Full wwPDB EM Validation Report (i)

Sep 10, 2026 – 10:24 am BST

PDB ID	:	2YBB / pdb_00002ybb
EMDB ID	:	EMD-1876
Title	:	Fitted model for bovine mitochondrial supercomplex I1III2IV1 by single particle cryo-EM (EMD-1876)
Authors	:	Althoff, T.; Mills, D.J.; Popot, J.-L.; Kuehlbrandt, W.
Deposited on	:	2011-03-02
Resolution	:	19.00 Å(reported)
Based on initial models	:	1PP9, 2B4Z, 3M9C, 3IAM, 1OCC, 1BGY

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 (i) 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 (i)) were used in the production of this report:

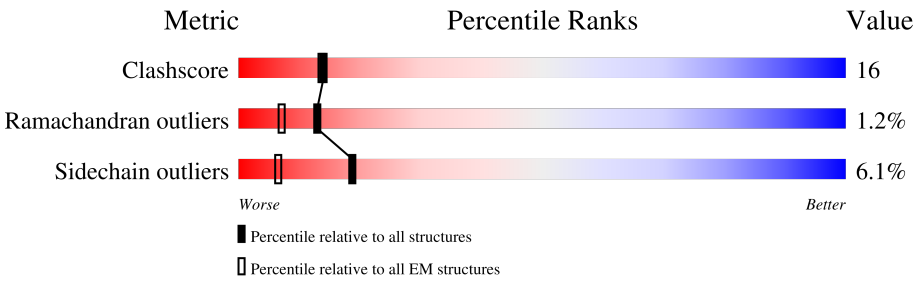
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

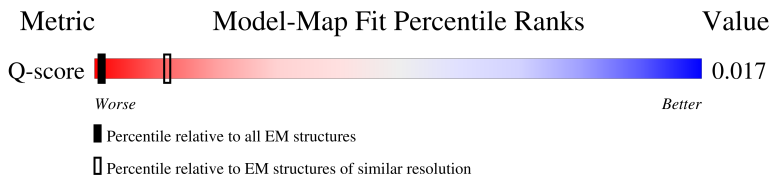
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 19.00 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	17 (18.70 - 19.50)

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	1	438	9% 53% 39% 8%
2	2	181	23% 52% 40% 7% •
3	3	783	15% 48% 40% 8% •
4	4	409	17% 42% 42% 9% 8%

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Mol	Chain	Length	Quality of chain
5	5	207	13% 48% 37% 9% 5%
6	6	181	7% 36% 36% 7% 20%
7	7	129	36% 64% 32%
8	8	182	42% 36% 7% 15%
9	A	446	9% 76% 21%
9	a	446	79% 18%
10	B	439	10% 77% 19%
10	b	439	5% 79% 16%
11	C	379	16% 79% 16%
11	c	379	16% 78% 17%
12	D	241	85% 14%
12	d	241	5% 80% 18%
13	E	196	30% 77% 21%
13	e	196	37% 80% 19%
14	F	110	72% 15% 10%
14	f	110	31% 71% 15% 10%
15	G	81	62% 27% 7%
15	g	81	11% 64% 25% 5% 6%
16	H	78	12% 62% 19% 15%
16	h	78	65% 19% 15%
17	I	65	12% 31% 32% 35%
17	i	65	5% 34% 28% 35%
18	J	62	5% 69% 27%
18	j	62	15% 69% 24% 6%
19	K	56	18% 12% 21% 5% 61%

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Mol	Chain	Length	Quality of chain
19	k	56	11% 18% 9% 61%
20	L	514	18% 69% 26% 5%
21	M	227	61% 34%
22	N	261	9% 71% 24% 5%
23	O	147	12% 70% 25%
24	P	109	16% 75% 21%
25	Q	98	53% 61% 30% 9%
26	R	84	11% 61% 26% 12%
27	S	85	36% 54% 29% 5% 12%
28	T	73	71% 23% 5%
29	U	59	14% 68% 17% 10%
30	V	56	20% 57% 29% 12%
31	W	47	11% 74% 23%
32	X	46	30% 63% 28% 7%
33	Y	104	56% 76% 24%
34	m	474	24% 95% 5%
35	n	391	28% 96%
36	o	378	26% 97%
37	p	281	20% 98%

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
38	SF4	8	183	-	-	X	-
47	HEC	D	501	X	-	-	-
47	HEC	d	501	X	-	-	-

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 72626 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 NADH-QUINONE OXIDOREDUCTASE SUBUNIT 1.

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

- Molecule 2 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 2.

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

- Molecule 3 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 3.

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

- Molecule 4 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 4.

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

- Molecule 5 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 5.

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

- Molecule 6 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 6.

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

- Molecule 7 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 15.

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

- Molecule 8 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	154	1193	759	201	222	11	0	0

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	443	3403	2121	602	660	20	0	1
9	a	443	3403	2121	602	660	20	0	1

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	424	3177	1996	562	612	7	0	1
10	b	424	3180	1998	562	613	7	0	0

- Molecule 11 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	365	2892	1940	450	485	17	0	0
11	c	370	2931	1968	455	490	18	0	0

- Molecule 12 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	241	1919	1225	330	349	15	0	0

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

- Molecule 13 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	196	1519	957	263	291	8	0	0
			Total	C	N	O	S		
13	e	196	1519	957	263	291	8	0	0

- Molecule 14 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	99	861	545	155	159	2	0	0
			Total	C	N	O	S		
14	f	99	861	545	155	159	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	engineered mutation	UNP P00129
f	56	ASP	ASN	engineered mutation	UNP P00129

- Molecule 15 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	75	621	406	117	97	1	0	2
			Total	C	N	O	S		
15	g	76	626	409	118	98	1	0	2

- Molecule 16 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	66	539	327	98	109	5	0	0
			Total	C	N	O	S		
16	h	66	539	327	98	109	5	0	0

- Molecule 17 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	42	285	174	55	55	1	0	0
17	i	42	285	174	55	55	1	0	0

- Molecule 18 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	J	62	507	333	88	86	0	0
18	j	62	507	333	88	86	0	0

- Molecule 19 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 10.

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

- Molecule 20 is a protein called CYTOCHROME C OXIDASE SUBUNIT 1.

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

- Molecule 21 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2.

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

- Molecule 22 is a protein called CYTOCHROME C OXIDASE SUBUNIT 3.

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

- Molecule 23 is a protein called CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1,

MITOCHONDRIAL.

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

- Molecule 24 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5A, MITOCHONDRIAL.

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

- Molecule 25 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5B, MITOCHONDRIAL.

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

- Molecule 26 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE VIA, CYTOCHROME C OXIDASE POLYPEPTIDE VB.

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

- Molecule 27 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6B1.

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

- Molecule 28 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6C.

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

- Molecule 29 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7A1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	U	57	442	285	74	80	3	0	1

- Molecule 30 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7B, MITOCHONDRIAL.

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

- Molecule 31 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7C, MITOCHONDRIAL.

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

- Molecule 32 is a protein called CYTOCHROME C OXIDASE SUBUNIT 8B, MITOCHONDRIAL.

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

- Molecule 33 is a protein called CYTOCHROME C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Y	104	875	552	155	163	5	7	0

- Molecule 34 is a protein called NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT L,.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
34	m	474	1422	948	474	0	0

- Molecule 35 is a protein called NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT M,.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
35	n	391	1173	782	391	0	0

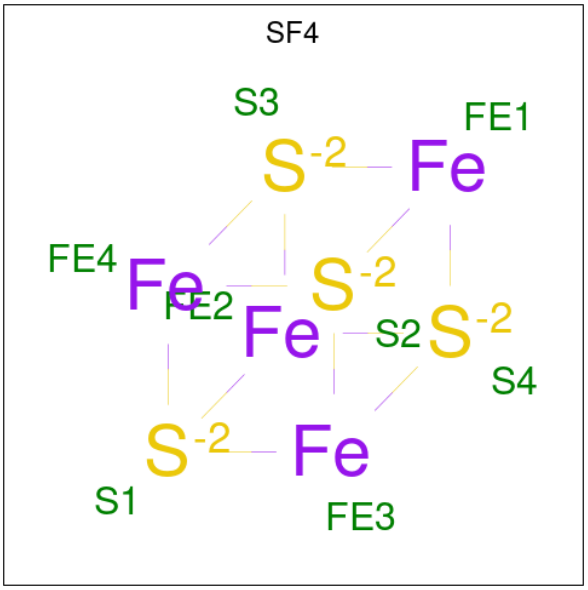
- Molecule 36 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT N.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
36	o	378	1134	756	378	0	0

- Molecule 37 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT K.

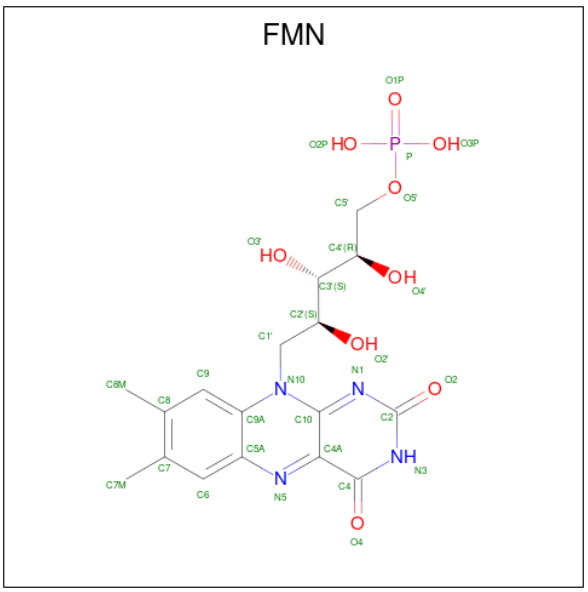
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
37	p	281	843	562	281	0	0

- Molecule 38 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



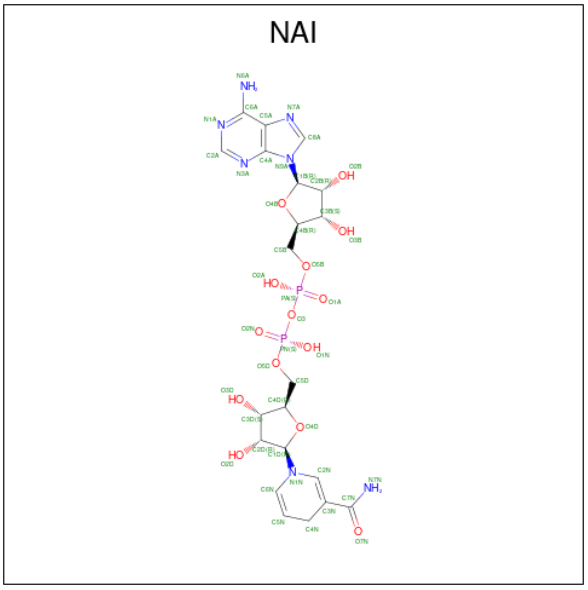
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
38	1	1	8	4	4	0
38	3	1	8	4	4	0
38	3	1	8	4	4	0
38	3	1	8	4	4	0
38	6	1	8	4	4	0
38	8	1	8	4	4	0
38	8	1	8	4	4	0

- Molecule 39 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	1	1	31	17	4	9	1	0

- Molecule 40 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

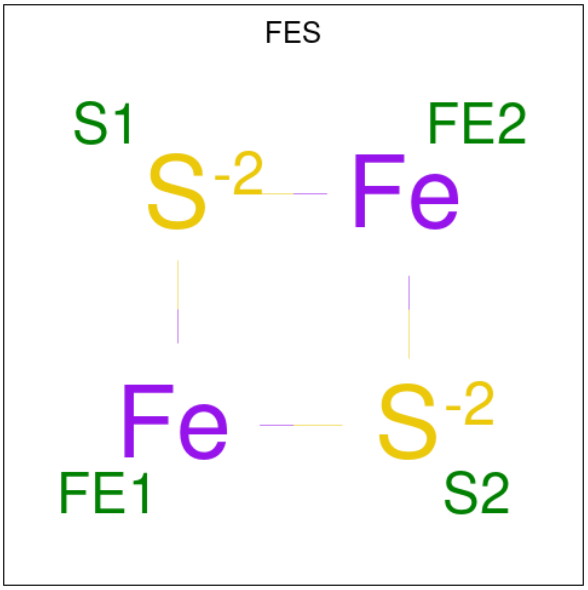


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
40	1	1	44	21	7	14	2	0

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
41	1	1	1	1	0
41	2	1	1	1	0
41	3	2	2	2	0
41	4	1	1	1	0
41	5	1	1	1	0
41	L	1	1	1	0

- Molecule 42 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

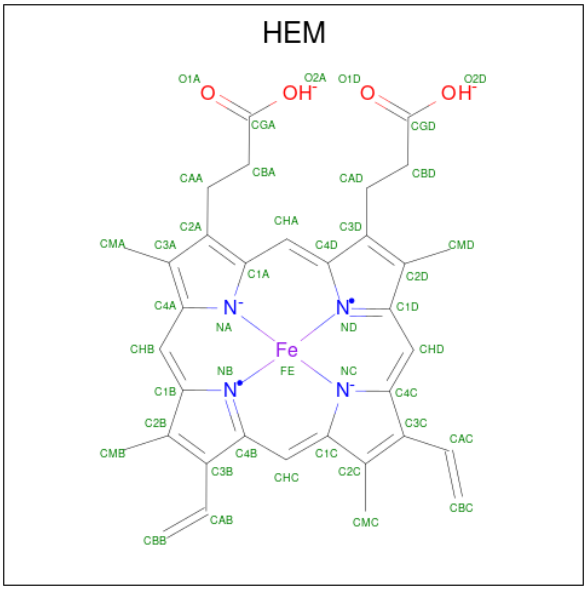


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
42	2	1	4	2	2	0
42	3	1	4	2	2	0
42	E	1	4	2	2	0
42	e	1	4	2	2	0

- Molecule 43 is CALCIUM ION (CCD ID: CA) (formula: Ca).

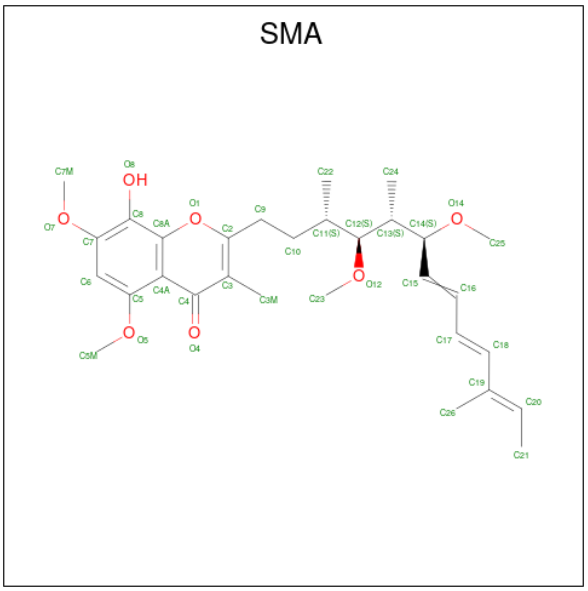
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
43	7	1	1	1	0

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



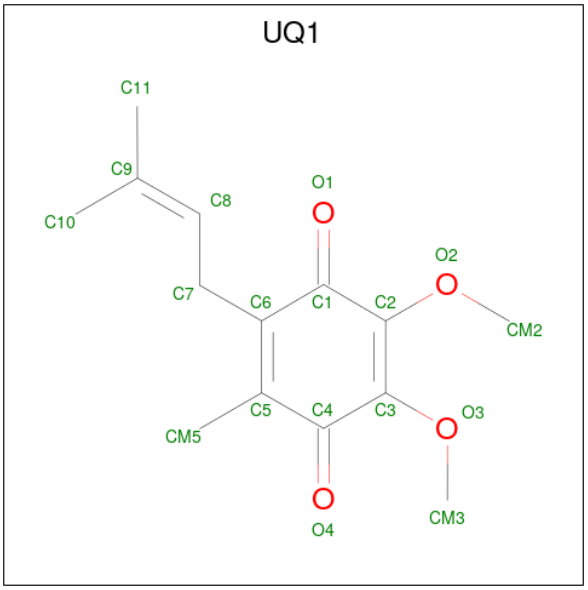
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
44	C	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
44	C	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
44	Y	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
44	c	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
44	c	1	43	34	1	4	4	0

- Molecule 45 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



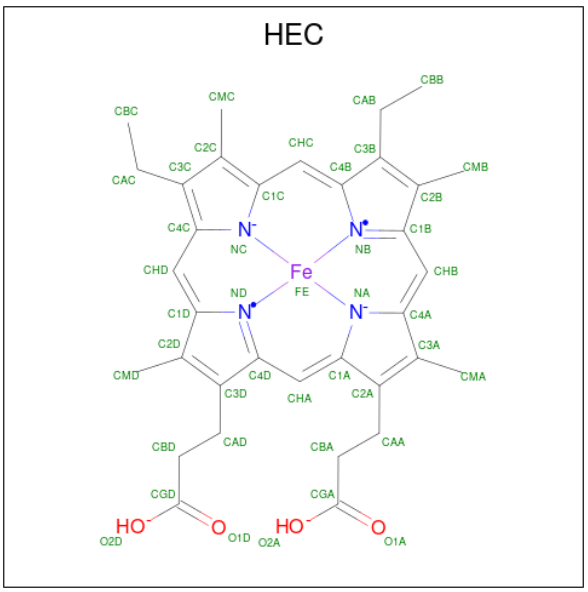
Mol	Chain	Residues	Atoms			AltConf
45	C	1	Total	C	O	0
			37	30	7	
45	c	1	Total	C	O	0
			37	30	7	

- Molecule 46 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



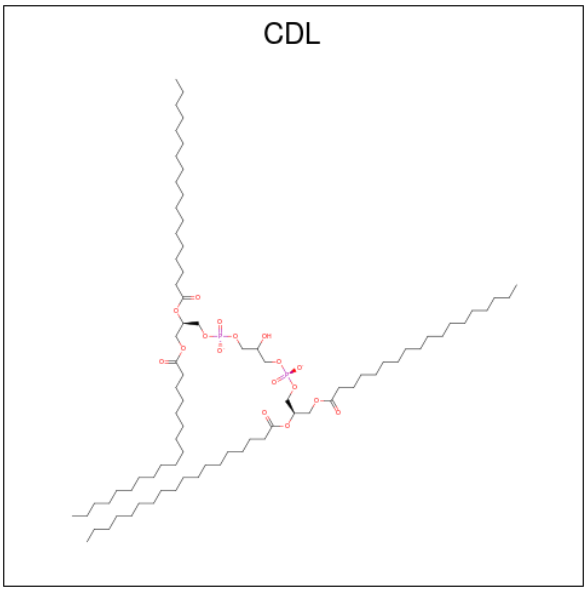
Mol	Chain	Residues	Atoms			AltConf
46	C	1	Total	C	O	0
			14	10	4	
46	c	1	Total	C	O	0
			14	10	4	

- Molecule 47 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 48 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
48	G	1	Total	C	O	P	0
			50	31	17	2	

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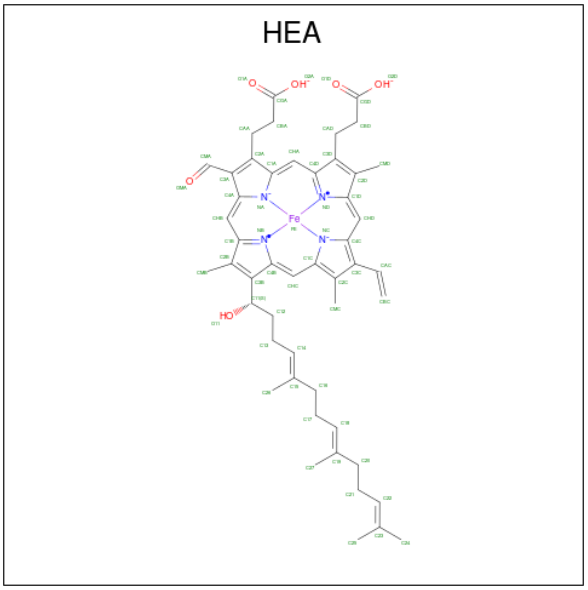
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
48	G	1	44	25	17	2	0
			Total	C	O	P	
48	d	1	50	31	17	2	0
			Total	C	O	P	
48	g	1	49	30	17	2	0

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



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

- Molecule 50 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
50	L	1	1	1	0
			Total	Cu	
50	M	2	2	2	0

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
51	Q	1	1	1	0

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
52	A	187	187	187	0
			Total	O	
52	B	149	149	149	0
			Total	O	
52	C	125	125	125	0
			Total	O	
52	D	118	118	118	0
			Total	O	
52	E	54	54	54	0
			Total	O	
52	F	57	57	57	0
			Total	O	
52	G	24	24	24	0
			Total	O	
52	H	14	14	14	0
			Total	O	
52	I	16	16	16	0
			Total	O	
52	J	5	5	5	0
			Total	O	
52	Y	161	161	161	0
			Total	O	
52	a	134	134	134	0
			Total	O	
52	b	130	130	130	0
			Total	O	
52	c	122	122	122	0
			Total	O	
52	d	109	109	109	0
			Total	O	
52	e	64	64	64	0
			Total	O	
52	f	73	73	73	0
			Total	O	
52	g	21	21	21	0
			Total	O	
52	h	16	16	16	0

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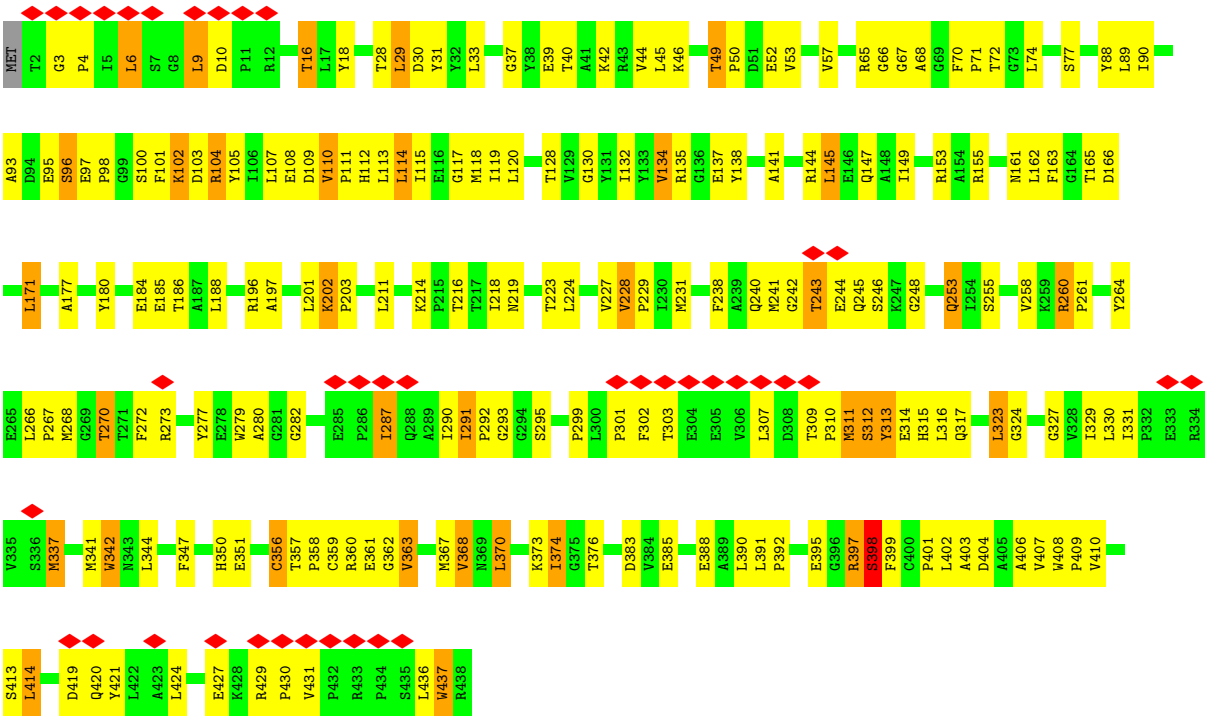
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
52	i	10	10	10	0
			Total	O	
52	j	9	9	9	0

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.

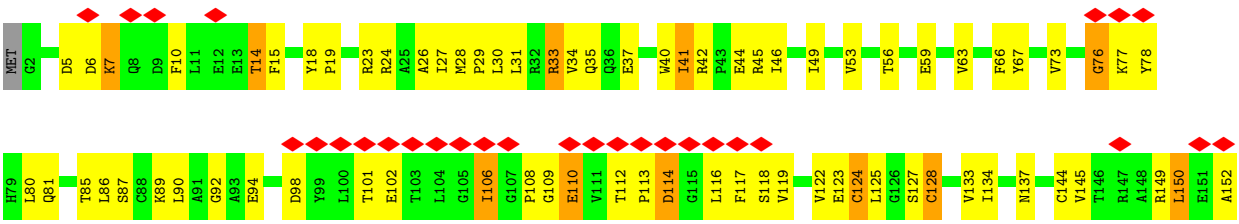
• Molecule 1: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 1

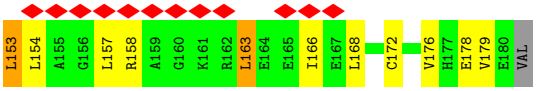
Chain 1:



• Molecule 2: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 2

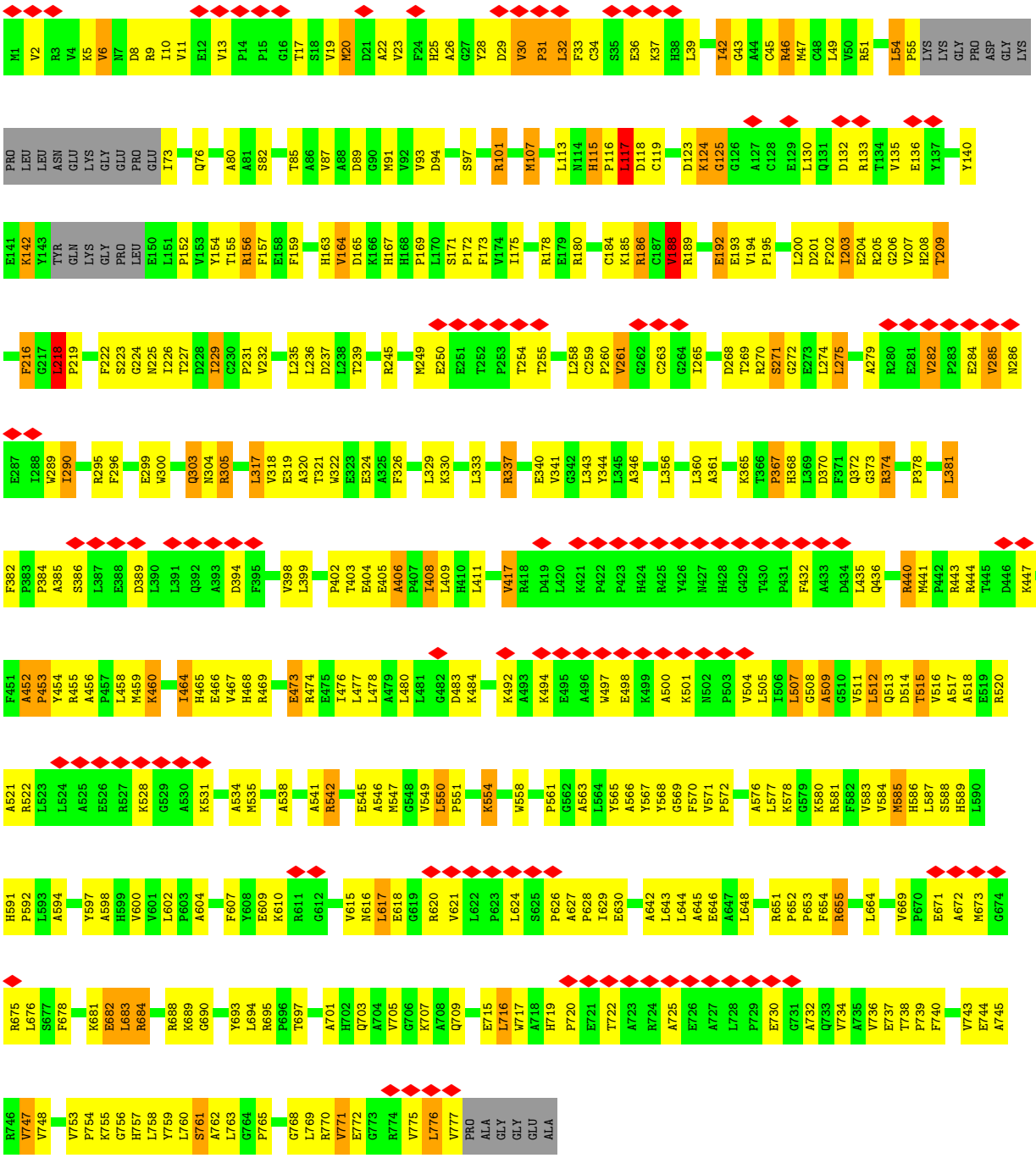
Chain 2:





