	GLU
23	o	75	ASN
48	l	71	LEU
48	l	249	SER
50	t	29	TYR
58	Al	52	HIS
11	b	107	GLY
33	I	96	SER
43	U	255	CYS
7	x	247	PRO
67	M	41	LEU
12	c	163	TYR
21	m	125	TRP
24	p	213	VAL
26	r	66	SER
29	D	122	ARG
46	Y	48	PRO
48	l	208	CYS
58	Al	158	ASP
65	G	136	GLU
28	C	203	MET
49	s	232	GLU
12	c	155	PRO
24	p	188	PRO
26	r	37	PRO
39	Q	122	VAL
21	m	63	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	65/85 (76%)	59 (91%)	6 (9%)	8	29
1	Ab	63/85 (74%)	57 (90%)	6 (10%)	8	28
2	1	49/52 (94%)	49 (100%)	0	100	100
2	Ac	48/52 (92%)	48 (100%)	0	100	100
3	2	166/245 (68%)	161 (97%)	5 (3%)	36	59
3	4	166/245 (68%)	157 (95%)	9 (5%)	20	46
3	Ae	29/245 (12%)	26 (90%)	3 (10%)	7	24
3	Af	23/245 (9%)	23 (100%)	0	100	100
4	3	40/46 (87%)	37 (92%)	3 (8%)	12	37
4	Ad	41/46 (89%)	39 (95%)	2 (5%)	22	48
5	6	329/355 (93%)	315 (96%)	14 (4%)	26	50
5	v	329/355 (93%)	317 (96%)	12 (4%)	31	55
6	7	332/332 (100%)	328 (99%)	4 (1%)	63	72
6	w	332/332 (100%)	325 (98%)	7 (2%)	47	64
7	8	204/259 (79%)	197 (97%)	7 (3%)	32	56
7	x	203/259 (78%)	195 (96%)	8 (4%)	28	53
8	9	93/99 (94%)	91 (98%)	2 (2%)	45	63
8	y	93/99 (94%)	89 (96%)	4 (4%)	26	50
9	A	49/61 (80%)	47 (96%)	2 (4%)	27	52
10	a	121/158 (77%)	119 (98%)	2 (2%)	53	67
11	b	95/121 (78%)	87 (92%)	8 (8%)	10	33
12	c	136/160 (85%)	130 (96%)	6 (4%)	25	50
13	d	152/156 (97%)	143 (94%)	9 (6%)	18	43
14	e	90/129 (70%)	81 (90%)	9 (10%)	7	25
15	f	41/66 (62%)	39 (95%)	2 (5%)	22	48
16	g	108/109 (99%)	98 (91%)	10 (9%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	h	93/94 (99%)	88 (95%)	5 (5%)	20	46
18	i	311/311 (100%)	296 (95%)	15 (5%)	23	48
19	j	78/100 (78%)	68 (87%)	10 (13%)	4	16
20	k	85/85 (100%)	79 (93%)	6 (7%)	13	38
21	m	129/141 (92%)	118 (92%)	11 (8%)	10	32
22	n	49/55 (89%)	46 (94%)	3 (6%)	17	42
23	o	113/114 (99%)	105 (93%)	8 (7%)	13	38
24	p	159/190 (84%)	152 (96%)	7 (4%)	25	50
25	q	409/409 (100%)	386 (94%)	23 (6%)	19	45
26	r	267/275 (97%)	254 (95%)	13 (5%)	22	48
27	B	345/368 (94%)	327 (95%)	18 (5%)	21	47
28	C	371/398 (93%)	349 (94%)	22 (6%)	18	43
29	D	188/228 (82%)	181 (96%)	7 (4%)	30	54
30	E	183/207 (88%)	177 (97%)	6 (3%)	33	57
31	F	79/97 (81%)	77 (98%)	2 (2%)	42	61
32	H	151/176 (86%)	141 (93%)	10 (7%)	15	40
33	I	132/217 (61%)	124 (94%)	8 (6%)	17	42
34	J	107/152 (70%)	105 (98%)	2 (2%)	50	66
35	K	130/131 (99%)	126 (97%)	4 (3%)	35	58
36	N	99/101 (98%)	93 (94%)	6 (6%)	17	42
37	O	79/132 (60%)	71 (90%)	8 (10%)	7	25
37	X	79/132 (60%)	70 (89%)	9 (11%)	5	20
38	P	74/82 (90%)	70 (95%)	4 (5%)	20	46
39	Q	105/134 (78%)	100 (95%)	5 (5%)	23	48
40	R	34/92 (37%)	33 (97%)	1 (3%)	37	59
41	S	58/58 (100%)	56 (97%)	2 (3%)	32	56
42	T	69/134 (52%)	66 (96%)	3 (4%)	26	50
43	U	278/307 (91%)	269 (97%)	9 (3%)	34	57
44	V	101/102 (99%)	99 (98%)	2 (2%)	48	65
45	W	122/124 (98%)	119 (98%)	3 (2%)	42	61
46	Y	54/84 (64%)	46 (85%)	8 (15%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	Z	60/90 (67%)	54 (90%)	6 (10%)	7	25
48	l	535/540 (99%)	502 (94%)	33 (6%)	16	42
49	s	153/206 (74%)	145 (95%)	8 (5%)	21	47
50	t	97/120 (81%)	83 (86%)	14 (14%)	3	13
51	5	363/397 (91%)	357 (98%)	6 (2%)	53	67
51	u	372/397 (94%)	359 (96%)	13 (4%)	32	55
52	Aa	70/73 (96%)	64 (91%)	6 (9%)	10	32
52	z	70/73 (96%)	65 (93%)	5 (7%)	13	38
53	Ag	37/57 (65%)	37 (100%)	0	100	100
54	Ah	47/68 (69%)	45 (96%)	2 (4%)	26	50
55	Ai	38/66 (58%)	36 (95%)	2 (5%)	20	46
56	Aj	39/55 (71%)	38 (97%)	1 (3%)	40	60
57	Ak	422/425 (99%)	405 (96%)	17 (4%)	28	52
58	Al	206/212 (97%)	199 (97%)	7 (3%)	32	56
59	Am	223/225 (99%)	220 (99%)	3 (1%)	61	71
60	An	123/149 (83%)	117 (95%)	6 (5%)	22	48
61	Ao	91/124 (73%)	86 (94%)	5 (6%)	19	45
62	Ap	77/101 (76%)	75 (97%)	2 (3%)	40	60
63	Aq	64/80 (80%)	63 (98%)	1 (2%)	55	68
64	Ar	73/76 (96%)	68 (93%)	5 (7%)	14	39
65	G	576/610 (94%)	561 (97%)	15 (3%)	40	60
66	L	268/320 (84%)	254 (95%)	14 (5%)	21	47
67	M	85/98 (87%)	78 (92%)	7 (8%)	10	34
All	All	12017/14188 (85%)	11459 (95%)	558 (5%)	25	49

All (558) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	ASP
1	0	35	GLU
1	0	44	ILE
1	0	54	ASP
1	0	66	ASP
1	0	71	LEU

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Mol	Chain	Res	Type
3	2	205	ILE
3	2	222	ASP
3	2	238	CYS
3	2	287	THR
3	2	292	VAL
4	3	18	ILE
4	3	39	ARG
4	3	42	LEU
3	4	119	ASP
3	4	177	LEU
3	4	212	GLU
3	4	224	GLU
3	4	232	VAL
3	4	240	HIS
3	4	251	ASP
3	4	283	THR
3	4	285	GLU
5	6	83	LEU
5	6	122	THR
5	6	129	ASP
5	6	134	MET
5	6	218	MET
5	6	230	LEU
5	6	235	GLU
5	6	244	LEU
5	6	260	ASP
5	6	309	LEU
5	6	323	VAL
5	6	365	ASN
5	6	378	LEU
5	6	450	VAL
6	7	2	THR
6	7	97	HIS
6	7	124	MET
6	7	264	THR
7	8	121	VAL
7	8	136	LEU
7	8	201	ILE
7	8	255	GLU
7	8	258	ASP
7	8	263	THR
7	8	297	MET

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Mol	Chain	Res	Type
8	9	43	ASP
8	9	75	ILE
9	A	29	LEU
9	A	45	LYS
10	a	57	ILE
10	a	130	GLU
11	b	18	LEU
11	b	23	LEU
11	b	24	LYS
11	b	35	LEU
11	b	60	VAL
11	b	104	ILE
11	b	119	LEU
11	b	120	MET
12	c	81	ARG
12	c	110	ASP
12	c	119	THR
12	c	139	PHE
12	c	156	VAL
12	c	166	LEU
13	d	17	THR
13	d	24	THR
13	d	33	LEU
13	d	63	TYR
13	d	68	PHE
13	d	83	LEU
13	d	146	LEU
13	d	155	CYS
13	d	163	MET
14	e	55	LEU
14	e	63	ASP
14	e	65	ASN
14	e	83	ASP
14	e	100	VAL
14	e	116	GLU
14	e	136	LEU
14	e	145	ASN
14	e	146	LYS
15	f	29	PHE
15	f	48	LEU
16	g	3	MET
16	g	16	LEU

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Mol	Chain	Res	Type
16	g	28	LEU
16	g	52	ARG
16	g	64	LEU
16	g	89	ASP
16	g	90	HIS
16	g	115	LEU
16	g	116	GLU
16	g	121	VAL
17	h	18	MET
17	h	72	THR
17	h	75	ARG
17	h	86	LEU
17	h	101	LYS
18	i	17	THR
18	i	149	ILE
18	i	154	MET
18	i	193	VAL
18	i	204	ASN
18	i	228	LEU
18	i	244	MET
18	i	258	SER
18	i	278	MET
18	i	290	LEU
18	i	311	MET
18	i	313	MET
18	i	336	VAL
18	i	343	LEU
18	i	346	LEU
19	j	13	LEU
19	j	16	LEU
19	j	53	MET
19	j	57	LEU
19	j	58	VAL
19	j	68	GLU
19	j	69	ILE
19	j	73	LEU
19	j	82	ASN
19	j	86	THR
20	k	10	MET
20	k	29	SER
20	k	43	MET
20	k	64	LEU

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Mol	Chain	Res	Type
20	k	70	GLU
20	k	76	SER
21	m	1	MET
21	m	2	THR
21	m	45	LEU
21	m	61	LEU
21	m	65	LEU
21	m	66	VAL
21	m	111	GLU
21	m	113	VAL
21	m	122	LEU
21	m	139	GLU
21	m	168	ILE
22	n	13	VAL
22	n	14	HIS
22	n	56	THR
23	o	30	ARG
23	o	37	LEU
23	o	45	ARG
23	o	56	ARG
23	o	60	ILE
23	o	102	TYR
23	o	104	VAL
23	o	127	ILE
24	p	75	HIS
24	p	97	LYS
24	p	147	ASP
24	p	164	ARG
24	p	170	LEU
24	p	171	ARG
24	p	177	ARG
25	q	11	LEU
25	q	14	MET
25	q	19	LYS
25	q	36	LEU
25	q	47	GLU
25	q	61	LEU
25	q	66	LEU
25	q	98	MET
25	q	179	ILE
25	q	195	MET
25	q	231	LEU

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Mol	Chain	Res	Type
25	q	252	PRO
25	q	266	MET
25	q	282	LEU
25	q	375	LEU
25	q	400	MET
25	q	409	TYR
25	q	420	THR
25	q	423	ILE
25	q	437	MET
25	q	441	ILE
25	q	444	LEU
25	q	452	LYS
26	r	13	ILE
26	r	70	MET
26	r	106	LEU
26	r	111	LEU
26	r	136	VAL
26	r	150	LEU
26	r	151	LEU
26	r	213	VAL
26	r	222	MET
26	r	253	GLU
26	r	279	ARG
26	r	282	TYR
26	r	310	MET
27	B	41	ILE
27	B	102	MET
27	B	131	ILE
27	B	134	ASP
27	B	170	GLN
27	B	171	VAL
27	B	195	VAL
27	B	226	LYS
27	B	232	ASP
27	B	277	ASN
27	B	278	ILE
27	B	282	VAL
27	B	294	VAL
27	B	317	VAL
27	B	327	ILE
27	B	349	LEU
27	B	405	ARG

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Mol	Chain	Res	Type
27	B	457	HIS
28	C	57	VAL
28	C	72	TRP
28	C	81	THR
28	C	88	LEU
28	C	107	LEU
28	C	139	LEU
28	C	143	ASP
28	C	167	ILE
28	C	191	MET
28	C	194	THR
28	C	195	THR
28	C	228	MET
28	C	238	VAL
28	C	244	LEU
28	C	247	LEU
28	C	284	VAL
28	C	304	ILE
28	C	362	ILE
28	C	418	VAL
28	C	446	LYS
28	C	462	ILE
28	C	466	GLU
29	D	47	ILE
29	D	104	THR
29	D	119	VAL
29	D	121	THR
29	D	148	ASP
29	D	216	VAL
29	D	234	ASP
30	E	95	ILE
30	E	137	THR
30	E	150	GLU
30	E	190	ASP
30	E	201	ILE
30	E	203	GLU
31	F	29	VAL
31	F	46	ASP
32	H	48	MET
32	H	54	THR
32	H	73	THR
32	H	114	ILE

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Mol	Chain	Res	Type
32	H	119	CYS
32	H	128	ILE
32	H	133	GLU
32	H	135	ARG
32	H	150	THR
32	H	175	PHE
33	I	42	ARG
33	I	65	MET
33	I	71	CYS
33	I	84	TYR
33	I	93	PHE
33	I	117	LEU
33	I	154	ASP
33	I	192	ILE
34	J	86	ASN
34	J	147	VAL
35	K	7	LEU
35	K	11	LEU
35	K	88	ARG
35	K	129	THR
36	N	5	LEU
36	N	11	LEU
36	N	19	THR
36	N	70	GLU
36	N	88	LEU
36	N	95	LEU
37	O	74	LEU
37	O	76	LEU
37	O	87	LEU
37	O	94	ASP
37	O	108	LEU
37	O	113	LEU
37	O	138	LEU
37	O	154	VAL
38	P	16	LEU
38	P	19	ILE
38	P	57	GLU
38	P	58	CYS
39	Q	68	GLU
39	Q	72	THR
39	Q	107	LEU
39	Q	117	GLU

