Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:23 am GMT

PDB ID	:	5LUF
EMDB ID	:	EMD-4107
Title	:	Cryo-EM of bovine respirasome
Authors	:	Sousa, J.S.; Mills, D.J.; Vonck, J.; Kuehlbrandt, W.
Deposited on	:	2016-09-08
Resolution	:	9.10 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:

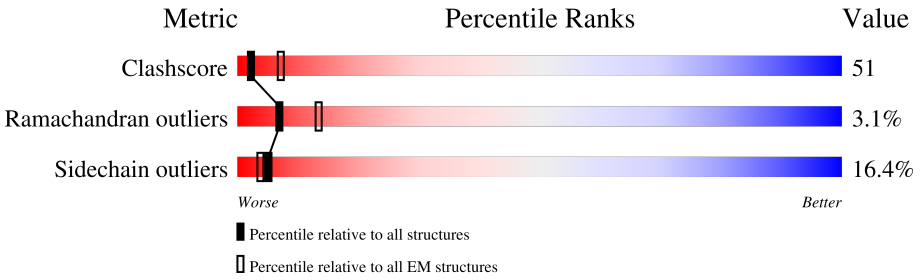
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	c	446	15% 70% 26% ·
1	l	446	13% 70% 26% ·
2	m	439	13% 73% 20% · 5%
2	n	439	9% 75% 19% · 5%
3	b	379	28% 69% 28% ·
3	o	379	31% 74% 23% ·
4	d	241	21% 78% 18% ·
4	p	241	22% 76% 22% ·

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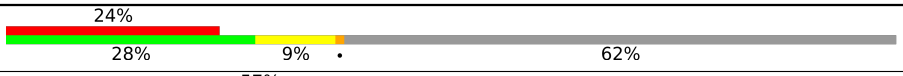
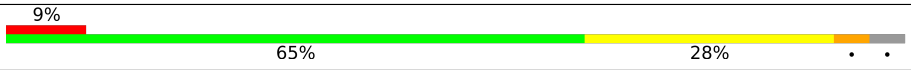
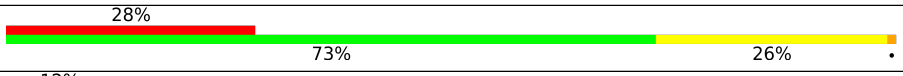
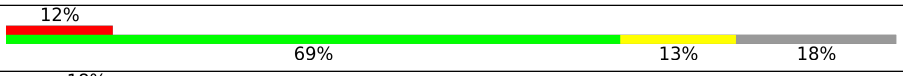
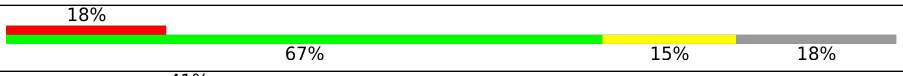
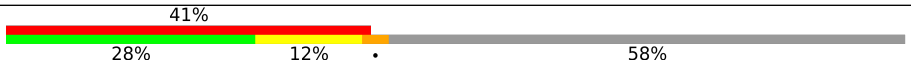
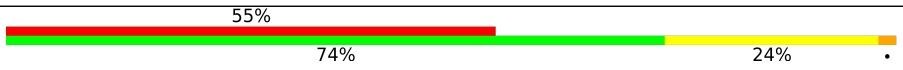
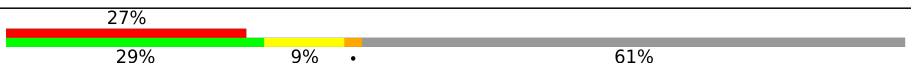
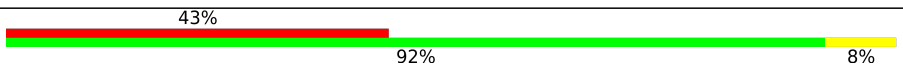
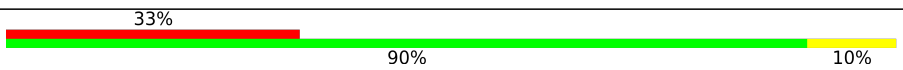
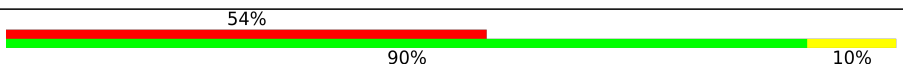
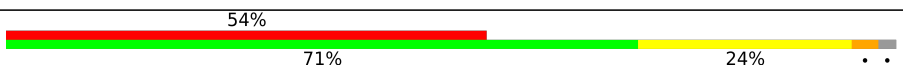
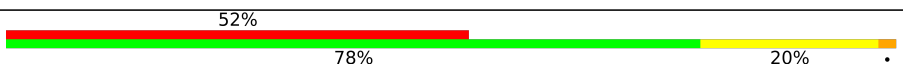
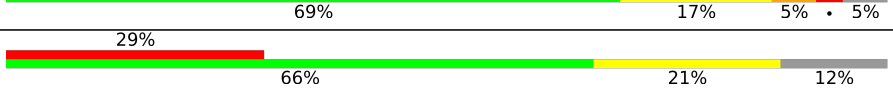
Mol	Chain	Length	Quality of chain
5	e	196	
5	q	196	
6	f	110	
6	r	110	
7	g	81	
7	s	81	
8	h	78	
8	t	78	
9	i	78	
9	u	78	
10	j	62	
10	v	62	
11	k	56	
11	w	56	
12	x	514	
13	y	227	
14	z	261	
15	1	147	
16	2	109	
17	3	98	
18	4	84	
19	5	85	
20	6	73	
21	7	59	
22	8	56	

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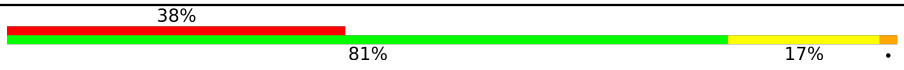
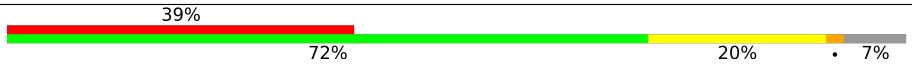
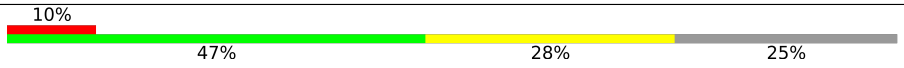
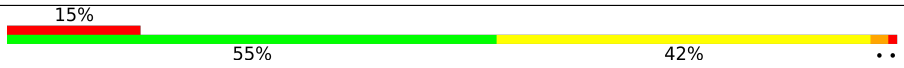
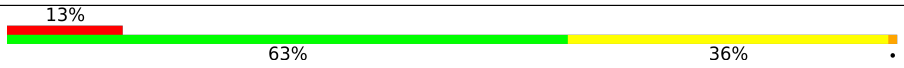
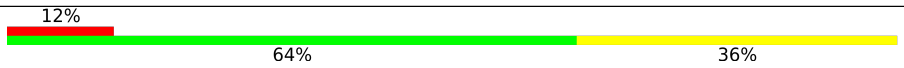
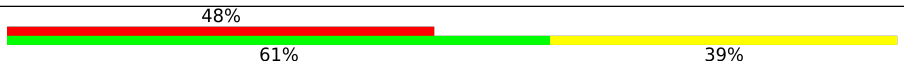
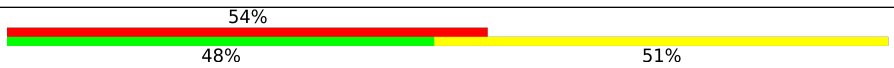
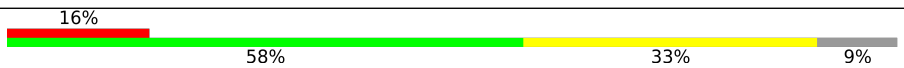
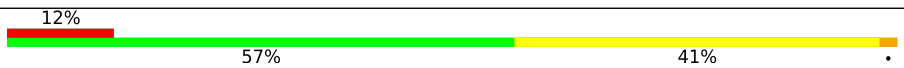
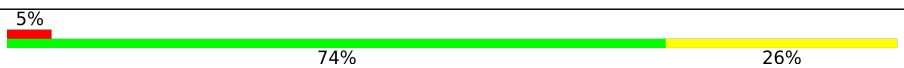
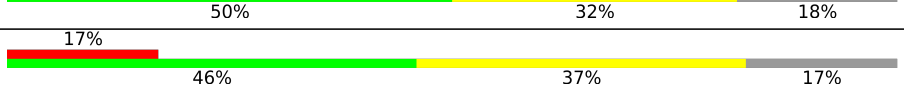
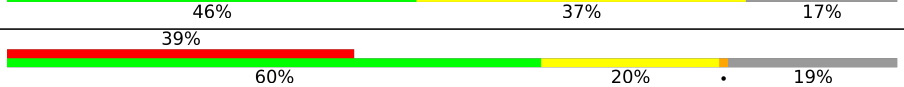
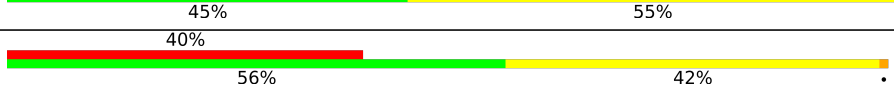
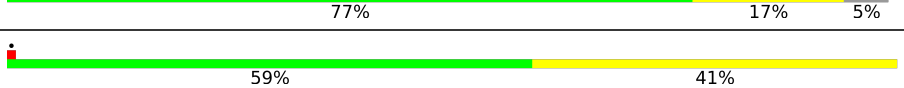
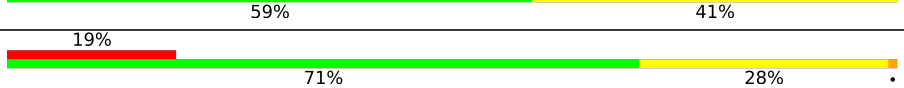
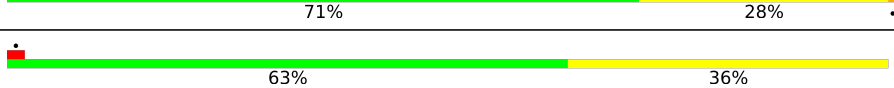
Mol	Chain	Length	Quality of chain
23	9	47	
24	0	46	
25	A	111	
26	B	143	
27	C	154	
28	D	384	
29	E	159	
30	F	411	
31	G	538	
32	H	313	
33	I	162	
34	J	171	
35	K	84	
36	L	601	
37	M	453	
38	N	345	
39	O	220	
40	P	303	
41	Q	85	
42	R	47	
43	S	80	
44	T	75	
45	V	71	
46	W	72	
47	X	330	

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Mol	Chain	Length	Quality of chain
48	Y	106	13% 66% 34%
49	a	142	9% 50% 50%
50	U	828	22% 8% 70%
51	Z	625	29% 13% 57%

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
54	FES	G	803	-	-	X	-
57	HEA	x	603	X	-	-	-
57	HEA	x	604	X	-	-	-
59	SF4	B	201	-	-	X	-
59	SF4	I	201	-	-	X	-
59	SF4	I	202	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 74493 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 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	446	Total	C	N	O	S	0	0
			3458	2161	609	668	20		
1	l	446	Total	C	N	O	S	0	0
			3458	2161	609	668	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		
2	n	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		
3	o	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		
4	p	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	75	Total	C	N	O	S	0	0
			566	352	94	118	2		
5	q	196	Total	C	N	O	S	0	0
			1518	956	263	291	8		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	106	Total	C	N	O	S	0	0
			916	579	166	169	2		
6	r	106	Total	C	N	O	S	0	0
			916	579	166	169	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	56	ASP	ASN	conflict	UNP P00129
r	56	ASP	ASN	conflict	UNP P00129

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	81	Total	C	N	O	S	0	0
			682	441	128	112	1		
7	s	81	Total	C	N	O	S	0	0
			682	441	128	112	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	64	Total	C	N	O	S	0	0
			524	316	96	107	5		
8	t	64	Total	C	N	O	S	0	0
			524	316	96	107	5		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	33	Total	C	N	O	S	0	0
			248	152	51	44	1		
9	u	33	Total	C	N	O	S	0	0
			248	152	51	44	1		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	62	Total	C	N	O	0	0
			512	335	89	88		
10	v	62	Total	C	N	O	0	0
			512	335	89	88		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	k	22	Total	C	N	O	0	0
			159	103	29	27		
11	w	22	Total	C	N	O	0	0
			159	103	29	27		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	22	GLN	SER	conflict	UNP P07552
k	34	SER	TRP	conflict	UNP P07552
k	38	SER	TRP	conflict	UNP P07552
w	22	GLN	SER	conflict	UNP P07552
w	34	SER	TRP	conflict	UNP P07552
w	38	SER	TRP	conflict	UNP P07552

- Molecule 12 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	x	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	y	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	z	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	238	GLY	ALA	conflict	UNP P00415

- Molecule 15 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	5	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	6	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	7	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	8	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	9	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 24 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	0	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 25 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	A	83	Total	C	N	O	0	0
			415	249	83	83		

- Molecule 26 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	143	Total	C	N	O	S	0	0
			719	429	143	143	4		

- Molecule 27 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	C	154	Total	C	N	O	0	0
			770	462	154	154		

- Molecule 28 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	D	384	Total	C	N	O	0	0
			1920	1152	384	384		

- Molecule 29 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	E	159	Total	C	N	O	S	0	0
			799	477	159	159	4		

- Molecule 30 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	411	Total	C	N	O	S	0	0
			2059	1233	411	411	4		

- Molecule 31 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	527	Total	C	N	O	S	0	0
			2651	1584	529	527	11		

- Molecule 32 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	H	285	Total	C	N	O	0	0
			1425	855	285	285		

- Molecule 33 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	162	Total	C	N	O	S	0	0
			818	486	162	162	8		

- Molecule 34 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	J	131	Total	C	N	O	0	0
			655	393	131	131		

- Molecule 35 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	K	84	Total	C	N	O	0	0
			420	252	84	84		

- Molecule 36 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L	558	Total	C	N	O	0	0
			2790	1674	558	558		

- Molecule 37 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	M	439	Total	C	N	O	0	0
			2195	1317	439	439		

- Molecule 38 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	N	326	Total	C	N	O	0	0
			1630	978	326	326		

- Molecule 39 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	O	181	Total	C	N	O	0	0
			905	543	181	181		

- Molecule 40 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	P	252	Total	C	N	O	0	0
			1260	756	252	252		

- Molecule 41 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Q	69	Total	C	N	O	0	0
			345	207	69	69		

- Molecule 42 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	R	47	Total 235	C 141	N 47	O 47	0	0

- Molecule 43 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	S	80	Total 400	C 240	N 80	O 80	0	0

- Molecule 44 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	T	71	Total 355	C 213	N 71	O 71	0	0

- Molecule 45 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	V	71	Total 355	C 213	N 71	O 71	0	0

- Molecule 46 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	W	72	Total 360	C 216	N 72	O 72	0	0

- Molecule 47 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	X	329	Total 1645	C 987	N 329	O 329	0	0

- Molecule 48 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Y	106	Total 530	C 318	N 106	O 106	0	0

- Molecule 49 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	a	71	Total	C	N	O	0	0
			355	213	71	71		

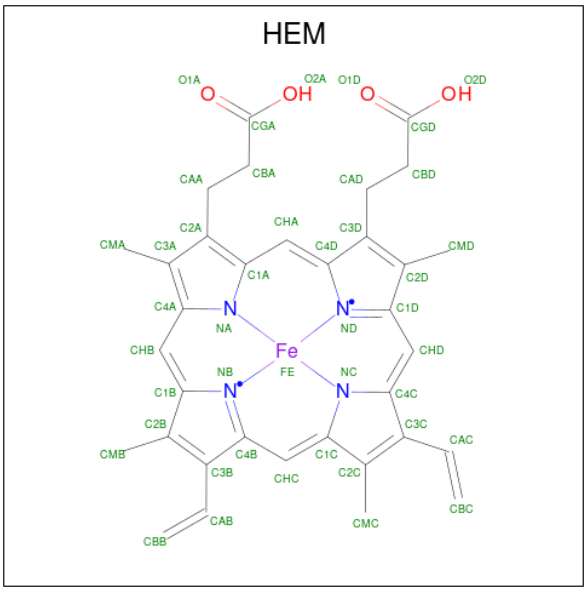
- Molecule 50 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	U	250	Total	C	N	O	0	0
			1250	750	250	250		

- Molecule 51 is a protein called complex I.

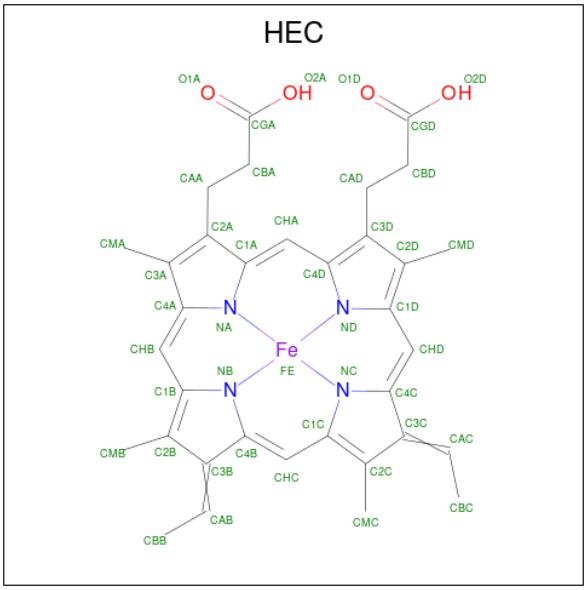
Mol	Chain	Residues	Atoms				AltConf	Trace
51	Z	266	Total	C	N	O	0	0
			1329	798	265	266		

- Molecule 52 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



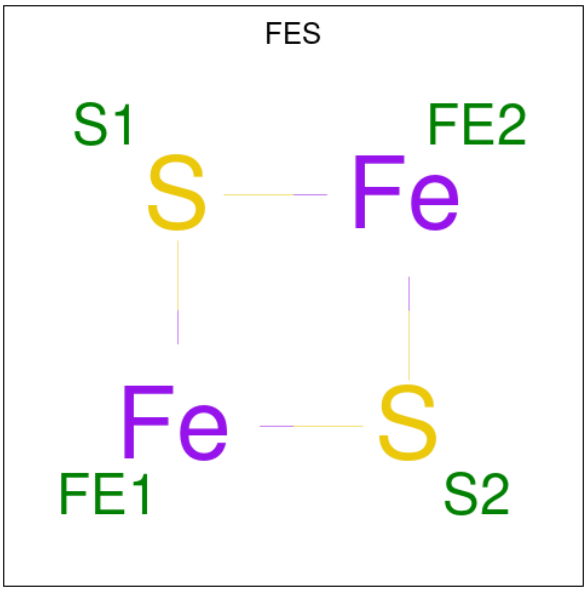
Mol	Chain	Residues	Atoms					AltConf
52	b	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
52	b	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
52	o	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
52	o	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 53 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
53	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
53	p	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

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

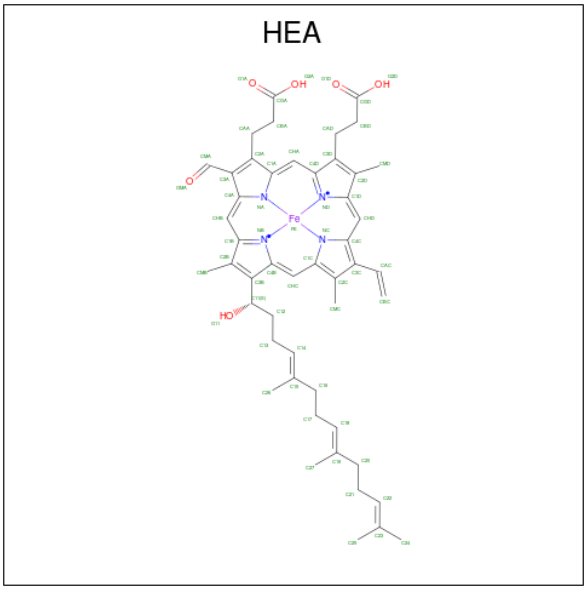
- Molecule 55 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
55	x	1	Total Cu 1 1	0
55	y	2	Total Cu 2 2	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	x	1	Total Mg 1 1	0

- Molecule 57 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

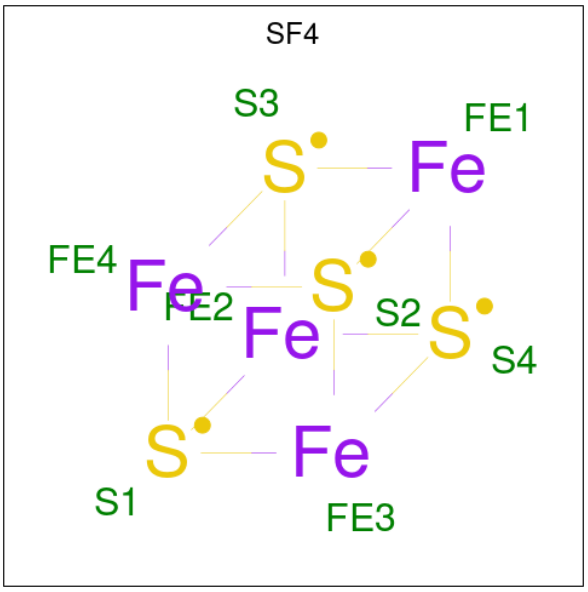


Mol	Chain	Residues	Atoms	AltConf
57	x	1	Total C Fe N O 120 98 2 8 12	0
57	x	1	Total C Fe N O 120 98 2 8 12	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
58	3	1	Total Zn 1 1	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



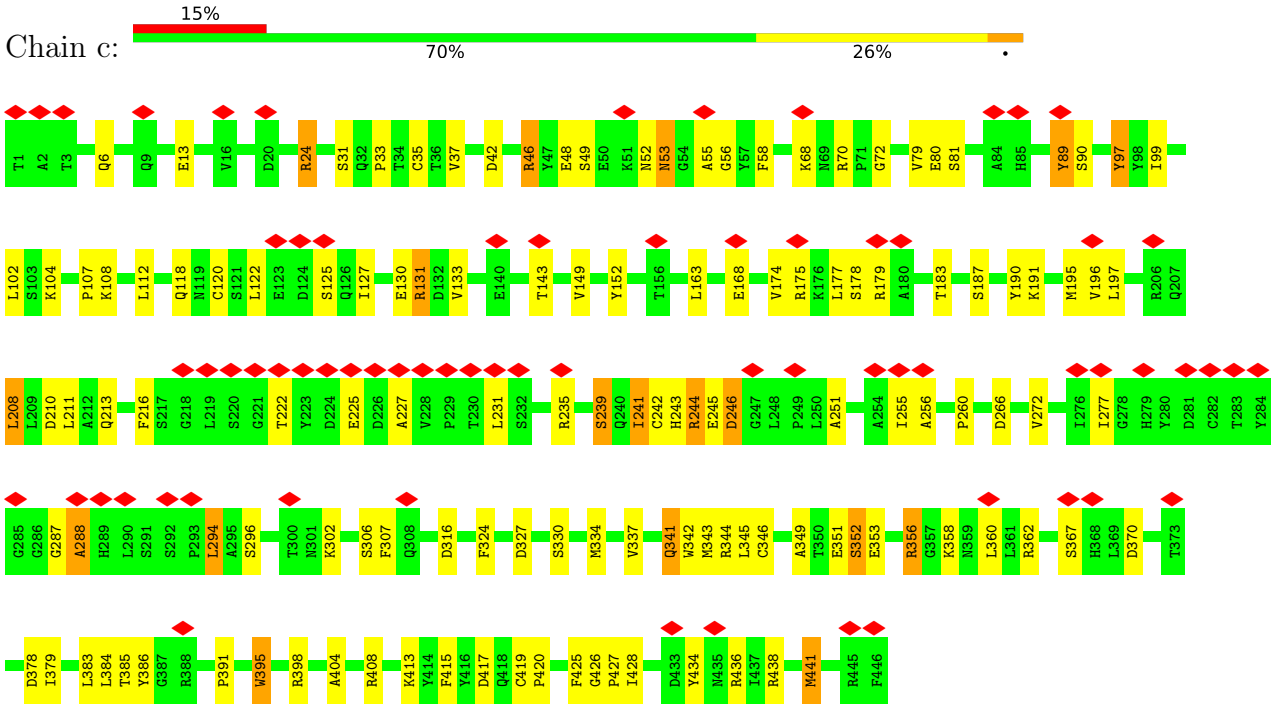
Mol	Chain	Residues	Atoms	AltConf
59	B	1	Total Fe S 8 4 4	0
59	F	1	Total Fe S 8 4 4	0
59	G	1	Total Fe S 16 8 8	0
59	G	1	Total Fe S 16 8 8	0
59	I	1	Total Fe S 16 8 8	0
59	I	1	Total Fe S 16 8 8	0

3 Residue-property plots (i)

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

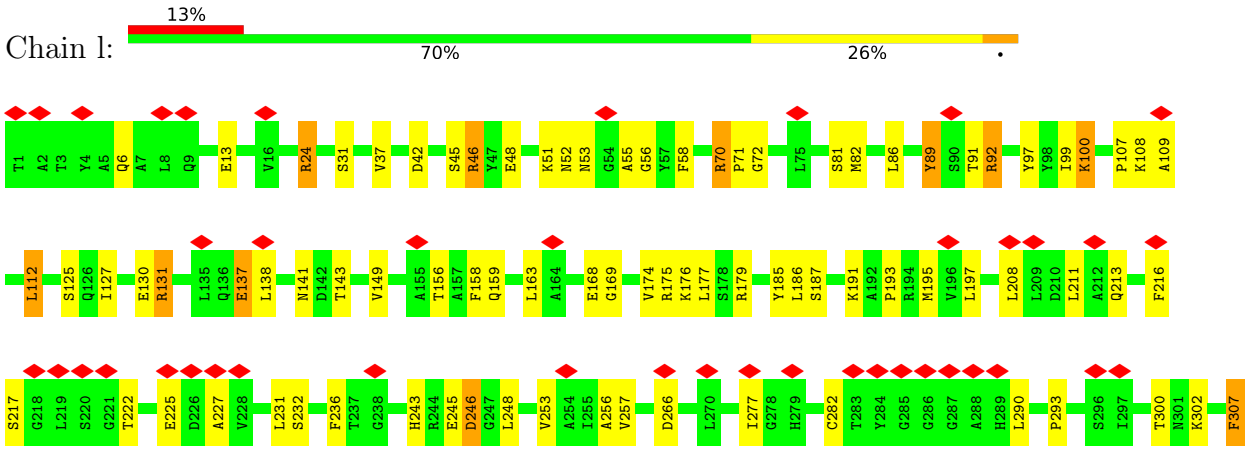
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

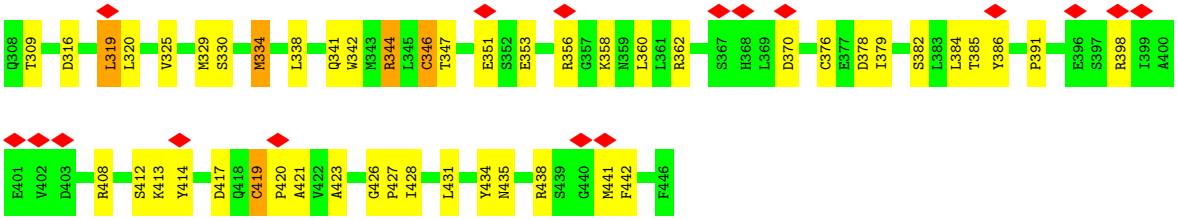
Chain c:



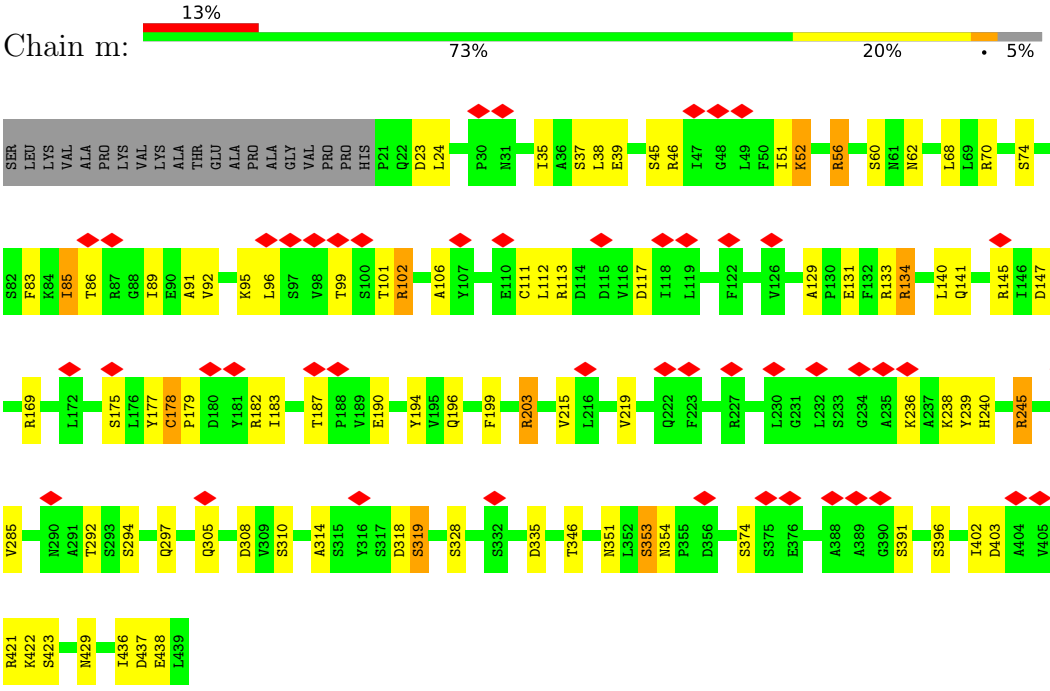
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain l:

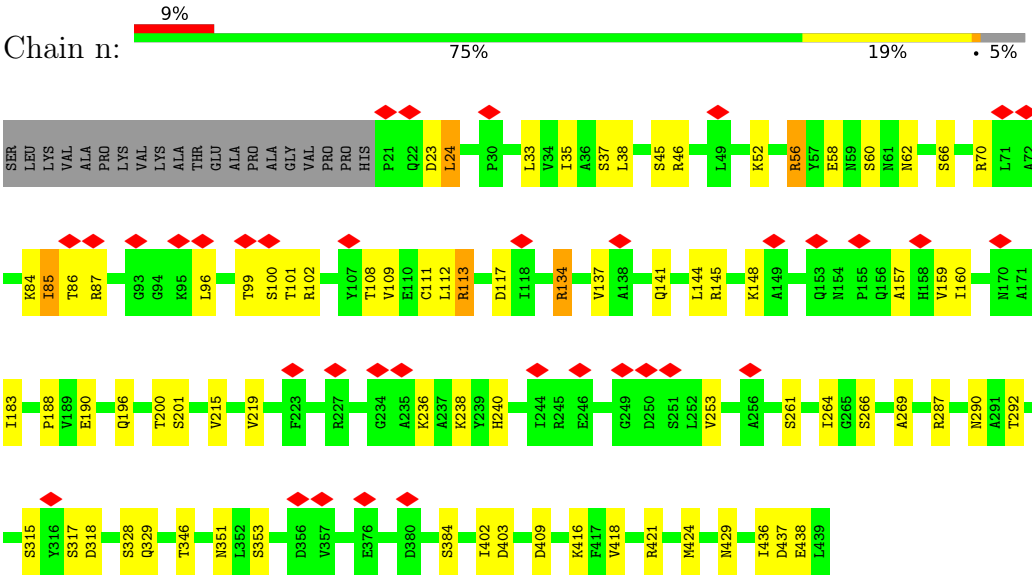




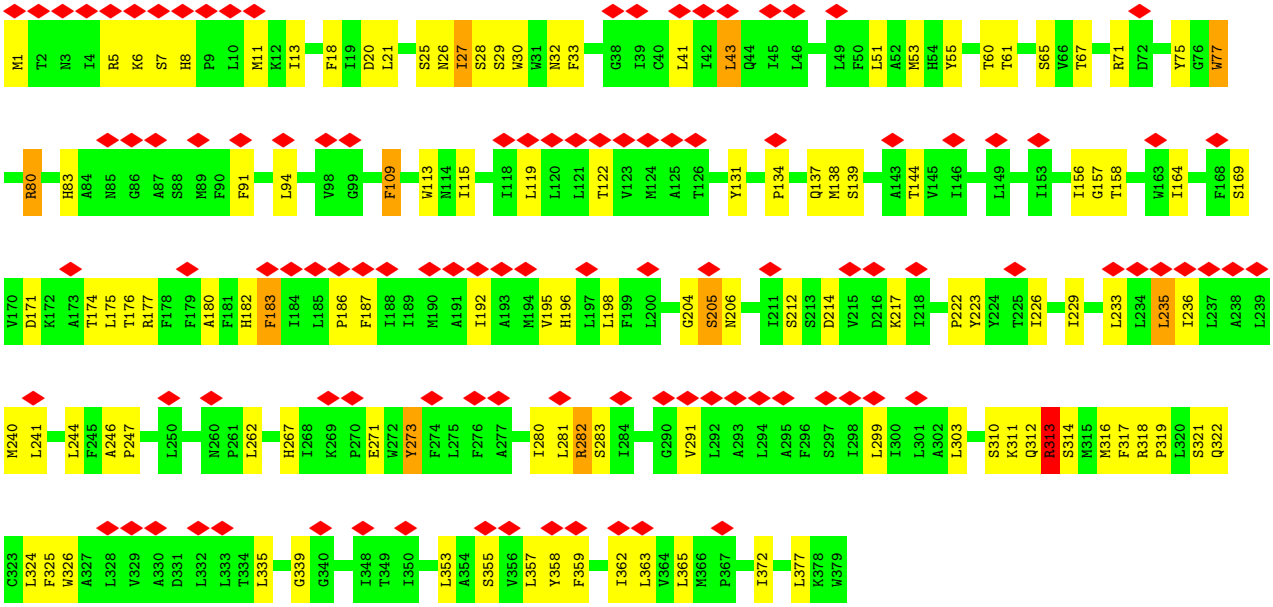
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



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

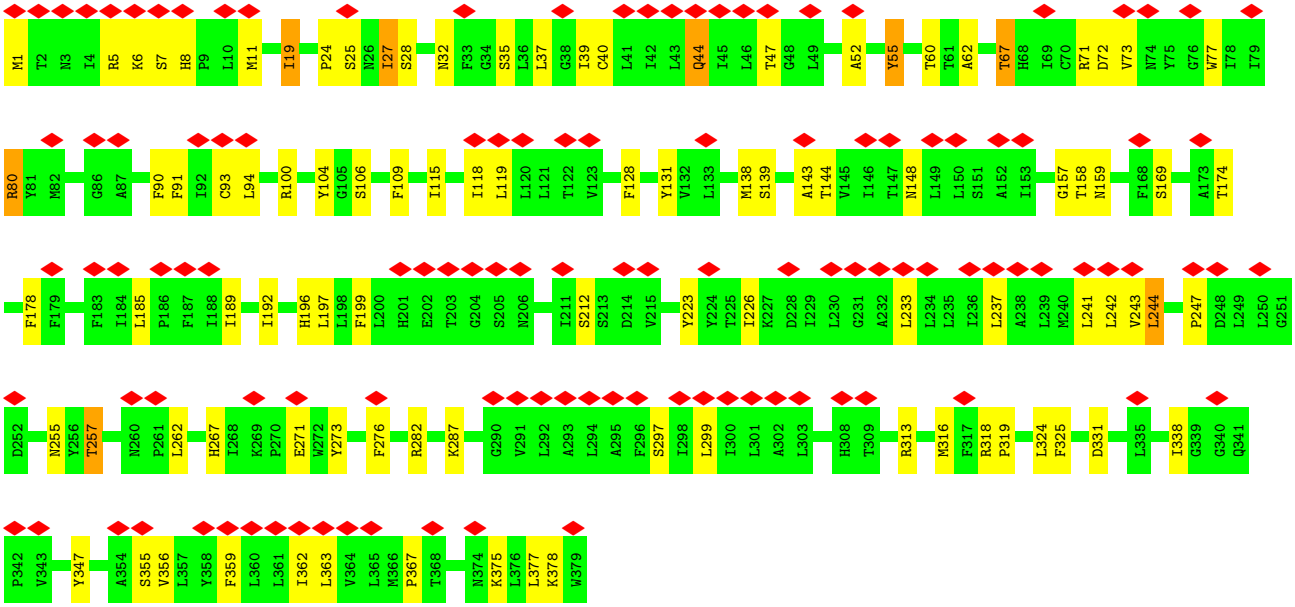


• Molecule 3: Cytochrome b



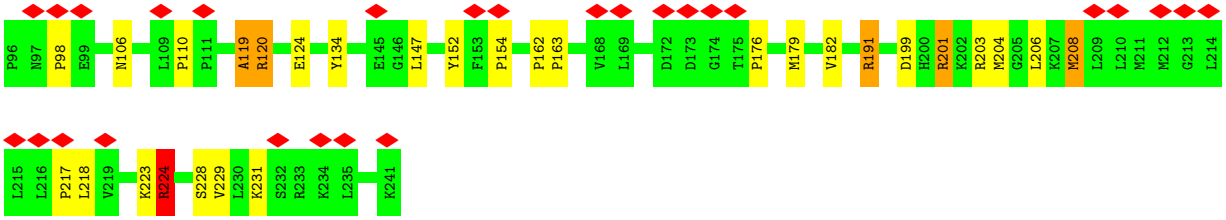
• Molecule 3: Cytochrome b

Chain o:



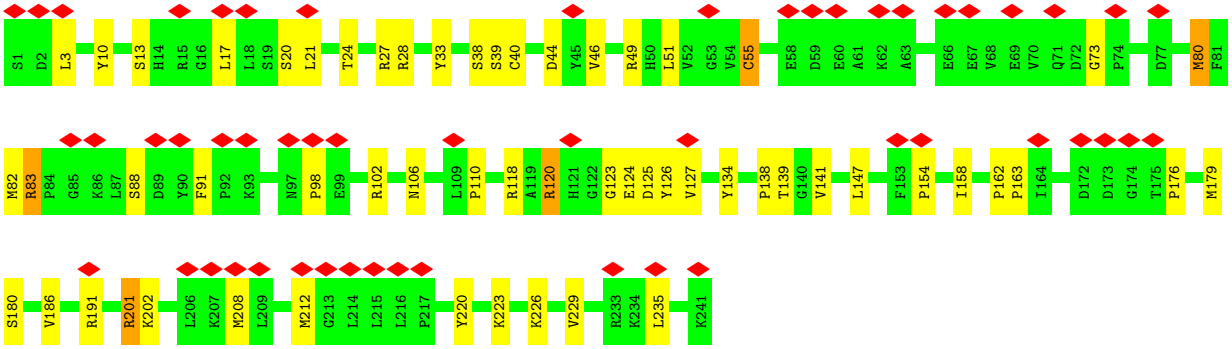
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain d:



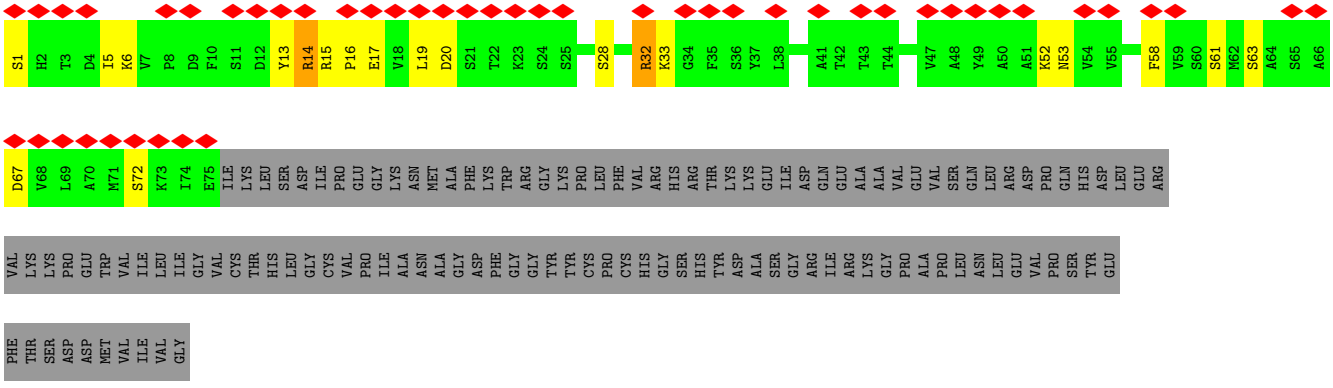
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain p:



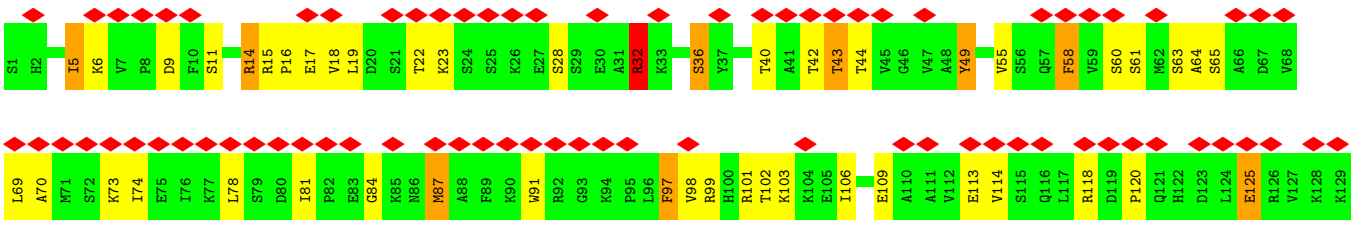
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

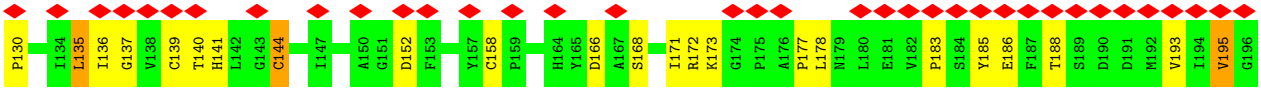
Chain e:



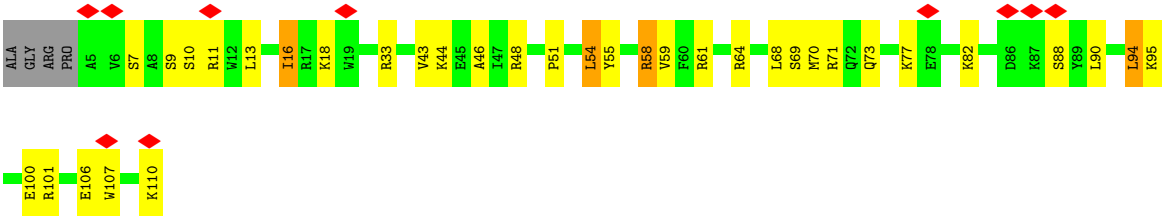
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain q:

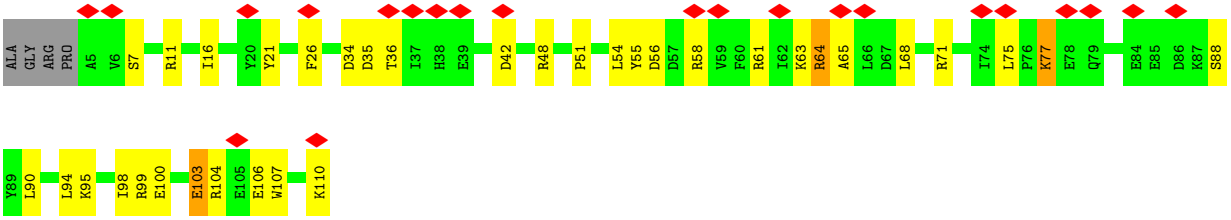




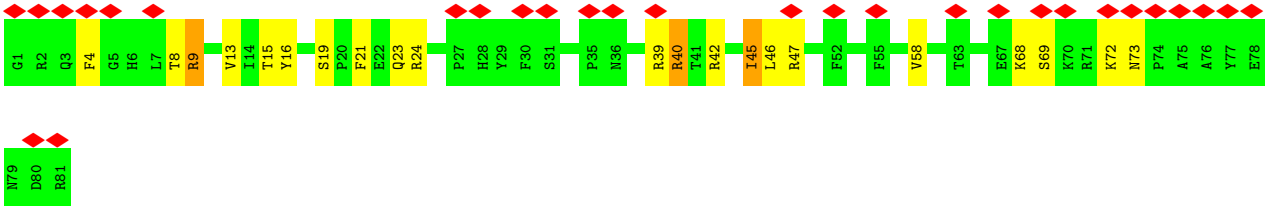
• Molecule 6: Cytochrome b-c1 complex subunit 7



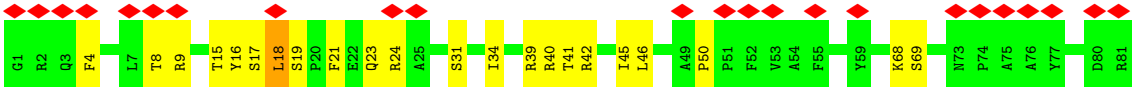
• Molecule 6: Cytochrome b-c1 complex subunit 7



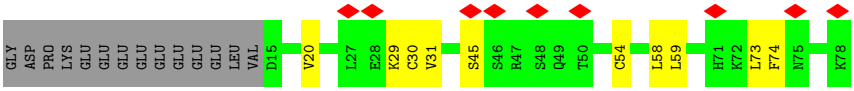
• Molecule 7: Cytochrome b-c1 complex subunit 8



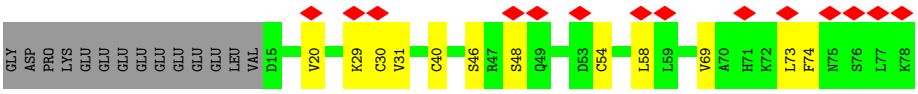
• Molecule 7: Cytochrome b-c1 complex subunit 8



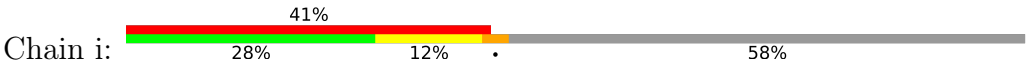
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

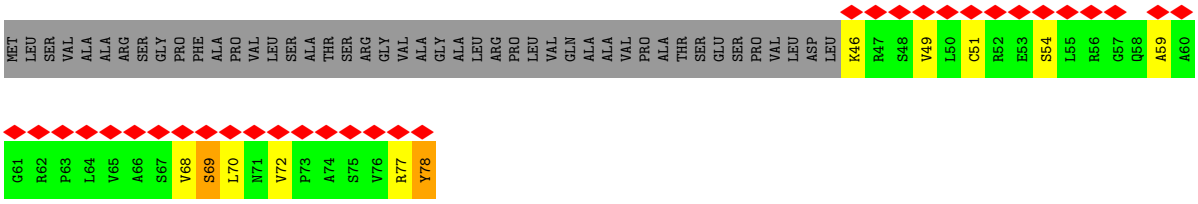


• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

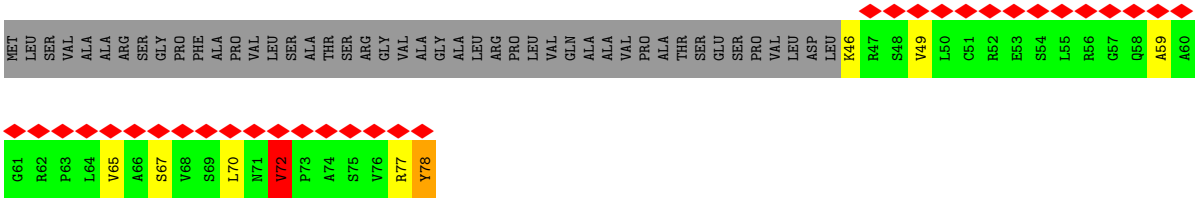


• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

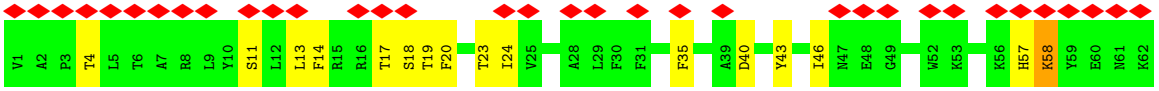




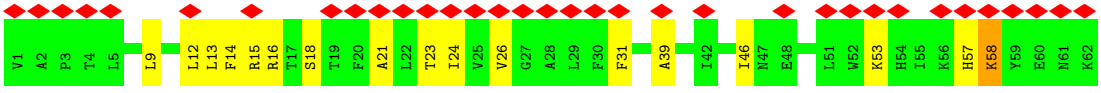
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 10: Cytochrome b-c1 complex subunit 9

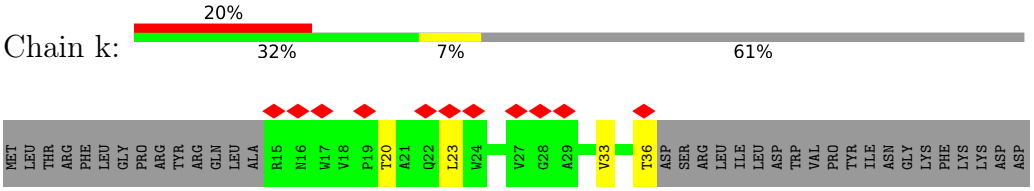


• Molecule 10: Cytochrome b-c1 complex subunit 9



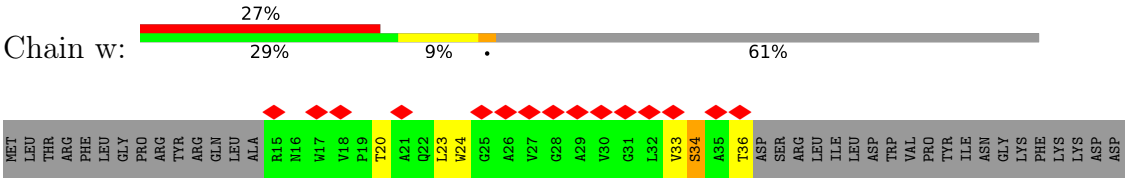
• Molecule 11: Cytochrome b-c1 complex subunit 10

Chain k:



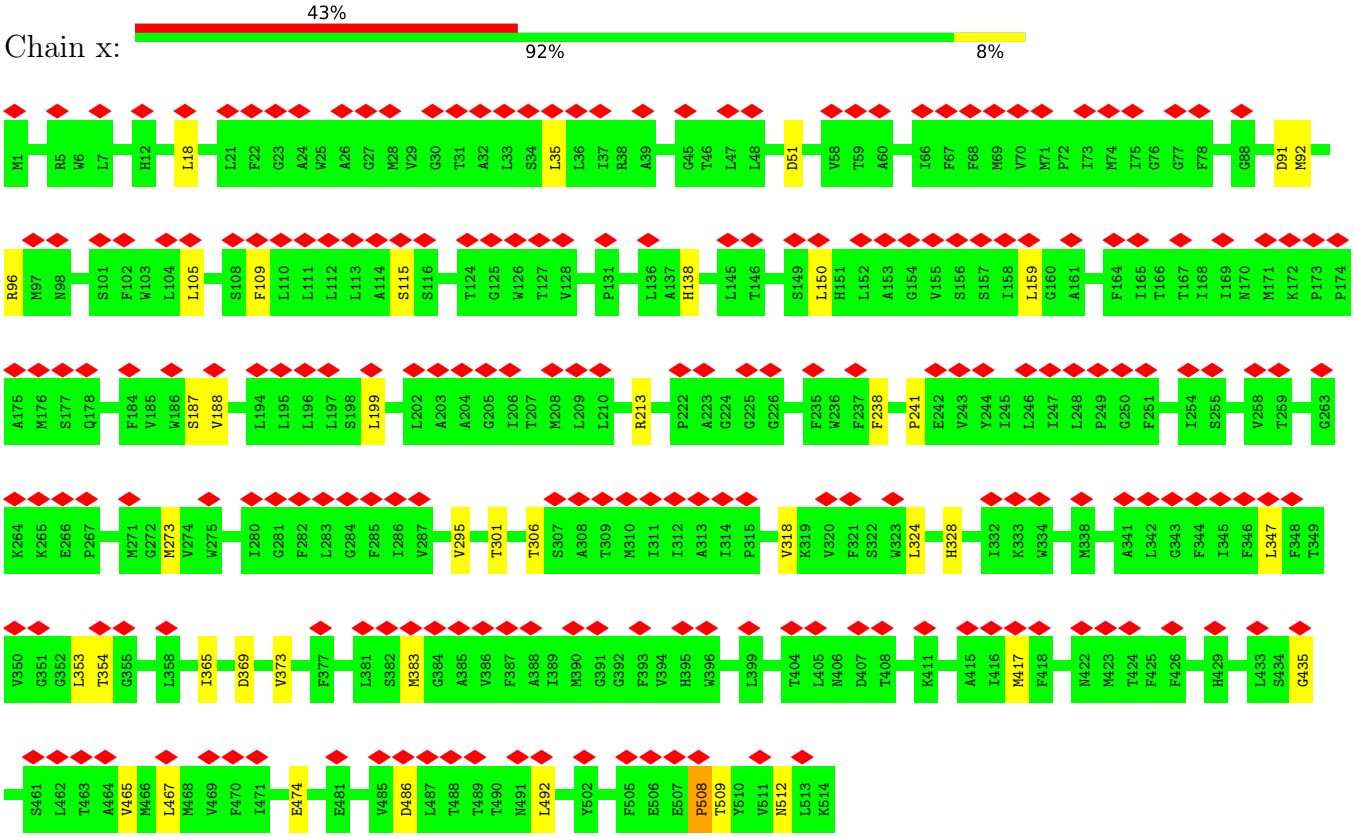
• Molecule 11: Cytochrome b-c1 complex subunit 10

Chain w:



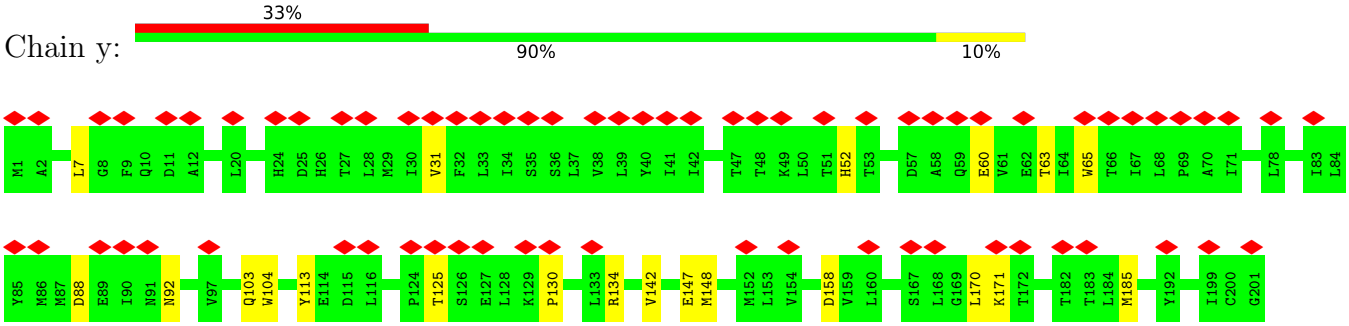
• Molecule 12: Cytochrome c oxidase subunit 1

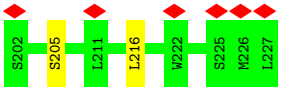
Chain x:



• Molecule 13: Cytochrome c oxidase subunit 2

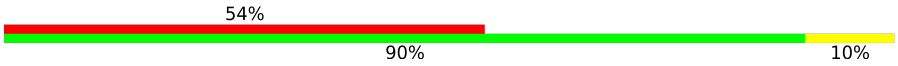
Chain y:

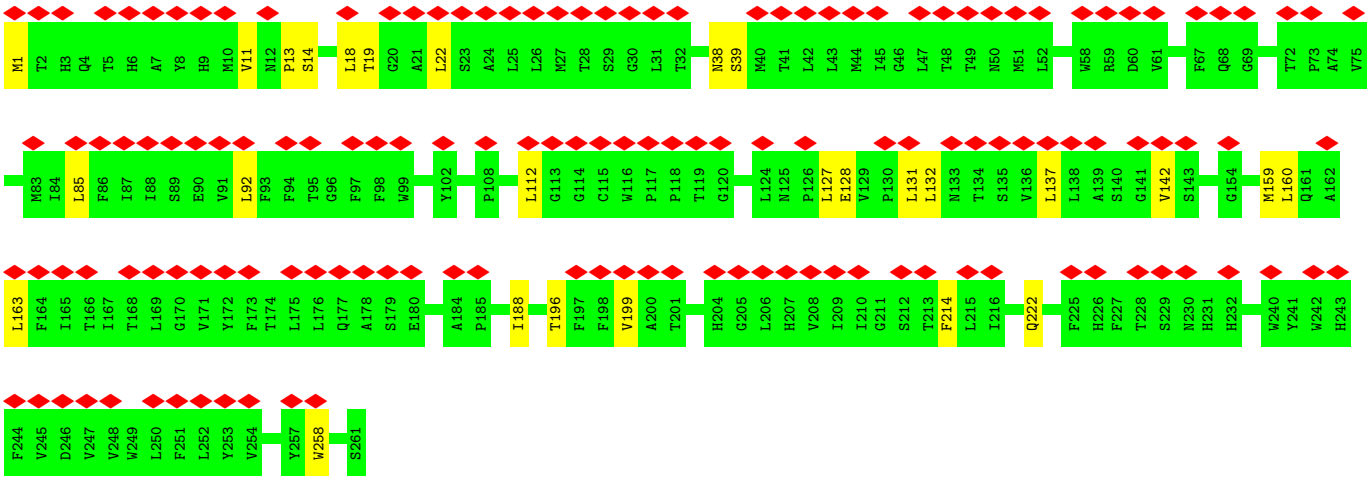




• Molecule 14: Cytochrome c oxidase subunit 3

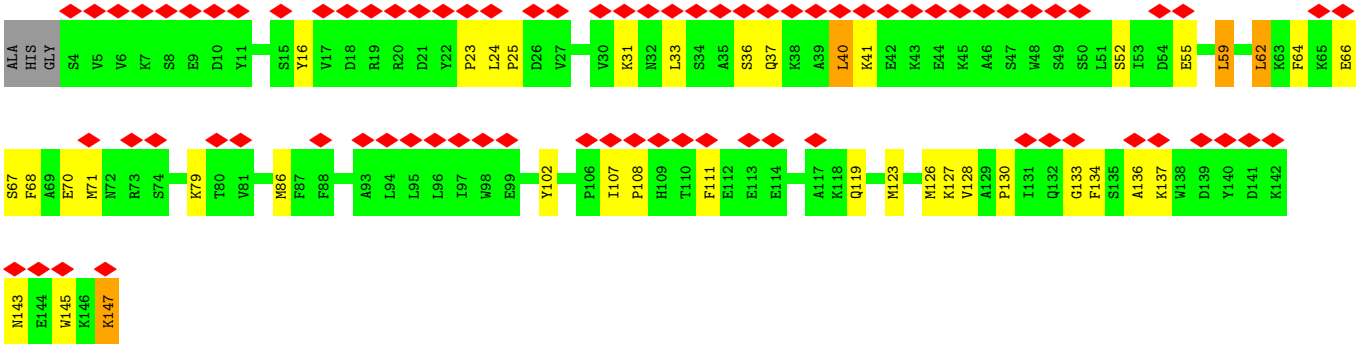
Chain z:





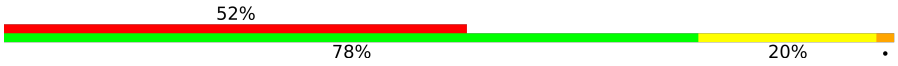
• Molecule 15: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

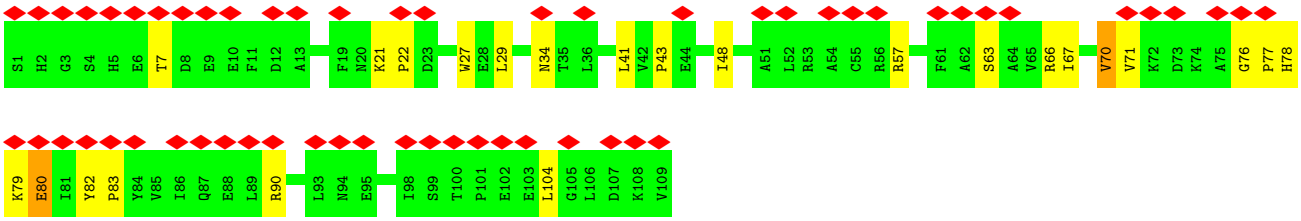
Chain 1:



• Molecule 16: Cytochrome c oxidase subunit 5A, mitochondrial

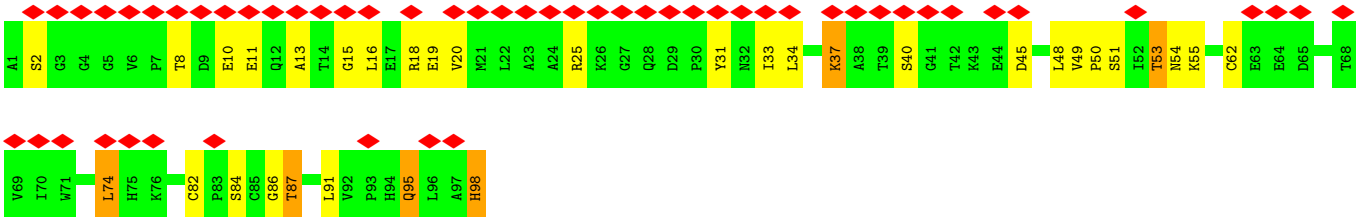
Chain 2:





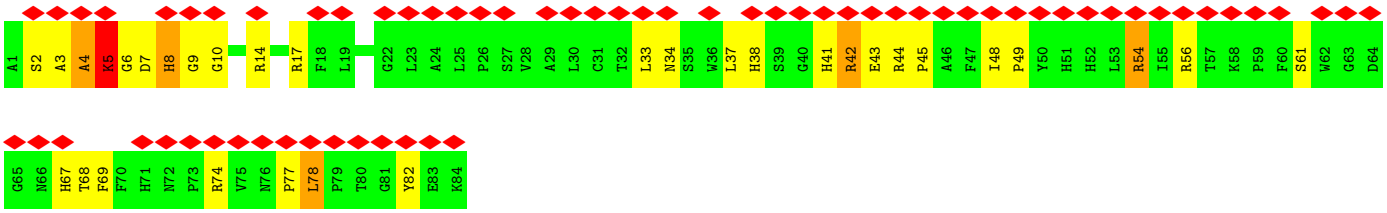
• Molecule 17: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 3:



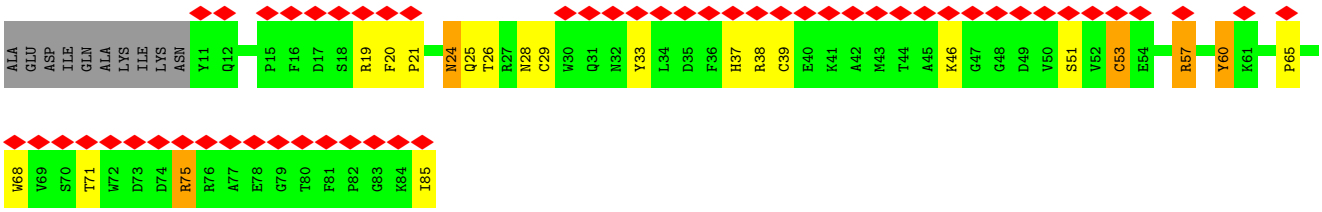
• Molecule 18: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain 4:



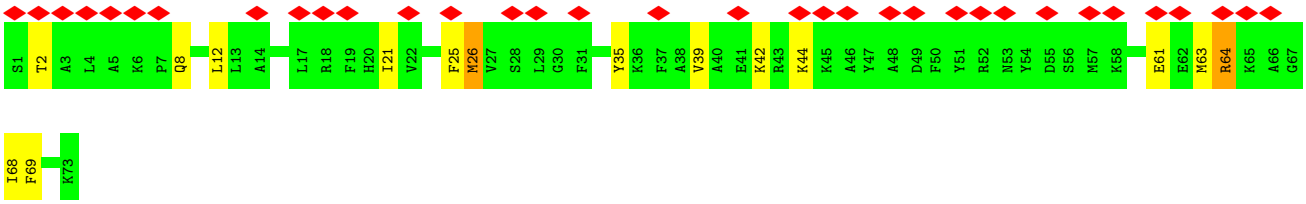
• Molecule 19: Cytochrome c oxidase subunit 6B1

Chain 5:



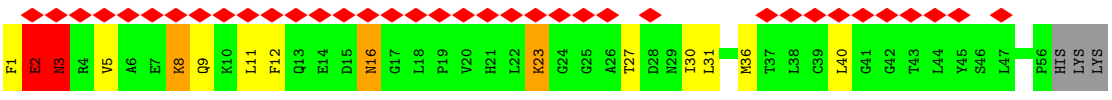
• Molecule 20: Cytochrome c oxidase subunit 6C

Chain 6:



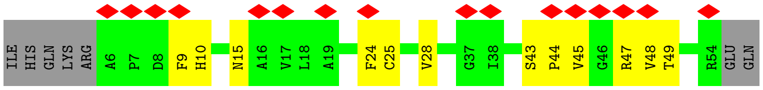
• Molecule 21: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 7:



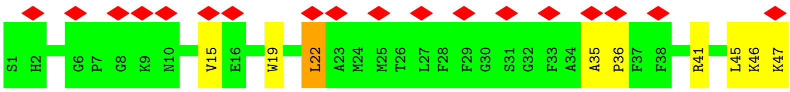
• Molecule 22: Cytochrome c oxidase subunit 7B, mitochondrial

Chain 8:



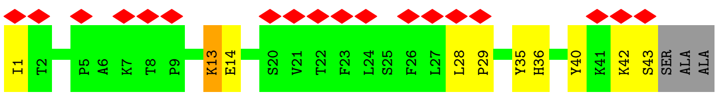
• Molecule 23: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 9:



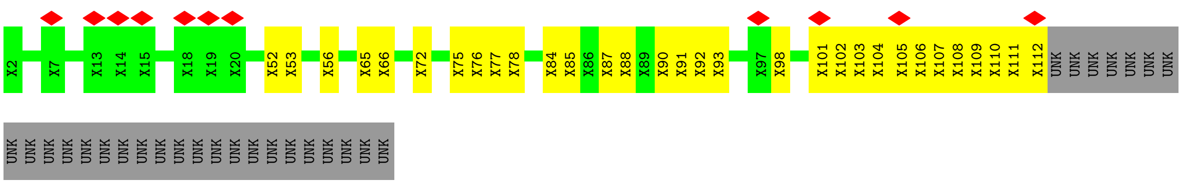
• Molecule 24: Cytochrome c oxidase subunit 8B, mitochondrial

Chain 0:



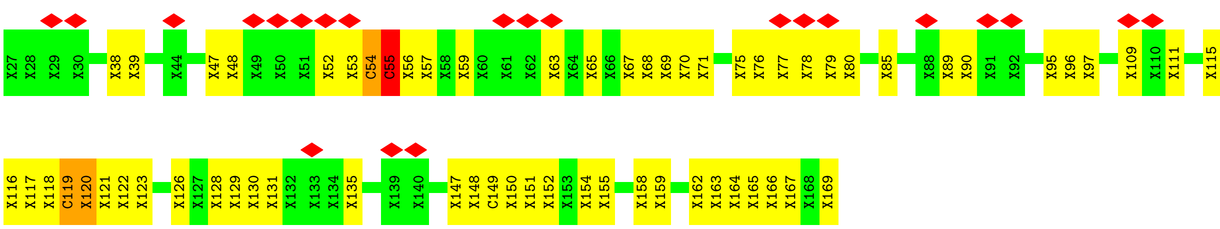
• Molecule 25: complex I

Chain A:



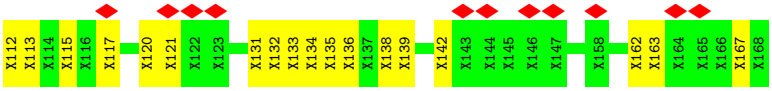
• Molecule 26: complex I

Chain B:



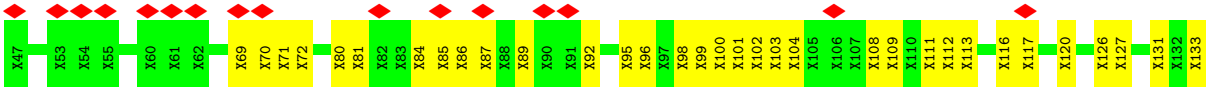
• Molecule 27: complex I

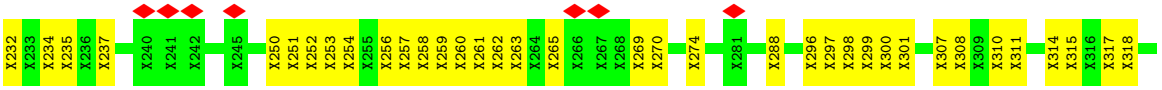
Chain C:

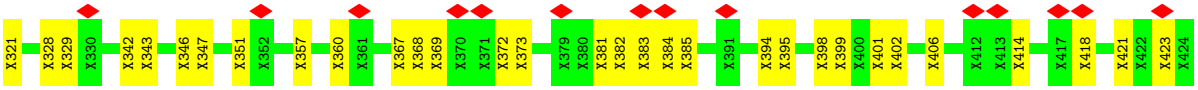


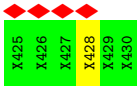
• Molecule 28: complex I

Chain D:



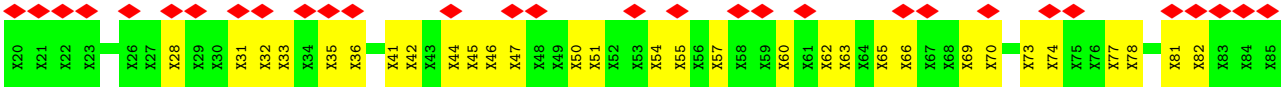


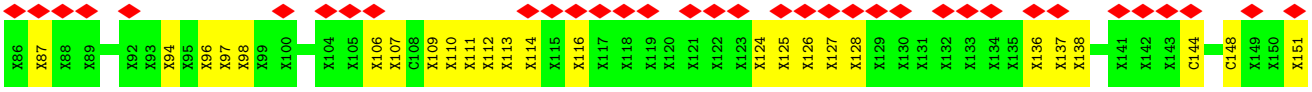


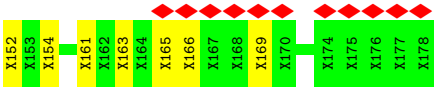


• Molecule 29: complex I

Chain E:

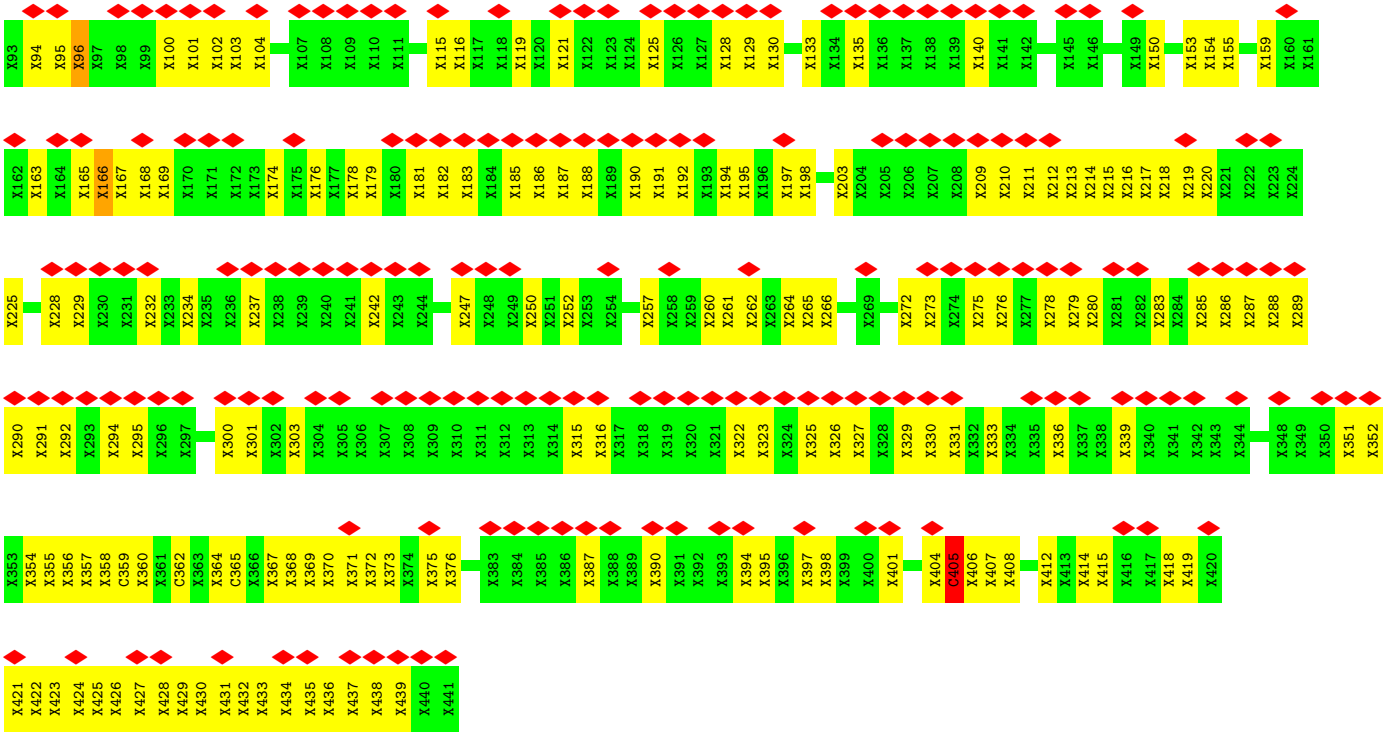






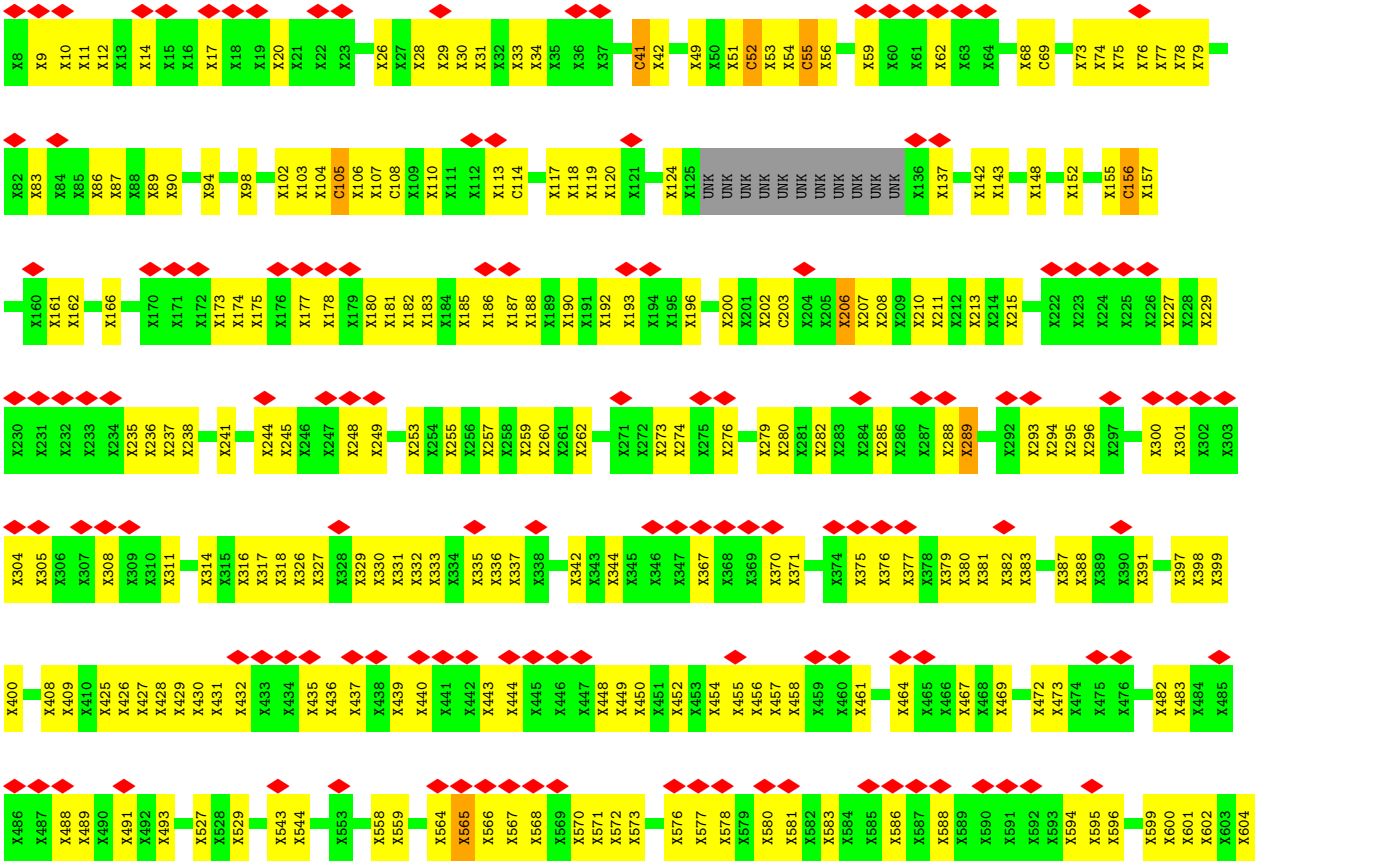
• Molecule 30: complex I

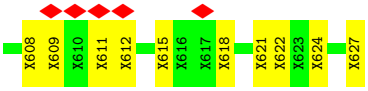
Chain F:



• Molecule 31: complex I

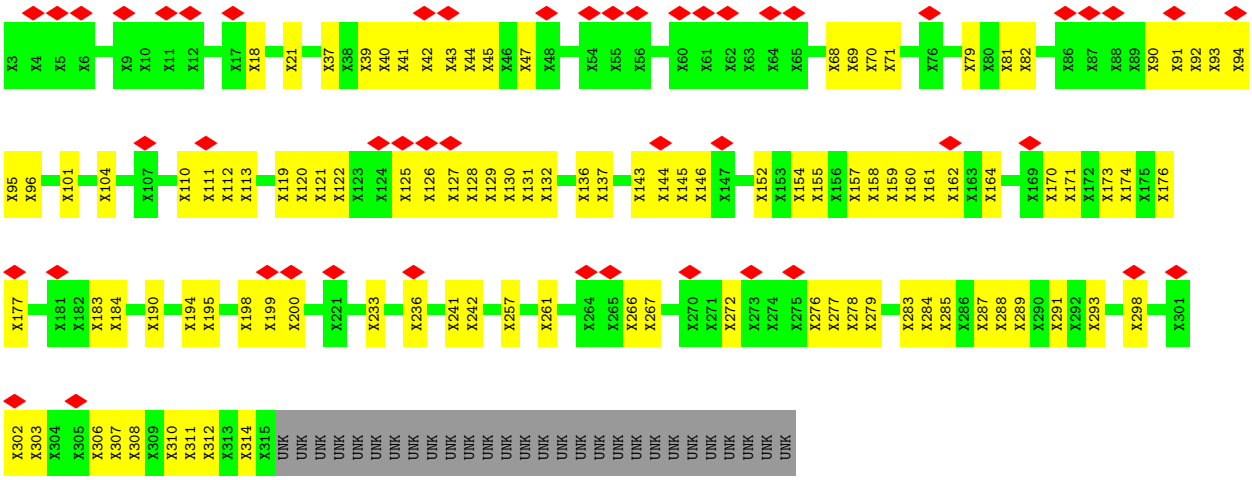
Chain G:





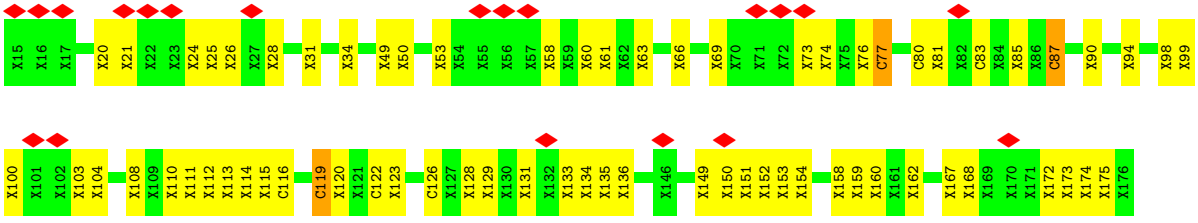
• Molecule 32: complex I

Chain H:



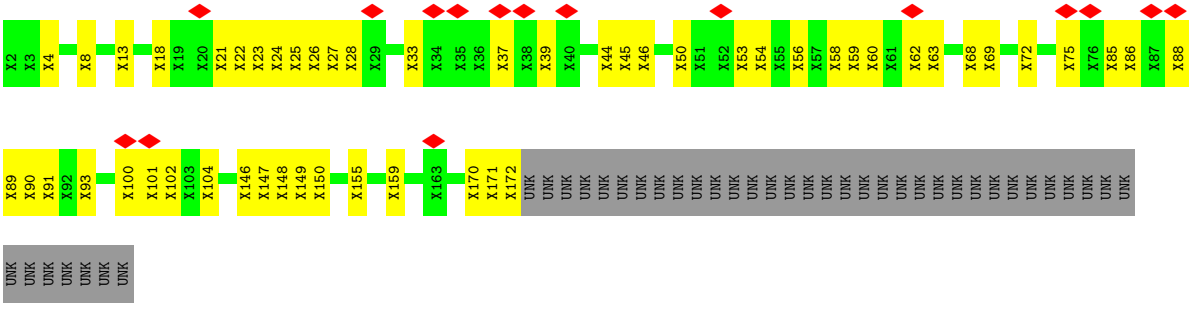
• Molecule 33: complex I

Chain I:



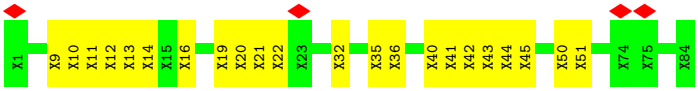
• Molecule 34: complex I

Chain J:



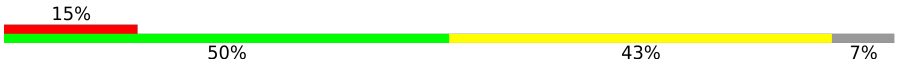
• Molecule 35: complex I

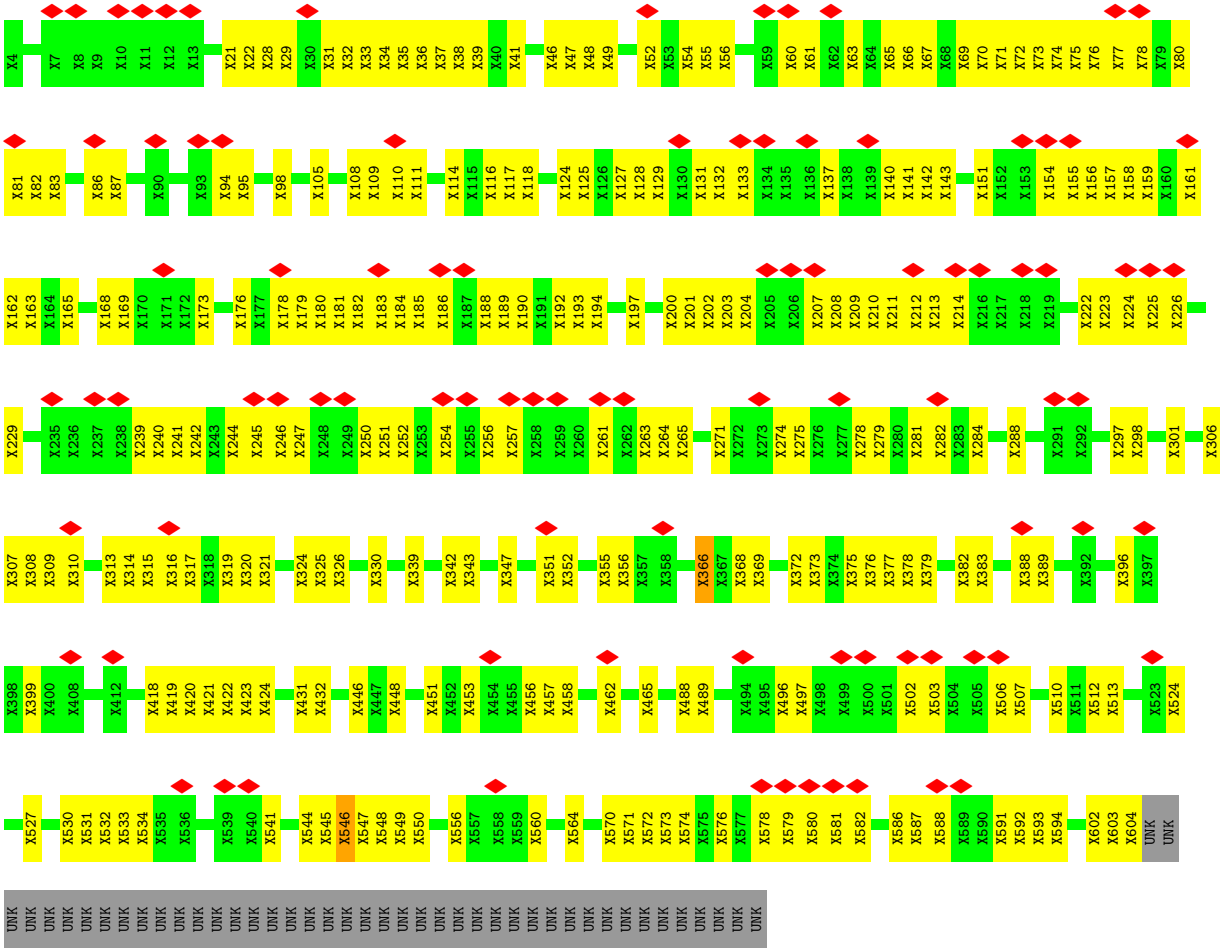
Chain K:



• Molecule 36: complex I

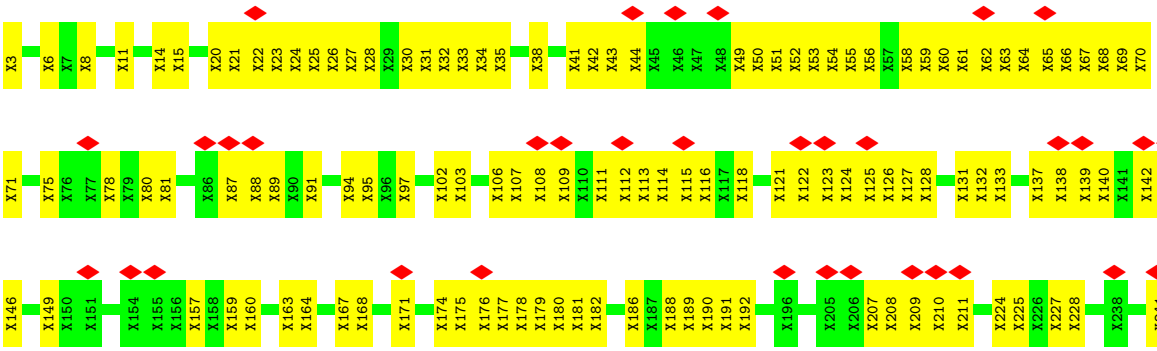
Chain L:

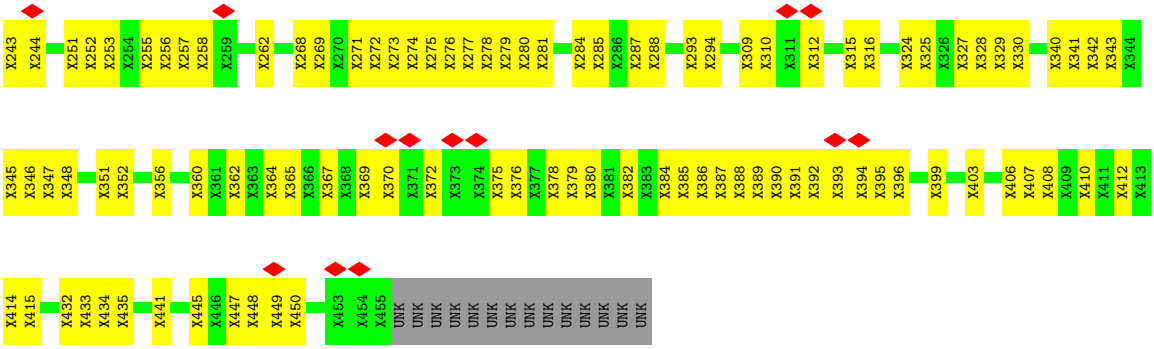




• Molecule 37: complex I

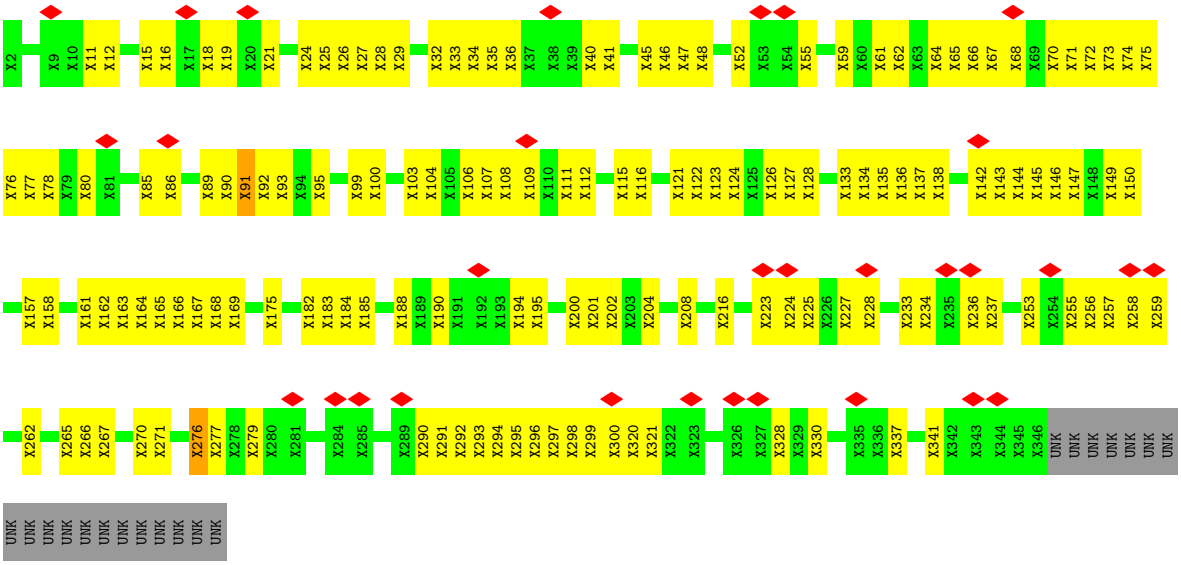
Chain M:





• Molecule 38: complex I

Chain N:

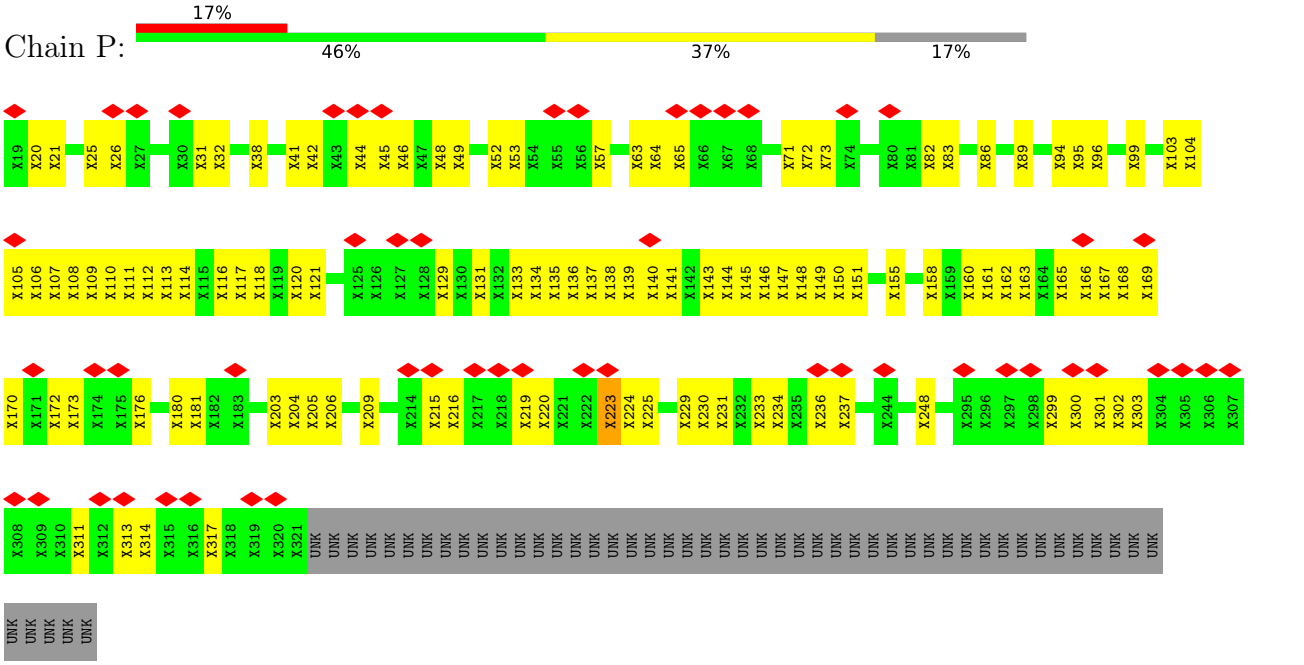


• Molecule 39: complex I

Chain O:

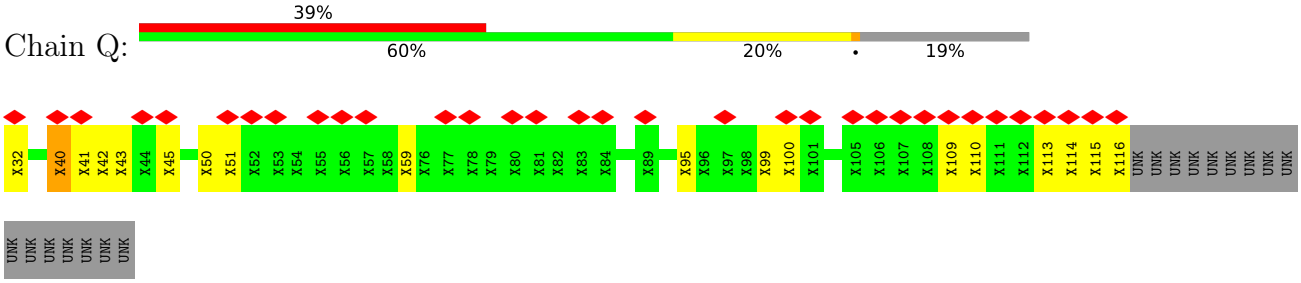
• Molecule 40: complex I

Chain P:



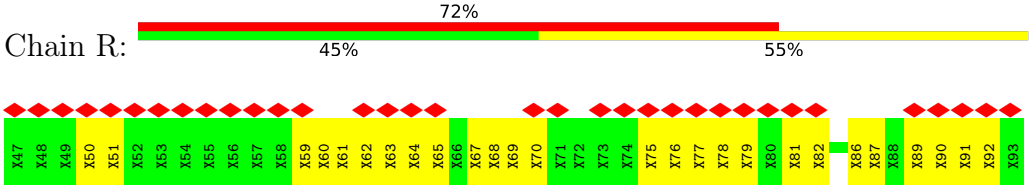
• Molecule 41: complex I

Chain Q:



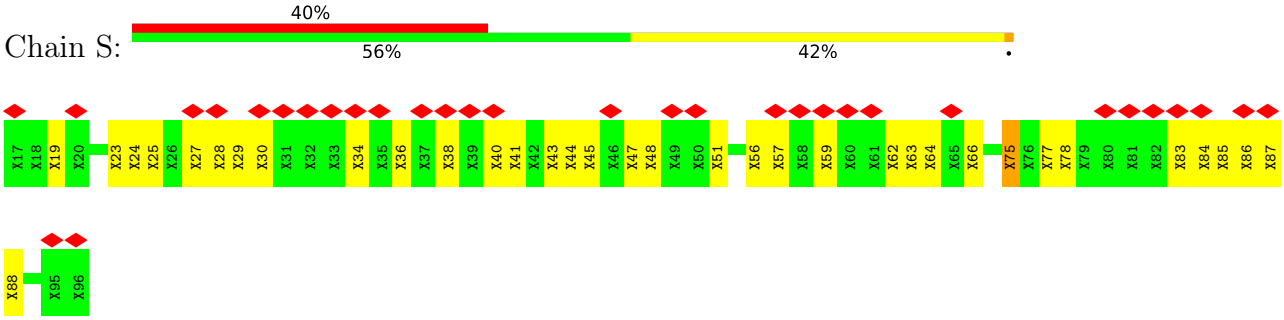
• Molecule 42: complex I

Chain R:



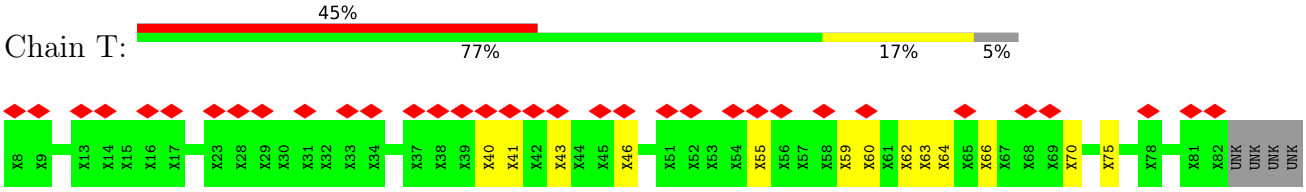
• Molecule 43: complex I

Chain S:



• Molecule 44: complex I

Chain T:



• Molecule 45: complex I

Chain V:

• Molecule 46: complex I

Chain W:

• Molecule 47: complex I

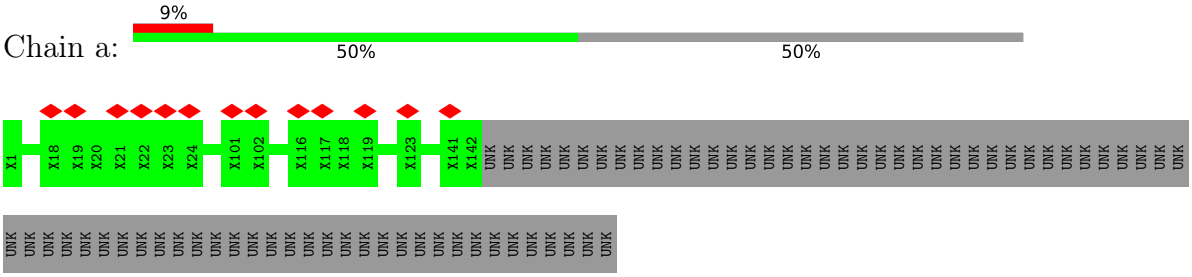
Chain X:

• Molecule 48: complex I

Chain Y:

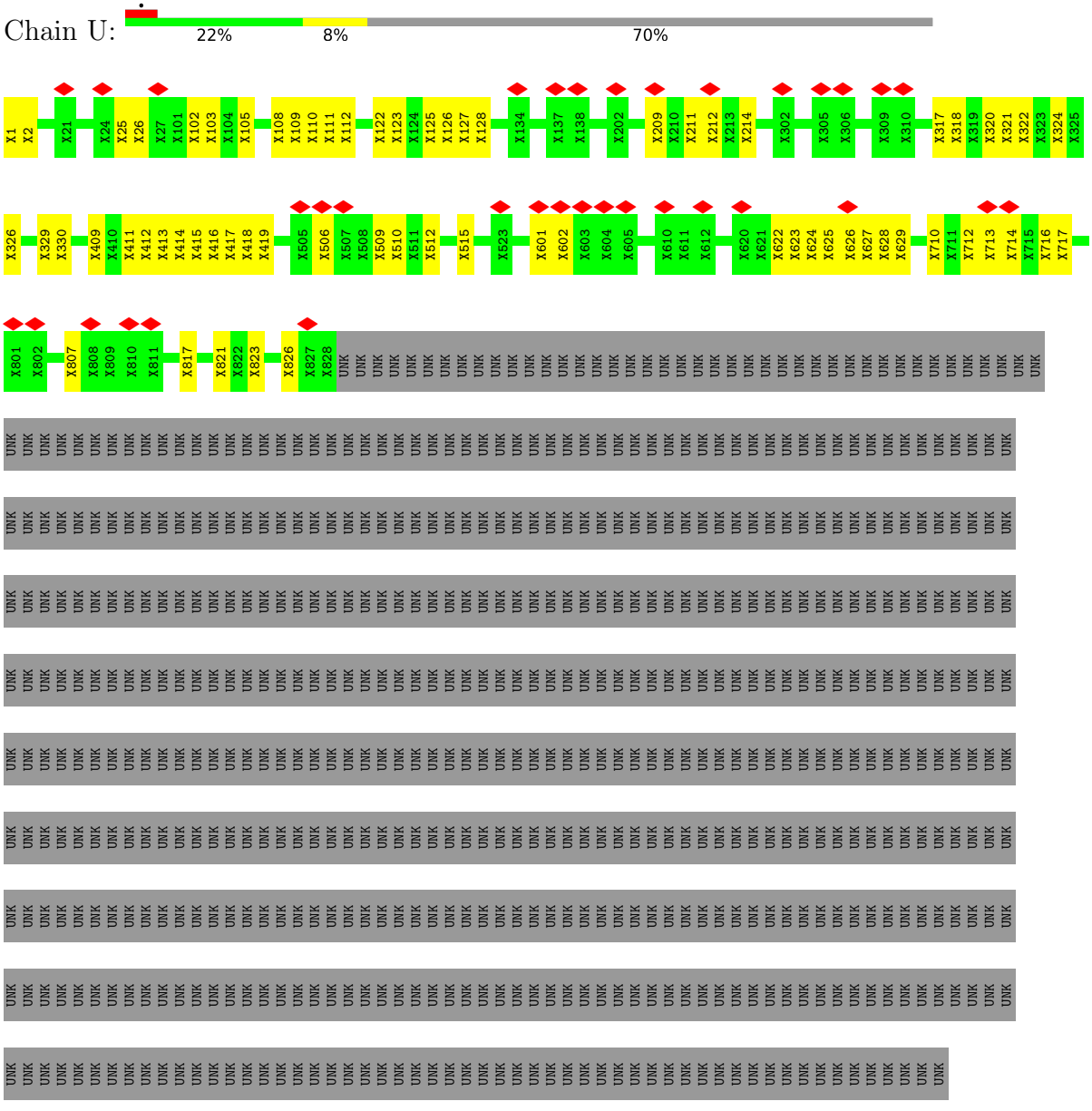
• Molecule 49: complex I

Chain a:



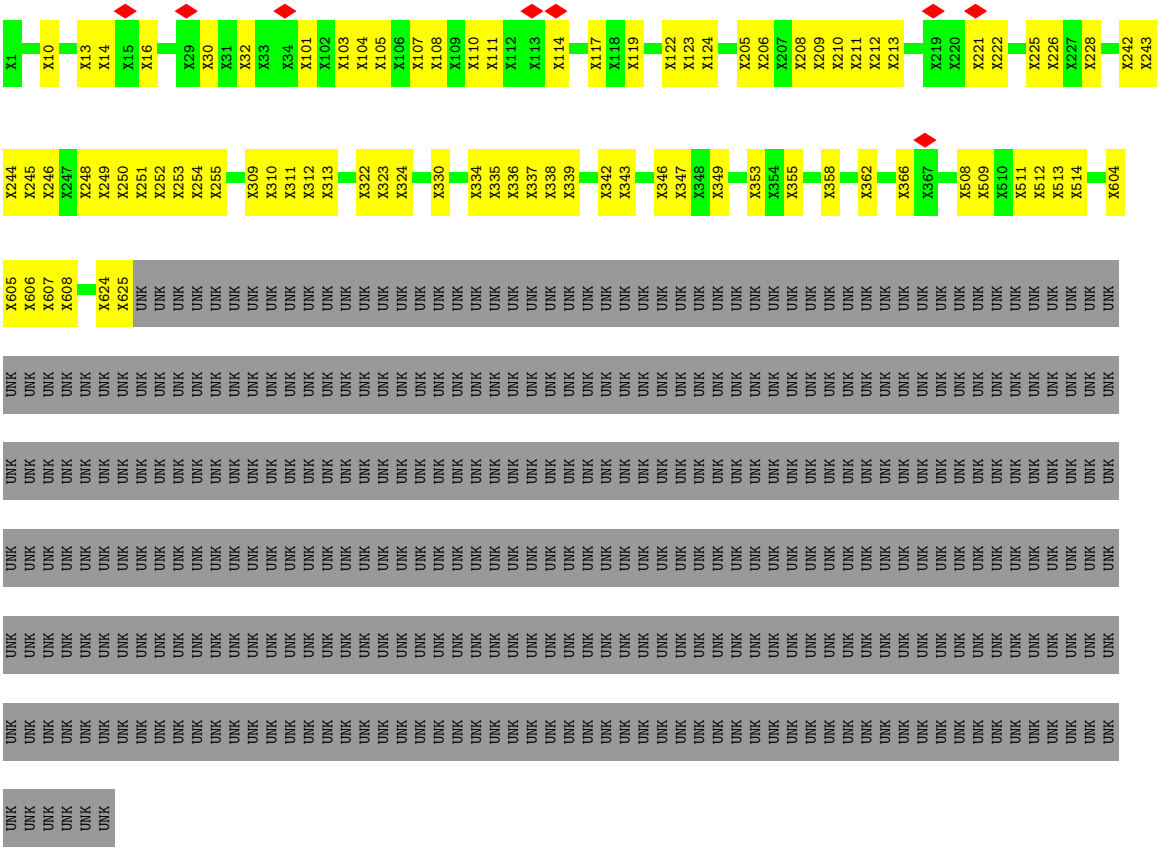
• Molecule 50: complex I

Chain U:



• Molecule 51: complex I

Chain Z:


X1 X10 X13 X14 X15 X16 X29 X30 X31 X32 X33 X34 X101 X102 X103 X104 X105 X106 X107 X108 X109 X110 X111 X112 X113 X114 X117 X118 X119 X122 X123 X124 X205 X206 X207 X208 X209 X210 X211 X212 X213 X219 X220 X221 X222 X225 X226 X227 X228 X242 X243
X244 X245 X246 X247 X248 X249 X250 X251 X252 X253 X254 X255 X309 X310 X311 X312 X313 X322 X323 X324 X330 X334 X335 X336 X337 X338 X339 X342 X343 X346 X347 X348 X349 X353 X354 X355 X358 X362 X366 X367 X508 X509 X510 X511 X512 X513 X514 X604
X605 X606 X607 X608 X624 X625
UNK

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17093	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	57797	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.368	Depositor
Minimum map value	-0.164	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.081	Depositor
Map size (Å)	509.76, 509.76, 509.76	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.77, 1.77, 1.77	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, MG, HEC, CU, FES, HEA, ZN, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	c	0.60	2/3531 (0.1%)	1.58	43/4792 (0.9%)
1	l	0.63	3/3531 (0.1%)	1.61	58/4792 (1.2%)
2	m	0.51	0/3198	1.46	31/4336 (0.7%)
2	n	0.51	0/3198	1.33	11/4336 (0.3%)
3	b	0.71	2/3108 (0.1%)	1.73	62/4252 (1.5%)
3	o	0.69	3/3108 (0.1%)	1.62	50/4252 (1.2%)
4	d	0.55	0/1978	1.50	23/2684 (0.9%)
4	p	0.55	0/1978	1.40	24/2684 (0.9%)
5	e	0.60	0/574	1.62	7/775 (0.9%)
5	q	0.61	0/1551	1.68	28/2097 (1.3%)
6	f	0.57	0/935	1.56	18/1253 (1.4%)
6	r	0.57	0/935	1.66	24/1253 (1.9%)
7	g	0.61	1/704 (0.1%)	1.41	9/951 (0.9%)
7	s	0.59	0/704	1.30	5/951 (0.5%)
8	h	0.41	0/529	1.12	0/708
8	t	0.39	0/529	1.06	0/708
9	i	0.48	0/250	1.31	2/335 (0.6%)
9	u	0.48	0/250	1.32	1/335 (0.3%)
10	j	0.51	0/525	1.31	5/707 (0.7%)
10	v	0.51	0/525	1.42	6/707 (0.8%)
11	k	0.42	0/163	1.01	0/225
11	w	0.46	0/163	1.17	0/225
12	x	0.60	0/4164	0.76	1/5688 (0.0%)
13	y	0.57	0/1868	0.79	0/2544
14	z	0.56	0/2211	0.68	0/3023
15	1	0.57	0/1229	0.64	1/1658 (0.1%)
16	2	0.50	0/898	0.66	0/1218
17	3	0.56	0/765	0.81	0/1038
18	4	0.54	0/699	0.73	1/950 (0.1%)
19	5	0.55	0/648	0.73	0/877
20	6	0.60	0/611	0.65	0/810
21	7	0.61	0/451	0.72	0/610

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
22	8	0.57	0/398	0.66	0/546
23	9	0.63	0/399	0.62	0/534
24	0	0.51	0/345	0.65	0/470
26	B	1.57	1/21 (4.8%)	2.68	2/23 (8.7%)
29	E	0.77	0/20	1.58	0/20
30	F	2.57	1/20 (5.0%)	2.24	0/20
31	G	1.04	0/65	1.60	0/67
33	I	2.33	2/40 (5.0%)	1.47	0/40
All	All	0.59	15/46819 (0.0%)	1.33	412/63494 (0.6%)

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
1	c	0	13
1	l	0	3
2	m	0	9
2	n	0	5
3	b	0	14
3	o	0	6
4	d	0	5
4	p	0	4
5	e	0	1
5	q	0	9
6	f	0	2
7	g	0	2
7	s	0	3
8	t	0	1
9	i	0	1
9	u	0	1
10	j	0	1
11	w	0	1
26	B	0	2
27	C	0	1
28	D	0	1
30	F	0	2
31	G	0	6
33	I	0	1
36	L	0	4
38	N	0	2

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	O	0	2
40	P	0	3
41	Q	0	1
43	S	0	1
46	W	0	1
47	X	0	1
All	All	0	109