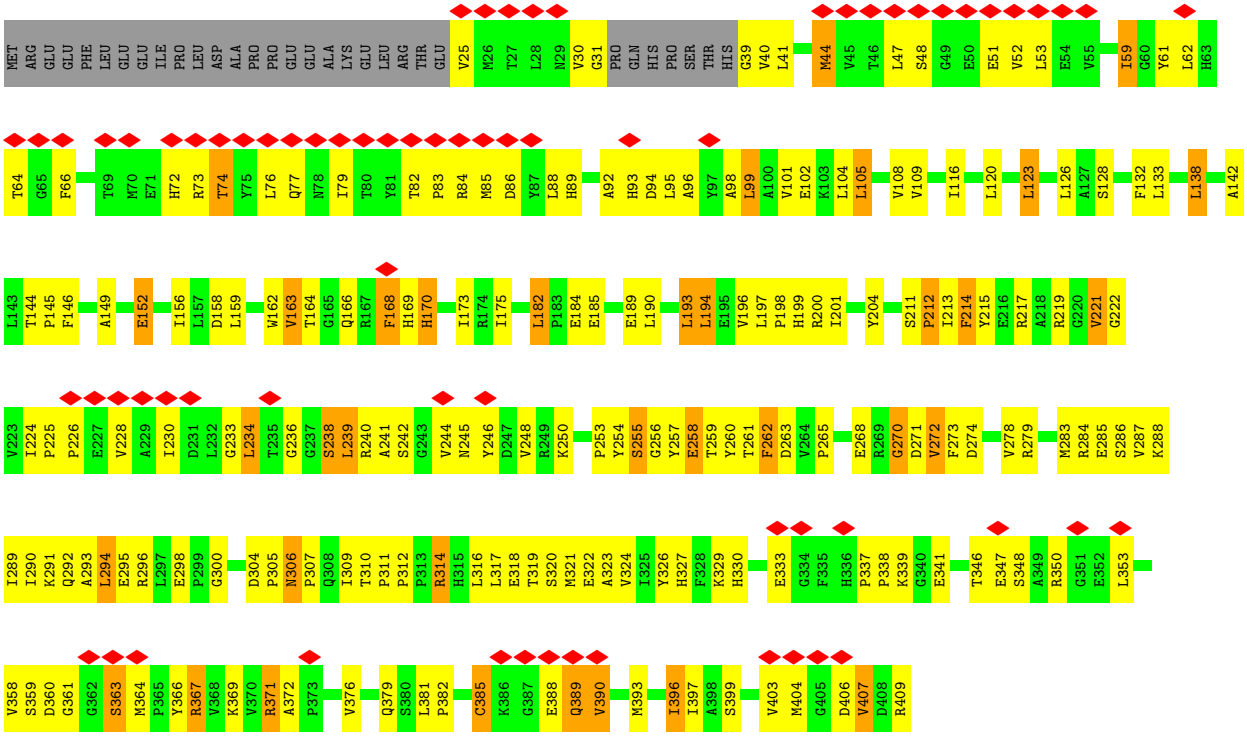
• Molecule 3: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 3

Chain 3:



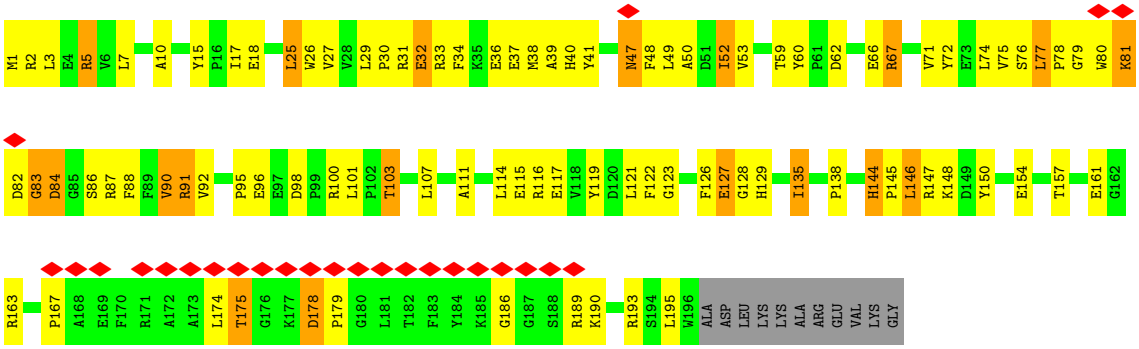
• Molecule 4: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 4

Chain 4:



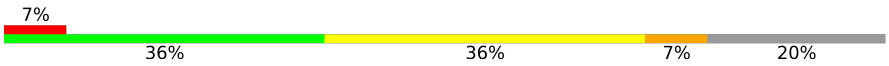
- Molecule 5: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 5

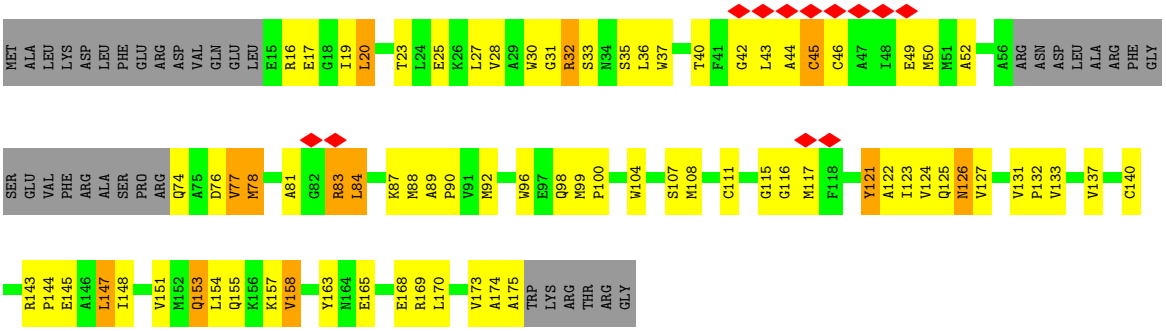
Chain 5:



- Molecule 6: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 6

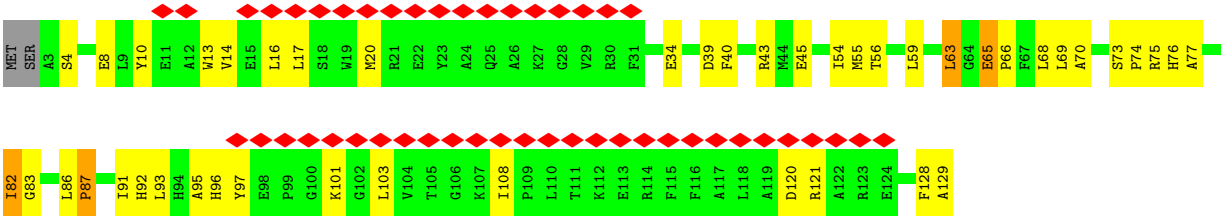
Chain 6:





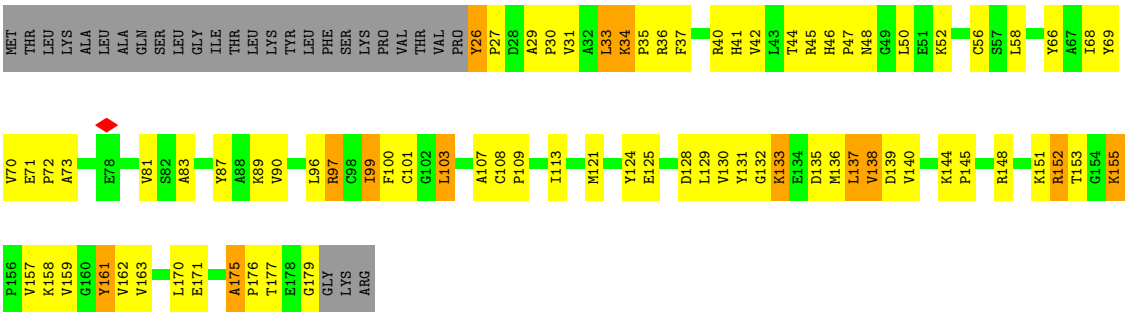
• Molecule 7: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 15

Chain 7:



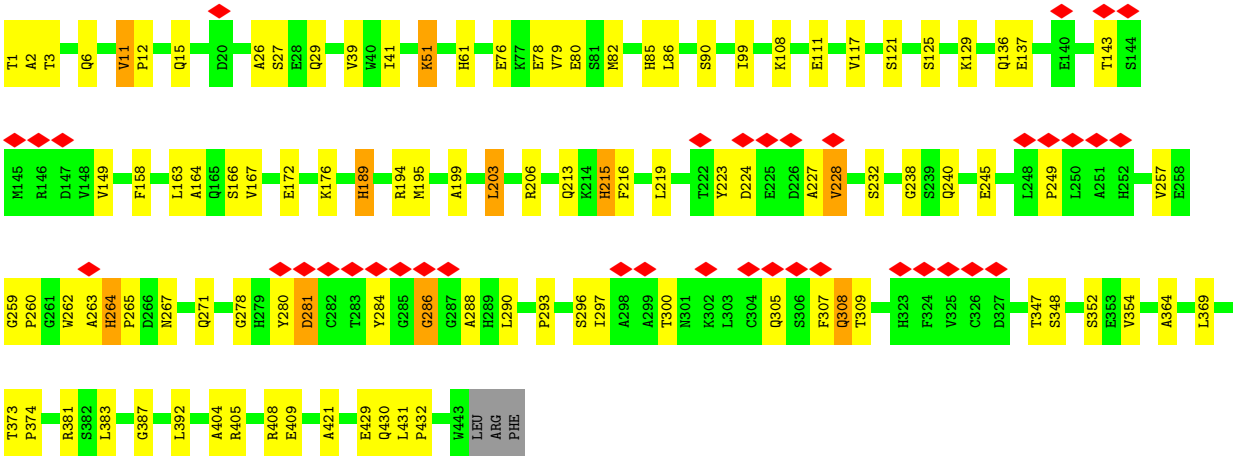
• Molecule 8: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 9

Chain 8:



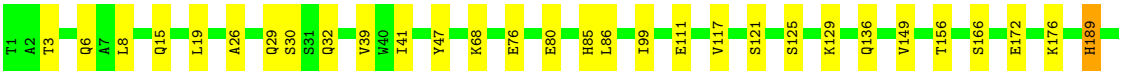
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

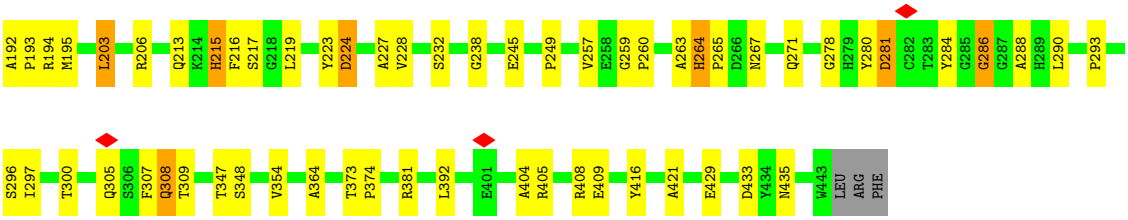
Chain A:



• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

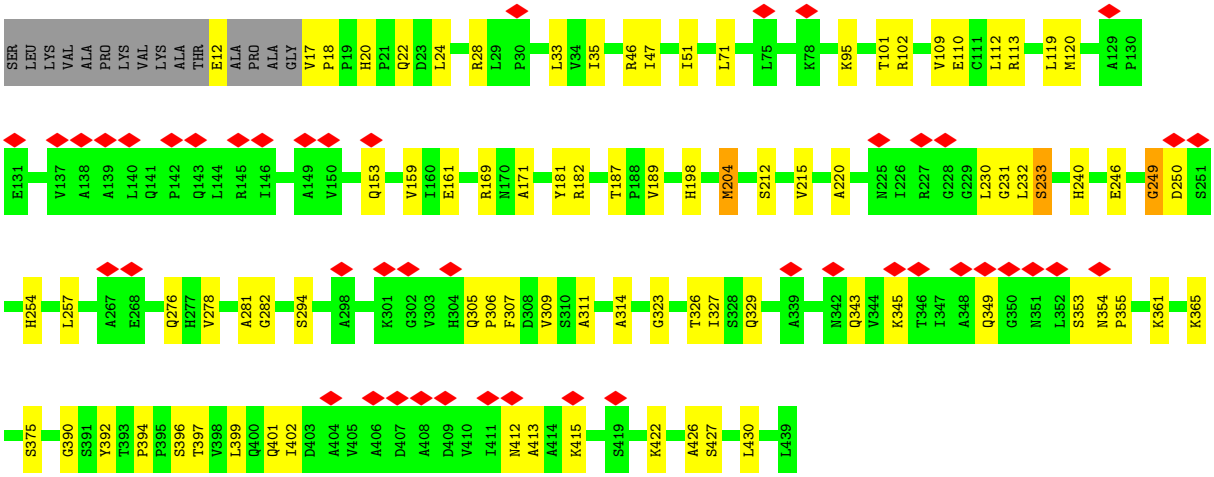
Chain a:





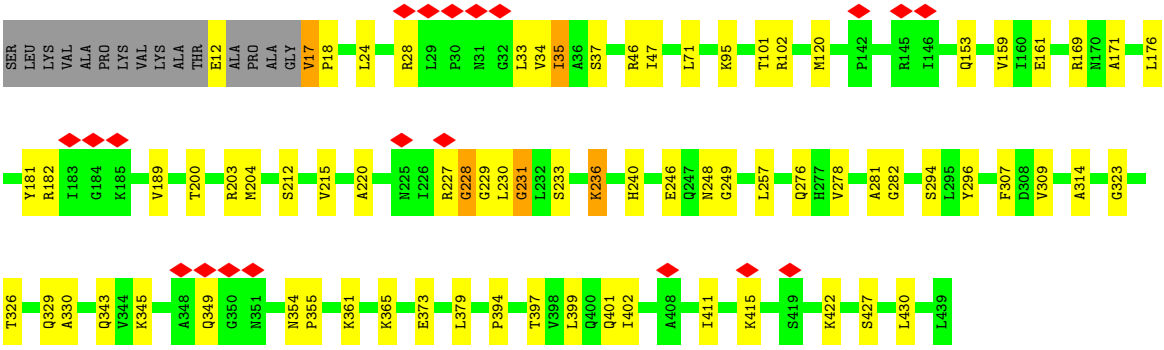
• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

Chain B:



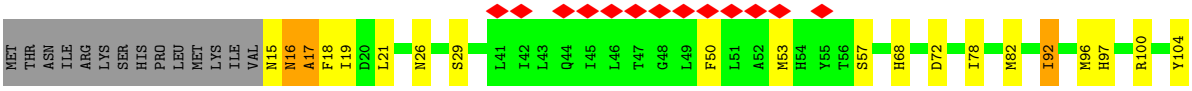
• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

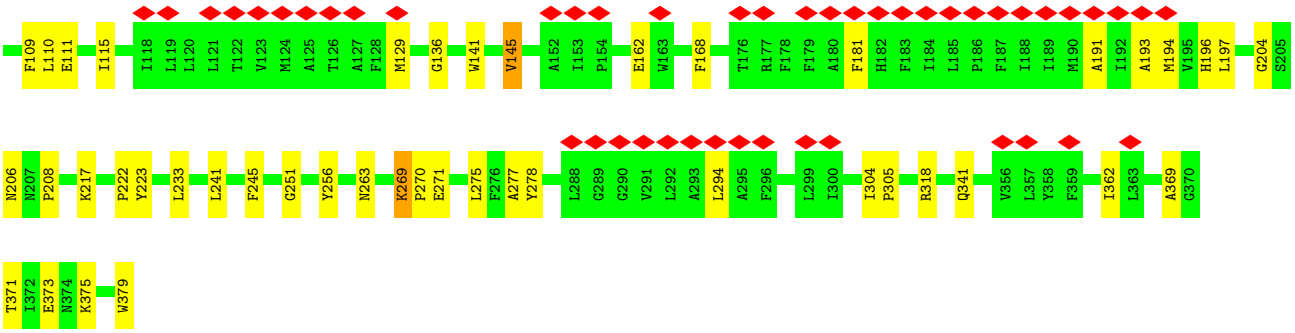
Chain b:



• Molecule 11: CYTOCHROME B

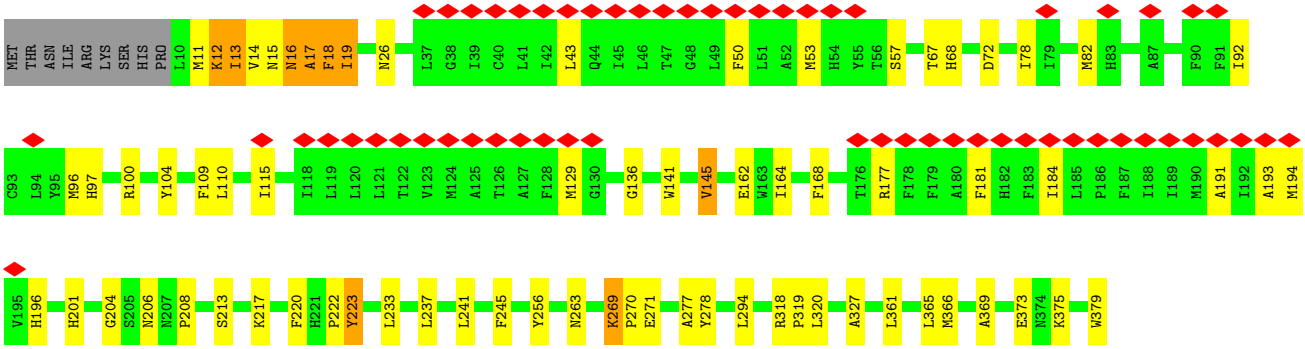
Chain C:





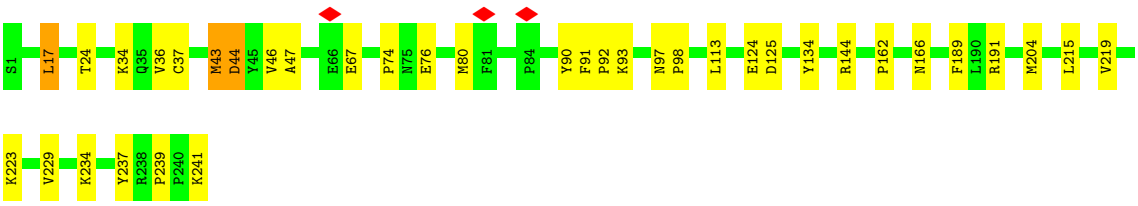
• Molecule 11: CYTOCHROME B

Chain c:



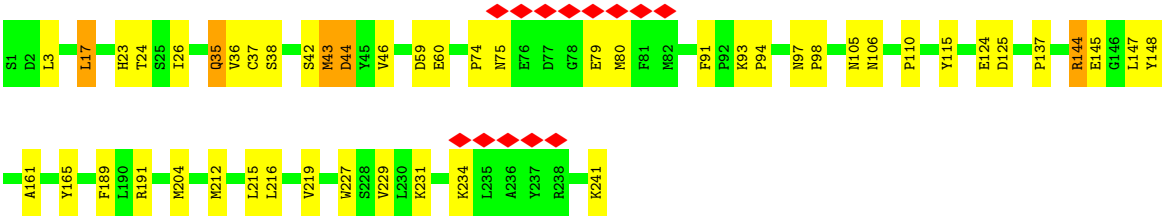
• Molecule 12: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

Chain D:



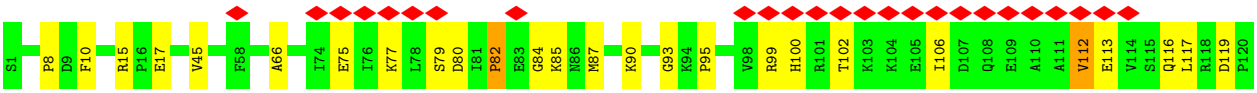
• Molecule 12: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

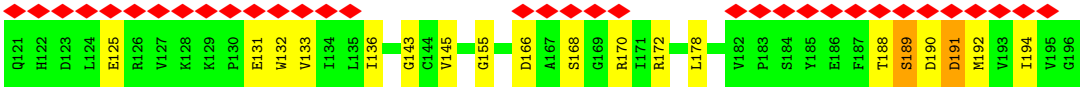
Chain d:



• Molecule 13: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

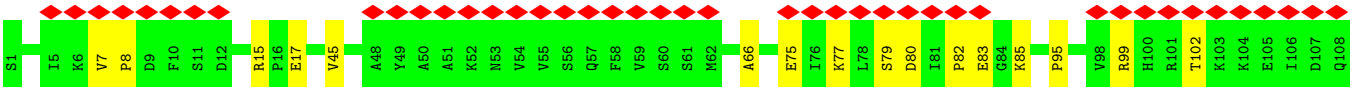
Chain E:

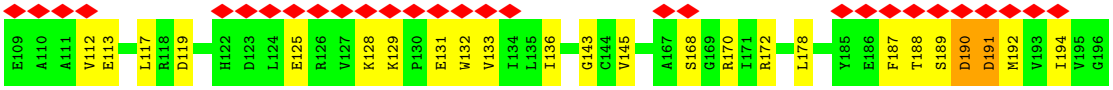




• Molecule 13: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain e:



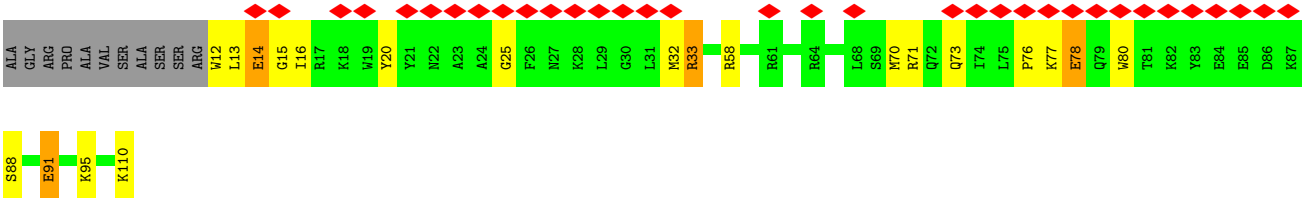


• Molecule 14: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain F:

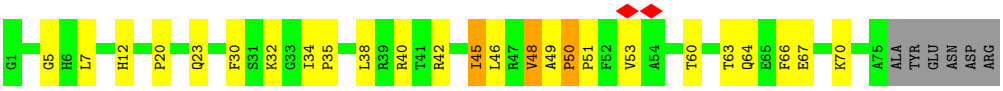
• Molecule 14: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain f:



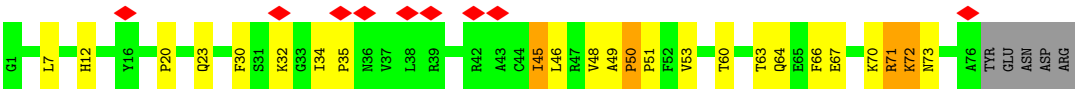
• Molecule 15: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

Chain G:



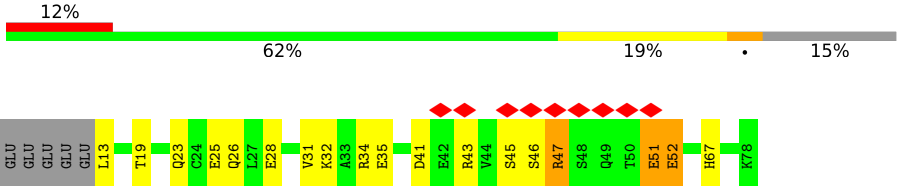
• Molecule 15: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

Chain g:



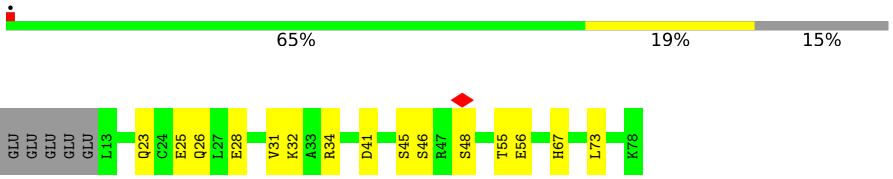
• Molecule 16: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

Chain H:



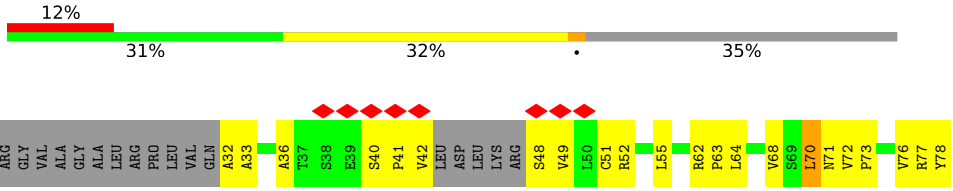
• Molecule 16: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

Chain h:



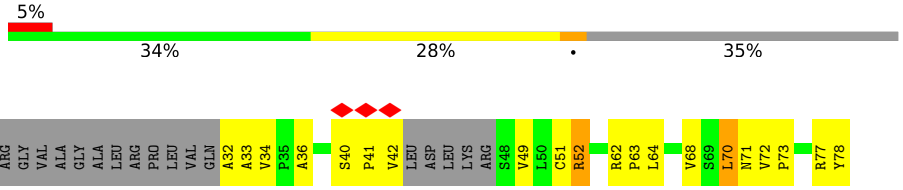
• Molecule 17: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain I:



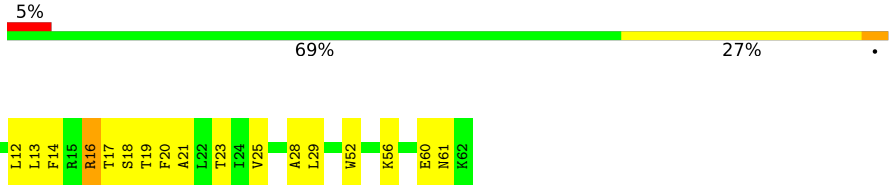
• Molecule 17: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain i:



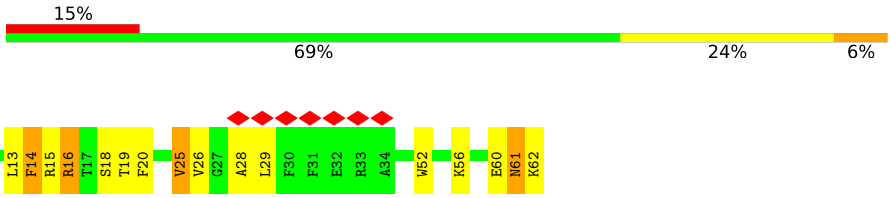
• Molecule 18: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain J:



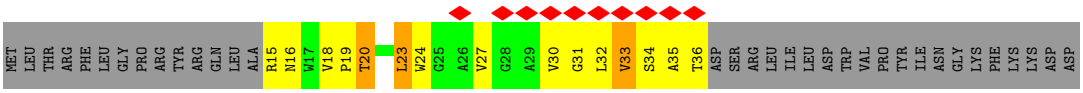
• Molecule 18: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain j:



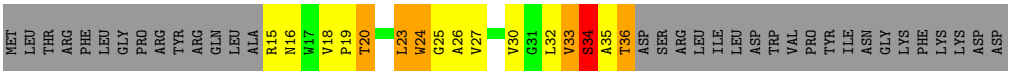
• Molecule 19: CYTOCHROME B-C1 COMPLEX SUBUNIT 10

Chain K:



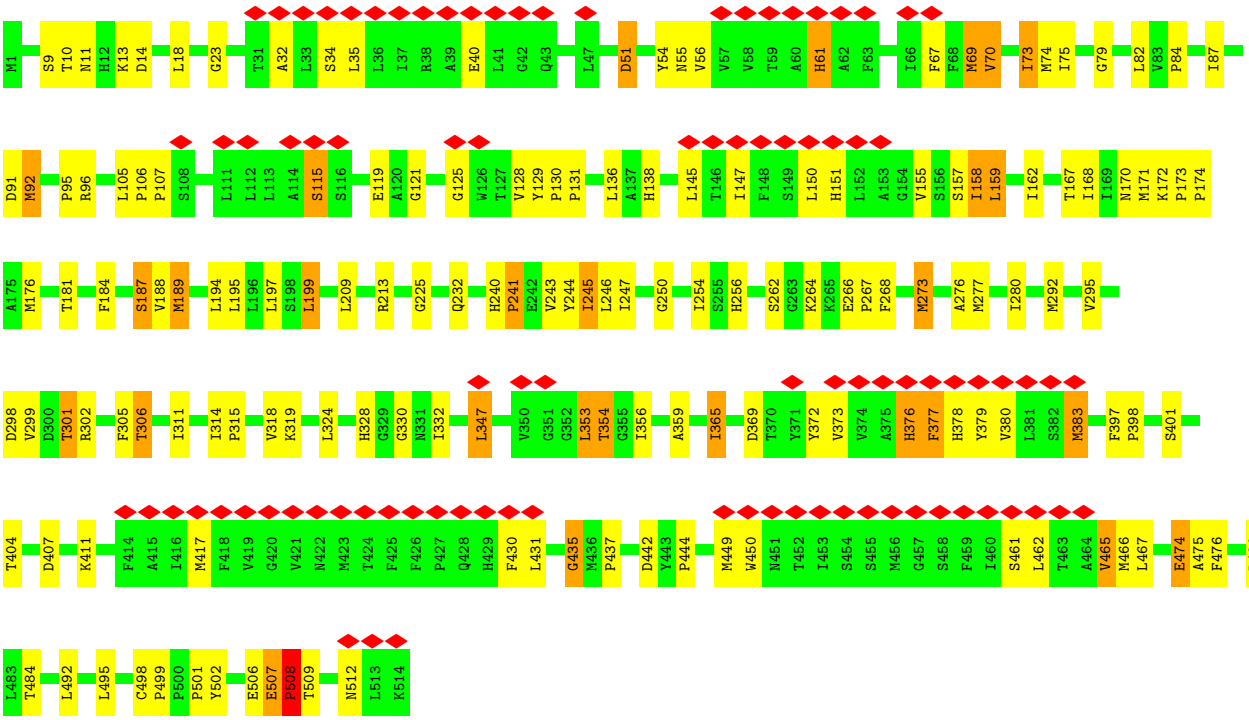
• Molecule 19: CYTOCHROME B-C1 COMPLEX SUBUNIT 10

Chain k:



• Molecule 20: CYTOCHROME C OXIDASE SUBUNIT 1

Chain L:

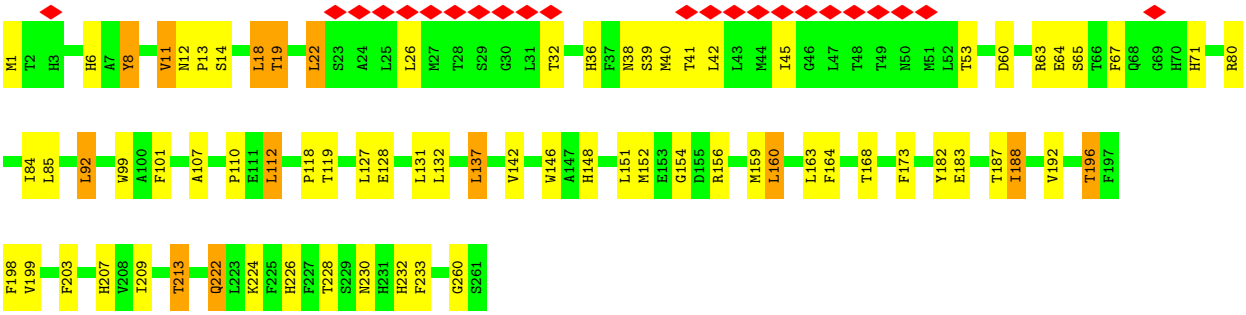


• Molecule 21: CYTOCHROME C OXIDASE SUBUNIT 2

Chain M:

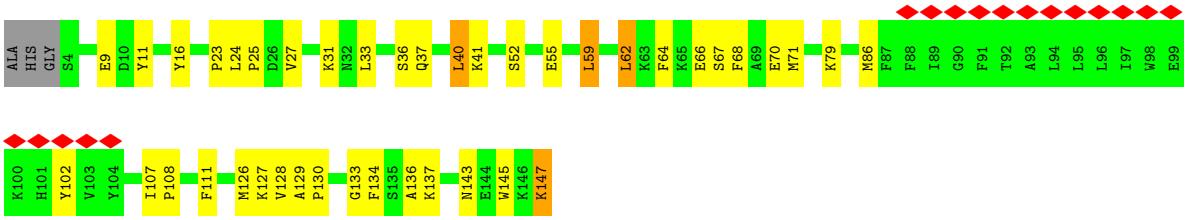
• Molecule 22: CYTOCHROME C OXIDASE SUBUNIT 3

Chain N: 9% 71% 24% 5%



• Molecule 23: CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1, MITOCHONDRIAL

Chain O: 12% 70% 25%

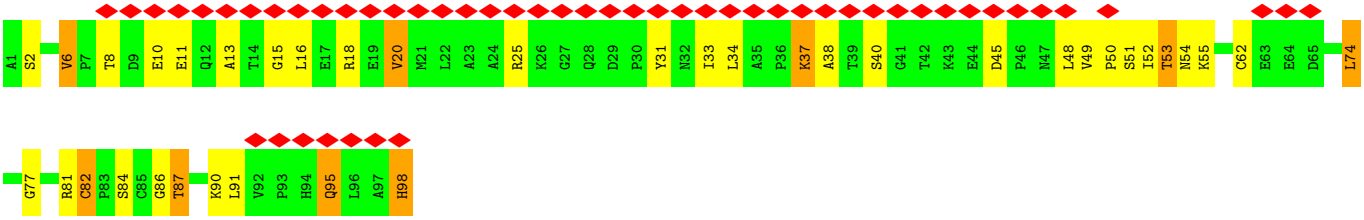


• Molecule 24: CYTOCHROME C OXIDASE SUBUNIT 5A, MITOCHONDRIAL

Chain P: 16% 75% 21%

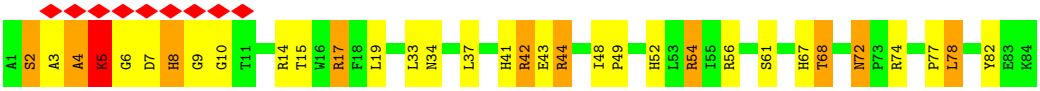
• Molecule 25: CYTOCHROME C OXIDASE SUBUNIT 5B, MITOCHONDRIAL

Chain Q: 53% 61% 30% 9%



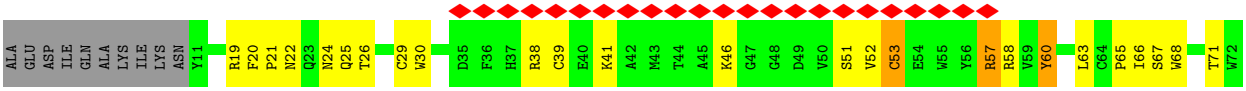
• Molecule 26: CYTOCHROME C OXIDASE POLYPEPTIDE VIA, CYTOCHROME C OXIDASE POLYPEPTIDE VB

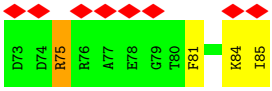
Chain R: 11% 61% 26% 12%



• Molecule 27: CYTOCHROME C OXIDASE SUBUNIT 6B1

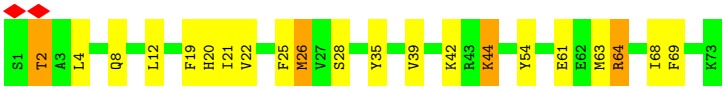
Chain S:





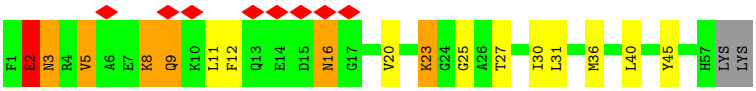
• Molecule 28: CYTOCHROME C OXIDASE SUBUNIT 6C

Chain T:



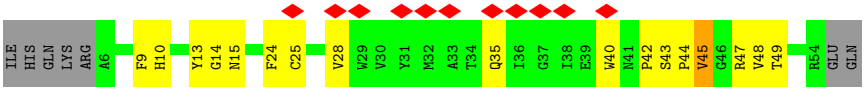
• Molecule 29: CYTOCHROME C OXIDASE SUBUNIT 7A1, MITOCHONDRIAL

Chain U:



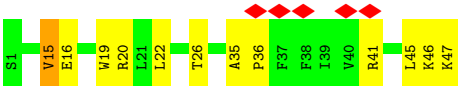
• Molecule 30: CYTOCHROME C OXIDASE SUBUNIT 7B, MITOCHONDRIAL

Chain V:



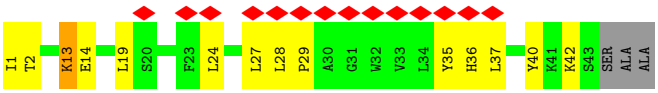
• Molecule 31: CYTOCHROME C OXIDASE SUBUNIT 7C, MITOCHONDRIAL

Chain W:



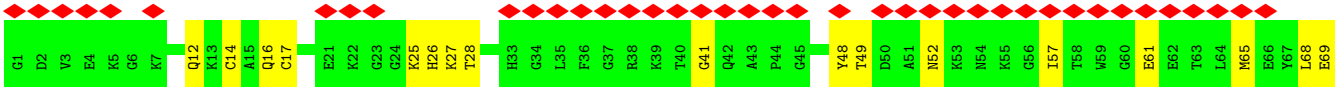
• Molecule 32: CYTOCHROME C OXIDASE SUBUNIT 8B, MITOCHONDRIAL

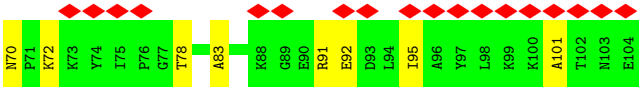
Chain X:



• Molecule 33: CYTOCHROME C

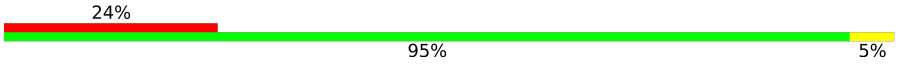
Chain Y:

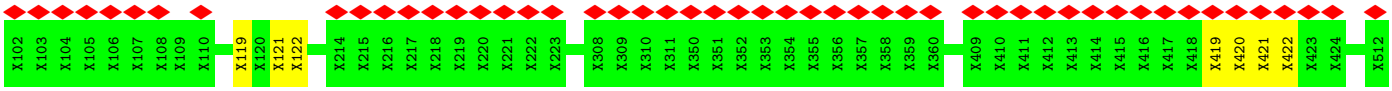


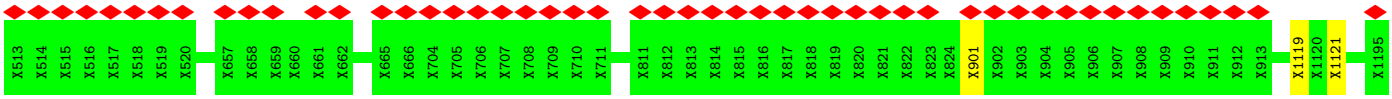


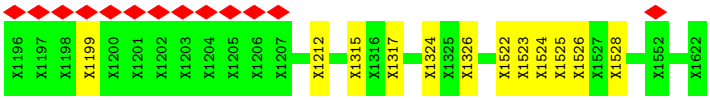
• Molecule 34: NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT L,

Chain m:



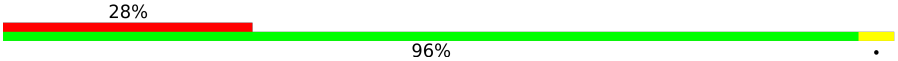


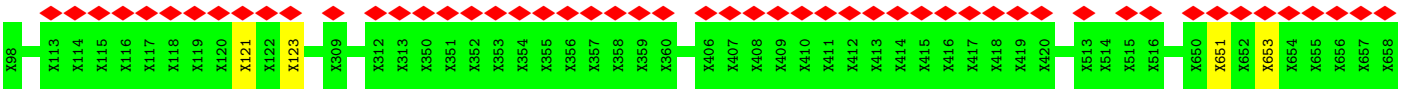


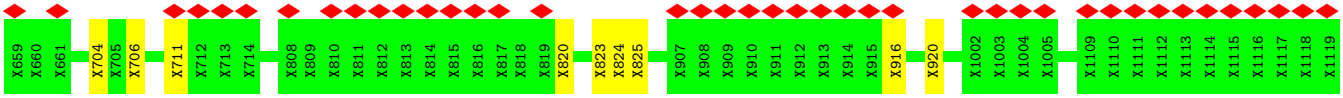


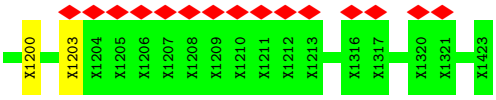
• Molecule 35: NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT M,

Chain n:



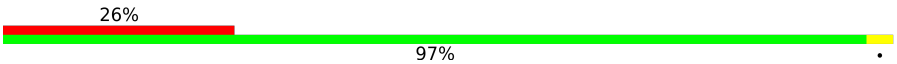


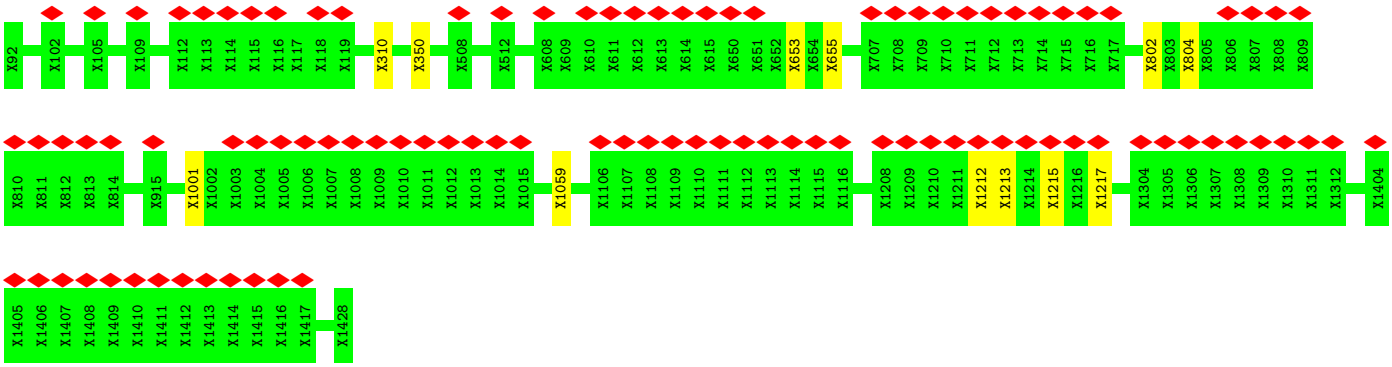




• Molecule 36: NADH-QUINONE OXIDOREDUCTASE SUBUNIT N

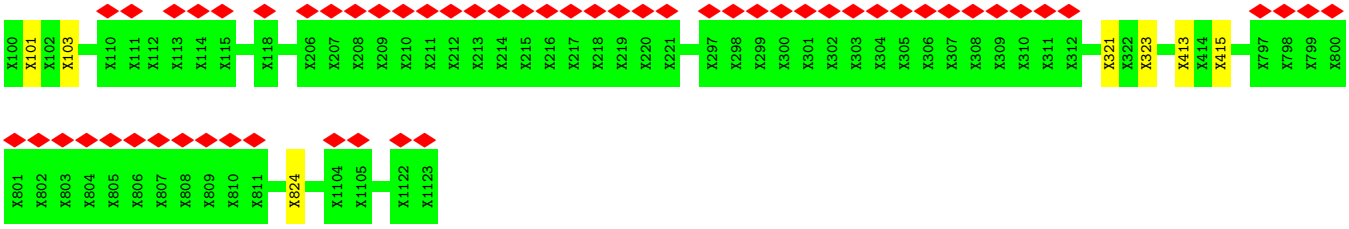
Chain o:





• Molecule 37: NADH-QUINONE OXIDOREDUCTASE SUBUNIT K

Chain p: 20% 98%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10684	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE-FLIPPPING ON EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	58829	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	18.839	Depositor
Minimum map value	-8.249	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.3	Depositor
Map size (Å)	533.12, 533.12, 533.12	wwPDB
Map dimensions	112, 112, 112	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	4.76, 4.76, 4.76	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: FMN, CU, UQ1, SF4, SMA, HEC, CDL, FES, HEM, NAI, MG, ZN, HEA, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1	0.58	0/3506	1.00	17/4745 (0.4%)
2	2	0.55	0/1443	1.03	8/1958 (0.4%)
3	3	0.57	1/6019 (0.0%)	0.99	19/8163 (0.2%)
4	4	0.55	0/3096	0.93	8/4207 (0.2%)
5	5	0.57	0/1656	1.03	13/2246 (0.6%)
6	6	0.61	0/1126	1.05	5/1528 (0.3%)
7	7	0.55	0/1059	0.99	3/1429 (0.2%)
8	8	0.59	0/1224	1.10	8/1663 (0.5%)
9	A	0.43	0/3472	1.03	23/4714 (0.5%)
9	a	0.43	0/3472	1.01	21/4714 (0.4%)
10	B	0.43	0/3235	0.99	20/4387 (0.5%)
10	b	0.42	0/3239	1.01	17/4393 (0.4%)
11	C	0.49	0/2986	1.04	25/4089 (0.6%)
11	c	0.47	0/3024	1.02	23/4137 (0.6%)
12	D	0.45	0/1978	1.02	7/2684 (0.3%)
12	d	0.44	0/1978	1.04	13/2684 (0.5%)
13	E	0.41	0/1553	1.00	9/2100 (0.4%)
13	e	0.45	0/1553	1.01	11/2100 (0.5%)
14	F	0.40	0/878	0.96	5/1175 (0.4%)
14	f	0.42	0/878	0.98	6/1175 (0.5%)
15	G	0.39	0/642	1.01	7/869 (0.8%)
15	g	0.42	0/647	1.02	7/876 (0.8%)
16	H	0.40	0/544	0.93	3/729 (0.4%)
16	h	0.39	0/544	0.89	2/729 (0.3%)
17	I	0.49	0/285	1.14	3/384 (0.8%)
17	i	0.48	0/285	1.24	4/384 (1.0%)
18	J	0.41	0/520	0.94	0/699
18	j	0.43	0/520	0.94	1/699 (0.1%)
19	K	0.54	0/163	1.34	0/225
19	k	0.59	0/163	1.52	1/225 (0.4%)
20	L	0.86	7/4164 (0.2%)
21	M	0.77	0/1868	1.12	10/2544 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
22	N	0.74	0/2211	1.02	7/3023 (0.2%)
23	O	0.67	0/1229	0.96	3/1658 (0.2%)
24	P	0.64	0/898	1.02	6/1218 (0.5%)
25	Q	0.72	0/765	1.13	4/1038 (0.4%)
26	R	0.69	0/699	1.10	6/950 (0.6%)
27	S	0.68	0/648	1.18	5/877 (0.6%)
28	T	0.71	0/611	0.94	2/810 (0.2%)
29	U	0.70	0/451	1.04	3/610 (0.5%)
30	V	0.75	0/398	1.01	1/546 (0.2%)
31	W	0.77	0/399	0.97	2/534 (0.4%)
32	X	0.69	0/345	0.98	1/470 (0.2%)
33	Y	0.34	0/891	0.91	4/1186 (0.3%)
All	All	0.56	8/67265 (0.0%)	1.02	378/91262 (0.4%)

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
19	k	0	1
34	m	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	61	HIS	CG-CD2	7.56	1.44	1.35
20	L	378	HIS	ND1-CE1	7.07	1.39	1.32
20	L	378	HIS	CE1-NE2	-6.57	1.25	1.32
20	L	69	MET	SD-CE	-6.25	1.64	1.79
20	L	61	HIS	ND1-CE1	5.68	1.38	1.32
3	3	188	VAL	CA-CB	5.63	1.60	1.54
20	L	378	HIS	CG-CD2	5.53	1.42	1.35
20	L	376	HIS	ND1-CE1	5.49	1.38	1.32