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Mol	Chain	Res	Type
39	Q	127	THR
40	R	89	LEU
41	S	12	MET
41	S	40	HIS
42	T	120	LEU
42	T	150	ASP
42	T	151	VAL
43	U	43	LEU
43	U	78	GLU
43	U	229	MET
43	U	243	TYR
43	U	250	GLU
43	U	263	ARG
43	U	278	LEU
43	U	281	ASP
43	U	312	ILE
44	V	99	LEU
44	V	115	CYS
45	W	88	ARG
45	W	120	MET
45	W	129	THR
37	X	75	THR
37	X	105	MET
37	X	108	LEU
37	X	114	ASP
37	X	120	MET
37	X	122	MET
37	X	138	LEU
37	X	140	CYS
37	X	153	ASP
46	Y	40	ILE
46	Y	46	GLN
46	Y	50	LEU
46	Y	51	THR
46	Y	65	MET
46	Y	70	LEU
46	Y	75	HIS
46	Y	88	ASP
47	Z	32	LEU
47	Z	48	VAL
47	Z	55	ARG
47	Z	57	LEU

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Mol	Chain	Res	Type
47	Z	73	PHE
47	Z	104	LEU
48	l	7	LEU
48	l	9	LEU
48	l	55	MET
48	l	61	MET
48	l	65	ASN
48	l	69	MET
48	l	70	THR
48	l	105	MET
48	l	129	MET
48	l	210	ASN
48	l	217	LEU
48	l	233	LEU
48	l	238	GLU
48	l	246	LEU
48	l	252	MET
48	l	268	GLU
48	l	286	LEU
48	l	313	MET
48	l	340	PHE
48	l	373	LEU
48	l	396	ILE
48	l	410	LEU
48	l	426	ILE
48	l	482	MET
48	l	488	MET
48	l	489	THR
48	l	491	LEU
48	l	504	LEU
48	l	512	LYS
48	l	525	MET
48	l	544	MET
48	l	572	LYS
48	l	589	LEU
49	s	90	LEU
49	s	97	VAL
49	s	101	VAL
49	s	125	TRP
49	s	186	GLU
49	s	235	LEU
49	s	236	LYS

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Mol	Chain	Res	Type
49	s	249	MET
50	t	20	LEU
50	t	22	MET
50	t	33	GLU
50	t	40	VAL
50	t	43	GLN
50	t	46	MET
50	t	47	ASN
50	t	52	MET
50	t	54	GLN
50	t	58	TYR
50	t	65	GLN
50	t	67	LEU
50	t	93	LEU
50	t	110	GLN
51	u	54	ASP
51	u	68	THR
51	u	95	HIS
51	u	116	MET
51	u	153	ASN
51	u	157	GLU
51	u	190	THR
51	u	253	LEU
51	u	258	VAL
51	u	341	PHE
51	u	342	GLN
51	u	403	LEU
51	u	417	LEU
5	v	43	LEU
5	v	130	ILE
5	v	134	MET
5	v	168	ASN
5	v	175	GLU
5	v	184	ASN
5	v	200	VAL
5	v	225	VAL
5	v	238	LEU
5	v	308	SER
5	v	421	ASP
5	v	451	ASP
6	w	97	HIS
6	w	102	LEU

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Mol	Chain	Res	Type
6	w	212	SER
6	w	214	ASP
6	w	233	LEU
6	w	281	LEU
6	w	379	TRP
7	x	91	HIS
7	x	122	CYS
7	x	164	GLU
7	x	172	LEU
7	x	209	GLU
7	x	258	ASP
7	x	293	MET
7	x	320	LEU
8	y	33	MET
8	y	75	ILE
8	y	99	ILE
8	y	103	LYS
52	z	16	THR
52	z	19	LEU
52	z	39	LEU
52	z	72	ARG
52	z	79	GLU
52	Aa	5	PHE
52	Aa	12	ARG
52	Aa	19	LEU
52	Aa	32	THR
52	Aa	35	ILE
52	Aa	71	LYS
1	Ab	35	GLU
1	Ab	48	GLU
1	Ab	51	GLU
1	Ab	52	LEU
1	Ab	54	ASP
1	Ab	69	GLU
4	Ad	6	LEU
4	Ad	18	ILE
54	Ah	32	ILE
54	Ah	49	ASP
55	Ai	72	VAL
55	Ai	73	THR
56	Aj	43	LEU
57	Ak	28	MET

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Mol	Chain	Res	Type
57	Ak	35	LEU
57	Ak	100	MET
57	Ak	117	MET
57	Ak	119	GLU
57	Ak	136	LEU
57	Ak	138	HIS
57	Ak	238	PHE
57	Ak	243	VAL
57	Ak	300	ASP
57	Ak	376	HIS
57	Ak	417	MET
57	Ak	440	TYR
57	Ak	462	LEU
57	Ak	465	VAL
57	Ak	468	MET
57	Ak	513	LEU
58	Al	29	MET
58	Al	30	ILE
58	Al	44	LEU
58	Al	73	LEU
58	Al	89	GLU
58	Al	133	MET
58	Al	160	LEU
59	Am	40	MET
59	Am	45	LEU
59	Am	246	ASP
60	An	65	LYS
60	An	76	ASP
60	An	114	THR
60	An	129	ILE
60	An	145	MET
60	An	148	MET
61	Ao	74	LYS
61	Ao	104	PHE
61	Ao	114	VAL
61	Ao	129	ILE
61	Ao	143	THR
62	Ap	43	GLN
62	Ap	56	ARG
63	Aq	81	LEU
64	Ar	8	LYS
64	Ar	30	CYS

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Mol	Chain	Res	Type
64	Ar	42	LYS
64	Ar	61	TYR
64	Ar	67	ILE
51	5	96	LEU
51	5	266	THR
51	5	359	VAL
51	5	368	MET
51	5	433	ILE
51	5	467	ASP
65	G	56	VAL
65	G	137	CYS
65	G	197	THR
65	G	225	ILE
65	G	241	ARG
65	G	346	VAL
65	G	366	LEU
65	G	367	CYS
65	G	473	MET
65	G	559	ASP
65	G	637	ASP
65	G	652	ASN
65	G	671	LEU
65	G	679	LEU
65	G	680	LEU
66	L	32	HIS
66	L	52	THR
66	L	92	MET
66	L	102	GLU
66	L	113	LYS
66	L	119	ASN
66	L	132	LYS
66	L	158	LYS
66	L	175	TYR
66	L	232	LYS
66	L	235	VAL
66	L	312	ASP
66	L	354	TYR
66	L	360	GLU
67	M	10	LEU
67	M	11	LEU
67	M	25	GLN
67	M	31	ILE

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Mol	Chain	Res	Type
67	M	41	LEU
67	M	69	VAL
67	M	106	LEU
3	Ae	62	THR
3	Ae	67	VAL
3	Ae	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (214) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	88	ASN
3	2	240	HIS
4	3	16	ASN
3	4	185	ASN
3	4	220	GLN
3	4	221	HIS
5	6	36	GLN
5	6	75	ASN
5	6	155	GLN
5	6	168	ASN
5	6	170	GLN
5	6	311	GLN
5	6	318	HIS
5	6	319	GLN
5	6	343	GLN
5	6	357	GLN
5	6	443	ASN
6	7	97	HIS
7	8	91	HIS
7	8	116	GLN
7	8	241	GLN
7	8	251	ASN
7	8	310	HIS
8	9	23	ASN
10	a	141	GLN
10	a	181	HIS
10	a	189	ASN
11	b	14	GLN
11	b	83	HIS
12	c	115	ASN
13	d	23	GLN
13	d	123	GLN

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Mol	Chain	Res	Type
13	d	140	GLN
13	d	149	HIS
14	e	86	ASN
16	g	14	GLN
16	g	48	ASN
16	g	63	GLN
17	h	7	GLN
17	h	27	HIS
17	h	45	HIS
17	h	97	HIS
17	h	98	HIS
18	i	83	GLN
18	i	134	GLN
18	i	147	GLN
18	i	204	ASN
18	i	221	HIS
18	i	289	ASN
19	j	26	GLN
21	m	46	ASN
21	m	175	ASN
22	n	11	HIS
23	o	123	GLN
24	p	54	HIS
24	p	75	HIS
24	p	108	GLN
24	p	118	HIS
24	p	211	HIS
25	q	30	HIS
25	q	44	GLN
25	q	48	ASN
25	q	83	HIS
25	q	103	GLN
25	q	169	ASN
25	q	188	ASN
25	q	251	ASN
25	q	279	GLN
25	q	349	GLN
25	q	374	ASN
25	q	415	GLN
25	q	422	HIS
26	r	5	ASN
26	r	138	GLN

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Mol	Chain	Res	Type
26	r	169	GLN
26	r	247	HIS
26	r	250	HIS
26	r	304	HIS
27	B	170	GLN
27	B	244	ASN
27	B	381	GLN
27	B	418	GLN
28	C	42	GLN
28	C	85	ASN
28	C	93	GLN
28	C	196	HIS
28	C	239	HIS
28	C	240	GLN
28	C	271	ASN
28	C	276	ASN
28	C	460	GLN
29	D	63	GLN
29	D	124	ASN
29	D	181	HIS
29	D	236	ASN
30	E	41	HIS
30	E	47	ASN
30	E	99	ASN
30	E	144	ASN
30	E	153	GLN
30	E	189	ASN
31	F	74	GLN
32	H	159	GLN
33	I	123	GLN
33	I	138	ASN
34	J	85	ASN
34	J	86	ASN
35	K	59	HIS
35	K	69	ASN
35	K	112	ASN
35	K	113	HIS
35	K	123	GLN
35	K	135	GLN
36	N	41	ASN
37	O	103	HIS
37	O	142	GLN

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Mol	Chain	Res	Type
38	P	31	GLN
38	P	81	ASN
39	Q	77	GLN
39	Q	96	ASN
39	Q	152	HIS
40	R	78	HIS
40	R	90	ASN
41	S	68	ASN
44	V	89	ASN
45	W	61	GLN
45	W	112	HIS
46	Y	54	GLN
47	Z	49	GLN
47	Z	64	ASN
48	l	136	ASN
48	l	139	GLN
48	l	175	ASN
48	l	192	HIS
48	l	205	ASN
48	l	323	HIS
48	l	354	GLN
48	l	400	ASN
48	l	446	ASN
48	l	506	ASN
48	l	580	GLN
49	s	108	HIS
49	s	112	GLN
49	s	141	ASN
49	s	240	HIS
50	t	47	ASN
50	t	84	GLN
50	t	92	HIS
51	u	49	GLN
51	u	160	GLN
51	u	247	GLN
51	u	277	HIS
51	u	469	ASN
5	v	75	ASN
5	v	170	GLN
5	v	184	ASN
5	v	188	ASN
5	v	239	ASN

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Mol	Chain	Res	Type
5	v	372	GLN
5	v	443	ASN
6	w	255	ASN
7	x	91	HIS
7	x	190	ASN
7	x	283	HIS
8	y	23	ASN
52	z	29	HIS
52	Aa	65	GLN
1	Ab	36	GLN
1	Ab	76	HIS
54	Ah	34	GLN
57	Ak	55	ASN
57	Ak	61	HIS
57	Ak	138	HIS
57	Ak	151	HIS
57	Ak	178	GLN
57	Ak	214	ASN
57	Ak	422	ASN
57	Ak	451	ASN
57	Ak	491	ASN
58	Al	10	GLN
58	Al	203	ASN
58	Al	204	HIS
59	Am	56	GLN
59	Am	68	GLN
59	Am	149	HIS
59	Am	161	GLN
60	An	54	ASN
60	An	165	ASN
61	Ao	121	HIS
62	Ap	63	ASN
62	Ap	97	ASN
62	Ap	119	HIS
64	Ar	26	GLN
64	Ar	33	ASN
64	Ar	38	HIS
51	5	152	GLN
51	5	207	ASN
51	5	247	GLN
51	5	469	ASN
65	G	59	GLN

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Mol	Chain	Res	Type
65	G	142	GLN
65	G	202	ASN
65	G	304	GLN
65	G	498	GLN
65	G	652	ASN
65	G	666	GLN
65	G	688	GLN
66	L	74	GLN
66	L	117	HIS
66	L	133	ASN
66	L	145	HIS
66	L	149	GLN
67	M	25	GLN
3	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
72	SF4	H	302	32	0,12,12	-	-	-		
69	HEM	w	402	6	50,50,50	1.45	6 (12%)	67,82,82	0.96	1 (1%)
71	FMN	B	501	-	33,33,33	0.61	0	48,50,50	0.64	1 (2%)
69	HEM	7	402	-	50,50,50	1.58	9 (18%)	67,82,82	1.63	12 (17%)
70	HEC	8	401	7	50,50,50	1.73	5 (10%)	68,82,82	1.50	8 (11%)
74	HEA	Ak	601	57	67,67,67	2.53	29 (43%)	81,103,103	2.49	33 (40%)
68	FES	G	803	65	0,4,4	-	-	-		
68	FES	4	301	3	0,4,4	-	-	-		
74	HEA	Ak	602	57	67,67,67	2.45	25 (37%)	81,103,103	2.56	36 (44%)
72	SF4	B	502	27	0,12,12	-	-	-		
70	HEC	x	401	7	50,50,50	1.72	5 (10%)	68,82,82	1.33	7 (10%)
72	SF4	H	301	-	0,12,12	-	-	-		
72	SF4	I	201	33	0,12,12	-	-	-		
68	FES	E	301	30	0,4,4	-	-	-		
72	SF4	G	802	65	0,12,12	-	-	-		
75	NDP	L	401	-	51,52,52	0.50	0	71,80,80	0.79	1 (1%)
73	ZMP	Q	201	-	27,29,36	0.32	0	34,38,45	1.20	1 (2%)
68	FES	2	301	3	0,4,4	-	-	-		
72	SF4	G	801	65	0,12,12	-	-	-		
69	HEM	w	401	-	50,50,50	1.33	6 (12%)	67,82,82	1.10	3 (4%)
69	HEM	7	401	6	50,50,50	1.46	6 (12%)	67,82,82	1.19	3 (4%)