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	F	405	CYS	CA-CB	-9.00	1.34	1.53
33	I	87	CYS	CA-CB	7.93	1.71	1.53
1	c	419	CYS	CB-SG	-7.15	1.70	1.82
33	I	77	CYS	CA-CB	6.97	1.69	1.53
1	l	253	VAL	C-O	6.79	1.36	1.23
1	c	104	LYS	CD-CE	6.55	1.67	1.51
1	l	169	GLY	N-CA	-6.53	1.36	1.46
3	o	106	SER	CB-OG	-6.42	1.33	1.42
7	g	16	TYR	CD2-CE2	-6.07	1.30	1.39
1	l	434	TYR	CG-CD2	-5.38	1.32	1.39
26	B	55	CYS	CA-CB	5.37	1.65	1.53
3	o	40	CYS	CB-SG	-5.32	1.73	1.81
3	b	75	TYR	CG-CD1	-5.09	1.32	1.39
3	o	37	LEU	C-N	-5.07	1.24	1.33
3	b	183	PHE	CG-CD1	-5.04	1.31	1.38

All (412) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	l	46	ARG	NE-CZ-NH2	-19.32	110.64	120.30
2	m	70	ARG	NE-CZ-NH2	16.29	128.45	120.30
1	c	419	CYS	CA-CB-SG	16.22	143.19	114.00
4	d	120	ARG	NE-CZ-NH2	-16.20	112.20	120.30
2	m	245	ARG	NE-CZ-NH2	14.94	127.77	120.30
1	l	253	VAL	O-C-N	-14.86	98.92	122.70
3	b	91	PHE	CB-CG-CD2	-14.46	110.68	120.80
1	c	434	TYR	CB-CG-CD1	13.97	129.38	121.00
3	o	199	PHE	CB-CG-CD2	13.41	130.19	120.80
2	m	133	ARG	NE-CZ-NH1	13.04	126.82	120.30
3	o	71	ARG	NE-CZ-NH1	-12.58	114.01	120.30
4	d	201	ARG	NE-CZ-NH1	-12.43	114.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	o	55	TYR	CB-CG-CD1	12.04	128.22	121.00
1	c	46	ARG	NE-CZ-NH2	-11.98	114.31	120.30
3	b	33	PHE	CG-CD2-CE2	11.87	133.85	120.80
6	r	34	ASP	CB-CG-OD1	-11.79	107.69	118.30
1	l	414	TYR	CB-CG-CD1	11.78	128.07	121.00
1	l	344	ARG	NE-CZ-NH1	11.74	126.17	120.30
1	l	398	ARG	NE-CZ-NH1	11.74	126.17	120.30
2	n	70	ARG	NE-CZ-NH2	-11.71	114.45	120.30
1	c	438	ARG	NE-CZ-NH2	11.69	126.15	120.30
2	m	70	ARG	NE-CZ-NH1	-11.35	114.62	120.30
1	c	244	ARG	NE-CZ-NH2	11.23	125.92	120.30
5	q	14	ARG	NE-CZ-NH1	-11.20	114.70	120.30
5	q	166	ASP	CB-CG-OD1	11.15	128.33	118.30
1	l	256	ALA	CB-CA-C	-11.08	93.48	110.10
3	b	313	ARG	NE-CZ-NH2	11.01	125.81	120.30
7	s	15	THR	CA-CB-CG2	-10.67	97.46	112.40
3	o	80	ARG	NE-CZ-NH1	-10.50	115.05	120.30
1	c	438	ARG	NE-CZ-NH1	-10.46	115.07	120.30
1	l	168	GLU	C-N-CA	10.45	144.25	122.30
10	v	26	VAL	CA-CB-CG1	10.38	126.47	110.90
1	l	398	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	l	414	TYR	CB-CG-CD2	-10.35	114.79	121.00
6	f	58	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	c	24	ARG	NE-CZ-NH1	-10.26	115.17	120.30
6	f	61	ARG	NE-CZ-NH2	10.20	125.40	120.30
3	b	187	PHE	CB-CG-CD2	-9.94	113.84	120.80
2	m	102	ARG	NE-CZ-NH2	9.82	125.21	120.30
2	n	56	ARG	CD-NE-CZ	9.77	137.28	123.60
5	q	193	VAL	CG1-CB-CG2	9.75	126.51	110.90
5	e	32	ARG	NE-CZ-NH1	-9.67	115.47	120.30
4	p	118	ARG	NE-CZ-NH2	-9.66	115.47	120.30
3	b	131	TYR	CB-CG-CD1	-9.64	115.22	121.00
3	b	196	HIS	CA-CB-CG	9.62	129.95	113.60
2	m	102	ARG	NE-CZ-NH1	-9.61	115.49	120.30
26	B	55	CYS	CA-CB-SG	-9.61	96.70	114.00
3	b	183	PHE	CB-CG-CD1	9.51	127.45	120.80
1	l	92	ARG	NE-CZ-NH1	9.38	124.99	120.30
2	m	199	PHE	CB-CG-CD2	-9.36	114.25	120.80
3	o	196	HIS	CA-CB-CG	9.32	129.44	113.60
3	b	71	ARG	NE-CZ-NH1	-9.32	115.64	120.30
6	r	26	PHE	CB-CG-CD2	9.29	127.30	120.80
3	b	282	ARG	NE-CZ-NH1	-9.20	115.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	m	245	ARG	NE-CZ-NH1	-9.19	115.70	120.30
1	c	408	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	c	434	TYR	CB-CG-CD2	-8.97	115.62	121.00
6	r	21	TYR	CB-CG-CD2	-8.90	115.66	121.00
6	r	58	ARG	NE-CZ-NH2	8.74	124.67	120.30
5	q	55	VAL	CA-CB-CG1	8.74	124.01	110.90
6	r	64	ARG	NE-CZ-NH2	-8.72	115.94	120.30
3	o	55	TYR	CB-CG-CD2	-8.57	115.86	121.00
6	r	77	LYS	CG-CD-CE	8.49	137.38	111.90
5	q	99	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	c	441	MET	CA-CB-CG	-8.42	98.98	113.30
3	b	33	PHE	CB-CG-CD1	8.41	126.68	120.80
3	b	359	PHE	CB-CG-CD1	8.36	126.65	120.80
3	b	171	ASP	CB-CG-OD1	8.35	125.81	118.30
3	o	104	TYR	CB-CG-CD1	8.35	126.01	121.00
2	m	199	PHE	CB-CG-CD1	8.30	126.61	120.80
4	d	152	TYR	CB-CG-CD1	8.24	125.95	121.00
3	o	223	TYR	CB-CG-CD2	8.23	125.94	121.00
1	l	253	VAL	CA-C-O	8.22	137.36	120.10
2	m	177	TYR	O-C-N	8.19	135.80	122.70
3	b	204	GLY	C-N-CA	8.15	142.08	121.70
2	m	56	ARG	CD-NE-CZ	8.10	134.94	123.60
3	o	185	LEU	CA-CB-CG	8.06	133.85	115.30
6	r	55	TYR	CB-CG-CD1	-8.05	116.17	121.00
6	r	35	ASP	CB-CG-OD2	7.99	125.49	118.30
10	v	31	PHE	CB-CG-CD2	-7.96	115.23	120.80
6	f	61	ARG	NE-CZ-NH1	-7.93	116.33	120.30
5	e	13	TYR	CB-CG-CD2	-7.93	116.24	121.00
5	e	13	TYR	CB-CG-CD1	7.91	125.74	121.00
3	b	235	LEU	CB-CG-CD2	7.90	124.44	111.00
1	c	343	MET	CA-CB-CG	-7.90	99.87	113.30
1	l	344	ARG	NE-CZ-NH2	-7.89	116.35	120.30
3	o	128	PHE	CB-CG-CD2	-7.89	115.28	120.80
10	v	31	PHE	CB-CG-CD1	7.88	126.31	120.80
7	g	9	ARG	NE-CZ-NH1	-7.86	116.37	120.30
3	b	131	TYR	CB-CG-CD2	7.83	125.70	121.00
10	v	14	PHE	CB-CG-CD1	7.81	126.27	120.80
1	l	342	TRP	CH2-CZ2-CE2	7.80	125.20	117.40
1	c	324	PHE	CB-CG-CD2	-7.73	115.39	120.80
1	c	436	ARG	NE-CZ-NH1	-7.68	116.46	120.30
3	o	325	PHE	CG-CD2-CE2	7.67	129.24	120.80
1	c	235	ARG	NE-CZ-NH1	7.67	124.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	c	395	TRP	NE1-CE2-CZ2	-7.65	121.99	130.40
2	m	319	SER	N-CA-CB	7.63	121.94	110.50
10	j	14	PHE	CB-CG-CD1	7.62	126.14	120.80
1	l	334	MET	O-C-N	-7.59	110.55	122.70
6	f	64	ARG	CD-NE-CZ	-7.59	112.98	123.60
3	o	19	ILE	O-C-N	-7.58	110.56	122.70
3	b	313	ARG	NE-CZ-NH1	-7.57	116.52	120.30
6	f	55	TYR	CB-CG-CD1	7.47	125.48	121.00
4	p	220	TYR	CB-CG-CD1	7.43	125.46	121.00
2	m	134	ARG	NE-CZ-NH1	-7.43	116.58	120.30
6	f	58	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	l	431	LEU	CB-CG-CD1	7.32	123.44	111.00
1	l	307	PHE	CA-C-O	7.31	135.45	120.10
4	d	206	LEU	CB-CA-C	-7.30	96.32	110.20
1	c	425	PHE	CB-CG-CD1	7.28	125.90	120.80
1	c	89	TYR	CB-CG-CD1	7.27	125.36	121.00
1	c	168	GLU	CA-C-O	7.25	135.32	120.10
3	o	44	GLN	C-N-CA	7.22	139.76	121.70
3	b	317	PHE	CB-CG-CD2	7.20	125.84	120.80
3	b	80	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	l	408	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	c	408	ARG	NH1-CZ-NH2	7.18	127.30	119.40
3	o	273	TYR	CB-CG-CD2	7.15	125.29	121.00
1	l	423	ALA	CB-CA-C	-7.12	99.41	110.10
4	p	125	ASP	CB-CG-OD2	7.12	124.70	118.30
1	l	362	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	l	419	CYS	CA-CB-SG	7.08	126.75	114.00
7	s	16	TYR	CG-CD1-CE1	7.07	126.95	121.30
2	m	147	ASP	CB-CG-OD2	7.05	124.65	118.30
3	b	273	TYR	CB-CG-CD2	7.04	125.23	121.00
3	b	75	TYR	CB-CG-CD1	7.03	125.22	121.00
3	b	214	ASP	CB-CG-OD2	7.03	124.62	118.30
5	q	97	PHE	CB-CG-CD1	7.00	125.70	120.80
6	r	61	ARG	NE-CZ-NH1	-7.00	116.80	120.30
4	p	28	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	l	376	CYS	CA-CB-SG	-6.94	101.50	114.00
6	r	21	TYR	CB-CG-CD1	6.93	125.16	121.00
1	l	174	VAL	CA-CB-CG1	6.92	121.28	110.90
3	b	33	PHE	CZ-CE2-CD2	-6.92	111.80	120.10
1	l	70	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	l	46	ARG	NH1-CZ-NH2	6.90	126.99	119.40
4	d	208	MET	CA-CB-CG	6.89	125.02	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	r	55	TYR	CB-CG-CD2	6.86	125.12	121.00
3	o	47	THR	O-C-N	-6.86	111.54	123.20
2	n	87	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	c	415	PHE	O-C-N	-6.81	111.81	122.70
3	o	80	ARG	CD-NE-CZ	-6.80	114.08	123.60
3	o	325	PHE	CB-CG-CD2	6.79	125.55	120.80
3	b	55	TYR	CB-CG-CD2	6.75	125.05	121.00
1	l	417	ASP	CB-CG-OD2	-6.74	112.23	118.30
7	g	47	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	c	408	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	l	342	TRP	CD1-NE1-CE2	-6.72	102.95	109.00
3	b	75	TYR	CB-CG-CD2	-6.71	116.98	121.00
6	r	65	ALA	CA-C-O	6.69	134.16	120.10
7	s	16	TYR	CB-CG-CD1	6.68	125.01	121.00
3	b	41	LEU	N-CA-CB	6.67	123.74	110.40
1	l	319	LEU	CB-CG-CD2	6.67	122.34	111.00
6	f	101	ARG	NE-CZ-NH1	-6.65	116.97	120.30
6	r	63	LYS	CB-CA-C	6.63	123.66	110.40
3	o	276	PHE	CB-CG-CD1	-6.62	116.16	120.80
5	q	14	ARG	NE-CZ-NH2	6.61	123.61	120.30
7	g	40	ARG	NE-CZ-NH2	-6.60	117.00	120.30
5	q	15	ARG	NE-CZ-NH1	6.60	123.60	120.30
3	o	72	ASP	CB-CG-OD2	6.57	124.21	118.30
4	p	235	LEU	CA-C-O	6.56	133.87	120.10
10	j	40	ASP	CB-CG-OD2	6.55	124.20	118.30
3	o	178	PHE	CB-CG-CD2	-6.54	116.22	120.80
4	p	27	ARG	NE-CZ-NH1	6.53	123.56	120.30
3	b	180	ALA	N-CA-CB	6.51	119.22	110.10
3	b	175	LEU	N-CA-CB	6.50	123.41	110.40
1	c	404	ALA	CB-CA-C	6.50	119.86	110.10
2	n	177	TYR	CB-CG-CD1	-6.49	117.10	121.00
4	d	134	TYR	CB-CG-CD1	6.47	124.89	121.00
5	q	99	ARG	NE-CZ-NH1	-6.47	117.06	120.30
6	r	36	THR	CA-CB-CG2	6.46	121.44	112.40
1	l	131	ARG	NE-CZ-NH2	-6.43	117.08	120.30
15	1	133	GLY	N-CA-C	6.42	129.16	113.10
3	b	267	HIS	CA-CB-CG	-6.41	102.71	113.60
1	l	300	THR	CA-CB-CG2	-6.39	103.45	112.40
1	c	441	MET	CG-SD-CE	6.39	110.42	100.20
3	o	359	PHE	CB-CG-CD1	6.36	125.25	120.80
3	b	359	PHE	CB-CG-CD2	-6.36	116.35	120.80
1	c	208	LEU	CA-CB-CG	6.35	129.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	l	421	ALA	CB-CA-C	6.35	119.62	110.10
1	c	190	TYR	CB-CG-CD2	6.35	124.81	121.00
1	l	435	ASN	OD1-CG-ND2	6.34	136.48	121.90
4	d	120	ARG	NE-CZ-NH1	6.33	123.47	120.30
3	o	242	LEU	CB-CA-C	-6.33	98.18	110.20
3	o	91	PHE	CB-CG-CD2	-6.32	116.38	120.80
7	s	21	PHE	CB-CG-CD2	-6.32	116.38	120.80
6	r	42	ASP	CB-CG-OD1	6.31	123.98	118.30
3	b	246	ALA	N-CA-CB	-6.31	101.26	110.10
3	o	40	CYS	CA-CB-SG	6.30	125.34	114.00
3	o	276	PHE	CB-CG-CD2	6.30	125.21	120.80
2	m	177	TYR	CB-CG-CD1	6.26	124.76	121.00
3	o	223	TYR	CZ-CE2-CD2	-6.26	114.17	119.80
7	s	21	PHE	CB-CG-CD1	6.24	125.17	120.80
4	p	118	ARG	NE-CZ-NH1	6.24	123.42	120.30
3	b	325	PHE	CB-CG-CD1	-6.23	116.44	120.80
1	c	97	TYR	CG-CD1-CE1	6.21	126.27	121.30
3	o	331	ASP	CB-CG-OD2	6.20	123.88	118.30
6	r	104	ARG	NE-CZ-NH1	-6.18	117.21	120.30
3	b	43	LEU	O-C-N	-6.18	112.81	122.70
5	q	91	TRP	CB-CG-CD1	-6.15	119.00	127.00
2	n	188	PRO	O-C-N	-6.15	112.86	122.70
3	o	73	VAL	CG1-CB-CG2	-6.14	101.07	110.90
3	o	223	TYR	CB-CG-CD1	-6.14	117.31	121.00
3	o	223	TYR	CG-CD2-CE2	6.14	126.21	121.30
5	q	91	TRP	CB-CG-CD2	6.13	134.57	126.60
6	f	107	TRP	CD1-NE1-CE2	6.13	114.51	109.00
3	o	52	ALA	N-CA-CB	6.12	118.67	110.10
5	q	97	PHE	CB-CG-CD2	-6.11	116.53	120.80
6	r	26	PHE	CG-CD2-CE2	6.09	127.50	120.80
1	l	24	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	l	112	LEU	CB-CG-CD2	-6.07	100.69	111.00
1	c	378	ASP	CB-CG-OD1	6.05	123.75	118.30
7	g	16	TYR	CZ-CE2-CD2	6.05	125.25	119.80
10	j	20	PHE	CZ-CE2-CD2	6.05	127.36	120.10
3	o	237	LEU	CB-CG-CD2	6.04	121.27	111.00
2	m	83	PHE	CB-CG-CD1	-6.04	116.57	120.80
4	d	49	ARG	NE-CZ-NH1	-6.04	117.28	120.30
3	o	104	TYR	CB-CG-CD2	-6.04	117.38	121.00
6	f	71	ARG	NE-CZ-NH2	-6.01	117.29	120.30
3	b	183	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	l	158	PHE	CB-CG-CD1	-6.00	116.60	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	14	ARG	CD-NE-CZ	-6.00	115.21	123.60
10	j	14	PHE	CB-CG-CD2	-5.98	116.61	120.80
6	f	33	ARG	NE-CZ-NH2	-5.98	117.31	120.30
6	f	73	GLN	CB-CA-C	5.98	122.36	110.40
1	l	89	TYR	CB-CG-CD1	5.98	124.59	121.00
1	c	168	GLU	O-C-N	-5.97	113.04	123.20
3	b	115	ILE	C-N-CA	-5.97	109.76	122.30
2	n	157	ALA	N-CA-CB	5.96	118.44	110.10
4	d	204	MET	CA-CB-CG	5.95	123.41	113.30
1	c	251	ALA	CA-C-O	5.93	132.56	120.10
2	m	134	ARG	NE-CZ-NH2	5.93	123.27	120.30
3	b	205	SER	O-C-N	-5.93	113.22	122.70
3	o	90	PHE	CB-CG-CD2	5.93	124.95	120.80
2	m	179	PRO	N-CA-CB	5.92	110.41	103.30
3	o	267	HIS	CA-CB-CG	-5.91	103.55	113.60
4	p	138	PRO	N-CD-CG	-5.91	94.34	103.20
2	m	308	ASP	CB-CG-OD2	5.91	123.61	118.30
1	l	236	PHE	CB-CG-CD1	5.91	124.93	120.80
5	q	183	PRO	O-C-N	5.90	132.14	122.70
4	d	182	VAL	CA-CB-CG1	5.90	119.75	110.90
5	q	144	CYS	CA-CB-SG	5.90	124.62	114.00
1	c	362	ARG	NE-CZ-NH2	5.89	123.25	120.30
10	v	39	ALA	O-C-N	5.89	132.12	122.70
3	o	199	PHE	CD1-CG-CD2	-5.88	110.66	118.30
1	l	325	VAL	CA-C-N	5.87	130.12	117.20
3	o	257	THR	N-CA-CB	5.87	121.46	110.30
4	p	201	ARG	NE-CZ-NH2	5.87	123.23	120.30
7	g	16	TYR	CB-CG-CD2	5.86	124.52	121.00
1	l	89	TYR	CA-CB-CG	5.86	124.54	113.40
4	p	134	TYR	CB-CG-CD1	5.85	124.51	121.00
2	m	194	TYR	CB-CG-CD1	-5.85	117.49	121.00
3	b	77	TRP	CD2-CE3-CZ3	-5.83	111.22	118.80
1	c	425	PHE	N-CA-CB	5.83	121.09	110.60
3	b	18	PHE	CB-CG-CD1	5.83	124.88	120.80
4	d	28	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	c	288	ALA	N-CA-CB	5.82	118.25	110.10
3	b	358	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	l	334	MET	N-CA-CB	-5.79	100.18	110.60
1	l	435	ASN	CB-CG-OD1	-5.79	110.03	121.60
4	p	220	TYR	CB-CG-CD2	-5.78	117.53	121.00
3	b	357	LEU	CB-CG-CD2	5.77	120.81	111.00
3	b	223	TYR	CB-CG-CD2	5.77	124.46	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	p	55	CYS	CA-CB-SG	-5.75	103.64	114.00
4	p	91	PHE	CZ-CE2-CD2	5.75	127.00	120.10
1	l	137	GLU	OE1-CD-OE2	-5.73	116.42	123.30
4	d	14	HIS	CA-CB-CG	5.73	123.34	113.60
2	n	287	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	c	131	ARG	NE-CZ-NH2	-5.72	117.44	120.30
4	p	235	LEU	O-C-N	-5.70	113.59	122.70
1	c	294	LEU	O-C-N	-5.69	113.60	122.70
3	b	53	MET	CA-CB-CG	5.68	122.95	113.30
5	q	135	LEU	O-C-N	-5.67	113.63	122.70
2	m	314	ALA	N-CA-CB	-5.67	102.17	110.10
6	r	34	ASP	OD1-CG-OD2	5.67	134.07	123.30
4	d	119	ALA	CB-CA-C	-5.64	101.63	110.10
5	q	14	ARG	CD-NE-CZ	-5.64	115.70	123.60
4	d	224	ARG	NE-CZ-NH1	5.64	123.12	120.30
3	b	122	THR	CA-CB-CG2	-5.62	104.53	112.40
3	b	187	PHE	CG-CD1-CE1	-5.61	114.63	120.80
2	m	178	CYS	O-C-N	5.60	131.75	121.10
3	o	347	TYR	CB-CG-CD2	5.60	124.36	121.00
3	b	303	LEU	N-CA-CB	5.60	121.59	110.40
3	o	143	ALA	CB-CA-C	5.60	118.50	110.10
4	d	199	ASP	CB-CG-OD1	5.59	123.33	118.30
2	n	66	SER	N-CA-CB	5.58	118.88	110.50
4	p	27	ARG	NE-CZ-NH2	-5.58	117.51	120.30
6	r	71	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	c	417	ASP	CB-CG-OD2	-5.57	113.29	118.30
2	m	203	ARG	NE-CZ-NH1	5.56	123.08	120.30
10	v	21	ALA	CB-CA-C	5.56	118.44	110.10
1	l	408	ARG	NH1-CZ-NH2	5.54	125.50	119.40
1	l	342	TRP	NE1-CE2-CD2	5.53	112.83	107.30
4	d	201	ARG	CA-CB-CG	5.53	125.56	113.40
3	o	244	LEU	O-C-N	5.53	131.54	122.70
3	o	128	PHE	CB-CG-CD1	5.52	124.67	120.80
6	r	56	ASP	CB-CG-OD1	5.52	123.27	118.30
4	p	49	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	l	346	CYS	CA-CB-SG	5.50	123.90	114.00
5	q	185	TYR	CB-CG-CD2	5.49	124.30	121.00
4	d	224	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	l	92	ARG	NE-CZ-NH2	-5.49	117.56	120.30
4	p	120	ARG	CD-NE-CZ	5.49	131.28	123.60
1	c	241	ILE	CA-CB-CG1	-5.48	100.58	111.00
4	d	191	ARG	NE-CZ-NH2	5.48	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	b	109	PHE	CG-CD1-CE1	5.48	126.83	120.80
3	b	18	PHE	CB-CG-CD2	-5.46	116.98	120.80
4	d	201	ARG	NH1-CZ-NH2	5.45	125.40	119.40
1	l	442	PHE	CB-CG-CD1	5.45	124.62	120.80
6	r	103	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	c	341	GLN	O-C-N	5.45	131.42	122.70
6	r	65	ALA	O-C-N	-5.44	113.99	122.70
3	o	25	SER	N-CA-CB	-5.44	102.34	110.50
6	f	94	LEU	CB-CG-CD1	5.41	120.19	111.00
3	o	72	ASP	CB-CG-OD1	-5.41	113.44	118.30
6	f	59	VAL	CA-CB-CG1	-5.39	102.81	110.90
5	e	53	ASN	CB-CG-OD1	-5.38	110.83	121.60
2	m	254	HIS	CA-CB-CG	5.38	122.75	113.60
1	l	420	PRO	N-CA-CB	5.38	109.76	103.30
7	g	21	PHE	CB-CG-CD1	-5.38	117.03	120.80
6	r	77	LYS	CD-CE-NZ	5.38	124.07	111.70
1	c	356	ARG	NE-CZ-NH1	-5.38	117.61	120.30
4	p	44	ASP	CB-CG-OD2	-5.37	113.47	118.30
3	b	109	PHE	O-C-N	-5.36	114.12	122.70
3	b	282	ARG	CD-NE-CZ	-5.34	116.12	123.60
1	l	217	SER	N-CA-CB	-5.34	102.49	110.50
5	q	40	THR	CA-CB-CG2	5.33	119.87	112.40
3	o	131	TYR	CB-CG-CD1	-5.33	117.80	121.00
3	b	206	ASN	CB-CG-OD1	-5.33	110.95	121.60
9	u	78	TYR	CA-CB-CG	5.32	123.51	113.40
5	q	193	VAL	CA-CB-CG2	-5.32	102.92	110.90
3	o	67	THR	CA-CB-CG2	-5.31	104.96	112.40
5	q	49	TYR	CB-CG-CD1	5.31	124.19	121.00
5	q	118	ARG	NE-CZ-NH1	-5.29	117.65	120.30
6	f	54	LEU	CB-CG-CD1	5.29	119.99	111.00
2	m	157	ALA	CB-CA-C	5.29	118.03	110.10
6	f	71	ARG	NE-CZ-NH1	5.28	122.94	120.30
3	b	91	PHE	CD1-CG-CD2	5.27	125.15	118.30
4	d	191	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	l	131	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	m	85	ILE	CB-CA-C	-5.27	101.07	111.60
6	r	99	ARG	CD-NE-CZ	5.26	130.97	123.60
4	d	40	CYS	CA-CB-SG	5.26	123.46	114.00
1	l	434	TYR	O-C-N	-5.26	114.29	122.70
5	q	5	ILE	CB-CA-C	-5.25	101.09	111.60
3	b	325	PHE	CB-CG-CD2	5.24	124.47	120.80
2	m	169	ARG	NE-CZ-NH1	5.23	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	203	ARG	CD-NE-CZ	5.23	130.92	123.60
6	f	43	VAL	CA-C-O	5.22	131.07	120.10
3	o	242	LEU	N-CA-CB	5.22	120.84	110.40
7	g	47	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	l	325	VAL	O-C-N	-5.20	114.38	122.70
3	b	30	TRP	O-C-N	-5.20	114.38	122.70
3	b	196	HIS	O-C-N	5.19	131.01	122.70
7	g	13	VAL	O-C-N	-5.19	114.39	122.70
18	4	5	LYS	N-CA-C	5.19	125.01	111.00
1	c	294	LEU	C-N-CA	5.19	134.67	121.70
3	b	195	VAL	CG1-CB-CG2	-5.19	102.60	110.90
12	x	435	GLY	N-CA-C	5.19	126.07	113.10
2	n	113	ARG	NE-CZ-NH1	5.18	122.89	120.30
3	o	325	PHE	CZ-CE2-CD2	-5.18	113.89	120.10
3	b	183	PHE	CZ-CE2-CD2	5.17	126.31	120.10
4	p	208	MET	CA-CB-CG	5.17	122.10	113.30
26	B	55	CYS	CB-CA-C	-5.17	100.05	110.40
1	l	378	ASP	CB-CG-OD1	5.17	122.96	118.30
5	q	87	MET	CA-CB-CG	5.17	122.09	113.30
6	f	55	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	l	320	LEU	O-C-N	-5.16	114.42	123.20
2	m	346	THR	CA-CB-OG1	5.16	119.84	109.00
1	l	421	ALA	N-CA-CB	-5.15	102.89	110.10
5	q	58	PHE	CB-CG-CD1	5.15	124.40	120.80
4	p	191	ARG	NE-CZ-NH2	-5.14	117.73	120.30
3	o	93	CYS	N-CA-CB	5.14	119.85	110.60
2	m	89	ILE	CA-CB-CG2	5.14	121.17	110.90
2	m	92	VAL	O-C-N	-5.12	114.49	123.20
5	q	70	ALA	CB-CA-C	-5.12	102.42	110.10
4	p	33	TYR	CB-CG-CD2	-5.12	117.93	121.00
9	i	68	VAL	CB-CA-C	-5.11	101.69	111.40
7	g	13	VAL	CA-C-O	5.11	130.83	120.10
1	c	420	PRO	N-CA-CB	5.11	109.43	103.30
5	e	61	SER	CA-CB-OG	-5.11	97.41	111.20
1	l	438	ARG	CA-CB-CG	-5.11	102.17	113.40
4	p	126	TYR	CB-CG-CD2	5.10	124.06	121.00
3	b	13	ILE	CB-CA-C	-5.10	101.40	111.60
4	p	212	MET	CA-CB-CG	5.10	121.97	113.30
3	b	13	ILE	CA-CB-CG1	5.09	120.68	111.00
2	m	102	ARG	CD-NE-CZ	-5.09	116.47	123.60
4	p	102	ARG	NE-CZ-NH1	-5.08	117.76	120.30
3	b	113	TRP	O-C-N	-5.08	114.57	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	b	51	LEU	CB-CG-CD1	5.08	119.63	111.00
5	q	101	ARG	NE-CZ-NH2	-5.08	117.76	120.30
9	i	78	TYR	CA-CB-CG	5.07	123.03	113.40
3	b	91	PHE	CZ-CE2-CD2	-5.05	114.03	120.10
1	l	423	ALA	N-CA-CB	5.05	117.18	110.10
5	q	18	VAL	CB-CA-C	-5.05	101.80	111.40
5	e	14	ARG	NE-CZ-NH2	-5.05	117.78	120.30
3	b	182	HIS	CA-CB-CG	5.04	122.18	113.60
2	n	134	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	c	419	CYS	N-CA-CB	5.04	119.68	110.60
3	b	186	PRO	O-C-N	-5.04	114.64	122.70
3	o	90	PHE	CB-CG-CD1	-5.04	117.28	120.80
3	o	19	ILE	C-N-CA	5.03	134.28	121.70
1	l	431	LEU	CB-CG-CD2	5.03	119.56	111.00
1	c	349	ALA	CB-CA-C	5.03	117.64	110.10
6	f	54	LEU	CA-CB-CG	5.03	126.87	115.30
5	q	32	ARG	CB-CA-C	5.03	120.46	110.40
1	l	408	ARG	NE-CZ-NH1	-5.02	117.79	120.30
2	n	172	LEU	CA-CB-CG	5.02	126.85	115.30
10	j	19	THR	CA-CB-CG2	-5.02	105.37	112.40
1	c	89	TYR	CA-CB-CG	5.01	122.93	113.40
4	d	134	TYR	CB-CG-CD2	-5.01	117.99	121.00

There are no chirality outliers.

All (109) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	B	120	UNK	Peptide
26	B	130	UNK	Peptide
27	C	56	UNK	Peptide
28	D	195	UNK	Peptide
30	F	166	UNK	Mainchain
30	F	96	UNK	Peptide
31	G	177	UNK	Peptide
31	G	178	UNK	Mainchain
31	G	206	UNK	Peptide
31	G	289	UNK	Peptide
31	G	399	UNK	Mainchain
31	G	565	UNK	Mainchain
33	I	160	UNK	Mainchain
36	L	133	UNK	Peptide
36	L	366	UNK	Peptide

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Mol	Chain	Res	Type	Group
36	L	446	UNK	Peptide
36	L	546	UNK	Mainchain
38	N	276	UNK	Peptide
38	N	91	UNK	Peptide
39	O	229	UNK	Peptide
39	O	92	UNK	Peptide
40	P	223	UNK	Peptide
40	P	225	UNK	Peptide
40	P	42	UNK	Peptide
41	Q	40	UNK	Peptide
43	S	75	UNK	Mainchain
46	W	40	UNK	Peptide
47	X	56	UNK	Peptide
3	b	134	PRO	Mainchain
3	b	164	ILE	Mainchain
3	b	20	ASP	Mainchain
3	b	21	LEU	Mainchain
3	b	222	PRO	Mainchain
3	b	235	LEU	Mainchain
3	b	281	LEU	Mainchain
3	b	322	GLN	Mainchain
3	b	326	TRP	Mainchain
3	b	335	LEU	Mainchain
3	b	355	SER	Mainchain
3	b	362	ILE	Mainchain
3	b	77	TRP	Mainchain
3	b	83	HIS	Mainchain
1	c	118	GLN	Mainchain
1	c	122	LEU	Mainchain
1	c	196	VAL	Mainchain
1	c	210	ASP	Mainchain
1	c	239	SER	Mainchain
1	c	242	CYS	Mainchain
1	c	244	ARG	Mainchain
1	c	256	ALA	Mainchain
1	c	294	LEU	Mainchain
1	c	306	SER	Mainchain
1	c	345	LEU	Mainchain
1	c	383	LEU	Mainchain
1	c	53	ASN	Mainchain
4	d	191	ARG	Mainchain
4	d	217	PRO	Mainchain

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Mol	Chain	Res	Type	Group
4	d	224	ARG	Mainchain
4	d	229	VAL	Mainchain
4	d	54	VAL	Mainchain
5	e	20	ASP	Mainchain
6	f	16	ILE	Mainchain
6	f	46	ALA	Mainchain
7	g	15	THR	Mainchain
7	g	73	ASN	Mainchain
9	i	69	SER	Mainchain
10	j	43	TYR	Mainchain
1	l	100	LYS	Mainchain
1	l	141	ASN	Mainchain
1	l	290	LEU	Mainchain
2	m	106	ALA	Mainchain
2	m	159	VAL	Mainchain
2	m	178	CYS	Mainchain
2	m	239	TYR	Mainchain
2	m	285	VAL	Mainchain
2	m	335	ASP	Mainchain
2	m	353	SER	Mainchain
2	m	68	LEU	Mainchain
2	m	99	THR	Mainchain
2	n	137	VAL	Mainchain
2	n	144	LEU	Mainchain
2	n	200	THR	Mainchain
2	n	290	ASN	Mainchain
2	n	353	SER	Mainchain
3	o	148	ASN	Mainchain
3	o	159	ASN	Mainchain
3	o	19	ILE	Mainchain
3	o	355	SER	Mainchain
3	o	55	TYR	Mainchain
3	o	77	TRP	Mainchain
4	p	202	LYS	Mainchain
4	p	229	VAL	Mainchain
4	p	24	THR	Mainchain
4	p	46	VAL	Mainchain
5	q	125	GLU	Mainchain
5	q	135	LEU	Mainchain
5	q	186	GLU	Mainchain
5	q	195	VAL	Mainchain
5	q	32	ARG	Mainchain

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Mol	Chain	Res	Type	Group
5	q	36	SER	Mainchain
5	q	49	TYR	Mainchain
5	q	9	ASP	Mainchain
5	q	97	PHE	Mainchain
7	s	17	SER	Mainchain
7	s	18	LEU	Mainchain
7	s	34	ILE	Mainchain
8	t	40	CYS	Mainchain
9	u	72	VAL	Mainchain
11	w	24	TRP	Mainchain

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	c	3458	0	3356	0	0
1	l	3458	0	3353	0	0
2	m	3141	0	3123	0	0
2	n	3141	0	3123	0	0
3	b	3011	0	3076	0	0
3	o	3011	0	3076	0	0
4	d	1919	0	1868	0	0
4	p	1919	0	1868	0	0
5	e	566	0	564	0	0
5	q	1518	0	1499	0	0
6	f	916	0	909	0	0
6	r	916	0	909	0	0
7	g	682	0	679	0	0
7	s	682	0	679	0	0
8	h	524	0	504	0	0
8	t	524	0	504	0	0
9	i	248	0	265	0	0
9	u	248	0	265	0	0
10	j	512	0	518	0	0
10	v	512	0	518	0	0
11	k	159	0	159	0	0
11	w	159	0	159	0	0
12	x	4025	0	4003	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	y	1822	0	1834	0	0
14	z	2124	0	2044	0	0
15	1	1195	0	1183	30	0
16	2	878	0	868	20	0
17	3	748	0	728	21	0
18	4	672	0	645	23	0
19	5	628	0	582	18	0
20	6	598	0	612	10	0
21	7	441	0	437	11	0
22	8	384	0	366	6	0
23	9	386	0	388	7	0
24	0	335	0	352	11	0
25	A	415	0	88	27	0
26	B	719	0	161	91	0
27	C	770	0	163	63	0
28	D	1920	0	402	126	0
29	E	799	0	176	56	0
30	F	2059	0	444	263	0
31	G	2651	0	606	226	0
32	H	1425	0	295	99	0
33	I	818	0	195	65	0
34	J	655	0	138	44	0
35	K	420	0	89	14	0
36	L	2790	0	583	255	0
37	M	2195	0	455	208	0
38	N	1630	0	340	147	0
39	O	905	0	197	65	0
40	P	1260	0	271	144	0
41	Q	345	0	80	14	0
42	R	235	0	54	22	0
43	S	400	0	86	46	0
44	T	355	0	76	12	0
45	V	355	0	77	23	0
46	W	360	0	75	18	0
47	X	1645	0	351	102	0
48	Y	530	0	111	30	0
49	a	355	0	75	0	0
50	U	1250	0	272	63	0
51	Z	1329	0	280	70	0
52	b	86	0	60	0	0
52	o	86	0	60	0	0
53	d	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	p	43	0	30	0	0
54	E	4	0	0	0	0
54	G	4	0	0	3	0
54	q	4	0	0	0	0
55	x	1	0	0	0	0
55	y	2	0	0	0	0
56	x	1	0	0	0	0
57	x	120	0	108	0	0
58	3	1	0	0	0	0
59	B	8	0	0	6	0
59	F	8	0	0	1	0
59	G	16	0	0	0	0
59	I	16	0	0	5	0
All	All	74493	0	51444	2394	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 51.