All (378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	228	GLY	N-CA-C	-14.09	95.71	115.30
3	3	115	HIS	CA-C-N	11.56	131.00	118.97
3	3	115	HIS	C-N-CA	11.56	131.00	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	218	LEU	CA-C-N	11.46	131.89	119.28
3	3	218	LEU	C-N-CA	11.46	131.89	119.28
1	1	291	ILE	CA-C-N	10.96	130.37	118.97
1	1	291	ILE	C-N-CA	10.96	130.37	118.97
12	d	36	VAL	N-CA-C	10.72	120.78	111.56
20	L	376	HIS	ND1-CE1-NE2	10.42	118.82	108.40
9	A	223	TYR	N-CA-C	-9.13	100.46	111.69
27	S	52	VAL	N-CA-C	8.92	121.19	108.17
13	e	143	GLY	N-CA-C	8.71	127.33	115.32
27	S	81	PHE	CA-C-N	8.70	128.34	119.56
27	S	81	PHE	C-N-CA	8.70	128.34	119.56
1	1	295	SER	N-CA-C	-8.38	103.50	114.31
17	I	40	SER	CA-C-N	8.34	130.26	119.84
17	I	40	SER	C-N-CA	8.34	130.26	119.84
17	i	40	SER	CA-C-N	8.17	130.06	119.84
17	i	40	SER	C-N-CA	8.17	130.06	119.84
6	6	123	ILE	N-CA-C	8.13	119.50	108.11
13	E	143	GLY	N-CA-C	8.13	126.54	115.32
13	E	15	ARG	N-CA-C	-8.13	98.86	110.08
31	W	20	ARG	N-CA-C	-8.08	102.55	111.36
20	L	378	HIS	ND1-CE1-NE2	8.06	116.46	108.40
5	5	144	HIS	CA-C-N	8.04	127.97	119.05
5	5	144	HIS	C-N-CA	8.04	127.97	119.05
20	L	82	LEU	N-CA-C	8.03	122.34	112.23
15	G	49	ALA	N-CA-C	7.96	123.58	112.75
11	C	318	ARG	CA-C-N	7.94	127.50	119.24
11	C	318	ARG	C-N-CA	7.94	127.50	119.24
17	i	34	VAL	N-CA-C	7.74	115.58	107.76
11	C	19	ILE	N-CA-C	7.72	118.25	110.23
15	g	49	ALA	N-CA-C	7.70	123.22	112.75
9	A	260	PRO	N-CA-C	7.67	123.62	113.57
11	c	318	ARG	CA-C-N	7.65	127.20	119.24
11	c	318	ARG	C-N-CA	7.65	127.20	119.24
1	1	110	VAL	CA-C-N	7.61	127.49	119.05
1	1	110	VAL	C-N-CA	7.61	127.49	119.05
20	L	435	GLY	N-CA-C	7.61	125.99	115.27
9	A	286	GLY	N-CA-C	7.55	121.25	112.50
13	e	15	ARG	N-CA-C	-7.50	99.74	110.08
10	B	305	GLN	N-CA-C	-7.48	101.33	110.31
4	4	182	LEU	CA-C-N	7.43	127.39	120.03
4	4	182	LEU	C-N-CA	7.43	127.39	120.03
9	A	259	GLY	CA-C-N	7.43	127.07	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	259	GLY	C-N-CA	7.43	127.07	119.19
20	L	330	GLY	N-CA-C	7.39	120.46	112.33
32	X	27	LEU	N-CA-C	7.37	119.40	111.36
1	1	282	GLY	CA-C-N	7.35	128.34	120.11
1	1	282	GLY	C-N-CA	7.35	128.34	120.11
20	L	56	VAL	N-CA-C	-7.35	103.30	110.72
9	a	223	TYR	N-CA-C	-7.32	102.47	111.40
11	c	223	TYR	N-CA-C	7.25	118.83	111.07
20	L	376	HIS	CE1-NE2-CD2	-7.22	101.78	109.00
20	L	9	SER	N-CA-C	7.14	119.79	110.43
11	c	26	ASN	N-CA-C	7.13	121.29	112.59
20	L	332	ILE	N-CA-C	7.13	118.99	109.37
13	e	125	GLU	N-CA-C	-7.12	104.62	113.38
24	P	42	VAL	N-CA-C	-7.12	99.65	108.05
10	b	249	GLY	N-CA-C	7.12	124.98	115.59
24	P	76	GLY	CA-C-N	7.09	128.32	120.45
24	P	76	GLY	C-N-CA	7.09	128.32	120.45
6	6	37	TRP	CA-C-N	7.08	128.94	120.23
6	6	37	TRP	C-N-CA	7.08	128.94	120.23
9	A	11	VAL	N-CA-C	7.06	115.87	108.95
5	5	60	TYR	CA-C-N	7.04	126.56	119.24
5	5	60	TYR	C-N-CA	7.04	126.56	119.24
11	c	19	ILE	N-CA-C	7.04	117.55	110.23
13	E	168	SER	N-CA-C	-7.03	104.59	113.72
11	C	206	ASN	N-CA-C	-7.00	99.51	110.36
9	a	260	PRO	N-CA-C	7.00	122.74	113.57
11	C	26	ASN	N-CA-C	6.99	121.90	112.88
11	C	110	LEU	N-CA-C	6.97	119.48	111.11
20	L	130	PRO	N-CA-C	-6.97	102.20	110.70
13	e	168	SER	N-CA-C	-6.92	104.72	113.72
22	N	36	HIS	N-CA-C	6.91	122.13	113.43
10	B	249	GLY	N-CA-C	6.88	124.15	115.42
11	c	110	LEU	N-CA-C	6.86	119.34	111.11
9	a	121	SER	N-CA-C	6.86	118.41	111.07
9	A	309	THR	N-CA-C	-6.86	100.65	110.59
11	C	223	TYR	N-CA-C	6.82	119.30	111.11
11	c	206	ASN	N-CA-C	-6.81	99.81	110.36
9	A	305	GLN	N-CA-C	-6.76	104.04	112.90
3	3	186	ARG	N-CA-C	6.76	119.22	111.11
23	O	133	GLY	N-CA-C	6.75	129.19	113.18
15	g	48	VAL	N-CA-C	6.75	117.36	110.82
4	4	39	GLY	N-CA-C	-6.73	93.79	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	507	GLU	N-CA-C	-6.71	97.94	109.15
14	F	25	GLY	N-CA-C	6.71	124.96	115.30
26	R	5	LYS	N-CA-C	6.71	125.09	110.80
11	c	241	LEU	N-CA-C	-6.71	104.05	111.36
10	b	278	VAL	N-CA-C	-6.70	104.23	110.53
12	D	215	LEU	N-CA-C	6.69	118.57	111.28
11	C	109	PHE	N-CA-C	-6.68	96.93	108.56
24	P	81	ILE	N-CA-C	6.67	116.80	110.53
3	3	406	ALA	CA-C-N	6.65	128.16	119.84
3	3	406	ALA	C-N-CA	6.65	128.16	119.84
3	3	229	ILE	CB-CA-C	-6.64	103.05	112.22
9	a	286	GLY	N-CA-C	6.64	120.68	112.64
11	c	136	GLY	N-CA-C	-6.64	103.47	112.57
15	g	50	PRO	N-CA-C	6.61	118.77	110.70
20	L	74	MET	N-CA-C	6.57	118.10	111.07
10	b	282	GLY	CA-C-N	6.55	126.53	119.78
10	b	282	GLY	C-N-CA	6.55	126.53	119.78
11	C	57	SER	N-CA-C	6.55	120.88	113.02
20	L	61	HIS	CB-CG-CD2	-6.55	122.69	131.20
18	j	14	PHE	N-CA-C	6.55	120.48	112.23
11	C	269	LYS	CA-C-N	6.53	126.47	120.21
11	C	269	LYS	C-N-CA	6.53	126.47	120.21
12	d	24	THR	N-CA-C	-6.52	104.26	111.36
1	1	260	ARG	CA-C-N	6.51	126.48	120.03
1	1	260	ARG	C-N-CA	6.51	126.48	120.03
20	L	506	GLU	N-CA-C	-6.49	104.21	111.28
13	E	125	GLU	N-CA-C	-6.48	105.38	113.28
12	D	44	ASP	N-CA-C	6.45	120.24	112.38
10	b	422	LYS	N-CA-C	6.45	120.06	110.52
15	G	50	PRO	N-CA-C	6.44	118.56	110.70
10	b	101	THR	N-CA-C	-6.43	100.04	109.18
20	L	61	HIS	ND1-CE1-NE2	6.43	114.83	108.40
11	c	72	ASP	N-CA-C	6.43	122.20	113.97
11	c	204	GLY	N-CA-C	-6.42	101.92	112.83
10	B	101	THR	N-CA-C	-6.39	100.10	109.18
9	a	238	GLY	N-CA-C	-6.38	101.02	110.97
9	a	309	THR	N-CA-C	-6.37	101.35	110.59
12	d	215	LEU	N-CA-C	6.37	118.22	111.28
13	E	136	ILE	N-CA-C	-6.35	99.15	108.54
11	c	109	PHE	N-CA-C	-6.35	97.52	108.56
14	f	32	MET	N-CA-C	-6.34	99.86	109.95
9	a	348	SER	N-CA-C	6.33	122.09	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	24	THR	N-CA-C	-6.29	104.52	111.82
26	R	2	SER	N-CA-C	6.27	119.57	109.79
11	C	72	ASP	N-CA-C	6.26	121.99	113.97
9	A	121	SER	N-CA-C	6.25	117.75	111.07
20	L	10	THR	N-CA-C	-6.24	103.86	112.03
24	P	21	LYS	CA-C-N	6.23	126.42	119.32
24	P	21	LYS	C-N-CA	6.23	126.42	119.32
9	a	278	GLY	N-CA-C	6.22	123.60	112.02
11	C	136	GLY	N-CA-C	-6.21	103.09	112.41
9	a	421	ALA	N-CA-C	-6.21	99.07	109.07
10	B	282	GLY	CA-C-N	6.19	126.16	119.78
10	B	282	GLY	C-N-CA	6.19	126.16	119.78
9	A	348	SER	N-CA-C	6.17	121.85	112.54
11	C	241	LEU	N-CA-C	-6.16	104.65	111.36
10	B	204	MET	N-CA-C	6.16	119.58	109.85
9	a	305	GLN	N-CA-C	-6.15	104.85	112.90
11	C	275	LEU	N-CA-C	6.14	117.97	111.28
20	L	170	ASN	N-CA-C	6.13	120.84	113.23
9	A	249	PRO	N-CA-C	6.13	121.93	113.65
9	A	166	SER	N-CA-C	-6.12	102.63	110.53
9	A	278	GLY	N-CA-C	6.10	123.37	112.02
12	d	44	ASP	N-CA-C	6.10	119.82	112.38
13	e	136	ILE	N-CA-C	-6.09	98.91	108.23
21	M	47	THR	N-CA-C	6.08	120.00	112.59
8	8	175	ALA	CA-C-N	6.05	127.41	119.84
8	8	175	ALA	C-N-CA	6.05	127.41	119.84
20	L	157	SER	N-CA-C	6.04	118.83	111.82
27	S	63	LEU	N-CA-C	6.03	119.11	111.69
9	a	249	PRO	N-CA-C	6.03	121.47	113.57
10	B	233	SER	N-CA-C	6.02	118.30	110.53
12	d	216	LEU	CA-C-N	-6.01	112.82	119.19
12	d	216	LEU	C-N-CA	-6.01	112.82	119.19
20	L	125	GLY	N-CA-C	-6.00	104.14	112.18
5	5	98	ASP	CA-C-N	6.00	127.34	119.84
5	5	98	ASP	C-N-CA	6.00	127.34	119.84
6	6	170	LEU	CA-C-N	5.99	126.55	120.38
6	6	170	LEU	C-N-CA	5.99	126.55	120.38
10	B	422	LYS	N-CA-C	5.96	119.24	110.59
22	N	8	TYR	N-CA-C	5.96	118.22	110.53
11	c	271	GLU	N-CA-C	-5.93	102.28	110.35
21	M	207	MET	CA-C-N	5.93	127.25	119.84
21	M	207	MET	C-N-CA	5.93	127.25	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	R	44	ARG	CA-C-N	5.93	125.95	119.90
26	R	44	ARG	C-N-CA	5.93	125.95	119.90
4	4	300	GLY	CA-C-N	5.92	125.83	119.85
4	4	300	GLY	C-N-CA	5.92	125.83	119.85
11	C	204	GLY	N-CA-C	-5.91	101.94	112.58
15	g	53	VAL	N-CA-C	-5.91	104.75	110.72
12	d	125	ASP	N-CA-C	-5.90	104.93	111.36
13	E	178	LEU	N-CA-C	5.90	118.66	109.52
8	8	103	LEU	N-CA-C	-5.89	104.86	111.28
20	L	67	PHE	N-CA-C	5.89	119.65	112.23
11	c	57	SER	N-CA-C	5.88	120.07	113.02
9	a	166	SER	N-CA-C	-5.87	102.96	110.53
16	H	52	GLU	N-CA-C	5.86	118.32	110.35
9	a	264	HIS	CA-C-N	5.86	125.73	119.28
9	a	264	HIS	C-N-CA	5.86	125.73	119.28
5	5	178	ASP	CA-C-N	5.84	125.39	119.19
5	5	178	ASP	C-N-CA	5.84	125.39	119.19
14	f	25	GLY	N-CA-C	5.84	123.71	115.30
20	L	119	GLU	CB-CA-C	-5.84	109.83	116.54
21	M	134	ARG	N-CA-C	5.84	123.23	110.80
12	D	36	VAL	N-CA-C	5.83	121.47	109.34
20	L	171	MET	N-CA-C	5.83	120.09	111.87
9	A	262	TRP	N-CA-C	5.82	120.92	111.37
12	D	113	LEU	N-CA-C	5.82	120.50	113.17
9	A	264	HIS	CA-C-N	5.80	125.66	119.28
9	A	264	HIS	C-N-CA	5.80	125.66	119.28
7	7	4	SER	N-CA-C	-5.78	105.89	113.17
12	D	37	CYS	N-CA-C	5.78	118.52	111.82
10	b	17	VAL	CA-C-N	5.78	126.33	120.38
10	b	17	VAL	C-N-CA	5.78	126.33	120.38
21	M	190	GLY	N-CA-C	5.77	117.76	110.38
11	c	184	ILE	N-CA-C	5.77	119.17	111.44
22	N	198	PHE	N-CA-C	5.76	117.56	111.28
14	f	14	GLU	N-CA-C	-5.76	104.98	112.23
23	O	129	ALA	CA-C-N	5.74	127.01	119.84
23	O	129	ALA	C-N-CA	5.74	127.01	119.84
11	c	263	ASN	N-CA-C	5.73	117.99	108.13
9	A	189	HIS	N-CA-C	5.73	120.40	113.41
16	h	67	HIS	N-CA-C	-5.73	105.04	111.28
29	U	25	GLY	N-CA-C	5.72	118.96	110.60
12	d	26	ILE	N-CA-C	-5.72	105.15	110.53
13	e	178	LEU	N-CA-C	5.71	118.37	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	53	VAL	N-CA-C	-5.70	104.96	110.72
20	L	129	TYR	CB-CA-C	-5.70	100.47	109.42
11	C	271	GLU	N-CA-C	-5.69	102.61	110.35
10	B	430	LEU	N-CA-C	5.68	119.30	112.93
12	D	125	ASP	N-CA-C	-5.68	105.17	111.36
10	b	153	GLN	N-CA-C	-5.68	105.84	112.89
2	2	73	VAL	CA-C-N	5.67	126.92	119.84
2	2	73	VAL	C-N-CA	5.67	126.92	119.84
3	3	441	MET	CA-C-N	5.66	125.84	119.90
3	3	441	MET	C-N-CA	5.66	125.84	119.90
15	g	12	HIS	N-CA-C	5.66	119.48	112.24
9	A	238	GLY	N-CA-C	-5.65	102.15	110.97
15	g	23	GLN	N-CA-C	5.65	118.00	109.41
11	C	115	ILE	N-CA-C	-5.65	105.01	110.72
21	M	104	TRP	N-CA-C	5.65	122.83	110.80
5	5	67	ARG	N-CA-C	5.64	117.43	111.28
9	A	263	ALA	N-CA-C	5.64	119.90	113.19
11	C	82	MET	N-CA-C	-5.64	105.22	111.36
33	Y	49	THR	N-CA-C	-5.63	102.95	110.55
11	c	82	MET	N-CA-C	-5.62	105.23	111.36
25	Q	82	CYS	CA-C-N	5.60	125.44	119.28
25	Q	82	CYS	C-N-CA	5.60	125.44	119.28
10	B	394	PRO	CA-C-N	5.58	125.04	119.24
10	B	394	PRO	C-N-CA	5.58	125.04	119.24
28	T	20	HIS	N-CA-C	5.57	118.11	111.71
1	1	331	ILE	CA-C-N	5.57	125.54	120.03
1	1	331	ILE	C-N-CA	5.57	125.54	120.03
11	C	263	ASN	N-CA-C	5.57	117.71	108.13
11	C	145	VAL	N-CA-C	5.56	115.69	110.30
13	E	119	ASP	CA-C-N	5.56	126.79	119.84
13	E	119	ASP	C-N-CA	5.56	126.79	119.84
26	R	72	ASN	CA-C-N	5.55	125.91	119.47
26	R	72	ASN	C-N-CA	5.55	125.91	119.47
10	b	394	PRO	CA-C-N	5.55	125.01	119.24
10	b	394	PRO	C-N-CA	5.55	125.01	119.24
11	C	17	ALA	N-CA-C	-5.54	98.99	110.80
9	a	232	SER	N-CA-C	-5.53	102.94	110.36
11	C	256	TYR	N-CA-C	-5.52	106.12	112.92
9	a	257	VAL	N-CA-C	-5.52	101.45	109.29
2	2	109	GLY	N-CA-C	5.51	120.52	114.40
8	8	161	TYR	N-CA-C	5.51	115.82	108.38
1	1	356	CYS	CB-CA-C	-5.51	100.09	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	119	ASP	CA-C-N	5.51	126.37	119.98
13	e	119	ASP	C-N-CA	5.51	126.37	119.98
29	U	2	GLU	N-CA-C	5.51	122.53	110.80
22	N	188	ILE	CB-CA-C	-5.50	104.71	112.14
9	a	259	GLY	CA-C-N	5.50	125.02	119.19
9	a	259	GLY	C-N-CA	5.50	125.02	119.19
3	3	30	VAL	CA-C-N	5.50	126.72	119.84
3	3	30	VAL	C-N-CA	5.50	126.72	119.84
31	W	16	GLU	N-CA-C	5.49	117.35	111.36
11	C	362	ILE	N-CA-C	5.46	115.66	110.53
15	G	23	GLN	N-CA-C	5.46	117.70	109.41
9	A	257	VAL	N-CA-C	-5.45	101.55	109.29
9	a	189	HIS	N-CA-C	5.45	120.80	114.04
15	G	48	VAL	N-CA-C	5.45	116.51	111.45
11	C	92	ILE	N-CA-C	-5.44	105.20	110.42
17	i	49	VAL	N-CA-C	5.44	116.14	108.36
33	Y	26	HIS	N-CA-C	-5.44	102.43	110.48
20	L	305	PHE	N-CA-C	5.43	119.01	112.38
11	c	145	VAL	N-CA-C	5.43	115.56	110.30
11	c	269	LYS	CA-C-N	5.41	125.40	120.21
11	c	269	LYS	C-N-CA	5.41	125.40	120.21
20	L	245	ILE	N-CA-C	-5.40	104.29	111.05
3	3	76	GLN	CA-C-N	5.40	124.92	119.19
3	3	76	GLN	C-N-CA	5.40	124.92	119.19
14	F	76	PRO	N-CA-C	-5.40	102.71	111.14
11	c	365	LEU	N-CA-C	5.39	116.84	111.07
5	5	77	LEU	CA-C-N	5.38	126.57	119.84
5	5	77	LEU	C-N-CA	5.38	126.57	119.84
20	L	159	LEU	N-CA-C	-5.37	105.50	111.36
1	1	312	SER	N-CA-C	5.37	117.14	109.14
9	A	421	ALA	N-CA-C	-5.36	100.44	109.07
9	A	215	HIS	N-CA-C	5.36	120.83	113.97
14	f	91	GLU	CA-C-N	-5.36	113.39	119.28
14	f	91	GLU	C-N-CA	-5.36	113.39	119.28
13	E	66	ALA	N-CA-C	5.33	117.78	111.33
8	8	155	LYS	CA-C-N	5.32	126.48	119.84
8	8	155	LYS	C-N-CA	5.32	126.48	119.84
11	c	256	TYR	N-CA-C	-5.32	106.38	112.92
14	f	76	PRO	N-CA-C	-5.31	102.85	111.14
9	a	215	HIS	N-CA-C	5.31	120.76	113.97
16	h	73	LEU	N-CA-C	5.31	120.07	111.37
13	e	191	ASP	N-CA-C	-5.30	99.74	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	8	ASP	N-CA-C	-5.30	106.70	114.39
1	1	70	PHE	CA-C-N	5.29	126.45	119.84
1	1	70	PHE	C-N-CA	5.29	126.45	119.84
20	L	372	TYR	N-CA-C	-5.28	105.42	111.07
4	4	306	ASN	CA-C-N	5.27	124.89	119.56
4	4	306	ASN	C-N-CA	5.27	124.89	119.56
2	2	18	TYR	CA-C-N	5.27	125.81	120.38
2	2	18	TYR	C-N-CA	5.27	125.81	120.38
12	d	37	CYS	N-CA-C	5.26	118.86	112.23
10	B	278	VAL	N-CA-C	-5.26	105.41	110.72
10	B	198	HIS	N-CA-C	5.25	121.08	114.31
10	b	330	ALA	N-CA-C	5.25	117.68	111.33
9	A	232	SER	N-CA-C	-5.24	103.53	110.40
11	c	115	ILE	N-CA-C	-5.24	105.43	110.72
3	3	452	ALA	CA-C-N	5.23	126.38	119.84
3	3	452	ALA	C-N-CA	5.23	126.38	119.84
20	L	262	SER	N-CA-C	-5.23	106.58	113.17
25	Q	38	ALA	N-CA-C	5.21	117.85	110.50
15	G	12	HIS	N-CA-C	5.21	118.91	112.24
10	b	176	LEU	N-CA-C	-5.21	106.88	113.18
33	Y	28	THR	N-CA-C	-5.21	105.61	111.28
13	e	66	ALA	N-CA-C	5.20	117.62	111.33
15	G	5	GLY	N-CA-C	-5.19	107.83	114.37
20	L	353	LEU	N-CA-C	-5.19	105.70	111.36
3	3	566	ALA	N-CA-C	5.19	117.27	109.23
10	B	413	ALA	N-CA-C	-5.18	105.63	111.28
10	b	159	VAL	N-CA-C	5.17	115.39	110.42
20	L	377	PHE	N-CA-C	5.17	119.44	113.18
20	L	401	SER	N-CA-C	5.17	119.71	113.41
10	B	159	VAL	N-CA-C	5.16	115.37	110.42
2	2	19	PRO	CA-C-N	5.16	125.20	119.32
2	2	19	PRO	C-N-CA	5.16	125.20	119.32
10	b	430	LEU	N-CA-C	5.15	119.28	113.15
27	S	22	ASN	N-CA-C	5.15	117.69	109.81
1	1	342	TRP	CA-CB-CG	5.14	123.36	113.60
29	U	9	GLN	N-CA-C	-5.14	105.57	111.07
22	N	99	TRP	N-CA-C	-5.14	105.58	111.07
22	N	107	ALA	CA-C-N	5.14	125.94	119.98
22	N	107	ALA	C-N-CA	5.14	125.94	119.98
8	8	34	LYS	CA-C-N	5.13	124.93	119.28
8	8	34	LYS	C-N-CA	5.13	124.93	119.28
10	B	112	LEU	N-CA-C	-5.13	103.27	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	329	GLN	N-CA-C	-5.12	103.28	110.50
7	7	65	GLU	CA-C-N	5.11	125.27	119.90
7	7	65	GLU	C-N-CA	5.11	125.27	119.90
14	F	13	LEU	N-CA-C	-5.11	104.79	111.02
10	B	311	ALA	N-CA-C	-5.10	103.30	110.50
9	a	263	ALA	N-CA-C	5.10	119.26	113.19
3	3	765	PRO	N-CA-C	-5.09	109.39	114.68
21	M	66	THR	N-CA-C	-5.09	107.73	114.04
12	d	137	PRO	CA-C-N	-5.08	115.33	120.21
12	d	137	PRO	C-N-CA	-5.08	115.33	120.21
33	Y	101	ALA	N-CA-C	5.08	117.56	111.71
28	T	2	THR	N-CA-C	5.08	116.13	108.46
15	g	71	ARG	N-CA-C	5.07	121.61	110.80
10	B	187	THR	N-CA-C	5.07	117.04	110.40
21	M	165	VAL	CA-C-N	5.07	126.17	119.84
21	M	165	VAL	C-N-CA	5.07	126.17	119.84
4	4	238	SER	N-CA-C	-5.06	106.93	113.01
17	I	49	VAL	N-CA-C	5.06	115.59	108.36
19	k	36	THR	CA-C-O	5.06	129.40	120.80
1	1	398	SER	N-CA-C	-5.05	102.10	109.63
2	2	41	ILE	N-CA-C	5.05	115.04	107.51
10	b	329	GLN	N-CA-C	-5.05	102.80	110.28
12	d	38	SER	N-CA-C	5.05	118.55	112.38
20	L	378	HIS	CB-CG-CD2	-5.05	124.64	131.20
14	F	32	MET	N-CA-C	-5.04	102.05	110.17
21	M	12	ALA	N-CA-C	5.04	117.47	109.96
5	5	62	ASP	CA-C-N	5.04	124.94	119.85
5	5	62	ASP	C-N-CA	5.04	124.94	119.85
10	B	153	GLN	N-CA-C	-5.04	106.64	112.89
14	F	24	ALA	N-CA-C	-5.03	105.79	111.28
16	H	67	HIS	N-CA-C	-5.03	105.80	111.28
30	V	35	GLN	N-CA-C	5.02	119.17	113.19
13	e	85	LYS	N-CA-C	5.02	117.99	109.76
25	Q	81	ARG	N-CA-C	5.02	117.62	109.24
20	L	378	HIS	N-CA-C	-5.01	106.34	112.90
12	d	23	HIS	N-CA-C	5.01	118.65	112.54
20	L	73	ILE	N-CA-C	5.00	115.15	110.30
16	H	46	SER	N-CA-C	5.00	119.10	113.15
20	L	70	VAL	N-CA-C	5.00	115.43	110.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	k	24	TRP	Mainchain
34	m	1212	UNK	Peptide

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	1	3417	0	3388	181	0
2	2	1410	0	1376	74	0
3	3	5880	0	5911	373	0
4	4	3018	0	3009	209	0
5	5	1607	0	1574	98	0
6	6	1102	0	1108	84	0
7	7	1031	0	1029	40	0
8	8	1193	0	1160	71	0
9	A	3403	0	3301	72	0
9	a	3403	0	3302	65	0
10	B	3177	0	3152	64	0
10	b	3180	0	3156	54	0
11	C	2892	0	2938	38	0
11	c	2931	0	2989	55	0
12	D	1919	0	1868	29	0
12	d	1919	0	1867	56	0
13	E	1519	0	1503	29	0
13	e	1519	0	1503	23	0
14	F	861	0	854	13	0
14	f	861	0	854	19	0
15	G	621	0	626	17	0
15	g	626	0	631	23	0
16	H	539	0	524	15	0
16	h	539	0	524	10	0
17	I	285	0	288	41	0
17	i	285	0	288	32	0
18	J	507	0	512	52	0
18	j	507	0	512	34	0
19	K	159	0	159	25	0
19	k	159	0	159	46	0
20	L	4025	0	4003	89	0
21	M	1822	0	1834	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	N	2124	0	2042	48	0
23	O	1195	0	1183	33	0
24	P	878	0	868	21	0
25	Q	748	0	728	25	0
26	R	672	0	645	30	0
27	S	628	0	582	22	0
28	T	598	0	612	14	0
29	U	442	0	439	16	0
30	V	384	0	366	11	0
31	W	386	0	388	8	0
32	X	335	0	352	13	0
33	Y	875	0	885	42	0
34	m	1422	0	52	11	0
35	n	1173	0	37	13	0
36	o	1134	0	36	10	0
37	p	843	0	24	6	0
38	1	8	0	0	0	0
38	3	24	0	0	3	0
38	6	8	0	0	1	0
38	8	16	0	0	2	0
39	1	31	0	19	7	0
40	1	44	0	27	5	0
41	1	1	0	0	0	0
41	2	1	0	0	0	0
41	3	2	0	0	0	0
41	4	1	0	0	0	0
41	5	1	0	0	0	0
41	L	1	0	0	0	0
42	2	4	0	0	0	0
42	3	4	0	0	1	0
42	E	4	0	0	0	0
42	e	4	0	0	0	0
43	7	1	0	0	0	0
44	C	86	0	60	5	0
44	Y	43	0	30	7	0
44	c	86	0	60	3	0
45	C	37	0	42	1	0
45	c	37	0	42	1	0
46	C	14	0	9	2	0
46	c	14	0	9	5	0
47	D	43	0	30	0	0
47	d	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	G	94	0	76	5	0
48	d	50	0	44	0	0
48	g	49	0	42	0	0
49	L	120	0	108	4	0
50	L	1	0	0	0	0
50	M	2	0	0	0	0
51	Q	1	0	0	0	0
52	A	187	0	0	11	0
52	B	149	0	0	2	0
52	C	125	0	0	4	0
52	D	118	0	0	2	0
52	E	54	0	0	2	0
52	F	57	0	0	3	0
52	G	24	0	0	1	0
52	H	14	0	0	0	0
52	I	16	0	0	2	0
52	J	5	0	0	0	0
52	Y	161	0	0	18	0
52	a	134	0	0	1	0
52	b	130	0	0	1	0
52	c	122	0	0	6	0
52	d	109	0	0	1	0
52	e	64	0	0	0	0
52	f	73	0	0	3	0
52	g	21	0	0	1	0
52	h	16	0	0	0	0
52	i	10	0	0	1	0
52	j	9	0	0	0	0
All	All	72626	0	65769	2146	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 16.