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
72	SF4	H	302	32	-	-	0/6/5/5
69	HEM	w	402	6	-	3/14/54/54	-
71	FMN	B	501	-	-	2/18/18/18	0/3/3/3
69	HEM	7	402	-	-	6/14/54/54	-
70	HEC	8	401	7	1/1/3/7	2/14/54/54	-
74	HEA	Ak	601	57	-	14/36/76/76	-
68	FES	G	803	65	-	-	0/1/1/1
68	FES	4	301	3	-	-	0/1/1/1
74	HEA	Ak	602	57	-	6/36/76/76	-
72	SF4	B	502	27	-	-	0/6/5/5
70	HEC	x	401	7	1/1/3/7	9/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	SF4	H	301	-	-	-	0/6/5/5
72	SF4	I	201	33	-	-	0/6/5/5
68	FES	E	301	30	-	-	0/1/1/1
72	SF4	G	802	65	-	-	0/6/5/5
75	NDP	L	401	-	-	7/34/77/77	0/5/5/5
73	ZMP	Q	201	-	-	8/36/36/43	-
68	FES	2	301	3	-	-	0/1/1/1
72	SF4	G	801	65	-	-	0/6/5/5
69	HEM	w	401	-	-	3/14/54/54	-
69	HEM	7	401	6	-	8/14/54/54	-

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	8	401	HEC	C3D-C2D	7.98	1.54	1.36
70	x	401	HEC	C3D-C2D	7.69	1.53	1.36
74	Ak	601	HEA	C3B-C2B	5.69	1.47	1.34
74	Ak	602	HEA	FE-ND	5.59	2.12	1.94
74	Ak	602	HEA	FE-NB	5.58	2.12	1.94
74	Ak	602	HEA	C3B-C2B	5.30	1.46	1.34
74	Ak	601	HEA	FE-ND	5.20	2.10	1.94
74	Ak	601	HEA	C3D-C2D	5.18	1.47	1.36
69	7	402	HEM	FE-NB	5.12	2.10	1.94
74	Ak	601	HEA	CHD-C1D	5.03	1.48	1.38
74	Ak	601	HEA	C3A-C2A	4.99	1.48	1.37
74	Ak	601	HEA	FE-NB	4.99	2.10	1.94
74	Ak	602	HEA	FE-NC	4.96	2.11	1.95
74	Ak	602	HEA	C3D-C2D	4.90	1.47	1.36
74	Ak	601	HEA	CHB-C4A	4.89	1.48	1.38
74	Ak	602	HEA	C3A-C2A	4.63	1.47	1.37
74	Ak	601	HEA	CHC-C4B	4.54	1.47	1.38
74	Ak	602	HEA	C1A-NA	4.50	1.48	1.39
74	Ak	602	HEA	CHD-C1D	4.47	1.47	1.38
70	8	401	HEC	FE-ND	4.45	2.08	1.94
74	Ak	601	HEA	CHA-C1A	4.44	1.47	1.38
74	Ak	601	HEA	FE-NC	4.41	2.09	1.95
74	Ak	602	HEA	C4A-NA	4.24	1.47	1.39
74	Ak	602	HEA	CHB-C4A	4.23	1.46	1.38
74	Ak	602	HEA	CHC-C4B	4.19	1.46	1.38
69	7	402	HEM	FE-NC	4.18	2.09	1.95
74	Ak	602	HEA	CHA-C1A	4.04	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	Ak	601	HEA	C1A-NA	3.91	1.47	1.39
74	Ak	601	HEA	CHD-C4C	3.91	1.48	1.39
74	Ak	601	HEA	C4A-NA	3.87	1.46	1.39
70	x	401	HEC	FE-ND	3.83	2.06	1.94
74	Ak	601	HEA	CHB-C1B	3.83	1.47	1.39
70	8	401	HEC	FE-NB	3.83	2.06	1.94
74	Ak	601	HEA	CHA-C4D	3.79	1.47	1.39
69	7	401	HEM	FE-ND	3.71	2.06	1.94
69	7	401	HEM	FE-NB	3.65	2.06	1.94
69	7	401	HEM	FE-NC	3.64	2.07	1.95
69	w	402	HEM	FE-NB	3.63	2.06	1.94
70	x	401	HEC	FE-NA	3.63	2.07	1.95
69	w	402	HEM	FE-ND	3.58	2.05	1.94
74	Ak	602	HEA	CHD-C4C	3.57	1.47	1.39
74	Ak	601	HEA	CHC-C1C	3.44	1.47	1.39
69	w	402	HEM	FE-NC	3.44	2.06	1.95
70	x	401	HEC	FE-NB	3.43	2.05	1.94
69	7	402	HEM	C1B-NB	-3.40	1.34	1.40
74	Ak	602	HEA	CHB-C1B	3.40	1.46	1.39
69	7	402	HEM	C4D-ND	-3.36	1.34	1.40
69	w	401	HEM	FE-ND	3.28	2.05	1.94
70	x	401	HEC	FE-NC	3.27	2.05	1.95
74	Ak	602	HEA	CHC-C1C	3.26	1.46	1.39
74	Ak	602	HEA	CHA-C4D	3.13	1.46	1.39
69	w	401	HEM	CAC-C3C	3.06	1.55	1.47
74	Ak	601	HEA	C4B-NB	-3.05	1.35	1.40
69	w	402	HEM	CAB-C3B	2.99	1.55	1.47
69	w	401	HEM	CAB-C3B	2.98	1.55	1.47
69	w	402	HEM	CAC-C3C	2.98	1.55	1.47
69	7	401	HEM	FE-NA	2.96	2.04	1.95
74	Ak	601	HEA	C1D-ND	-2.91	1.35	1.40
69	w	402	HEM	FE-NA	2.89	2.04	1.95
69	7	401	HEM	CAC-C3C	2.89	1.55	1.47
69	7	401	HEM	CAB-C3B	2.81	1.54	1.47
70	8	401	HEC	FE-NC	2.79	2.04	1.95
74	Ak	601	HEA	C4D-C3D	2.77	1.49	1.45
74	Ak	602	HEA	C4B-NB	-2.66	1.35	1.40
74	Ak	601	HEA	C4B-C3B	2.62	1.49	1.44
69	w	401	HEM	FE-NA	2.61	2.03	1.95
74	Ak	602	HEA	C1D-ND	-2.61	1.35	1.40
69	w	401	HEM	FE-NB	2.60	2.02	1.94
69	7	402	HEM	FE-ND	-2.56	1.87	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	8	401	HEC	FE-NA	2.56	2.03	1.95
74	Ak	601	HEA	C4C-NC	-2.53	1.34	1.39
74	Ak	602	HEA	C4B-C3B	2.48	1.49	1.44
69	7	402	HEM	C1C-C2C	-2.46	1.40	1.45
74	Ak	602	HEA	C1C-C2C	2.43	1.48	1.43
69	w	401	HEM	FE-NC	2.38	2.03	1.95
74	Ak	602	HEA	C1D-C2D	2.37	1.49	1.44
74	Ak	601	HEA	C1C-NC	-2.32	1.35	1.39
74	Ak	601	HEA	C1C-C2C	2.27	1.48	1.43
69	7	402	HEM	C1D-ND	-2.26	1.34	1.38
74	Ak	602	HEA	C1B-C2B	2.25	1.49	1.44
74	Ak	601	HEA	C1A-C2A	2.18	1.49	1.45
69	7	402	HEM	C4B-NB	-2.17	1.34	1.38
74	Ak	601	HEA	C1D-C2D	2.13	1.48	1.44
69	7	402	HEM	C3C-C4C	-2.12	1.42	1.46
74	Ak	601	HEA	C1B-NB	-2.11	1.34	1.38
74	Ak	601	HEA	C3C-C4C	2.11	1.48	1.42
74	Ak	602	HEA	C3C-C4C	2.08	1.48	1.42
74	Ak	601	HEA	C1B-C2B	2.08	1.48	1.44
74	Ak	601	HEA	C11-C3B	-2.06	1.48	1.51
74	Ak	602	HEA	C4C-NC	-2.04	1.35	1.39
74	Ak	602	HEA	C11-C3B	-2.02	1.48	1.51

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	Ak	601	HEA	CHA-C4D-ND	-6.96	116.93	124.42
74	Ak	602	HEA	C3D-C4D-ND	6.78	116.90	110.35
73	Q	201	ZMP	C11-S1-C10	6.15	120.03	101.84
74	Ak	602	HEA	C3B-C4B-NB	5.84	116.56	109.84
74	Ak	601	HEA	C3C-C2C-C1C	-5.69	100.47	107.17
74	Ak	602	HEA	C3C-C2C-C1C	-5.65	100.51	107.17
70	8	401	HEC	C1D-ND-C4D	5.50	111.72	105.21
74	Ak	602	HEA	C2A-C1A-NA	5.48	115.61	110.32
74	Ak	602	HEA	C2D-C1D-ND	5.40	116.05	109.84
74	Ak	602	HEA	C3C-C4C-NC	5.39	114.34	109.80
74	Ak	602	HEA	C2B-C1B-NB	5.39	116.13	109.90
74	Ak	601	HEA	C1A-CHA-C4D	-5.36	114.63	126.02
75	L	401	NDP	P2B-O2B-C2B	-5.21	109.53	123.43
70	x	401	HEC	C1D-ND-C4D	5.06	111.20	105.21
69	7	402	HEM	CHC-C4B-NB	5.01	129.82	124.42
74	Ak	601	HEA	CHA-C1A-NA	-4.86	119.17	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	Ak	601	HEA	C3D-C4D-ND	4.84	115.03	110.35
74	Ak	601	HEA	C2A-C1A-NA	4.74	114.90	110.32
74	Ak	601	HEA	C3B-C4B-NB	4.67	115.20	109.84
70	8	401	HEC	CAC-C3C-C4C	4.49	131.09	124.91
74	Ak	602	HEA	C2C-C1C-NC	4.49	117.34	110.14
69	7	402	HEM	CHD-C1D-ND	4.49	129.25	124.42
74	Ak	602	HEA	C1D-C2D-C3D	-4.39	102.37	106.98
74	Ak	601	HEA	CAD-C3D-C4D	4.17	131.96	124.70
74	Ak	601	HEA	C2D-C1D-ND	4.11	114.56	109.84
74	Ak	601	HEA	C2B-C1B-NB	4.09	114.63	109.90
74	Ak	601	HEA	C3A-C2A-C1A	-4.02	103.24	107.05
74	Ak	602	HEA	C3A-C2A-C1A	-4.02	103.24	107.05
74	Ak	601	HEA	C2C-C1C-NC	3.72	116.11	110.14
74	Ak	601	HEA	CHC-C4B-NB	-3.57	119.95	124.37
74	Ak	602	HEA	C1B-C2B-C3B	-3.43	102.82	106.80
74	Ak	602	HEA	C4A-NA-C1A	-3.41	100.25	105.82
74	Ak	601	HEA	C26-C15-C16	3.39	121.10	115.23
74	Ak	601	HEA	C27-C19-C20	3.35	121.04	115.23
69	7	402	HEM	CHB-C1B-NB	3.34	128.49	124.37
69	7	402	HEM	C1B-NB-C4B	3.31	109.12	105.21
74	Ak	601	HEA	C1D-C2D-C3D	-3.30	103.50	106.98
74	Ak	601	HEA	CHB-C1B-NB	-3.29	120.89	124.42
69	7	402	HEM	CHA-C4D-ND	3.27	128.41	124.37
74	Ak	601	HEA	C4D-C3D-C2D	-3.27	102.14	106.89
74	Ak	602	HEA	CMB-C2B-C1B	3.26	130.13	125.03
74	Ak	601	HEA	C4B-C3B-C2B	-3.21	102.04	107.44
74	Ak	602	HEA	C4D-C3D-C2D	-3.16	102.30	106.89
74	Ak	602	HEA	C4B-C3B-C2B	-3.16	102.13	107.44
74	Ak	602	HEA	CHB-C1B-NB	-3.13	121.06	124.42
74	Ak	602	HEA	C13-C14-C15	-3.02	120.70	127.62
74	Ak	601	HEA	C3C-C4C-NC	3.00	112.33	109.80
74	Ak	601	HEA	C13-C12-C11	-2.90	109.76	114.39
74	Ak	601	HEA	C1B-C2B-C3B	-2.89	103.44	106.80
70	8	401	HEC	CAC-C3C-C2C	-2.88	122.34	126.89
69	w	401	HEM	C4D-ND-C1D	2.77	108.49	105.21
74	Ak	601	HEA	C13-C14-C15	-2.76	121.30	127.62
69	7	402	HEM	CHD-C4C-NC	2.76	127.45	124.45
74	Ak	602	HEA	CHC-C1C-C2C	-2.74	119.46	127.43
74	Ak	602	HEA	C27-C19-C20	2.74	119.99	115.23
74	Ak	602	HEA	C17-C18-C19	-2.69	121.46	127.62
74	Ak	602	HEA	C26-C15-C16	2.69	119.89	115.23
74	Ak	602	HEA	CAD-CBD-CGD	-2.64	106.66	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	7	402	HEM	CHD-C1D-C2D	-2.62	120.89	125.03
74	Ak	601	HEA	CMC-C2C-C1C	2.59	129.37	125.42
74	Ak	602	HEA	CHB-C4A-NA	-2.58	121.64	124.45
69	7	402	HEM	C3B-C4B-NB	-2.57	107.62	109.47
74	Ak	602	HEA	OMA-CMA-C3A	-2.54	119.89	125.62
74	Ak	602	HEA	C13-C12-C11	-2.53	110.34	114.39
74	Ak	602	HEA	CHA-C4D-ND	-2.52	121.71	124.42
74	Ak	601	HEA	CHB-C4A-NA	-2.52	121.71	124.45
69	7	401	HEM	C3B-C2B-C1B	2.46	108.25	106.41
74	Ak	602	HEA	C25-C23-C24	2.44	120.21	114.59
69	w	401	HEM	C3D-C4D-ND	-2.43	107.50	110.17
74	Ak	602	HEA	C4B-NB-C1B	-2.40	102.36	105.21
74	Ak	602	HEA	C1D-ND-C4D	-2.38	102.38	105.21
74	Ak	601	HEA	C17-C18-C19	-2.38	122.19	127.62
74	Ak	601	HEA	C4A-NA-C1A	-2.37	101.96	105.82
74	Ak	602	HEA	CMD-C2D-C1D	2.36	128.72	125.03
70	x	401	HEC	C2A-C1A-NA	-2.35	108.06	110.32
69	7	402	HEM	C4C-CHD-C1D	-2.33	121.07	126.02
74	Ak	602	HEA	CHA-C4D-C3D	-2.32	121.39	124.77
70	x	401	HEC	CHA-C4D-ND	2.31	126.91	124.42
70	8	401	HEC	C2A-C1A-NA	-2.31	108.09	110.32
74	Ak	601	HEA	C25-C23-C24	2.29	119.85	114.59
74	Ak	602	HEA	C21-C22-C23	-2.27	120.06	127.64
74	Ak	601	HEA	CMB-C2B-C1B	2.27	128.58	125.03
74	Ak	601	HEA	CHA-C4D-C3D	2.24	128.04	124.77
69	w	401	HEM	C2A-C1A-NA	-2.24	107.67	110.15
74	Ak	601	HEA	OMA-CMA-C3A	-2.23	120.59	125.62
69	7	402	HEM	C4A-CHB-C1B	-2.21	121.04	126.25
74	Ak	602	HEA	CHA-C1A-NA	-2.21	122.05	124.45
70	8	401	HEC	C3B-C4B-NB	-2.20	107.76	110.17
70	8	401	HEC	C2C-C1C-NC	-2.20	106.62	110.14
74	Ak	602	HEA	CMC-C2C-C1C	2.20	128.76	125.42
70	x	401	HEC	CAB-C3B-C4B	-2.17	121.96	124.79
69	7	402	HEM	CAD-CBD-CGD	-2.16	107.94	113.67
69	7	401	HEM	C4D-ND-C1D	2.16	107.76	105.21
70	x	401	HEC	CAA-C2A-C3A	-2.16	123.83	127.87
70	x	401	HEC	CMB-C2B-C1B	-2.12	121.72	125.03
71	B	501	FMN	C4-N3-C2	-2.12	121.87	125.64
74	Ak	601	HEA	CMD-C2D-C1D	2.11	128.34	125.03
74	Ak	602	HEA	CHC-C4B-C3B	-2.10	120.50	125.80
69	7	402	HEM	O2D-CGD-CBD	2.08	120.57	114.00
74	Ak	602	HEA	CHD-C1D-C2D	-2.08	121.04	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	x	401	HEC	CAD-CBD-CGD	-2.06	108.21	113.67
70	8	401	HEC	CAA-CBA-CGA	-2.06	108.21	113.67
70	8	401	HEC	CHA-C1A-NA	2.05	126.69	124.45
69	w	402	HEM	C4D-ND-C1D	2.05	107.63	105.21
69	7	401	HEM	C1B-NB-C4B	2.04	107.63	105.21
74	Ak	601	HEA	C27-C19-C18	-2.00	118.49	123.63