All (2394) 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)
26:B:148:UNK:CB	26:B:151:UNK:CA	1.77	1.59
30:F:405:CYS:CB	30:F:406:UNK:CB	1.78	1.56
30:F:405:CYS:HB2	30:F:406:UNK:CB	1.04	1.48
36:L:321:UNK:CB	36:L:324:UNK:CB	1.92	1.45
29:E:148:CYS:SG	30:F:103:UNK:CB	2.04	1.44
26:B:119:CYS:N	26:B:122:UNK:CB	1.81	1.44
31:G:55:CYS:HB2	31:G:68:UNK:CB	1.49	1.40
36:L:247:UNK:HA	36:L:251:UNK:CB	1.52	1.37
29:E:148:CYS:CB	30:F:103:UNK:CB	2.07	1.32
29:E:148:CYS:HB2	30:F:103:UNK:CB	1.59	1.30
30:F:405:CYS:CA	30:F:406:UNK:CB	2.07	1.29
30:F:100:UNK:O	30:F:102:UNK:N	1.67	1.27
31:G:10:UNK:O	31:G:76:UNK:HA	1.33	1.27
29:E:148:CYS:SG	30:F:102:UNK:O	1.91	1.27
31:G:376:UNK:N	31:G:449:UNK:N	1.83	1.27
43:S:25:UNK:CA	43:S:57:UNK:CB	2.13	1.26
36:L:65:UNK:CB	36:L:67:UNK:N	1.98	1.26
26:B:119:CYS:CA	26:B:122:UNK:CB	2.18	1.21
36:L:161:UNK:HA	36:L:162:UNK:C	1.65	1.21
30:F:408:UNK:CB	59:F:501:SF4:S4	2.29	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:55:CYS:CB	31:G:68:UNK:CB	2.19	1.20
40:P:170:UNK:CB	40:P:204:UNK:HA	1.70	1.20
33:I:151:UNK:O	33:I:154:UNK:N	1.75	1.18
43:S:25:UNK:N	43:S:57:UNK:CB	2.06	1.18
36:L:161:UNK:HA	36:L:163:UNK:N	1.59	1.17
32:H:158:UNK:CB	32:H:314:UNK:O	1.93	1.17
31:G:152:UNK:CB	31:G:206:UNK:CB	2.23	1.16
36:L:225:UNK:HA	36:L:229:UNK:CB	1.73	1.16
37:M:58:UNK:HA	37:M:59:UNK:CB	1.71	1.15
37:M:347:UNK:O	37:M:351:UNK:N	1.81	1.14
30:F:405:CYS:HA	30:F:406:UNK:CB	1.69	1.12
38:N:103:UNK:O	38:N:107:UNK:N	1.83	1.12
31:G:10:UNK:O	31:G:76:UNK:CA	1.99	1.11
32:H:40:UNK:C	32:H:47:UNK:CB	2.28	1.10
31:G:41:CYS:N	54:G:803:FES:S2	2.23	1.10
40:P:103:UNK:O	40:P:107:UNK:N	1.84	1.10
26:B:119:CYS:HA	26:B:122:UNK:CB	1.80	1.09
47:X:77:UNK:O	47:X:79:UNK:N	1.84	1.09
31:G:377:UNK:H	31:G:449:UNK:HA	0.99	1.08
26:B:118:UNK:O	26:B:122:UNK:N	1.85	1.08
32:H:143:UNK:O	32:H:146:UNK:N	1.86	1.08
30:F:423:UNK:O	30:F:427:UNK:N	1.87	1.08
36:L:32:UNK:O	36:L:36:UNK:N	1.87	1.08
39:O:229:UNK:CB	39:O:231:UNK:CA	2.32	1.07
40:P:203:UNK:HA	40:P:234:UNK:HA	1.34	1.07
48:Y:102:UNK:O	48:Y:105:UNK:CB	2.01	1.07
40:P:105:UNK:O	40:P:109:UNK:N	1.87	1.07
31:G:175:UNK:N	31:G:182:UNK:O	1.87	1.07
34:J:101:UNK:O	34:J:104:UNK:N	1.86	1.07
48:Y:11:UNK:HA	48:Y:48:UNK:CB	1.84	1.06
50:U:506:UNK:O	50:U:510:UNK:CB	2.02	1.06
27:C:34:UNK:O	27:C:38:UNK:N	1.88	1.06
36:L:209:UNK:O	36:L:212:UNK:N	1.88	1.06
40:P:106:UNK:O	40:P:110:UNK:N	1.87	1.06
31:G:227:UNK:O	31:G:238:UNK:O	1.72	1.06
34:J:68:UNK:O	34:J:72:UNK:N	1.87	1.06
36:L:29:UNK:O	36:L:33:UNK:N	1.88	1.06
43:S:40:UNK:O	43:S:44:UNK:N	1.88	1.06
31:G:435:UNK:C	31:G:437:UNK:HA	1.86	1.06
32:H:177:UNK:HA	47:X:146:UNK:CB	1.86	1.06
51:Z:104:UNK:O	51:Z:108:UNK:N	1.88	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:21:UNK:N	40:P:44:UNK:O	1.88	1.05
31:G:376:UNK:N	31:G:448:UNK:C	2.17	1.05
39:O:229:UNK:CB	39:O:231:UNK:N	2.19	1.05
29:E:70:UNK:O	29:E:74:UNK:N	1.89	1.04
30:F:261:UNK:O	30:F:286:UNK:O	1.75	1.04
36:L:33:UNK:O	36:L:37:UNK:N	1.90	1.04
31:G:241:UNK:O	31:G:248:UNK:N	1.88	1.04
40:P:133:UNK:N	40:P:166:UNK:O	1.91	1.03
31:G:142:UNK:O	31:G:190:UNK:HA	1.59	1.03
30:F:262:UNK:CB	30:F:286:UNK:N	2.21	1.03
43:S:25:UNK:CB	43:S:57:UNK:CB	2.36	1.03
29:E:148:CYS:SG	30:F:102:UNK:C	2.45	1.03
36:L:28:UNK:O	36:L:32:UNK:N	1.92	1.03
30:F:294:UNK:N	30:F:339:UNK:CB	2.23	1.02
30:F:422:UNK:O	30:F:426:UNK:N	1.92	1.02
47:X:302:UNK:O	47:X:305:UNK:N	1.92	1.02
36:L:181:UNK:O	36:L:184:UNK:N	1.92	1.02
28:D:133:UNK:CB	28:D:321:UNK:CB	2.39	1.01
30:F:51:UNK:HA	30:F:52:UNK:CB	1.90	1.01
48:Y:103:UNK:O	48:Y:106:UNK:N	1.92	1.01
26:B:148:UNK:CB	26:B:151:UNK:C	2.38	1.01
40:P:170:UNK:O	40:P:205:UNK:N	1.94	1.01
48:Y:55:UNK:O	48:Y:58:UNK:CB	2.08	1.01
31:G:435:UNK:CB	31:G:440:UNK:CB	2.38	1.01
40:P:300:UNK:HA	40:P:302:UNK:CB	1.90	1.01
42:R:77:UNK:O	42:R:78:UNK:C	2.09	1.01
40:P:172:UNK:N	40:P:205:UNK:O	1.93	1.01
40:P:108:UNK:O	40:P:112:UNK:N	1.94	1.00
30:F:74:UNK:CB	30:F:77:UNK:CB	2.38	1.00
36:L:239:UNK:O	36:L:240:UNK:C	2.07	1.00
30:F:369:UNK:O	30:F:370:UNK:O	1.77	1.00
31:G:380:UNK:CB	31:G:408:UNK:CB	2.39	1.00
31:G:604:UNK:CB	31:G:609:UNK:O	2.08	1.00
26:B:118:UNK:C	26:B:122:UNK:CB	2.40	0.99
36:L:131:UNK:HA	36:L:143:UNK:CB	1.92	0.99
30:F:288:UNK:CB	30:F:291:UNK:CB	2.41	0.99
30:F:423:UNK:HA	30:F:426:UNK:CB	1.92	0.99
43:S:63:UNK:C	43:S:78:UNK:CB	2.40	0.99
36:L:247:UNK:O	36:L:252:UNK:N	1.95	0.99
36:L:82:UNK:O	36:L:87:UNK:N	1.96	0.99
47:X:93:UNK:CB	47:X:94:UNK:CB	2.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:55:CYS:SG	31:G:68:UNK:CB	2.50	0.99
32:H:40:UNK:O	32:H:47:UNK:CA	2.12	0.98
37:M:387:UNK:C	37:M:389:UNK:HA	1.93	0.98
34:J:147:UNK:O	34:J:149:UNK:N	1.95	0.98
29:E:144:CYS:SG	30:F:102:UNK:HA	2.03	0.98
36:L:246:UNK:O	36:L:251:UNK:N	1.96	0.98
26:B:118:UNK:O	26:B:121:UNK:N	1.97	0.98
29:E:87:UNK:CB	30:F:181:UNK:CB	2.40	0.98
41:Q:99:UNK:HA	41:Q:100:UNK:CB	1.90	0.98
32:H:40:UNK:O	32:H:47:UNK:CB	2.12	0.97
50:U:509:UNK:O	50:U:512:UNK:CB	2.13	0.97
36:L:189:UNK:O	36:L:194:UNK:N	1.98	0.97
38:N:293:UNK:O	38:N:294:UNK:C	2.09	0.97
27:C:64:UNK:O	27:C:70:UNK:CB	2.13	0.96
39:O:188:UNK:O	39:O:192:UNK:N	1.99	0.96
31:G:377:UNK:N	31:G:449:UNK:HA	1.80	0.96
39:O:87:UNK:CB	39:O:88:UNK:HA	1.96	0.96
42:R:63:UNK:O	42:R:64:UNK:C	2.14	0.96
30:F:166:UNK:O	30:F:169:UNK:N	1.99	0.95
45:V:55:UNK:O	45:V:57:UNK:N	1.98	0.95
38:N:276:UNK:O	38:N:279:UNK:N	1.98	0.95
39:O:129:UNK:O	39:O:132:UNK:CB	2.14	0.95
43:S:25:UNK:HA	43:S:57:UNK:CB	1.93	0.95
37:M:58:UNK:CA	37:M:59:UNK:CB	2.42	0.95
28:D:162:UNK:HA	32:H:279:UNK:CB	1.95	0.95
31:G:14:UNK:N	31:G:79:UNK:O	1.99	0.95
26:B:48:UNK:CB	26:B:80:UNK:HA	1.96	0.95
31:G:142:UNK:O	31:G:190:UNK:CB	2.14	0.95
38:N:100:UNK:O	38:N:104:UNK:N	2.00	0.95
37:M:388:UNK:N	37:M:389:UNK:HA	1.79	0.95
31:G:435:UNK:HA	31:G:440:UNK:CB	1.96	0.95
31:G:483:UNK:HA	31:G:576:UNK:CB	1.96	0.95
36:L:161:UNK:CA	36:L:162:UNK:C	2.41	0.95
30:F:51:UNK:CA	30:F:52:UNK:CB	2.46	0.94
30:F:190:UNK:CB	30:F:203:UNK:HA	1.96	0.94
34:J:58:UNK:O	34:J:62:UNK:N	2.00	0.94
47:X:90:UNK:O	47:X:92:UNK:N	2.01	0.94
30:F:289:UNK:HA	30:F:290:UNK:C	1.93	0.94
26:B:52:UNK:CB	26:B:89:UNK:O	2.15	0.94
31:G:52:CYS:O	31:G:53:UNK:C	2.13	0.94
39:O:49:UNK:HA	39:O:50:UNK:CB	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:319:UNK:O	36:L:320:UNK:CB	2.13	0.94
30:F:155:UNK:O	30:F:159:UNK:N	2.00	0.93
36:L:83:UNK:HA	36:L:87:UNK:CB	1.97	0.93
36:L:55:UNK:N	36:L:56:UNK:O	2.02	0.93
45:V:45:UNK:O	45:V:48:UNK:N	2.02	0.93
27:C:21:UNK:O	27:C:24:UNK:N	2.02	0.93
31:G:237:UNK:O	31:G:253:UNK:N	2.02	0.93
30:F:34:UNK:O	30:F:38:UNK:N	2.02	0.93
36:L:210:UNK:O	36:L:214:UNK:N	2.01	0.93
51:Z:243:UNK:O	51:Z:246:UNK:N	2.01	0.93
18:4:5:LYS:HZ3	18:4:6:GLY:H	1.01	0.92
30:F:426:UNK:HA	30:F:429:UNK:CB	2.00	0.92
37:M:103:UNK:O	37:M:107:UNK:N	2.02	0.92
38:N:142:UNK:O	38:N:145:UNK:CB	2.18	0.92
46:W:49:UNK:HA	46:W:52:UNK:CB	2.00	0.92
47:X:426:UNK:O	47:X:428:UNK:O	1.85	0.92
36:L:321:UNK:O	36:L:324:UNK:CB	2.18	0.92
30:F:60:UNK:O	30:F:64:UNK:N	2.02	0.92
37:M:51:UNK:CB	37:M:58:UNK:CB	2.46	0.92
27:C:83:UNK:O	27:C:85:UNK:N	2.02	0.92
26:B:148:UNK:CB	26:B:151:UNK:CB	2.48	0.92
31:G:142:UNK:O	31:G:190:UNK:CA	2.18	0.92
40:P:109:UNK:O	40:P:113:UNK:N	2.03	0.92
28:D:101:UNK:O	28:D:102:UNK:C	2.09	0.92
30:F:121:UNK:CB	30:F:229:UNK:HA	1.99	0.92
50:U:25:UNK:O	50:U:26:UNK:O	1.88	0.92
30:F:372:UNK:O	30:F:376:UNK:N	2.03	0.91
48:Y:102:UNK:O	48:Y:105:UNK:N	2.03	0.91
37:M:189:UNK:N	37:M:191:UNK:O	2.03	0.91
44:T:55:UNK:CB	44:T:60:UNK:O	2.19	0.91
46:W:39:UNK:C	46:W:41:UNK:CB	2.49	0.91
47:X:203:UNK:O	47:X:206:UNK:N	2.03	0.91
27:C:131:UNK:O	27:C:132:UNK:C	2.18	0.91
40:P:52:UNK:HA	40:P:72:UNK:CB	2.00	0.91
31:G:193:UNK:HA	31:G:196:UNK:CB	2.01	0.91
33:I:113:UNK:O	33:I:115:UNK:O	1.89	0.91
31:G:604:UNK:O	31:G:608:UNK:N	2.04	0.90
30:F:287:UNK:O	30:F:291:UNK:O	1.87	0.90
42:R:77:UNK:O	42:R:78:UNK:O	1.89	0.90
36:L:247:UNK:CA	36:L:251:UNK:CB	2.47	0.90
30:F:33:UNK:O	30:F:37:UNK:N	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:52:UNK:O	30:F:56:UNK:N	2.05	0.90
27:C:83:UNK:O	27:C:84:UNK:C	2.16	0.89
31:G:377:UNK:H	31:G:449:UNK:CA	1.83	0.89
45:V:44:UNK:O	45:V:47:UNK:CB	2.19	0.89
27:C:133:UNK:HA	27:C:136:UNK:CB	2.01	0.89
51:Z:205:UNK:O	51:Z:208:UNK:N	2.05	0.89
37:M:348:UNK:HA	37:M:351:UNK:CB	2.03	0.89
39:O:234:UNK:O	39:O:237:UNK:CB	2.20	0.89
40:P:71:UNK:O	40:P:72:UNK:C	2.18	0.89
36:L:151:UNK:O	36:L:155:UNK:CB	2.21	0.89
36:L:263:UNK:O	36:L:265:UNK:N	2.05	0.88
37:M:347:UNK:O	37:M:351:UNK:CB	2.20	0.88
26:B:121:UNK:HA	26:B:135:UNK:CB	2.03	0.88
28:D:96:UNK:N	28:D:385:UNK:CB	2.35	0.88
33:I:111:UNK:O	33:I:113:UNK:N	2.06	0.88
31:G:318:UNK:O	31:G:529:UNK:N	2.07	0.88
31:G:436:UNK:N	31:G:437:UNK:HA	1.82	0.88
30:F:212:UNK:HA	30:F:220:UNK:O	1.74	0.88
36:L:29:UNK:HA	36:L:32:UNK:CB	2.03	0.88
30:F:294:UNK:CA	30:F:339:UNK:CB	2.52	0.87
38:N:33:UNK:O	38:N:36:UNK:N	2.06	0.87
37:M:68:UNK:O	37:M:69:UNK:C	2.19	0.87
27:C:89:UNK:N	27:C:112:UNK:O	2.07	0.87
28:D:395:UNK:O	28:D:399:UNK:N	2.07	0.87
30:F:359:CYS:O	30:F:360:UNK:CB	2.22	0.87
31:G:435:UNK:CA	31:G:440:UNK:CB	2.53	0.87
38:N:146:UNK:N	38:N:147:UNK:HA	1.89	0.87
40:P:106:UNK:HA	40:P:109:UNK:CB	2.05	0.87
47:X:177:UNK:O	47:X:180:UNK:N	2.08	0.87
51:Z:323:UNK:CB	51:Z:324:UNK:HA	2.03	0.87
31:G:174:UNK:HA	31:G:183:UNK:HA	1.55	0.87
31:G:52:CYS:O	31:G:54:UNK:N	2.08	0.87
33:I:123:UNK:CB	33:I:131:UNK:O	2.23	0.87
37:M:176:UNK:N	37:M:177:UNK:HA	1.89	0.87
30:F:323:UNK:O	30:F:326:UNK:N	2.08	0.86
40:P:21:UNK:CB	40:P:45:UNK:HA	2.04	0.86
40:P:21:UNK:O	40:P:46:UNK:N	2.08	0.86
37:M:49:UNK:HA	37:M:50:UNK:CB	2.05	0.86
40:P:99:UNK:CB	40:P:103:UNK:CB	2.53	0.86
42:R:67:UNK:C	42:R:69:UNK:N	2.33	0.86
30:F:369:UNK:O	30:F:370:UNK:C	2.21	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:380:UNK:O	31:G:409:UNK:N	2.08	0.86
40:P:301:UNK:HA	40:P:302:UNK:CB	2.06	0.86
37:M:281:UNK:O	37:M:284:UNK:CB	2.24	0.86
36:L:316:UNK:O	36:L:319:UNK:N	2.09	0.86
36:L:321:UNK:O	36:L:324:UNK:N	2.08	0.86
31:G:187:UNK:N	31:G:188:UNK:HA	1.88	0.86
46:W:47:UNK:CB	46:W:50:UNK:CB	2.54	0.86
50:U:320:UNK:O	50:U:324:UNK:N	2.08	0.85
39:O:229:UNK:CB	39:O:231:UNK:HA	2.04	0.85
30:F:419:UNK:HA	30:F:423:UNK:CB	2.05	0.85
36:L:67:UNK:CB	36:L:76:UNK:HA	2.05	0.85
30:F:60:UNK:O	30:F:63:UNK:CB	2.24	0.85
30:F:300:UNK:CB	30:F:329:UNK:HA	2.06	0.85
38:N:72:UNK:O	38:N:75:UNK:CB	2.24	0.85
25:A:103:UNK:HA	25:A:106:UNK:CB	2.07	0.85
38:N:89:UNK:C	38:N:91:UNK:HA	2.07	0.85
50:U:122:UNK:O	50:U:125:UNK:N	2.10	0.85
31:G:192:UNK:HA	31:G:193:UNK:CB	2.05	0.85
25:A:102:UNK:O	25:A:106:UNK:N	2.10	0.84
36:L:34:UNK:O	36:L:38:UNK:N	2.10	0.84
36:L:46:UNK:O	36:L:49:UNK:CB	2.25	0.84
38:N:128:UNK:CB	38:N:216:UNK:CB	2.55	0.84
37:M:146:UNK:O	37:M:149:UNK:N	2.09	0.84
50:U:712:UNK:HA	50:U:807:UNK:CB	2.07	0.84
32:H:43:UNK:N	32:H:44:UNK:HA	1.91	0.84
32:H:120:UNK:CB	32:H:132:UNK:CB	2.54	0.84
36:L:297:UNK:HA	36:L:356:UNK:N	1.92	0.84
31:G:594:UNK:HA	31:G:595:UNK:CB	2.07	0.84
43:S:63:UNK:O	43:S:78:UNK:HA	1.78	0.84
30:F:56:UNK:O	30:F:59:UNK:CB	2.26	0.84
43:S:43:UNK:O	43:S:47:UNK:N	2.10	0.84
50:U:326:UNK:O	50:U:329:UNK:CB	2.25	0.84
36:L:288:UNK:CB	36:L:308:UNK:CB	2.55	0.84
40:P:63:UNK:C	40:P:65:UNK:CB	2.55	0.84
44:T:55:UNK:O	44:T:59:UNK:N	2.11	0.83
36:L:197:UNK:O	36:L:201:UNK:N	2.11	0.83
47:X:333:UNK:O	47:X:336:UNK:CB	2.25	0.83
26:B:148:UNK:CB	26:B:152:UNK:N	2.41	0.83
30:F:365:CYS:HA	30:F:368:UNK:CB	2.08	0.83
38:N:233:UNK:O	38:N:236:UNK:CB	2.25	0.83
47:X:334:UNK:O	47:X:337:UNK:N	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:131:UNK:O	27:C:134:UNK:N	2.12	0.83
43:S:24:UNK:CB	43:S:59:UNK:O	2.27	0.83
31:G:577:UNK:O	31:G:578:UNK:CB	2.25	0.83
43:S:27:UNK:O	43:S:28:UNK:CB	2.24	0.83
27:C:23:UNK:HA	27:C:26:UNK:CB	2.08	0.83
31:G:104:UNK:O	31:G:107:UNK:N	2.12	0.82
30:F:303:UNK:O	30:F:414:UNK:CB	2.26	0.82
28:D:250:UNK:O	28:D:253:UNK:N	2.12	0.82
28:D:258:UNK:O	28:D:262:UNK:N	2.12	0.82
30:F:426:UNK:O	30:F:429:UNK:N	2.12	0.82
33:I:98:UNK:O	33:I:103:UNK:O	1.98	0.82
39:O:229:UNK:CB	39:O:231:UNK:CB	2.57	0.82
51:Z:210:UNK:O	51:Z:213:UNK:N	2.12	0.82
31:G:595:UNK:O	31:G:599:UNK:N	2.12	0.82
40:P:172:UNK:O	40:P:206:UNK:HA	1.80	0.82
41:Q:109:UNK:HA	41:Q:110:UNK:CB	2.09	0.82
50:U:622:UNK:O	50:U:625:UNK:N	2.13	0.82
37:M:210:UNK:HA	37:M:268:UNK:CB	2.10	0.82
40:P:131:UNK:O	40:P:165:UNK:HA	1.80	0.82
30:F:44:UNK:O	30:F:47:UNK:N	2.13	0.81
36:L:321:UNK:O	36:L:325:UNK:N	2.12	0.81
30:F:405:CYS:SG	30:F:407:UNK:N	2.53	0.81
36:L:77:UNK:HA	36:L:78:UNK:CB	2.09	0.81
37:M:281:UNK:O	37:M:285:UNK:N	2.13	0.81
18:4:5:LYS:NZ	18:4:6:GLY:H	1.78	0.81
26:B:78:UNK:N	26:B:79:UNK:HA	1.94	0.81
30:F:265:UNK:O	30:F:266:UNK:CB	2.29	0.81
37:M:118:UNK:O	37:M:122:UNK:N	2.13	0.81
29:E:98:UNK:O	29:E:137:UNK:HA	1.80	0.81
30:F:264:UNK:CB	30:F:283:UNK:O	2.29	0.81
40:P:103:UNK:O	40:P:106:UNK:N	2.13	0.81
31:G:10:UNK:O	31:G:76:UNK:N	2.14	0.81
47:X:182:UNK:O	47:X:186:UNK:N	2.14	0.80
51:Z:103:UNK:O	51:Z:107:UNK:N	2.14	0.80
30:F:294:UNK:C	30:F:339:UNK:CB	2.52	0.80
40:P:223:UNK:HA	40:P:224:UNK:CB	2.10	0.80
40:P:139:UNK:HA	40:P:140:UNK:CB	2.12	0.80
42:R:87:UNK:O	42:R:89:UNK:N	2.14	0.80
43:S:84:UNK:O	43:S:88:UNK:N	2.14	0.80
33:I:128:UNK:O	33:I:129:UNK:C	2.29	0.80
37:M:108:UNK:HA	37:M:111:UNK:CB	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S:41:UNK:HA	43:S:44:UNK:CB	2.11	0.80
30:F:133:UNK:CB	30:F:174:UNK:CB	2.60	0.80
40:P:145:UNK:O	40:P:148:UNK:CB	2.30	0.80
26:B:154:UNK:O	26:B:158:UNK:N	2.15	0.80
31:G:381:UNK:HA	31:G:409:UNK:O	1.82	0.80
31:G:428:UNK:O	31:G:432:UNK:N	2.14	0.80
40:P:170:UNK:CB	40:P:204:UNK:CA	2.57	0.80
29:E:165:UNK:O	29:E:169:UNK:N	2.14	0.80
36:L:225:UNK:CA	36:L:229:UNK:CB	2.58	0.80
40:P:64:UNK:N	40:P:65:UNK:CB	2.43	0.80
51:Z:335:UNK:CB	51:Z:338:UNK:CB	2.60	0.80
19:5:39:CYS:SG	19:5:53:CYS:CB	2.70	0.80
30:F:212:UNK:O	30:F:220:UNK:N	2.15	0.80
31:G:41:CYS:HB2	54:G:803:FES:S2	2.20	0.80
36:L:321:UNK:O	36:L:324:UNK:CA	2.30	0.80
37:M:241:UNK:O	37:M:244:UNK:N	2.15	0.79
46:W:49:UNK:O	46:W:53:UNK:N	2.15	0.79
40:P:53:UNK:CB	40:P:57:UNK:CB	2.60	0.79
43:S:83:UNK:O	43:S:87:UNK:N	2.15	0.79
33:I:94:UNK:HA	33:I:108:UNK:O	1.82	0.79
38:N:163:UNK:O	38:N:166:UNK:N	2.15	0.79
40:P:146:UNK:O	40:P:149:UNK:N	2.15	0.79
47:X:203:UNK:O	47:X:204:UNK:C	2.31	0.79
30:F:61:UNK:O	30:F:64:UNK:N	2.16	0.79
40:P:203:UNK:HA	40:P:234:UNK:CA	2.12	0.79
26:B:95:UNK:O	26:B:97:UNK:N	2.16	0.79
26:B:121:UNK:C	26:B:135:UNK:HA	2.12	0.79
45:V:1:UNK:O	45:V:2:UNK:C	2.30	0.79
34:J:24:UNK:O	34:J:25:UNK:CB	2.31	0.79
40:P:136:UNK:HA	40:P:137:UNK:CB	2.11	0.79
40:P:311:UNK:O	40:P:314:UNK:N	2.16	0.79
44:T:62:UNK:CB	44:T:66:UNK:CB	2.60	0.79
19:5:39:CYS:SG	19:5:53:CYS:HB3	2.22	0.79
51:Z:101:UNK:O	51:Z:105:UNK:N	2.15	0.79
31:G:120:UNK:O	31:G:124:UNK:O	2.01	0.79
40:P:203:UNK:HA	40:P:233:UNK:CB	2.13	0.79
36:L:578:UNK:O	36:L:579:UNK:C	2.28	0.78
40:P:135:UNK:HA	40:P:168:UNK:N	1.98	0.78
30:F:262:UNK:CB	30:F:285:UNK:HA	2.13	0.78
31:G:311:UNK:CB	31:G:314:UNK:CB	2.61	0.78
37:M:207:UNK:O	37:M:208:UNK:CB	2.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:174:UNK:O	28:D:177:UNK:N	2.15	0.78
32:H:68:UNK:O	32:H:69:UNK:C	2.24	0.78
42:R:81:UNK:CB	42:R:91:UNK:O	2.31	0.78
30:F:65:UNK:O	30:F:75:UNK:N	2.16	0.78
26:B:116:UNK:O	26:B:117:UNK:CB	2.31	0.78
32:H:101:UNK:N	32:H:161:UNK:HA	1.99	0.78
50:U:416:UNK:O	50:U:419:UNK:N	2.17	0.78
37:M:113:UNK:HA	37:M:114:UNK:CB	2.13	0.78
37:M:191:UNK:CB	37:M:192:UNK:HA	2.14	0.78
41:Q:95:UNK:O	41:Q:99:UNK:N	2.17	0.78
36:L:223:UNK:CB	36:L:256:UNK:CB	2.62	0.78
50:U:713:UNK:O	50:U:716:UNK:N	2.17	0.78
28:D:163:UNK:CA	32:H:278:UNK:HA	2.14	0.77
31:G:11:UNK:CB	31:G:77:UNK:O	2.32	0.77
36:L:142:UNK:HA	37:M:370:UNK:CB	2.14	0.77
25:A:84:UNK:O	25:A:85:UNK:C	2.32	0.77
36:L:67:UNK:CB	36:L:76:UNK:CB	2.63	0.77
19:5:75:ARG:HG2	19:5:75:ARG:HH11	1.48	0.77
31:G:316:UNK:HA	31:G:342:UNK:O	1.85	0.77
31:G:227:UNK:O	31:G:238:UNK:C	2.33	0.77
37:M:258:UNK:O	37:M:262:UNK:N	2.17	0.77
36:L:580:UNK:N	36:L:581:UNK:HA	1.98	0.77
37:M:25:UNK:O	37:M:28:UNK:N	2.18	0.77
38:N:257:UNK:O	38:N:259:UNK:N	2.18	0.77
30:F:426:UNK:O	30:F:430:UNK:N	2.18	0.77
50:U:109:UNK:O	50:U:110:UNK:C	2.31	0.77
31:G:382:UNK:CB	31:G:454:UNK:HA	2.15	0.77
38:N:204:UNK:O	38:N:208:UNK:N	2.18	0.77
30:F:61:UNK:O	30:F:64:UNK:CA	2.33	0.76
47:X:171:UNK:O	47:X:175:UNK:CB	2.33	0.76
26:B:147:UNK:O	26:B:148:UNK:CB	2.33	0.76
36:L:453:UNK:O	36:L:456:UNK:N	2.19	0.76
51:Z:114:UNK:O	51:Z:117:UNK:CB	2.32	0.76
27:C:21:UNK:O	27:C:24:UNK:CB	2.33	0.76
32:H:194:UNK:O	32:H:195:UNK:CB	2.34	0.76
40:P:203:UNK:CA	40:P:234:UNK:HA	2.15	0.76
36:L:181:UNK:O	36:L:182:UNK:C	2.32	0.76
38:N:165:UNK:CB	38:N:185:UNK:CB	2.63	0.76
51:Z:111:UNK:O	51:Z:114:UNK:N	2.19	0.76
27:C:62:UNK:O	27:C:66:UNK:N	2.18	0.76
30:F:352:UNK:O	30:F:355:UNK:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:190:UNK:HA	36:L:194:UNK:HA	1.68	0.76
37:M:62:UNK:N	37:M:63:UNK:HA	2.00	0.76
40:P:223:UNK:CA	40:P:224:UNK:CB	2.63	0.76
47:X:426:UNK:O	47:X:427:UNK:C	2.29	0.76
28:D:234:UNK:O	28:D:237:UNK:N	2.18	0.76
40:P:53:UNK:CA	40:P:57:UNK:CB	2.64	0.76
26:B:155:UNK:O	26:B:159:UNK:N	2.19	0.76
38:N:175:UNK:CB	38:N:225:UNK:O	2.33	0.76
28:D:193:UNK:O	28:D:194:UNK:CB	2.34	0.75
37:M:447:UNK:O	37:M:450:UNK:O	2.04	0.75
28:D:218:UNK:O	28:D:222:UNK:CB	2.34	0.75
31:G:148:UNK:CB	31:G:207:UNK:O	2.34	0.75
46:W:41:UNK:O	46:W:42:UNK:CB	2.33	0.75
27:C:111:UNK:CB	27:C:113:UNK:CB	2.64	0.75
29:E:28:UNK:O	29:E:32:UNK:N	2.20	0.75
37:M:347:UNK:O	37:M:351:UNK:CA	2.34	0.75
30:F:322:UNK:O	30:F:327:UNK:N	2.19	0.75
32:H:195:UNK:O	32:H:198:UNK:CB	2.34	0.75
26:B:119:CYS:H	26:B:122:UNK:CB	1.94	0.75
28:D:139:UNK:O	28:D:143:UNK:N	2.20	0.75
30:F:405:CYS:SG	30:F:408:UNK:N	2.60	0.75
37:M:372:UNK:O	37:M:376:UNK:N	2.20	0.75
42:R:60:UNK:O	42:R:61:UNK:C	2.35	0.75
30:F:352:UNK:O	30:F:355:UNK:CB	2.35	0.75
31:G:317:UNK:HA	31:G:527:UNK:O	1.87	0.75
29:E:106:UNK:O	29:E:110:UNK:N	2.20	0.74
31:G:210:UNK:O	31:G:213:UNK:N	2.20	0.74
37:M:275:UNK:O	37:M:278:UNK:CB	2.35	0.74
31:G:185:UNK:O	31:G:188:UNK:CB	2.35	0.74
40:P:38:UNK:O	40:P:41:UNK:O	2.05	0.74
43:S:63:UNK:CB	43:S:78:UNK:CB	2.66	0.74
36:L:503:UNK:O	36:L:507:UNK:N	2.19	0.74
30:F:421:UNK:O	30:F:425:UNK:N	2.20	0.74
33:I:73:UNK:O	33:I:74:UNK:CB	2.34	0.74
36:L:165:UNK:O	36:L:169:UNK:N	2.20	0.74
36:L:224:UNK:N	36:L:256:UNK:CB	2.51	0.74
37:M:23:UNK:O	37:M:25:UNK:N	2.20	0.74
38:N:90:UNK:N	38:N:91:UNK:HA	2.01	0.74
36:L:207:UNK:HA	36:L:208:UNK:CB	2.18	0.74
37:M:241:UNK:O	37:M:242:UNK:C	2.35	0.74
36:L:71:UNK:O	36:L:72:UNK:CB	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:152:UNK:O	29:E:163:UNK:N	2.21	0.74
31:G:12:UNK:O	31:G:78:UNK:HA	1.87	0.74
42:R:78:UNK:O	42:R:79:UNK:C	2.36	0.74
48:Y:35:UNK:O	48:Y:39:UNK:N	2.21	0.74
30:F:82:UNK:O	30:F:83:UNK:C	2.34	0.74
30:F:300:UNK:CA	30:F:329:UNK:HA	2.18	0.74
45:V:66:UNK:O	45:V:69:UNK:CB	2.36	0.74
32:H:40:UNK:O	32:H:47:UNK:HA	1.88	0.73
41:Q:40:UNK:CB	41:Q:41:UNK:HA	2.17	0.73
30:F:163:UNK:O	30:F:165:UNK:O	2.06	0.73
37:M:87:UNK:CB	37:M:88:UNK:HA	2.17	0.73
50:U:329:UNK:O	50:U:330:UNK:CB	2.37	0.73
31:G:52:CYS:C	31:G:54:UNK:N	2.41	0.73
45:V:45:UNK:C	45:V:47:UNK:N	2.50	0.73
18:4:54:ARG:HD3	18:4:54:ARG:N	2.04	0.73
25:A:103:UNK:O	25:A:107:UNK:N	2.21	0.73
26:B:128:UNK:O	26:B:131:UNK:CB	2.36	0.73
26:B:121:UNK:HA	26:B:135:UNK:CA	2.18	0.73
36:L:530:UNK:O	36:L:534:UNK:N	2.21	0.73
30:F:61:UNK:C	30:F:64:UNK:N	2.51	0.73
31:G:565:UNK:O	31:G:568:UNK:N	2.22	0.73
27:C:111:UNK:C	27:C:113:UNK:CB	2.67	0.73
30:F:140:UNK:CB	30:F:182:UNK:HA	2.18	0.73
34:J:58:UNK:O	34:J:62:UNK:CB	2.37	0.73
36:L:209:UNK:O	36:L:212:UNK:CB	2.37	0.73
36:L:239:UNK:O	36:L:240:UNK:O	2.06	0.73
46:W:68:UNK:O	46:W:72:UNK:CB	2.37	0.73
50:U:713:UNK:O	50:U:714:UNK:C	2.35	0.73
31:G:469:UNK:O	31:G:473:UNK:N	2.21	0.72
32:H:177:UNK:CA	47:X:146:UNK:CB	2.67	0.72
34:J:22:UNK:CB	34:J:24:UNK:O	2.37	0.72
37:M:27:UNK:O	37:M:30:UNK:N	2.22	0.72
47:X:188:UNK:O	47:X:191:UNK:N	2.22	0.72
30:F:74:UNK:O	30:F:78:UNK:N	2.22	0.72
43:S:23:UNK:O	43:S:56:UNK:O	2.07	0.72
28:D:360:UNK:CB	28:D:381:UNK:HA	2.19	0.72
29:E:98:UNK:N	29:E:136:UNK:O	2.23	0.72
36:L:223:UNK:C	36:L:256:UNK:CB	2.66	0.72
15:1:23:PRO:O	16:2:66:ARG:HD3	1.89	0.72
33:I:149:UNK:HA	33:I:150:UNK:CB	2.19	0.72
40:P:236:UNK:O	40:P:237:UNK:CB	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S:84:UNK:O	43:S:87:UNK:N	2.22	0.72
27:C:113:UNK:O	27:C:115:UNK:N	2.22	0.72
31:G:375:UNK:CB	31:G:376:UNK:HA	2.18	0.72
39:O:130:UNK:O	39:O:131:UNK:C	2.35	0.72
36:L:580:UNK:N	36:L:581:UNK:CA	2.51	0.72
40:P:137:UNK:CB	40:P:138:UNK:HA	2.19	0.72
15:1:147:LYS:HA	15:1:147:LYS:HE3	1.72	0.72
38:N:223:UNK:HA	38:N:224:UNK:C	2.19	0.72
31:G:332:UNK:O	31:G:336:UNK:N	2.23	0.72
30:F:362:CYS:SG	30:F:404:UNK:CB	2.78	0.71
38:N:61:UNK:O	38:N:64:UNK:N	2.23	0.71
45:V:27:UNK:O	45:V:31:UNK:N	2.23	0.71
45:V:45:UNK:O	45:V:46:UNK:C	2.38	0.71
30:F:398:UNK:O	30:F:401:UNK:CB	2.39	0.71
31:G:12:UNK:O	31:G:79:UNK:N	2.23	0.71
40:P:104:UNK:O	40:P:108:UNK:N	2.22	0.71
26:B:166:UNK:HA	26:B:169:UNK:O	1.90	0.71
30:F:214:UNK:HA	30:F:218:UNK:O	1.90	0.71
33:I:151:UNK:O	33:I:154:UNK:CB	2.38	0.71
37:M:31:UNK:O	37:M:32:UNK:C	2.37	0.71
38:N:123:UNK:HA	38:N:124:UNK:CB	2.18	0.71
45:V:44:UNK:O	45:V:47:UNK:N	2.24	0.71
48:Y:102:UNK:O	48:Y:105:UNK:CA	2.39	0.71
43:S:41:UNK:O	43:S:45:UNK:N	2.23	0.71
26:B:122:UNK:HA	26:B:123:UNK:CB	2.21	0.71
38:N:33:UNK:O	38:N:34:UNK:C	2.38	0.71
40:P:52:UNK:CA	40:P:72:UNK:CB	2.68	0.71
43:S:44:UNK:O	43:S:48:UNK:N	2.24	0.71
48:Y:103:UNK:O	48:Y:104:UNK:C	2.36	0.71
36:L:182:UNK:O	36:L:186:UNK:N	2.24	0.71
37:M:32:UNK:O	37:M:35:UNK:N	2.23	0.71
40:P:146:UNK:O	40:P:150:UNK:N	2.24	0.71
47:X:353:UNK:O	47:X:356:UNK:O	2.07	0.71
31:G:59:UNK:CB	31:G:62:UNK:CB	2.69	0.71
38:N:158:UNK:O	38:N:161:UNK:CB	2.39	0.71
18:4:5:LYS:HZ3	18:4:5:LYS:HB3	1.55	0.70
30:F:70:UNK:CB	30:F:330:UNK:CB	2.69	0.70
30:F:370:UNK:O	30:F:372:UNK:N	2.24	0.70
31:G:367:UNK:O	31:G:370:UNK:N	2.24	0.70
51:Z:13:UNK:O	51:Z:16:UNK:CB	2.39	0.70
38:N:158:UNK:O	38:N:162:UNK:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:351:UNK:O	30:F:354:UNK:N	2.23	0.70
31:G:367:UNK:O	31:G:370:UNK:CB	2.40	0.70
36:L:67:UNK:CB	36:L:76:UNK:CA	2.68	0.70
38:N:258:UNK:CB	38:N:330:UNK:O	2.39	0.70
31:G:73:UNK:O	31:G:74:UNK:CB	2.39	0.70
36:L:34:UNK:HA	36:L:37:UNK:CB	2.22	0.70
37:M:279:UNK:CB	37:M:280:UNK:HA	2.20	0.70
39:O:24:UNK:HA	39:O:122:UNK:O	1.90	0.70
40:P:64:UNK:N	40:P:65:UNK:CA	2.54	0.70
30:F:323:UNK:HA	30:F:327:UNK:O	1.92	0.70
33:I:100:UNK:N	33:I:103:UNK:O	2.24	0.70
36:L:530:UNK:O	36:L:533:UNK:N	2.23	0.70
38:N:142:UNK:O	38:N:145:UNK:N	2.24	0.70
39:O:130:UNK:O	39:O:133:UNK:N	2.24	0.70
31:G:288:UNK:HA	31:G:289:UNK:C	2.20	0.70
39:O:50:UNK:CB	39:O:123:UNK:O	2.39	0.70
47:X:177:UNK:O	47:X:180:UNK:CB	2.40	0.70
27:C:132:UNK:O	27:C:136:UNK:N	2.25	0.70
31:G:367:UNK:O	31:G:371:UNK:N	2.25	0.70
38:N:190:UNK:CB	38:N:204:UNK:CB	2.69	0.70
34:J:58:UNK:O	34:J:62:UNK:CA	2.40	0.70
28:D:182:UNK:O	28:D:186:UNK:N	2.25	0.70
30:F:150:UNK:O	30:F:154:UNK:N	2.25	0.70
36:L:161:UNK:CA	36:L:163:UNK:N	2.46	0.69
36:L:321:UNK:CA	36:L:324:UNK:CB	2.70	0.69
34:J:85:UNK:O	34:J:88:UNK:N	2.25	0.69
35:K:32:UNK:O	35:K:35:UNK:CB	2.39	0.69
26:B:121:UNK:CA	26:B:135:UNK:HA	2.22	0.69
42:R:81:UNK:CB	42:R:92:UNK:HA	2.22	0.69
51:Z:511:UNK:O	51:Z:514:UNK:N	2.25	0.69
31:G:94:UNK:O	31:G:98:UNK:N	2.25	0.69
36:L:151:UNK:O	36:L:155:UNK:N	2.26	0.69
37:M:274:UNK:O	37:M:278:UNK:CB	2.40	0.69
47:X:156:UNK:O	47:X:159:UNK:CB	2.41	0.69
36:L:180:UNK:O	36:L:181:UNK:C	2.37	0.69
37:M:21:UNK:O	37:M:22:UNK:C	2.41	0.69
38:N:73:UNK:O	38:N:74:UNK:C	2.38	0.69
32:H:127:UNK:O	32:H:131:UNK:CB	2.41	0.69
36:L:35:UNK:O	36:L:39:UNK:N	2.25	0.69
50:U:416:UNK:O	50:U:417:UNK:C	2.38	0.69
36:L:314:UNK:O	36:L:317:UNK:CB	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:703:UNK:C	47:X:705:UNK:N	2.54	0.69
25:A:109:UNK:O	25:A:110:UNK:CB	2.38	0.69
38:N:77:UNK:O	38:N:80:UNK:O	2.11	0.69
38:N:108:UNK:O	38:N:109:UNK:C	2.41	0.69
40:P:112:UNK:O	40:P:116:UNK:N	2.26	0.69
30:F:92:UNK:O	30:F:220:UNK:HA	1.92	0.68
31:G:229:UNK:N	31:G:238:UNK:CB	2.56	0.68
33:I:113:UNK:O	33:I:114:UNK:C	2.37	0.68
38:N:158:UNK:O	38:N:161:UNK:N	2.26	0.68
30:F:34:UNK:O	30:F:38:UNK:CB	2.41	0.68
36:L:369:UNK:O	36:L:373:UNK:N	2.26	0.68
38:N:204:UNK:O	38:N:208:UNK:CB	2.41	0.68
27:C:131:UNK:C	27:C:133:UNK:N	2.54	0.68
32:H:285:UNK:O	32:H:289:UNK:N	2.26	0.68
38:N:108:UNK:O	38:N:112:UNK:N	2.26	0.68
39:O:41:UNK:O	39:O:44:UNK:CB	2.42	0.68
40:P:160:UNK:N	40:P:162:UNK:N	2.42	0.68
40:P:311:UNK:O	40:P:314:UNK:CB	2.42	0.68
47:X:77:UNK:C	47:X:79:UNK:N	2.56	0.68
29:E:96:UNK:O	29:E:98:UNK:O	2.10	0.68
30:F:294:UNK:CB	30:F:339:UNK:CB	2.72	0.68
37:M:167:UNK:O	37:M:171:UNK:N	2.26	0.68
38:N:52:UNK:O	38:N:55:UNK:N	2.27	0.68
23:9:19:TRP:HZ2	24:0:14:GLU:HG2	1.58	0.68
30:F:51:UNK:CB	30:F:52:UNK:CB	2.72	0.68
37:M:24:UNK:O	37:M:27:UNK:CB	2.42	0.68
32:H:143:UNK:O	32:H:144:UNK:C	2.42	0.68
36:L:419:UNK:O	36:L:422:UNK:CB	2.42	0.68
47:X:334:UNK:O	47:X:335:UNK:C	2.41	0.68
48:Y:11:UNK:CA	48:Y:48:UNK:CB	2.69	0.68
51:Z:343:UNK:O	51:Z:347:UNK:N	2.26	0.68
40:P:134:UNK:O	40:P:167:UNK:HA	1.93	0.68
50:U:626:UNK:O	50:U:628:UNK:O	2.12	0.68
26:B:117:UNK:O	26:B:120:UNK:N	2.27	0.68
36:L:46:UNK:O	36:L:49:UNK:N	2.27	0.68
39:O:28:UNK:O	39:O:172:UNK:CB	2.41	0.68
48:Y:103:UNK:C	48:Y:105:UNK:N	2.56	0.68
18:4:5:LYS:HZ3	18:4:6:GLY:N	1.85	0.67
33:I:173:UNK:HA	33:I:174:UNK:C	2.23	0.67
37:M:60:UNK:C	37:M:63:UNK:N	2.57	0.67
28:D:357:UNK:HA	28:D:384:UNK:CB	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:50:UNK:O	34:J:54:UNK:N	2.27	0.67
37:M:60:UNK:C	37:M:62:UNK:C	2.72	0.67
50:U:25:UNK:C	50:U:26:UNK:O	2.42	0.67
36:L:281:UNK:CB	36:L:315:UNK:HA	2.25	0.67
47:X:93:UNK:CA	47:X:94:UNK:CB	2.71	0.67
26:B:148:UNK:CA	26:B:151:UNK:CA	2.58	0.67
38:N:293:UNK:O	38:N:296:UNK:N	2.27	0.67
30:F:194:UNK:O	30:F:197:UNK:CB	2.42	0.67
36:L:178:UNK:CB	36:L:222:UNK:CB	2.73	0.67
27:C:131:UNK:O	27:C:133:UNK:N	2.27	0.67
36:L:297:UNK:HA	36:L:355:UNK:HA	1.77	0.67
30:F:289:UNK:CA	30:F:290:UNK:C	2.66	0.67
36:L:226:UNK:HA	36:L:284:UNK:CB	2.24	0.67
38:N:224:UNK:N	38:N:225:UNK:HA	2.08	0.67
39:O:87:UNK:CB	39:O:88:UNK:CA	2.73	0.67
28:D:234:UNK:O	28:D:237:UNK:CB	2.43	0.67
42:R:51:UNK:HA	42:R:92:UNK:O	1.95	0.67
50:U:411:UNK:O	50:U:412:UNK:C	2.43	0.67
19:5:38:ARG:HG2	19:5:85:ILE:HG23	1.77	0.67
26:B:65:UNK:HA	26:B:68:UNK:CB	2.25	0.67
36:L:207:UNK:CB	36:L:209:UNK:HA	2.25	0.67
38:N:135:UNK:O	38:N:136:UNK:C	2.43	0.67
30:F:291:UNK:O	30:F:292:UNK:C	2.43	0.66
25:A:76:UNK:O	25:A:77:UNK:C	2.38	0.66
31:G:380:UNK:O	31:G:409:UNK:O	2.13	0.66
46:W:47:UNK:O	46:W:50:UNK:CB	2.42	0.66
47:X:703:UNK:O	47:X:704:UNK:C	2.41	0.66
34:J:101:UNK:O	34:J:102:UNK:C	2.44	0.66
37:M:32:UNK:O	37:M:33:UNK:C	2.42	0.66
15:1:24:LEU:H	16:2:34:ASN:HD21	1.44	0.66
30:F:429:UNK:O	30:F:432:UNK:CB	2.44	0.66
33:I:172:UNK:O	33:I:175:UNK:HA	1.95	0.66
37:M:102:UNK:O	37:M:106:UNK:CB	2.43	0.66
40:P:134:UNK:O	40:P:167:UNK:CB	2.43	0.66
51:Z:511:UNK:O	51:Z:512:UNK:C	2.44	0.66
30:F:262:UNK:CB	30:F:285:UNK:CA	2.74	0.66
31:G:12:UNK:HA	31:G:17:UNK:HA	1.77	0.66
31:G:388:UNK:CB	31:G:391:UNK:CB	2.74	0.66
31:G:426:UNK:O	31:G:430:UNK:N	2.29	0.66
28:D:296:UNK:O	28:D:299:UNK:N	2.28	0.66
28:D:383:UNK:CB	28:D:385:UNK:O	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:H:152:UNK:O	32:H:155:UNK:N	2.29	0.66
28:D:218:UNK:O	28:D:222:UNK:N	2.28	0.66
30:F:101:UNK:O	30:F:102:UNK:CB	2.43	0.66
38:N:24:UNK:O	38:N:28:UNK:N	2.28	0.66
38:N:142:UNK:O	38:N:145:UNK:CA	2.43	0.66
39:O:130:UNK:C	39:O:132:UNK:N	2.59	0.66
47:X:187:UNK:O	47:X:190:UNK:N	2.28	0.66
51:Z:243:UNK:O	51:Z:244:UNK:C	2.42	0.66
26:B:48:UNK:HA	26:B:78:UNK:CB	2.26	0.66
31:G:311:UNK:O	31:G:314:UNK:CB	2.43	0.66
36:L:61:UNK:HA	36:L:80:UNK:CB	2.26	0.66
16:2:43:PRO:HB2	16:2:48:ILE:HD11	1.76	0.66
28:D:229:UNK:O	28:D:232:UNK:N	2.29	0.66
37:M:271:UNK:O	37:M:272:UNK:C	2.44	0.66
38:N:45:UNK:O	38:N:46:UNK:C	2.45	0.65
27:C:31:UNK:O	27:C:33:UNK:N	2.30	0.65
31:G:114:CYS:O	31:G:118:UNK:N	2.30	0.65
31:G:375:UNK:C	31:G:449:UNK:N	2.58	0.65
37:M:278:UNK:O	37:M:279:UNK:CB	2.43	0.65
31:G:26:UNK:O	31:G:29:UNK:CB	2.45	0.65
37:M:281:UNK:O	37:M:284:UNK:N	2.29	0.65
25:A:111:UNK:O	25:A:112:UNK:CB	2.43	0.65
38:N:227:UNK:O	38:N:228:UNK:C	2.39	0.65
26:B:95:UNK:C	26:B:97:UNK:N	2.55	0.65
31:G:26:UNK:O	31:G:29:UNK:N	2.30	0.65
34:J:4:UNK:O	34:J:8:UNK:N	2.30	0.65
51:Z:244:UNK:O	51:Z:248:UNK:N	2.29	0.65
30:F:121:UNK:HA	30:F:232:UNK:CB	2.26	0.65
31:G:155:UNK:C	31:G:156:CYS:O	2.41	0.65
31:G:615:UNK:O	31:G:618:UNK:N	2.30	0.65
33:I:21:UNK:O	33:I:25:UNK:N	2.29	0.65
36:L:579:UNK:CB	36:L:581:UNK:CB	2.74	0.65
23:9:45:LEU:HD21	24:0:40:TYR:HA	1.78	0.65
43:S:84:UNK:HA	43:S:87:UNK:CB	2.27	0.65
30:F:166:UNK:O	30:F:167:UNK:C	2.45	0.65
37:M:432:UNK:O	37:M:435:UNK:CB	2.45	0.65
38:N:99:UNK:O	38:N:103:UNK:N	2.30	0.65
38:N:124:UNK:O	38:N:127:UNK:N	2.29	0.65
36:L:321:UNK:C	36:L:324:UNK:CB	2.73	0.65
37:M:180:UNK:O	37:M:181:UNK:C	2.44	0.65
37:M:375:UNK:O	37:M:379:UNK:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:U:411:UNK:O	50:U:414:UNK:N	2.30	0.65
27:C:133:UNK:O	27:C:136:UNK:N	2.30	0.64
31:G:241:UNK:O	31:G:248:UNK:CB	2.44	0.64
38:N:328:UNK:CB	50:U:209:UNK:HA	2.27	0.64
28:D:163:UNK:N	32:H:278:UNK:HA	2.12	0.64
40:P:147:UNK:O	40:P:151:UNK:N	2.29	0.64
47:X:306:UNK:O	47:X:307:UNK:C	2.44	0.64
27:C:68:UNK:O	27:C:69:UNK:CB	2.45	0.64
27:C:112:UNK:N	27:C:113:UNK:CB	2.61	0.64
28:D:347:UNK:O	28:D:351:UNK:N	2.31	0.64
31:G:55:CYS:O	31:G:56:UNK:C	2.45	0.64
31:G:543:UNK:O	31:G:558:UNK:O	2.16	0.64
33:I:26:UNK:O	33:I:28:UNK:N	2.29	0.64
36:L:116:UNK:O	36:L:117:UNK:C	2.45	0.64
37:M:271:UNK:O	37:M:274:UNK:N	2.30	0.64
37:M:342:UNK:O	37:M:343:UNK:CB	2.45	0.64
31:G:102:UNK:O	31:G:103:UNK:CB	2.43	0.64
37:M:382:UNK:O	37:M:385:UNK:N	2.30	0.64
47:X:321:UNK:O	47:X:323:UNK:N	2.30	0.64
36:L:420:UNK:O	36:L:424:UNK:N	2.31	0.64
41:Q:42:UNK:O	41:Q:45:UNK:N	2.30	0.64
26:B:56:UNK:O	26:B:59:UNK:N	2.31	0.64
30:F:39:UNK:O	30:F:40:UNK:CB	2.45	0.64
30:F:103:UNK:CB	30:F:104:UNK:HA	2.27	0.64
36:L:326:UNK:O	36:L:330:UNK:N	2.29	0.64
47:X:157:UNK:O	47:X:160:UNK:N	2.30	0.64
30:F:188:UNK:O	30:F:192:UNK:N	2.31	0.64
30:F:289:UNK:HA	30:F:291:UNK:N	2.11	0.64
36:L:375:UNK:O	36:L:376:UNK:C	2.43	0.64
37:M:60:UNK:O	37:M:62:UNK:O	2.15	0.64
38:N:157:UNK:O	38:N:161:UNK:CB	2.46	0.64
51:Z:604:UNK:O	51:Z:608:UNK:N	2.31	0.64
28:D:382:UNK:C	28:D:384:UNK:HA	2.28	0.64
34:J:85:UNK:O	34:J:88:UNK:CB	2.46	0.64
37:M:32:UNK:O	37:M:34:UNK:N	2.30	0.64
29:E:151:UNK:HA	29:E:152:UNK:C	2.28	0.64
36:L:571:UNK:O	36:L:574:UNK:N	2.31	0.64
40:P:167:UNK:O	40:P:230:UNK:N	2.31	0.64
32:H:40:UNK:O	32:H:47:UNK:N	2.31	0.63
36:L:210:UNK:O	36:L:211:UNK:C	2.45	0.63
47:X:156:UNK:O	47:X:159:UNK:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:M:281:UNK:O	37:M:284:UNK:CA	2.46	0.63
40:P:134:UNK:C	40:P:136:UNK:H2	2.11	0.63
51:Z:10:UNK:O	51:Z:14:UNK:N	2.32	0.63
19:5:39:CYS:HG	19:5:53:CYS:HG	0.67	0.63
26:B:71:UNK:C	32:H:37:UNK:CB	2.77	0.63
29:E:124:UNK:O	29:E:125:UNK:CB	2.46	0.63
30:F:370:UNK:O	30:F:371:UNK:C	2.45	0.63
37:M:68:UNK:O	37:M:70:UNK:N	2.32	0.63
31:G:332:UNK:O	31:G:336:UNK:CB	2.46	0.63
35:K:14:UNK:CB	35:K:36:UNK:CB	2.76	0.63
36:L:376:UNK:O	36:L:377:UNK:C	2.46	0.63
39:O:87:UNK:N	39:O:88:UNK:CB	2.62	0.63
28:D:99:UNK:O	28:D:100:UNK:C	2.44	0.63
30:F:434:UNK:O	30:F:437:UNK:N	2.32	0.63
31:G:330:UNK:CB	31:G:600:UNK:CB	2.77	0.63
36:L:209:UNK:O	36:L:212:UNK:CA	2.46	0.63
37:M:123:UNK:O	37:M:126:UNK:N	2.31	0.63
37:M:441:UNK:O	37:M:445:UNK:N	2.32	0.63
40:P:167:UNK:CB	40:P:229:UNK:HA	2.29	0.63
33:I:99:UNK:HA	33:I:104:UNK:HA	1.79	0.63
38:N:77:UNK:O	38:N:78:UNK:C	2.44	0.63
33:I:126:CYS:HA	59:I:202:SF4:S3	2.39	0.62
33:I:151:UNK:O	33:I:154:UNK:CA	2.47	0.62
39:O:160:UNK:O	39:O:163:UNK:N	2.32	0.62
26:B:163:UNK:O	26:B:164:UNK:C	2.47	0.62
30:F:288:UNK:O	30:F:289:UNK:CB	2.45	0.62
30:F:434:UNK:O	30:F:438:UNK:N	2.32	0.62
40:P:64:UNK:N	40:P:65:UNK:HA	2.14	0.62
28:D:360:UNK:CB	28:D:381:UNK:CA	2.77	0.62
30:F:428:UNK:O	30:F:431:UNK:CB	2.47	0.62
38:N:262:UNK:O	38:N:265:UNK:N	2.32	0.62
40:P:53:UNK:HA	40:P:57:UNK:CB	2.28	0.62
19:5:57:ARG:HB3	19:5:57:ARG:HH11	1.64	0.62
25:A:52:UNK:O	25:A:56:UNK:N	2.31	0.62
26:B:118:UNK:CB	59:B:201:SF4:S3	2.88	0.62
27:C:112:UNK:N	27:C:113:UNK:CA	2.62	0.62
29:E:60:UNK:CB	29:E:94:UNK:HA	2.30	0.62
48:Y:92:UNK:O	48:Y:95:UNK:CB	2.48	0.62
51:Z:362:UNK:CB	51:Z:366:UNK:CB	2.77	0.62
31:G:464:UNK:O	31:G:467:UNK:N	2.33	0.62
40:P:113:UNK:O	40:P:117:UNK:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:U:509:UNK:O	50:U:512:UNK:N	2.32	0.62
28:D:80:UNK:O	28:D:81:UNK:CB	2.47	0.62
30:F:116:UNK:O	30:F:119:UNK:N	2.31	0.62
28:D:126:UNK:O	28:D:127:UNK:CB	2.45	0.62
31:G:624:UNK:O	31:G:627:UNK:N	2.32	0.62
40:P:103:UNK:HA	40:P:106:UNK:CB	2.29	0.62
40:P:135:UNK:O	40:P:136:UNK:C	2.48	0.62
43:S:84:UNK:O	43:S:87:UNK:CB	2.47	0.62
15:1:16:TYR:CE1	15:1:25:PRO:HG3	2.34	0.62
30:F:44:UNK:O	30:F:47:UNK:CB	2.48	0.62
30:F:103:UNK:HA	30:F:104:UNK:C	2.30	0.62
30:F:325:UNK:O	30:F:326:UNK:CB	2.45	0.62
17:3:13:ALA:O	17:3:18:ARG:HD2	2.00	0.61
30:F:294:UNK:CB	30:F:295:UNK:HA	2.30	0.61
31:G:296:UNK:O	31:G:300:UNK:CB	2.48	0.61
31:G:367:UNK:O	31:G:370:UNK:CA	2.47	0.61
33:I:87:CYS:SG	33:I:90:UNK:N	2.73	0.61
36:L:376:UNK:O	36:L:378:UNK:N	2.33	0.61
46:W:1:UNK:O	46:W:2:UNK:CB	2.46	0.61
30:F:60:UNK:O	30:F:63:UNK:CA	2.48	0.61
25:A:103:UNK:O	25:A:106:UNK:N	2.33	0.61
32:H:154:UNK:O	32:H:157:UNK:O	2.18	0.61
37:M:26:UNK:O	37:M:27:UNK:C	2.47	0.61
38:N:100:UNK:HA	38:N:103:UNK:CB	2.30	0.61
40:P:155:UNK:O	40:P:158:UNK:CB	2.48	0.61
26:B:89:UNK:O	26:B:90:UNK:CB	2.47	0.61
27:C:23:UNK:O	27:C:26:UNK:N	2.33	0.61
27:C:27:UNK:O	27:C:30:UNK:N	2.34	0.61
28:D:70:UNK:O	28:D:71:UNK:C	2.48	0.61
30:F:166:UNK:O	30:F:168:UNK:N	2.33	0.61
30:F:262:UNK:HA	30:F:286:UNK:CB	2.31	0.61
30:F:44:UNK:O	30:F:48:UNK:N	2.34	0.61
30:F:370:UNK:O	30:F:373:UNK:N	2.32	0.61
31:G:331:UNK:O	31:G:335:UNK:N	2.33	0.61
36:L:383:UNK:O	36:L:389:UNK:CB	2.48	0.61
27:C:79:UNK:O	27:C:93:UNK:N	2.33	0.61
30:F:428:UNK:O	30:F:431:UNK:N	2.33	0.61
47:X:203:UNK:O	47:X:205:UNK:N	2.32	0.61
27:C:44:UNK:O	27:C:47:UNK:N	2.33	0.61
30:F:272:UNK:O	30:F:273:UNK:CB	2.49	0.61
32:H:128:UNK:O	32:H:132:UNK:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:M:168:UNK:CB	37:M:174:UNK:HA	2.30	0.61
47:X:503:UNK:O	47:X:506:UNK:N	2.33	0.61
36:L:546:UNK:O	36:L:549:UNK:N	2.34	0.61
51:Z:252:UNK:O	51:Z:255:UNK:N	2.34	0.61
28:D:211:UNK:O	28:D:214:UNK:N	2.34	0.61
31:G:104:UNK:O	31:G:106:UNK:N	2.33	0.61
31:G:565:UNK:O	31:G:566:UNK:C	2.48	0.61
47:X:423:UNK:O	47:X:426:UNK:CB	2.49	0.61
16:2:82:TYR:HB3	16:2:83:PRO:HD3	1.81	0.61
26:B:119:CYS:SG	59:B:201:SF4:FE1	1.90	0.61
39:O:225:UNK:C	39:O:227:UNK:O	2.49	0.61
47:X:108:UNK:O	47:X:111:UNK:CB	2.49	0.61
51:Z:119:UNK:O	51:Z:122:UNK:O	2.19	0.61
28:D:360:UNK:HA	28:D:381:UNK:HA	1.81	0.60
39:O:229:UNK:C	39:O:231:UNK:N	2.55	0.60
24:0:13:LYS:H	24:0:13:LYS:HD3	1.65	0.60
28:D:383:UNK:CB	28:D:385:UNK:C	2.79	0.60
37:M:113:UNK:HA	37:M:114:UNK:C	2.31	0.60
51:Z:225:UNK:O	51:Z:226:UNK:C	2.45	0.60
51:Z:221:UNK:O	51:Z:222:UNK:CB	2.48	0.60
31:G:425:UNK:O	31:G:428:UNK:CB	2.49	0.60
17:3:62:CYS:SG	17:3:84:SER:OG	2.60	0.60
42:R:77:UNK:C	42:R:78:UNK:O	2.45	0.60
31:G:333:UNK:O	31:G:337:UNK:N	2.33	0.60
36:L:321:UNK:C	36:L:324:UNK:N	2.64	0.60
36:L:502:UNK:O	36:L:506:UNK:N	2.35	0.60
26:B:67:UNK:N	26:B:68:UNK:HA	2.17	0.60
27:C:138:UNK:O	27:C:139:UNK:CB	2.50	0.60
43:S:83:UNK:O	43:S:86:UNK:CB	2.50	0.60
45:V:52:UNK:O	45:V:53:UNK:CB	2.50	0.60
27:C:56:UNK:O	27:C:57:UNK:C	2.49	0.60
28:D:165:UNK:O	28:D:166:UNK:CB	2.49	0.60
36:L:128:UNK:O	36:L:131:UNK:N	2.35	0.60
37:M:68:UNK:O	37:M:71:UNK:N	2.34	0.60
51:Z:209:UNK:O	51:Z:212:UNK:N	2.35	0.60
37:M:137:UNK:O	37:M:138:UNK:CB	2.50	0.60
23:9:46:LYS:O	23:9:47:LYS:HB2	2.02	0.60
30:F:129:UNK:O	30:F:130:UNK:CB	2.48	0.60
31:G:119:UNK:O	31:G:120:UNK:C	2.48	0.60
33:I:99:UNK:O	33:I:104:UNK:CB	2.50	0.60
38:N:144:UNK:O	38:N:145:UNK:C	2.46	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:298:UNK:O	38:N:300:UNK:N	2.35	0.60
43:S:84:UNK:O	43:S:87:UNK:CA	2.50	0.60
26:B:121:UNK:HA	26:B:135:UNK:HA	1.82	0.59
26:B:166:UNK:O	26:B:169:UNK:O	2.19	0.59
27:C:80:UNK:HA	27:C:91:UNK:O	2.01	0.59
31:G:186:UNK:HA	31:G:187:UNK:C	2.31	0.59
37:M:324:UNK:O	37:M:328:UNK:CB	2.50	0.59
31:G:383:UNK:O	31:G:387:UNK:CB	2.49	0.59
36:L:211:UNK:O	36:L:214:UNK:CB	2.50	0.59
39:O:25:UNK:O	39:O:123:UNK:HA	2.02	0.59
40:P:143:UNK:C	40:P:145:UNK:N	2.65	0.59
41:Q:32:UNK:CB	41:Q:59:UNK:C	2.80	0.59
47:X:172:UNK:O	47:X:176:UNK:CB	2.51	0.59
50:U:623:UNK:O	50:U:626:UNK:CB	2.50	0.59
37:M:356:UNK:O	37:M:360:UNK:N	2.35	0.59
26:B:122:UNK:CA	26:B:123:UNK:CB	2.80	0.59
50:U:823:UNK:O	50:U:826:UNK:CB	2.51	0.59
51:Z:309:UNK:O	51:Z:312:UNK:CB	2.51	0.59
30:F:212:UNK:C	30:F:220:UNK:H	2.16	0.59
31:G:33:UNK:O	31:G:34:UNK:CB	2.50	0.59
50:U:122:UNK:O	50:U:123:UNK:C	2.47	0.59
30:F:352:UNK:HA	30:F:355:UNK:CB	2.33	0.59
32:H:79:UNK:O	32:H:81:UNK:N	2.36	0.59
47:X:720:UNK:O	47:X:724:UNK:N	2.35	0.59
30:F:163:UNK:H	30:F:166:UNK:CB	2.16	0.59
36:L:576:UNK:CB	38:N:167:UNK:CB	2.80	0.59
38:N:45:UNK:O	38:N:47:UNK:N	2.35	0.59
36:L:547:UNK:O	36:L:550:UNK:N	2.35	0.59
37:M:42:UNK:O	37:M:44:UNK:N	2.36	0.59
42:R:64:UNK:O	42:R:65:UNK:C	2.51	0.59
19:5:57:ARG:HG3	19:5:60:TYR:CE2	2.38	0.59
37:M:80:UNK:O	37:M:81:UNK:C	2.48	0.59
36:L:316:UNK:O	36:L:319:UNK:CB	2.51	0.58
38:N:91:UNK:H	38:N:92:UNK:C	2.16	0.58
43:S:63:UNK:O	43:S:78:UNK:CA	2.49	0.58
30:F:212:UNK:HA	30:F:220:UNK:C	2.33	0.58
31:G:377:UNK:N	31:G:449:UNK:CA	2.53	0.58
38:N:143:UNK:O	38:N:145:UNK:O	2.21	0.58
39:O:26:UNK:HA	39:O:124:UNK:O	2.03	0.58
50:U:714:UNK:O	50:U:717:UNK:CB	2.51	0.58
22:8:43:SER:OG	22:8:45:VAL:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:28:LEU:HB2	24:0:29:PRO:HD3	1.83	0.58
27:C:83:UNK:C	27:C:85:UNK:N	2.64	0.58
31:G:114:CYS:O	31:G:118:UNK:CB	2.52	0.58
34:J:101:UNK:O	34:J:104:UNK:CA	2.51	0.58
37:M:340:UNK:O	37:M:342:UNK:N	2.36	0.58
47:X:309:UNK:O	47:X:312:UNK:N	2.36	0.58
29:E:96:UNK:C	29:E:98:UNK:O	2.52	0.58
31:G:379:UNK:O	31:G:452:UNK:N	2.37	0.58
38:N:276:UNK:O	38:N:279:UNK:CB	2.51	0.58
51:Z:205:UNK:O	51:Z:206:UNK:C	2.48	0.58
31:G:439:UNK:O	31:G:443:UNK:N	2.37	0.58
36:L:38:UNK:O	36:L:41:UNK:N	2.37	0.58
38:N:59:UNK:O	38:N:62:UNK:N	2.37	0.58
39:O:119:UNK:C	39:O:121:UNK:H	2.16	0.58
44:T:55:UNK:CA	44:T:60:UNK:O	2.51	0.58
30:F:60:UNK:O	30:F:63:UNK:C	2.52	0.58
30:F:352:UNK:O	30:F:355:UNK:CA	2.51	0.58
30:F:387:UNK:O	30:F:390:UNK:N	2.37	0.58
32:H:136:UNK:O	32:H:137:UNK:C	2.50	0.58
51:Z:243:UNK:C	51:Z:245:UNK:N	2.59	0.58
51:Z:323:UNK:CB	51:Z:324:UNK:CA	2.81	0.58
26:B:77:UNK:CB	26:B:78:UNK:C	2.82	0.58
31:G:210:UNK:O	31:G:211:UNK:C	2.52	0.58
47:X:302:UNK:O	47:X:303:UNK:C	2.52	0.58
51:Z:322:UNK:O	51:Z:323:UNK:CB	2.52	0.58
26:B:71:UNK:CB	32:H:37:UNK:CB	2.82	0.58
26:B:166:UNK:O	26:B:169:UNK:C	2.52	0.58
29:E:97:UNK:N	29:E:136:UNK:O	2.37	0.58
33:I:159:UNK:O	33:I:162:UNK:CB	2.52	0.58
36:L:604:UNK:CB	38:N:93:UNK:N	2.67	0.58
37:M:75:UNK:O	37:M:78:UNK:N	2.37	0.58
38:N:32:UNK:O	38:N:35:UNK:CB	2.51	0.58
51:Z:209:UNK:O	51:Z:212:UNK:CB	2.52	0.58
26:B:54:CYS:O	26:B:57:UNK:N	2.37	0.58
30:F:183:UNK:O	30:F:186:UNK:N	2.37	0.58
30:F:209:UNK:CA	30:F:210:UNK:C	2.82	0.58
31:G:180:UNK:O	31:G:181:UNK:C	2.47	0.58
40:P:103:UNK:O	40:P:106:UNK:CA	2.51	0.58
50:U:624:UNK:O	50:U:627:UNK:CB	2.52	0.58
37:M:108:UNK:CA	37:M:111:UNK:CB	2.80	0.57
28:D:163:UNK:HA	32:H:278:UNK:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:269:UNK:CB	28:D:368:UNK:CB	2.82	0.57
30:F:435:UNK:O	30:F:439:UNK:N	2.36	0.57
31:G:594:UNK:CB	31:G:595:UNK:C	2.82	0.57
38:N:85:UNK:O	38:N:86:UNK:CB	2.51	0.57
40:P:170:UNK:CB	40:P:203:UNK:O	2.52	0.57
30:F:371:UNK:O	30:F:375:UNK:CB	2.52	0.57
36:L:419:UNK:O	36:L:422:UNK:N	2.37	0.57
37:M:31:UNK:O	37:M:32:UNK:O	2.23	0.57
39:O:43:UNK:O	39:O:46:UNK:N	2.38	0.57
40:P:25:UNK:CB	40:P:95:UNK:CB	2.82	0.57
40:P:147:UNK:O	40:P:150:UNK:CB	2.52	0.57
42:R:63:UNK:O	42:R:64:UNK:O	2.22	0.57
31:G:604:UNK:O	31:G:608:UNK:CA	2.51	0.57
33:I:69:UNK:CB	33:I:74:UNK:O	2.53	0.57
34:J:170:UNK:O	34:J:171:UNK:C	2.53	0.57
36:L:137:UNK:O	36:L:140:UNK:N	2.38	0.57
36:L:579:UNK:C	36:L:581:UNK:CB	2.83	0.57
37:M:94:UNK:O	37:M:95:UNK:C	2.48	0.57
40:P:103:UNK:O	40:P:104:UNK:C	2.52	0.57
40:P:136:UNK:HA	40:P:137:UNK:C	2.33	0.57
27:C:23:UNK:CA	27:C:26:UNK:CB	2.81	0.57
30:F:150:UNK:O	30:F:153:UNK:CB	2.52	0.57
31:G:333:UNK:O	31:G:337:UNK:CB	2.53	0.57
35:K:13:UNK:O	35:K:16:UNK:CB	2.52	0.57
40:P:133:UNK:CA	40:P:166:UNK:O	2.52	0.57
28:D:188:UNK:O	28:D:189:UNK:CB	2.52	0.57
31:G:318:UNK:HA	31:G:344:UNK:O	2.03	0.57
31:G:425:UNK:O	31:G:428:UNK:N	2.38	0.57
32:H:176:UNK:O	47:X:146:UNK:CB	2.53	0.57
36:L:368:UNK:O	36:L:372:UNK:N	2.37	0.57
36:L:382:UNK:CB	36:L:389:UNK:HA	2.34	0.57
40:P:111:UNK:HA	40:P:151:UNK:CB	2.35	0.57
50:U:817:UNK:O	50:U:821:UNK:N	2.38	0.57
19:5:71:THR:O	19:5:75:ARG:HD3	2.05	0.57
21:7:3:ASN:C	21:7:3:ASN:HD22	2.08	0.57
28:D:369:UNK:N	28:D:372:UNK:O	2.38	0.57
30:F:315:UNK:HA	30:F:316:UNK:O	2.04	0.57
31:G:11:UNK:CB	31:G:77:UNK:N	2.67	0.57
31:G:202:UNK:O	31:G:203:CYS:C	2.43	0.57
32:H:41:UNK:CB	32:H:44:UNK:CB	2.82	0.57
34:J:59:UNK:O	34:J:63:UNK:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:207:UNK:CA	36:L:208:UNK:C	2.82	0.57
37:M:180:UNK:C	37:M:182:UNK:N	2.65	0.57
45:V:30:UNK:O	45:V:33:UNK:N	2.38	0.57
36:L:21:UNK:O	36:L:22:UNK:C	2.52	0.57
47:X:320:UNK:O	47:X:321:UNK:CB	2.50	0.57
28:D:224:UNK:O	28:D:227:UNK:N	2.38	0.56
32:H:93:UNK:N	32:H:94:UNK:HA	2.20	0.56
33:I:81:UNK:N	59:I:202:SF4:S1	2.77	0.56
35:K:9:UNK:O	35:K:12:UNK:N	2.38	0.56
37:M:91:UNK:O	37:M:94:UNK:N	2.38	0.56
37:M:328:UNK:O	37:M:329:UNK:C	2.52	0.56
30:F:315:UNK:HA	30:F:316:UNK:CB	2.34	0.56
48:Y:25:UNK:O	48:Y:28:UNK:O	2.23	0.56
16:2:78:HIS:ND1	20:6:12:LEU:HD22	2.21	0.56
19:5:75:ARG:HG2	19:5:75:ARG:NH1	2.19	0.56
23:9:41:ARG:HG3	24:0:40:TYR:CE2	2.40	0.56
28:D:234:UNK:HA	28:D:237:UNK:CB	2.35	0.56
28:D:383:UNK:N	28:D:384:UNK:HA	2.21	0.56
28:D:394:UNK:O	28:D:398:UNK:N	2.38	0.56
30:F:275:UNK:CB	30:F:278:UNK:CB	2.83	0.56
32:H:79:UNK:O	32:H:82:UNK:N	2.38	0.56
35:K:50:UNK:O	35:K:51:UNK:C	2.52	0.56
36:L:546:UNK:O	36:L:547:UNK:C	2.52	0.56
37:M:410:UNK:O	37:M:414:UNK:N	2.38	0.56
38:N:122:UNK:O	38:N:124:UNK:HA	2.05	0.56
39:O:109:UNK:O	39:O:112:UNK:N	2.38	0.56
40:P:103:UNK:O	40:P:106:UNK:C	2.53	0.56
43:S:28:UNK:C	43:S:30:UNK:N	2.62	0.56
43:S:66:UNK:HA	43:S:75:UNK:O	2.04	0.56
47:X:72:UNK:O	47:X:73:UNK:CB	2.53	0.56
50:U:506:UNK:O	50:U:510:UNK:N	2.38	0.56
51:Z:349:UNK:O	51:Z:353:UNK:N	2.39	0.56
28:D:117:UNK:CB	28:D:367:UNK:CB	2.83	0.56
36:L:65:UNK:CB	36:L:66:UNK:CA	2.83	0.56
36:L:512:UNK:O	36:L:513:UNK:C	2.53	0.56
30:F:100:UNK:O	30:F:101:UNK:C	2.48	0.56
36:L:457:UNK:O	36:L:458:UNK:C	2.51	0.56
42:R:75:UNK:O	42:R:76:UNK:CB	2.53	0.56
25:A:65:UNK:O	25:A:66:UNK:C	2.52	0.56
28:D:402:UNK:O	28:D:406:UNK:N	2.38	0.56
37:M:121:UNK:O	37:M:124:UNK:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:169:UNK:CB	40:P:231:UNK:CB	2.83	0.56
28:D:163:UNK:CB	32:H:278:UNK:CB	2.83	0.56
28:D:357:UNK:CA	28:D:384:UNK:CB	2.84	0.56
30:F:69:UNK:O	30:F:70:UNK:CB	2.53	0.56
33:I:149:UNK:CA	33:I:150:UNK:CB	2.84	0.56
30:F:44:UNK:O	30:F:47:UNK:CA	2.54	0.56
30:F:214:UNK:HA	30:F:218:UNK:C	2.36	0.56
30:F:215:UNK:C	30:F:217:UNK:N	2.63	0.56
30:F:303:UNK:HA	30:F:414:UNK:CB	2.36	0.56
36:L:156:UNK:O	36:L:157:UNK:CB	2.54	0.56
37:M:42:UNK:O	37:M:43:UNK:C	2.53	0.56
43:S:62:UNK:O	43:S:78:UNK:CB	2.54	0.56
51:Z:310:UNK:O	51:Z:313:UNK:CB	2.54	0.56
34:J:101:UNK:O	34:J:104:UNK:CB	2.54	0.56
36:L:366:UNK:O	36:L:369:UNK:N	2.39	0.56
37:M:176:UNK:CB	37:M:179:UNK:N	2.69	0.56
38:N:26:UNK:CB	38:N:27:UNK:CB	2.84	0.56
26:B:123:UNK:N	26:B:126:UNK:O	2.40	0.56
28:D:259:UNK:O	28:D:261:UNK:N	2.39	0.56
30:F:212:UNK:O	30:F:219:UNK:HA	2.05	0.56
31:G:273:UNK:O	31:G:276:UNK:N	2.39	0.56
38:N:55:UNK:CB	38:N:121:UNK:CB	2.84	0.56
38:N:158:UNK:O	38:N:161:UNK:CA	2.53	0.56
39:O:234:UNK:O	39:O:237:UNK:N	2.39	0.56
27:C:135:UNK:O	27:C:139:UNK:HA	2.06	0.55
31:G:456:UNK:CB	31:G:457:UNK:CA	2.83	0.55
36:L:510:UNK:O	36:L:513:UNK:CB	2.54	0.55
45:V:45:UNK:O	45:V:47:UNK:N	2.39	0.55
48:Y:56:UNK:C	48:Y:58:UNK:N	2.66	0.55
30:F:214:UNK:CB	30:F:218:UNK:HA	2.36	0.55
30:F:300:UNK:O	30:F:333:UNK:N	2.39	0.55
30:F:367:UNK:O	30:F:371:UNK:N	2.40	0.55
33:I:66:UNK:HA	33:I:158:UNK:CB	2.36	0.55
36:L:181:UNK:O	36:L:183:UNK:N	2.39	0.55
36:L:207:UNK:CB	36:L:208:UNK:C	2.84	0.55
38:N:253:UNK:HA	38:N:259:UNK:CB	2.36	0.55
39:O:84:UNK:O	39:O:85:UNK:C	2.53	0.55
50:U:710:UNK:O	50:U:713:UNK:N	2.39	0.55
31:G:527:UNK:HA	31:G:544:UNK:O	2.06	0.55
36:L:351:UNK:O	36:L:352:UNK:CB	2.53	0.55
38:N:108:UNK:O	38:N:111:UNK:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:293:UNK:C	38:N:295:UNK:N	2.63	0.55
40:P:82:UNK:O	40:P:86:UNK:N	2.39	0.55
30:F:322:UNK:CB	30:F:327:UNK:CB	2.85	0.55
30:F:433:UNK:O	30:F:436:UNK:N	2.40	0.55
33:I:80:CYS:N	59:I:202:SF4:S1	2.79	0.55
33:I:150:UNK:CB	33:I:154:UNK:CB	2.83	0.55
36:L:383:UNK:C	36:L:389:UNK:CB	2.84	0.55
38:N:32:UNK:O	38:N:35:UNK:N	2.40	0.55
40:P:160:UNK:N	40:P:161:UNK:C	2.70	0.55
25:A:72:UNK:O	25:A:75:UNK:N	2.40	0.55
29:E:154:UNK:N	29:E:161:UNK:O	2.39	0.55
30:F:52:UNK:O	30:F:55:UNK:CB	2.54	0.55
31:G:215:UNK:CB	33:I:99:UNK:CB	2.85	0.55
37:M:61:UNK:CA	37:M:62:UNK:C	2.85	0.55
37:M:188:UNK:CB	37:M:189:UNK:CB	2.84	0.55
51:Z:245:UNK:O	51:Z:249:UNK:N	2.38	0.55
26:B:118:UNK:C	26:B:120:UNK:N	2.69	0.55
28:D:137:UNK:O	28:D:140:UNK:N	2.39	0.55
30:F:260:UNK:CB	30:F:336:UNK:CB	2.85	0.55
32:H:173:UNK:O	32:H:174:UNK:C	2.54	0.55
36:L:61:UNK:CB	36:L:80:UNK:CB	2.85	0.55
36:L:593:UNK:O	36:L:594:UNK:C	2.52	0.55
37:M:209:UNK:O	37:M:211:UNK:O	2.25	0.55
37:M:227:UNK:CA	37:M:228:UNK:CB	2.85	0.55
38:N:107:UNK:CB	38:N:108:UNK:HA	2.35	0.55
50:U:622:UNK:O	50:U:623:UNK:C	2.54	0.55
15:1:108:PRO:HG2	15:1:111:PHE:CE2	2.42	0.55
20:6:63:MET:HB3	20:6:68:ILE:HD11	1.89	0.55
26:B:65:UNK:C	26:B:68:UNK:CB	2.85	0.55
29:E:96:UNK:N	29:E:138:UNK:CB	2.70	0.55
30:F:209:UNK:CB	30:F:210:UNK:C	2.85	0.55
30:F:351:UNK:O	30:F:352:UNK:C	2.54	0.55
31:G:9:UNK:N	31:G:20:UNK:O	2.40	0.55
33:I:63:UNK:CB	33:I:133:UNK:CB	2.84	0.55
36:L:77:UNK:CA	36:L:78:UNK:CB	2.84	0.55
37:M:94:UNK:O	37:M:97:UNK:N	2.40	0.55
42:R:68:UNK:CB	42:R:86:UNK:CB	2.84	0.55
43:S:64:UNK:HA	43:S:78:UNK:CA	2.37	0.55
51:Z:330:UNK:CB	51:Z:334:UNK:CB	2.85	0.55
31:G:200:UNK:CB	31:G:208:UNK:CB	2.85	0.55
36:L:488:UNK:O	36:L:489:UNK:C	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:5:LYS:HD2	18:4:6:GLY:N	2.21	0.55
29:E:46:UNK:O	29:E:47:UNK:C	2.55	0.55
30:F:31:UNK:N	30:F:35:UNK:CB	2.70	0.55
30:F:209:UNK:HA	30:F:210:UNK:C	2.36	0.55
32:H:42:UNK:C	32:H:44:UNK:HA	2.37	0.55
36:L:65:UNK:CB	36:L:66:UNK:C	2.83	0.55
36:L:242:UNK:O	36:L:245:UNK:N	2.39	0.55
37:M:372:UNK:CB	37:M:375:UNK:CB	2.85	0.55
38:N:70:UNK:O	38:N:71:UNK:C	2.52	0.55
30:F:31:UNK:H	30:F:35:UNK:CB	2.20	0.55
30:F:125:UNK:O	30:F:128:UNK:N	2.40	0.55
31:G:436:UNK:N	31:G:437:UNK:CA	2.62	0.55
32:H:159:UNK:CB	32:H:164:UNK:CB	2.85	0.55
38:N:107:UNK:CB	38:N:108:UNK:CA	2.85	0.55
40:P:138:UNK:CB	40:P:149:UNK:CB	2.85	0.55
40:P:233:UNK:CB	40:P:234:UNK:HA	2.37	0.55
44:T:55:UNK:HA	44:T:60:UNK:O	2.07	0.55
51:Z:250:UNK:O	51:Z:251:UNK:C	2.52	0.55
16:2:80:GLU:H	16:2:80:GLU:CD	2.10	0.54
28:D:360:UNK:CB	28:D:381:UNK:CB	2.85	0.54
32:H:92:UNK:C	32:H:94:UNK:CB	2.85	0.54
32:H:183:UNK:O	32:H:184:UNK:C	2.51	0.54
37:M:25:UNK:O	37:M:26:UNK:C	2.55	0.54
37:M:113:UNK:CA	37:M:114:UNK:C	2.85	0.54
37:M:133:UNK:CA	37:M:224:UNK:CB	2.85	0.54
40:P:20:UNK:CB	40:P:89:UNK:CB	2.85	0.54
43:S:48:UNK:CB	43:S:51:UNK:CB	2.85	0.54
28:D:186:UNK:CB	33:I:60:UNK:C	2.85	0.54
30:F:398:UNK:O	30:F:401:UNK:N	2.40	0.54
32:H:101:UNK:O	32:H:104:UNK:N	2.40	0.54
33:I:113:UNK:C	33:I:115:UNK:N	2.65	0.54
36:L:28:UNK:CB	36:L:31:UNK:CB	2.86	0.54
36:L:38:UNK:O	36:L:39:UNK:C	2.55	0.54
40:P:203:UNK:CA	40:P:234:UNK:C	2.85	0.54
40:P:215:UNK:O	40:P:219:UNK:N	2.40	0.54
40:P:301:UNK:CB	40:P:303:UNK:CB	2.86	0.54
51:Z:210:UNK:C	51:Z:212:UNK:N	2.66	0.54
26:B:47:UNK:CB	26:B:85:UNK:CB	2.85	0.54
29:E:60:UNK:CB	29:E:94:UNK:CA	2.85	0.54
30:F:195:UNK:O	30:F:198:UNK:N	2.40	0.54
30:F:397:UNK:O	30:F:401:UNK:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:137:UNK:CB	42:R:75:UNK:O	2.55	0.54
36:L:310:UNK:O	36:L:313:UNK:CB	2.55	0.54
36:L:448:UNK:CB	36:L:451:UNK:CB	2.85	0.54
36:L:531:UNK:O	36:L:532:UNK:C	2.53	0.54
37:M:176:UNK:O	47:X:418:UNK:CB	2.55	0.54
37:M:279:UNK:CB	37:M:280:UNK:CA	2.85	0.54
40:P:140:UNK:N	40:P:141:UNK:HA	2.20	0.54
44:T:43:UNK:CB	44:T:46:UNK:CB	2.86	0.54
30:F:103:UNK:CB	30:F:104:UNK:CA	2.85	0.54
30:F:301:UNK:CB	30:F:331:UNK:CB	2.85	0.54
32:H:40:UNK:CB	32:H:47:UNK:CB	2.86	0.54
32:H:143:UNK:C	32:H:145:UNK:N	2.66	0.54
36:L:197:UNK:CB	36:L:200:UNK:CB	2.85	0.54
38:N:24:UNK:C	38:N:28:UNK:CB	2.86	0.54
40:P:137:UNK:CB	40:P:138:UNK:CA	2.84	0.54
26:B:78:UNK:N	26:B:79:UNK:CA	2.70	0.54
28:D:178:UNK:O	28:D:182:UNK:N	2.41	0.54
28:D:395:UNK:CB	28:D:428:UNK:CB	2.85	0.54
31:G:210:UNK:CB	31:G:213:UNK:CB	2.85	0.54
31:G:464:UNK:O	31:G:467:UNK:CB	2.56	0.54
36:L:176:UNK:O	36:L:179:UNK:CB	2.56	0.54
38:N:24:UNK:CB	38:N:28:UNK:CB	2.86	0.54
38:N:91:UNK:CB	38:N:92:UNK:CB	2.85	0.54
38:N:134:UNK:O	38:N:137:UNK:CB	2.56	0.54
39:O:43:UNK:C	39:O:45:UNK:N	2.65	0.54
39:O:102:UNK:O	39:O:106:UNK:CB	2.55	0.54
28:D:163:UNK:CB	32:H:278:UNK:CA	2.85	0.54
30:F:53:UNK:O	30:F:54:UNK:C	2.55	0.54
30:F:100:UNK:C	30:F:102:UNK:N	2.57	0.54
30:F:242:UNK:O	30:F:252:UNK:HA	2.07	0.54
31:G:375:UNK:CB	31:G:376:UNK:CA	2.85	0.54
31:G:456:UNK:CB	31:G:457:UNK:HA	2.37	0.54
36:L:188:UNK:CB	36:L:211:UNK:CB	2.84	0.54
36:L:376:UNK:C	36:L:378:UNK:N	2.68	0.54
38:N:25:UNK:C	38:N:27:UNK:C	2.85	0.54
38:N:253:UNK:CB	38:N:259:UNK:CB	2.85	0.54
41:Q:50:UNK:CB	41:Q:51:UNK:C	2.85	0.54
27:C:34:UNK:CB	27:C:38:UNK:CB	2.85	0.54
36:L:111:UNK:CB	36:L:114:UNK:CB	2.85	0.54
37:M:293:UNK:O	37:M:294:UNK:C	2.52	0.54
39:O:32:UNK:C	39:O:34:UNK:N	2.67	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:U:122:UNK:O	50:U:125:UNK:CB	2.55	0.54
36:L:55:UNK:CB	36:L:56:UNK:CB	2.86	0.54
50:U:416:UNK:C	50:U:418:UNK:N	2.67	0.54
50:U:601:UNK:O	50:U:602:UNK:C	2.56	0.54
51:Z:343:UNK:CB	51:Z:346:UNK:CB	2.85	0.54
30:F:294:UNK:CB	30:F:295:UNK:CA	2.85	0.54
37:M:343:UNK:C	37:M:345:UNK:N	2.70	0.54
38:N:135:UNK:O	38:N:138:UNK:N	2.41	0.54
39:O:103:UNK:O	39:O:107:UNK:CB	2.56	0.54
41:Q:113:UNK:O	41:Q:114:UNK:CB	2.55	0.54
48:Y:98:UNK:O	48:Y:101:UNK:N	2.41	0.54
26:B:78:UNK:CB	26:B:79:UNK:C	2.86	0.54
28:D:96:UNK:O	28:D:99:UNK:CB	2.55	0.54
32:H:93:UNK:CA	32:H:94:UNK:CB	2.86	0.54
34:J:86:UNK:O	34:J:89:UNK:N	2.41	0.54
36:L:587:UNK:O	36:L:591:UNK:N	2.41	0.54
40:P:94:UNK:O	40:P:95:UNK:CB	2.54	0.54
43:S:36:UNK:CB	43:S:84:UNK:CB	2.85	0.54
17:3:82:CYS:N	17:3:86:GLY:O	2.40	0.53
27:C:73:UNK:O	28:D:252:UNK:HA	2.07	0.53
31:G:285:UNK:CB	31:G:288:UNK:CB	2.86	0.53
34:J:13:UNK:CB	34:J:39:UNK:CB	2.87	0.53
36:L:127:UNK:O	36:L:131:UNK:N	2.41	0.53
37:M:241:UNK:O	37:M:243:UNK:N	2.40	0.53
38:N:66:UNK:O	38:N:67:UNK:C	2.55	0.53
38:N:72:UNK:O	38:N:76:UNK:N	2.41	0.53
38:N:292:UNK:O	38:N:295:UNK:CB	2.55	0.53
43:S:83:UNK:O	43:S:86:UNK:N	2.41	0.53
27:C:21:UNK:O	27:C:24:UNK:CA	2.56	0.53
30:F:183:UNK:CB	30:F:186:UNK:CB	2.86	0.53
31:G:108:CYS:SG	31:G:110:UNK:CB	2.96	0.53
31:G:570:UNK:HA	31:G:583:UNK:O	2.07	0.53
36:L:210:UNK:O	36:L:213:UNK:N	2.41	0.53
37:M:364:UNK:O	37:M:367:UNK:N	2.42	0.53
39:O:188:UNK:CB	39:O:191:UNK:CB	2.85	0.53
16:2:41:LEU:O	16:2:41:LEU:HD12	2.08	0.53
29:E:96:UNK:O	29:E:98:UNK:C	2.56	0.53
30:F:300:UNK:CB	30:F:329:UNK:CA	2.84	0.53
31:G:10:UNK:C	31:G:76:UNK:HA	2.28	0.53
33:I:135:UNK:O	33:I:136:UNK:C	2.56	0.53
36:L:117:UNK:O	36:L:118:UNK:C	2.53	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:M:364:UNK:O	37:M:367:UNK:CB	2.56	0.53
47:X:302:UNK:O	47:X:305:UNK:CB	2.57	0.53
50:U:411:UNK:C	50:U:413:UNK:N	2.69	0.53
15:1:67:SER:OG	15:1:70:GLU:HG3	2.08	0.53
36:L:31:UNK:O	36:L:35:UNK:N	2.41	0.53
47:X:334:UNK:C	47:X:336:UNK:N	2.68	0.53
50:U:317:UNK:O	50:U:321:UNK:N	2.42	0.53
15:1:128:VAL:O	15:1:134:PHE:HB3	2.09	0.53
17:3:51:SER:HB2	17:3:91:LEU:HD11	1.90	0.53
26:B:77:UNK:N	26:B:78:UNK:HA	2.23	0.53
27:C:113:UNK:C	27:C:115:UNK:N	2.66	0.53