All (2146) 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)
18:J:29:LEU:HD21	19:k:34:SER:CB	1.16	1.63
36:o:1001:UNK:CA	36:o:1059:UNK:C	1.85	1.52
18:J:29:LEU:CD2	19:k:34:SER:HB2	1.46	1.42
19:K:15:ARG:HG2	9:a:408:ARG:NH2	1.33	1.38
52:Y:350:HOH:O	12:d:106:ASN:HB2	1.24	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y:27:LYS:HD3	12:d:145:GLU:OE1	1.23	1.28
18:J:29:LEU:HD21	19:k:34:SER:OG	1.35	1.25
18:J:29:LEU:CD2	19:k:34:SER:CB	2.09	1.25
19:K:15:ARG:CG	9:a:408:ARG:HH22	1.54	1.20
35:n:920:UNK:CA	35:n:1200:UNK:N	2.03	1.20
33:Y:14:CYS:SG	44:Y:500:HEM:HAB	1.85	1.16
52:Y:269:HOH:O	12:d:145:GLU:CD	1.85	1.16
10:b:95:LYS:HB2	17:i:32:ALA:HB2	1.20	1.16
1:1:104:ARG:HH21	2:2:127:SER:HB3	1.04	1.15
18:J:17:THR:HG22	19:k:24:TRP:HZ2	1.03	1.13
3:3:474:ARG:HH21	3:3:516:VAL:HG21	1.03	1.11
18:J:17:THR:HG22	19:k:24:TRP:CZ2	1.85	1.11
15:g:45:ILE:HG22	15:g:46:LEU:HD22	1.31	1.11
33:Y:14:CYS:SG	44:Y:500:HEM:CAB	2.40	1.10
33:Y:65[B]:MET:HE1	33:Y:92:GLU:HA	1.29	1.09
36:o:310:UNK:CA	36:o:350:UNK:CA	2.31	1.08
6:6:83:ARG:HH11	6:6:83:ARG:HG3	1.13	1.07
10:B:12:GLU:HG2	10:B:17:VAL:H	1.15	1.07
10:B:47:ILE:HG21	10:B:120:MET:HE1	1.35	1.06
33:Y:25:LYS:HE2	12:d:145:GLU:OE2	1.56	1.06
3:3:11:VAL:HG11	3:3:25:HIS:HD2	1.16	1.05
18:J:18:SER:HB2	19:k:23:LEU:HB2	1.08	1.05
1:1:97:GLU:HB2	40:1:441:NAI:H42N	1.37	1.04
10:b:47:ILE:HG21	10:b:120:MET:HE1	1.37	1.04
1:1:104:ARG:NH2	2:2:127:SER:HB3	1.73	1.04
11:C:129:MET:HE1	11:C:181:PHE:HD2	1.19	1.03
12:d:74:PRO:HG3	12:d:80:MET:HE1	1.40	1.03
3:3:31:PRO:HB3	3:3:47:MET:HE3	1.38	1.02
52:A:4099:HOH:O	19:k:15:ARG:NE	1.77	1.02
3:3:474:ARG:NH2	3:3:516:VAL:HG21	1.75	1.01
10:b:200:THR:HB	10:b:229:GLY:HA2	1.36	1.01
18:J:18:SER:CB	19:k:23:LEU:HB2	1.90	1.01
13:E:166:ASP:HA	52:E:541:HOH:O	1.59	1.00
5:5:66:GLU:HG2	5:5:95:PRO:HA	1.40	1.00
36:o:1001:UNK:C	36:o:1059:UNK:C	2.40	1.00
5:5:52:ILE:CG2	5:5:114:LEU:HB3	1.92	0.99
5:5:34:PHE:HE1	5:5:38:MET:HE2	1.22	0.99
5:5:175:THR:HG23	5:5:178:ASP:HB2	1.42	0.99
11:c:129:MET:HE1	11:c:181:PHE:HD2	1.29	0.97
18:J:25:VAL:HG11	19:k:30:VAL:HB	1.45	0.97
33:Y:27:LYS:CD	12:d:145:GLU:OE1	2.12	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:129:MET:HE1	11:C:181:PHE:CD2	2.00	0.96
35:n:920:UNK:C	35:n:1200:UNK:H2	1.78	0.96
3:3:373:GLY:HA3	3:3:538:ALA:HB2	1.48	0.96
20:L:365:ILE:HD12	21:M:87:MET:HE1	1.48	0.95
19:K:34:SER:OG	18:j:29:LEU:HD21	1.65	0.95
18:J:18:SER:HB2	19:k:23:LEU:CB	1.96	0.95
33:Y:83:ALA:HB3	12:d:165:TYR:OH	1.67	0.95
12:D:74:PRO:HG3	12:D:80:MET:HE1	1.47	0.95
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.48	0.94
26:R:5:LYS:HZ3	26:R:6:GLY:H	0.94	0.94
3:3:405:GLU:HB2	3:3:535:MET:HE2	1.49	0.94
6:6:117:MET:HE3	8:8:99:ILE:HG12	1.49	0.94
35:n:920:UNK:CA	35:n:1200:UNK:H2	1.77	0.93
1:1:16:THR:HG21	1:1:229:PRO:HB3	1.50	0.93
18:J:29:LEU:CD2	19:k:34:SER:OG	2.12	0.92
3:3:701:ALA:HB2	3:3:763:LEU:HB2	1.49	0.92
9:A:136:GLN:HE21	17:I:51:CYS:HB3	1.34	0.92
1:1:184:GLU:OE1	1:1:186:THR:HG22	1.69	0.92
2:2:114:ASP:HB2	2:2:116:LEU:HD22	1.52	0.92
20:L:449:MET:SD	21:M:5:MET:HE2	2.09	0.92
10:b:229:GLY:C	10:b:231:GLY:H	1.76	0.92
3:3:117:LEU:N	4:4:321:MET:HE1	1.84	0.91
3:3:522:ARG:HH12	3:3:681:LYS:HE3	1.35	0.91
3:3:459:MET:HE2	3:3:465:HIS:HB2	1.51	0.91
52:Y:308:HOH:O	47:d:501:HEC:CBC	2.17	0.91
5:5:121:LEU:HB3	5:5:146:LEU:HB2	1.52	0.91
12:d:59:ASP:OD2	18:j:62:LYS:HB3	1.71	0.91
3:3:117:LEU:HD12	4:4:321:MET:HE2	1.52	0.91
3:3:165:ASP:HB3	3:3:178:ARG:HD2	1.52	0.91
4:4:40:VAL:HG13	4:4:404:MET:HG3	1.52	0.90
3:3:11:VAL:HG11	3:3:25:HIS:CD2	2.06	0.90
11:c:129:MET:HE1	11:c:181:PHE:CD2	2.06	0.90
14:f:13:LEU:HD12	14:f:16:ILE:HD11	1.52	0.90
34:m:119:UNK:C	34:m:121:UNK:N	2.34	0.90
4:4:250:LYS:HE2	4:4:262:PHE:HB3	1.54	0.90
33:Y:25:LYS:HE2	12:d:145:GLU:CD	1.95	0.90
3:3:20:MET:HE1	3:3:432:PHE:HB2	1.55	0.89
9:A:293:PRO:O	9:A:297:ILE:HG12	1.71	0.89
3:3:115:HIS:CG	3:3:116:PRO:HD2	2.07	0.89
9:A:1:THR:HG21	10:B:212:SER:HB3	1.54	0.89
17:I:32:ALA:N	17:I:72:VAL:HG23	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.55	0.88
19:K:15:ARG:HG3	9:a:408:ARG:HH12	1.35	0.88
3:3:738:THR:HG22	3:3:740:PHE:H	1.39	0.88
22:N:112:LEU:HG	22:N:118:PRO:HB3	1.55	0.88
52:Y:236:HOH:O	12:d:161:ALA:HB3	1.73	0.88
17:i:64:LEU:HD12	17:i:77:ARG:O	1.73	0.88
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.55	0.88
18:j:16:ARG:HB2	18:j:19:THR:HG22	1.56	0.87
5:5:5:ARG:HH11	5:5:5:ARG:HG3	1.37	0.87
9:a:136:GLN:HE21	17:i:51:CYS:HB3	1.37	0.87
10:B:12:GLU:HG2	10:B:17:VAL:N	1.90	0.87
1:1:149:ILE:HD13	1:1:171:LEU:HB3	1.57	0.86
18:J:29:LEU:HD21	19:k:34:SER:HB2	0.88	0.86
4:4:96:ALA:HB2	4:4:346:THR:HG21	1.58	0.86
10:B:95:LYS:HB2	17:I:32:ALA:HB2	1.57	0.86
3:3:237:ASP:OD1	3:3:239:THR:HG22	1.75	0.86
17:i:52:ARG:HB3	17:i:52:ARG:HH11	1.40	0.86
18:J:17:THR:CG2	19:k:24:TRP:HZ2	1.88	0.85
1:1:242:GLY:HA2	1:1:268:MET:O	1.76	0.85
3:3:561:PRO:HB3	3:3:576:ALA:HA	1.58	0.85
6:6:46:CYS:HB3	6:6:81:ALA:HB1	1.58	0.85
18:J:16:ARG:HB2	18:J:19:THR:HG22	1.58	0.85
21:M:78:LEU:HB2	21:M:79:PRO:HD3	1.58	0.85
3:3:494:LYS:O	3:3:498:GLU:HG2	1.76	0.84
12:D:43:MET:HE3	12:D:46:VAL:HG21	1.59	0.84
3:3:116:PRO:O	3:3:117:LEU:HB2	1.78	0.84
4:4:367:ARG:HG2	4:4:367:ARG:HH11	1.43	0.84
9:a:293:PRO:O	9:a:297:ILE:HG12	1.78	0.84
1:1:293:GLY:HA3	1:1:324:GLY:H	1.42	0.84
5:5:34:PHE:CE1	5:5:38:MET:HE2	2.11	0.84
52:Y:308:HOH:O	47:d:501:HEC:HBC3	1.77	0.84
3:3:522:ARG:NH1	3:3:681:LYS:HE3	1.92	0.84
1:1:118:MET:HG2	1:1:224:LEU:HD13	1.60	0.83
19:K:15:ARG:HG2	9:a:408:ARG:CZ	2.07	0.83
5:5:52:ILE:HG21	5:5:114:LEU:HB3	1.57	0.83
6:6:83:ARG:HG3	6:6:83:ARG:NH1	1.93	0.83
35:n:704:UNK:C	35:n:706:UNK:N	2.40	0.83
10:b:236:LYS:H	10:b:236:LYS:HD2	1.42	0.83
20:L:187:SER:HB2	20:L:277:MET:HE1	1.60	0.82
52:A:4099:HOH:O	19:k:15:ARG:CZ	2.17	0.82
7:7:101:LYS:HE2	7:7:101:LYS:HA	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:12:LYS:HE2	11:c:16:ASN:H	1.42	0.82
1:1:185:GLU:HB2	1:1:218:ILE:HD12	1.62	0.82
3:3:515:THR:HG23	3:3:683:LEU:HD12	1.60	0.82
17:I:64:LEU:HD12	17:I:77:ARG:O	1.78	0.82
17:I:36:ALA:HB2	17:I:73:PRO:HD2	1.61	0.82
1:1:246:SER:HB3	1:1:268:MET:HG2	1.62	0.82
17:i:52:ARG:HB3	17:i:52:ARG:NH1	1.94	0.82
1:1:337:MET:HE2	1:1:337:MET:HA	1.59	0.81
33:Y:72:LYS:HD2	52:Y:358:HOH:O	1.79	0.81
9:a:29:GLN:HB3	10:b:12:GLU:O	1.80	0.81
10:b:95:LYS:CB	17:i:32:ALA:HB2	2.06	0.81
15:g:72:LYS:HG3	16:h:56:GLU:OE2	1.81	0.81
26:R:5:LYS:HZ3	26:R:6:GLY:N	1.77	0.81
3:3:501:LYS:H	3:3:501:LYS:HD2	1.43	0.81
52:Y:269:HOH:O	12:d:145:GLU:CG	2.23	0.81
3:3:642:ALA:HB1	3:3:652:PRO:HG3	1.63	0.81
19:K:30:VAL:HG11	18:j:25:VAL:HG11	1.62	0.81
3:3:384:PRO:HG3	3:3:542:ARG:HH21	1.45	0.81
4:4:212:PRO:HB2	4:4:213:ILE:HD12	1.63	0.80
4:4:363:SER:HB2	5:5:174:LEU:H	1.46	0.80
1:1:344:LEU:O	1:1:347:PHE:HB3	1.80	0.80
11:c:12:LYS:HA	11:c:12:LYS:HE3	1.62	0.80
52:A:4099:HOH:O	19:k:15:ARG:NH2	2.12	0.80
27:S:39:CYS:SG	27:S:53:CYS:HB3	2.22	0.79
3:3:279:ALA:HB2	3:3:290:ILE:HG12	1.64	0.79
4:4:310:THR:HG22	4:4:311:PRO:O	1.83	0.79
4:4:254:TYR:HD1	4:4:255:SER:H	1.30	0.79
27:S:75:ARG:HG2	27:S:75:ARG:HH11	1.48	0.79
3:3:171:SER:HB2	3:3:172:PRO:HD2	1.64	0.79
5:5:186:GLY:HA2	5:5:190:LYS:HD3	1.65	0.79
9:A:2:ALA:HB1	9:A:6:GLN:HB2	1.65	0.79
3:3:370:ASP:OD1	3:3:551:PRO:HD3	1.82	0.79
27:S:39:CYS:SG	27:S:53:CYS:CB	2.70	0.79
10:b:200:THR:CB	10:b:229:GLY:HA2	2.11	0.79
34:m:420:UNK:C	34:m:422:UNK:N	2.44	0.79
4:4:222:GLY:HA3	4:4:396:ILE:HD11	1.63	0.78
12:D:43:MET:HE1	12:D:189:PHE:CZ	2.18	0.78
12:d:43:MET:HE1	12:d:189:PHE:CZ	2.17	0.78
12:d:43:MET:HE3	12:d:46:VAL:HG21	1.66	0.78
3:3:19:VAL:HG22	3:3:91:MET:HE1	1.66	0.78
18:J:16:ARG:NH1	18:J:19:THR:HG21	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:104:LEU:O	5:5:193:ARG:HD2	1.84	0.78
5:5:47:ASN:H	5:5:47:ASN:HD22	1.32	0.78
9:A:1:THR:HG21	10:B:212:SER:CB	2.13	0.78
1:1:162:LEU:O	1:1:165:THR:HG22	1.84	0.78
3:3:55:PRO:HB3	3:3:73:ILE:HA	1.66	0.78
18:j:13:LEU:O	18:j:19:THR:HG23	1.84	0.78
3:3:194:VAL:HB	3:3:195:PRO:HD3	1.66	0.77
52:Y:247:HOH:O	12:d:145:GLU:OE2	2.02	0.77
8:8:26:TYR:N	8:8:27:PRO:HD3	1.98	0.77
4:4:213:ILE:HD12	4:4:213:ILE:H	1.48	0.77
7:7:8:GLU:HG2	7:7:97:TYR:CZ	2.19	0.77
3:3:655:ARG:HB2	3:3:655:ARG:HH11	1.47	0.77
19:K:34:SER:CB	18:j:29:LEU:HD21	2.13	0.77
26:R:5:LYS:NZ	26:R:6:GLY:H	1.78	0.77
33:Y:17:CYS:HG	44:Y:500:HEM:CAC	1.98	0.77
34:m:1526:UNK:C	34:m:1528:UNK:N	2.48	0.77
17:I:32:ALA:N	17:I:71:ASN:HB3	1.99	0.76
21:M:5:MET:HE3	30:V:42:PRO:HA	1.67	0.76
3:3:542:ARG:HB2	3:3:542:ARG:HH11	1.51	0.76
4:4:261:THR:N	4:4:292:GLN:HE22	1.83	0.76
18:J:29:LEU:HD22	19:k:34:SER:HB2	1.65	0.76
4:4:105:LEU:HD13	4:4:309:ILE:HD13	1.67	0.76
7:7:121:ARG:HH11	7:7:121:ARG:HG3	1.50	0.76
22:N:187:THR:HG21	26:R:68:THR:HG21	1.68	0.76
21:M:59:GLN:H	21:M:62:GLU:HG3	1.51	0.75
8:8:131:TYR:CB	8:8:136:MET:HE2	2.17	0.75
8:8:40:ARG:HB2	8:8:121:MET:HE1	1.69	0.75
1:1:358:PRO:HD3	3:3:107:MET:CE	2.16	0.75
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.66	0.75
3:3:184:CYS:O	3:3:184:CYS:SG	2.45	0.75
3:3:218:LEU:N	3:3:219:PRO:HD3	2.01	0.75
4:4:346:THR:HG23	4:4:353:LEU:HB3	1.69	0.75
3:3:509:ALA:HB1	3:3:768:GLY:HA3	1.68	0.75
5:5:5:ARG:HG3	5:5:5:ARG:NH1	2.00	0.75
3:3:402:PRO:HA	3:3:535:MET:CE	2.17	0.74
5:5:66:GLU:HG2	5:5:95:PRO:CA	2.16	0.74
3:3:101:ARG:NH1	3:3:140:TYR:CD1	2.55	0.74
4:4:274:ASP:O	4:4:278:VAL:HG23	1.87	0.74
5:5:47:ASN:H	5:5:47:ASN:ND2	1.80	0.74
11:c:379:TRP:CZ3	14:f:33:ARG:HD3	2.22	0.74
4:4:261:THR:H	4:4:292:GLN:HE22	1.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:384:PRO:HG3	3:3:542:ARG:NH2	2.01	0.74
11:c:78:ILE:CD1	12:d:204:MET:HE1	2.18	0.74
18:j:3:PRO:HB2	18:j:8:ARG:NH1	2.01	0.74
21:M:184:LEU:HD11	21:M:211:LEU:HD21	1.69	0.74
3:3:405:GLU:HB2	3:3:535:MET:CE	2.17	0.74
19:K:15:ARG:CG	9:a:408:ARG:NH2	2.29	0.74
1:1:40:THR:O	1:1:44:VAL:HG23	1.87	0.74
2:2:101:THR:HG22	7:7:108:ILE:HD11	1.69	0.74
9:A:3:THR:OG1	9:A:6:GLN:HG3	1.87	0.74
36:o:310:UNK:CA	36:o:350:UNK:N	2.51	0.74
4:4:47:LEU:HD12	4:4:48:SER:N	2.03	0.73
10:b:71:LEU:HD23	17:i:68:VAL:HG21	1.69	0.73
2:2:101:THR:HG23	2:2:106:ILE:O	1.87	0.73
3:3:156:ARG:HH11	3:3:156:ARG:HG3	1.53	0.73
19:K:15:ARG:CG	9:a:408:ARG:HH12	2.02	0.73
3:3:567:TYR:HA	3:3:584:VAL:HG23	1.69	0.73
23:O:23:PRO:O	24:P:66:ARG:HD3	1.89	0.73
6:6:77:VAL:HG22	6:6:104:TRP:HB2	1.69	0.73
17:I:32:ALA:N	17:I:71:ASN:CB	2.51	0.73
1:1:50:PRO:O	1:1:53:VAL:HG12	1.89	0.73
9:A:117:VAL:HG11	9:A:195:MET:HE1	1.69	0.73
10:B:71:LEU:HD23	17:I:68:VAL:HG21	1.70	0.73
26:R:54:ARG:HD3	26:R:54:ARG:N	2.04	0.73
3:3:20:MET:CE	3:3:432:PHE:HB2	2.18	0.72
6:6:148:ILE:HG21	8:8:27:PRO:HG3	1.71	0.72
2:2:81:GLN:HB3	2:2:122:VAL:HG21	1.70	0.72
18:j:16:ARG:HH11	18:j:19:THR:HG21	1.53	0.72
5:5:10:ALA:HB1	5:5:15:TYR:HB2	1.72	0.72
4:4:126:LEU:HD21	4:4:286:SER:HB2	1.71	0.72
16:h:28:GLU:O	16:h:31:VAL:HG22	1.89	0.72
36:o:653:UNK:C	36:o:655:UNK:N	2.51	0.72
3:3:31:PRO:CB	3:3:47:MET:HE3	2.18	0.72
18:J:13:LEU:O	18:J:19:THR:HG23	1.90	0.72
52:Y:308:HOH:O	47:d:501:HEC:HBC2	1.83	0.72
4:4:262:PHE:CE1	4:4:289:ILE:HD11	2.24	0.72
9:A:352:SER:HB3	14:f:110:LYS:HD2	1.71	0.72
1:1:253:GLN:N	1:1:253:GLN:HE21	1.87	0.72
20:L:176:MET:HE3	20:L:181:THR:HG22	1.71	0.72
6:6:163:TYR:HB2	8:8:152:ARG:NH1	2.05	0.72
8:8:96:LEU:HD21	8:8:129:LEU:HD13	1.71	0.72
19:k:18:VAL:HB	19:k:19:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:55:PRO:HB3	3:3:73:ILE:CA	2.18	0.71
8:8:131:TYR:HB2	8:8:136:MET:HE2	1.72	0.71
1:1:253:GLN:HE21	1:1:253:GLN:H	1.39	0.71
14:F:13:LEU:O	14:F:16:ILE:HG12	1.89	0.71
18:J:16:ARG:HB2	18:J:16:ARG:HH11	1.55	0.71
33:Y:17:CYS:SG	44:Y:500:HEM:CAC	2.78	0.71
35:n:651:UNK:C	35:n:653:UNK:N	2.50	0.71
13:E:113:GLU:HB3	13:E:116:GLN:NE2	2.05	0.71
39:1:440:FMN:N1	39:1:440:FMN:O3'	2.20	0.71
9:A:408:ARG:HH22	19:k:15:ARG:HB2	1.53	0.71
16:H:43:ARG:O	16:H:47:ARG:HD2	1.89	0.71
3:3:583:VAL:CG2	3:3:598:ALA:HA	2.21	0.71
6:6:108:MET:HA	6:6:137:VAL:CG1	2.21	0.71
4:4:371:ARG:NH1	5:5:50:ALA:O	2.24	0.71
1:1:90:ILE:HD11	1:1:211:LEU:HD22	1.72	0.71
3:3:11:VAL:CG1	3:3:25:HIS:HD2	2.00	0.71
23:O:147:LYS:HA	23:O:147:LYS:HE3	1.72	0.70
33:Y:25:LYS:CE	12:d:145:GLU:CD	2.64	0.70
4:4:318:GLU:HB2	7:7:39:ASP:HA	1.73	0.70
20:L:11:ASN:HD22	20:L:14:ASP:H	1.39	0.70
37:p:413:UNK:C	37:p:415:UNK:N	2.54	0.70
1:1:395:GLU:HB2	1:1:407:VAL:HG21	1.72	0.70
2:2:106:ILE:HG23	2:2:110:GLU:HB2	1.73	0.70
10:B:231:GLY:N	10:B:233:SER:H	1.90	0.70
3:3:386:SER:HB2	3:3:675:ARG:HH12	1.57	0.70
21:M:13:THR:HB	21:M:168:LEU:HD23	1.74	0.70
35:n:820:UNK:C	35:n:824:UNK:N	2.55	0.70
9:A:136:GLN:HE21	17:I:51:CYS:CB	2.04	0.69
52:Y:269:HOH:O	12:d:145:GLU:HG2	1.90	0.69
11:c:78:ILE:HD12	12:d:204:MET:HE1	1.74	0.69
2:2:27:ILE:O	2:2:31:LEU:HD23	1.92	0.69
6:6:77:VAL:HA	6:6:104:TRP:O	1.92	0.69
16:H:28:GLU:O	16:H:31:VAL:HG22	1.92	0.69
12:d:35:GLN:HG3	52:d:3086:HOH:O	1.91	0.69
12:d:74:PRO:CG	12:d:80:MET:HE1	2.20	0.69
1:1:267:PRO:O	1:1:270:THR:HG23	1.93	0.69
2:2:144:CYS:O	2:2:149:ARG:HD2	1.93	0.69
3:3:402:PRO:HA	3:3:535:MET:HE1	1.74	0.69
9:A:352:SER:HB3	14:f:110:LYS:CD	2.23	0.69
11:c:68:HIS:HD2	52:c:3131:HOH:O	1.75	0.69
4:4:254:TYR:CE2	4:4:346:THR:HA	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:29:LEU:O	5:5:92:VAL:HG12	1.93	0.69
3:3:737:GLU:HB2	3:3:776:LEU:HD21	1.74	0.68
3:3:261:VAL:HG22	38:3:786:SF4:S2	2.33	0.68
4:4:272:VAL:HG23	4:4:399:SER:HB3	1.74	0.68
11:C:379:TRP:CZ3	14:F:33:ARG:HD3	2.28	0.68
20:L:69:MET:HE2	20:L:70:VAL:HG23	1.74	0.68
22:N:154:GLY:HA2	25:Q:6:VAL:HG22	1.75	0.68
22:N:156:ARG:HH11	22:N:156:ARG:HG3	1.56	0.68
3:3:20:MET:HE1	3:3:432:PHE:CB	2.23	0.68
4:4:219:ARG:HG2	37:p:824:UNK:C	2.23	0.68
8:8:71:GLU:HB2	8:8:90:VAL:HB	1.74	0.68
10:B:353:SER:HB3	10:B:355:PRO:HD2	1.76	0.68
9:a:117:VAL:HG11	9:a:195:MET:HE1	1.76	0.68
1:1:219:ASN:ND2	39:1:440:FMN:O2P	2.27	0.68
1:1:18:TYR:OH	1:1:105:TYR:HB2	1.94	0.68
1:1:49:THR:HG23	1:1:52:GLU:HG3	1.75	0.68
1:1:272:PHE:CE1	1:1:311:MET:HE3	2.29	0.68
1:1:341:MET:HE3	1:1:413:SER:HB3	1.76	0.68
11:C:78:ILE:CD1	12:D:204:MET:HE1	2.23	0.68
34:m:1522:UNK:C	34:m:1524:UNK:N	2.54	0.68
22:N:12:ASN:HD22	29:U:20:VAL:H	1.39	0.68
13:e:79:SER:HB3	13:e:191:ASP:OD2	1.93	0.68
3:3:2:VAL:CG1	3:3:89:ASP:HA	2.24	0.68
5:5:47:ASN:HD22	5:5:47:ASN:N	1.87	0.68
5:5:123:GLY:H	5:5:147:ARG:NH1	1.92	0.68
9:a:29:GLN:HG3	9:a:203:LEU:O	1.94	0.68
1:1:363:VAL:HA	1:1:367:MET:HB2	1.76	0.68
10:b:236:LYS:H	10:b:236:LYS:CD	2.07	0.68
5:5:145:PRO:HA	5:5:150:TYR:CD1	2.27	0.68
2:2:110:GLU:HA	7:7:121:ARG:HH12	1.59	0.68
17:I:36:ALA:CB	17:I:73:PRO:HD2	2.23	0.68
1:1:104:ARG:HD2	1:1:108:GLU:OE2	1.94	0.67
6:6:108:MET:HA	6:6:137:VAL:HG13	1.75	0.67
9:a:32:GLN:OE1	10:b:373:GLU:HB2	1.94	0.67
4:4:85:MET:CE	4:4:409:ARG:HB2	2.24	0.67
27:S:38:ARG:HG2	27:S:85:ILE:HG23	1.77	0.67
20:L:151:HIS:O	20:L:155:VAL:HG23	1.95	0.67
4:4:372:ALA:HB1	4:4:406:ASP:OD1	1.94	0.67
13:E:113:GLU:HB3	13:E:116:GLN:HE21	1.55	0.67
2:2:134:ILE:HG13	2:2:145:VAL:HG21	1.77	0.67
10:b:95:LYS:HB2	17:i:32:ALA:CB	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:16:THR:CG2	1:1:229:PRO:HB3	2.22	0.67
3:3:378:PRO:O	3:3:381:LEU:HB2	1.93	0.67
24:P:43:PRO:HB2	24:P:48:ILE:HD11	1.76	0.67
10:b:169:ARG:HG3	10:b:240:HIS:HB2	1.76	0.67
8:8:40:ARG:HB2	8:8:121:MET:CE	2.25	0.67
9:A:2:ALA:O	10:B:113:ARG:NE	2.28	0.67
15:G:60:THR:O	15:G:64:GLN:HG3	1.95	0.67
19:K:30:VAL:HG11	18:j:25:VAL:CG1	2.24	0.67
52:Y:236:HOH:O	12:d:161:ALA:CB	2.38	0.67
3:3:216:PHE:CZ	7:7:128:PHE:HD2	2.13	0.66
12:d:74:PRO:HG3	12:d:80:MET:CE	2.22	0.66
1:1:110:VAL:N	1:1:111:PRO:HD3	2.11	0.66
3:3:42:ILE:HD11	3:3:189:ARG:CD	2.26	0.66
4:4:215:TYR:OH	37:p:824:UNK:C	2.41	0.66
52:A:4185:HOH:O	17:I:73:PRO:HG3	1.94	0.66
12:d:75:ASN:HD21	12:d:79:GLU:HG2	1.58	0.66
10:B:95:LYS:HD3	10:B:110:GLU:OE2	1.94	0.66
18:J:29:LEU:CG	19:k:34:SER:HB2	2.25	0.66
20:L:298:ASP:HB2	20:L:301:THR:HG23	1.77	0.66
31:W:19:TRP:HZ2	32:X:14:GLU:HG2	1.59	0.66
1:1:437:TRP:CB	2:2:92:GLY:HA3	2.25	0.66
3:3:405:GLU:OE1	3:3:508:GLY:HA3	1.95	0.66
11:C:129:MET:CE	11:C:181:PHE:HD2	2.02	0.66