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
70	8	401	HEC	NA
70	x	401	HEC	NA

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	7	402	HEM	C1A-C2A-CAA-CBA
69	7	402	HEM	C2B-C3B-CAB-CBB
69	7	402	HEM	C2C-C3C-CAC-CBC
69	7	402	HEM	C4C-C3C-CAC-CBC
73	Q	201	ZMP	O3-C16-C17-C18
73	Q	201	ZMP	N2-C16-C17-O4
73	Q	201	ZMP	C17-C16-N2-C15
73	Q	201	ZMP	O3-C16-N2-C15
74	Ak	601	HEA	C2A-C3A-CMA-OMA
74	Ak	601	HEA	C4A-C3A-CMA-OMA
74	Ak	601	HEA	C4C-C3C-CAC-CBC
74	Ak	602	HEA	C2A-C3A-CMA-OMA
70	x	401	HEC	C4B-C3B-CAB-CBB
70	x	401	HEC	C2B-C3B-CAB-CBB
70	8	401	HEC	C2C-C3C-CAC-CBC
70	8	401	HEC	C4C-C3C-CAC-CBC
74	Ak	601	HEA	C4D-C3D-CAD-CBD
74	Ak	601	HEA	C26-C15-C16-C17
74	Ak	601	HEA	C14-C15-C16-C17
75	L	401	NDP	C3B-C4B-C5B-O5B
75	L	401	NDP	C2D-C1D-N1N-C2N
75	L	401	NDP	C2D-C1D-N1N-C6N
74	Ak	601	HEA	C2D-C3D-CAD-CBD
74	Ak	601	HEA	C2C-C3C-CAC-CBC
69	7	401	HEM	C3D-CAD-CBD-CGD
74	Ak	602	HEA	C2A-CAA-CBA-CGA

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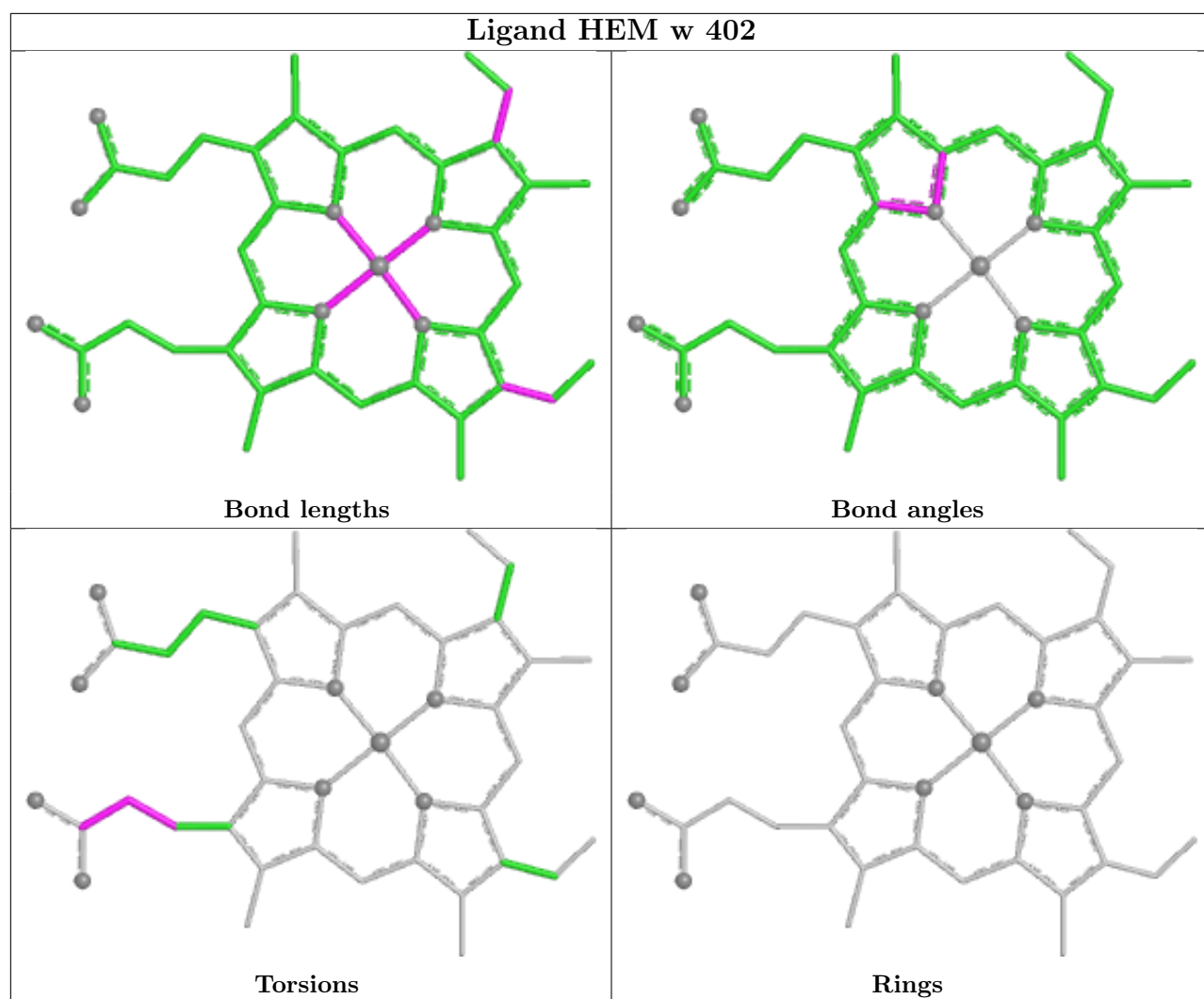
Mol	Chain	Res	Type	Atoms
70	x	401	HEC	C1A-C2A-CAA-CBA
75	L	401	NDP	O4B-C4B-C5B-O5B
69	7	402	HEM	C3A-C2A-CAA-CBA
69	7	401	HEM	C4C-C3C-CAC-CBC
69	7	402	HEM	C4B-C3B-CAB-CBB
73	Q	201	ZMP	O3-C16-C17-O4
70	x	401	HEC	C3A-C2A-CAA-CBA
74	Ak	601	HEA	C3B-C11-C12-C13
73	Q	201	ZMP	N2-C16-C17-C18
69	7	401	HEM	C2A-CAA-CBA-CGA
69	7	401	HEM	C4B-C3B-CAB-CBB
74	Ak	601	HEA	O11-C11-C12-C13
75	L	401	NDP	O4D-C1D-N1N-C2N
69	w	402	HEM	C2A-CAA-CBA-CGA
73	Q	201	ZMP	C12-C11-S1-C10
74	Ak	602	HEA	C4A-C3A-CMA-OMA
75	L	401	NDP	O4D-C1D-N1N-C6N
73	Q	201	ZMP	C11-C12-N1-C13
75	L	401	NDP	C5B-O5B-PA-O1A
71	B	501	FMN	C4'-C5'-O5'-P
74	Ak	601	HEA	C12-C11-C3B-C4B
74	Ak	601	HEA	C12-C11-C3B-C2B
69	7	401	HEM	CAA-CBA-CGA-O1A
69	7	401	HEM	CAA-CBA-CGA-O2A
74	Ak	602	HEA	CAD-CBD-CGD-O1D
69	w	401	HEM	CAA-CBA-CGA-O1A
69	w	402	HEM	CAA-CBA-CGA-O1A
69	w	402	HEM	CAA-CBA-CGA-O2A
74	Ak	602	HEA	CAD-CBD-CGD-O2D
74	Ak	602	HEA	C26-C15-C16-C17
74	Ak	601	HEA	C11-C12-C13-C14
70	x	401	HEC	C4C-C3C-CAC-CBC
69	w	401	HEM	CAA-CBA-CGA-O2A
70	x	401	HEC	CAD-CBD-CGD-O2D
69	w	401	HEM	C4D-C3D-CAD-CBD
70	x	401	HEC	C2C-C3C-CAC-CBC
70	x	401	HEC	CAD-CBD-CGD-O1D
69	7	401	HEM	CAD-CBD-CGD-O1D
69	7	401	HEM	CAD-CBD-CGD-O2D
71	B	501	FMN	N10-C1'-C2'-O2'
74	Ak	601	HEA	O11-C11-C3B-C4B
70	x	401	HEC	CAA-CBA-CGA-O2A

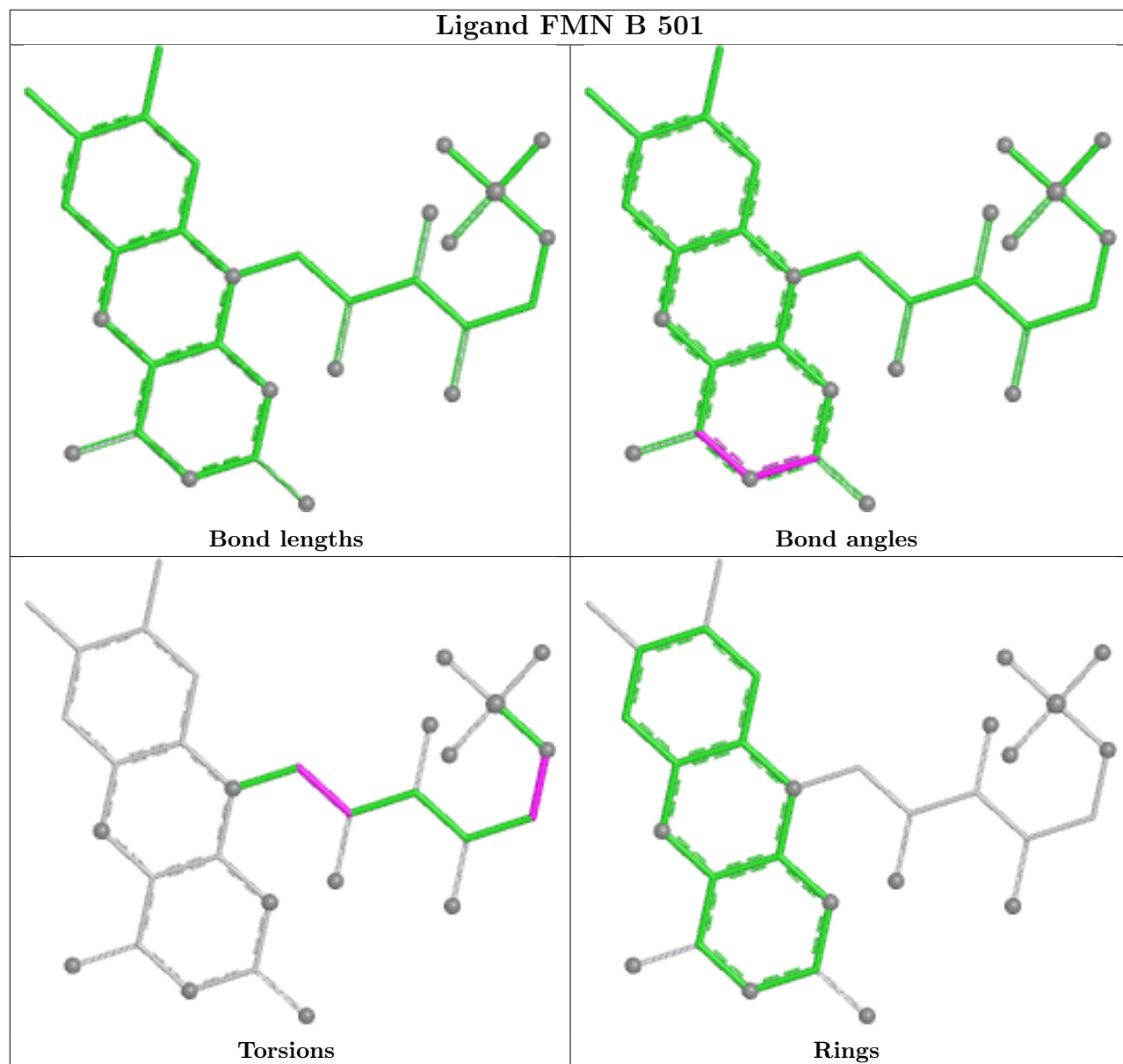
There are no ring outliers.