30:F:426:UNK:C	30:F:429:UNK:N	2.72	0.53
31:G:235:UNK:O	31:G:236:UNK:CB	2.56	0.53
32:H:307:UNK:O	32:H:310:UNK:CB	2.56	0.53
33:I:63:UNK:CB	33:I:134:UNK:N	2.71	0.53
36:L:181:UNK:C	36:L:183:UNK:N	2.71	0.53
36:L:201:UNK:O	36:L:202:UNK:C	2.54	0.53
45:V:8:UNK:O	45:V:12:UNK:N	2.42	0.53
15:1:23:PRO:HD2	16:2:34:ASN:HD22	1.74	0.53
15:1:52:SER:OG	15:1:55:GLU:HG3	2.09	0.53
17:3:48:LEU:O	17:3:50:PRO:HD3	2.08	0.53
30:F:140:UNK:CB	30:F:182:UNK:CA	2.86	0.53
31:G:114:CYS:SG	31:G:117:UNK:CB	2.97	0.53
31:G:329:UNK:O	31:G:333:UNK:N	2.42	0.53
31:G:440:UNK:O	31:G:444:UNK:N	2.41	0.53
36:L:55:UNK:N	36:L:56:UNK:C	2.71	0.53
39:O:102:UNK:O	39:O:106:UNK:N	2.41	0.53
40:P:203:UNK:N	40:P:234:UNK:O	2.41	0.53
47:X:187:UNK:O	47:X:190:UNK:CB	2.56	0.53
50:U:211:UNK:O	50:U:214:UNK:N	2.41	0.53
18:4:2:SER:OG	18:4:3:ALA:N	2.41	0.53
18:4:8:HIS:O	18:4:10:GLY:N	2.42	0.53
28:D:383:UNK:N	28:D:384:UNK:CA	2.72	0.53
30:F:60:UNK:O	30:F:63:UNK:N	2.41	0.53
37:M:391:UNK:O	37:M:392:UNK:CB	2.56	0.53
40:P:49:UNK:N	40:P:73:UNK:CB	2.71	0.53
29:E:154:UNK:O	29:E:161:UNK:N	2.42	0.53
30:F:94:UNK:CB	30:F:135:UNK:O	2.57	0.53
30:F:433:UNK:O	30:F:434:UNK:C	2.55	0.53
40:P:95:UNK:O	40:P:96:UNK:CB	2.57	0.53
40:P:203:UNK:HA	40:P:234:UNK:C	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Z:337:UNK:HA	51:Z:342:UNK:CB	2.39	0.53
26:B:95:UNK:O	26:B:96:UNK:C	2.57	0.53
28:D:163:UNK:N	32:H:278:UNK:CB	2.72	0.53
29:E:109:UNK:O	29:E:112:UNK:N	2.42	0.53
30:F:209:UNK:CB	30:F:211:UNK:HA	2.39	0.53
31:G:31:UNK:O	31:G:34:UNK:N	2.42	0.53
37:M:3:UNK:H	37:M:6:UNK:CB	2.22	0.53
40:P:143:UNK:O	40:P:145:UNK:N	2.42	0.53
40:P:216:UNK:O	40:P:220:UNK:N	2.42	0.53
44:T:70:UNK:HA	44:T:75:UNK:CB	2.39	0.53
46:W:56:UNK:O	46:W:59:UNK:CB	2.56	0.53
48:Y:59:UNK:O	48:Y:60:UNK:C	2.56	0.53
17:3:55:LYS:HA	17:3:74:LEU:O	2.08	0.53
27:C:133:UNK:CA	27:C:136:UNK:CB	2.82	0.53
28:D:95:UNK:N	28:D:98:UNK:CB	2.72	0.53
28:D:360:UNK:CA	28:D:381:UNK:HA	2.39	0.53
47:X:414:UNK:O	47:X:418:UNK:N	2.41	0.53
51:Z:101:UNK:N	51:Z:104:UNK:CB	2.72	0.53
18:4:42:ARG:HH11	18:4:42:ARG:HG3	1.74	0.52
27:C:88:UNK:HA	27:C:112:UNK:HA	1.91	0.52
31:G:110:UNK:O	31:G:113:UNK:O	2.26	0.52
33:I:110:UNK:HA	33:I:150:UNK:O	2.10	0.52
34:J:21:UNK:O	34:J:22:UNK:C	2.55	0.52
34:J:59:UNK:HA	34:J:63:UNK:CB	2.39	0.52
36:L:67:UNK:CB	36:L:75:UNK:O	2.57	0.52
37:M:114:UNK:N	37:M:177:UNK:CB	2.72	0.52
37:M:325:UNK:O	37:M:329:UNK:N	2.41	0.52
38:N:26:UNK:CA	38:N:27:UNK:CB	2.87	0.52
43:S:34:UNK:O	43:S:38:UNK:N	2.42	0.52
46:W:49:UNK:CA	46:W:52:UNK:CB	2.81	0.52
30:F:262:UNK:CB	30:F:285:UNK:C	2.87	0.52
33:I:151:UNK:C	33:I:153:UNK:N	2.68	0.52
36:L:207:UNK:CB	36:L:209:UNK:N	2.72	0.52
37:M:362:UNK:O	37:M:365:UNK:N	2.42	0.52
38:N:293:UNK:O	38:N:295:UNK:N	2.41	0.52
40:P:140:UNK:N	40:P:141:UNK:CA	2.72	0.52
51:Z:244:UNK:O	51:Z:245:UNK:C	2.55	0.52
31:G:282:UNK:O	31:G:293:UNK:HA	2.09	0.52
32:H:101:UNK:N	32:H:161:UNK:CB	2.72	0.52
36:L:383:UNK:N	36:L:389:UNK:CB	2.72	0.52
37:M:378:UNK:C	37:M:380:UNK:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:91:UNK:N	38:N:92:UNK:CB	2.73	0.52
15:1:40:LEU:HD13	15:1:59:LEU:HD13	1.90	0.52
25:A:90:UNK:O	25:A:93:UNK:CB	2.58	0.52
26:B:54:CYS:C	26:B:56:UNK:N	2.61	0.52
28:D:163:UNK:N	32:H:278:UNK:CA	2.72	0.52
28:D:258:UNK:N	28:D:261:UNK:CB	2.72	0.52
30:F:290:UNK:O	30:F:291:UNK:CB	2.57	0.52
30:F:421:UNK:N	30:F:424:UNK:CB	2.73	0.52
37:M:190:UNK:N	37:M:191:UNK:C	2.73	0.52
37:M:309:UNK:O	37:M:312:UNK:N	2.43	0.52
47:X:503:UNK:O	47:X:504:UNK:C	2.56	0.52
47:X:721:UNK:O	47:X:725:UNK:N	2.43	0.52
51:Z:111:UNK:O	51:Z:114:UNK:CB	2.57	0.52
30:F:300:UNK:CB	30:F:330:UNK:N	2.73	0.52
34:J:147:UNK:C	34:J:149:UNK:N	2.71	0.52
36:L:69:UNK:CB	36:L:74:UNK:HA	2.39	0.52
36:L:161:UNK:CB	36:L:162:UNK:HA	2.40	0.52
36:L:241:UNK:O	36:L:244:UNK:CB	2.57	0.52
36:L:279:UNK:O	36:L:282:UNK:N	2.43	0.52
39:O:141:UNK:O	39:O:142:UNK:CB	2.58	0.52
40:P:223:UNK:N	40:P:224:UNK:CB	2.73	0.52
30:F:276:UNK:O	30:F:280:UNK:N	2.43	0.52
33:I:21:UNK:O	33:I:24:UNK:CB	2.58	0.52
33:I:21:UNK:HA	33:I:24:UNK:CB	2.40	0.52
36:L:82:UNK:N	36:L:86:UNK:CB	2.73	0.52
37:M:393:UNK:O	37:M:394:UNK:C	2.57	0.52
38:N:26:UNK:N	38:N:27:UNK:C	2.73	0.52
38:N:276:UNK:O	38:N:277:UNK:C	2.57	0.52
31:G:227:UNK:O	31:G:238:UNK:CA	2.58	0.52
31:G:282:UNK:N	31:G:293:UNK:CB	2.73	0.52
37:M:115:UNK:N	37:M:175:UNK:CB	2.73	0.52
38:N:26:UNK:N	38:N:27:UNK:CB	2.73	0.52
40:P:114:UNK:O	40:P:118:UNK:N	2.43	0.52
40:P:134:UNK:O	40:P:167:UNK:CA	2.57	0.52
28:D:229:UNK:HA	28:D:232:UNK:CB	2.40	0.52
30:F:257:UNK:O	30:F:333:UNK:HA	2.09	0.52
31:G:448:UNK:O	31:G:449:UNK:CB	2.58	0.52
32:H:190:UNK:O	32:H:194:UNK:CB	2.57	0.52
37:M:392:UNK:C	37:M:394:UNK:N	2.68	0.52
41:Q:50:UNK:N	41:Q:51:UNK:HA	2.25	0.52
28:D:307:UNK:O	28:D:308:UNK:C	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:46:UNK:O	29:E:50:UNK:N	2.43	0.52
30:F:121:UNK:CB	30:F:232:UNK:CB	2.88	0.52
30:F:300:UNK:N	30:F:329:UNK:HA	2.25	0.52
38:N:25:UNK:C	38:N:28:UNK:N	2.72	0.52
40:P:203:UNK:C	40:P:233:UNK:CB	2.88	0.52
47:X:353:UNK:O	47:X:354:UNK:C	2.58	0.52
16:2:63:SER:O	16:2:67:ILE:HG13	2.10	0.52
28:D:211:UNK:O	28:D:214:UNK:CB	2.58	0.52
33:I:119:CYS:O	33:I:120:UNK:CB	2.58	0.52
36:L:580:UNK:N	36:L:581:UNK:CB	2.73	0.52
37:M:22:UNK:HA	37:M:23:UNK:CB	2.40	0.52
37:M:61:UNK:N	37:M:62:UNK:C	2.73	0.52
37:M:62:UNK:CB	37:M:64:UNK:N	2.73	0.52
37:M:68:UNK:C	37:M:70:UNK:N	2.66	0.52
40:P:117:UNK:O	40:P:120:UNK:N	2.43	0.52
47:X:88:UNK:O	47:X:91:UNK:CB	2.58	0.52
28:D:162:UNK:CB	32:H:279:UNK:N	2.73	0.51
28:D:174:UNK:O	28:D:175:UNK:C	2.57	0.51
28:D:259:UNK:C	28:D:261:UNK:N	2.71	0.51
30:F:322:UNK:CA	30:F:327:UNK:CB	2.87	0.51
36:L:207:UNK:CB	36:L:209:UNK:CA	2.89	0.51
15:1:40:LEU:HD22	15:1:59:LEU:HD13	1.92	0.51
31:G:565:UNK:O	31:G:567:UNK:N	2.43	0.51
36:L:47:UNK:O	36:L:48:UNK:C	2.53	0.51
36:L:524:UNK:HA	36:L:527:UNK:CB	2.40	0.51
36:L:602:UNK:C	36:L:604:UNK:N	2.72	0.51
43:S:25:UNK:N	43:S:57:UNK:CA	2.73	0.51
47:X:605:UNK:O	47:X:608:UNK:N	2.43	0.51
51:Z:225:UNK:O	51:Z:228:UNK:N	2.43	0.51
51:Z:310:UNK:O	51:Z:313:UNK:N	2.43	0.51
28:D:163:UNK:CB	32:H:278:UNK:HA	2.41	0.51
29:E:113:UNK:O	29:E:114:UNK:C	2.57	0.51
32:H:93:UNK:N	32:H:94:UNK:CA	2.73	0.51
33:I:111:UNK:C	33:I:113:UNK:N	2.72	0.51
35:K:42:UNK:O	35:K:45:UNK:CB	2.58	0.51
37:M:227:UNK:N	37:M:228:UNK:CB	2.72	0.51
38:N:163:UNK:O	38:N:166:UNK:CB	2.58	0.51
39:O:33:UNK:CB	39:O:36:UNK:CB	2.89	0.51
39:O:43:UNK:O	39:O:45:UNK:N	2.43	0.51
44:T:63:UNK:O	44:T:66:UNK:N	2.43	0.51
47:X:333:UNK:O	47:X:336:UNK:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:94:UNK:O	36:L:95:UNK:C	2.56	0.51
38:N:224:UNK:N	38:N:225:UNK:CA	2.73	0.51
17:3:8:THR:OG1	17:3:11:GLU:HG2	2.09	0.51
28:D:195:UNK:O	28:D:198:UNK:O	2.28	0.51
30:F:103:UNK:CA	30:F:104:UNK:C	2.89	0.51
36:L:47:UNK:C	36:L:49:UNK:N	2.71	0.51
36:L:60:UNK:O	36:L:81:UNK:N	2.43	0.51
37:M:347:UNK:HA	37:M:415:UNK:HA	1.92	0.51
40:P:170:UNK:O	40:P:172:UNK:N	2.43	0.51
44:T:62:UNK:C	44:T:63:UNK:O	2.56	0.51
28:D:108:UNK:O	28:D:109:UNK:C	2.58	0.51
30:F:102:UNK:O	30:F:103:UNK:CB	2.58	0.51
31:G:594:UNK:CA	31:G:595:UNK:C	2.87	0.51
34:J:90:UNK:O	34:J:93:UNK:N	2.44	0.51
36:L:190:UNK:HA	36:L:194:UNK:CA	2.40	0.51
36:L:321:UNK:O	36:L:324:UNK:C	2.58	0.51
37:M:341:UNK:O	37:M:342:UNK:C	2.56	0.51
37:M:348:UNK:N	37:M:415:UNK:CB	2.74	0.51
38:N:33:UNK:C	38:N:35:UNK:N	2.67	0.51
40:P:135:UNK:HA	40:P:167:UNK:C	2.41	0.51
40:P:139:UNK:CB	40:P:140:UNK:C	2.88	0.51
50:U:623:UNK:O	50:U:626:UNK:N	2.44	0.51
26:B:129:UNK:O	26:B:131:UNK:N	2.43	0.51
32:H:93:UNK:HA	32:H:94:UNK:CB	2.40	0.51
33:I:100:UNK:CB	33:I:103:UNK:N	2.74	0.51
36:L:70:UNK:O	36:L:73:UNK:O	2.28	0.51
37:M:241:UNK:C	37:M:243:UNK:N	2.71	0.51
44:T:40:UNK:O	44:T:41:UNK:CB	2.58	0.51
47:X:703:UNK:O	47:X:705:UNK:N	2.43	0.51
29:E:112:UNK:C	29:E:114:UNK:N	2.72	0.51
36:L:556:UNK:O	36:L:560:UNK:N	2.43	0.51
38:N:145:UNK:CB	38:N:147:UNK:CB	2.88	0.51
38:N:234:UNK:O	38:N:237:UNK:O	2.28	0.51
40:P:248:UNK:CB	40:P:317:UNK:CB	2.89	0.51
48:Y:94:UNK:O	48:Y:97:UNK:N	2.43	0.51
51:Z:253:UNK:O	51:Z:254:UNK:C	2.59	0.51
29:E:62:UNK:O	29:E:63:UNK:C	2.58	0.51
30:F:370:UNK:C	30:F:372:UNK:N	2.74	0.51
36:L:246:UNK:O	36:L:250:UNK:N	2.44	0.51
37:M:139:UNK:HA	37:M:140:UNK:CB	2.39	0.51
40:P:203:UNK:CA	40:P:233:UNK:CB	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:183:UNK:O	47:X:184:UNK:C	2.54	0.51
47:X:702:UNK:O	47:X:705:UNK:CB	2.59	0.51
48:Y:29:UNK:O	48:Y:30:UNK:CB	2.58	0.51
26:B:129:UNK:C	26:B:131:UNK:N	2.73	0.51
28:D:357:UNK:N	28:D:384:UNK:CB	2.74	0.51
31:G:227:UNK:O	31:G:238:UNK:CB	2.59	0.51
34:J:26:UNK:O	34:J:27:UNK:CB	2.59	0.51
37:M:341:UNK:C	37:M:342:UNK:O	2.56	0.51
39:O:125:UNK:O	39:O:126:UNK:CB	2.59	0.51
40:P:49:UNK:O	40:P:73:UNK:N	2.44	0.51
40:P:155:UNK:O	40:P:158:UNK:N	2.44	0.51
40:P:203:UNK:N	40:P:234:UNK:C	2.73	0.51
45:V:1:UNK:C	45:V:3:UNK:N	2.67	0.51
45:V:23:UNK:O	45:V:24:UNK:CB	2.58	0.51
45:V:55:UNK:C	45:V:57:UNK:N	2.74	0.51
28:D:101:UNK:O	28:D:103:UNK:N	2.42	0.50
31:G:573:UNK:O	31:G:580:UNK:HA	2.11	0.50
36:L:263:UNK:O	36:L:264:UNK:C	2.59	0.50
27:C:23:UNK:O	27:C:27:UNK:N	2.44	0.50
29:E:112:UNK:O	29:E:113:UNK:C	2.57	0.50
30:F:419:UNK:CA	30:F:423:UNK:CB	2.84	0.50
39:O:33:UNK:O	39:O:36:UNK:N	2.44	0.50
40:P:25:UNK:CB	40:P:95:UNK:CA	2.89	0.50
40:P:170:UNK:O	40:P:205:UNK:CA	2.59	0.50
32:H:110:UNK:O	32:H:113:UNK:N	2.44	0.50
32:H:284:UNK:O	32:H:288:UNK:N	2.45	0.50
35:K:9:UNK:O	35:K:12:UNK:CB	2.60	0.50
37:M:63:UNK:O	37:M:67:UNK:N	2.44	0.50
39:O:129:UNK:O	39:O:132:UNK:N	2.44	0.50
47:X:69:UNK:O	47:X:70:UNK:C	2.59	0.50
47:X:526:UNK:O	47:X:527:UNK:C	2.57	0.50
26:B:71:UNK:O	32:H:37:UNK:CB	2.60	0.50
30:F:234:UNK:O	30:F:237:UNK:O	2.30	0.50
32:H:79:UNK:C	32:H:81:UNK:N	2.73	0.50
36:L:257:UNK:O	36:L:261:UNK:N	2.43	0.50
36:L:547:UNK:O	36:L:550:UNK:CB	2.60	0.50
38:N:297:UNK:C	38:N:299:UNK:N	2.72	0.50
40:P:203:UNK:H2	40:P:234:UNK:C	2.23	0.50
43:S:63:UNK:O	43:S:78:UNK:CB	2.58	0.50
47:X:714:UNK:O	47:X:717:UNK:CB	2.59	0.50
51:Z:13:UNK:O	51:Z:16:UNK:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Z:30:UNK:C	51:Z:32:UNK:N	2.73	0.50
17:3:37:LYS:HD3	17:3:37:LYS:N	2.27	0.50
37:M:256:UNK:O	37:M:257:UNK:C	2.56	0.50
38:N:184:UNK:O	38:N:188:UNK:N	2.44	0.50
51:Z:110:UNK:O	51:Z:111:UNK:C	2.59	0.50
15:1:64:PHE:CE1	16:2:66:ARG:HD2	2.47	0.50
18:4:5:LYS:HD2	18:4:5:LYS:C	2.32	0.50
28:D:270:UNK:O	28:D:274:UNK:HA	2.11	0.50
33:I:120:UNK:N	59:I:201:SF4:S4	2.85	0.50
37:M:106:UNK:O	37:M:109:UNK:N	2.45	0.50
38:N:194:UNK:O	38:N:195:UNK:C	2.58	0.50
26:B:119:CYS:HG	59:B:201:SF4:FE1	1.29	0.50
26:B:129:UNK:CB	27:C:167:UNK:O	2.59	0.50
28:D:86:UNK:O	28:D:87:UNK:C	2.59	0.50
30:F:91:UNK:HA	30:F:219:UNK:O	2.12	0.50
36:L:241:UNK:O	36:L:244:UNK:N	2.45	0.50
37:M:23:UNK:C	37:M:25:UNK:N	2.73	0.50
37:M:27:UNK:O	37:M:28:UNK:C	2.58	0.50
26:B:150:UNK:HA	59:B:201:SF4:S1	2.51	0.50
30:F:95:UNK:O	30:F:96:UNK:C	2.57	0.50
38:N:26:UNK:N	38:N:27:UNK:CA	2.74	0.50
18:4:44:ARG:HD2	18:4:74:ARG:O	2.12	0.50
29:E:111:UNK:C	29:E:113:UNK:N	2.72	0.50
31:G:469:UNK:HA	31:G:472:UNK:CB	2.42	0.50
34:J:50:UNK:O	34:J:54:UNK:CB	2.60	0.50
36:L:105:UNK:O	36:L:109:UNK:N	2.45	0.50
47:X:411:UNK:O	47:X:414:UNK:CB	2.60	0.50
51:Z:252:UNK:O	51:Z:255:UNK:CB	2.60	0.50
26:B:121:UNK:CA	26:B:135:UNK:CB	2.85	0.49
33:I:20:UNK:O	33:I:24:UNK:N	2.45	0.49
36:L:137:UNK:O	36:L:140:UNK:CB	2.60	0.49
36:L:288:UNK:CB	36:L:308:UNK:CA	2.89	0.49
37:M:189:UNK:N	37:M:191:UNK:C	2.75	0.49
37:M:227:UNK:CB	37:M:228:UNK:CB	2.90	0.49
38:N:123:UNK:CA	38:N:124:UNK:CB	2.90	0.49
40:P:53:UNK:C	40:P:57:UNK:CB	2.89	0.49
48:Y:103:UNK:O	48:Y:106:UNK:CA	2.60	0.49
51:Z:205:UNK:O	51:Z:208:UNK:CB	2.60	0.49
31:G:104:UNK:O	31:G:105:CYS:C	2.49	0.49
50:U:109:UNK:O	50:U:112:UNK:N	2.46	0.49
28:D:257:UNK:O	28:D:259:UNK:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:126:UNK:O	29:E:127:UNK:C	2.55	0.49
30:F:92:UNK:N	30:F:219:UNK:O	2.45	0.49
30:F:365:CYS:O	30:F:368:UNK:N	2.45	0.49
31:G:28:UNK:O	31:G:29:UNK:C	2.60	0.49
32:H:143:UNK:O	32:H:145:UNK:N	2.46	0.49
33:I:98:UNK:C	33:I:103:UNK:O	2.60	0.49
37:M:396:UNK:O	37:M:399:UNK:N	2.45	0.49
38:N:169:UNK:CB	38:N:292:UNK:CB	2.90	0.49
39:O:119:UNK:C	39:O:121:UNK:N	2.73	0.49
25:A:91:UNK:O	25:A:92:UNK:C	2.61	0.49
26:B:166:UNK:O	26:B:167:UNK:C	2.60	0.49
30:F:352:UNK:O	30:F:356:UNK:N	2.45	0.49
31:G:236:UNK:CB	31:G:259:UNK:CB	2.90	0.49
31:G:611:UNK:O	31:G:612:UNK:CB	2.60	0.49
33:I:49:UNK:O	33:I:53:UNK:N	2.45	0.49
47:X:179:UNK:O	47:X:180:UNK:C	2.56	0.49
18:4:42:ARG:HD2	18:4:42:ARG:O	2.12	0.49
33:I:85:UNK:C	33:I:87:CYS:H	2.24	0.49
47:X:714:UNK:O	47:X:718:UNK:N	2.45	0.49
51:Z:107:UNK:O	51:Z:108:UNK:C	2.60	0.49
31:G:193:UNK:CA	31:G:196:UNK:CB	2.85	0.49
32:H:39:UNK:C	32:H:41:UNK:N	2.72	0.49
36:L:161:UNK:HA	36:L:163:UNK:CA	2.37	0.49
36:L:163:UNK:C	36:L:165:UNK:N	2.69	0.49
36:L:239:UNK:C	36:L:240:UNK:O	2.60	0.49
36:L:602:UNK:O	36:L:604:UNK:N	2.45	0.49
39:O:191:UNK:O	39:O:192:UNK:C	2.60	0.49
40:P:82:UNK:O	40:P:83:UNK:C	2.60	0.49
47:X:187:UNK:O	47:X:188:UNK:C	2.60	0.49
30:F:194:UNK:O	30:F:198:UNK:N	2.45	0.49
30:F:423:UNK:O	30:F:426:UNK:N	2.46	0.49
31:G:301:UNK:O	31:G:304:UNK:CB	2.61	0.49
36:L:580:UNK:CB	36:L:581:UNK:HA	2.43	0.49
38:N:61:UNK:O	38:N:62:UNK:C	2.60	0.49
40:P:204:UNK:N	40:P:233:UNK:CB	2.75	0.49
31:G:570:UNK:O	31:G:571:UNK:CB	2.61	0.49
37:M:384:UNK:C	37:M:386:UNK:N	2.72	0.49
27:C:117:UNK:O	27:C:142:UNK:HA	2.13	0.49
29:E:109:UNK:C	29:E:111:UNK:N	2.73	0.49
30:F:300:UNK:CA	30:F:329:UNK:CA	2.90	0.49
31:G:425:UNK:O	31:G:429:UNK:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:H:257:UNK:O	32:H:261:UNK:N	2.46	0.49
36:L:281:UNK:CB	36:L:315:UNK:CA	2.91	0.49
47:X:46:UNK:C	47:X:48:UNK:N	2.72	0.49
27:C:31:UNK:C	27:C:33:UNK:N	2.75	0.49
30:F:191:UNK:O	30:F:195:UNK:N	2.46	0.49
47:X:41:UNK:O	47:X:44:UNK:N	2.46	0.49
17:3:49:VAL:HG21	17:3:74:LEU:HD12	1.95	0.48
19:5:24:ASN:ND2	19:5:26:THR:H	2.11	0.48
27:C:112:UNK:N	27:C:113:UNK:HA	2.27	0.48
28:D:116:UNK:O	28:D:120:UNK:N	2.46	0.48
31:G:75:UNK:C	31:G:77:UNK:N	2.73	0.48
31:G:173:UNK:O	31:G:183:UNK:O	2.30	0.48
35:K:40:UNK:O	35:K:43:UNK:CB	2.61	0.48
38:N:267:UNK:O	38:N:271:UNK:N	2.45	0.48
47:X:40:UNK:O	47:X:44:UNK:N	2.46	0.48
18:4:42:ARG:NH1	18:4:74:ARG:HH21	2.10	0.48
27:C:56:UNK:O	27:C:58:UNK:N	2.47	0.48
29:E:62:UNK:O	29:E:65:UNK:N	2.46	0.48
30:F:150:UNK:O	30:F:153:UNK:N	2.47	0.48
31:G:30:UNK:O	31:G:33:UNK:CB	2.61	0.48
35:K:11:UNK:O	35:K:12:UNK:C	2.61	0.48
36:L:161:UNK:CB	36:L:162:UNK:CA	2.90	0.48
36:L:306:UNK:O	36:L:307:UNK:C	2.60	0.48
37:M:275:UNK:C	37:M:278:UNK:CB	2.91	0.48
40:P:203:UNK:CA	40:P:234:UNK:CA	2.86	0.48
41:Q:115:UNK:O	41:Q:116:UNK:C	2.61	0.48
27:C:28:UNK:O	27:C:31:UNK:N	2.46	0.48
28:D:183:UNK:HA	33:I:58:UNK:CB	2.43	0.48
32:H:241:UNK:O	32:H:242:UNK:CB	2.61	0.48
46:W:24:UNK:O	46:W:25:UNK:CB	2.56	0.48
47:X:90:UNK:C	47:X:92:UNK:N	2.76	0.48
29:E:33:UNK:O	29:E:36:UNK:N	2.47	0.48
30:F:45:UNK:O	30:F:48:UNK:CB	2.61	0.48
30:F:315:UNK:HA	30:F:316:UNK:C	2.42	0.48
38:N:201:UNK:O	38:N:202:UNK:C	2.57	0.48
28:D:84:UNK:O	28:D:85:UNK:CB	2.62	0.48
28:D:234:UNK:O	28:D:237:UNK:CA	2.61	0.48
30:F:190:UNK:CB	30:F:203:UNK:CA	2.83	0.48
30:F:262:UNK:CA	30:F:286:UNK:N	2.76	0.48
30:F:412:UNK:O	30:F:415:UNK:CB	2.61	0.48
30:F:426:UNK:C	30:F:428:UNK:N	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:49:UNK:C	31:G:51:UNK:N	2.76	0.48
40:P:145:UNK:O	40:P:149:UNK:N	2.47	0.48
50:U:415:UNK:O	50:U:418:UNK:CB	2.60	0.48
20:6:39:VAL:O	20:6:42:LYS:HE2	2.14	0.48
30:F:431:UNK:O	30:F:434:UNK:CB	2.60	0.48
36:L:297:UNK:CA	36:L:356:UNK:N	2.73	0.48
37:M:287:UNK:O	37:M:288:UNK:C	2.57	0.48
38:N:16:UNK:O	38:N:19:UNK:N	2.45	0.48
38:N:137:UNK:O	38:N:138:UNK:C	2.56	0.48
39:O:229:UNK:CA	39:O:231:UNK:N	2.75	0.48
50:U:512:UNK:O	50:U:515:UNK:CB	2.62	0.48
18:4:5:LYS:NZ	18:4:5:LYS:HB3	2.27	0.48
19:5:39:CYS:HG	19:5:53:CYS:CB	2.11	0.48
25:A:90:UNK:O	25:A:93:UNK:N	2.47	0.48
27:C:28:UNK:O	27:C:31:UNK:CB	2.61	0.48
34:J:171:UNK:O	34:J:172:UNK:C	2.62	0.48
37:M:63:UNK:O	37:M:66:UNK:N	2.46	0.48
38:N:72:UNK:C	38:N:75:UNK:CB	2.92	0.48
38:N:168:UNK:O	38:N:169:UNK:C	2.61	0.48
40:P:206:UNK:O	40:P:209:UNK:N	2.47	0.48
47:X:72:UNK:CB	47:X:75:UNK:HA	2.43	0.48
28:D:310:UNK:O	28:D:314:UNK:N	2.46	0.48
31:G:285:UNK:HA	31:G:289:UNK:O	2.13	0.48
36:L:52:UNK:C	36:L:54:UNK:N	2.73	0.48
21:7:8:LYS:NZ	21:7:8:LYS:HB3	2.29	0.48
30:F:322:UNK:HA	30:F:327:UNK:CB	2.43	0.48
30:F:364:UNK:O	30:F:367:UNK:CB	2.62	0.48
36:L:571:UNK:C	36:L:573:UNK:N	2.76	0.48
38:N:223:UNK:CB	38:N:224:UNK:HA	2.43	0.48
26:B:150:UNK:CA	59:B:201:SF4:S1	3.02	0.48
32:H:195:UNK:HA	32:H:198:UNK:HA	1.96	0.48
37:M:386:UNK:HA	37:M:390:UNK:HA	1.96	0.48
38:N:133:UNK:O	38:N:136:UNK:CB	2.62	0.48
38:N:149:UNK:O	38:N:150:UNK:C	2.61	0.48
43:S:19:UNK:HA	43:S:66:UNK:O	2.13	0.48
36:L:48:UNK:O	36:L:52:UNK:N	2.46	0.47
36:L:111:UNK:O	36:L:114:UNK:N	2.47	0.47
36:L:604:UNK:CB	38:N:92:UNK:C	2.92	0.47
37:M:133:UNK:HA	37:M:224:UNK:CB	2.44	0.47
37:M:351:UNK:O	37:M:352:UNK:CB	2.62	0.47
38:N:157:UNK:O	38:N:158:UNK:C	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:255:UNK:HA	38:N:256:UNK:HA	1.66	0.47
50:U:318:UNK:O	50:U:322:UNK:N	2.47	0.47
26:B:115:UNK:CB	26:B:120:UNK:CB	2.91	0.47
26:B:119:CYS:SG	59:B:201:SF4:S4	3.09	0.47
28:D:367:UNK:O	28:D:373:UNK:HA	2.14	0.47
30:F:125:UNK:O	30:F:128:UNK:CB	2.62	0.47
31:G:87:UNK:O	31:G:90:UNK:N	2.48	0.47
40:P:135:UNK:CA	40:P:168:UNK:N	2.72	0.47
42:R:59:UNK:O	42:R:70:UNK:HA	2.13	0.47
26:B:123:UNK:N	26:B:126:UNK:C	2.72	0.47
35:K:41:UNK:O	35:K:42:UNK:C	2.58	0.47
36:L:339:UNK:O	36:L:342:UNK:N	2.47	0.47
37:M:133:UNK:C	37:M:224:UNK:CB	2.92	0.47
38:N:163:UNK:O	38:N:164:UNK:C	2.62	0.47
47:X:165:UNK:O	47:X:166:UNK:C	2.57	0.47
15:1:68:PHE:HA	15:1:71:MET:HG2	1.95	0.47
30:F:163:UNK:N	30:F:166:UNK:CB	2.77	0.47
34:J:22:UNK:C	34:J:24:UNK:N	2.77	0.47
29:E:77:UNK:O	29:E:81:UNK:N	2.48	0.47
30:F:433:UNK:O	30:F:436:UNK:CB	2.63	0.47
31:G:377:UNK:N	31:G:449:UNK:CB	2.77	0.47
31:G:382:UNK:CB	31:G:454:UNK:CA	2.90	0.47
38:N:134:UNK:O	38:N:137:UNK:N	2.47	0.47
47:X:516:UNK:O	47:X:520:UNK:N	2.47	0.47
15:1:33:LEU:HD13	15:1:41:LYS:HG3	1.97	0.47
30:F:209:UNK:CB	30:F:211:UNK:N	2.77	0.47
30:F:212:UNK:C	30:F:219:UNK:HA	2.44	0.47
32:H:126:UNK:O	32:H:130:UNK:CB	2.63	0.47
38:N:328:UNK:CB	50:U:209:UNK:CB	2.92	0.47
40:P:21:UNK:CB	40:P:45:UNK:CA	2.86	0.47
48:Y:62:UNK:O	48:Y:63:UNK:CB	2.63	0.47
21:7:16:ASN:H	21:7:16:ASN:ND2	2.12	0.47
27:C:67:UNK:O	27:C:68:UNK:C	2.59	0.47
31:G:305:UNK:O	31:G:308:UNK:CB	2.63	0.47
31:G:564:UNK:CB	31:G:568:UNK:CB	2.93	0.47
32:H:199:UNK:O	32:H:200:UNK:CB	2.63	0.47
33:I:119:CYS:N	59:I:201:SF4:S4	2.88	0.47
37:M:168:UNK:CB	37:M:174:UNK:CB	2.93	0.47
38:N:73:UNK:C	38:N:75:UNK:N	2.72	0.47
45:V:26:UNK:O	45:V:30:UNK:N	2.48	0.47
50:U:25:UNK:O	50:U:26:UNK:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:U:622:UNK:C	50:U:624:UNK:N	2.71	0.47
15:1:41:LYS:HD3	15:1:62:LEU:HD23	1.97	0.47
28:D:85:UNK:O	28:D:86:UNK:C	2.63	0.47
30:F:63:UNK:O	30:F:64:UNK:C	2.62	0.47
30:F:212:UNK:CA	30:F:220:UNK:H	2.28	0.47
33:I:99:UNK:C	33:I:104:UNK:CB	2.93	0.47
34:J:33:UNK:O	34:J:37:UNK:N	2.48	0.47
34:J:155:UNK:O	34:J:159:UNK:N	2.47	0.47
37:M:273:UNK:O	37:M:277:UNK:N	2.48	0.47
50:U:627:UNK:C	50:U:628:UNK:O	2.56	0.47
51:Z:511:UNK:C	51:Z:513:UNK:N	2.76	0.47
15:1:33:LEU:HD22	15:1:37:GLN:HB3	1.97	0.47
19:5:60:TYR:CD1	19:5:60:TYR:C	2.88	0.47
36:L:396:UNK:O	36:L:399:UNK:N	2.48	0.47
15:1:102:TYR:CD2	24:0:35:TYR:HE1	2.34	0.47
25:A:76:UNK:C	25:A:78:UNK:N	2.71	0.47
31:G:248:UNK:O	31:G:249:UNK:CB	2.63	0.47
37:M:49:UNK:CA	37:M:50:UNK:CB	2.84	0.47
37:M:106:UNK:HA	37:M:109:UNK:CB	2.45	0.47
37:M:131:UNK:O	37:M:132:UNK:C	2.63	0.47
42:R:50:UNK:O	42:R:91:UNK:HA	2.15	0.47
51:Z:210:UNK:O	51:Z:213:UNK:CB	2.63	0.47
15:1:108:PRO:HG2	15:1:111:PHE:CD2	2.50	0.46
17:3:31:TYR:HE1	17:3:98:HIS:HE1	1.62	0.46
28:D:89:UNK:O	28:D:92:UNK:N	2.48	0.46
28:D:234:UNK:O	28:D:235:UNK:C	2.63	0.46
28:D:328:UNK:O	28:D:329:UNK:C	2.58	0.46
30:F:423:UNK:C	30:F:425:UNK:N	2.72	0.46
31:G:455:UNK:O	31:G:456:UNK:CB	2.62	0.46
31:G:488:UNK:O	31:G:489:UNK:C	2.61	0.46
36:L:225:UNK:C	36:L:229:UNK:CB	2.93	0.46
37:M:157:UNK:O	37:M:160:UNK:N	2.48	0.46
37:M:188:UNK:CB	37:M:189:UNK:CA	2.93	0.46
39:O:25:UNK:O	39:O:124:UNK:N	2.48	0.46
39:O:114:UNK:O	39:O:117:UNK:O	2.33	0.46
43:S:24:UNK:C	43:S:57:UNK:CB	2.87	0.46
45:V:32:UNK:O	45:V:36:UNK:N	2.48	0.46
18:4:67:HIS:CD2	18:4:78:LEU:HD11	2.50	0.46
28:D:250:UNK:C	28:D:252:UNK:N	2.73	0.46
32:H:101:UNK:N	32:H:161:UNK:CA	2.73	0.46
34:J:45:UNK:O	34:J:46:UNK:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:147:UNK:O	34:J:148:UNK:C	2.57	0.46
36:L:95:UNK:O	36:L:98:UNK:N	2.48	0.46
37:M:133:UNK:CB	37:M:224:UNK:CB	2.92	0.46
37:M:273:UNK:O	37:M:276:UNK:N	2.48	0.46
43:S:64:UNK:HA	43:S:77:UNK:C	2.44	0.46
50:U:411:UNK:O	50:U:413:UNK:N	2.48	0.46
15:1:23:PRO:HB3	16:2:70:VAL:CG2	2.45	0.46
24:0:1:ILE:HG23	24:0:1:ILE:O	2.15	0.46
25:A:88:UNK:O	25:A:91:UNK:N	2.48	0.46
29:E:28:UNK:HA	29:E:31:UNK:CB	2.46	0.46
31:G:155:UNK:O	31:G:156:CYS:O	2.33	0.46
34:J:85:UNK:O	34:J:86:UNK:C	2.61	0.46
37:M:281:UNK:O	37:M:284:UNK:C	2.64	0.46
38:N:25:UNK:O	38:N:28:UNK:N	2.48	0.46
38:N:45:UNK:O	38:N:48:UNK:N	2.48	0.46
40:P:136:UNK:CA	40:P:137:UNK:C	2.93	0.46
40:P:301:UNK:CB	40:P:303:UNK:N	2.78	0.46
42:R:63:UNK:C	42:R:65:UNK:N	2.72	0.46
47:X:157:UNK:O	47:X:160:UNK:CB	2.64	0.46
27:C:89:UNK:CA	27:C:112:UNK:O	2.63	0.46
28:D:70:UNK:C	28:D:72:UNK:N	2.74	0.46
30:F:352:UNK:C	30:F:355:UNK:N	2.79	0.46
31:G:427:UNK:O	31:G:431:UNK:N	2.48	0.46
43:S:64:UNK:HA	43:S:78:UNK:CB	2.45	0.46
21:7:11:LEU:O	21:7:11:LEU:HD23	2.15	0.46
28:D:101:UNK:O	28:D:104:UNK:N	2.48	0.46
36:L:545:UNK:O	36:L:548:UNK:N	2.49	0.46
38:N:40:UNK:O	38:N:41:UNK:C	2.61	0.46
47:X:719:UNK:O	47:X:723:UNK:N	2.49	0.46
48:Y:43:UNK:O	48:Y:44:UNK:C	2.57	0.46
50:U:1:UNK:O	50:U:2:UNK:C	2.64	0.46
15:1:66:GLU:O	16:2:66:ARG:NH2	2.49	0.46
17:3:40:SER:OG	17:3:45:ASP:HB3	2.16	0.46
26:B:90:UNK:C	26:B:119:CYS:HB3	2.46	0.46
33:I:26:UNK:C	33:I:28:UNK:N	2.78	0.46
36:L:169:UNK:O	36:L:173:UNK:N	2.49	0.46
37:M:127:UNK:O	37:M:128:UNK:C	2.60	0.46
37:M:140:UNK:C	37:M:142:UNK:N	2.74	0.46
37:M:255:UNK:O	37:M:258:UNK:CB	2.63	0.46
38:N:72:UNK:HA	38:N:75:UNK:CB	2.46	0.46
45:V:56:UNK:O	45:V:60:UNK:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:423:UNK:O	47:X:426:UNK:N	2.49	0.46
51:Z:605:UNK:C	51:Z:607:UNK:N	2.78	0.46
17:3:31:TYR:HE1	17:3:98:HIS:CE1	2.34	0.46
25:A:103:UNK:C	25:A:106:UNK:N	2.79	0.46
32:H:125:UNK:O	32:H:129:UNK:CB	2.64	0.46
35:K:19:UNK:O	35:K:20:UNK:CB	2.61	0.46
36:L:108:UNK:O	36:L:111:UNK:N	2.49	0.46
36:L:316:UNK:O	36:L:319:UNK:CA	2.64	0.46
40:P:161:UNK:O	40:P:162:UNK:O	2.34	0.46
40:P:173:UNK:O	40:P:176:UNK:CB	2.63	0.46
26:B:147:UNK:O	26:B:151:UNK:CB	2.64	0.46
32:H:43:UNK:N	32:H:44:UNK:CA	2.70	0.46
36:L:128:UNK:O	36:L:129:UNK:C	2.61	0.46
36:L:314:UNK:O	36:L:317:UNK:N	2.49	0.46
37:M:432:UNK:O	37:M:435:UNK:N	2.49	0.46
40:P:233:UNK:N	40:P:234:UNK:HA	2.31	0.46
42:R:82:UNK:O	42:R:90:UNK:HA	2.16	0.46
47:X:93:UNK:HA	47:X:94:UNK:CB	2.46	0.46
47:X:111:UNK:O	47:X:112:UNK:C	2.63	0.46
48:Y:98:UNK:O	48:Y:99:UNK:C	2.64	0.46
22:8:9:PHE:HD1	22:8:10:HIS:HD2	1.64	0.46
26:B:149:CYS:CA	26:B:150:UNK:C	2.93	0.46
28:D:146:UNK:O	28:D:147:UNK:C	2.62	0.46
30:F:61:UNK:O	30:F:64:UNK:CB	2.64	0.46
31:G:260:UNK:C	31:G:262:UNK:N	2.78	0.46
34:J:56:UNK:O	34:J:60:UNK:CB	2.64	0.46
37:M:38:UNK:O	37:M:41:UNK:N	2.49	0.46
38:N:91:UNK:CA	38:N:92:UNK:CB	2.94	0.46
47:X:710:UNK:O	47:X:713:UNK:N	2.49	0.46
48:Y:69:UNK:CB	48:Y:98:UNK:CB	2.93	0.46
25:A:106:UNK:O	25:A:108:UNK:N	2.93	0.45
26:B:65:UNK:CA	26:B:68:UNK:CB	2.94	0.45
28:D:179:UNK:O	28:D:183:UNK:N	2.50	0.45
30:F:178:UNK:C	30:F:179:UNK:O	2.58	0.45
31:G:162:UNK:O	31:G:166:UNK:N	2.49	0.45
31:G:229:UNK:O	31:G:235:UNK:HA	2.16	0.45
36:L:61:UNK:CA	36:L:80:UNK:CB	2.93	0.45
36:L:544:UNK:O	36:L:545:UNK:C	2.61	0.45
37:M:113:UNK:CA	37:M:114:UNK:CB	2.89	0.45
40:P:139:UNK:CA	40:P:140:UNK:CB	2.88	0.45
41:Q:99:UNK:CA	41:Q:100:UNK:CB	2.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:309:UNK:O	47:X:310:UNK:C	2.62	0.45
50:U:320:UNK:O	50:U:324:UNK:CB	2.64	0.45
18:4:42:ARG:HG3	18:4:42:ARG:NH1	2.32	0.45
28:D:117:UNK:O	28:D:120:UNK:N	2.49	0.45
39:O:185:UNK:O	39:O:186:UNK:C	2.55	0.45
44:T:62:UNK:O	44:T:63:UNK:C	2.64	0.45
50:U:125:UNK:O	50:U:128:UNK:CB	2.64	0.45
18:4:44:ARG:HA	18:4:45:PRO:HD2	1.75	0.45
28:D:101:UNK:C	28:D:103:UNK:N	2.75	0.45
39:O:85:UNK:O	39:O:86:UNK:C	2.61	0.45
40:P:136:UNK:CA	40:P:137:UNK:CB	2.85	0.45
40:P:145:UNK:O	40:P:148:UNK:CA	2.64	0.45
40:P:145:UNK:O	40:P:148:UNK:N	2.49	0.45
43:S:64:UNK:N	43:S:78:UNK:CB	2.78	0.45
51:Z:205:UNK:O	51:Z:208:UNK:CA	2.65	0.45
28:D:300:UNK:O	28:D:301:UNK:C	2.63	0.45
30:F:351:UNK:O	30:F:354:UNK:CB	2.63	0.45
35:K:44:UNK:O	35:K:45:UNK:C	2.61	0.45
36:L:203:UNK:HA	36:L:204:UNK:HA	1.87	0.45
36:L:207:UNK:HA	36:L:208:UNK:C	2.45	0.45
37:M:87:UNK:HA	37:M:89:UNK:HA	1.98	0.45
37:M:225:UNK:CB	37:M:228:UNK:CB	2.95	0.45
37:M:448:UNK:O	37:M:449:UNK:C	2.61	0.45
38:N:135:UNK:C	38:N:137:UNK:N	2.78	0.45
39:O:138:UNK:O	39:O:141:UNK:N	2.49	0.45
48:Y:94:UNK:O	48:Y:97:UNK:CB	2.65	0.45
50:U:409:UNK:O	50:U:412:UNK:CB	2.64	0.45
16:2:70:VAL:HG12	16:2:71:VAL:N	2.31	0.45
17:3:98:HIS:ND1	17:3:98:HIS:N	2.64	0.45
28:D:109:UNK:O	28:D:111:UNK:N	2.50	0.45
31:G:601:UNK:O	31:G:602:UNK:C	2.63	0.45
34:J:44:UNK:CB	34:J:53:UNK:CB	2.94	0.45
36:L:316:UNK:O	36:L:317:UNK:C	2.63	0.45
37:M:42:UNK:C	37:M:44:UNK:N	2.76	0.45
37:M:327:UNK:O	37:M:330:UNK:N	2.49	0.45
43:S:84:UNK:O	43:S:85:UNK:C	2.64	0.45
47:X:94:UNK:O	47:X:95:UNK:C	2.64	0.45
31:G:491:UNK:C	31:G:493:UNK:N	2.78	0.45
34:J:72:UNK:HA	34:J:75:UNK:CB	2.46	0.45
36:L:151:UNK:O	36:L:155:UNK:CA	2.64	0.45
36:L:271:UNK:O	36:L:274:UNK:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:304:UNK:O	47:X:307:UNK:N	2.49	0.45
47:X:603:UNK:C	47:X:605:UNK:N	2.79	0.45
48:Y:81:UNK:O	48:Y:84:UNK:O	2.34	0.45
18:4:3:ALA:O	18:4:4:ALA:HB2	2.17	0.45
28:D:228:UNK:O	28:D:232:UNK:CB	2.65	0.45
43:S:64:UNK:CA	43:S:78:UNK:CB	2.94	0.45
51:Z:355:UNK:O	51:Z:358:UNK:O	2.34	0.45
21:7:2:GLU:CG	21:7:3:ASN:H	2.30	0.45
37:M:14:UNK:O	37:M:15:UNK:C	2.60	0.45
37:M:61:UNK:N	37:M:63:UNK:N	2.65	0.45
39:O:26:UNK:CB	39:O:124:UNK:O	2.65	0.45
47:X:188:UNK:O	47:X:191:UNK:CB	2.65	0.45
16:2:78:HIS:CE1	20:6:12:LEU:HD22	2.52	0.45
26:B:163:UNK:C	26:B:165:UNK:N	2.78	0.45
29:E:33:UNK:C	29:E:35:UNK:N	2.74	0.45
30:F:405:CYS:SG	30:F:406:UNK:CB	2.98	0.45
30:F:430:UNK:O	30:F:433:UNK:N	2.50	0.45
31:G:41:CYS:SG	31:G:49:UNK:O	2.74	0.45
31:G:621:UNK:O	31:G:622:UNK:C	2.64	0.45
36:L:545:UNK:C	36:L:547:UNK:N	2.74	0.45
37:M:114:UNK:CA	37:M:177:UNK:CB	2.95	0.45
40:P:180:UNK:O	40:P:181:UNK:C	2.65	0.45
30:F:247:UNK:O	30:F:250:UNK:O	2.35	0.45
37:M:347:UNK:C	37:M:351:UNK:CB	2.92	0.45
25:A:78:UNK:CB	34:J:146:UNK:O	2.65	0.44
25:A:106:UNK:O	25:A:107:UNK:C	2.63	0.44
28:D:296:UNK:O	28:D:299:UNK:CB	2.64	0.44
28:D:298:UNK:O	28:D:299:UNK:C	2.65	0.44
29:E:113:UNK:O	29:E:116:UNK:N	2.50	0.44
31:G:11:UNK:CB	31:G:76:UNK:C	2.95	0.44
31:G:311:UNK:O	31:G:314:UNK:N	2.50	0.44
37:M:52:UNK:HA	37:M:53:UNK:HA	1.71	0.44
43:S:63:UNK:CA	43:S:78:UNK:CB	2.94	0.44
50:U:326:UNK:O	50:U:329:UNK:N	2.50	0.44
27:C:133:UNK:O	27:C:136:UNK:CB	2.65	0.44
28:D:95:UNK:CB	28:D:98:UNK:CB	2.96	0.44
28:D:342:UNK:O	28:D:343:UNK:C	2.65	0.44
29:E:165:UNK:O	29:E:166:UNK:C	2.65	0.44
30:F:426:UNK:CA	30:F:429:UNK:CB	2.83	0.44
31:G:89:UNK:O	31:G:90:UNK:C	2.64	0.44
31:G:305:UNK:O	31:G:308:UNK:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:K:21:UNK:O	35:K:22:UNK:C	2.64	0.44
36:L:29:UNK:CA	36:L:32:UNK:CB	2.85	0.44
36:L:288:UNK:CB	36:L:308:UNK:HA	2.47	0.44
37:M:123:UNK:CB	38:N:255:UNK:CB	2.96	0.44
50:U:108:UNK:O	50:U:111:UNK:CB	2.66	0.44
21:7:3:ASN:ND2	21:7:5:VAL:HG13	2.33	0.44
27:C:120:UNK:O	27:C:121:UNK:C	2.64	0.44
29:E:107:UNK:O	29:E:110:UNK:N	2.50	0.44
30:F:275:UNK:O	30:F:279:UNK:N	2.50	0.44
31:G:175:UNK:CB	31:G:182:UNK:N	2.80	0.44
31:G:572:UNK:HA	31:G:581:UNK:O	2.17	0.44
36:L:155:UNK:O	36:L:239:UNK:CB	2.65	0.44
37:M:32:UNK:C	37:M:34:UNK:N	2.79	0.44
37:M:406:UNK:O	37:M:407:UNK:C	2.64	0.44
38:N:91:UNK:O	38:N:95:UNK:CB	2.65	0.44
38:N:146:UNK:N	38:N:147:UNK:CA	2.72	0.44
40:P:106:UNK:CA	40:P:109:UNK:CB	2.85	0.44
46:W:71:UNK:O	46:W:72:UNK:C	2.65	0.44
47:X:203:UNK:C	47:X:205:UNK:N	2.73	0.44
17:3:33:ILE:HG22	17:3:34:LEU:HD12	1.98	0.44
28:D:70:UNK:O	28:D:72:UNK:N	2.50	0.44
28:D:137:UNK:O	28:D:138:UNK:C	2.63	0.44
30:F:351:UNK:O	30:F:355:UNK:N	2.51	0.44
31:G:482:UNK:O	31:G:576:UNK:CB	2.66	0.44
32:H:298:UNK:O	32:H:302:UNK:N	2.50	0.44
33:I:50:UNK:HA	33:I:53:UNK:O	2.18	0.44
36:L:124:UNK:O	36:L:125:UNK:C	2.63	0.44
37:M:118:UNK:O	37:M:121:UNK:N	2.49	0.44
47:X:172:UNK:O	47:X:176:UNK:N	2.51	0.44
47:X:503:UNK:O	47:X:506:UNK:CB	2.65	0.44
50:U:102:UNK:O	50:U:103:UNK:C	2.59	0.44
50:U:714:UNK:O	50:U:717:UNK:N	2.50	0.44
27:C:21:UNK:O	27:C:22:UNK:C	2.66	0.44
28:D:383:UNK:CB	28:D:384:UNK:C	2.95	0.44
30:F:76:UNK:O	30:F:80:UNK:CB	2.66	0.44
30:F:300:UNK:CB	30:F:329:UNK:C	2.95	0.44
30:F:423:UNK:C	30:F:426:UNK:N	2.81	0.44
35:K:10:UNK:O	35:K:13:UNK:N	2.51	0.44
37:M:159:UNK:O	37:M:160:UNK:C	2.64	0.44
38:N:320:UNK:O	38:N:321:UNK:C	2.62	0.44
38:N:337:UNK:O	38:N:341:UNK:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:704:UNK:O	47:X:705:UNK:C	2.65	0.44
15:1:79:LYS:NZ	22:8:15:ASN:HD21	2.15	0.44
26:B:118:UNK:C	26:B:122:UNK:N	2.73	0.44
27:C:132:UNK:O	27:C:133:UNK:C	2.63	0.44
27:C:162:UNK:O	27:C:163:UNK:C	2.65	0.44
32:H:41:UNK:CB	32:H:44:UNK:C	2.96	0.44
33:I:112:UNK:O	33:I:115:UNK:CB	2.66	0.44
33:I:112:UNK:O	33:I:115:UNK:N	2.50	0.44
36:L:211:UNK:HA	36:L:214:UNK:CB	2.47	0.44
36:L:246:UNK:O	36:L:250:UNK:CA	2.65	0.44
36:L:541:UNK:O	36:L:545:UNK:N	2.50	0.44
37:M:30:UNK:O	37:M:33:UNK:N	2.50	0.44
37:M:91:UNK:O	37:M:94:UNK:CB	2.66	0.44
39:O:130:UNK:O	39:O:132:UNK:N	2.50	0.44
47:X:42:UNK:O	47:X:45:UNK:CB	2.66	0.44
20:6:61:GLU:OE1	20:6:64:ARG:NH1	2.51	0.44
27:C:23:UNK:O	27:C:26:UNK:CB	2.65	0.44
28:D:254:UNK:O	28:D:256:UNK:N	2.50	0.44
28:D:421:UNK:C	28:D:423:UNK:N	2.79	0.44
30:F:52:UNK:O	30:F:55:UNK:CA	2.66	0.44
31:G:30:UNK:O	31:G:34:UNK:N	2.51	0.44
47:X:421:UNK:O	47:X:422:UNK:C	2.61	0.44
15:1:40:LEU:HD22	15:1:59:LEU:CD1	2.47	0.44
21:7:36:MET:O	21:7:40:LEU:HG	2.18	0.44
31:G:567:UNK:O	31:G:586:UNK:CB	2.66	0.44
32:H:18:UNK:O	32:H:21:UNK:N	2.50	0.44
33:I:31:UNK:O	33:I:34:UNK:CB	2.66	0.44
36:L:165:UNK:HA	36:L:168:UNK:CB	2.47	0.44
39:O:105:UNK:O	39:O:108:UNK:N	2.50	0.44
40:P:64:UNK:CB	40:P:65:UNK:HA	2.46	0.44
47:X:46:UNK:O	47:X:49:UNK:N	2.51	0.44
51:Z:104:UNK:HA	51:Z:107:UNK:CB	2.47	0.44
16:2:76:GLY:HA3	16:2:77:PRO:HD2	1.85	0.44
21:7:30:ILE:HG13	21:7:31:LEU:N	2.32	0.44
26:B:162:UNK:O	26:B:165:UNK:CB	2.65	0.44
31:G:86:UNK:O	31:G:87:UNK:C	2.65	0.44
33:I:151:UNK:O	33:I:152:UNK:C	2.66	0.44
39:O:38:UNK:O	39:O:41:UNK:N	2.51	0.44
39:O:101:UNK:O	39:O:105:UNK:N	2.50	0.44
40:P:48:UNK:CB	40:P:73:UNK:CB	2.95	0.44
40:P:158:UNK:O	40:P:161:UNK:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S:84:UNK:C	43:S:87:UNK:N	2.80	0.44
47:X:306:UNK:C	47:X:308:UNK:N	2.79	0.44
50:U:512:UNK:O	50:U:515:UNK:N	2.51	0.44
50:U:622:UNK:O	50:U:624:UNK:N	2.51	0.44
51:Z:309:UNK:O	51:Z:312:UNK:N	2.50	0.44
23:9:35:ALA:HB3	23:9:36:PRO:HD3	1.99	0.43
30:F:315:UNK:CA	30:F:316:UNK:C	2.95	0.43
31:G:185:UNK:C	31:G:188:UNK:CB	2.96	0.43
32:H:283:UNK:O	32:H:287:UNK:N	2.51	0.43
40:P:129:UNK:O	40:P:163:UNK:CB	2.66	0.43
25:A:53:UNK:O	25:A:56:UNK:N	2.50	0.43
26:B:117:UNK:O	26:B:118:UNK:C	2.62	0.43
30:F:56:UNK:C	30:F:59:UNK:CB	2.96	0.43
30:F:433:UNK:O	30:F:437:UNK:N	2.51	0.43
32:H:110:UNK:C	32:H:112:UNK:N	2.78	0.43
33:I:76:UNK:O	33:I:77:CYS:C	2.54	0.43
36:L:343:UNK:O	36:L:347:UNK:N	2.51	0.43
27:C:22:UNK:O	27:C:26:UNK:CB	2.66	0.43
29:E:69:UNK:O	29:E:73:UNK:N	2.51	0.43
29:E:96:UNK:C	29:E:136:UNK:O	2.67	0.43
30:F:58:UNK:O	30:F:61:UNK:N	2.51	0.43
31:G:586:UNK:C	31:G:588:UNK:N	2.80	0.43
36:L:309:UNK:O	36:L:313:UNK:N	2.50	0.43
38:N:65:UNK:O	38:N:68:UNK:N	2.51	0.43
46:W:58:UNK:O	46:W:59:UNK:C	2.66	0.43
48:Y:103:UNK:O	48:Y:105:UNK:N	2.51	0.43
50:U:510:UNK:C	50:U:512:UNK:N	2.77	0.43
20:6:26:MET:N	20:6:26:MET:SD	2.91	0.43
27:C:110:UNK:O	27:C:111:UNK:C	2.65	0.43
30:F:115:UNK:O	30:F:116:UNK:C	2.67	0.43
30:F:150:UNK:O	30:F:153:UNK:CA	2.67	0.43
31:G:380:UNK:O	31:G:409:UNK:C	2.67	0.43
34:J:18:UNK:HA	34:J:21:UNK:CB	2.49	0.43
34:J:149:UNK:O	34:J:150:UNK:C	2.65	0.43
40:P:203:UNK:CB	40:P:234:UNK:HA	2.48	0.43
50:U:126:UNK:O	50:U:127:UNK:C	2.67	0.43
51:Z:335:UNK:CB	51:Z:339:UNK:N	2.82	0.43
15:1:37:GLN:O	15:1:41:LYS:HG2	2.18	0.43
23:9:22:LEU:HD23	23:9:22:LEU:HA	1.83	0.43
28:D:297:UNK:O	28:D:298:UNK:C	2.63	0.43
30:F:74:UNK:O	30:F:77:UNK:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:43:UNK:O	39:O:44:UNK:C	2.67	0.43
48:Y:14:UNK:CB	48:Y:44:UNK:O	2.66	0.43
50:U:625:UNK:O	50:U:628:UNK:CB	2.66	0.43
23:9:41:ARG:HD2	24:0:40:TYR:CZ	2.54	0.43
29:E:54:UNK:O	29:E:57:UNK:N	2.51	0.43
31:G:41:CYS:CA	54:G:803:FES:S2	3.01	0.43
31:G:187:UNK:N	31:G:188:UNK:CA	2.73	0.43
38:N:253:UNK:CA	38:N:259:UNK:CB	2.96	0.43
39:O:42:UNK:C	39:O:44:UNK:N	2.76	0.43
40:P:48:UNK:C	40:P:73:UNK:CB	2.97	0.43
47:X:331:UNK:O	47:X:332:UNK:C	2.65	0.43
51:Z:508:UNK:O	51:Z:509:UNK:C	2.64	0.43
26:B:55:CYS:SG	26:B:117:UNK:CB	3.06	0.43
29:E:96:UNK:CB	29:E:98:UNK:O	2.66	0.43
30:F:73:UNK:O	30:F:74:UNK:C	2.67	0.43
31:G:31:UNK:O	31:G:34:UNK:HA	2.18	0.43
31:G:259:UNK:C	31:G:260:UNK:O	2.58	0.43
31:G:558:UNK:O	31:G:559:UNK:CB	2.67	0.43
32:H:195:UNK:HA	32:H:198:UNK:CA	2.48	0.43
36:L:209:UNK:O	36:L:210:UNK:C	2.66	0.43
37:M:393:UNK:C	37:M:395:UNK:N	2.79	0.43
40:P:313:UNK:O	40:P:314:UNK:C	2.67	0.43
20:6:21:ILE:O	20:6:25:PHE:HD2	2.02	0.43
20:6:68:ILE:HG13	20:6:69:PHE:N	2.33	0.43
26:B:63:UNK:HA	26:B:69:UNK:CB	2.48	0.43
29:E:106:UNK:O	29:E:109:UNK:N	2.51	0.43
32:H:272:UNK:O	32:H:276:UNK:CB	2.67	0.43
36:L:63:UNK:CB	36:L:78:UNK:CB	2.97	0.43
36:L:379:UNK:O	36:L:388:UNK:CB	2.66	0.43
37:M:348:UNK:CA	37:M:351:UNK:CB	2.85	0.43
39:O:25:UNK:O	39:O:123:UNK:CA	2.66	0.43
41:Q:50:UNK:N	41:Q:51:UNK:CA	2.82	0.43
26:B:166:UNK:O	26:B:169:UNK:N	2.52	0.43
28:D:151:UNK:O	28:D:152:UNK:C	2.66	0.43
28:D:311:UNK:O	28:D:315:UNK:N	2.52	0.43
30:F:303:UNK:O	30:F:414:UNK:CA	2.67	0.43
37:M:62:UNK:CB	37:M:65:UNK:N	2.82	0.43
48:Y:18:UNK:CB	48:Y:44:UNK:CB	2.97	0.43
51:Z:30:UNK:O	51:Z:32:UNK:N	2.51	0.43
16:2:27:TRP:CH2	17:3:86:GLY:HA2	2.54	0.43
20:6:42:LYS:HE2	20:6:42:LYS:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:H:291:UNK:C	32:H:293:UNK:N	2.81	0.43
36:L:544:UNK:O	36:L:547:UNK:CB	2.67	0.43
39:O:209:UNK:O	39:O:210:UNK:C	2.66	0.43
40:P:71:UNK:O	40:P:73:UNK:N	2.50	0.43
40:P:134:UNK:C	40:P:136:UNK:N	2.74	0.43
43:S:83:UNK:O	43:S:86:UNK:CA	2.67	0.43
51:Z:311:UNK:O	51:Z:312:UNK:C	2.67	0.43
25:A:98:UNK:O	25:A:101:UNK:N	2.52	0.42
31:G:192:UNK:CA	31:G:193:UNK:CB	2.83	0.42
31:G:398:UNK:C	31:G:400:UNK:N	2.77	0.42
31:G:425:UNK:O	31:G:428:UNK:CA	2.66	0.42
32:H:68:UNK:O	32:H:71:UNK:N	2.52	0.42
32:H:170:UNK:O	32:H:171:UNK:C	2.65	0.42
34:J:100:UNK:O	34:J:101:UNK:C	2.63	0.42
36:L:250:UNK:O	36:L:254:UNK:CB	2.67	0.42
25:A:103:UNK:O	25:A:106:UNK:CA	2.67	0.42
27:C:112:UNK:CB	27:C:113:UNK:HA	2.49	0.42
28:D:296:UNK:O	28:D:297:UNK:C	2.66	0.42
29:E:50:UNK:O	29:E:51:UNK:C	2.67	0.42
31:G:12:UNK:HA	31:G:17:UNK:CA	2.47	0.42
31:G:426:UNK:HA	31:G:429:UNK:CB	2.50	0.42
36:L:141:UNK:O	36:L:142:UNK:C	2.67	0.42
37:M:168:UNK:CB	37:M:174:UNK:CA	2.97	0.42
19:5:24:ASN:HD22	19:5:25:GLN:N	2.18	0.42
21:7:31:LEU:HA	21:7:31:LEU:HD23	1.83	0.42
30:F:394:UNK:O	30:F:395:UNK:C	2.66	0.42
36:L:108:UNK:O	36:L:111:UNK:CB	2.67	0.42
36:L:140:UNK:O	36:L:143:UNK:N	2.53	0.42
36:L:241:UNK:O	36:L:242:UNK:C	2.68	0.42
36:L:462:UNK:O	36:L:465:UNK:N	2.52	0.42
37:M:408:UNK:O	37:M:412:UNK:N	2.52	0.42
40:P:160:UNK:N	40:P:161:UNK:CA	2.83	0.42
27:C:78:UNK:HA	27:C:93:UNK:O	2.18	0.42
30:F:215:UNK:O	30:F:216:UNK:C	2.64	0.42
33:I:113:UNK:O	33:I:115:UNK:N	2.53	0.42
36:L:32:UNK:HA	36:L:35:UNK:CB	2.48	0.42
37:M:22:UNK:CA	37:M:23:UNK:CB	2.97	0.42
48:Y:92:UNK:O	48:Y:95:UNK:N	2.52	0.42
17:3:86:GLY:O	17:3:87:THR:O	2.37	0.42
18:4:77:PRO:HA	18:4:82:TYR:HA	2.02	0.42
39:O:22:UNK:CB	39:O:23:UNK:CA	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:331:UNK:O	47:X:334:UNK:N	2.52	0.42
18:4:5:LYS:CD	18:4:6:GLY:N	2.81	0.42
19:5:57:ARG:HA	19:5:60:TYR:CD2	2.55	0.42
22:8:44:PRO:HA	22:8:47:ARG:NH1	2.34	0.42
26:B:75:UNK:O	26:B:76:UNK:CB	2.68	0.42
26:B:166:UNK:CA	26:B:169:UNK:O	2.63	0.42
30:F:34:UNK:O	30:F:38:UNK:CA	2.67	0.42
30:F:286:UNK:HA	30:F:287:UNK:HA	1.55	0.42
31:G:456:UNK:CB	31:G:457:UNK:C	2.98	0.42
32:H:95:UNK:HA	32:H:96:UNK:HA	1.81	0.42
33:I:83:CYS:HB2	33:I:122:CYS:HB2	2.02	0.42
36:L:582:UNK:O	36:L:586:UNK:N	2.53	0.42
37:M:315:UNK:O	37:M:316:UNK:C	2.64	0.42
50:U:627:UNK:O	50:U:628:UNK:C	2.65	0.42
26:B:117:UNK:O	26:B:120:UNK:CA	2.67	0.42
30:F:56:UNK:O	30:F:59:UNK:N	2.53	0.42
34:J:58:UNK:O	34:J:63:UNK:N	2.52	0.42
34:J:69:UNK:HA	34:J:72:UNK:CB	2.50	0.42
34:J:88:UNK:O	34:J:91:UNK:CB	2.67	0.42
36:L:82:UNK:O	36:L:86:UNK:N	2.52	0.42
36:L:128:UNK:O	36:L:132:UNK:N	2.53	0.42
36:L:369:UNK:O	36:L:372:UNK:N	2.53	0.42
37:M:168:UNK:HA	37:M:174:UNK:HA	2.02	0.42
37:M:175:UNK:C	37:M:177:UNK:HA	2.47	0.42
38:N:76:UNK:O	38:N:80:UNK:N	2.52	0.42
40:P:301:UNK:C	40:P:303:UNK:N	2.82	0.42
47:X:303:UNK:O	47:X:304:UNK:C	2.68	0.42
15:1:126:MET:HG3	15:1:128:VAL:HG23	2.00	0.42
17:3:53:THR:HG22	17:3:54:ASN:OD1	2.19	0.42
25:A:84:UNK:O	25:A:87:UNK:N	2.52	0.42
28:D:317:UNK:O	28:D:318:UNK:C	2.68	0.42
30:F:185:UNK:C	30:F:187:UNK:N	2.81	0.42
31:G:326:UNK:O	31:G:327:UNK:C	2.67	0.42
34:J:25:UNK:O	34:J:28:UNK:CB	2.68	0.42
36:L:158:UNK:O	36:L:159:UNK:C	2.64	0.42
37:M:164:UNK:O	37:M:167:UNK:N	2.52	0.42
37:M:369:UNK:O	37:M:372:UNK:CB	2.68	0.42
39:O:80:UNK:O	39:O:83:UNK:N	2.53	0.42
39:O:231:UNK:O	39:O:234:UNK:N	2.53	0.42
45:V:30:UNK:O	45:V:31:UNK:C	2.67	0.42
31:G:12:UNK:N	31:G:77:UNK:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:565:UNK:C	31:G:567:UNK:N	2.78	0.42
31:G:604:UNK:O	31:G:609:UNK:N	2.53	0.42
32:H:110:UNK:O	32:H:111:UNK:C	2.68	0.42
32:H:277:UNK:O	32:H:278:UNK:CB	2.66	0.42
45:V:33:UNK:O	45:V:37:UNK:N	2.53	0.42
45:V:51:UNK:O	45:V:52:UNK:CB	2.68	0.42
47:X:322:UNK:HA	47:X:325:UNK:CB	2.50	0.42
26:B:109:UNK:O	26:B:111:UNK:N	2.53	0.42
26:B:149:CYS:HA	26:B:150:UNK:HA	1.94	0.42
28:D:182:UNK:O	28:D:186:UNK:HA	2.20	0.42
30:F:183:UNK:CB	30:F:186:UNK:N	2.82	0.42
31:G:143:UNK:CB	31:G:190:UNK:CB	2.98	0.42
31:G:273:UNK:O	31:G:274:UNK:C	2.67	0.42
31:G:288:UNK:CA	31:G:289:UNK:C	2.89	0.42
31:G:491:UNK:O	31:G:493:UNK:N	2.53	0.42
36:L:34:UNK:O	36:L:37:UNK:N	2.52	0.42
36:L:297:UNK:HA	36:L:355:UNK:CA	2.48	0.42
37:M:139:UNK:CA	37:M:140:UNK:CB	2.98	0.42
38:N:12:UNK:O	38:N:16:UNK:N	2.52	0.42
38:N:124:UNK:C	38:N:126:UNK:N	2.78	0.42
47:X:212:UNK:O	47:X:213:UNK:C	2.68	0.42
51:Z:245:UNK:O	51:Z:249:UNK:CB	2.68	0.42
25:A:105:UNK:O	25:A:109:UNK:HA	2.20	0.41
29:E:54:UNK:O	29:E:55:UNK:C	2.65	0.41
31:G:594:UNK:CB	31:G:596:UNK:N	2.83	0.41
36:L:274:UNK:O	36:L:275:UNK:C	2.67	0.41
37:M:54:UNK:HA	37:M:55:UNK:HA	1.65	0.41
37:M:178:UNK:O	37:M:179:UNK:C	2.62	0.41
37:M:179:UNK:O	37:M:180:UNK:C	2.68	0.41
40:P:53:UNK:O	40:P:57:UNK:N	2.53	0.41
40:P:120:UNK:O	40:P:121:UNK:C	2.67	0.41
40:P:229:UNK:N	40:P:299:UNK:CB	2.83	0.41
50:U:103:UNK:C	50:U:105:UNK:N	2.82	0.41
19:5:57:ARG:HB3	19:5:57:ARG:NH1	2.31	0.41
26:B:71:UNK:CB	32:H:37:UNK:N	2.83	0.41
28:D:95:UNK:O	28:D:98:UNK:N	2.54	0.41
30:F:181:UNK:O	30:F:182:UNK:CB	2.69	0.41
30:F:213:UNK:HA	30:F:214:UNK:HA	1.67	0.41
33:I:100:UNK:O	33:I:103:UNK:C	2.69	0.41
36:L:109:UNK:O	36:L:110:UNK:CB	2.67	0.41
36:L:161:UNK:CB	36:L:163:UNK:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:184:UNK:O	36:L:188:UNK:N	2.54	0.41
37:M:124:UNK:O	37:M:125:UNK:C	2.64	0.41
37:M:433:UNK:O	37:M:434:UNK:C	2.63	0.41
38:N:11:UNK:O	38:N:15:UNK:N	2.53	0.41
38:N:124:UNK:O	38:N:127:UNK:CB	2.68	0.41
15:1:130:PRO:O	15:1:136:ALA:HB2	2.20	0.41
26:B:38:UNK:O	26:B:39:UNK:C	2.68	0.41
26:B:118:UNK:O	26:B:122:UNK:CA	2.63	0.41
28:D:250:UNK:O	28:D:251:UNK:C	2.68	0.41
29:E:78:UNK:HA	29:E:81:UNK:CB	2.50	0.41
32:H:266:UNK:O	32:H:267:UNK:C	2.69	0.41
38:N:290:UNK:O	38:N:294:UNK:N	2.54	0.41
46:W:56:UNK:O	46:W:59:UNK:N	2.52	0.41
47:X:156:UNK:O	47:X:157:UNK:C	2.66	0.41
47:X:413:UNK:O	47:X:417:UNK:N	2.54	0.41
18:4:5:LYS:NZ	18:4:6:GLY:N	2.54	0.41
21:7:5:VAL:O	21:7:9:GLN:HG3	2.21	0.41
30:F:365:CYS:CA	30:F:368:UNK:CB	2.91	0.41
33:I:100:UNK:O	33:I:104:UNK:N	2.52	0.41
36:L:182:UNK:O	36:L:185:UNK:N	2.54	0.41
36:L:418:UNK:O	36:L:421:UNK:CB	2.69	0.41
36:L:431:UNK:O	36:L:432:UNK:CB	2.67	0.41
36:L:588:UNK:O	36:L:592:UNK:N	2.53	0.41
37:M:111:UNK:O	37:M:112:UNK:CB	2.68	0.41
37:M:209:UNK:O	37:M:210:UNK:C	2.69	0.41
37:M:327:UNK:O	37:M:330:UNK:CB	2.69	0.41
47:X:426:UNK:O	47:X:428:UNK:N	2.52	0.41
51:Z:624:UNK:O	51:Z:625:UNK:C	2.66	0.41
15:1:86:MET:O	22:8:25:CYS:HB2	2.20	0.41
15:1:137:LYS:O	15:1:145:TRP:HE3	2.03	0.41
16:2:21:LYS:O	16:2:57:ARG:NH1	2.53	0.41
16:2:21:LYS:HA	16:2:22:PRO:HD2	1.84	0.41
18:4:78:LEU:HD12	18:4:78:LEU:HA	1.75	0.41
21:7:12:PHE:O	21:7:23:LYS:HE2	2.21	0.41
26:B:48:UNK:CB	26:B:80:UNK:CA	2.84	0.41
26:B:121:UNK:C	26:B:135:UNK:CA	2.92	0.41
27:C:23:UNK:C	27:C:26:UNK:CB	2.98	0.41
30:F:322:UNK:CB	30:F:327:UNK:C	2.98	0.41
31:G:41:CYS:O	31:G:42:UNK:CB	2.69	0.41
32:H:94:UNK:O	32:H:95:UNK:C	2.68	0.41
36:L:420:UNK:O	36:L:423:UNK:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:530:UNK:C	36:L:532:UNK:N	2.78	0.41
36:L:570:UNK:O	36:L:573:UNK:N	2.53	0.41
38:N:200:UNK:O	38:N:201:UNK:C	2.68	0.41
39:O:50:UNK:O	39:O:51:UNK:CB	2.68	0.41
48:Y:33:UNK:C	48:Y:35:UNK:N	2.81	0.41
17:3:16:LEU:O	17:3:20:VAL:HG13	2.21	0.41
27:C:25:UNK:O	27:C:28:UNK:N	2.54	0.41
30:F:87:UNK:O	30:F:88:UNK:C	2.68	0.41
30:F:183:UNK:O	30:F:186:UNK:CB	2.69	0.41
30:F:315:UNK:CA	30:F:316:UNK:O	2.69	0.41
31:G:157:UNK:O	31:G:161:UNK:CB	2.69	0.41
31:G:461:UNK:O	31:G:464:UNK:N	2.54	0.41
37:M:50:UNK:O	37:M:51:UNK:CB	2.68	0.41
45:V:44:UNK:O	45:V:47:UNK:CA	2.68	0.41
47:X:177:UNK:O	47:X:178:UNK:C	2.69	0.41
51:Z:101:UNK:H	51:Z:104:UNK:CB	2.34	0.41
18:4:42:ARG:NH1	18:4:74:ARG:NH2	2.68	0.41
28:D:263:UNK:HA	28:D:288:UNK:CB	2.51	0.41
28:D:342:UNK:O	28:D:346:UNK:N	2.54	0.41
30:F:225:UNK:O	30:F:228:UNK:N	2.54	0.41
30:F:428:UNK:O	30:F:429:UNK:C	2.68	0.41
31:G:377:UNK:O	31:G:450:UNK:N	2.53	0.41
32:H:41:UNK:CB	32:H:45:UNK:N	2.84	0.41
40:P:31:UNK:O	40:P:32:UNK:C	2.68	0.41
43:S:36:UNK:O	43:S:40:UNK:N	2.54	0.41
47:X:302:UNK:O	47:X:305:UNK:CA	2.65	0.41
28:D:95:UNK:HA	28:D:385:UNK:CB	2.51	0.41
28:D:414:UNK:O	28:D:418:UNK:N	2.54	0.41
31:G:244:UNK:O	31:G:245:UNK:CB	2.65	0.41
31:G:255:UNK:C	31:G:257:UNK:N	2.79	0.41
31:G:567:UNK:O	31:G:586:UNK:N	2.54	0.41
32:H:160:UNK:O	32:H:161:UNK:CB	2.69	0.41
32:H:233:UNK:O	32:H:236:UNK:N	2.54	0.41
36:L:297:UNK:CA	36:L:355:UNK:HA	2.49	0.41
37:M:115:UNK:O	37:M:116:UNK:CB	2.69	0.41
37:M:189:UNK:C	37:M:191:UNK:O	2.69	0.41
37:M:225:UNK:O	37:M:228:UNK:C	2.69	0.41
37:M:399:UNK:O	37:M:403:UNK:N	2.53	0.41
42:R:60:UNK:O	42:R:62:UNK:N	2.54	0.41
15:1:102:TYR:HD2	24:0:35:TYR:HE1	1.68	0.41
15:1:127:LYS:O	15:1:130:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:20:PHE:N	19:5:21:PRO:HD3	2.35	0.41
19:5:65:PRO:HG2	19:5:68:TRP:CG	2.55	0.41
22:8:24:PHE:CE1	22:8:28:VAL:HG21	2.56	0.41
24:0:13:LYS:HD3	24:0:13:LYS:N	2.35	0.41
24:0:35:TYR:HD2	24:0:36:HIS:CE1	2.39	0.41
25:A:104:UNK:O	25:A:105:UNK:C	2.87	0.41
26:B:47:UNK:HA	26:B:85:UNK:O	2.20	0.41
26:B:53:UNK:N	26:B:90:UNK:CB	2.82	0.41
26:B:68:UNK:O	26:B:70:UNK:N	2.54	0.41
27:C:28:UNK:O	27:C:29:UNK:C	2.69	0.41
28:D:131:UNK:O	28:D:135:UNK:N	2.54	0.41
30:F:61:UNK:O	30:F:64:UNK:HA	2.15	0.41
30:F:71:UNK:O	30:F:72:UNK:CB	2.69	0.41
30:F:72:UNK:O	30:F:73:UNK:C	2.65	0.41
30:F:90:UNK:O	30:F:218:UNK:CB	2.68	0.41
30:F:303:UNK:C	30:F:414:UNK:CB	2.99	0.41
31:G:83:UNK:O	31:G:86:UNK:N	2.54	0.41
31:G:210:UNK:O	31:G:213:UNK:C	2.69	0.41
31:G:241:UNK:O	31:G:248:UNK:CA	2.65	0.41
31:G:279:UNK:O	31:G:280:UNK:CB	2.69	0.41
32:H:101:UNK:CB	32:H:162:UNK:N	2.84	0.41
32:H:101:UNK:CA	32:H:161:UNK:HA	2.51	0.41
33:I:63:UNK:CB	33:I:134:UNK:O	2.69	0.41
36:L:275:UNK:O	36:L:278:UNK:N	2.54	0.41
36:L:298:UNK:O	36:L:301:UNK:CB	2.69	0.41
36:L:496:UNK:O	36:L:497:UNK:C	2.68	0.41
36:L:560:UNK:O	36:L:564:UNK:N	2.54	0.41
37:M:108:UNK:O	37:M:111:UNK:CB	2.69	0.41
37:M:133:UNK:O	37:M:224:UNK:CB	2.69	0.41
37:M:163:UNK:O	37:M:164:UNK:C	2.69	0.41
37:M:390:UNK:O	37:M:391:UNK:C	2.69	0.41
38:N:72:UNK:O	38:N:75:UNK:N	2.54	0.41
38:N:126:UNK:O	38:N:127:UNK:C	2.67	0.41
38:N:276:UNK:O	38:N:279:UNK:CA	2.68	0.41
39:O:114:UNK:O	39:O:117:UNK:N	2.53	0.41
40:P:143:UNK:O	40:P:144:UNK:CB	2.68	0.41
41:Q:42:UNK:O	41:Q:43:UNK:C	2.69	0.41
43:S:83:UNK:O	43:S:84:UNK:C	2.68	0.41
46:W:71:UNK:O	46:W:72:UNK:O	2.38	0.41
50:U:628:UNK:O	50:U:629:UNK:CB	2.69	0.41
51:Z:605:UNK:O	51:Z:606:UNK:C	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:10:GLU:HG2	17:3:25:ARG:HH22	1.86	0.41
29:E:41:UNK:O	29:E:42:UNK:CB	2.69	0.41
30:F:52:UNK:O	30:F:55:UNK:C	2.68	0.41
30:F:62:UNK:C	30:F:64:UNK:N	2.79	0.41
30:F:262:UNK:HA	30:F:286:UNK:N	2.36	0.41
32:H:152:UNK:O	32:H:155:UNK:CB	2.69	0.41
33:I:167:UNK:O	33:I:168:UNK:C	2.69	0.41
37:M:186:UNK:O	37:M:253:UNK:CB	2.69	0.41
38:N:291:UNK:O	38:N:292:UNK:C	2.69	0.41
47:X:605:UNK:O	47:X:608:UNK:CB	2.69	0.41
51:Z:208:UNK:O	51:Z:211:UNK:CB	2.69	0.41
17:3:19:GLU:HB3	17:3:98:HIS:CE1	2.57	0.40
27:C:27:UNK:O	27:C:30:UNK:CB	2.69	0.40
28:D:138:UNK:O	28:D:142:UNK:CB	2.69	0.40
28:D:250:UNK:O	28:D:253:UNK:CB	2.69	0.40
29:E:78:UNK:O	29:E:82:UNK:N	2.54	0.40
29:E:127:UNK:O	29:E:128:UNK:C	2.70	0.40
30:F:276:UNK:N	30:F:315:UNK:O	2.54	0.40
31:G:49:UNK:O	31:G:51:UNK:N	2.54	0.40
32:H:68:UNK:C	32:H:70:UNK:N	2.79	0.40
36:L:34:UNK:O	36:L:37:UNK:CB	2.69	0.40
47:X:43:UNK:HA	47:X:59:UNK:CB	2.51	0.40
16:2:43:PRO:HB2	16:2:48:ILE:CD1	2.48	0.40
16:2:104:LEU:HD23	16:2:104:LEU:HA	1.87	0.40
20:6:35:TYR:O	20:6:39:VAL:HB	2.19	0.40
29:E:44:UNK:O	29:E:45:UNK:C	2.69	0.40
30:F:242:UNK:O	30:F:252:UNK:CB	2.69	0.40
31:G:12:UNK:O	31:G:78:UNK:CA	2.65	0.40
31:G:294:UNK:O	31:G:295:UNK:C	2.69	0.40
31:G:397:UNK:O	31:G:400:UNK:CB	2.69	0.40
32:H:283:UNK:O	32:H:284:UNK:C	2.70	0.40
32:H:308:UNK:HA	32:H:312:UNK:CB	2.51	0.40
32:H:310:UNK:O	32:H:311:UNK:CB	2.68	0.40
33:I:60:UNK:O	33:I:61:UNK:C	2.69	0.40
36:L:192:UNK:O	36:L:193:UNK:C	2.69	0.40
37:M:345:UNK:O	37:M:346:UNK:CB	2.69	0.40
38:N:18:UNK:O	38:N:21:UNK:N	2.54	0.40
38:N:90:UNK:HA	38:N:91:UNK:CB	2.50	0.40
38:N:115:UNK:O	38:N:116:UNK:C	2.70	0.40
38:N:182:UNK:O	38:N:183:UNK:C	2.69	0.40
38:N:266:UNK:O	38:N:270:UNK:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:145:UNK:O	40:P:146:UNK:C	2.70	0.40
43:S:28:UNK:O	43:S:29:UNK:CB	2.69	0.40
46:W:53:UNK:O	46:W:56:UNK:N	2.54	0.40
47:X:604:UNK:C	47:X:606:UNK:N	2.82	0.40
48:Y:90:UNK:C	48:Y:92:UNK:N	2.84	0.40
17:3:49:VAL:O	17:3:91:LEU:HD12	2.21	0.40
26:B:67:UNK:N	26:B:68:UNK:CA	2.83	0.40
28:D:112:UNK:O	28:D:113:UNK:C	2.69	0.40
30:F:35:UNK:O	30:F:39:UNK:N	2.55	0.40
30:F:121:UNK:CA	30:F:232:UNK:CB	2.97	0.40
30:F:135:UNK:HA	30:F:176:UNK:O	2.21	0.40
30:F:418:UNK:O	30:F:423:UNK:CB	2.68	0.40
31:G:142:UNK:O	31:G:143:UNK:CB	2.69	0.40
31:G:624:UNK:O	31:G:627:UNK:CA	2.68	0.40
36:L:570:UNK:O	36:L:571:UNK:C	2.70	0.40
36:L:571:UNK:O	36:L:572:UNK:C	2.69	0.40
36:L:603:UNK:O	36:L:604:UNK:CB	2.70	0.40
37:M:8:UNK:O	37:M:11:UNK:N	2.55	0.40
37:M:55:UNK:HA	37:M:56:UNK:HA	1.82	0.40
37:M:66:UNK:O	37:M:67:UNK:C	2.70	0.40
37:M:174:UNK:O	37:M:175:UNK:C	2.69	0.40
38:N:29:UNK:O	38:N:32:UNK:N	2.54	0.40
40:P:146:UNK:O	40:P:149:UNK:CA	2.69	0.40
42:R:87:UNK:C	42:R:89:UNK:N	2.84	0.40
46:W:43:UNK:O	46:W:44:UNK:CB	2.69	0.40
51:Z:123:UNK:O	51:Z:124:UNK:C	2.69	0.40
51:Z:242:UNK:O	51:Z:243:UNK:CB	2.69	0.40
28:D:182:UNK:O	28:D:186:UNK:CA	2.69	0.40
28:D:253:UNK:O	28:D:254:UNK:CB	2.70	0.40
28:D:260:UNK:O	28:D:265:UNK:CB	2.70	0.40
28:D:401:UNK:O	28:D:402:UNK:C	2.69	0.40
29:E:65:UNK:O	29:E:66:UNK:C	2.63	0.40
30:F:82:UNK:O	30:F:84:UNK:N	2.54	0.40
30:F:357:UNK:O	30:F:358:UNK:C	2.70	0.40
31:G:435:UNK:CB	31:G:437:UNK:HA	2.51	0.40
32:H:90:UNK:CB	32:H:95:UNK:O	2.70	0.40
33:I:110:UNK:CB	33:I:150:UNK:O	2.70	0.40
36:L:65:UNK:CB	36:L:66:UNK:HA	2.50	0.40
37:M:268:UNK:O	37:M:269:UNK:C	2.70	0.40
38:N:12:UNK:O	38:N:15:UNK:CB	2.69	0.40
39:O:187:UNK:O	39:O:188:UNK:C	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:26:UNK:O	40:P:31:UNK:CB	2.70	0.40
41:Q:40:UNK:CB	41:Q:41:UNK:CA	2.93	0.40
44:T:63:UNK:O	44:T:64:UNK:C	2.66	0.40
46:W:40:UNK:N	46:W:41:UNK:CB	2.82	0.40
50:U:211:UNK:O	50:U:212:UNK:C	2.69	0.40
50:U:622:UNK:O	50:U:625:UNK:CB	2.69	0.40
51:Z:336:UNK:O	51:Z:342:UNK:CB	2.70	0.40
15:1:119:GLN:O	15:1:123:MET:HG3	2.22	0.40
19:5:33:TYR:O	19:5:37:HIS:HD2	2.05	0.40
25:A:76:UNK:O	25:A:78:UNK:N	2.55	0.40
28:D:69:UNK:O	28:D:70:UNK:CB	2.70	0.40
28:D:262:UNK:O	28:D:263:UNK:C	2.69	0.40
28:D:394:UNK:O	28:D:398:UNK:CB	2.70	0.40
30:F:44:UNK:O	30:F:45:UNK:C	2.70	0.40
30:F:322:UNK:O	30:F:327:UNK:CA	2.70	0.40
31:G:457:UNK:O	31:G:458:UNK:CB	2.68	0.40
32:H:90:UNK:O	32:H:91:UNK:CB	2.70	0.40
32:H:119:UNK:O	32:H:120:UNK:C	2.70	0.40
32:H:119:UNK:O	32:H:122:UNK:CB	2.69	0.40
32:H:120:UNK:O	32:H:121:UNK:C	2.70	0.40
32:H:303:UNK:O	32:H:306:UNK:N	2.54	0.40
33:I:63:UNK:CB	33:I:133:UNK:CA	3.00	0.40
34:J:22:UNK:O	34:J:23:UNK:CB	2.69	0.40
36:L:111:UNK:O	36:L:114:UNK:CB	2.70	0.40
36:L:154:UNK:O	36:L:155:UNK:C	2.70	0.40
36:L:182:UNK:O	36:L:183:UNK:C	2.69	0.40
37:M:20:UNK:O	37:M:21:UNK:CB	2.70	0.40
37:M:251:UNK:O	37:M:252:UNK:CB	2.69	0.40
37:M:309:UNK:O	37:M:310:UNK:C	2.70	0.40
38:N:74:UNK:O	38:N:75:UNK:C	2.70	0.40
38:N:106:UNK:O	38:N:107:UNK:CB	2.68	0.40
39:O:129:UNK:O	39:O:132:UNK:CA	2.67	0.40
39:O:234:UNK:O	39:O:237:UNK:CA	2.69	0.40
40:P:146:UNK:O	40:P:149:UNK:CB	2.69	0.40
47:X:177:UNK:O	47:X:180:UNK:CA	2.69	0.40
47:X:204:UNK:O	47:X:205:UNK:C	2.70	0.40
51:Z:243:UNK:O	51:Z:245:UNK:N	2.53	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	c	444/446 (100%)	355 (80%)	66 (15%)	23 (5%)	2 19
1	l	444/446 (100%)	370 (83%)	54 (12%)	20 (4%)	2 22
2	m	417/439 (95%)	341 (82%)	67 (16%)	9 (2%)	6 35
2	n	417/439 (95%)	344 (82%)	62 (15%)	11 (3%)	5 31
3	b	377/379 (100%)	303 (80%)	60 (16%)	14 (4%)	3 24
3	o	377/379 (100%)	316 (84%)	50 (13%)	11 (3%)	4 29
4	d	239/241 (99%)	188 (79%)	36 (15%)	15 (6%)	1 17
4	p	239/241 (99%)	195 (82%)	32 (13%)	12 (5%)	2 20
5	e	73/196 (37%)	57 (78%)	14 (19%)	2 (3%)	5 31
5	q	194/196 (99%)	148 (76%)	35 (18%)	11 (6%)	1 18
6	f	104/110 (94%)	89 (86%)	13 (12%)	2 (2%)	8 38
6	r	104/110 (94%)	87 (84%)	15 (14%)	2 (2%)	8 38
7	g	79/81 (98%)	63 (80%)	13 (16%)	3 (4%)	3 24
7	s	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	3 24
8	h	62/78 (80%)	52 (84%)	10 (16%)	0	100 100
8	t	62/78 (80%)	51 (82%)	10 (16%)	1 (2%)	9 44
9	i	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1 16
9	u	31/78 (40%)	17 (55%)	11 (36%)	3 (10%)	0 10
10	j	60/62 (97%)	41 (68%)	13 (22%)	6 (10%)	0 9
10	v	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1 15
11	k	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	2 20
11	w	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0 9
12	x	512/514 (100%)	480 (94%)	28 (6%)	4 (1%)	19 60
13	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	12 48
14	z	259/261 (99%)	249 (96%)	10 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	1	142/147 (97%)	135 (95%)	7 (5%)	0	100 100
16	2	107/109 (98%)	104 (97%)	3 (3%)	0	100 100
17	3	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3 22
18	4	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1 17
19	5	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	11 46
20	6	71/73 (97%)	65 (92%)	6 (8%)	0	100 100
21	7	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	3 24
22	8	47/56 (84%)	41 (87%)	6 (13%)	0	100 100
23	9	45/47 (96%)	42 (93%)	3 (7%)	0	100 100
24	0	41/46 (89%)	39 (95%)	2 (5%)	0	100 100
26	B	4/143 (3%)	3 (75%)	0	1 (25%)	0 1
29	E	4/159 (2%)	3 (75%)	1 (25%)	0	100 100
30	F	4/411 (1%)	4 (100%)	0	0	100 100
31	G	12/538 (2%)	9 (75%)	1 (8%)	2 (17%)	0 3
33	I	8/162 (5%)	7 (88%)	0	1 (12%)	0 5
All	All	5719/7551 (76%)	4821 (84%)	718 (13%)	180 (3%)	7 27