23:O:24:LEU:H	24:P:34:ASN:HD21	1.44	0.66
18:j:8:ARG:HG2	18:j:8:ARG:HH11	1.60	0.66
18:j:16:ARG:NH1	18:j:19:THR:HG21	2.10	0.66
33:Y:65[B]:MET:HE1	33:Y:92:GLU:CA	2.17	0.66
3:3:305:ARG:HH22	3:3:609:GLU:CD	2.04	0.66
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.75	0.66
21:M:186:SER:HB3	21:M:213:LEU:HD22	1.76	0.66
33:Y:52[B]:ASN:HD22	33:Y:52[B]:ASN:C	2.04	0.66
22:N:209:ILE:O	22:N:213:THR:HG23	1.95	0.66
3:3:738:THR:HG23	3:3:739:PRO:HD2	1.77	0.66
5:5:66:GLU:CG	5:5:95:PRO:HA	2.19	0.66
9:A:86:LEU:HD13	9:A:99:ILE:HG12	1.77	0.66
22:N:101:PHE:HZ	22:N:260:GLY:HA3	1.61	0.65
1:1:370:LEU:O	1:1:374:ILE:HG22	1.96	0.65
3:3:591:HIS:ND1	3:3:592:PRO:HD2	2.11	0.65
22:N:160:LEU:HD13	22:N:222:GLN:HG2	1.78	0.65
3:3:578:LYS:HG2	3:3:597:TYR:HE2	1.62	0.65
1:1:115:ILE:O	1:1:119:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:54:LEU:N	3:3:55:PRO:CD	2.60	0.65
4:4:279:ARG:HH11	4:4:279:ARG:HG3	1.60	0.65
14:f:13:LEU:HA	14:f:16:ILE:HG12	1.78	0.65
9:A:408:ARG:HH22	19:k:15:ARG:CB	1.98	0.65
20:L:172:LYS:HB2	20:L:172:LYS:NZ	2.12	0.65
31:W:45:LEU:HD21	32:X:40:TYR:HA	1.78	0.65
3:3:31:PRO:HB3	3:3:47:MET:CE	2.20	0.65
3:3:249:MET:HE3	3:3:268:ASP:HB3	1.77	0.65
3:3:285:VAL:HG22	3:3:286:ASN:H	1.61	0.65
10:b:365:LYS:HG2	10:b:399:LEU:HD22	1.78	0.65
3:3:739:PRO:HG2	3:3:771:VAL:CG1	2.27	0.65
10:B:95:LYS:HD2	17:I:32:ALA:HB2	1.79	0.65
18:J:16:ARG:HH11	18:J:16:ARG:CB	2.10	0.65
4:4:98:ALA:O	4:4:102:GLU:HG3	1.97	0.64
3:3:206:GLY:O	3:3:209:THR:HG23	1.98	0.64
3:3:722:THR:HG21	3:3:756:GLY:N	2.12	0.64
11:C:191:ALA:HA	11:C:194:MET:HE2	1.78	0.64
19:K:23:LEU:HB2	18:j:18:SER:HB2	1.78	0.64
3:3:671:GLU:HG2	3:3:672:ALA:H	1.62	0.64
4:4:236:GLY:C	4:4:238:SER:H	2.05	0.64
17:I:36:ALA:HB3	17:I:73:PRO:HG2	1.78	0.64
15:g:71:ARG:HH11	15:g:72:LYS:HZ2	1.45	0.64
18:J:16:ARG:HB2	18:J:19:THR:CG2	2.26	0.64
21:M:120:SER:OG	21:M:138:VAL:HG21	1.97	0.64
10:B:231:GLY:N	10:B:232:LEU:N	2.46	0.64
1:1:16:THR:HG21	1:1:229:PRO:CB	2.25	0.64
3:3:279:ALA:CB	3:3:290:ILE:HG12	2.28	0.64
2:2:26:ALA:O	2:2:29:PRO:HG2	1.97	0.64
5:5:47:ASN:HD21	5:5:76:SER:HA	1.61	0.64
10:b:227:ARG:C	10:b:229:GLY:N	2.50	0.64
1:1:350:HIS:O	3:3:205:ARG:NH1	2.31	0.64
10:B:412:ASN:HA	10:B:415:LYS:HD2	1.80	0.64
2:2:122:VAL:HG12	2:2:123:GLU:N	2.12	0.64
2:2:106:ILE:CG2	2:2:110:GLU:HB2	2.27	0.64
13:E:45:VAL:HG13	18:J:28:ALA:HA	1.80	0.64
16:H:25:GLU:HG2	16:H:34:ARG:HH22	1.62	0.64
27:S:39:CYS:HG	27:S:53:CYS:HG	0.73	0.64
12:d:75:ASN:ND2	12:d:79:GLU:HG2	2.14	0.64
5:5:18:GLU:HB2	5:5:26:TRP:HB2	1.80	0.63
1:1:120:LEU:HD13	1:1:227:VAL:HG12	1.79	0.63
10:B:95:LYS:CB	17:I:32:ALA:HB2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:10:TYR:O	7:7:14:VAL:HG23	1.98	0.63
20:L:195:LEU:HD23	20:L:245:ILE:HD13	1.79	0.63
12:d:110:PRO:HG3	47:d:501:HEC:HMD2	1.79	0.63
1:1:357:THR:N	1:1:358:PRO:HD2	2.12	0.63
3:3:739:PRO:HG2	3:3:771:VAL:HG12	1.79	0.63
6:6:36:LEU:HD22	6:6:77:VAL:HG21	1.79	0.63
13:e:190:ASP:HB2	13:e:192:MET:HG2	1.79	0.63
3:3:30:VAL:CG2	3:3:31:PRO:HD2	2.28	0.63
3:3:184:CYS:O	38:3:785:SF4:S3	2.57	0.63
24:P:82:TYR:HB3	24:P:83:PRO:HD3	1.81	0.63
4:4:59:ILE:HD11	5:5:135:ILE:HG23	1.79	0.63
8:8:56:CYS:SG	8:8:58:LEU:HB2	2.39	0.63
27:S:57:ARG:HB3	27:S:57:ARG:HH11	1.64	0.63
9:a:136:GLN:NE2	17:i:51:CYS:HB3	2.12	0.63
1:1:358:PRO:HD3	3:3:107:MET:HE1	1.79	0.63
3:3:55:PRO:CB	3:3:73:ILE:HA	2.29	0.63
23:O:16:TYR:CE1	23:O:25:PRO:HG3	2.34	0.63
37:p:101:UNK:C	37:p:103:UNK:N	2.59	0.63
3:3:205:ARG:C	3:3:209:THR:HG22	2.24	0.63
3:3:101:ARG:NH1	3:3:140:TYR:CE1	2.67	0.62
11:c:191:ALA:HA	11:c:194:MET:HE2	1.80	0.62
11:C:50:PHE:HA	11:C:53:MET:HE3	1.81	0.62
14:F:28:LYS:HE3	52:F:4052:HOH:O	1.98	0.62
1:1:53:VAL:HG23	1:1:231:MET:HE2	1.80	0.62
4:4:85:MET:HE2	4:4:409:ARG:HB2	1.80	0.62
11:c:201:HIS:NE2	46:c:3002:UQ1:O4	2.28	0.62
4:4:230:ILE:HG22	4:4:230:ILE:O	2.00	0.62
11:C:29:SER:HB2	48:G:2004:CDL:HA31	1.81	0.62
15:g:60:THR:O	15:g:64:GLN:HG3	1.98	0.62
1:1:253:GLN:HG2	1:1:327:GLY:HA2	1.81	0.62
1:1:397:ARG:HD2	1:1:397:ARG:N	2.14	0.62
2:2:33:ARG:HH21	2:2:37:GLU:HG2	1.64	0.62
4:4:367:ARG:HG2	4:4:367:ARG:NH1	2.10	0.62
19:k:26:ALA:O	19:k:30:VAL:HG23	1.99	0.62
3:3:154:TYR:CZ	4:4:312:PRO:HB3	2.34	0.62
5:5:59:THR:O	5:5:59:THR:HG22	1.99	0.62
17:i:32:ALA:N	17:i:71:ASN:CB	2.63	0.62
3:3:736:VAL:HG22	3:3:775:VAL:HG22	1.80	0.62
4:4:47:LEU:HD12	4:4:48:SER:H	1.63	0.62
4:4:190:LEU:O	4:4:194:LEU:HB2	1.99	0.62
8:8:44:THR:HA	8:8:138:VAL:HG13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:M:16:ILE:HD12	21:M:17:MET:N	2.15	0.62
10:b:227:ARG:C	10:b:229:GLY:H	2.02	0.62
2:2:10:PHE:CZ	2:2:33:ARG:HG3	2.34	0.62
2:2:114:ASP:HB2	2:2:116:LEU:CD2	2.26	0.62
3:3:117:LEU:HD12	4:4:321:MET:CE	2.28	0.62
4:4:393:MET:HA	4:4:396:ILE:HG22	1.81	0.62
12:D:74:PRO:HG3	12:D:80:MET:CE	2.27	0.62
33:Y:72:LYS:HD3	33:Y:78:THR:HG22	1.82	0.62
3:3:545:GLU:HA	3:3:550:LEU:HD11	1.81	0.62
3:3:583:VAL:HG21	3:3:598:ALA:HA	1.80	0.62
6:6:76:ASP:O	6:6:77:VAL:HB	2.00	0.62
20:L:84:PRO:HG3	20:L:92:MET:HE3	1.80	0.62
20:L:128:VAL:O	20:L:128:VAL:HG22	1.99	0.62
1:1:104:ARG:NH2	2:2:127:SER:CB	2.57	0.62
4:4:89:HIS:CE1	4:4:92:ALA:HB2	2.35	0.62
6:6:154:LEU:O	6:6:158:VAL:HG13	1.99	0.62
9:A:51:LYS:HZ2	9:A:51:LYS:H	1.48	0.62
18:J:3:PRO:HD2	18:J:8:ARG:CZ	2.30	0.62
9:A:29:GLN:HG3	9:A:203:LEU:O	2.00	0.61
3:3:346:ALA:HB2	3:3:569:GLY:O	1.99	0.61
12:d:60:GLU:HG3	18:j:62:LYS:NZ	2.15	0.61
2:2:44:GLU:CD	2:2:44:GLU:H	2.09	0.61
3:3:185:LYS:HG3	3:3:202:PHE:HE2	1.65	0.61
3:3:285:VAL:HG22	3:3:286:ASN:N	2.14	0.61
4:4:64:THR:OG1	6:6:83:ARG:NH1	2.33	0.61
6:6:143:ARG:HG2	6:6:144:PRO:HD2	1.82	0.61
13:E:113:GLU:CB	13:E:116:GLN:HE21	2.13	0.61
19:K:15:ARG:CG	9:a:408:ARG:NH1	2.64	0.61
29:U:3:ASN:C	29:U:3:ASN:HD22	2.08	0.61
1:1:266:LEU:HB3	1:1:270:THR:HG21	1.83	0.61
3:3:333:LEU:HB3	3:3:648:LEU:HD21	1.82	0.61
6:6:153:GLN:HG3	8:8:124:TYR:OH	2.00	0.61
18:J:14:PHE:HA	18:J:20:PHE:HD1	1.64	0.61
32:X:13:LYS:H	32:X:13:LYS:HD3	1.65	0.61
10:b:296:TYR:OH	17:i:52:ARG:NE	2.33	0.61
3:3:259:CYS:SG	3:3:261:VAL:HG13	2.40	0.61
3:3:282:VAL:HG22	3:3:285:VAL:HG12	1.80	0.61
4:4:83:PRO:HB2	4:4:169:HIS:HA	1.82	0.61
20:L:11:ASN:HD21	20:L:13:LYS:HB2	1.64	0.61
22:N:154:GLY:HA2	25:Q:6:VAL:CG2	2.30	0.61
33:Y:65[B]:MET:SD	33:Y:95:ILE:HD12	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:435:LEU:HD22	3:3:435:LEU:H	1.65	0.61
20:L:92:MET:CE	20:L:167:THR:HG21	2.31	0.61
20:L:273:MET:HG3	20:L:319:LYS:HZ1	1.64	0.61
21:M:122:MET:HB2	21:M:208:PRO:HD2	1.81	0.61
1:1:66:GLY:O	40:1:441:NAI:H2N	2.01	0.61
3:3:722:THR:HG21	3:3:756:GLY:H	1.66	0.61
7:7:34:GLU:HB3	7:7:56:THR:HG22	1.83	0.61
12:D:74:PRO:CG	12:D:80:MET:HE1	2.26	0.61
20:L:187:SER:CB	20:L:277:MET:HE1	2.28	0.61
10:b:229:GLY:C	10:b:231:GLY:N	2.47	0.61
8:8:73:ALA:HB2	8:8:89:LYS:HB2	1.80	0.61
1:1:270:THR:O	1:1:311:MET:HG3	2.00	0.61
1:1:385:GLU:O	1:1:388:GLU:HB3	2.00	0.61
3:3:304:ASN:O	3:3:589:HIS:CD2	2.54	0.61
10:B:397:THR:O	10:B:401:GLN:HG3	2.00	0.61
22:N:192:VAL:O	22:N:196:THR:HB	2.01	0.61
1:1:356:CYS:HB3	1:1:358:PRO:HD2	1.83	0.61
3:3:453:PRO:HD3	3:3:468:HIS:CE1	2.36	0.61
20:L:92:MET:HE2	20:L:167:THR:HG21	1.82	0.61
22:N:148:HIS:O	22:N:152:MET:HG3	2.01	0.61
25:Q:13:ALA:O	25:Q:18:ARG:HD2	2.00	0.61
10:b:397:THR:O	10:b:401:GLN:HG3	2.01	0.61
1:1:267:PRO:HG2	1:1:270:THR:HG22	1.83	0.60
2:2:78:TYR:HA	2:2:137:ASN:HD21	1.66	0.60
3:3:615:VAL:HG22	3:3:621:VAL:HG12	1.82	0.60
1:1:145:LEU:O	1:1:149:ILE:HG13	2.01	0.60
21:M:59:GLN:HA	21:M:62:GLU:HB2	1.83	0.60
9:a:86:LEU:HD13	9:a:99:ILE:HG12	1.82	0.60
11:c:129:MET:CE	11:c:181:PHE:HD2	2.08	0.60
34:m:1324:UNK:C	34:m:1326:UNK:N	2.63	0.60
3:3:655:ARG:HB2	3:3:655:ARG:NH1	2.16	0.60
5:5:37:GLU:O	5:5:41:TYR:HD1	1.84	0.60
17:I:36:ALA:HB3	17:I:73:PRO:CG	2.31	0.60
27:S:39:CYS:HG	27:S:53:CYS:CB	2.07	0.60
18:J:16:ARG:HH11	18:J:16:ARG:CG	2.12	0.60
10:b:35:ILE:HD12	10:b:35:ILE:N	2.16	0.60
6:6:83:ARG:HH11	6:6:83:ARG:CG	1.97	0.60
18:J:25:VAL:HG12	19:k:30:VAL:CG1	2.31	0.60
17:i:36:ALA:HB2	17:i:73:PRO:HD2	1.84	0.60
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.84	0.60
3:3:2:VAL:HG13	3:3:89:ASP:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:116:PRO:O	3:3:117:LEU:CB	2.49	0.60
4:4:250:LYS:CE	4:4:262:PHE:HB3	2.31	0.60
9:A:296:SER:O	9:A:300:THR:HG23	2.02	0.60
3:3:216:PHE:HZ	7:7:128:PHE:HD2	1.47	0.60
4:4:200:ARG:HG3	4:4:204:TYR:HE1	1.67	0.60
10:b:203:ARG:HH12	10:b:233:SER:HA	1.65	0.60
39:1:440:FMN:HO3'	39:1:440:FMN:C2	2.13	0.60
3:3:385:ALA:HB2	3:3:531:LYS:HB3	1.84	0.60
3:3:513:GLN:HG2	3:3:769:LEU:HD23	1.84	0.60
4:4:164:THR:OG1	4:4:170:HIS:HB3	2.02	0.60
4:4:226:PRO:HG3	4:4:242:SER:O	2.02	0.60
4:4:234:LEU:HD21	4:4:238:SER:HB2	1.84	0.60
9:a:41:ILE:HG12	9:a:195:MET:HG2	1.83	0.60
9:a:308:GLN:HG2	52:a:3026:HOH:O	2.02	0.60
11:c:14:VAL:O	11:c:18:PHE:HB3	2.02	0.60
3:3:722:THR:HA	3:3:725:ALA:HB3	1.84	0.60
4:4:149:ALA:HA	4:4:152:GLU:OE1	2.00	0.60
6:6:99:MET:HG2	6:6:100:PRO:HD2	1.84	0.60
4:4:222:GLY:CA	4:4:396:ILE:HD11	2.32	0.60
4:4:389:GLN:HG3	4:4:390:VAL:H	1.67	0.60
18:J:29:LEU:HD21	19:k:34:SER:HG	1.64	0.60
32:X:28:LEU:HB2	32:X:29:PRO:HD3	1.84	0.60
11:c:145:VAL:HG21	45:c:3001:SMA:H6	1.84	0.60
15:g:71:ARG:HH11	15:g:72:LYS:NZ	1.99	0.60
17:i:32:ALA:N	17:i:71:ASN:HB2	2.15	0.60
19:K:34:SER:OG	18:j:29:LEU:CD2	2.46	0.59
22:N:119:THR:O	26:R:52:HIS:HE1	1.84	0.59
25:Q:62:CYS:SG	25:Q:84:SER:OG	2.60	0.59
3:3:337:ARG:HH12	3:3:581:ARG:NH1	2.00	0.59
4:4:221:VAL:O	4:4:272:VAL:HG12	2.02	0.59
1:1:138:TYR:HB3	1:1:141:ALA:HB3	1.84	0.59
3:3:515:THR:HG23	3:3:683:LEU:CD1	2.31	0.59
8:8:175:ALA:O	8:8:177:THR:HG23	2.02	0.59
21:M:179:LEU:HD21	27:S:65:PRO:HD3	1.85	0.59
2:2:149:ARG:NH1	2:2:168:LEU:HD13	2.16	0.59
3:3:583:VAL:HG21	3:3:597:TYR:O	2.02	0.59
3:3:586:HIS:CD2	3:3:604:ALA:HB2	2.37	0.59
19:K:32:LEU:O	19:K:33:VAL:C	2.46	0.59
9:a:172:GLU:OE2	9:a:176:LYS:HE3	2.01	0.59
1:1:184:GLU:CD	1:1:186:THR:HG22	2.28	0.59
1:1:301:PRO:HB2	1:1:303:THR:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:374:ILE:HG12	1:1:374:ILE:O	2.02	0.59
13:E:85:LYS:NZ	13:E:87:MET:SD	2.75	0.59
1:1:358:PRO:HD3	3:3:107:MET:HE3	1.83	0.59
3:3:343:LEU:HD12	3:3:361:ALA:HB2	1.84	0.59
6:6:92:MET:HE1	6:6:127:VAL:HG13	1.84	0.59
9:a:216:PHE:HD2	9:a:219:LEU:HD22	1.67	0.59
3:3:132:ASP:OD1	4:4:329:LYS:HE2	2.02	0.59
21:M:226:MET:O	21:M:227:LEU:HB2	2.02	0.59
27:S:57:ARG:HG3	27:S:60:TYR:CE2	2.38	0.59
3:3:511:VAL:O	3:3:518:ALA:HB2	2.03	0.59
4:4:74:THR:HB	4:4:77:GLN:H	1.67	0.59
4:4:163:VAL:HG22	4:4:164:THR:HG22	1.85	0.59
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.37	0.59
21:M:145:PRO:CG	21:M:148:MET:HE2	2.32	0.59
21:M:193:TYR:HE1	23:O:126:MET:HE1	1.68	0.59
22:N:6:HIS:HD2	22:N:8:TYR:H	1.49	0.59
9:a:8:LEU:HD22	9:a:392:LEU:HB3	1.84	0.59
4:4:40:VAL:O	4:4:40:VAL:HG22	2.03	0.59
11:C:145:VAL:HG21	45:C:2001:SMA:H6	1.84	0.59
13:E:77:LYS:HE3	13:E:79:SER:OG	2.03	0.59
18:J:3:PRO:HD2	18:J:8:ARG:NH2	2.18	0.59
26:R:5:LYS:HZ3	26:R:5:LYS:HB3	1.66	0.59
3:3:156:ARG:HG3	3:3:156:ARG:NH1	2.15	0.58
10:B:20:HIS:HB2	10:B:22:GLN:HG3	1.84	0.58
15:G:45:ILE:HG22	15:G:46:LEU:HD12	1.85	0.58
3:3:123:ASP:HB2	3:3:236:LEU:HD13	1.85	0.58
4:4:225:PRO:HG2	4:4:228:VAL:HB	1.85	0.58
31:W:46:LYS:O	31:W:47:LYS:HB2	2.02	0.58
1:1:33:LEU:HA	1:1:37:GLY:HA2	1.86	0.58
1:1:397:ARG:HD2	1:1:397:ARG:H	1.68	0.58
7:7:121:ARG:HG3	7:7:121:ARG:NH1	2.18	0.58
15:g:66:PHE:CZ	15:g:70:LYS:HD2	2.38	0.58
18:j:56:LYS:HG2	18:j:60:GLU:CD	2.28	0.58
3:3:227:THR:HG21	3:3:237:ASP:HB2	1.86	0.58
6:6:163:TYR:HB2	8:8:152:ARG:HH11	1.68	0.58
9:A:136:GLN:NE2	17:I:51:CYS:HB3	2.15	0.58
30:V:43:SER:OG	30:V:45:VAL:HG12	2.04	0.58
9:a:373:THR:HB	9:a:374:PRO:HD3	1.86	0.58
35:n:820:UNK:C	35:n:824:UNK:CA	2.80	0.58
3:3:279:ALA:HB2	3:3:290:ILE:CG1	2.31	0.58
10:B:309:VAL:HG23	10:B:326:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:32:ALA:N	17:i:72:VAL:HG23	2.18	0.58
35:n:121:UNK:C	35:n:123:UNK:N	2.66	0.58
5:5:123:GLY:H	5:5:147:ARG:HH11	1.51	0.58
10:B:169:ARG:HG3	10:B:240:HIS:HB2	1.84	0.58
10:B:412:ASN:HD22	10:B:415:LYS:HD2	1.67	0.58
4:4:219:ARG:CG	37:p:824:UNK:C	2.82	0.58
19:K:16:ASN:ND2	9:a:347:THR:O	2.32	0.58
3:3:185:LYS:HG2	3:3:188:VAL:HG22	1.86	0.58
8:8:131:TYR:HB3	8:8:136:MET:HE2	1.85	0.58
10:B:47:ILE:CG2	10:B:120:MET:HE1	2.24	0.58
13:E:99:ARG:HB3	13:E:133:VAL:CG1	2.33	0.58
11:c:100:ARG:HD2	11:c:100:ARG:C	2.28	0.58
34:m:1315:UNK:C	34:m:1317:UNK:N	2.67	0.58
10:B:354:ASN:N	10:B:355:PRO:CD	2.66	0.58
3:3:42:ILE:HD11	3:3:189:ARG:HD2	1.85	0.58
3:3:440:ARG:HG2	3:3:440:ARG:HH11	1.67	0.58
20:L:184:PHE:H	20:L:256:HIS:HE1	1.52	0.58
20:L:404:THR:O	20:L:480:ARG:NH1	2.37	0.58
4:4:363:SER:HB2	5:5:174:LEU:N	2.18	0.57
10:B:189:VAL:HG23	52:B:3089:HOH:O	2.03	0.57
6:6:78:MET:O	6:6:78:MET:HG3	2.03	0.57
17:I:32:ALA:N	17:I:71:ASN:HB2	2.19	0.57
2:2:77:LYS:H	2:2:116:LEU:HA	1.68	0.57
3:3:370:ASP:OD1	3:3:374:ARG:HD3	2.03	0.57
24:P:80:GLU:CD	24:P:80:GLU:H	2.10	0.57
18:j:16:ARG:HB2	18:j:19:THR:CG2	2.33	0.57
1:1:214:LYS:O	1:1:216:THR:HG23	2.03	0.57
3:3:398:VAL:HB	3:3:450:LEU:HD22	1.87	0.57
9:A:51:LYS:H	9:A:51:LYS:NZ	2.03	0.57
11:C:78:ILE:HD12	12:D:204:MET:HE1	1.86	0.57
13:E:190:ASP:O	13:E:192:MET:HG2	2.05	0.57
19:K:34:SER:HB2	18:j:29:LEU:HD21	1.84	0.57
21:M:193:TYR:CE1	23:O:126:MET:HE1	2.39	0.57
36:o:802:UNK:C	36:o:804:UNK:N	2.65	0.57
1:1:177:ALA:O	2:2:67:TYR:HB3	2.05	0.57
4:4:95:LEU:HG	4:4:99:LEU:HD23	1.87	0.57
33:Y:65[A]:MET:HE1	33:Y:92:GLU:CG	2.34	0.57
18:J:29:LEU:CD1	19:k:34:SER:HB2	2.34	0.57
1:1:6:LEU:HB2	1:1:241:MET:HA	1.86	0.57
3:3:394:ASP:OD2	3:3:501:LYS:HB2	2.05	0.57
3:3:689:LYS:HB2	3:3:772:GLU:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:239:LEU:HD22	4:4:244:VAL:HB	1.87	0.57
4:4:288:LYS:O	4:4:292:GLN:HB2	2.05	0.57
3:3:167:HIS:ND1	3:3:167:HIS:O	2.36	0.57
3:3:385:ALA:HB2	3:3:531:LYS:CB	2.35	0.57
3:3:466:GLU:CD	3:3:467:VAL:H	2.13	0.57
3:3:583:VAL:HG23	3:3:598:ALA:HA	1.87	0.57
4:4:144:THR:HB	4:4:145:PRO:HD3	1.84	0.57
5:5:32:GLU:CD	5:5:32:GLU:H	2.13	0.57
21:M:189:PRO:HD2	28:T:54:TYR:OH	2.05	0.57
31:W:41:ARG:HG3	32:X:40:TYR:CE2	2.40	0.57
9:a:30:SER:HA	10:b:18:PRO:HG3	1.85	0.57
3:3:469:ARG:HG2	3:3:754:PRO:HB3	1.85	0.57
14:F:82:LYS:HE3	52:F:4032:HOH:O	2.04	0.57
18:J:12:LEU:O	18:J:13:LEU:HD23	2.04	0.57
9:a:286:GLY:HA3	9:a:290:LEU:HD21	1.85	0.57
3:3:607:PHE:HA	3:3:610:LYS:HE2	1.87	0.57
15:G:40:ARG:HB3	48:G:2004:CDL:HB32	1.85	0.57
18:J:3:PRO:HB2	18:J:8:ARG:HD3	1.86	0.57
20:L:69:MET:HE2	20:L:70:VAL:CG2	2.35	0.57
27:S:71:THR:O	27:S:75:ARG:HD3	2.05	0.57
3:3:226:ILE:HD12	3:3:235:LEU:HD13	1.85	0.56
3:3:567:TYR:HA	3:3:584:VAL:CG2	2.36	0.56
9:A:136:GLN:NE2	17:I:51:CYS:CB	2.67	0.56
22:N:203:PHE:O	22:N:207:HIS:HD2	1.88	0.56
17:i:62:ARG:O	17:i:78:TYR:HB3	2.05	0.56
1:1:93:ALA:O	1:1:134:VAL:HA	2.05	0.56
3:3:140:TYR:CE2	3:3:142:LYS:HB3	2.40	0.56
10:B:365:LYS:HG2	10:B:399:LEU:HD22	1.86	0.56
21:M:132:GLU:HB3	21:M:137:GLU:HG3	1.87	0.56
33:Y:65[B]:MET:HE2	33:Y:95:ILE:HD12	1.86	0.56
11:c:319:PRO:HD2	52:c:3113:HOH:O	2.06	0.56
3:3:6:VAL:HG13	3:3:23:VAL:HG22	1.88	0.56
4:4:211:SER:HB2	4:4:214:PHE:HB3	1.87	0.56
5:5:37:GLU:O	5:5:41:TYR:CD1	2.58	0.56
6:6:83:ARG:HD3	38:6:182:SF4:S4	2.46	0.56
10:B:95:LYS:CG	17:I:32:ALA:HB2	2.35	0.56
13:E:189:SER:C	13:E:190:ASP:OD1	2.49	0.56
33:Y:69:GLU:HB2	33:Y:91[B]:ARG:NH1	2.20	0.56
6:6:81:ALA:HB1	6:6:108:MET:HE2	1.87	0.56
3:3:204:GLU:O	3:3:209:THR:HB	2.06	0.56
3:3:320:ALA:HB1	3:3:324:GLU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:440:ARG:HH11	3:3:440:ARG:CG	2.19	0.56
6:6:121:TYR:HD1	6:6:121:TYR:H	1.52	0.56
7:7:63:LEU:HD13	7:7:129:ALA:HB3	1.86	0.56
24:P:78:HIS:ND1	28:T:12:LEU:HD22	2.21	0.56
1:1:28:THR:HG22	1:1:30:ASP:H	1.70	0.56
3:3:469:ARG:HG2	3:3:754:PRO:CB	2.35	0.56
8:8:41:HIS:HB3	8:8:113:ILE:HD11	1.88	0.56
26:R:5:LYS:HD2	26:R:6:GLY:N	2.21	0.56
3:3:550:LEU:HD12	3:3:550:LEU:N	2.20	0.56
10:B:20:HIS:HB2	10:B:22:GLN:CG	2.36	0.56
1:1:437:TRP:C	1:1:437:TRP:CD1	2.84	0.56
3:3:11:VAL:CG1	3:3:25:HIS:CD2	2.81	0.56