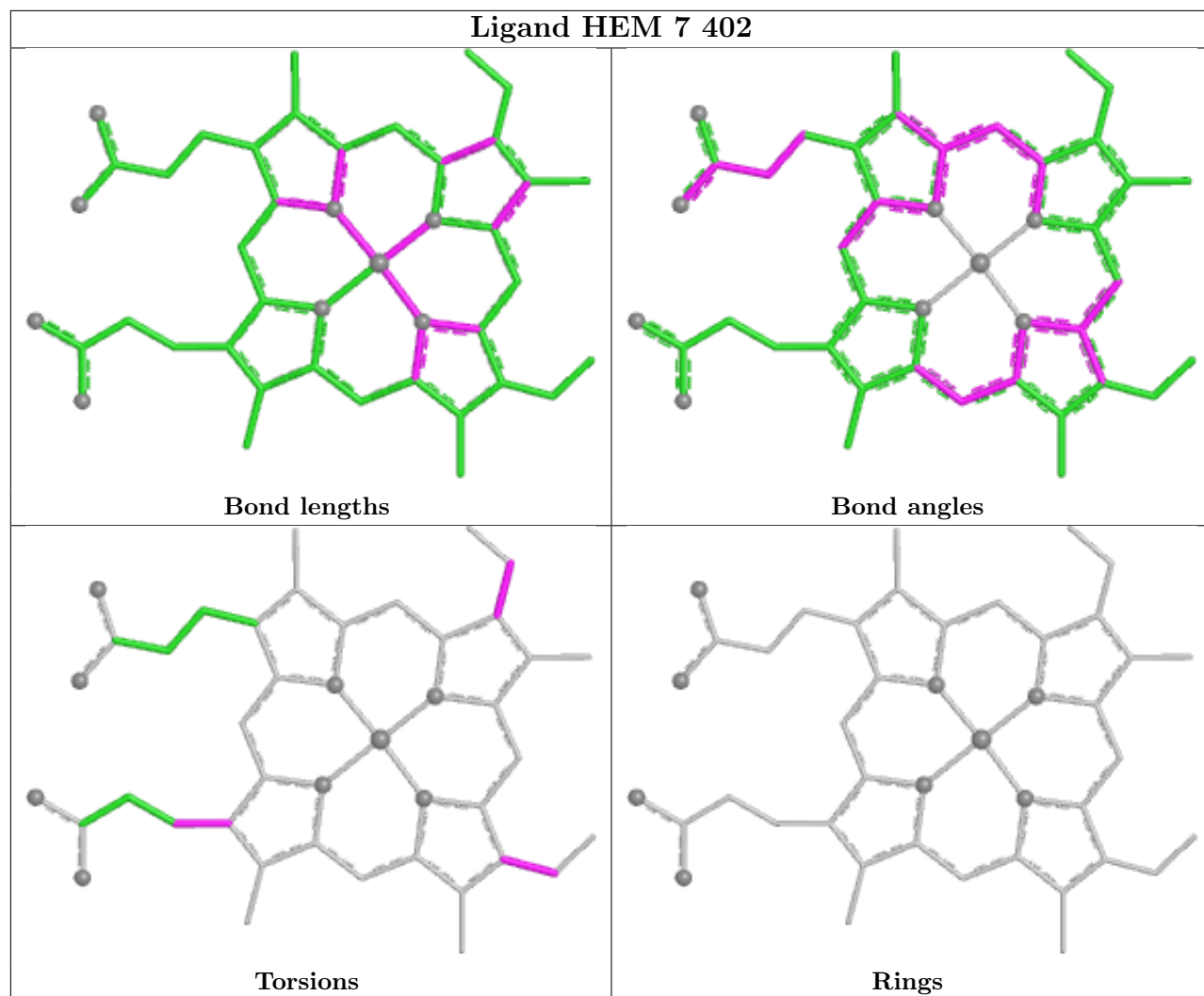
19 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	H	302	SF4	8	0
69	w	402	HEM	4	0
69	7	402	HEM	6	0
70	8	401	HEC	3	0
74	Ak	601	HEA	14	0
68	G	803	FES	8	0
68	4	301	FES	1	0
74	Ak	602	HEA	6	0
72	B	502	SF4	6	0
70	x	401	HEC	13	0
72	H	301	SF4	4	0
72	I	201	SF4	11	0
72	G	802	SF4	10	0
75	L	401	NDP	6	0
73	Q	201	ZMP	1	0
68	2	301	FES	6	0
72	G	801	SF4	1	0
69	w	401	HEM	4	0
69	7	401	HEM	6	0

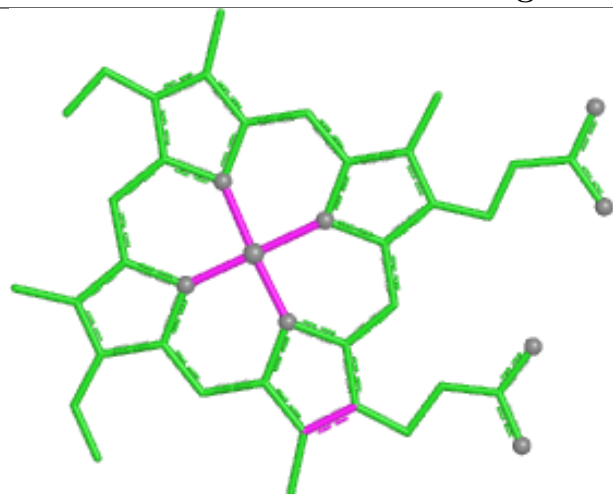
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