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	c	327	ASP
1	c	426	GLY
1	c	427	PRO
2	m	141	GLN
2	m	183	ILE
2	m	305	GLN
3	b	8	HIS
3	b	27	ILE
3	b	109	PHE
4	d	51	LEU
4	d	73	GLY
4	d	98	PRO
9	i	72	VAL
1	l	55	ALA
1	l	427	PRO
2	n	141	GLN
2	n	183	ILE

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Mol	Chain	Res	Type
2	n	351	ASN
3	o	8	HIS
3	o	27	ILE
3	o	157	GLY
4	p	51	LEU
4	p	73	GLY
5	q	114	VAL
5	q	141	HIS
9	u	72	VAL
10	v	58	LYS
12	x	328	HIS
12	x	508	PRO
17	3	2	SER
17	3	87	THR
17	3	95	GLN
18	4	4	ALA
18	4	9	GLY
19	5	46	LYS
21	7	2	GLU
26	B	119	CYS
31	G	105	CYS
1	c	55	ALA
1	c	56	GLY
1	c	72	GLY
1	c	80	GLU
1	c	81	SER
1	c	227	ALA
1	c	287	GLY
1	c	288	ALA
1	c	342	TRP
2	m	236	LYS
2	m	351	ASN
3	b	28	SER
3	b	137	GLN
3	b	157	GLY
3	b	313	ARG
4	d	119	ALA
4	d	154	PRO
7	g	68	LYS
9	i	59	ALA
10	j	58	LYS
1	l	52	ASN