6:6:49:GLU:OE1	6:6:49:GLU:HA	2.05	0.56
6:6:50:MET:C	6:6:52:ALA:H	2.12	0.56
9:A:227:ALA:O	9:A:228:VAL:C	2.49	0.56
15:g:71:ARG:HD3	15:g:72:LYS:HZ3	1.70	0.56
4:4:138:LEU:HD13	4:4:146:PHE:CD1	2.41	0.56
15:G:30:PHE:O	15:G:34:ILE:HG12	2.06	0.56
18:J:25:VAL:HG11	19:k:30:VAL:CB	2.28	0.56
18:j:8:ARG:HH11	18:j:8:ARG:CG	2.18	0.56
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.88	0.55
4:4:25:VAL:HA	4:4:48:SER:HB3	1.88	0.55
6:6:83:ARG:HD3	6:6:83:ARG:H	1.71	0.55
13:E:90:LYS:HE2	13:E:93:GLY:HA2	1.87	0.55
1:1:359:CYS:HA	1:1:363:VAL:HG13	1.87	0.55
3:3:474:ARG:HA	3:3:517:ALA:HB2	1.89	0.55
4:4:254:TYR:O	4:4:256:GLY:N	2.35	0.55
5:5:52:ILE:HG22	5:5:114:LEU:HB3	1.86	0.55
11:C:217:LYS:HG3	15:G:7:LEU:HD13	1.88	0.55
12:d:241:LYS:OXT	12:d:241:LYS:HD3	2.06	0.55
15:g:34:ILE:HB	15:g:35:PRO:HD3	1.89	0.55
1:1:373:LYS:HD3	1:1:383:ASP:OD2	2.06	0.55
2:2:112:THR:OG1	2:2:113:PRO:HD2	2.05	0.55
3:3:115:HIS:ND1	3:3:116:PRO:HD2	2.21	0.55
3:3:270:ARG:O	3:3:271:SER:HB2	2.06	0.55
5:5:53:VAL:HG13	5:5:71:VAL:HB	1.86	0.55
15:G:63:THR:O	15:G:67:GLU:HG2	2.06	0.55
21:M:111:THR:HG21	27:S:66:ILE:HD11	1.88	0.55
22:N:42:LEU:HD13	29:U:45:TYR:CD2	2.41	0.55
33:Y:83:ALA:CB	12:d:165:TYR:OH	2.50	0.55
16:h:25:GLU:HG2	16:h:34:ARG:HH22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:47:MET:SD	3:3:107:MET:HB3	2.46	0.55
3:3:225:ASN:ND2	3:3:289:TRP:HB3	2.21	0.55
4:4:246:TYR:CD1	5:5:77:LEU:HD22	2.42	0.55
11:C:245:PHE:CD1	12:D:17:LEU:HD13	2.41	0.55
20:L:172:LYS:HB2	20:L:172:LYS:HZ2	1.71	0.55
21:M:145:PRO:HG3	21:M:148:MET:HE2	1.87	0.55
1:1:312:SER:C	1:1:314:GLU:H	2.15	0.55
4:4:193:LEU:HD22	4:4:197:LEU:HG	1.88	0.55
7:7:108:ILE:HD12	7:7:108:ILE:N	2.22	0.55
14:F:63:LYS:HE2	52:G:1280:HOH:O	2.06	0.55
2:2:98:ASP:O	2:2:102:GLU:HB2	2.07	0.55
3:3:507:LEU:HD22	3:3:511:VAL:HG11	1.88	0.55
5:5:175:THR:HG23	5:5:178:ASP:CB	2.26	0.55
20:L:95:PRO:HB2	22:N:11:VAL:HG13	1.87	0.55
22:N:222:GLN:HE21	22:N:222:GLN:HA	1.72	0.55
13:e:188:THR:HG21	13:e:194:ILE:CD1	2.37	0.55
18:j:25:VAL:HG12	18:j:26:VAL:N	2.20	0.55
3:3:30:VAL:HG22	3:3:31:PRO:HD2	1.87	0.55
4:4:263:ASP:O	4:4:265:PRO:HD3	2.07	0.55
9:A:172:GLU:OE2	9:A:176:LYS:HE3	2.06	0.55
9:A:216:PHE:HD2	9:A:219:LEU:HD22	1.71	0.55
9:a:364:ALA:HB2	17:i:33:ALA:HB1	1.89	0.55
12:d:231:LYS:HD3	14:f:70:MET:HE3	1.87	0.55
15:g:30:PHE:O	15:g:34:ILE:HG12	2.06	0.55
15:g:63:THR:O	15:g:67:GLU:HG2	2.07	0.55
3:3:101:ARG:NH1	3:3:140:TYR:HD1	2.00	0.55
4:4:44:MET:HE2	4:4:44:MET:HA	1.89	0.55
4:4:320:SER:O	4:4:324:VAL:HG23	2.07	0.55
3:3:34:CYS:HA	3:3:184:CYS:HB2	1.89	0.55
7:7:8:GLU:HG2	7:7:97:TYR:CE2	2.42	0.55
10:B:95:LYS:HD2	17:I:32:ALA:CB	2.36	0.55
26:R:5:LYS:HD2	26:R:5:LYS:C	2.32	0.55
1:1:337:MET:HA	1:1:337:MET:CE	2.33	0.55
3:3:456:ALA:HB3	3:3:459:MET:HG3	1.88	0.55
3:3:546:ALA:O	3:3:547:MET:HE2	2.07	0.55
4:4:213:ILE:HD12	4:4:213:ILE:N	2.20	0.55
13:e:77:LYS:HE3	13:e:79:SER:OG	2.07	0.55
3:3:402:PRO:HA	3:3:535:MET:HE3	1.90	0.54
6:6:83:ARG:NH1	6:6:83:ARG:CG	2.64	0.54
8:8:48:ASN:HB2	8:8:50:LEU:HD23	1.89	0.54
8:8:151:LYS:C	8:8:153:THR:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:96:MET:HE2	11:C:96:MET:HA	1.89	0.54
16:H:25:GLU:CG	16:H:34:ARG:HH22	2.19	0.54
22:N:151:LEU:HB2	22:N:159:MET:HG3	1.89	0.54
11:c:50:PHE:HA	11:c:53:MET:HE3	1.88	0.54
3:3:550:LEU:HD23	3:3:684:ARG:HH21	1.73	0.54
8:8:137:LEU:O	8:8:140:VAL:HG12	2.08	0.54
9:A:76:GLU:HG2	9:A:80:GLU:OE2	2.07	0.54
20:L:407:ASP:O	20:L:411:LYS:HG3	2.07	0.54
4:4:233:GLY:HA2	5:5:48:PHE:HE1	1.71	0.54
6:6:165:GLU:HG2	8:8:148:ARG:NH1	2.22	0.54
14:F:78:GLU:H	14:F:78:GLU:CD	2.15	0.54
9:a:136:GLN:HE21	17:i:51:CYS:CB	2.15	0.54
13:e:191:ASP:N	13:e:191:ASP:OD1	2.41	0.54
3:3:113:LEU:HD12	3:3:157:PHE:HB2	1.90	0.54
3:3:715:GLU:H	3:3:761:SER:HB2	1.72	0.54
4:4:193:LEU:CD2	4:4:197:LEU:HG	2.38	0.54
4:4:248:VAL:HB	4:4:347:GLU:HB2	1.89	0.54
4:4:409:ARG:NH2	5:5:117:GLU:OE2	2.40	0.54
7:7:82:ILE:HG23	7:7:95:ALA:HB3	1.90	0.54
17:I:62:ARG:O	17:I:78:TYR:HB3	2.07	0.54
23:O:108:PRO:HG2	23:O:111:PHE:CE2	2.42	0.54
33:Y:41:GLY:N	33:Y:52[A]:ASN:HD21	2.05	0.54
17:i:36:ALA:HB3	17:i:73:PRO:HG2	1.89	0.54
3:3:444:ARG:NH2	3:3:447:LYS:HG3	2.22	0.54
3:3:707:LYS:C	3:3:709:GLN:H	2.14	0.54
5:5:53:VAL:CG1	5:5:71:VAL:HB	2.37	0.54
4:4:241:ALA:HB2	4:4:278:VAL:HG21	1.90	0.54
11:C:341:GLN:NE2	52:C:2099:HOH:O	2.39	0.54
1:1:98:PRO:HA	2:2:124:CYS:SG	2.48	0.54
3:3:318:VAL:HG12	3:3:319:GLU:N	2.23	0.54
3:3:546:ALA:HA	3:3:678:PHE:CE2	2.43	0.54
3:3:629:ILE:HG22	3:3:630:GLU:N	2.23	0.54
25:Q:55:LYS:HA	25:Q:74:LEU:O	2.08	0.54
10:b:229:GLY:O	10:b:230:LEU:HB2	2.07	0.54
3:3:664:LEU:O	3:3:669:VAL:HG12	2.08	0.54
6:6:163:TYR:HD2	8:8:152:ARG:NH1	2.05	0.54
10:B:314:ALA:HA	17:I:63:PRO:HD3	1.90	0.54
28:T:63:MET:HB3	28:T:68:ILE:HD11	1.89	0.54
33:Y:65[B]:MET:CE	33:Y:95:ILE:HD12	2.38	0.54
1:1:406:ALA:O	1:1:410:VAL:HG23	2.08	0.54
4:4:337:PRO:O	4:4:361:GLY:HA2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:369:LYS:HG3	5:5:53:VAL:HG23	1.90	0.54
10:B:12:GLU:O	10:B:18:PRO:HD3	2.08	0.54
21:M:165:VAL:HB	21:M:170:LEU:HD12	1.90	0.54
10:b:47:ILE:CG2	10:b:120:MET:HE1	2.25	0.54
6:6:42:GLY:O	6:6:43:LEU:HD23	2.07	0.53
21:M:136:LEU:HB3	21:M:193:TYR:HD2	1.73	0.53
1:1:376:THR:O	1:1:376:THR:HG22	2.07	0.53
3:3:55:PRO:HB3	3:3:73:ILE:N	2.22	0.53
3:3:452:ALA:O	3:3:454:TYR:N	2.42	0.53
11:C:15:ASN:O	11:C:16:ASN:C	2.50	0.53
24:P:41:LEU:HD12	24:P:41:LEU:O	2.08	0.53
25:Q:48:LEU:O	25:Q:50:PRO:HD3	2.08	0.53
9:a:30:SER:CA	10:b:18:PRO:HG3	2.39	0.53
2:2:28:MET:HB2	2:2:29:PRO:CD	2.38	0.53
3:3:115:HIS:C	4:4:321:MET:HE3	2.33	0.53
5:5:121:LEU:HD13	5:5:146:LEU:HD23	1.91	0.53
21:M:203:ASN:HD22	21:M:206:PHE:HD2	1.55	0.53
33:Y:70:ASN:C	33:Y:70:ASN:HD22	2.16	0.53
2:2:153:LEU:O	2:2:153:LEU:HD22	2.09	0.53
3:3:356:LEU:HD13	3:3:654:PHE:HB2	1.91	0.53
3:3:501:LYS:HD2	3:3:501:LYS:N	2.19	0.53
18:J:25:VAL:CG1	19:k:30:VAL:CG1	2.86	0.53
18:J:25:VAL:CG1	19:k:30:VAL:HB	2.30	0.53
17:i:72:VAL:HG13	17:i:73:PRO:HD2	1.91	0.53
35:n:920:UNK:CA	35:n:1200:UNK:H	2.10	0.53
1:1:74:LEU:O	1:1:77:SER:HB3	2.09	0.53
1:1:161:ASN:ND2	1:1:166:ASP:HA	2.23	0.53
19:K:30:VAL:CG1	18:j:25:VAL:HG11	2.37	0.53
10:b:411:ILE:O	10:b:415:LYS:HG3	2.08	0.53
1:1:313:TYR:CE1	1:1:323:LEU:HD13	2.44	0.53
3:3:205:ARG:HH11	3:3:205:ARG:HG3	1.72	0.53
3:3:572:PRO:HG2	3:3:577:LEU:HD21	1.91	0.53
8:8:132:GLY:H	8:8:135:ASP:HB2	1.74	0.53
23:O:128:VAL:O	23:O:134:PHE:HB3	2.09	0.53
11:c:220:PHE:HE2	46:c:3002:UQ1:CM2	2.22	0.53
14:f:78:GLU:H	14:f:78:GLU:CD	2.16	0.53
3:3:386:SER:HB2	3:3:675:ARG:NH1	2.22	0.53
4:4:283:MET:O	4:4:287:VAL:HG23	2.08	0.53
10:B:353:SER:CB	10:B:355:PRO:HD2	2.38	0.53
16:H:41:ASP:O	16:H:45:SER:HB2	2.09	0.53
20:L:302:ARG:O	20:L:306:THR:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:40:LEU:HD13	23:O:59:LEU:HD13	1.90	0.53
27:S:75:ARG:HG2	27:S:75:ARG:NH1	2.19	0.53
11:c:12:LYS:CE	11:c:15:ASN:HB3	2.39	0.53
5:5:37:GLU:O	5:5:40:HIS:HB3	2.08	0.53
9:A:41:ILE:HG12	9:A:195:MET:HG2	1.89	0.53
33:Y:41:GLY:HA2	33:Y:48:TYR:CZ	2.43	0.53
9:a:136:GLN:NE2	17:i:51:CYS:CB	2.72	0.53
10:b:95:LYS:HG3	17:i:32:ALA:N	2.24	0.53
10:b:276:GLN:HG2	10:b:281:ALA:HB2	1.91	0.53
3:3:136:GLU:HG2	5:5:189:ARG:HG3	1.91	0.53
4:4:213:ILE:H	4:4:213:ILE:CD1	2.20	0.53
25:Q:82:CYS:N	25:Q:86:GLY:O	2.41	0.53
3:3:645:ALA:HB3	3:3:652:PRO:HD3	1.91	0.53
6:6:74:GLN:OE1	6:6:74:GLN:HA	2.09	0.53
6:6:96:TRP:O	6:6:99:MET:HB2	2.09	0.53
12:D:166:ASN:HB3	16:H:13:LEU:HD23	1.91	0.53
20:L:398:PRO:O	20:L:498:CYS:HB3	2.08	0.53
21:M:104:TRP:CG	21:M:203:ASN:HB2	2.44	0.53
23:O:52:SER:OG	23:O:55:GLU:HG3	2.08	0.53
1:1:397:ARG:HG3	3:3:49:LEU:HD13	1.91	0.52
4:4:327:HIS:HE1	8:8:107:ALA:O	1.92	0.52
9:A:51:LYS:HZ2	9:A:51:LYS:HB2	1.74	0.52
10:B:294:SER:OG	10:B:343:GLN:NE2	2.42	0.52
13:e:188:THR:HG21	13:e:194:ILE:HD12	1.91	0.52
2:2:40:TRP:CH2	2:2:42:ARG:HG2	2.45	0.52
5:5:5:ARG:HH11	5:5:5:ARG:CG	2.15	0.52
5:5:80:TRP:CD1	5:5:81:LYS:HG2	2.45	0.52
21:M:59:GLN:N	21:M:62:GLU:HG3	2.24	0.52
25:Q:8:THR:OG1	25:Q:11:GLU:HG2	2.10	0.52
9:a:206:ARG:HH11	9:a:206:ARG:HG3	1.75	0.52
11:c:220:PHE:HE2	46:c:3002:UQ1:HM22	1.74	0.52
17:i:32:ALA:N	17:i:71:ASN:HB3	2.24	0.52
18:j:61:ASN:C	18:j:62:LYS:HG3	2.35	0.52
34:m:1119:UNK:C	34:m:1121:UNK:N	2.72	0.52
1:1:196:ARG:NH2	3:3:203:ILE:O	2.42	0.52
4:4:381:LEU:HD11	4:4:397:ILE:HG12	1.91	0.52
6:6:163:TYR:CD1	6:6:169:ARG:HA	2.44	0.52
7:7:20:MET:HE3	7:7:59:LEU:HG	1.91	0.52
7:7:34:GLU:HB3	7:7:56:THR:CG2	2.40	0.52
13:E:90:LYS:CE	13:E:93:GLY:HA2	2.40	0.52
23:O:67:SER:OG	23:O:70:GLU:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:162:GLU:OE2	11:c:168:PHE:HD1	1.93	0.52
6:6:78:MET:HE2	6:6:99:MET:HE1	1.91	0.52
9:a:76:GLU:HG2	9:a:80:GLU:OE2	2.09	0.52
12:d:60:GLU:HG3	18:j:62:LYS:HZ3	1.74	0.52
36:o:310:UNK:CA	36:o:350:UNK:H2	2.19	0.52
1:1:188:LEU:HD23	1:1:188:LEU:C	2.34	0.52
1:1:358:PRO:O	1:1:362:GLY:HA3	2.08	0.52
5:5:87:ARG:O	5:5:88:PHE:HB3	2.09	0.52
6:6:116:GLY:O	8:8:97:ARG:NH1	2.42	0.52
22:N:18:LEU:HD22	22:N:22:LEU:HD22	1.92	0.52
25:Q:51:SER:HB2	25:Q:91:LEU:HD11	1.90	0.52
52:Y:269:HOH:O	12:d:145:GLU:OE1	2.11	0.52
11:c:379:TRP:CE3	14:f:33:ARG:HD3	2.44	0.52
36:o:1001:UNK:CA	36:o:1059:UNK:CA	2.81	0.52
20:L:225:GLY:HA3	22:N:112:LEU:HD13	1.92	0.52
26:R:8:HIS:O	26:R:10:GLY:N	2.42	0.52
1:1:37:GLY:C	1:1:39:GLU:H	2.18	0.52
3:3:600:VAL:HG12	3:3:602:LEU:CD1	2.40	0.52
4:4:123:LEU:HD13	4:4:290:ILE:HD12	1.92	0.52
5:5:161:GLU:CG	5:5:163:ARG:HH22	2.23	0.52
8:8:144:LYS:HB2	8:8:145:PRO:HD2	1.92	0.52
20:L:268:PHE:CZ	21:M:58:ALA:HA	2.44	0.52
26:R:42:ARG:HG3	26:R:42:ARG:HH11	1.74	0.52
11:c:12:LYS:HA	11:c:12:LYS:CE	2.37	0.52
1:1:29:LEU:HD23	1:1:112:HIS:CE1	2.45	0.52
1:1:363:VAL:O	1:1:368:VAL:HG12	2.09	0.52
3:3:218:LEU:H	3:3:219:PRO:HD3	1.71	0.52
3:3:688:ARG:HB3	3:3:770:ARG:HB2	1.91	0.52
24:P:63:SER:O	24:P:67:ILE:HG13	2.10	0.52
10:b:46:ARG:HG2	10:b:379:LEU:HD22	1.92	0.52
2:2:76:GLY:H	2:2:118:SER:HB2	1.74	0.52
4:4:404:MET:HA	4:4:407:VAL:CG1	2.40	0.52
12:D:34:LYS:HE3	52:D:4097:HOH:O	2.09	0.52
13:E:102:THR:O	13:E:106:ILE:HG13	2.09	0.52
20:L:240:HIS:HB3	20:L:241:PRO:HD3	1.92	0.52
21:M:102:HIS:O	21:M:104:TRP:N	2.42	0.52
23:O:23:PRO:HD2	24:P:34:ASN:HD22	1.74	0.52
11:c:14:VAL:C	11:c:15:ASN:CA	2.83	0.52
3:3:42:ILE:HG22	3:3:43:GLY:H	1.75	0.52
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.91	0.52
4:4:245:ASN:O	5:5:79:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:60:TYR:CD1	27:S:60:TYR:C	2.88	0.52
13:e:77:LYS:HD3	13:e:80:ASP:OD2	2.10	0.52
9:A:308:GLN:HG2	52:A:4140:HOH:O	2.10	0.51
10:B:276:GLN:HG2	10:B:281:ALA:HB2	1.91	0.51
10:B:306:PRO:HA	17:I:52:ARG:HE	1.74	0.51
21:M:33:LEU:HD23	28:T:28:SER:HB2	1.91	0.51
21:M:68:LEU:HB3	21:M:69:PRO:HD3	1.91	0.51
14:f:71:ARG:O	14:f:73:GLN:HG3	2.11	0.51
14:f:88:SER:OG	14:f:91:GLU:HB2	2.09	0.51
1:1:258:VAL:HG21	1:1:280:ALA:HB1	1.91	0.51
1:1:310:PRO:O	1:1:315:HIS:HB2	2.10	0.51
2:2:27:ILE:HG12	2:2:53:VAL:HG21	1.91	0.51
5:5:36:GLU:HG3	5:5:37:GLU:N	2.24	0.51
22:N:119:THR:O	26:R:52:HIS:CE1	2.63	0.51
10:b:189:VAL:HG23	52:b:3052:HOH:O	2.10	0.51
16:h:25:GLU:CG	16:h:34:ARG:HH22	2.24	0.51
1:1:93:ALA:HB1	1:1:107:LEU:HD11	1.91	0.51
3:3:132:ASP:O	3:3:135:VAL:HG12	2.09	0.51
7:7:66:PRO:O	7:7:87:PRO:HG2	2.11	0.51
8:8:26:TYR:N	8:8:27:PRO:CD	2.69	0.51
21:M:1:MET:SD	21:M:133:LEU:CD1	2.98	0.51
26:R:2:SER:OG	26:R:3:ALA:N	2.41	0.51
1:1:96:SER:HA	1:1:135:ARG:NH1	2.26	0.51
3:3:458:LEU:C	3:3:460:LYS:H	2.18	0.51
3:3:568:TYR:CD1	3:3:572:PRO:HG3	2.46	0.51
11:C:100:ARG:HD2	11:C:100:ARG:C	2.35	0.51
20:L:75:ILE:O	20:L:79:GLY:HA3	2.11	0.51
52:Y:350:HOH:O	12:d:105:ASN:C	2.53	0.51
2:2:31:LEU:HD12	2:2:41:ILE:HD13	1.92	0.51
8:8:45:ARG:NH2	8:8:137:LEU:HD23	2.26	0.51
9:A:373:THR:HB	9:A:374:PRO:HD3	1.92	0.51
20:L:250:GLY:O	20:L:254:ILE:HG12	2.11	0.51
21:M:100:MET:CE	21:M:157:GLU:HG3	2.40	0.51
23:O:40:LEU:HD22	23:O:59:LEU:HD13	1.92	0.51
10:b:181:TYR:CE1	10:b:182:ARG:HG2	2.44	0.51
12:d:229:VAL:CG2	15:g:20:PRO:HD3	2.40	0.51
1:1:197:ALA:HB3	2:2:66:PHE:CE1	2.46	0.51
6:6:23:THR:O	6:6:27:LEU:HD13	2.09	0.51
1:1:292:PRO:HB2	1:1:316:LEU:CD2	2.41	0.51
11:C:369:ALA:O	11:C:373:GLU:HG3	2.10	0.51
20:L:347:LEU:HG	20:L:383:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:71:ARG:HB2	15:g:72:LYS:HD3	1.93	0.51
1:1:260:ARG:HG3	1:1:264:TYR:OH	2.11	0.51
3:3:337:ARG:HD3	3:3:340:GLU:HG3	1.92	0.51
4:4:133:LEU:HD21	4:4:204:TYR:CD2	2.46	0.51
8:8:153:THR:HG22	8:8:155:LYS:H	1.76	0.51
44:C:502:HEM:HBA1	46:C:2002:UQ1:O2	2.11	0.51
18:J:13:LEU:HB3	18:J:23:THR:OG1	2.10	0.51
1:1:114:LEU:HD22	1:1:118:MET:HG3	1.93	0.51
3:3:94:ASP:OD2	3:3:97:SER:HB2	2.10	0.51
9:A:408:ARG:NH2	19:k:15:ARG:CB	2.65	0.51
1:1:29:LEU:O	1:1:29:LEU:HD22	2.10	0.51
1:1:149:ILE:O	1:1:153:ARG:HG3	2.11	0.51
3:3:617:LEU:HD23	3:3:618:GLU:N	2.26	0.51
4:4:381:LEU:N	4:4:382:PRO:CD	2.74	0.51
12:D:234:LYS:HD3	13:E:8:PRO:HB2	1.91	0.51
17:I:72:VAL:HG13	17:I:73:PRO:HD2	1.92	0.51
18:j:56:LYS:O	18:j:60:GLU:HG3	2.09	0.51
3:3:224:GLY:O	3:3:227:THR:HB	2.09	0.50
3:3:642:ALA:CB	3:3:652:PRO:HG3	2.39	0.50
4:4:333:GLU:OE2	5:5:189:ARG:HD2	2.11	0.50
5:5:101:LEU:O	5:5:126:PHE:HA	2.11	0.50
8:8:73:ALA:HB3	8:8:87:TYR:CE1	2.46	0.50
12:D:34:LYS:NZ	12:D:67:GLU:OE1	2.31	0.50
15:G:40:ARG:CB	48:G:2004:CDL:HB32	2.41	0.50
9:a:381:ARG:HG2	9:a:381:ARG:HH11	1.75	0.50
12:d:43:MET:HE1	12:d:189:PHE:HZ	1.74	0.50
2:2:149:ARG:O	2:2:152:ALA:HB3	2.11	0.50
3:3:43:GLY:HA2	42:3:787:FES:S2	2.52	0.50
4:4:126:LEU:HD21	4:4:286:SER:CB	2.40	0.50
4:4:257:TYR:C	4:4:259:THR:H	2.18	0.50
4:4:261:THR:H	4:4:292:GLN:NE2	2.04	0.50
4:4:346:THR:CG2	4:4:353:LEU:HB3	2.40	0.50
4:4:371:ARG:HH22	4:4:376:VAL:HG21	1.76	0.50
6:6:163:TYR:HD2	8:8:152:ARG:HH11	1.59	0.50
10:B:33:LEU:CD2	10:B:220:ALA:HB1	2.41	0.50
20:L:40:GLU:HG2	20:L:54:TYR:CD1	2.47	0.50
20:L:232:GLN:HB2	20:L:292:MET:HE3	1.93	0.50
33:Y:65[A]:MET:HE1	33:Y:92:GLU:HG3	1.93	0.50
9:a:39:VAL:HG11	9:a:195:MET:HE3	1.92	0.50
10:b:294:SER:OG	10:b:343:GLN:NE2	2.44	0.50
1:1:97:GLU:O	1:1:100:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:89:LYS:HE3	2:2:94:GLU:OE1	2.11	0.50
5:5:7:LEU:HD22	5:5:17:ILE:HD12	1.93	0.50
6:6:30:TRP:O	6:6:30:TRP:CD1	2.65	0.50
6:6:83:ARG:HA	6:6:111:CYS:HB3	1.92	0.50
33:Y:41:GLY:CA	33:Y:52[A]:ASN:ND2	2.74	0.50
13:e:80:ASP:O	13:e:82:PRO:HD3	2.12	0.50
1:1:132:ILE:HG21	1:1:145:LEU:HD11	1.94	0.50
1:1:243:THR:HG21	1:1:315:HIS:HE1	1.77	0.50
1:1:437:TRP:CD1	1:1:437:TRP:O	2.64	0.50
2:2:6:ASP:HB3	2:2:7:LYS:HD2	1.92	0.50
3:3:405:GLU:CB	3:3:535:MET:HE2	2.33	0.50
4:4:233:GLY:HA2	5:5:48:PHE:CE1	2.46	0.50
12:D:234:LYS:HE2	13:E:10:PHE:CE1	2.46	0.50
14:F:88:SER:OG	14:F:91:GLU:HB2	2.12	0.50
20:L:184:PHE:H	20:L:256:HIS:CE1	2.29	0.50
21:M:139:ASP:OD1	21:M:140:ASN:N	2.44	0.50
26:R:44:ARG:HD2	26:R:74:ARG:O	2.12	0.50
9:a:68:LYS:HA	9:a:68:LYS:HE3	1.93	0.50
18:j:52:TRP:O	18:j:56:LYS:HB2	2.11	0.50
1:1:401:PRO:O	1:1:404:ASP:HB2	2.12	0.50
3:3:326:PHE:CZ	3:3:330:LYS:HE3	2.47	0.50
3:3:549:VAL:HG12	3:3:549:VAL:O	2.12	0.50
4:4:73:ARG:O	4:4:364:MET:HB3	2.12	0.50
6:6:32:ARG:HA	6:6:35:SER:OG	2.10	0.50
7:7:40:PHE:HE1	8:8:83:ALA:HB2	1.76	0.50
8:8:68:ILE:HD11	38:8:183:SF4:S1	2.51	0.50
13:E:99:ARG:HB3	13:E:133:VAL:HG12	1.91	0.50
10:b:309:VAL:HG23	10:b:326:THR:HG22	1.93	0.50
2:2:113:PRO:HG2	2:2:114:ASP:OD1	2.11	0.50
4:4:271:ASP:OD1	4:4:274:ASP:N	2.39	0.50
9:a:125:SER:O	9:a:129:LYS:HG3	2.11	0.50
11:c:245:PHE:CG	12:d:17:LEU:HD13	2.47	0.50
12:d:124:GLU:OE2	12:d:191:ARG:CD	2.60	0.50
2:2:122:VAL:CG1	2:2:123:GLU:N	2.75	0.50
3:3:550:LEU:HB3	3:3:684:ARG:HH21	1.77	0.50
5:5:163:ARG:HD2	8:8:69:TYR:CD1	2.47	0.50
9:A:125:SER:O	9:A:129:LYS:HG3	2.12	0.50
9:A:206:ARG:HH11	9:A:206:ARG:HG3	1.76	0.50
10:B:109:VAL:HB	10:B:119:LEU:HD12	1.94	0.50
21:M:136:LEU:HB3	21:M:193:TYR:CD2	2.46	0.50
25:Q:37:LYS:HD3	25:Q:37:LYS:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:42:ARG:NH1	26:R:74:ARG:HH21	2.10	0.50
11:c:15:ASN:O	11:c:17:ALA:N	2.44	0.50
13:e:99:ARG:HB3	13:e:133:VAL:CG1	2.42	0.50
1:1:272:PHE:HZ	1:1:316:LEU:HD21	1.77	0.50