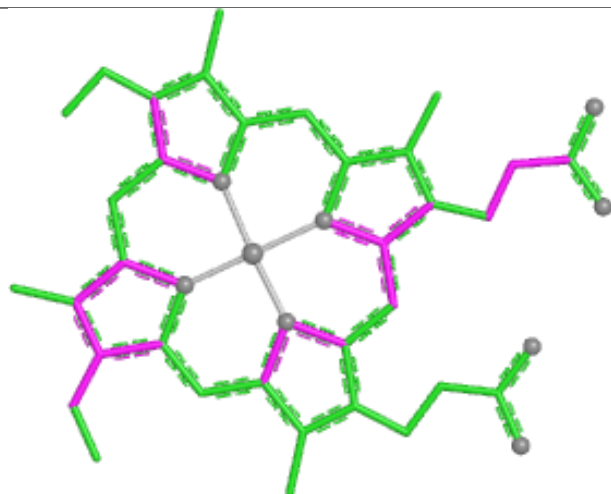




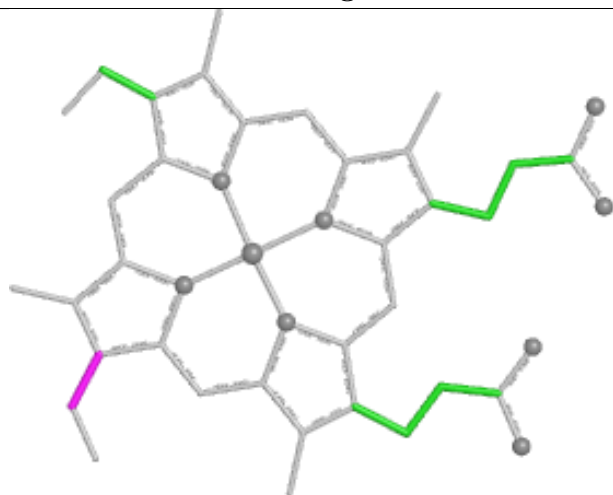
Ligand HEC 8 401



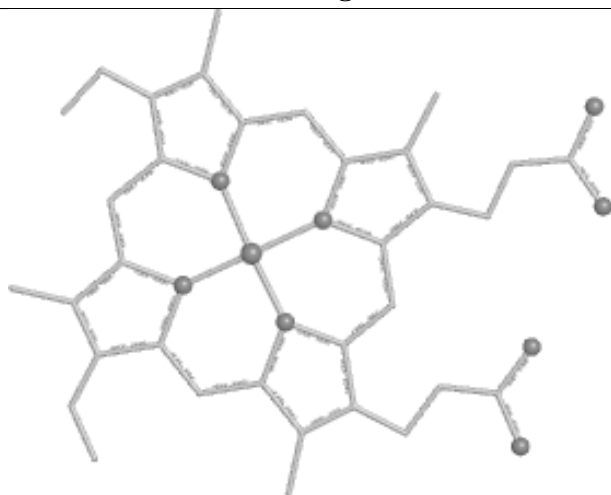
Bond lengths



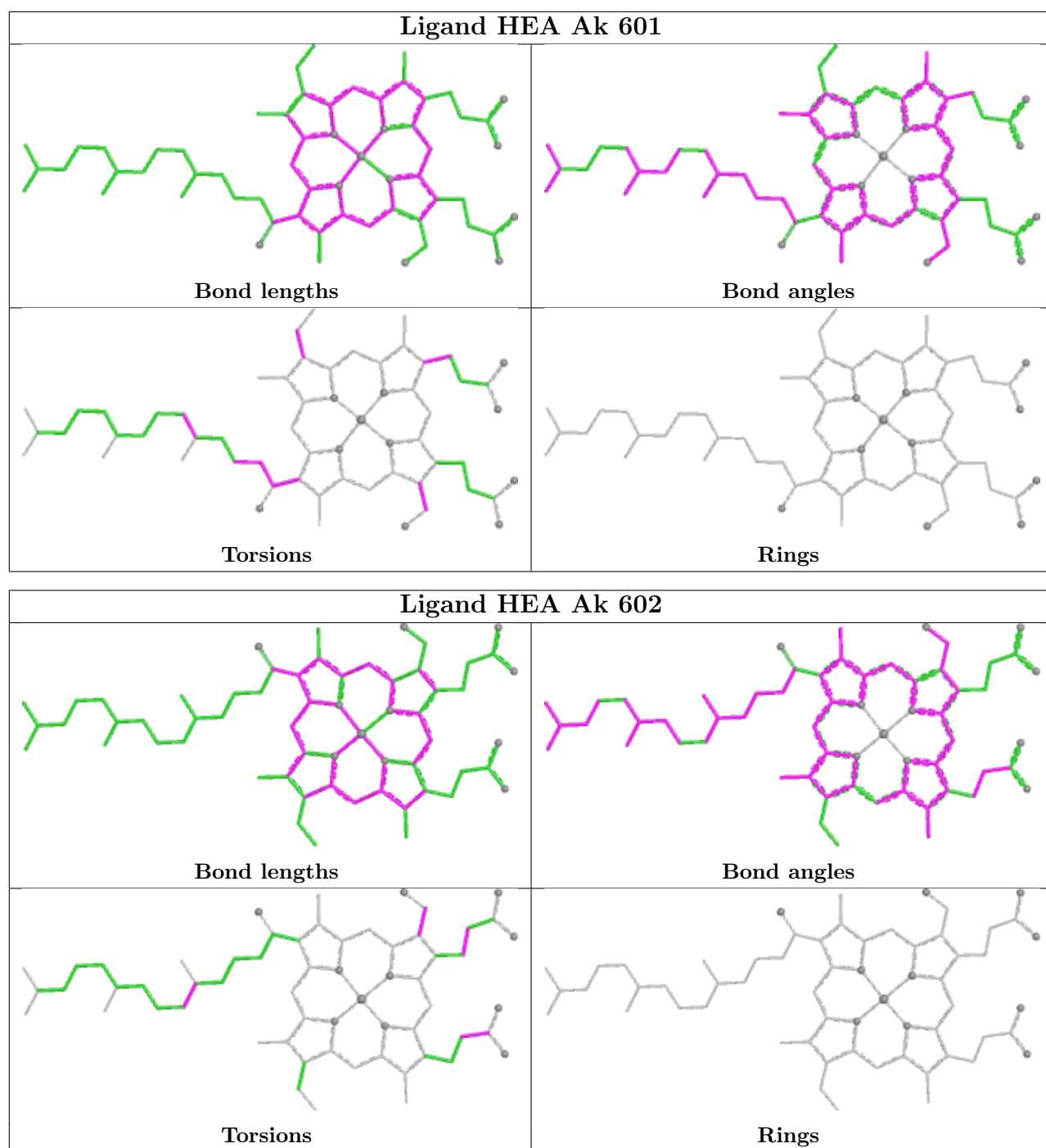
Bond angles



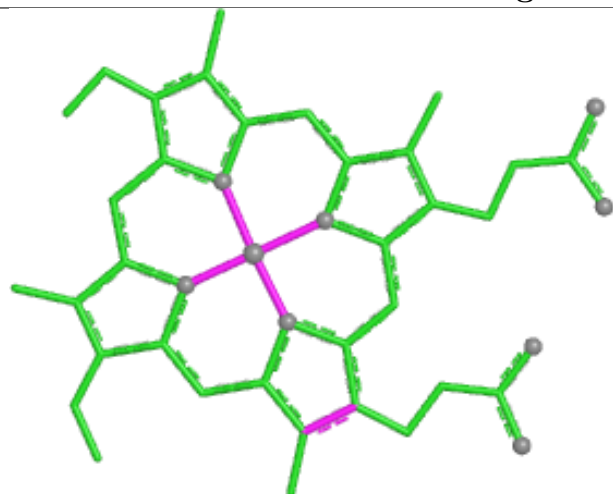
Torsions



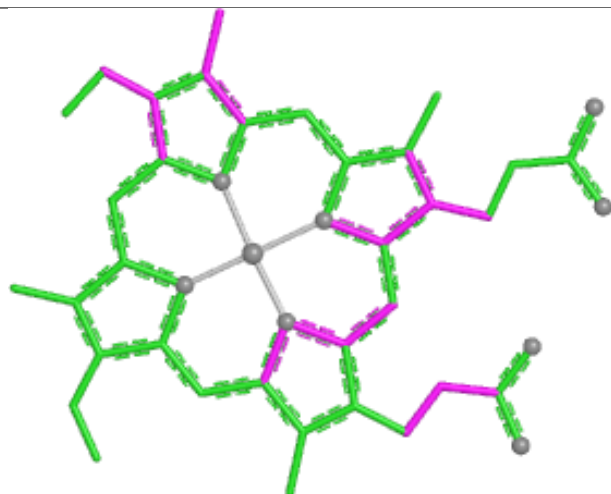
Rings



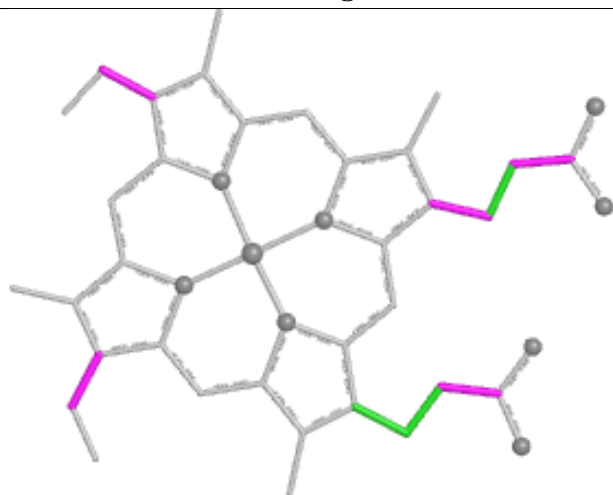
Ligand HEC x 401



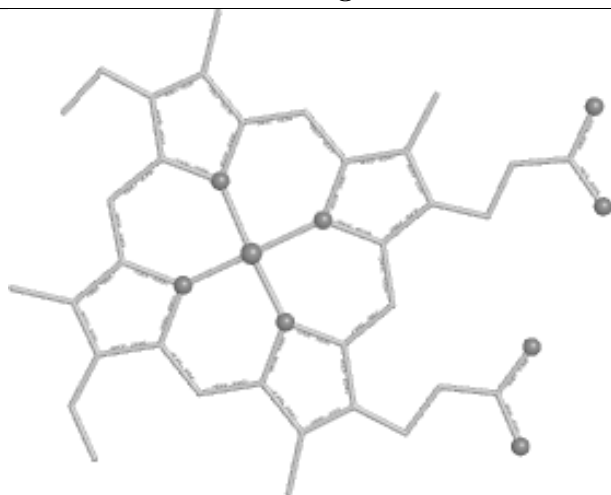
Bond lengths



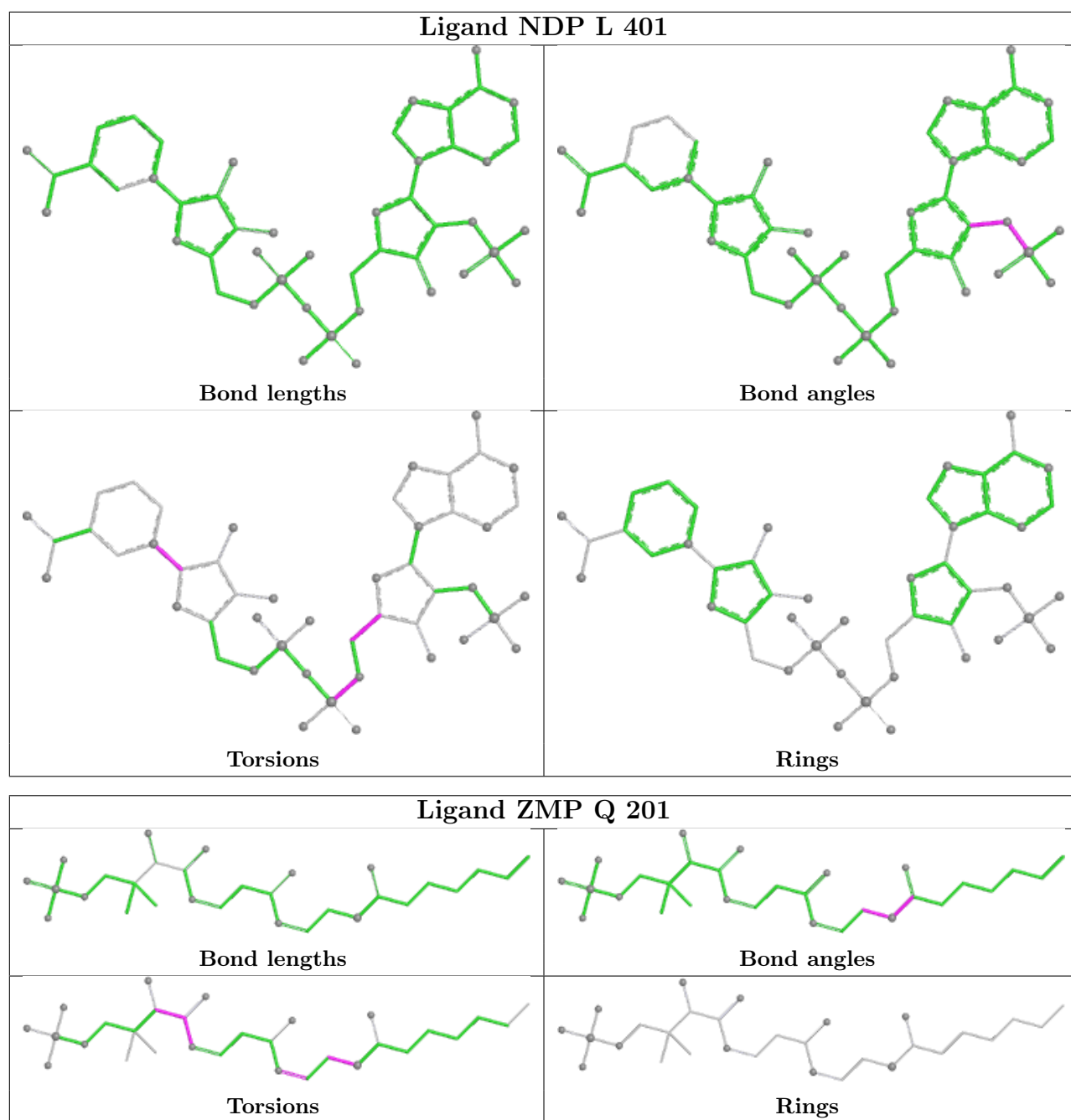
Bond angles

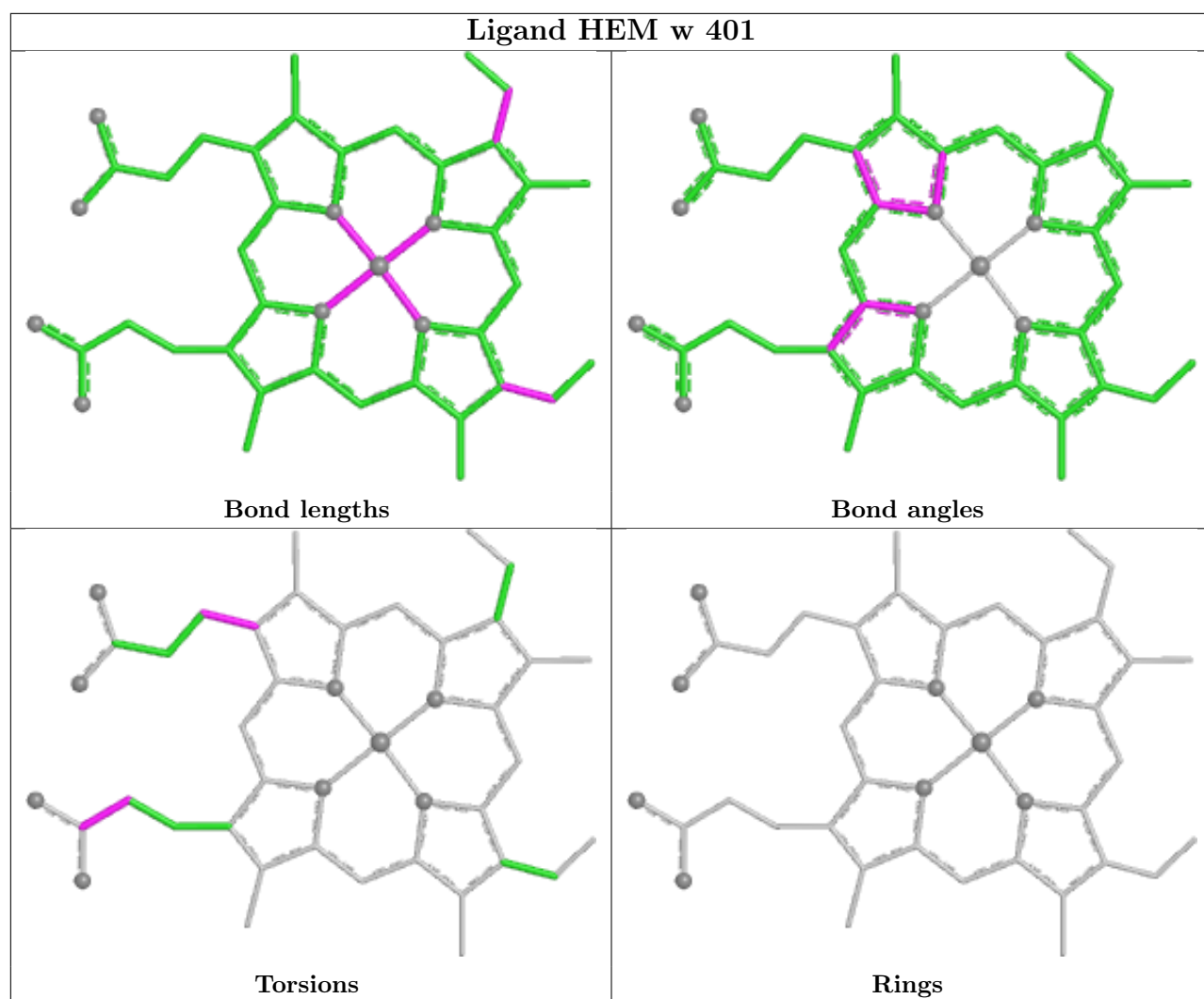


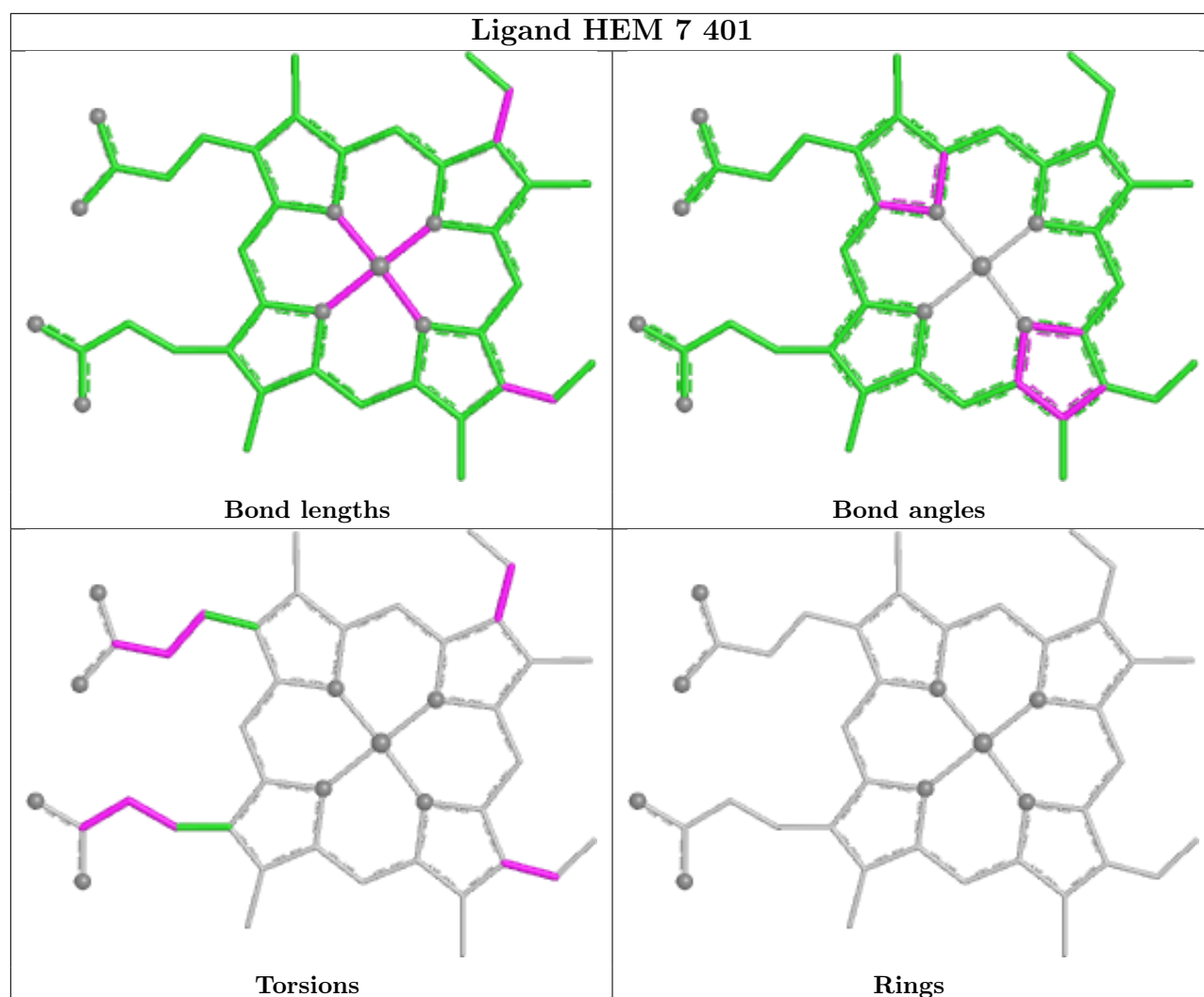
Torsions



Rings







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.

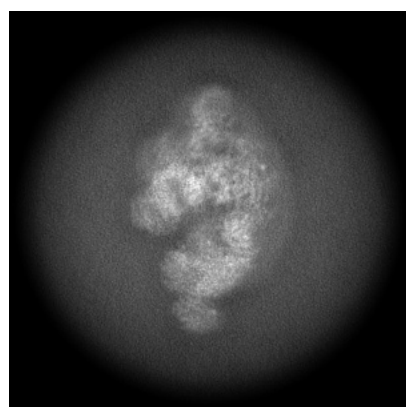
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45490. These allow visual inspection of the internal detail of the map and identification of artifacts.