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Mol	Chain	Res	Type
1	l	72	GLY
1	l	227	ALA
1	l	246	ASP
1	l	282	CYS
1	l	385	THR
2	n	236	LYS
5	q	137	GLY
9	u	59	ALA
10	v	23	THR
10	v	24	ILE
18	4	5	LYS
33	I	116	CYS
1	c	52	ASN
1	c	352	SER
1	c	385	THR
1	c	395	TRP
2	m	91	ALA
3	b	283	SER
3	b	319	PRO
4	d	27	ARG
4	d	162	PRO
4	d	218	LEU
5	e	16	PRO
5	e	72	SER
10	j	23	THR
10	j	35	PHE
1	l	81	SER
1	l	107	PRO
1	l	426	GLY
2	n	24	LEU
2	n	305	GLN
3	o	28	SER
3	o	62	ALA
3	o	316	MET
3	o	319	PRO
4	p	80	MET
4	p	162	PRO
5	q	64	ALA
5	q	177	PRO
7	s	68	LYS
10	v	57	HIS
11	w	33	VAL

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Mol	Chain	Res	Type
13	y	104	TRP
18	4	61	SER
31	G	156	CYS
1	c	107	PRO
1	c	246	ASP
1	c	391	PRO
3	b	236	ILE
3	b	365	LEU
4	d	80	MET
4	d	147	LEU
6	f	95	LYS
10	j	4	THR
10	j	57	HIS
1	l	6	GLN
1	l	109	ALA
2	n	269	ALA
2	n	409	ASP
3	o	24	PRO
3	o	109	PHE
4	p	147	LEU
5	q	130	PRO
6	r	95	LYS
12	x	51	ASP
1	c	6	GLN
1	c	152	TYR
2	m	39	GLU
3	b	316	MET
7	g	72	LYS
1	l	338	LEU
1	l	391	PRO
3	o	247	PRO
3	o	255	ASN
4	p	83	ARG
4	p	98	PRO
4	p	110	PRO
4	p	154	PRO
5	q	16	PRO
5	q	69	LEU
5	q	188	THR
7	s	50	PRO
11	w	34	SER
13	y	103	GLN

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Mol	Chain	Res	Type
21	7	3	ASN
1	c	33	PRO
2	m	52	LYS
4	d	110	PRO
4	d	163	PRO
4	d	176	PRO
7	g	45	ILE
1	l	185	TYR
2	n	52	LYS
4	p	176	PRO
5	q	43	THR
12	x	91	ASP
13	y	158	ASP
18	4	49	PRO
2	m	129	ALA
6	f	51	PRO
1	l	56	GLY
1	l	293	PRO
3	b	339	GLY
4	d	83	ARG
2	n	85	ILE
2	n	109	VAL
4	p	123	GLY
5	q	84	GLY
8	t	69	VAL
17	3	15	GLY
10	j	24	ILE
6	r	51	PRO
7	s	45	ILE
1	c	260	PRO
11	k	33	VAL
4	p	163	PRO
9	u	65	VAL
3	b	372	ILE
4	d	26	ILE
1	l	71	PRO
1	l	193	PRO

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	c	370/370 (100%)	289 (78%)	81 (22%)	1 5
1	l	370/370 (100%)	286 (77%)	84 (23%)	1 5
2	m	328/343 (96%)	260 (79%)	68 (21%)	1 6
2	n	328/343 (96%)	262 (80%)	66 (20%)	1 7
3	b	327/327 (100%)	269 (82%)	58 (18%)	2 10
3	o	327/327 (100%)	276 (84%)	51 (16%)	2 14
4	d	206/206 (100%)	179 (87%)	27 (13%)	4 18
4	p	206/206 (100%)	179 (87%)	27 (13%)	4 18
5	e	65/168 (39%)	51 (78%)	14 (22%)	1 6
5	q	167/168 (99%)	123 (74%)	44 (26%)	0 3
6	f	96/98 (98%)	74 (77%)	22 (23%)	1 4
6	r	96/98 (98%)	78 (81%)	18 (19%)	1 9
7	g	71/71 (100%)	58 (82%)	13 (18%)	1 10
7	s	71/71 (100%)	57 (80%)	14 (20%)	1 8
8	h	61/74 (82%)	51 (84%)	10 (16%)	2 12
8	t	61/74 (82%)	51 (84%)	10 (16%)	2 12
9	i	27/60 (45%)	19 (70%)	8 (30%)	0 2
9	u	27/60 (45%)	20 (74%)	7 (26%)	0 3
10	j	52/52 (100%)	46 (88%)	6 (12%)	5 21
10	v	52/52 (100%)	43 (83%)	9 (17%)	2 11
11	k	15/46 (33%)	12 (80%)	3 (20%)	1 7
11	w	15/46 (33%)	11 (73%)	4 (27%)	0 3
12	x	427/427 (100%)	389 (91%)	38 (9%)	9 30
13	y	211/211 (100%)	191 (90%)	20 (10%)	8 27
14	z	226/226 (100%)	199 (88%)	27 (12%)	5 20
15	1	128/129 (99%)	120 (94%)	8 (6%)	18 43
16	2	95/95 (100%)	89 (94%)	6 (6%)	18 43
17	3	81/81 (100%)	76 (94%)	5 (6%)	18 43
18	4	68/68 (100%)	50 (74%)	18 (26%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	5	67/75 (89%)	58 (87%)	9 (13%)	4 17
20	6	58/58 (100%)	53 (91%)	5 (9%)	10 32
21	7	47/50 (94%)	40 (85%)	7 (15%)	3 15
22	8	39/46 (85%)	37 (95%)	2 (5%)	24 48
23	9	40/40 (100%)	38 (95%)	2 (5%)	24 49
24	0	37/38 (97%)	34 (92%)	3 (8%)	11 35
26	B	4/4 (100%)	2 (50%)	2 (50%)	0 0
29	E	4/4 (100%)	4 (100%)	0	100 100
30	F	4/4 (100%)	3 (75%)	1 (25%)	0 3
31	G	12/12 (100%)	8 (67%)	4 (33%)	0 2
33	I	8/8 (100%)	7 (88%)	1 (12%)	4 19
All	All	4894/5206 (94%)	4092 (84%)	802 (16%)	5 12

All (802) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	13	GLU
1	c	24	ARG
1	c	31	SER
1	c	35	CYS
1	c	37	VAL
1	c	42	ASP
1	c	46	ARG
1	c	48	GLU
1	c	49	SER
1	c	53	ASN
1	c	58	PHE
1	c	68	LYS
1	c	70	ARG
1	c	79	VAL
1	c	89	TYR
1	c	90	SER
1	c	97	TYR
1	c	99	ILE
1	c	102	LEU
1	c	108	LYS
1	c	112	LEU
1	c	120	CYS

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Mol	Chain	Res	Type
1	c	125	SER
1	c	127	ILE
1	c	130	GLU
1	c	131	ARG
1	c	133	VAL
1	c	143	THR
1	c	149	VAL
1	c	163	LEU
1	c	174	VAL
1	c	175	ARG
1	c	177	LEU
1	c	178	SER
1	c	179	ARG
1	c	183	THR
1	c	187	SER
1	c	191	LYS
1	c	195	MET
1	c	197	LEU
1	c	208	LEU
1	c	211	LEU
1	c	213	GLN
1	c	216	PHE
1	c	222	THR
1	c	225	GLU
1	c	231	LEU
1	c	239	SER
1	c	241	ILE
1	c	243	HIS
1	c	245	GLU
1	c	246	ASP
1	c	255	ILE
1	c	266	ASP
1	c	272	VAL
1	c	277	ILE
1	c	296	SER
1	c	302	LYS
1	c	307	PHE
1	c	316	ASP
1	c	330	SER
1	c	334	MET
1	c	337	VAL
1	c	341	GLN

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Mol	Chain	Res	Type
1	c	344	ARG
1	c	346	CYS
1	c	351	GLU
1	c	352	SER
1	c	353	GLU
1	c	356	ARG
1	c	358	LYS
1	c	360	LEU
1	c	367	SER
1	c	370	ASP
1	c	379	ILE
1	c	384	LEU
1	c	386	TYR
1	c	398	ARG
1	c	413	LYS
1	c	428	ILE
1	c	441	MET
2	m	23	ASP
2	m	24	LEU
2	m	35	ILE
2	m	37	SER
2	m	38	LEU
2	m	45	SER
2	m	46	ARG
2	m	51	ILE
2	m	52	LYS
2	m	56	ARG
2	m	60	SER
2	m	62	ASN
2	m	74	SER
2	m	77	THR
2	m	81	SER
2	m	85	ILE
2	m	86	THR
2	m	95	LYS
2	m	96	LEU
2	m	101	THR
2	m	102	ARG
2	m	111	CYS
2	m	112	LEU
2	m	113	ARG
2	m	117	ASP

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Mol	Chain	Res	Type
2	m	131	GLU
2	m	134	ARG
2	m	140	LEU
2	m	145	ARG
2	m	159	VAL
2	m	160	ILE
2	m	175	SER
2	m	182	ARG
2	m	187	THR
2	m	190	GLU
2	m	196	GLN
2	m	203	ARG
2	m	215	VAL
2	m	219	VAL
2	m	238	LYS
2	m	240	HIS
2	m	245	ARG
2	m	253	VAL
2	m	283	PRO
2	m	292	THR
2	m	294	SER
2	m	297	GLN
2	m	310	SER
2	m	318	ASP
2	m	319	SER
2	m	328	SER
2	m	353	SER
2	m	354	ASN
2	m	374	SER
2	m	391	SER
2	m	396	SER
2	m	402	ILE
2	m	403	ASP
2	m	409	ASP
2	m	416	LYS
2	m	418	VAL
2	m	421	ARG
2	m	422	LYS
2	m	423	SER
2	m	429	ASN
2	m	436	ILE
2	m	437	ASP

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Mol	Chain	Res	Type
2	m	438	GLU
3	b	1	MET
3	b	5	ARG
3	b	6	LYS
3	b	7	SER
3	b	11	MET
3	b	25	SER
3	b	26	ASN
3	b	27	ILE
3	b	29	SER
3	b	32	ASN
3	b	43	LEU
3	b	60	THR
3	b	61	THR
3	b	65	SER
3	b	67	THR
3	b	80	ARG
3	b	94	LEU
3	b	119	LEU
3	b	138	MET
3	b	139	SER
3	b	144	THR
3	b	156	ILE
3	b	158	THR
3	b	169	SER
3	b	174	THR
3	b	176	THR
3	b	177	ARG
3	b	183	PHE
3	b	192	ILE
3	b	198	LEU
3	b	205	SER
3	b	212	SER
3	b	217	LYS
3	b	226	ILE
3	b	229	ILE
3	b	233	LEU
3	b	240	MET
3	b	241	LEU
3	b	244	LEU
3	b	247	PRO
3	b	262	LEU

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Mol	Chain	Res	Type
3	b	271	GLU
3	b	273	TYR
3	b	280	ILE
3	b	282	ARG
3	b	291	VAL
3	b	299	LEU
3	b	310	SER
3	b	311	LYS
3	b	312	GLN
3	b	313	ARG
3	b	314	SER
3	b	318	ARG
3	b	321	SER
3	b	324	LEU
3	b	353	LEU
3	b	363	LEU
3	b	377	LEU
4	d	3	LEU
4	d	9	SER
4	d	10	TYR
4	d	20	SER
4	d	21	LEU
4	d	27	ARG
4	d	32	VAL
4	d	40	CYS
4	d	42	SER
4	d	43	MET
4	d	52	VAL
4	d	55	CYS
4	d	80	MET
4	d	82	MET
4	d	83	ARG
4	d	87	LEU
4	d	95	TYR
4	d	106	ASN
4	d	120	ARG
4	d	124	GLU
4	d	179	MET
4	d	201	ARG
4	d	208	MET
4	d	223	LYS
4	d	224	ARG

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Mol	Chain	Res	Type
4	d	228	SER
4	d	231	LYS
5	e	1	SER
5	e	5	ILE
5	e	6	LYS
5	e	14	ARG
5	e	15	ARG
5	e	17	GLU
5	e	19	LEU
5	e	28	SER
5	e	32	ARG
5	e	33	LYS
5	e	52	LYS
5	e	58	PHE
5	e	63	SER
5	e	67	ASP
6	f	7	SER
6	f	9	SER
6	f	10	SER
6	f	11	ARG
6	f	13	LEU
6	f	16	ILE
6	f	18	LYS
6	f	44	LYS
6	f	48	ARG
6	f	54	LEU
6	f	58	ARG
6	f	68	LEU
6	f	69	SER
6	f	70	MET
6	f	77	LYS
6	f	82	LYS
6	f	88	SER
6	f	90	LEU
6	f	94	LEU
6	f	100	GLU
6	f	106	GLU
6	f	110	LYS
7	g	4	PHE
7	g	8	THR
7	g	9	ARG
7	g	19	SER

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Mol	Chain	Res	Type
7	g	23	GLN
7	g	24	ARG
7	g	39	ARG
7	g	40	ARG
7	g	42	ARG
7	g	45	ILE
7	g	46	LEU
7	g	58	VAL
7	g	69	SER
8	h	20	VAL
8	h	29	LYS
8	h	30	CYS
8	h	31	VAL
8	h	45	SER
8	h	54	CYS
8	h	58	LEU
8	h	59	LEU
8	h	73	LEU
8	h	74	PHE
9	i	46	LYS
9	i	49	VAL
9	i	51	CYS
9	i	54	SER
9	i	69	SER
9	i	70	LEU
9	i	77	ARG
9	i	78	TYR
10	j	11	SER
10	j	13	LEU
10	j	17	THR
10	j	18	SER
10	j	46	ILE
10	j	58	LYS
11	k	20	THR
11	k	23	LEU
11	k	36	THR
1	l	13	GLU
1	l	24	ARG
1	l	31	SER
1	l	37	VAL
1	l	42	ASP
1	l	45	SER

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Mol	Chain	Res	Type
1	l	46	ARG
1	l	48	GLU
1	l	51	LYS
1	l	53	ASN
1	l	58	PHE
1	l	70	ARG
1	l	82	MET
1	l	86	LEU
1	l	89	TYR
1	l	91	THR
1	l	92	ARG
1	l	97	TYR
1	l	99	ILE
1	l	100	LYS
1	l	108	LYS
1	l	112	LEU
1	l	125	SER
1	l	127	ILE
1	l	130	GLU
1	l	131	ARG
1	l	137	GLU
1	l	138	LEU
1	l	143	THR
1	l	149	VAL
1	l	156	THR
1	l	159	GLN
1	l	163	LEU
1	l	175	ARG
1	l	176	LYS
1	l	177	LEU
1	l	179	ARG
1	l	186	LEU
1	l	187	SER
1	l	191	LYS
1	l	195	MET
1	l	197	LEU
1	l	208	LEU
1	l	211	LEU
1	l	213	GLN
1	l	216	PHE
1	l	222	THR
1	l	225	GLU

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Mol	Chain	Res	Type
1	l	231	LEU
1	l	232	SER
1	l	243	HIS
1	l	245	GLU
1	l	246	ASP
1	l	248	LEU
1	l	257	VAL
1	l	266	ASP
1	l	277	ILE
1	l	302	LYS
1	l	307	PHE
1	l	309	THR
1	l	316	ASP
1	l	319	LEU
1	l	329	MET
1	l	330	SER
1	l	334	MET
1	l	341	GLN
1	l	344	ARG
1	l	346	CYS
1	l	347	THR
1	l	351	GLU
1	l	353	GLU
1	l	356	ARG
1	l	358	LYS
1	l	360	LEU
1	l	370	ASP
1	l	379	ILE
1	l	382	SER
1	l	384	LEU
1	l	386	TYR
1	l	412	SER
1	l	413	LYS
1	l	419	CYS
1	l	428	ILE
1	l	441	MET
2	n	23	ASP
2	n	24	LEU
2	n	33	LEU
2	n	35	ILE
2	n	37	SER
2	n	38	LEU

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Mol	Chain	Res	Type
2	n	45	SER
2	n	46	ARG
2	n	56	ARG
2	n	58	GLU
2	n	60	SER
2	n	62	ASN
2	n	73	SER
2	n	78	LYS
2	n	81	SER
2	n	84	LYS
2	n	85	ILE
2	n	86	THR
2	n	96	LEU
2	n	99	THR
2	n	100	SER
2	n	101	THR
2	n	102	ARG
2	n	108	THR
2	n	111	CYS
2	n	112	LEU
2	n	113	ARG
2	n	117	ASP
2	n	134	ARG
2	n	145	ARG
2	n	148	LYS
2	n	159	VAL
2	n	160	ILE
2	n	175	SER
2	n	182	ARG
2	n	190	GLU
2	n	196	GLN
2	n	201	SER
2	n	215	VAL
2	n	219	VAL
2	n	238	LYS
2	n	240	HIS
2	n	253	VAL
2	n	261	SER
2	n	264	ILE
2	n	266	SER
2	n	292	THR
2	n	295	LEU

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Mol	Chain	Res	Type
2	n	297	GLN
2	n	315	SER
2	n	317	SER
2	n	318	ASP
2	n	328	SER
2	n	329	GLN
2	n	346	THR
2	n	384	SER
2	n	402	ILE
2	n	403	ASP
2	n	416	LYS
2	n	418	VAL
2	n	421	ARG
2	n	424	MET
2	n	429	ASN
2	n	436	ILE
2	n	437	ASP
2	n	438	GLU
3	o	1	MET
3	o	5	ARG
3	o	6	LYS
3	o	7	SER
3	o	11	MET
3	o	27	ILE
3	o	32	ASN
3	o	35	SER
3	o	39	ILE
3	o	44	GLN
3	o	60	THR
3	o	67	THR
3	o	80	ARG
3	o	94	LEU
3	o	100	ARG
3	o	115	ILE
3	o	118	ILE
3	o	119	LEU
3	o	138	MET
3	o	139	SER
3	o	144	THR
3	o	158	THR
3	o	169	SER
3	o	174	THR

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Mol	Chain	Res	Type
3	o	189	ILE
3	o	192	ILE
3	o	197	LEU
3	o	212	SER
3	o	226	ILE
3	o	233	LEU
3	o	241	LEU
3	o	243	VAL
3	o	244	LEU
3	o	257	THR
3	o	262	LEU
3	o	271	GLU
3	o	282	ARG
3	o	287	LYS
3	o	297	SER
3	o	299	LEU
3	o	313	ARG
3	o	318	ARG
3	o	324	LEU
3	o	338	ILE
3	o	356	VAL
3	o	362	ILE
3	o	363	LEU
3	o	367	PRO
3	o	375	LYS
3	o	377	LEU
3	o	378	LYS
4	p	3	LEU
4	p	10	TYR
4	p	13	SER
4	p	17	LEU
4	p	20	SER
4	p	21	LEU
4	p	38	SER
4	p	39	SER
4	p	40	CYS
4	p	55	CYS
4	p	80	MET
4	p	82	MET
4	p	83	ARG
4	p	88	SER
4	p	106	ASN

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Mol	Chain	Res	Type
4	p	120	ARG
4	p	124	GLU
4	p	127	VAL
4	p	139	THR
4	p	141	VAL
4	p	158	ILE
4	p	179	MET
4	p	180	SER
4	p	186	VAL
4	p	201	ARG
4	p	223	LYS
4	p	226	LYS
5	q	5	ILE
5	q	6	LYS
5	q	11	SER
5	q	14	ARG
5	q	17	GLU
5	q	19	LEU
5	q	22	THR
5	q	23	LYS
5	q	28	SER
5	q	32	ARG
5	q	36	SER
5	q	42	THR
5	q	43	THR
5	q	44	THR
5	q	58	PHE
5	q	60	SER
5	q	61	SER
5	q	63	SER
5	q	65	SER
5	q	73	LYS
5	q	74	ILE
5	q	78	LEU
5	q	81	ILE
5	q	87	MET
5	q	98	VAL
5	q	102	THR
5	q	103	LYS
5	q	106	ILE
5	q	109	GLU
5	q	113	GLU

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Mol	Chain	Res	Type
5	q	120	PRO
5	q	125	GLU
5	q	136	ILE
5	q	139	CYS
5	q	140	THR
5	q	144	CYS
5	q	152	ASP
5	q	158	CYS
5	q	168	SER
5	q	171	ILE
5	q	172	ARG
5	q	173	LYS
5	q	178	LEU
5	q	195	VAL
6	r	7	SER
6	r	11	ARG
6	r	16	ILE
6	r	48	ARG
6	r	54	LEU
6	r	64	ARG
6	r	68	LEU
6	r	75	LEU
6	r	77	LYS
6	r	88	SER
6	r	90	LEU
6	r	94	LEU
6	r	98	ILE
6	r	100	GLU
6	r	103	GLU
6	r	106	GLU
6	r	107	TRP
6	r	110	LYS
7	s	4	PHE
7	s	8	THR
7	s	9	ARG
7	s	18	LEU
7	s	19	SER
7	s	23	GLN
7	s	24	ARG
7	s	31	SER
7	s	39	ARG
7	s	40	ARG

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Mol	Chain	Res	Type
7	s	41	THR
7	s	42	ARG
7	s	46	LEU
7	s	69	SER
8	t	20	VAL
8	t	29	LYS
8	t	30	CYS
8	t	31	VAL
8	t	46	SER
8	t	48	SER
8	t	54	CYS
8	t	58	LEU
8	t	73	LEU
8	t	74	PHE
9	u	46	LYS
9	u	49	VAL
9	u	67	SER
9	u	70	LEU
9	u	72	VAL
9	u	77	ARG
9	u	78	TYR
10	v	9	LEU
10	v	12	LEU
10	v	13	LEU
10	v	15	ARG
10	v	16	ARG
10	v	18	SER
10	v	46	ILE
10	v	53	LYS
10	v	58	LYS
11	w	20	THR
11	w	23	LEU
11	w	34	SER
11	w	36	THR
12	x	18	LEU
12	x	35	LEU
12	x	92	MET
12	x	96	ARG
12	x	105	LEU
12	x	109	PHE
12	x	115	SER
12	x	138	HIS

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Mol	Chain	Res	Type
12	x	150	LEU
12	x	159	LEU
12	x	187	SER
12	x	188	VAL
12	x	199	LEU
12	x	213	ARG
12	x	238	PHE
12	x	241	PRO
12	x	273	MET
12	x	295	VAL
12	x	301	THR
12	x	306	THR
12	x	318	VAL
12	x	324	LEU
12	x	347	LEU
12	x	353	LEU
12	x	354	THR
12	x	365	ILE
12	x	369	ASP
12	x	373	VAL
12	x	383	MET
12	x	417	MET
12	x	465	VAL
12	x	467	LEU
12	x	474	GLU
12	x	486	ASP
12	x	492	LEU
12	x	508	PRO
12	x	509	THR
12	x	512	ASN
13	y	7	LEU
13	y	31	VAL
13	y	52	HIS
13	y	60	GLU
13	y	63	THR
13	y	65	TRP
13	y	88	ASP
13	y	92	ASN
13	y	113	TYR
13	y	125	THR
13	y	130	PRO
13	y	134	ARG

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Mol	Chain	Res	Type
13	y	142	VAL
13	y	147	GLU
13	y	148	MET
13	y	170	LEU
13	y	171	LYS
13	y	185	MET
13	y	205	SER
13	y	216	LEU
14	z	1	MET
14	z	11	VAL
14	z	13	PRO
14	z	14	SER
14	z	18	LEU
14	z	19	THR
14	z	22	LEU
14	z	38	ASN
14	z	39	SER
14	z	85	LEU
14	z	92	LEU
14	z	112	LEU
14	z	127	LEU
14	z	128	GLU
14	z	131	LEU
14	z	132	LEU
14	z	137	LEU
14	z	142	VAL
14	z	159	MET
14	z	160	LEU
14	z	163	LEU
14	z	188	ILE
14	z	196	THR
14	z	199	VAL
14	z	214	PHE
14	z	222	GLN
14	z	258	TRP
15	1	31	LYS
15	1	36	SER
15	1	40	LEU
15	1	59	LEU
15	1	62	LEU
15	1	107	ILE
15	1	143	ASN

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Mol	Chain	Res	Type
15	1	147	LYS
16	2	7	THR
16	2	29	LEU
16	2	70	VAL
16	2	79	LYS
16	2	80	GLU
16	2	90	ARG
17	3	37	LYS
17	3	53	THR
17	3	74	LEU
17	3	95	GLN
17	3	98	HIS
18	4	5	LYS
18	4	7	ASP
18	4	8	HIS
18	4	14	ARG
18	4	17	ARG
18	4	33	LEU
18	4	34	ASN
18	4	37	LEU
18	4	38	HIS
18	4	41	HIS
18	4	42	ARG
18	4	43	GLU
18	4	48	ILE
18	4	54	ARG
18	4	56	ARG
18	4	68	THR
18	4	69	PHE
18	4	78	LEU
19	5	19	ARG
19	5	24	ASN
19	5	28	ASN
19	5	29	CYS
19	5	51	SER
19	5	53	CYS
19	5	57	ARG
19	5	60	TYR
19	5	75	ARG
20	6	2	THR
20	6	8	GLN
20	6	26	MET

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Mol	Chain	Res	Type
20	6	44	LYS
20	6	64	ARG
21	7	1	PHE
21	7	2	GLU
21	7	3	ASN
21	7	8	LYS
21	7	16	ASN
21	7	23	LYS
21	7	27	THR
22	8	48	VAL
22	8	49	THR
23	9	15	VAL
23	9	22	LEU
24	0	13	LYS
24	0	42	LYS
24	0	43	SER
26	B	54	CYS
26	B	55	CYS
30	F	405	CYS
31	G	41	CYS
31	G	52	CYS
31	G	55	CYS
31	G	69	CYS
33	I	119	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	18	GLN
1	c	32	GLN
1	c	73	ASN
1	c	85	HIS
1	c	136	GLN
1	c	151	ASN
1	c	154	HIS
1	c	189	HIS
1	c	213	GLN
1	c	240	GLN
1	c	243	HIS
1	c	252	HIS
1	c	308	GLN
1	c	323	HIS

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Mol	Chain	Res	Type
1	c	435	ASN
2	m	62	ASN
2	m	67	HIS
2	m	125	ASN
2	m	162	ASN
2	m	164	HIS
2	m	198	HIS
2	m	247	GLN
2	m	304	HIS
2	m	429	ASN
3	b	15	ASN
3	b	26	ASN
3	b	32	ASN
3	b	114	ASN
3	b	201	HIS
3	b	206	ASN
3	b	312	GLN
3	b	374	ASN
4	d	6	HIS
4	d	50	HIS
4	d	75	ASN
4	d	106	ASN
4	d	181	GLN
4	d	200	HIS
4	d	225	HIS
6	f	22	ASN
6	f	27	ASN
6	f	38	HIS
7	g	6	HIS
7	g	12	HIS
7	g	73	ASN
9	i	71	ASN
10	j	54	HIS
1	l	18	GLN
1	l	32	GLN
1	l	85	HIS
1	l	136	GLN
1	l	151	ASN
1	l	154	HIS
1	l	159	GLN
1	l	189	HIS
1	l	213	GLN

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Mol	Chain	Res	Type
1	l	240	GLN
1	l	243	HIS
1	l	308	GLN
1	l	323	HIS
1	l	435	ASN
2	n	62	ASN
2	n	67	HIS
2	n	125	ASN
2	n	141	GLN
2	n	164	HIS
2	n	198	HIS
2	n	247	GLN
2	n	304	HIS
2	n	429	ASN
3	o	15	ASN
3	o	26	ASN
3	o	32	ASN
3	o	114	ASN
3	o	206	ASN
3	o	374	ASN
4	p	6	HIS
4	p	50	HIS
4	p	75	ASN
4	p	106	ASN
4	p	181	GLN
4	p	225	HIS
5	q	121	GLN
6	r	38	HIS
6	r	73	GLN
7	s	6	HIS
10	v	54	HIS
12	x	11	ASN
12	x	12	HIS
12	x	43	GLN
12	x	99	ASN
12	x	170	ASN
12	x	256	HIS
12	x	360	ASN
12	x	413	HIS
12	x	512	ASN
13	y	103	GLN
13	y	203	ASN

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Mol	Chain	Res	Type
14	z	6	HIS
14	z	12	ASN
14	z	133	ASN
14	z	148	HIS
14	z	158	HIS
14	z	207	HIS
14	z	222	GLN
14	z	232	HIS
15	1	109	HIS
16	2	34	ASN
17	3	66	ASN
18	4	52	HIS
19	5	23	GLN
19	5	24	ASN
19	5	25	GLN
19	5	28	ASN
19	5	37	HIS
21	7	3	ASN
21	7	16	ASN
22	8	10	HIS
22	8	15	ASN
22	8	41	ASN
23	9	42	HIS
24	0	39	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	SF4	B	201	26	0,12,12	-	-	-		
54	FES	q	201	5	0,4,4	-	-	-		
52	HEM	b	402	3	41,50,50	1.39	4 (9%)	45,82,82	2.16	13 (28%)
53	HEC	p	301	4	32,50,50	2.24	5 (15%)	24,82,82	1.92	9 (37%)
54	FES	G	803	31	0,4,4	-	-	-		
52	HEM	o	401	3	41,50,50	1.59	5 (12%)	45,82,82	2.55	19 (42%)
57	HEA	x	604	12	57,67,67	1.47	6 (10%)	61,103,103	1.45	11 (18%)
59	SF4	F	501	30	0,12,12	-	-	-		
59	SF4	G	801	31	0,12,12	-	-	-		
54	FES	E	201	29	0,4,4	-	-	-		
53	HEC	d	301	4	32,50,50	2.20	4 (12%)	24,82,82	2.10	12 (50%)
59	SF4	G	802	31	0,12,12	-	-	-		
59	SF4	I	201	33	0,12,12	-	-	-		
57	HEA	x	603	12	57,67,67	1.25	6 (10%)	61,103,103	1.47	12 (19%)
52	HEM	b	401	3	41,50,50	1.48	4 (9%)	45,82,82	1.87	10 (22%)
59	SF4	I	202	33	0,12,12	-	-	-		
52	HEM	o	402	3	41,50,50	1.57	4 (9%)	45,82,82	1.96	14 (31%)

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
59	SF4	B	201	26	-	-	0/6/5/5
54	FES	q	201	5	-	-	0/1/1/1
52	HEM	b	402	3	-	6/12/54/54	-
53	HEC	p	301	4	-	6/10/54/54	-
54	FES	G	803	31	-	-	0/1/1/1
52	HEM	o	401	3	-	6/12/54/54	-
57	HEA	x	604	12	3/3/7/16	5/32/76/76	-
59	SF4	F	501	30	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	G	801	31	-	-	0/6/5/5
54	FES	E	201	29	-	-	0/1/1/1
53	HEC	d	301	4	-	3/10/54/54	-
59	SF4	G	802	31	-	-	0/6/5/5
59	SF4	I	201	33	-	-	0/6/5/5
57	HEA	x	603	12	3/3/7/16	7/32/76/76	-
52	HEM	b	401	3	-	4/12/54/54	-
59	SF4	I	202	33	-	-	0/6/5/5
52	HEM	o	402	3	-	4/12/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	p	301	HEC	C3C-C2C	-7.19	1.33	1.40
53	d	301	HEC	C2B-C3B	-7.02	1.33	1.40
53	p	301	HEC	C2B-C3B	-6.85	1.33	1.40
53	d	301	HEC	C3C-C2C	-6.55	1.33	1.40
57	x	604	HEA	C3A-C2A	-6.39	1.31	1.40
52	o	402	HEM	C3C-C2C	-5.11	1.33	1.40
52	o	401	HEM	C3C-C2C	-4.89	1.33	1.40
52	b	401	HEM	C3C-C2C	-4.11	1.34	1.40
52	o	402	HEM	C1A-NA	3.99	1.44	1.36
57	x	604	HEA	C3A-CMA	-3.97	1.37	1.46
53	d	301	HEC	CBB-CAB	-3.67	1.35	1.49
53	p	301	HEC	CBC-CAC	-3.62	1.35	1.49
53	d	301	HEC	CBC-CAC	-3.47	1.36	1.49
53	p	301	HEC	CBB-CAB	-3.44	1.36	1.49
52	o	402	HEM	C3C-CAC	3.35	1.54	1.47
52	b	401	HEM	CAB-C3B	3.33	1.56	1.47
52	o	401	HEM	CAB-C3B	3.29	1.56	1.47
57	x	603	HEA	C3C-C2C	-3.28	1.35	1.40
52	o	401	HEM	C3C-CAC	3.22	1.54	1.47
52	b	401	HEM	C3B-C2B	-3.08	1.31	1.37
52	b	402	HEM	C4A-CHB	-3.06	1.32	1.41
52	b	402	HEM	C3C-C2C	-3.00	1.36	1.40
52	b	401	HEM	C3C-CAC	2.97	1.53	1.47
52	b	402	HEM	C2C-C1C	2.96	1.49	1.42
57	x	603	HEA	C3A-CMA	-2.94	1.39	1.46
52	o	401	HEM	C1B-C2B	2.83	1.50	1.44
57	x	604	HEA	C1D-C2D	2.70	1.49	1.44
57	x	603	HEA	C4C-NC	2.69	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	x	604	HEA	C1D-ND	-2.68	1.35	1.40
57	x	604	HEA	C3C-C2C	-2.63	1.36	1.40
57	x	604	HEA	CMD-C2D	2.30	1.55	1.50
52	o	401	HEM	C3D-C2D	-2.25	1.31	1.36
57	x	603	HEA	C3A-C2A	-2.22	1.37	1.40
57	x	603	HEA	C1C-NC	2.18	1.40	1.36
52	o	402	HEM	CAB-C3B	2.17	1.53	1.47
52	b	402	HEM	CAB-C3B	2.13	1.53	1.47
57	x	603	HEA	CHD-C1D	2.09	1.40	1.35
53	p	301	HEC	CAD-C3D	2.01	1.55	1.52

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	o	401	HEM	CMA-C3A-C4A	-6.84	117.95	128.46
52	o	401	HEM	C3B-C2B-C1B	-5.58	102.35	106.49
52	b	402	HEM	CMA-C3A-C4A	-5.42	120.13	128.46
52	b	402	HEM	C4B-CHC-C1C	4.99	129.15	122.56
52	o	402	HEM	C3B-C2B-C1B	4.93	110.15	106.49
52	b	401	HEM	CBD-CAD-C3D	4.72	125.74	112.63
52	o	401	HEM	C4B-C3B-C2B	4.45	110.64	107.11
52	b	401	HEM	CMA-C3A-C4A	-4.37	121.75	128.46
52	o	402	HEM	CMC-C2C-C3C	4.27	132.66	124.68
52	o	401	HEM	C4C-CHD-C1D	4.13	128.01	122.56
52	o	402	HEM	CHC-C4B-NB	4.07	128.85	124.43
52	o	401	HEM	CMA-C3A-C2A	4.04	132.57	124.94
52	b	402	HEM	CMC-C2C-C3C	4.04	132.23	124.68
52	b	401	HEM	O1D-CGD-CBD	-4.01	110.19	123.08
53	d	301	HEC	CMD-C2D-C1D	-3.98	122.34	128.46
57	x	603	HEA	C17-C18-C19	-3.97	118.11	127.66
52	b	401	HEM	CBB-CAB-C3B	-3.90	108.23	127.62
52	o	402	HEM	CHB-C1B-NB	-3.82	119.66	124.38
52	b	402	HEM	C4D-ND-C1D	3.69	108.89	105.07
52	o	401	HEM	C2B-C1B-NB	3.62	114.13	109.84
52	b	402	HEM	CAA-CBA-CGA	3.60	123.86	113.76
57	x	604	HEA	C4A-CHB-C1B	3.57	127.28	122.56
52	b	402	HEM	CMA-C3A-C2A	3.57	131.68	124.94
52	o	401	HEM	O1D-CGD-CBD	-3.57	111.61	123.08
52	o	401	HEM	CHB-C1B-NB	-3.55	119.99	124.38
52	o	401	HEM	O2D-CGD-O1D	3.54	132.13	123.30
53	p	301	HEC	CMD-C2D-C1D	-3.49	123.09	128.46
52	o	401	HEM	C4A-C3A-C2A	3.47	109.41	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	d	301	HEC	CMB-C2B-C1B	-3.44	123.18	128.46
52	b	402	HEM	CHD-C1D-ND	3.35	128.07	124.43
52	o	401	HEM	C4B-CHC-C1C	3.34	126.97	122.56
52	b	402	HEM	CAD-CBD-CGD	3.29	120.68	113.60
53	d	301	HEC	CBD-CAD-C3D	3.17	118.04	112.62
57	x	603	HEA	C13-C14-C15	-3.17	120.03	127.66
52	o	402	HEM	CMA-C3A-C4A	-3.17	123.60	128.46
52	o	402	HEM	O1D-CGD-CBD	-3.04	113.32	123.08
53	p	301	HEC	CBD-CAD-C3D	3.02	117.78	112.62
52	b	402	HEM	O2A-CGA-CBA	3.00	123.66	114.03
53	p	301	HEC	CMA-C3A-C2A	2.99	130.58	124.94
52	b	402	HEM	O2A-CGA-O1A	-2.92	116.01	123.30
52	b	401	HEM	O2A-CGA-O1A	2.92	130.58	123.30
52	o	402	HEM	C4A-C3A-C2A	2.89	109.00	107.00
52	b	402	HEM	CHB-C1B-NB	-2.86	120.85	124.38
57	x	603	HEA	C1B-C2B-C3B	2.83	110.19	106.80
52	b	401	HEM	CMB-C2B-C1B	-2.83	120.73	125.04
57	x	604	HEA	CBA-CAA-C2A	2.82	117.36	112.60
52	o	401	HEM	C1B-NB-C4B	-2.81	102.17	105.07
52	o	401	HEM	CMD-C2D-C1D	-2.79	120.79	125.04
53	p	301	HEC	O1D-CGD-CBD	-2.67	114.50	123.08
53	p	301	HEC	CBA-CAA-C2A	2.66	117.09	112.60
53	p	301	HEC	CMB-C2B-C1B	-2.66	124.38	128.46
52	b	401	HEM	CMA-C3A-C2A	2.65	129.93	124.94
57	x	604	HEA	C4D-CHA-C1A	2.64	126.04	122.56
52	o	401	HEM	CBA-CAA-C2A	2.62	117.10	112.62
52	o	401	HEM	CAB-C3B-C2B	-2.61	119.99	128.60
57	x	604	HEA	CMD-C2D-C1D	2.59	128.98	125.04
53	d	301	HEC	CMB-C2B-C3B	2.57	128.84	125.82
53	d	301	HEC	C4C-C3C-C2C	2.56	109.12	106.35
52	b	402	HEM	CBD-CAD-C3D	2.55	119.72	112.63
53	d	301	HEC	O1A-CGA-CBA	-2.51	115.01	123.08
53	d	301	HEC	O2D-CGD-O1D	2.51	129.54	123.30
52	o	402	HEM	C4B-C3B-C2B	-2.49	105.14	107.11
52	o	401	HEM	CMB-C2B-C3B	2.48	134.36	128.30
52	b	401	HEM	O2D-CGD-CBD	2.47	121.96	114.03
52	o	402	HEM	C4C-CHD-C1D	2.46	125.80	122.56
52	o	401	HEM	CBD-CAD-C3D	2.45	119.43	112.63
57	x	604	HEA	CMC-C2C-C3C	2.44	129.25	124.68
52	o	401	HEM	CHA-C4D-ND	-2.44	121.37	124.38
57	x	604	HEA	C1D-C2D-C3D	-2.43	104.40	106.96
57	x	603	HEA	C17-C16-C15	-2.42	105.03	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	b	401	HEM	C4B-C3B-C2B	2.37	109.00	107.11
52	o	402	HEM	CMB-C2B-C3B	-2.37	122.50	128.30
52	o	402	HEM	CHC-C4B-C3B	-2.36	120.95	124.57
57	x	603	HEA	C16-C17-C18	-2.36	104.14	111.88
57	x	603	HEA	C20-C19-C18	2.36	125.88	121.12
57	x	604	HEA	CMB-C2B-C3B	-2.34	125.89	130.34
57	x	603	HEA	CAD-C3D-C4D	2.31	128.69	124.66
57	x	604	HEA	C25-C23-C24	2.30	119.69	114.60
53	d	301	HEC	CMD-C2D-C3D	2.29	129.26	124.94
53	d	301	HEC	O1D-CGD-CBD	-2.27	115.78	123.08
52	b	402	HEM	C3D-C4D-ND	-2.27	107.64	110.17
57	x	604	HEA	C13-C14-C15	-2.27	122.19	127.66
53	d	301	HEC	CMA-C3A-C2A	2.25	129.19	124.94
52	o	402	HEM	CBA-CAA-C2A	2.23	116.43	112.62
52	o	402	HEM	CMD-C2D-C1D	-2.23	121.64	125.04
52	o	402	HEM	O2D-CGD-CBD	2.22	121.15	114.03
53	p	301	HEC	CMD-C2D-C3D	2.20	129.09	124.94
57	x	603	HEA	C12-C13-C14	-2.19	106.46	112.23
57	x	604	HEA	C26-C15-C16	2.17	118.92	115.27
57	x	603	HEA	C4B-C3B-C2B	-2.14	103.75	107.41
57	x	603	HEA	C4A-CHB-C1B	2.09	125.32	122.56
53	p	301	HEC	C4C-C3C-C2C	2.08	108.60	106.35
57	x	603	HEA	C27-C19-C18	-2.08	118.35	123.68
52	o	401	HEM	O1A-CGA-CBA	-2.07	116.44	123.08
57	x	603	HEA	C3C-C4C-NC	2.04	111.85	109.21
53	d	301	HEC	CMC-C2C-C1C	-2.04	125.33	128.46
52	b	401	HEM	C4C-CHD-C1D	2.04	125.25	122.56
57	x	604	HEA	CBD-CAD-C3D	2.04	118.30	112.63
53	p	301	HEC	O1A-CGA-CBA	-2.01	116.62	123.08
53	d	301	HEC	C1D-C2D-C3D	2.01	108.39	107.00

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	x	603	HEA	NB
57	x	603	HEA	NA
57	x	603	HEA	ND
57	x	604	HEA	NB
57	x	604	HEA	NA
57	x	604	HEA	ND

All (41) torsion outliers are listed below:

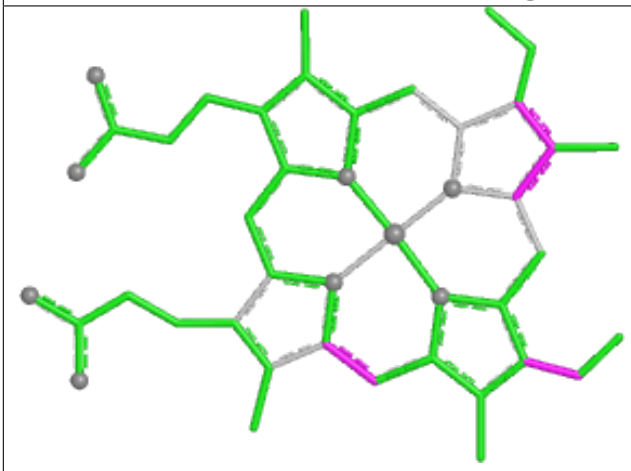
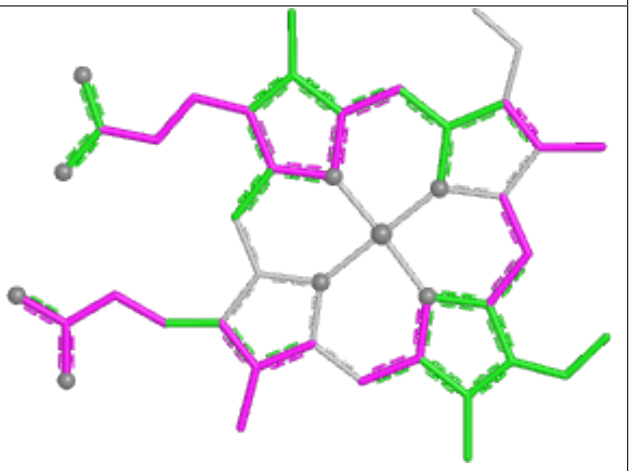
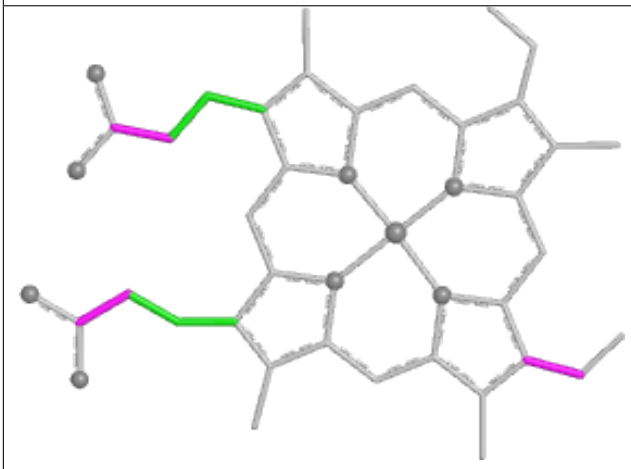
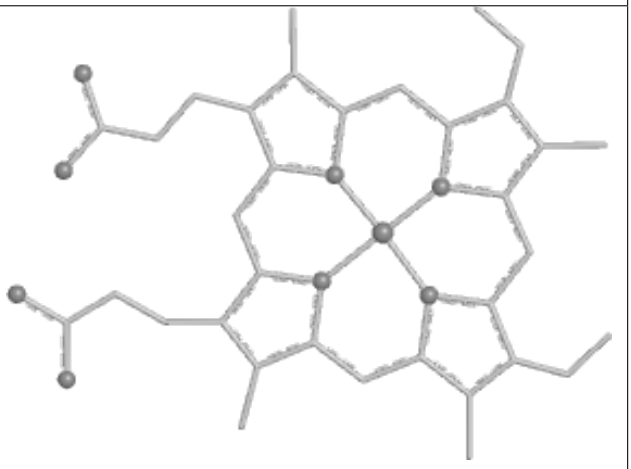
Mol	Chain	Res	Type	Atoms
52	o	401	HEM	C2B-C3B-CAB-CBB
57	x	603	HEA	C12-C11-C3B-C2B
57	x	603	HEA	C15-C16-C17-C18
52	o	401	HEM	C4B-C3B-CAB-CBB
52	b	402	HEM	C2B-C3B-CAB-CBB
53	p	301	HEC	C2A-CAA-CBA-CGA
53	p	301	HEC	C1A-C2A-CAA-CBA
53	p	301	HEC	C3A-C2A-CAA-CBA
52	o	401	HEM	CAD-CBD-CGD-O2D
52	b	402	HEM	CAA-CBA-CGA-O2A
52	o	401	HEM	CAD-CBD-CGD-O1D
57	x	603	HEA	CAD-CBD-CGD-O1D
52	o	402	HEM	CAA-CBA-CGA-O1A
52	b	401	HEM	CAD-CBD-CGD-O2D
53	d	301	HEC	CAA-CBA-CGA-O1A
53	p	301	HEC	CAA-CBA-CGA-O1A
52	b	401	HEM	CAD-CBD-CGD-O1D
52	b	402	HEM	CAA-CBA-CGA-O1A
57	x	604	HEA	CAD-CBD-CGD-O1D
53	d	301	HEC	CAA-CBA-CGA-O2A
52	b	402	HEM	CAD-CBD-CGD-O1D
57	x	604	HEA	CAD-CBD-CGD-O2D
52	o	402	HEM	CAA-CBA-CGA-O2A
53	p	301	HEC	CAA-CBA-CGA-O2A
57	x	603	HEA	CAA-CBA-CGA-O1A
52	o	401	HEM	CAA-CBA-CGA-O2A
52	o	402	HEM	CAD-CBD-CGD-O2D
57	x	603	HEA	CAD-CBD-CGD-O2D
52	b	402	HEM	CAD-CBD-CGD-O2D
52	o	402	HEM	CAD-CBD-CGD-O1D
52	b	401	HEM	CAA-CBA-CGA-O2A
52	o	401	HEM	CAA-CBA-CGA-O1A
52	b	402	HEM	C4B-C3B-CAB-CBB
57	x	604	HEA	CAA-CBA-CGA-O2A
52	b	401	HEM	CAA-CBA-CGA-O1A
57	x	604	HEA	CAA-CBA-CGA-O1A
57	x	603	HEA	CAA-CBA-CGA-O2A
53	p	301	HEC	CAD-CBD-CGD-O2D
57	x	604	HEA	C26-C15-C16-C17
53	d	301	HEC	C2A-CAA-CBA-CGA
57	x	603	HEA	O11-C11-C3B-C2B

There are no ring outliers.