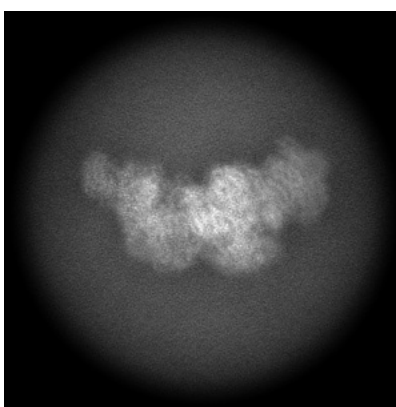
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

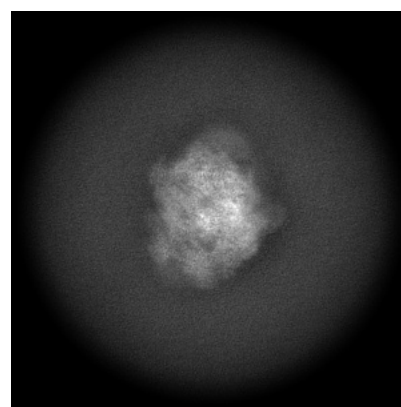
6.1.1 Primary map



X



Y

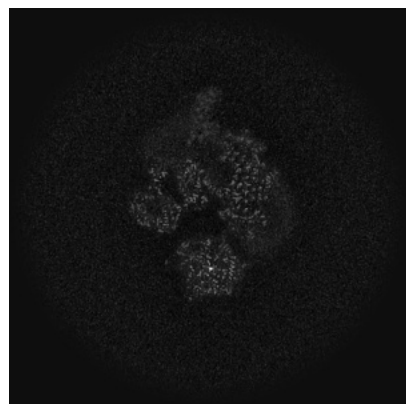


Z

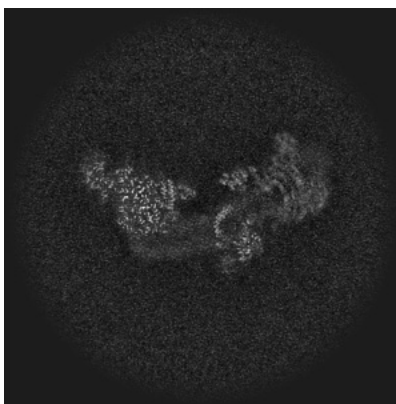
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

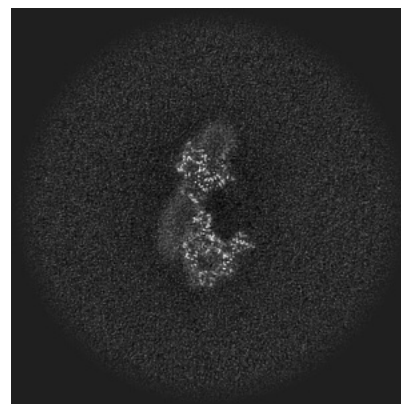
6.2.1 Primary map



X Index: 256



Y Index: 256

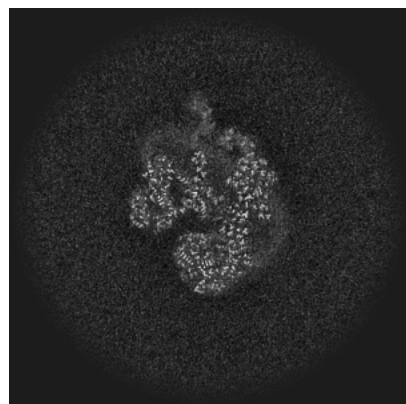


Z Index: 256

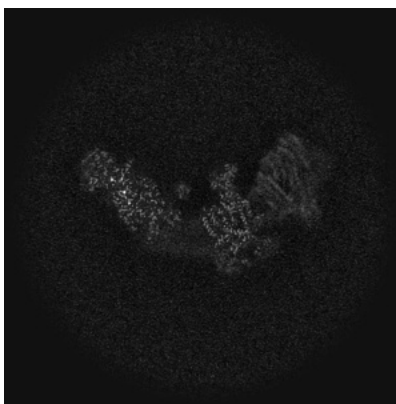
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

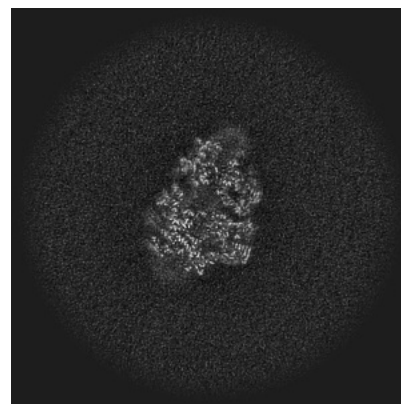
6.3.1 Primary map



X Index: 244



Y Index: 242

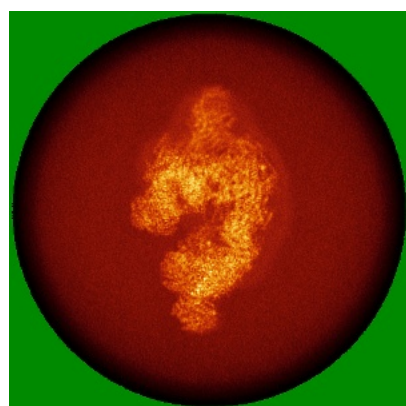


Z Index: 298

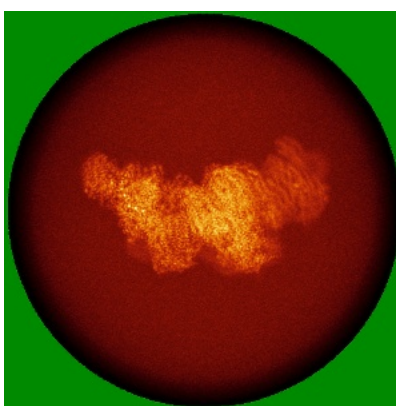
The images above show the largest variance slices of the map in three orthogonal directions.

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

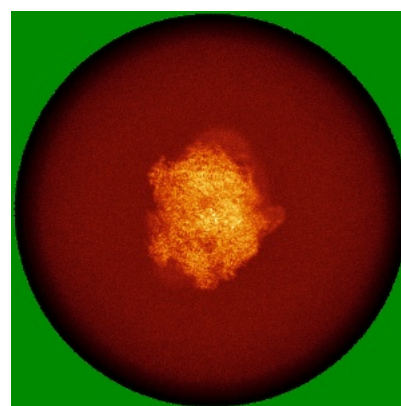
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

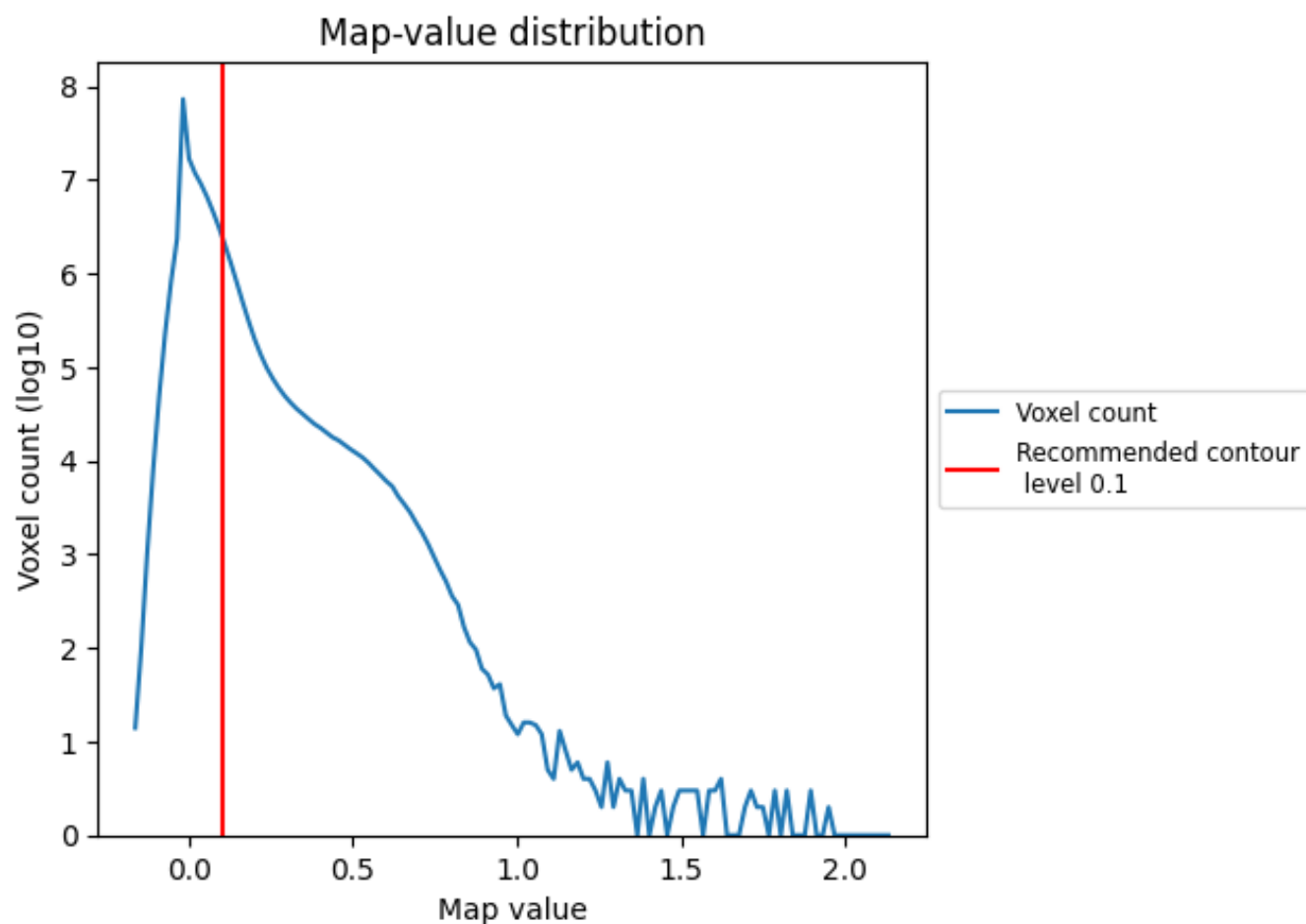
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

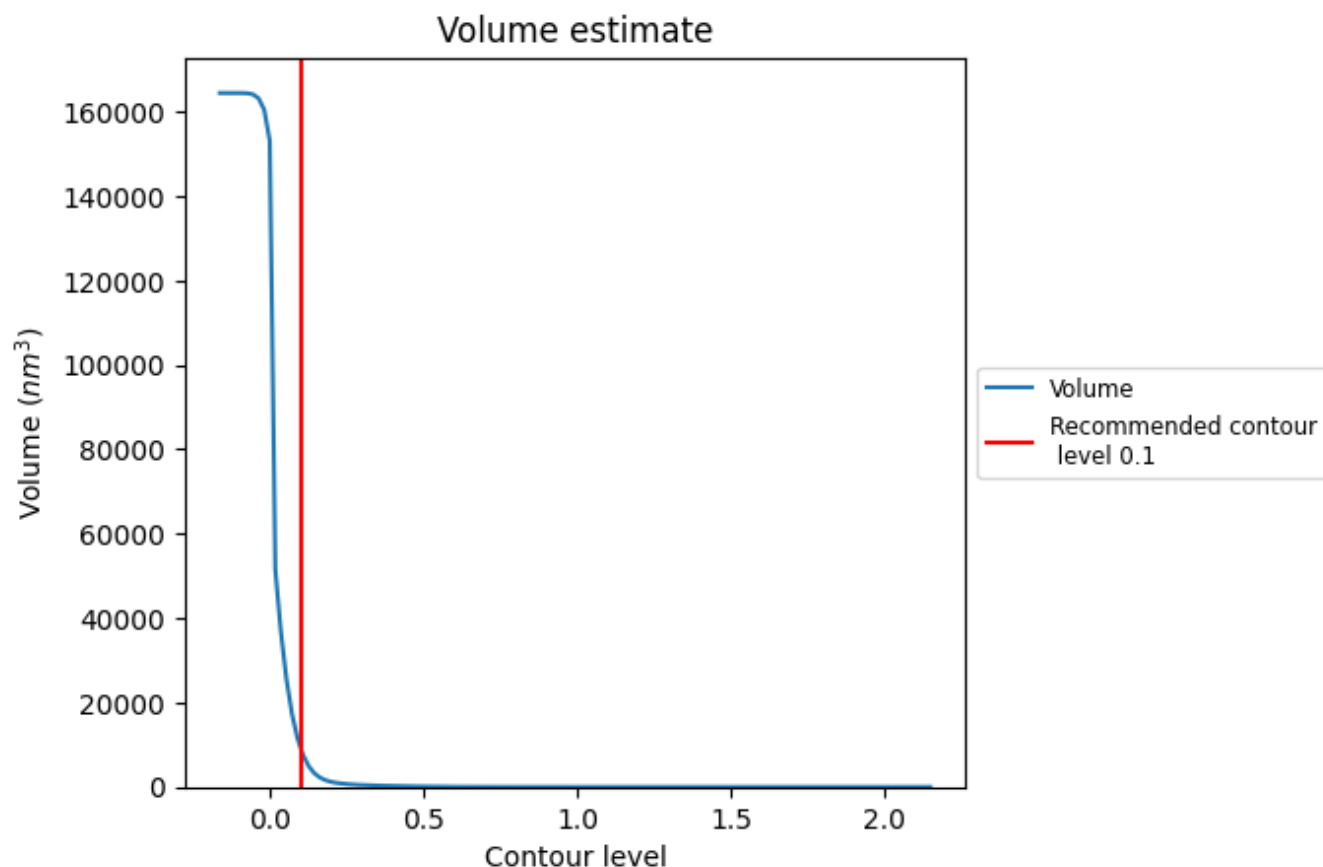
This section contains the results of statistical analysis of the map.

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.

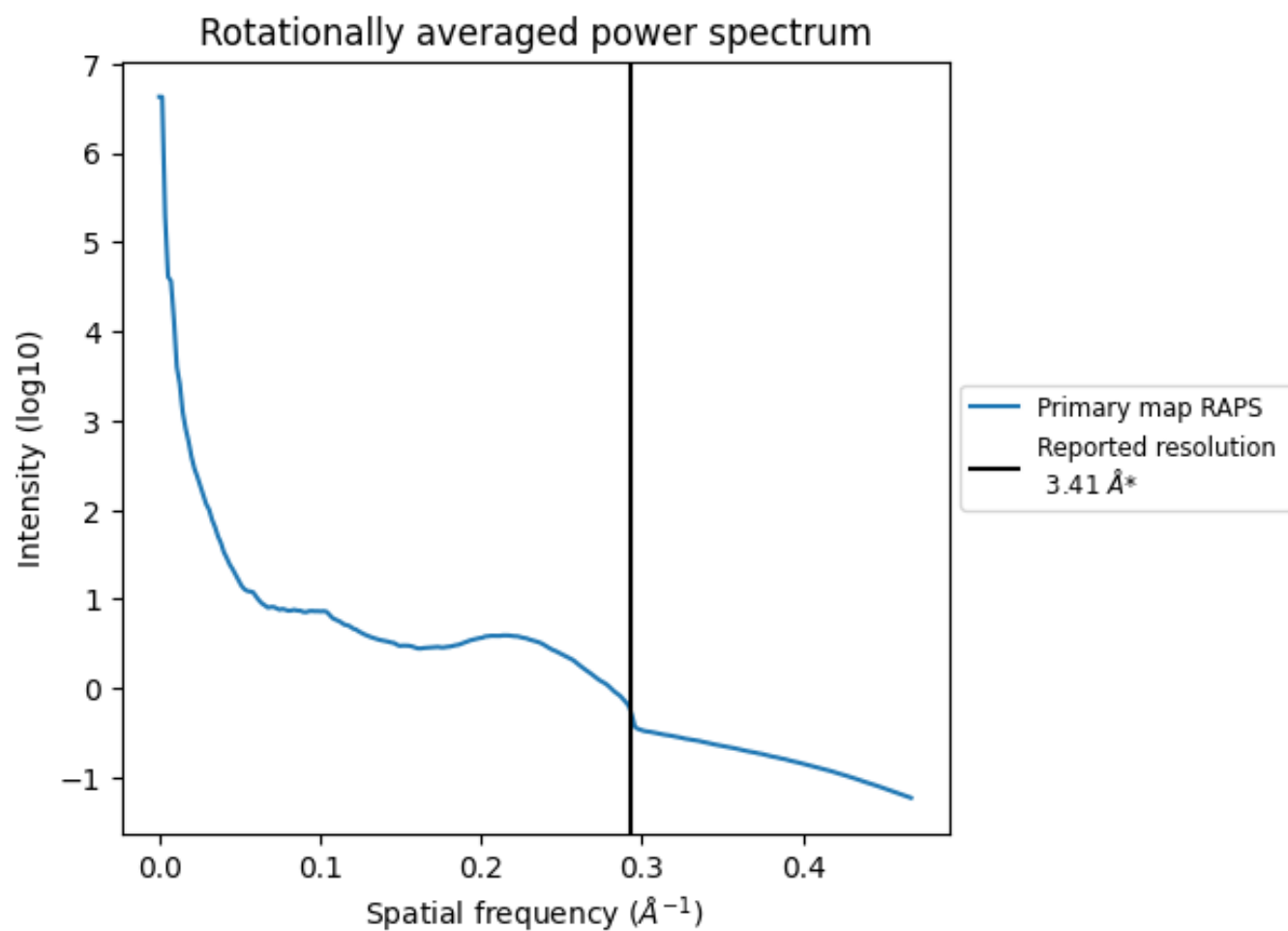
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9143 nm^3 ; this corresponds to an approximate mass of 8259 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 0.293 Å⁻¹

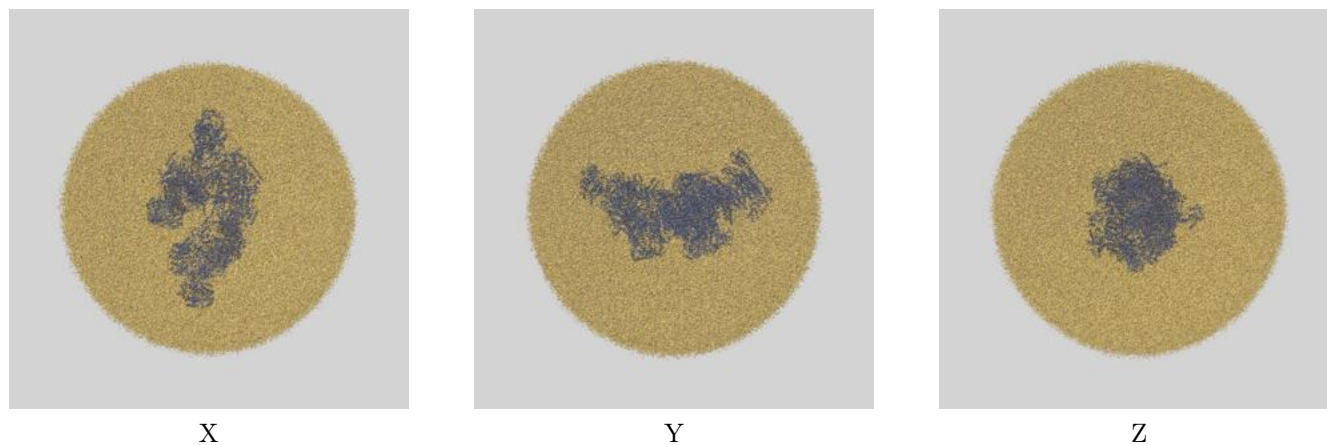
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

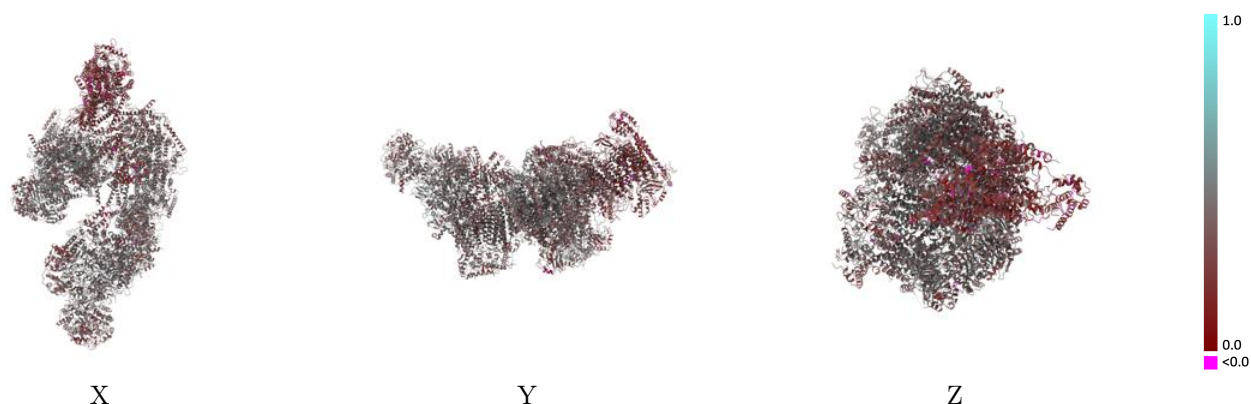
This section contains information regarding the fit between EMDB map EMD-45490 and PDB model 9CE2. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



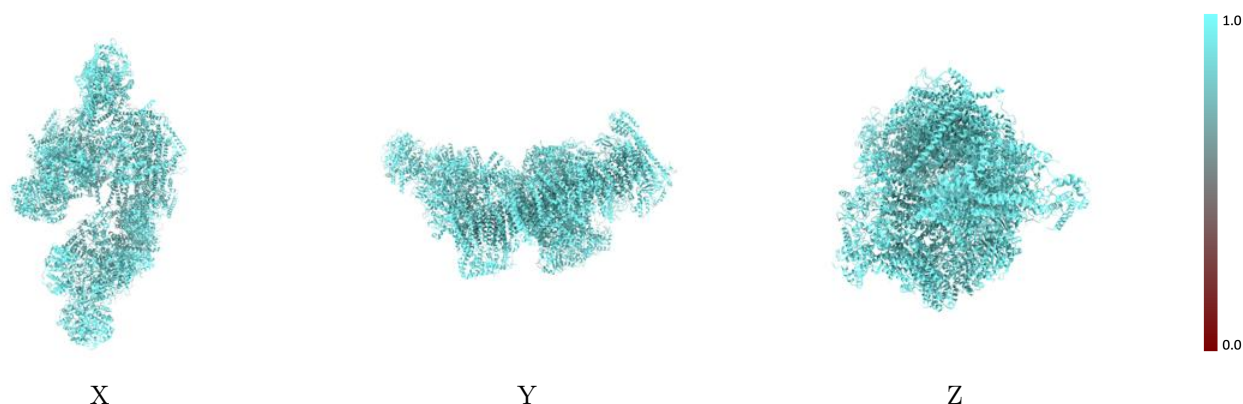
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



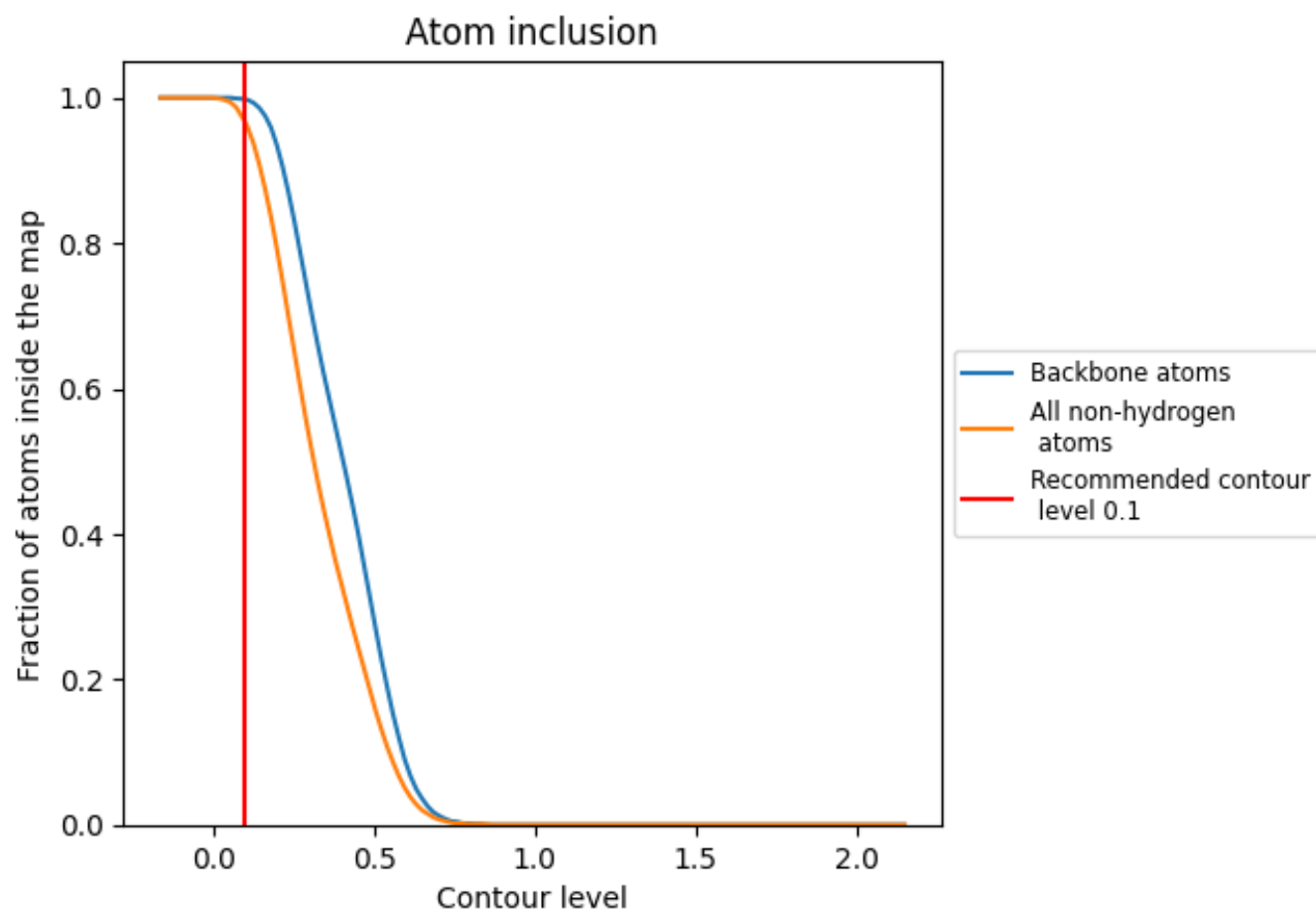
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 97% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.3770
0	 0.9580	 0.3210
1	 0.9880	 0.4190
2	 0.9480	 0.3390
3	 0.9830	 0.4170
4	 0.9590	 0.3310
5	 0.9820	 0.4210
6	 0.9770	 0.4170
7	 0.9740	 0.4400
8	 0.9780	 0.4210
9	 0.9540	 0.4050
A	 0.9700	 0.2370
Aa	 0.9720	 0.4120
Ab	 0.9510	 0.3380
Ac	 0.9830	 0.4040
Ad	 0.9750	 0.3950
Ae	 0.9180	 0.2260
Af	 0.8820	 0.2710
Ag	 0.9460	 0.2220
Ah	 0.9350	 0.2430
Ai	 0.9680	 0.2280
Aj	 0.9220	 0.2560
Ak	 0.9440	 0.2680
Al	 0.9660	 0.2470
Am	 0.9390	 0.2380
An	 0.9460	 0.2120
Ao	 0.9560	 0.1840
Ap	 0.9350	 0.2120
Aq	 0.9660	 0.1860
Ar	 0.9640	 0.2260
B	 0.9770	 0.3840
C	 0.9780	 0.4220
D	 0.9840	 0.4420
E	 0.9510	 0.3710
F	 0.9460	 0.4210



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Chain	Atom inclusion	Q-score
G	 0.9710	 0.4010
H	 0.9890	 0.4510
I	 0.9790	 0.4330
J	 0.9750	 0.4320
K	 0.9750	 0.4330
L	 0.9540	 0.3780
M	 0.9810	 0.4200
N	 0.9750	 0.3920
O	 0.9330	 0.2770
P	 0.9630	 0.3300
Q	 0.9670	 0.3860
R	 0.9480	 0.3290
S	 0.9910	 0.4140
T	 0.9760	 0.3900
U	 0.9570	 0.3770
V	 0.9700	 0.3820
W	 0.9790	 0.4080
X	 0.9580	 0.3020
Y	 0.9650	 0.3100
Z	 0.9460	 0.3060
a	 0.9760	 0.4160
b	 0.9750	 0.3310
c	 0.9610	 0.3670
d	 0.9720	 0.3620
e	 0.9550	 0.3670
f	 0.9810	 0.3730
g	 0.9620	 0.3970
h	 0.9550	 0.3850
i	 0.9740	 0.4390
j	 0.9270	 0.3790
k	 0.9680	 0.4130
l	 0.9590	 0.3940
m	 0.9420	 0.3540
n	 0.9500	 0.3750
o	 0.9500	 0.3380
p	 0.9650	 0.2680
q	 0.9680	 0.4410
r	 0.9630	 0.3960
s	 0.9740	 0.4030
t	 0.9780	 0.2980
u	 0.9730	 0.4200
v	 0.9770	 0.4190

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Chain	Atom inclusion	Q-score
w	 0.9830	 0.4390
x	 0.9790	 0.4240
y	 0.9690	 0.4150
z	 0.9780	 0.4120