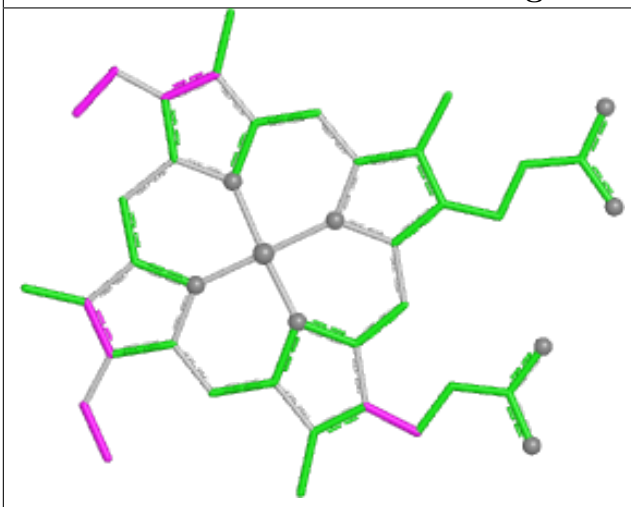
5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	B	201	SF4	6	0
54	G	803	FES	3	0
59	F	501	SF4	1	0
59	I	201	SF4	2	0
59	I	202	SF4	3	0

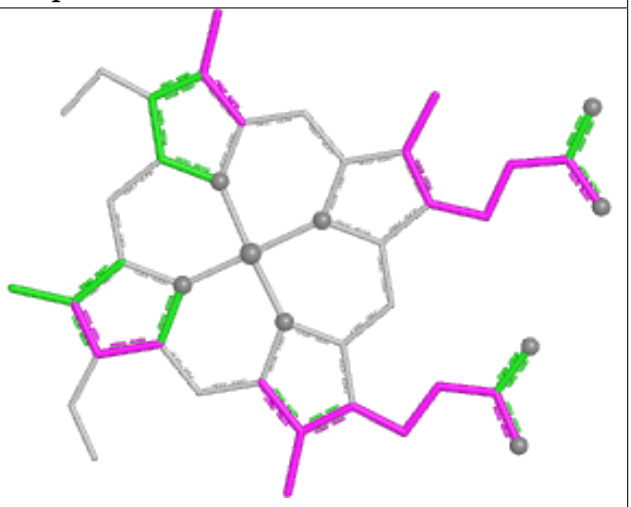
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand HEM b 402	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

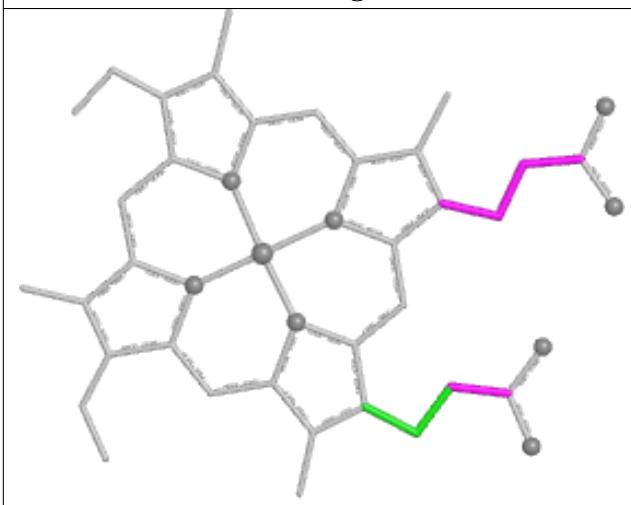
Ligand HEC p 301



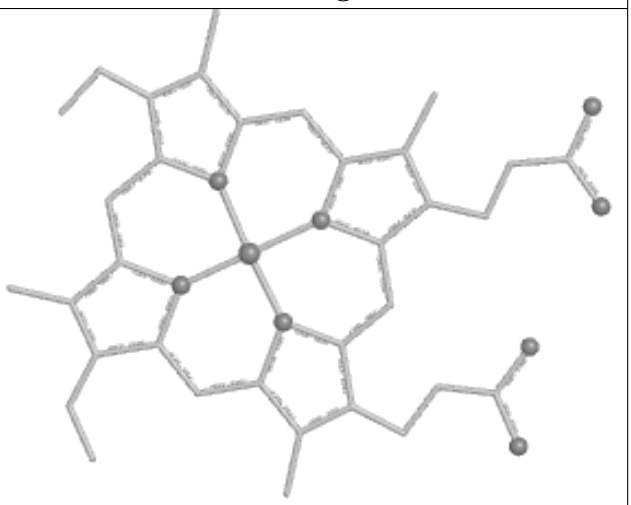
Bond lengths



Bond angles

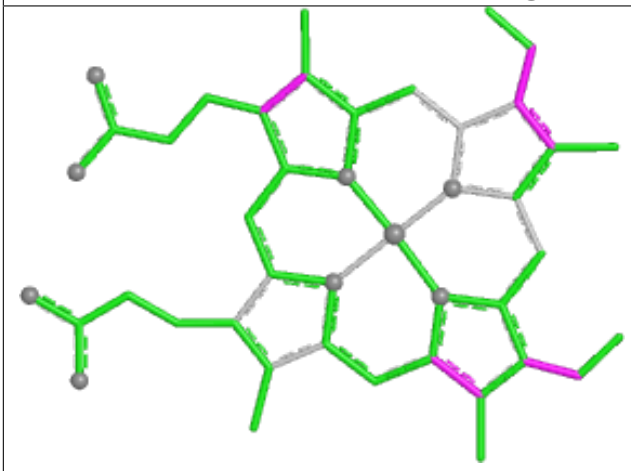


Torsions

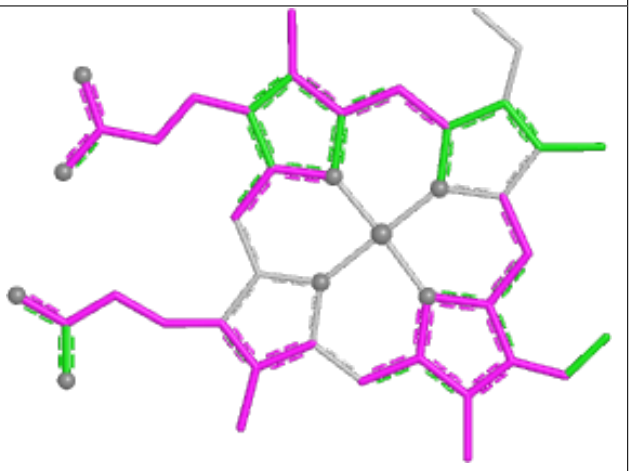


Rings

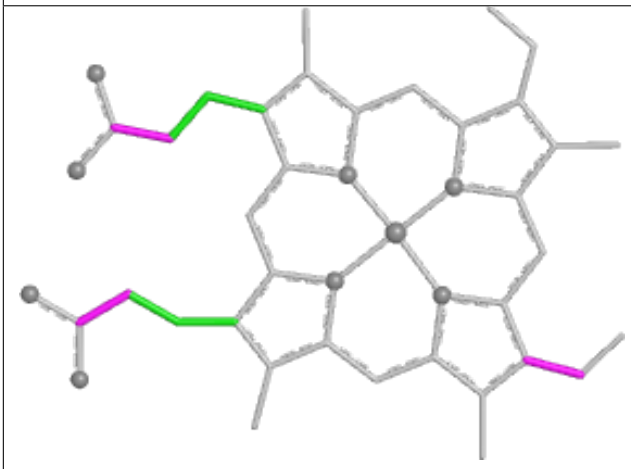
Ligand HEM o 401



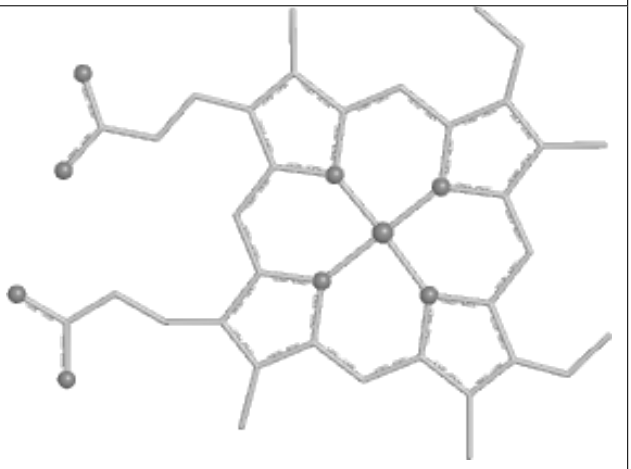
Bond lengths



Bond angles

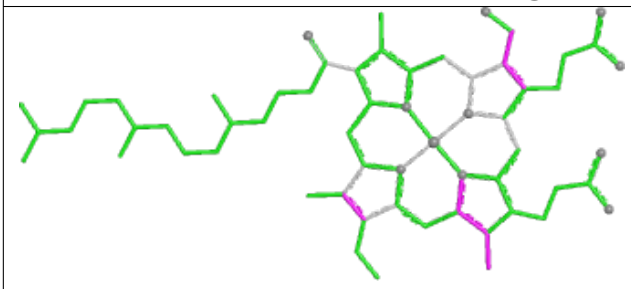


Torsions

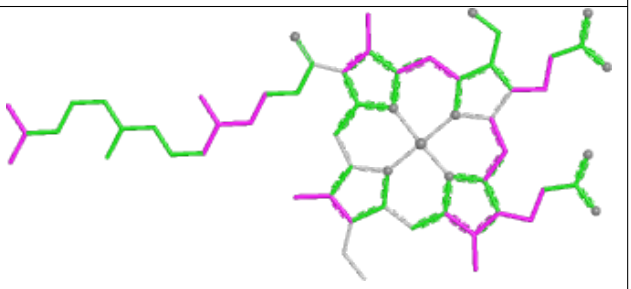


Rings

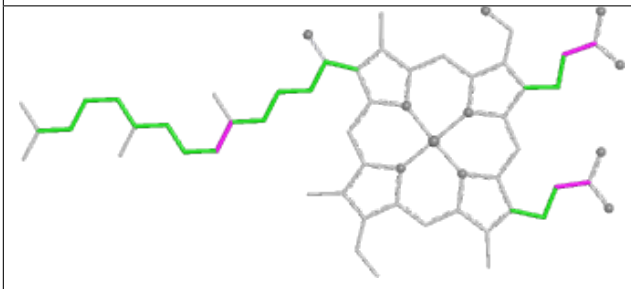
Ligand HEA x 604



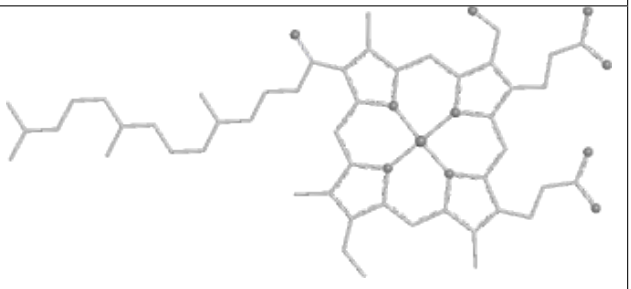
Bond lengths



Bond angles

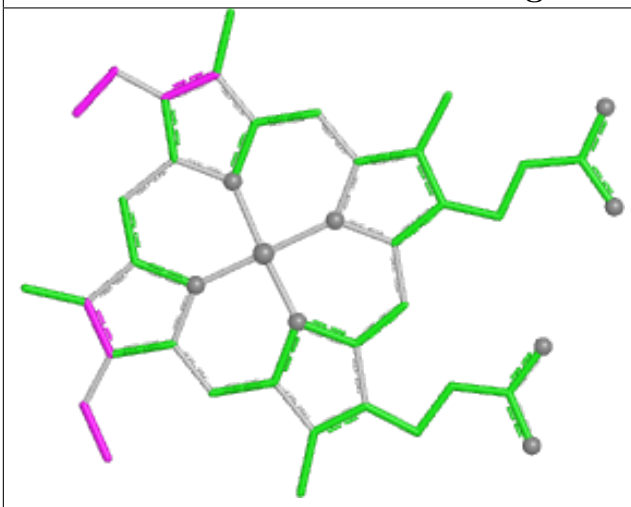


Torsions

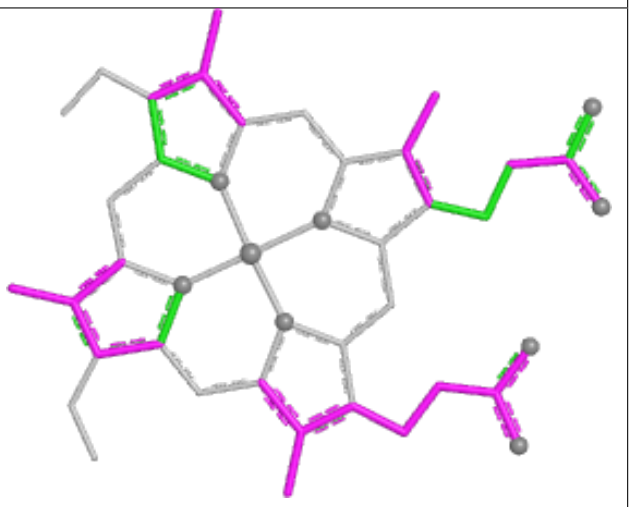


Rings

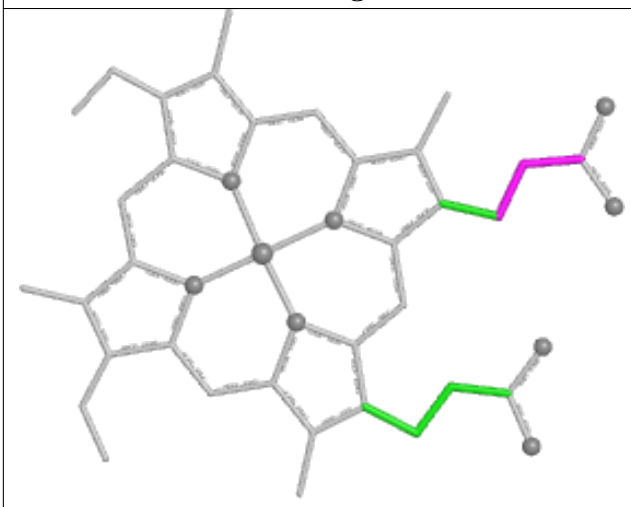
Ligand HEC d 301



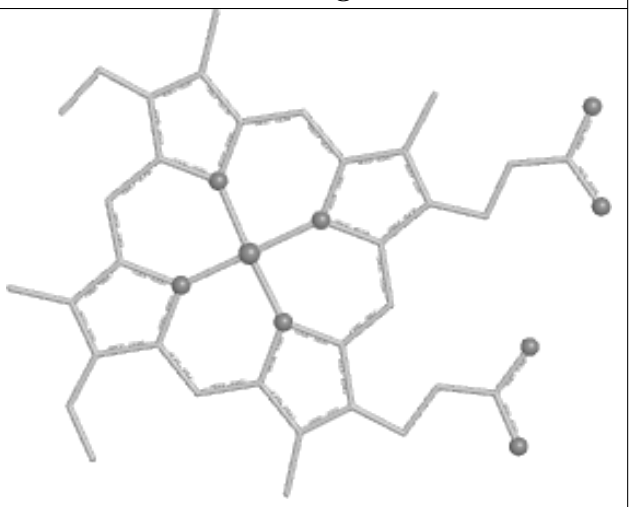
Bond lengths



Bond angles

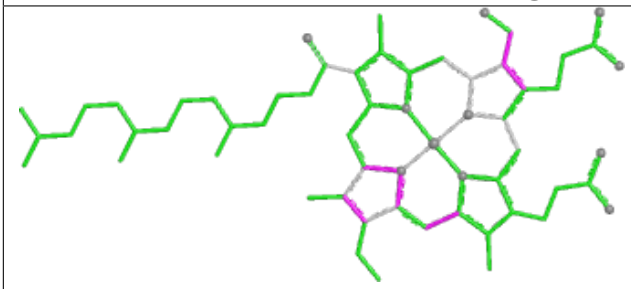


Torsions

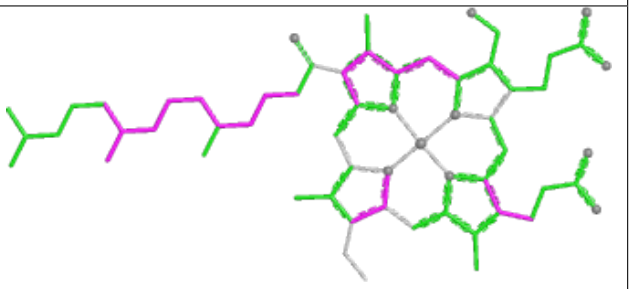


Rings

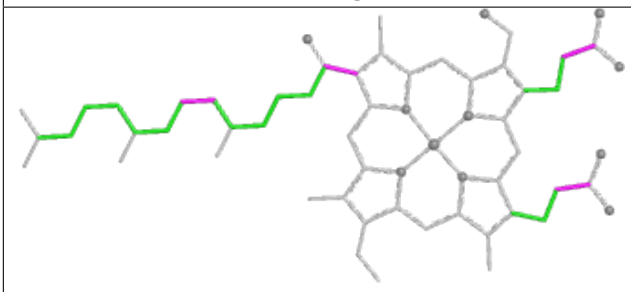
Ligand HEA x 603



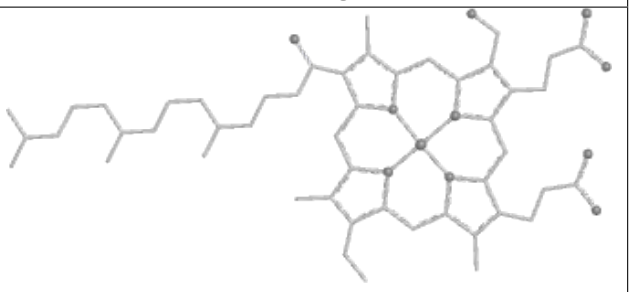
Bond lengths



Bond angles

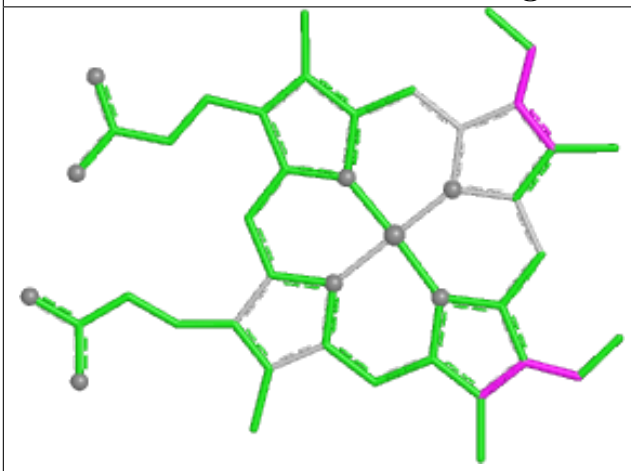


Torsions

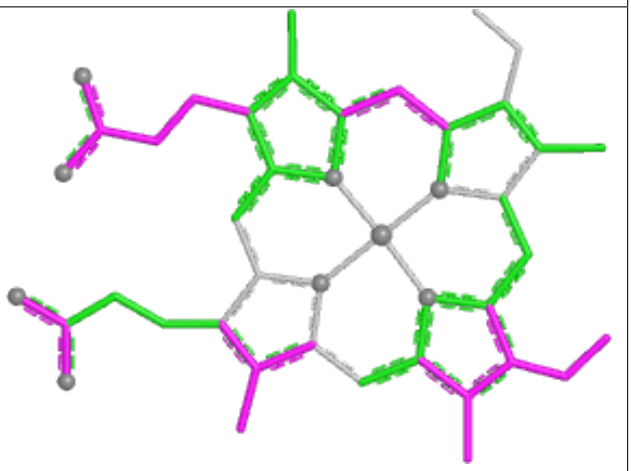


Rings

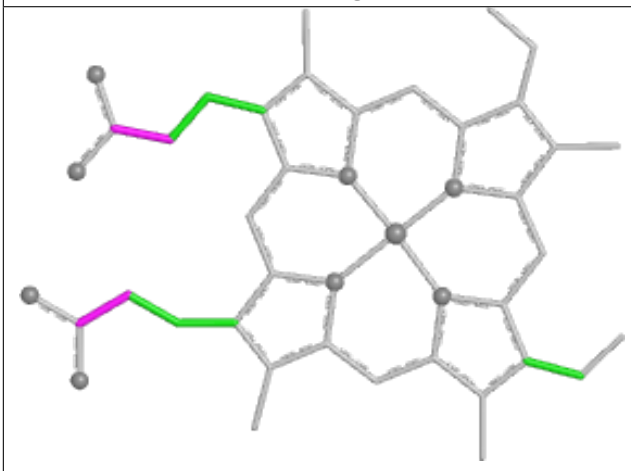
Ligand HEM b 401



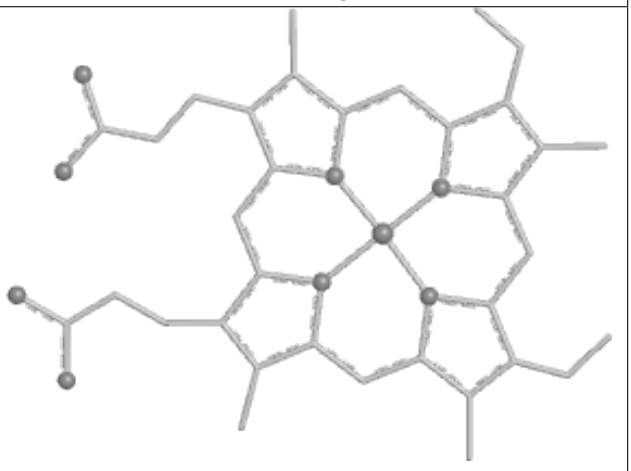
Bond lengths



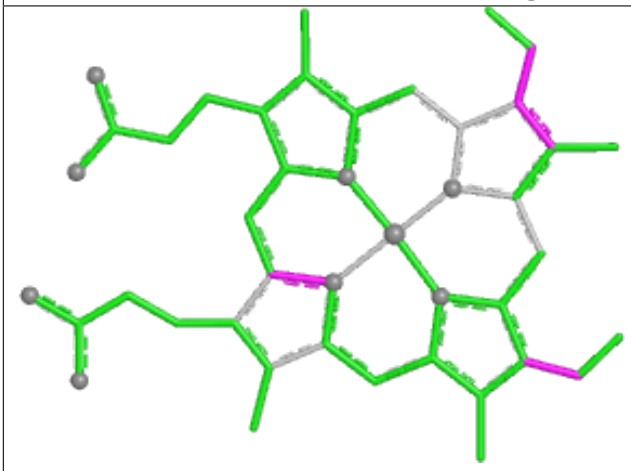
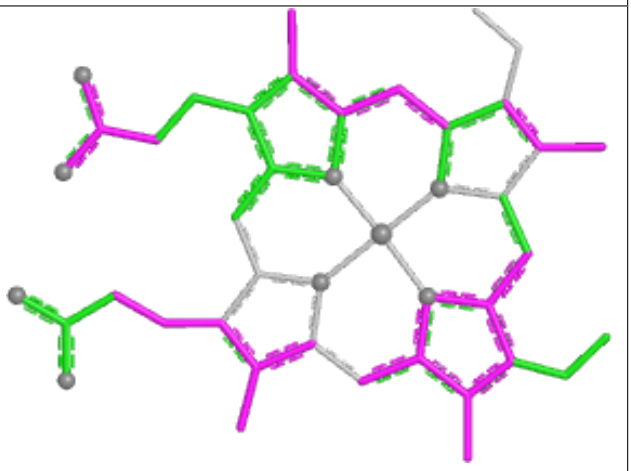
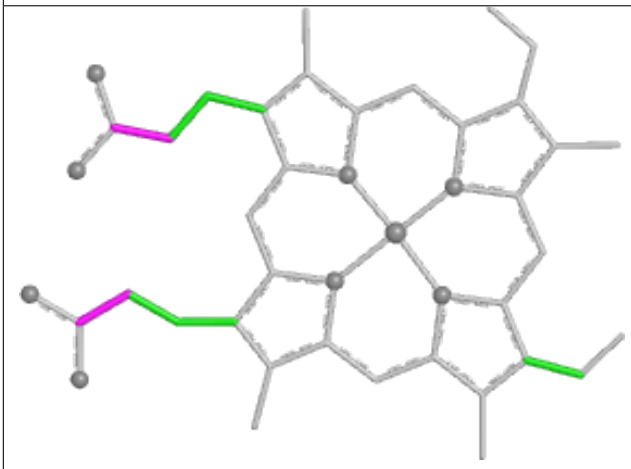
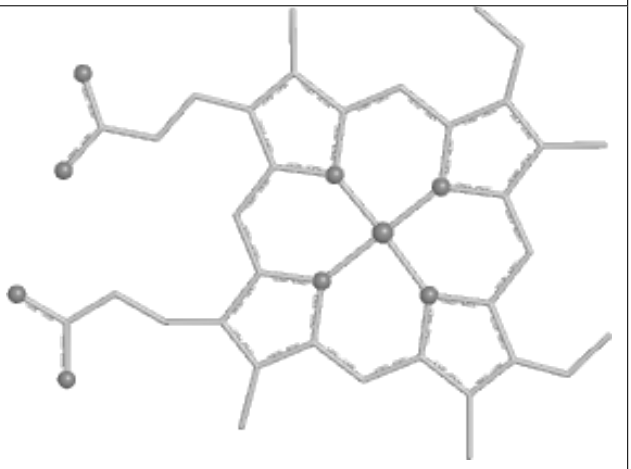
Bond angles



Torsions



Rings

Ligand HEM o 402	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
50	U	8
47	X	7
51	Z	6
31	G	6
36	L	5
39	O	3
34	J	2

Continued on next page...

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Mol	Chain	Number of breaks
40	P	2
32	H	2
44	T	2
49	a	1
25	A	1
38	N	1
37	M	1
41	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	226:UNK	C	301:UNK	N	71.67
1	X	113:UNK	C	133:UNK	N	66.39
1	U	27:UNK	C	101:UNK	N	63.89
1	a	29:UNK	C	101:UNK	N	61.67
1	U	630:UNK	C	701:UNK	N	57.60
1	Z	34:UNK	C	101:UNK	N	53.76
1	U	330:UNK	C	401:UNK	N	52.64
1	Z	124:UNK	C	201:UNK	N	45.23
1	U	530:UNK	C	601:UNK	N	42.27
1	A	23:UNK	C	52:UNK	N	39.81
1	X	615:UNK	C	701:UNK	N	36.95
1	U	220:UNK	C	301:UNK	N	35.63
1	Z	259:UNK	C	308:UNK	N	35.43
1	X	428:UNK	C	501:UNK	N	35.30
1	U	724:UNK	C	801:UNK	N	31.76
1	J	107:UNK	C	140:UNK	N	30.90
1	X	357:UNK	C	401:UNK	N	28.19
1	N	300:UNK	C	320:UNK	N	26.56
1	P	250:UNK	C	285:UNK	N	26.49
1	L	466:UNK	C	487:UNK	N	23.59
1	G	347:UNK	C	367:UNK	N	22.81
1	M	415:UNK	C	430:UNK	N	22.06
1	P	185:UNK	C	203:UNK	N	21.21
1	H	200:UNK	C	219:UNK	N	20.56
1	Z	421:UNK	C	501:UNK	N	20.30
1	J	76:UNK	C	85:UNK	N	19.66
1	Z	528:UNK	C	601:UNK	N	19.36
1	Z	382:UNK	C	401:UNK	N	19.30
1	H	242:UNK	C	253:UNK	N	18.95
1	U	139:UNK	C	201:UNK	N	18.89
1	G	495:UNK	C	525:UNK	N	18.00

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Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	513:UNK	C	520:UNK	N	17.41
1	G	530:UNK	C	542:UNK	N	16.15
1	U	422:UNK	C	501:UNK	N	15.81
1	L	400:UNK	C	408:UNK	N	14.38
1	Q	59:UNK	C	76:UNK	N	13.52
1	O	54:UNK	C	79:UNK	N	12.62
1	G	318:UNK	C	326:UNK	N	12.59
1	L	22:UNK	C	28:UNK	N	11.17
1	O	167:UNK	C	172:UNK	N	11.07
1	X	197:UNK	C	201:UNK	N	10.95
1	O	210:UNK	C	222:UNK	N	10.93
1	T	23:UNK	C	28:UNK	N	9.73
1	L	358:UNK	C	363:UNK	N	8.92
1	G	410:UNK	C	425:UNK	N	7.46
1	G	400:UNK	C	404:UNK	N	6.25
1	X	527:UNK	C	601:UNK	N	5.18
1	T	8:UNK	C	9:UNK	N	1.65

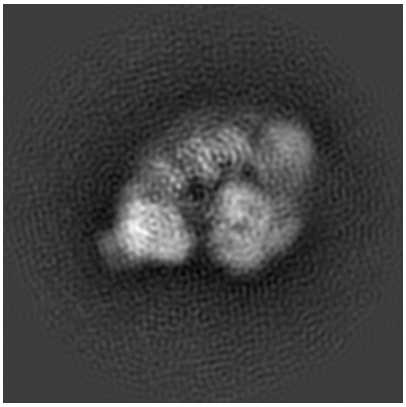
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4107. These allow visual inspection of the internal detail of the map and identification of artifacts.

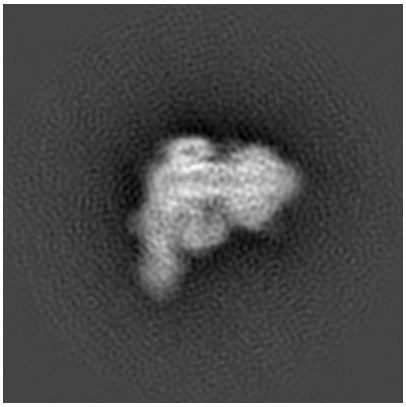
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

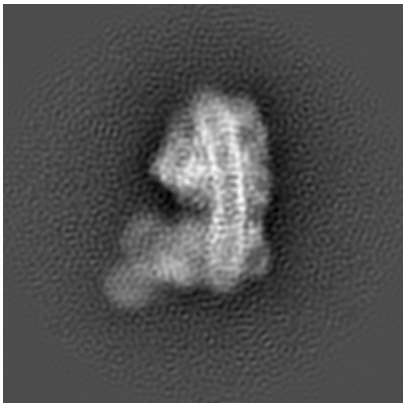
6.1.1 Primary map



X



Y

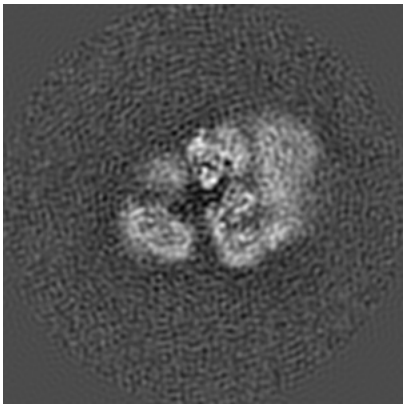


Z

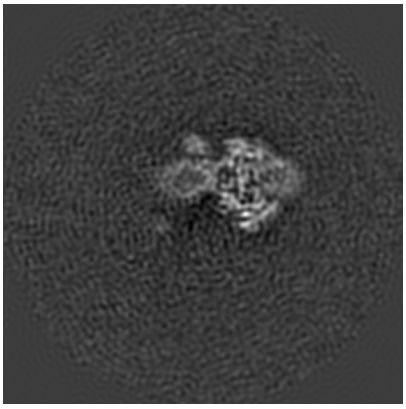
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 144



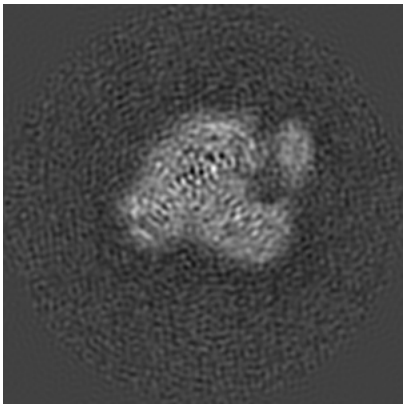
Y Index: 144

Z Index: 144

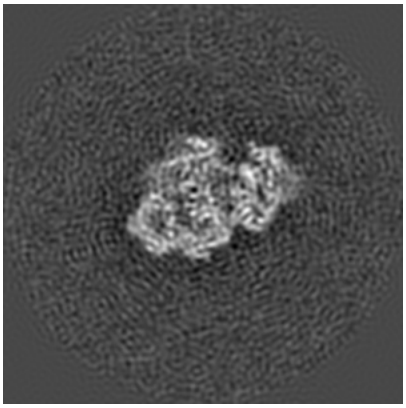
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

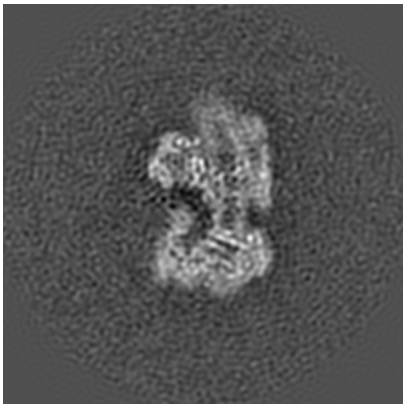
6.3.1 Primary map



X Index: 170



Y Index: 166

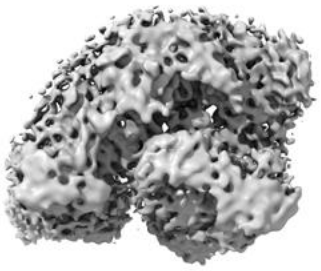


Z Index: 139

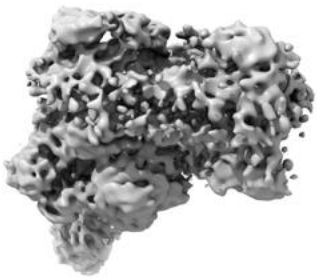
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.081. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

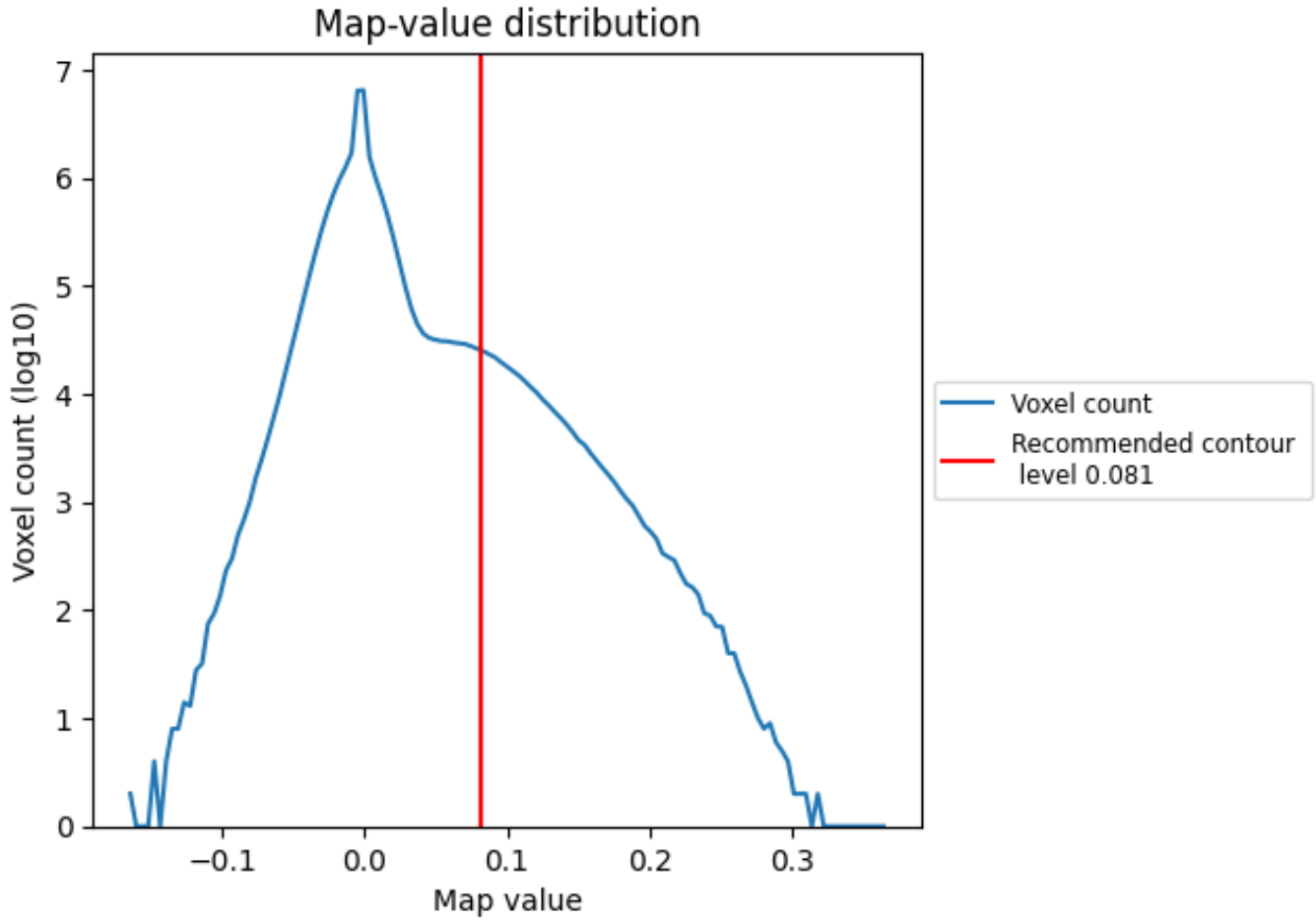
6.5 Mask visualisation (i)

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

7 Map analysis

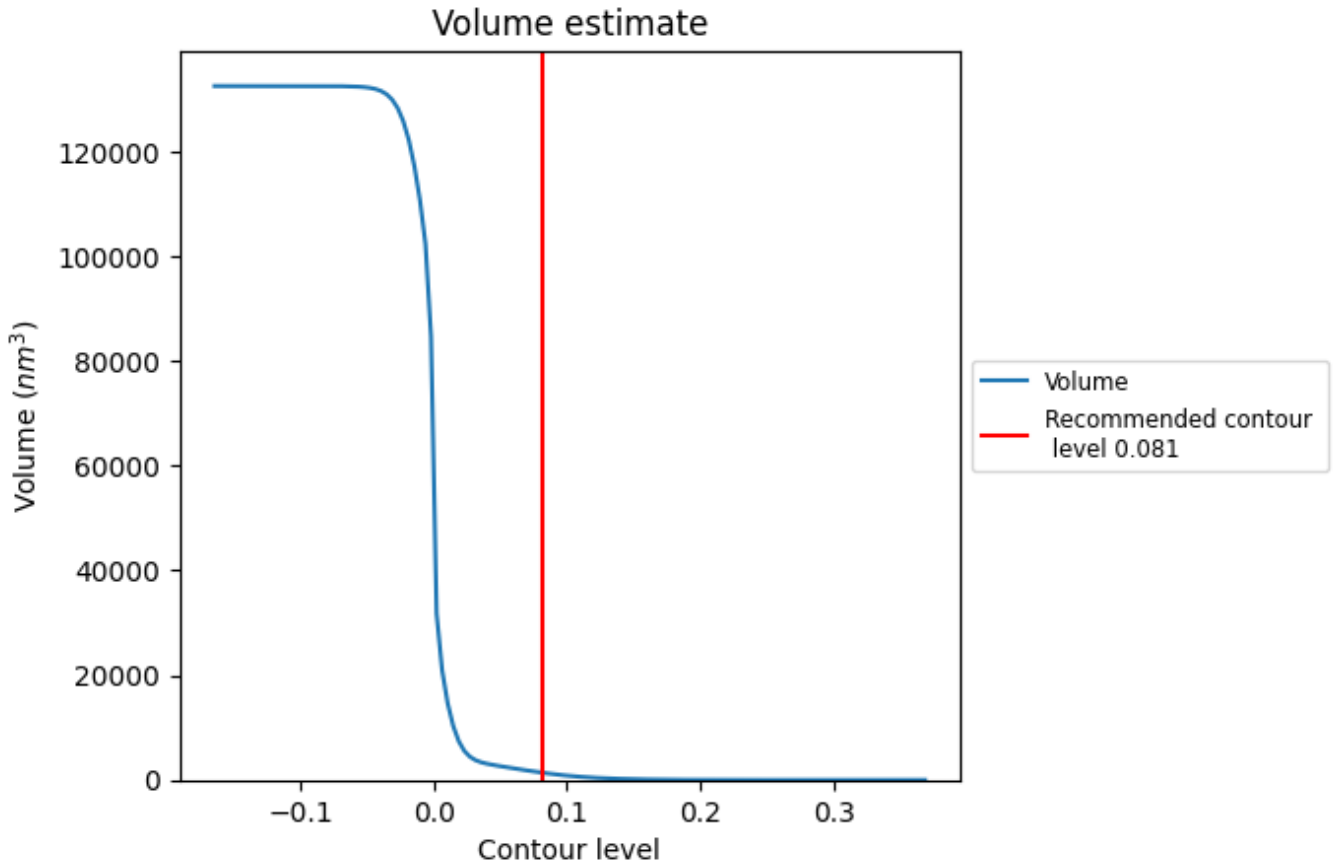
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

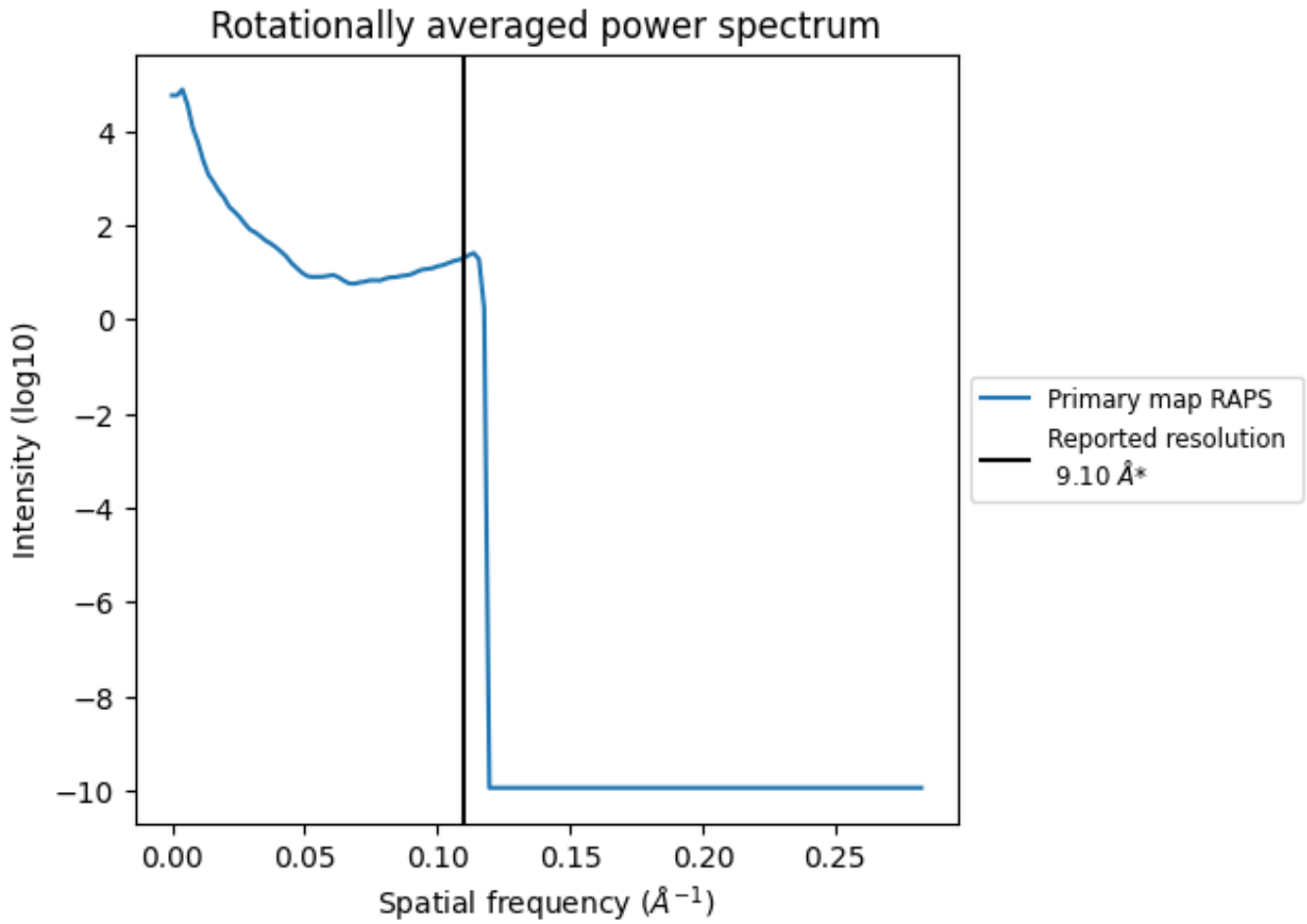
7.2 Volume estimate



The volume at the recommended contour level is 1405 nm^3; this corresponds to an approximate mass of 1269 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.110 Å^{-1}

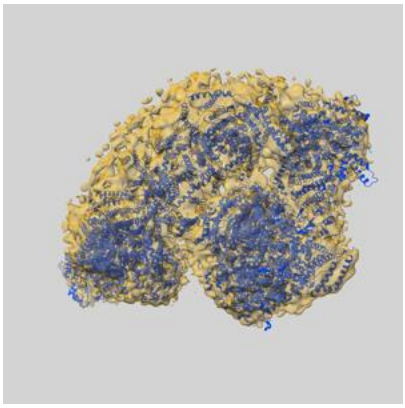
8 Fourier-Shell correlation

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

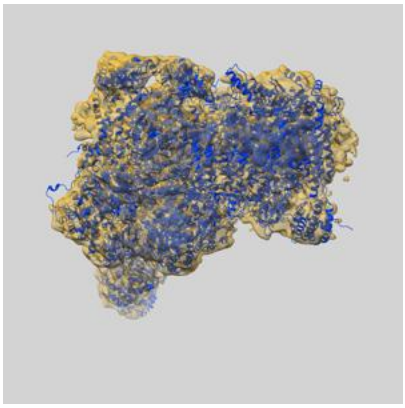
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4107 and PDB model 5LUF. Per-residue inclusion information can be found in section 3 on page 18.

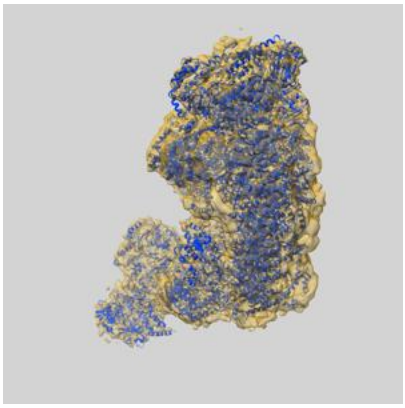
9.1 Map-model overlay



X



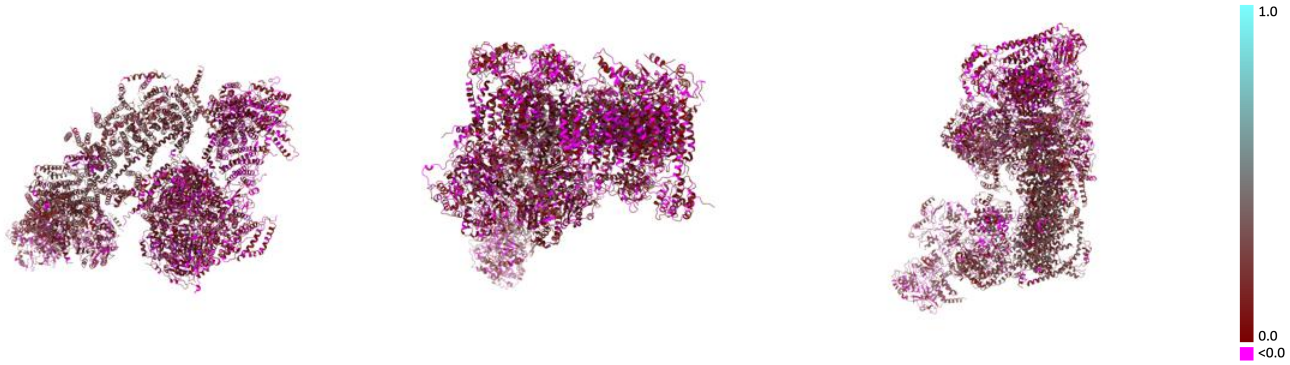
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.081 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

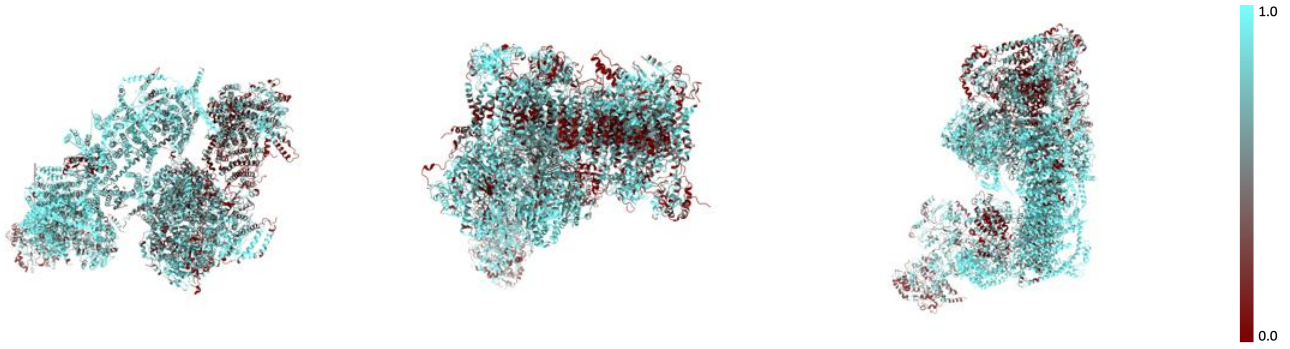
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

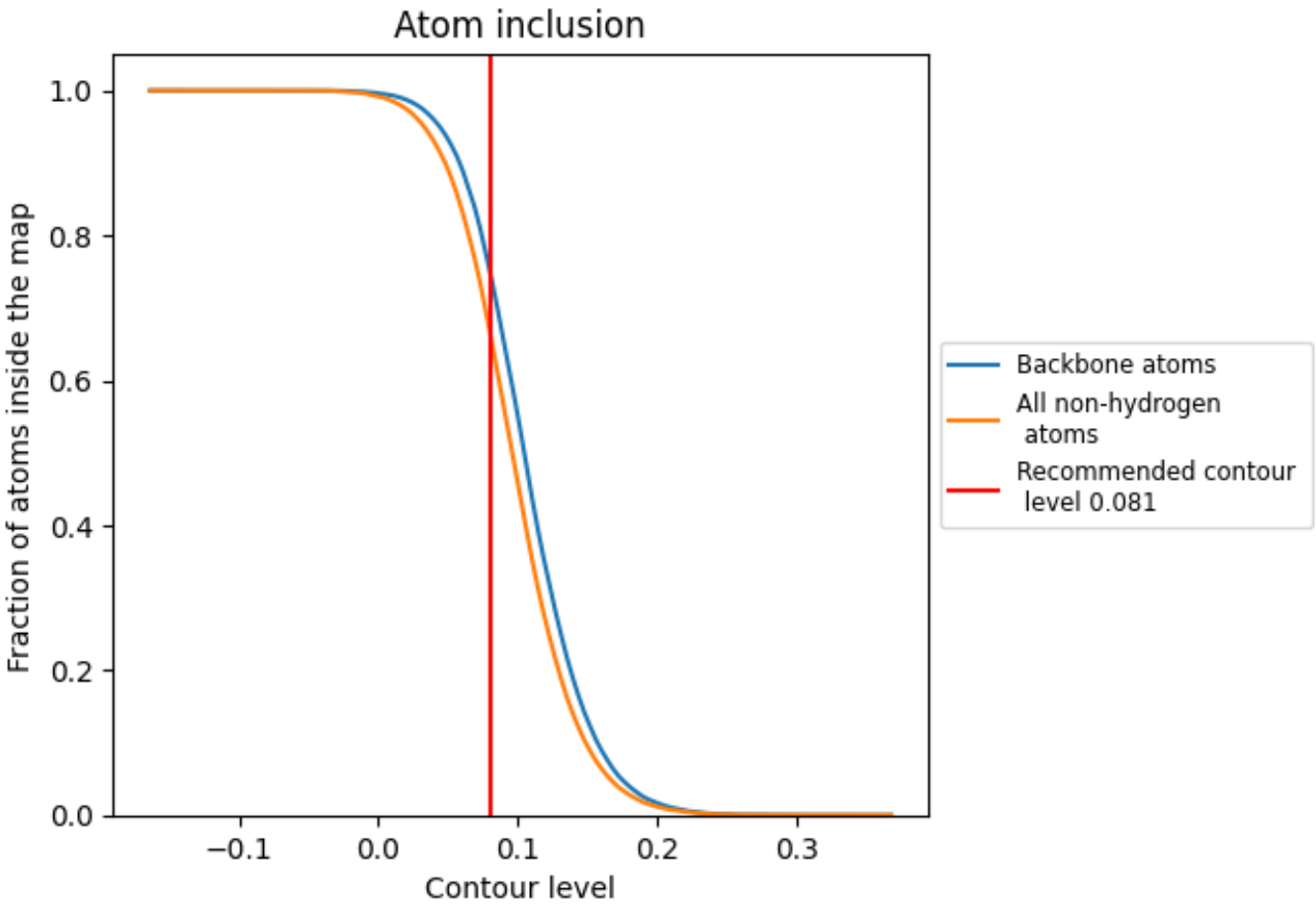
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.081).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 66% 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 (0.081) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6583	0.1160
0	0.5211	0.1040
1	0.4155	0.0580
2	0.4347	0.0580
3	0.4016	0.0310
4	0.2190	-0.0020
5	0.2607	0.0540
6	0.4552	0.0650
7	0.2794	0.0510
8	0.5333	0.0780
9	0.5000	0.0550
A	0.8096	0.2640
B	0.8171	0.1760
C	0.8442	0.1700
D	0.8536	0.1700
E	0.5044	0.0580
F	0.4688	0.0870
G	0.7286	0.1010
H	0.7986	0.2150
I	0.8669	0.1290
J	0.7832	0.2180
K	0.8571	0.2430
L	0.7946	0.2180
M	0.8387	0.2470
N	0.8620	0.2510
O	0.1381	0.0250
P	0.7627	0.1270
Q	0.5391	0.1060
R	0.3149	0.0480
S	0.6200	0.1160
T	0.5577	0.1320
U	0.8296	0.2110
V	0.9634	0.2470
W	0.7806	0.1910
X	0.9629	0.2400

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Chain	Atom inclusion	Q-score
Y	0.8396	0.2070
Z	0.9308	0.2490
a	0.8056	0.2040
b	0.6240	0.1050
c	0.7549	0.0740
d	0.7178	0.0810
e	0.3196	0.0120
f	0.7370	0.1280
g	0.5549	0.0720
h	0.7500	0.0750
i	0.0295	-0.0600
j	0.3780	0.0430
k	0.4452	0.1510
l	0.7209	0.1030
m	0.7675	0.1000
n	0.8218	0.1160
o	0.5954	0.1030
p	0.6712	0.0830
q	0.3811	0.0600
r	0.6440	0.1280
s	0.5884	0.0990
t	0.6738	0.0770
u	0.0549	-0.0640
v	0.4060	0.0980
w	0.3032	0.0900
x	0.5070	0.0580
y	0.6130	0.0520
z	0.4051	0.0220