3:3:192:GLU:HG3	3:3:193:GLU:HG3	1.92	0.50
11:C:68:HIS:HD2	52:C:2126:HOH:O	1.95	0.50
18:J:16:ARG:NH1	18:J:16:ARG:CG	2.75	0.50
21:M:186:SER:CB	21:M:213:LEU:HD22	2.40	0.50
23:O:64:PHE:CE1	24:P:66:ARG:HD2	2.46	0.50
3:3:171:SER:CB	3:3:172:PRO:HD2	2.39	0.50
3:3:697:THR:OG1	3:3:763:LEU:HD23	2.11	0.50
5:5:30:PRO:HG2	5:5:33:ARG:HB2	1.93	0.50
22:N:42:LEU:HD13	29:U:45:TYR:HD2	1.77	0.50
22:N:156:ARG:HG3	22:N:156:ARG:NH1	2.22	0.50
11:c:96:MET:HE2	11:c:96:MET:HA	1.93	0.50
1:1:238:PHE:CZ	1:1:248:GLY:HA3	2.47	0.49
3:3:55:PRO:HG3	3:3:73:ILE:HA	1.92	0.49
3:3:123:ASP:C	3:3:125:GLY:H	2.19	0.49
3:3:135:VAL:HG23	4:4:326:TYR:CE2	2.46	0.49
3:3:452:ALA:C	3:3:454:TYR:H	2.20	0.49
3:3:474:ARG:NH2	3:3:516:VAL:CG2	2.64	0.49
10:b:354:ASN:N	10:b:355:PRO:CD	2.76	0.49
11:c:164:ILE:O	11:c:177:ARG:HD2	2.12	0.49
36:o:1212:UNK:N	36:o:1213:UNK:CA	2.75	0.49
2:2:112:THR:HG22	2:2:117:PHE:H	1.76	0.49
2:2:122:VAL:HG12	2:2:123:GLU:H	1.77	0.49
4:4:132:PHE:CE2	4:4:279:ARG:HG3	2.47	0.49
4:4:385:CYS:HB3	4:4:396:ILE:HG21	1.94	0.49
11:C:379:TRP:CE3	14:F:33:ARG:HD3	2.47	0.49
20:L:266:GLU:HB2	20:L:267:PRO:HD2	1.94	0.49
20:L:508:PRO:HG3	22:N:6:HIS:HB3	1.94	0.49
26:R:5:LYS:NZ	26:R:5:LYS:HB3	2.27	0.49
1:1:219:ASN:ND2	1:1:223:THR:HG21	2.27	0.49
2:2:24:ARG:HA	2:2:53:VAL:CG1	2.42	0.49
3:3:19:VAL:O	3:3:22:ALA:HB3	2.12	0.49
3:3:42:ILE:HG22	3:3:43:GLY:N	2.27	0.49
3:3:208:HIS:ND1	7:7:92:HIS:CE1	2.80	0.49
3:3:693:TYR:HB3	3:3:759:TYR:CD1	2.48	0.49
4:4:61:TYR:HB3	6:6:88:MET:HE2	1.95	0.49
10:B:35:ILE:N	10:B:35:ILE:HD12	2.27	0.49
10:B:95:LYS:CD	17:I:32:ALA:HB2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:11:ASN:ND2	20:L:14:ASP:H	2.07	0.49
33:Y:41:GLY:CA	33:Y:52[A]:ASN:HD21	2.24	0.49
10:b:200:THR:O	10:b:204:MET:HG3	2.12	0.49
4:4:381:LEU:HB3	4:4:382:PRO:HD3	1.95	0.49
13:E:82:PRO:O	13:E:100:HIS:HB3	2.12	0.49
18:J:16:ARG:CB	18:J:19:THR:HG22	2.38	0.49
18:J:18:SER:CB	19:k:23:LEU:CB	2.68	0.49
20:L:377:PHE:HA	20:L:380:VAL:HG22	1.93	0.49
21:M:90:ILE:H	21:M:90:ILE:HD12	1.77	0.49
21:M:186:SER:HB3	21:M:213:LEU:CD2	2.42	0.49
2:2:28:MET:HB2	2:2:29:PRO:HD2	1.95	0.49
3:3:188:VAL:CG1	3:3:201:ASP:HA	2.42	0.49
3:3:367:PRO:CG	3:3:554:LYS:HB2	2.43	0.49
5:5:161:GLU:HB2	5:5:163:ARG:CZ	2.43	0.49
11:C:371:THR:O	11:C:375:LYS:HG2	2.13	0.49
13:E:155:GLY:N	52:E:541:HOH:O	2.46	0.49
20:L:168:ILE:HG21	20:L:189:MET:HG3	1.94	0.49
10:b:365:LYS:HG2	10:b:399:LEU:CD2	2.42	0.49
3:3:117:LEU:CA	4:4:321:MET:HE1	2.41	0.49
3:3:477:LEU:CD2	3:3:521:ALA:HB2	2.42	0.49
3:3:734:VAL:HG12	3:3:736:VAL:HG23	1.94	0.49
4:4:197:LEU:O	4:4:198:PRO:C	2.56	0.49
4:4:284:ARG:HH11	4:4:284:ARG:HG3	1.77	0.49
4:4:320:SER:HB3	4:4:323:ALA:HB3	1.95	0.49
9:A:189:HIS:ND1	9:A:194:ARG:NH2	2.59	0.49
16:H:28:GLU:O	16:H:32:LYS:HG2	2.13	0.49
20:L:145:LEU:HD21	22:N:32:THR:HG21	1.93	0.49
21:M:13:THR:HG22	21:M:13:THR:O	2.12	0.49
21:M:16:ILE:HD12	21:M:17:MET:H	1.78	0.49
26:R:42:ARG:O	26:R:42:ARG:HD2	2.13	0.49
13:e:129:LYS:HG3	13:e:187:PHE:CE2	2.47	0.49
3:3:130:LEU:HD23	38:3:784:SF4:S4	2.52	0.49
4:4:240:ARG:C	4:4:242:SER:H	2.19	0.49
9:A:90:SER:HB3	52:A:4116:HOH:O	2.11	0.49
12:D:239:PRO:HG2	12:D:241:LYS:HZ3	1.78	0.49
15:G:66:PHE:CZ	15:G:70:LYS:HD2	2.47	0.49
33:Y:41:GLY:HA2	33:Y:48:TYR:CE1	2.47	0.49
17:i:32:ALA:HA	17:i:71:ASN:HD22	1.78	0.49
4:4:234:LEU:O	4:4:239:LEU:HG	2.12	0.49
20:L:87:ILE:O	20:L:173:PRO:HD3	2.13	0.49
18:j:3:PRO:HB2	18:j:8:ARG:HH11	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:m:901:UNK:CA	34:m:1199:UNK:CA	2.91	0.49
1:1:359:CYS:HB2	1:1:403:ALA:HB2	1.93	0.49
3:3:218:LEU:N	3:3:219:PRO:CD	2.75	0.49
19:K:15:ARG:HG2	9:a:408:ARG:NH1	2.28	0.49
9:a:405:ARG:O	9:a:409:GLU:HG3	2.13	0.49
2:2:33:ARG:HH21	2:2:37:GLU:CG	2.26	0.49
4:4:62:LEU:HD23	4:4:62:LEU:HA	1.65	0.49
4:4:168:PHE:N	4:4:168:PHE:CD1	2.81	0.49
9:A:172:GLU:HG3	9:A:176:LYS:HE3	1.95	0.49
9:A:364:ALA:HB2	17:I:33:ALA:HB1	1.95	0.49
18:J:52:TRP:O	18:J:56:LYS:HB2	2.13	0.49
22:N:65:SER:HB3	22:N:71:HIS:CE1	2.48	0.49
10:b:229:GLY:O	10:b:231:GLY:N	2.44	0.49
1:1:9:LEU:HD13	1:1:279:TRP:CZ2	2.48	0.48
1:1:398:SER:C	3:3:46:ARG:HD2	2.38	0.48
3:3:719:HIS:ND1	3:3:720:PRO:HD2	2.28	0.48
5:5:175:THR:O	5:5:175:THR:OG1	2.31	0.48
9:A:143:THR:OG1	17:I:48:SER:HB3	2.13	0.48
11:C:251:GLY:HA3	52:C:2091:HOH:O	2.13	0.48
20:L:197:LEU:O	22:N:92:LEU:HD22	2.13	0.48
33:Y:65[A]:MET:HE1	33:Y:92:GLU:HG2	1.94	0.48
9:a:264:HIS:ND1	9:a:265:PRO:HD2	2.28	0.48
12:d:43:MET:HE1	12:d:189:PHE:CE2	2.48	0.48
1:1:299:PRO:HG3	1:1:341:MET:CE	2.43	0.48
3:3:518:ALA:O	3:3:521:ALA:HB3	2.13	0.48
3:3:629:ILE:HG22	3:3:630:GLU:H	1.77	0.48
4:4:236:GLY:C	4:4:238:SER:N	2.71	0.48
7:7:39:ASP:OD2	7:7:75:ARG:HD3	2.14	0.48
1:1:9:LEU:HD13	1:1:279:TRP:HZ2	1.78	0.48
3:3:250:GLU:CD	3:3:628:PRO:HG2	2.39	0.48
3:3:508:GLY:O	3:3:512:LEU:HB2	2.13	0.48
4:4:53:LEU:N	4:4:53:LEU:HD22	2.28	0.48
4:4:82:THR:N	4:4:83:PRO:HD2	2.29	0.48
4:4:341:GLU:OE1	5:5:91:ARG:NH2	2.46	0.48
5:5:31:ARG:O	5:5:34:PHE:HB3	2.12	0.48
5:5:163:ARG:HD2	8:8:69:TYR:CE1	2.48	0.48
6:6:50:MET:C	6:6:52:ALA:N	2.71	0.48
9:a:227:ALA:O	9:a:228:VAL:HB	2.13	0.48
12:d:3:LEU:HD12	16:h:55:THR:HG22	1.96	0.48
37:p:321:UNK:C	37:p:323:UNK:N	2.70	0.48
3:3:321:THR:HG22	3:3:322:TRP:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:333:LEU:HB3	3:3:648:LEU:CD2	2.43	0.48
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.94	0.48
4:4:102:GLU:HG2	4:4:175:ILE:O	2.14	0.48
11:C:21:LEU:HD21	46:C:2002:UQ1:HM32	1.95	0.48
29:U:16:ASN:H	29:U:16:ASN:ND2	2.12	0.48
1:1:72:THR:HG21	1:1:223:THR:HG23	1.94	0.48
1:1:273:ARG:HB2	1:1:307:LEU:O	2.13	0.48
2:2:24:ARG:HA	2:2:53:VAL:HG13	1.94	0.48
3:3:719:HIS:HB2	3:3:753:VAL:O	2.12	0.48
4:4:163:VAL:HG22	4:4:164:THR:CG2	2.43	0.48
4:4:219:ARG:NH1	4:4:273:PHE:CD2	2.81	0.48
5:5:167:PRO:HB3	8:8:66:TYR:CE2	2.48	0.48
7:7:14:VAL:HA	7:7:17:LEU:HD12	1.95	0.48
10:B:396:SER:HB3	52:B:3031:HOH:O	2.14	0.48
15:G:32:LYS:C	15:G:35:PRO:HD2	2.39	0.48
20:L:11:ASN:ND2	20:L:13:LYS:HB2	2.28	0.48
21:M:78:LEU:HB2	21:M:79:PRO:CD	2.38	0.48
27:S:24:ASN:ND2	27:S:26:THR:H	2.11	0.48
11:c:191:ALA:HA	11:c:194:MET:CE	2.43	0.48
1:1:367:MET:HE1	1:1:410:VAL:HG21	1.94	0.48
1:1:420:GLN:O	1:1:424:LEU:HD13	2.14	0.48
10:B:51:ILE:HG12	10:B:204:MET:HG2	1.95	0.48
11:C:97:HIS:CD2	44:C:502:HEM:NC	2.81	0.48
19:K:18:VAL:HB	19:K:19:PRO:HD3	1.95	0.48
21:M:22:HIS:CE1	28:T:44:LYS:HD3	2.49	0.48
13:e:99:ARG:HB3	13:e:133:VAL:HG12	1.94	0.48
15:g:46:LEU:HD23	52:g:3018:HOH:O	2.13	0.48
1:1:272:PHE:CD1	1:1:311:MET:HE3	2.49	0.48
1:1:311:MET:HA	1:1:316:LEU:HD11	1.94	0.48
20:L:115:SER:O	20:L:121:GLY:HA2	2.14	0.48
28:T:39:VAL:O	28:T:42:LYS:HE2	2.14	0.48
13:e:83:GLU:HG2	13:e:102:THR:HG22	1.96	0.48
1:1:188:LEU:HD23	1:1:188:LEU:O	2.13	0.48
4:4:88:LEU:HD12	4:4:403:VAL:HG22	1.94	0.48
4:4:94:ASP:HB3	4:4:173:ILE:HG21	1.96	0.48
6:6:121:TYR:CG	6:6:122:ALA:N	2.81	0.48
7:7:86:LEU:HD12	7:7:91:ILE:HD12	1.95	0.48
9:A:15:GLN:NE2	10:B:12:GLU:HB2	2.29	0.48
15:G:34:ILE:HB	15:G:35:PRO:HD3	1.95	0.48
17:I:36:ALA:HB2	17:I:73:PRO:CD	2.40	0.48
13:e:79:SER:CB	13:e:191:ASP:OD2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:120:LEU:HD22	1:1:231:MET:HG3	1.96	0.48
3:3:113:LEU:CD1	3:3:157:PHE:HB2	2.43	0.48
3:3:254:THR:OG1	3:3:624:LEU:HD12	2.12	0.48
3:3:341:VAL:HA	3:3:565:TYR:O	2.13	0.48
4:4:86:ASP:OD2	4:4:350:ARG:HD2	2.14	0.48
4:4:250:LYS:HE2	4:4:262:PHE:CB	2.33	0.48
10:B:24:LEU:HD13	10:B:392:TYR:CD2	2.49	0.48
21:M:4:PRO:HB2	30:V:43:SER:HA	1.96	0.48
21:M:59:GLN:O	21:M:62:GLU:HB2	2.13	0.48
12:d:59:ASP:OD2	18:j:62:LYS:CB	2.52	0.48
1:1:356:CYS:SG	1:1:399:PHE:HB2	2.53	0.48
2:2:145:VAL:CG1	2:2:150:LEU:HB2	2.44	0.48
6:6:104:TRP:NE1	6:6:173:VAL:HG22	2.29	0.48
6:6:140:CYS:SG	8:8:99:ILE:HG13	2.54	0.48
8:8:44:THR:HA	8:8:138:VAL:CG1	2.44	0.48
8:8:100:PHE:HA	38:8:183:SF4:S4	2.54	0.48
11:C:191:ALA:HA	11:C:194:MET:CE	2.43	0.48
18:J:16:ARG:HH12	18:J:19:THR:HG21	1.76	0.48
18:J:56:LYS:HG2	18:J:60:GLU:CD	2.39	0.48
20:L:397:PHE:HB3	20:L:398:PRO:HD3	1.95	0.48
29:U:8:LYS:NZ	29:U:8:LYS:HB3	2.29	0.48
11:c:14:VAL:O	11:c:15:ASN:O	2.32	0.48
3:3:382:PHE:CD1	3:3:382:PHE:N	2.81	0.47
3:3:465:HIS:O	3:3:465:HIS:CG	2.66	0.47
12:D:124:GLU:OE2	12:D:191:ARG:HD2	2.14	0.47
18:J:16:ARG:O	18:J:19:THR:HG22	2.14	0.47
1:1:109:ASP:O	1:1:110:VAL:HG13	2.13	0.47
1:1:358:PRO:HB3	3:3:107:MET:HE1	1.95	0.47
3:3:117:LEU:HG	4:4:324:VAL:HG21	1.96	0.47
3:3:473:GLU:O	3:3:477:LEU:HD12	2.14	0.47
3:3:571:VAL:HG11	3:3:591:HIS:CD2	2.50	0.47
4:4:215:TYR:CE1	4:4:219:ARG:HG2	2.49	0.47
4:4:238:SER:OG	4:4:279:ARG:NH2	2.47	0.47
9:A:286:GLY:HA3	9:A:290:LEU:HD21	1.95	0.47
10:B:46:ARG:HD2	10:B:375:SER:OG	2.14	0.47
10:B:345:LYS:O	10:B:349:GLN:HG3	2.14	0.47
13:E:131:GLU:HG2	13:E:132:TRP:CD1	2.49	0.47
22:N:164:PHE:O	22:N:168:THR:HG23	2.14	0.47
25:Q:49:VAL:HG21	25:Q:74:LEU:HD12	1.95	0.47
10:b:361:LYS:HE2	10:b:402:ILE:O	2.14	0.47
4:4:93:HIS:CE1	4:4:353:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:366:TYR:CZ	5:5:148:LYS:HE3	2.49	0.47
5:5:25:LEU:CD2	5:5:25:LEU:N	2.78	0.47
7:7:45:GLU:CD	7:7:45:GLU:H	2.21	0.47
8:8:133:LYS:O	8:8:137:LEU:HD13	2.14	0.47
20:L:476:PHE:CD1	31:W:15:VAL:HG21	2.48	0.47
23:O:68:PHE:HA	23:O:71:MET:HG2	1.95	0.47
9:a:172:GLU:HG3	9:a:176:LYS:HE3	1.97	0.47
15:g:45:ILE:HG22	15:g:46:LEU:CD2	2.22	0.47
35:n:653:UNK:CA	35:n:711:UNK:CA	2.92	0.47
35:n:920:UNK:C	35:n:1200:UNK:N	2.52	0.47
1:1:391:LEU:HB2	1:1:392:PRO:CD	2.43	0.47
3:3:47:MET:HE3	3:3:47:MET:HB3	1.66	0.47
3:3:224:GLY:HA3	3:3:295:ARG:HD2	1.96	0.47
3:3:440:ARG:CG	3:3:440:ARG:NH1	2.77	0.47
3:3:512:LEU:HD21	3:3:534:ALA:HB1	1.96	0.47
4:4:194:LEU:HD12	4:4:194:LEU:HA	1.71	0.47
9:A:429:GLU:OE2	15:G:7:LEU:HB2	2.14	0.47
52:A:4072:HOH:O	14:f:110:LYS:HD2	2.15	0.47
25:Q:31:TYR:HE1	25:Q:98:HIS:HE1	1.62	0.47
9:a:296:SER:O	9:a:300:THR:HG23	2.14	0.47
11:c:245:PHE:CD1	12:d:17:LEU:HD13	2.48	0.47
3:3:386:SER:HB3	3:3:389:ASP:CG	2.40	0.47
4:4:30:VAL:HG12	4:4:31:GLY:N	2.29	0.47
4:4:369:LYS:C	4:4:369:LYS:HD3	2.40	0.47
9:A:431:LEU:HD12	9:A:432:PRO:HD2	1.96	0.47
10:B:246:GLU:O	10:B:427:SER:HA	2.14	0.47
12:D:43:MET:HE1	12:D:189:PHE:HZ	1.75	0.47
18:J:17:THR:CG2	19:k:24:TRP:CZ2	2.75	0.47
21:M:63:THR:O	21:M:66:THR:HG22	2.15	0.47
13:e:131:GLU:HG2	13:e:132:TRP:CD1	2.49	0.47
3:3:591:HIS:ND1	3:3:592:PRO:CD	2.76	0.47
8:8:170:LEU:O	8:8:171:GLU:C	2.56	0.47
21:M:108:TYR:CD1	21:M:108:TYR:N	2.83	0.47
12:d:234:LYS:HD3	13:e:8:PRO:HB2	1.96	0.47
1:1:49:THR:HG23	1:1:52:GLU:CG	2.43	0.47
1:1:219:ASN:HD22	1:1:223:THR:HG21	1.78	0.47
3:3:717:TRP:HB2	3:3:759:TYR:HB2	1.97	0.47
3:3:732:ALA:O	3:3:747:VAL:HG12	2.15	0.47
5:5:3:LEU:HB2	5:5:86:SER:HB3	1.96	0.47
9:A:213:GLN:HG2	52:A:4055:HOH:O	2.15	0.47
10:B:12:GLU:CG	10:B:17:VAL:H	2.04	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:141:TRP:CH2	13:e:145:VAL:HG23	2.49	0.47
11:C:277:ALA:HB1	11:C:294:LEU:CD1	2.44	0.47
12:D:124:GLU:OE2	12:D:191:ARG:CD	2.63	0.47
20:L:172:LYS:HB3	20:L:176:MET:HE2	1.96	0.47
21:M:83:ILE:O	21:M:87:MET:HG3	2.14	0.47
21:M:148:MET:HE3	21:M:148:MET:HB3	1.78	0.47
10:b:17:VAL:HG13	10:b:18:PRO:HD2	1.96	0.47
11:c:361:LEU:O	11:c:366:MET:HG3	2.15	0.47
14:f:13:LEU:HB3	52:f:2070:HOH:O	2.13	0.47
15:g:46:LEU:HD22	15:g:46:LEU:N	2.30	0.47
16:h:28:GLU:O	16:h:32:LYS:HG2	2.15	0.47
3:3:124:LYS:HA	3:3:124:LYS:HD3	1.75	0.47
4:4:88:LEU:HD12	4:4:403:VAL:CG2	2.45	0.47
6:6:28:VAL:O	6:6:32:ARG:HG2	2.15	0.47
6:6:163:TYR:CD2	8:8:152:ARG:HD2	2.50	0.47
8:8:29:ALA:HA	8:8:30:PRO:HD2	1.72	0.47
10:B:212:SER:OG	10:B:215:VAL:HG23	2.15	0.47
19:K:19:PRO:O	19:K:23:LEU:HG	2.14	0.47
20:L:507:GLU:O	20:L:508:PRO:O	2.32	0.47
1:1:356:CYS:SG	1:1:399:PHE:CB	3.03	0.47
4:4:234:LEU:CD2	4:4:238:SER:HB2	2.45	0.47
4:4:279:ARG:HG3	4:4:279:ARG:NH1	2.29	0.47
10:B:95:LYS:HE3	17:I:72:VAL:HG21	1.97	0.47
19:K:31:GLY:O	19:K:35:ALA:N	2.46	0.47
33:Y:12[A]:GLN:HG3	52:Y:351:HOH:O	2.14	0.47
11:c:277:ALA:HB1	11:c:294:LEU:CD1	2.45	0.47
11:c:375:LYS:N	11:c:375:LYS:HD2	2.29	0.47
2:2:153:LEU:O	2:2:157:LEU:HG	2.15	0.47
3:3:54:LEU:N	3:3:55:PRO:HD3	2.30	0.47
4:4:211:SER:OG	4:4:215:TYR:HB2	2.15	0.47
6:6:99:MET:CG	6:6:100:PRO:HD2	2.44	0.47
10:B:365:LYS:HG2	10:B:399:LEU:CD2	2.45	0.47
23:O:41:LYS:HD3	23:O:62:LEU:HD23	1.97	0.47
26:R:67:HIS:CD2	26:R:78:LEU:HD11	2.50	0.47
29:U:11:LEU:O	29:U:11:LEU:HD23	2.15	0.47
11:c:97:HIS:CD2	44:c:502:HEM:NC	2.83	0.47
13:e:45:VAL:HG13	18:j:28:ALA:HA	1.97	0.47
15:g:32:LYS:C	15:g:35:PRO:HD2	2.40	0.47
1:1:42:LYS:O	1:1:46:LYS:HG3	2.15	0.46
2:2:10:PHE:O	2:2:14:THR:OG1	2.34	0.46
3:3:19:VAL:HG23	3:3:85:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:113:LEU:HD12	3:3:157:PHE:CB	2.44	0.46
3:3:370:ASP:OD2	3:3:558:TRP:HD1	1.98	0.46
4:4:108:VAL:HG23	4:4:108:VAL:O	2.15	0.46
11:C:162:GLU:OE2	11:C:168:PHE:HD1	1.98	0.46
21:M:1:MET:SD	21:M:133:LEU:HD11	2.56	0.46
22:N:173:PHE:CD1	22:N:173:PHE:C	2.92	0.46
16:h:31:VAL:HG23	16:h:32:LYS:N	2.30	0.46
1:1:245:GLN:HB2	1:1:314:GLU:OE2	2.15	0.46
4:4:291:LYS:O	4:4:295:GLU:HG3	2.14	0.46
4:4:348:SER:C	4:4:350:ARG:H	2.22	0.46
12:D:44:ASP:OD1	12:D:93:LYS:HE2	2.15	0.46
20:L:484:THR:HB	32:X:2:THR:OG1	2.15	0.46
22:N:80:ARG:O	22:N:84:ILE:HG12	2.14	0.46
23:O:102:TYR:CD2	32:X:35:TYR:HE1	2.33	0.46
44:c:502:HEM:HBA1	46:c:3002:UQ1:O2	2.15	0.46
12:d:97:ASN:HB2	12:d:98:PRO:HD2	1.96	0.46
1:1:161:ASN:HD22	1:1:166:ASP:HA	1.80	0.46
1:1:243:THR:HG22	1:1:244:GLU:H	1.79	0.46
3:3:269:THR:HG22	3:3:274:LEU:HA	1.97	0.46
5:5:71:VAL:HG22	5:5:91:ARG:HB2	1.97	0.46
9:A:15:GLN:O	9:A:26:ALA:HA	2.16	0.46
21:M:185:MET:C	21:M:185:MET:SD	2.99	0.46
23:O:108:PRO:HG2	23:O:111:PHE:CD2	2.50	0.46
11:c:92:ILE:O	11:c:96:MET:HG2	2.16	0.46
6:6:104:TRP:NE1	6:6:158:VAL:HG12	2.30	0.46
9:A:167:VAL:HG13	52:A:4111:HOH:O	2.15	0.46
20:L:299:VAL:HA	20:L:302:ARG:NH1	2.31	0.46
20:L:435:GLY:O	20:L:437:PRO:HD3	2.15	0.46
10:b:33:LEU:CD2	10:b:220:ALA:HB1	2.45	0.46
11:c:193:ALA:O	11:c:196:HIS:HB3	2.15	0.46
18:j:8:ARG:NH1	18:j:8:ARG:CG	2.75	0.46
1:1:110:VAL:O	1:1:113:LEU:HB3	2.15	0.46
3:3:33:PHE:O	3:3:186:ARG:NH2	2.48	0.46
3:3:326:PHE:CD1	3:3:643:LEU:HG	2.49	0.46
4:4:200:ARG:O	4:4:204:TYR:HD1	1.99	0.46
4:4:262:PHE:CD1	4:4:289:ILE:HD11	2.51	0.46
9:A:369:LEU:HD12	9:A:392:LEU:HD21	1.98	0.46
13:E:85:LYS:HZ3	13:E:87:MET:HA	1.80	0.46
25:Q:40:SER:OG	25:Q:45:ASP:HB3	2.16	0.46
10:b:354:ASN:HB3	10:b:355:PRO:HD3	1.96	0.46
3:3:459:MET:HE2	3:3:465:HIS:CB	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:571:VAL:HA	3:3:572:PRO:HD3	1.73	0.46
3:3:695:ARG:O	3:3:697:THR:HG23	2.14	0.46
4:4:320:SER:HB3	4:4:323:ALA:CB	2.46	0.46
4:4:393:MET:HA	4:4:396:ILE:CG2	2.44	0.46
11:C:104:TYR:CD1	11:C:208:PRO:HA	2.51	0.46
13:E:79:SER:HB3	13:E:191:ASP:OD2	2.15	0.46
23:O:66:GLU:O	24:P:66:ARG:NH2	2.49	0.46
18:j:56:LYS:HG2	18:j:60:GLU:CG	2.45	0.46
3:3:458:LEU:C	3:3:460:LYS:N	2.73	0.46
3:3:561:PRO:CB	3:3:576:ALA:HA	2.37	0.46
3:3:587:LEU:HD13	3:3:589:HIS:O	2.16	0.46
3:3:715:GLU:HA	3:3:745:ALA:HB1	1.97	0.46
9:A:86:LEU:HD13	9:A:99:ILE:CG1	2.45	0.46
11:C:233:LEU:HD11	12:D:219:VAL:HG21	1.98	0.46
20:L:195:LEU:CD2	20:L:245:ILE:HD13	2.45	0.46
19:k:18:VAL:CB	19:k:19:PRO:HD3	2.41	0.46
19:k:34:SER:OG	19:k:35:ALA:N	2.46	0.46
1:1:28:THR:HB	1:1:31:TYR:H	1.80	0.46
1:1:53:VAL:O	1:1:57:VAL:HG23	2.16	0.46
1:1:211:LEU:H	1:1:216:THR:HG21	1.78	0.46
3:3:478:LEU:HD22	3:3:484:LYS:HB2	1.97	0.46
5:5:116:ARG:HB3	5:5:135:ILE:HG13	1.97	0.46
20:L:147:ILE:HD11	20:L:209:LEU:HD23	1.98	0.46
23:O:23:PRO:HB3	24:P:70:VAL:CG2	2.45	0.46
30:V:9:PHE:HD1	30:V:10:HIS:HD2	1.64	0.46
9:a:47:TYR:HB3	9:a:189:HIS:CE1	2.51	0.46
12:d:124:GLU:OE2	12:d:191:ARG:HD2	2.16	0.46
3:3:192:GLU:HG3	3:3:193:GLU:N	2.31	0.46
3:3:398:VAL:C	3:3:399:LEU:HD12	2.41	0.46
6:6:31:GLY:C	6:6:33:SER:H	2.24	0.46
7:7:121:ARG:NH1	7:7:121:ARG:CG	2.78	0.46
9:A:264:HIS:HA	9:A:265:PRO:HD3	1.82	0.46
12:D:134:TYR:CG	12:D:162:PRO:HG3	2.51	0.46
16:H:31:VAL:HG23	16:H:32:LYS:N	2.30	0.46
32:X:1:ILE:HG23	32:X:1:ILE:O	2.15	0.46
9:a:213:GLN:O	9:a:217:SER:OG	2.25	0.46
10:b:24:LEU:HD12	10:b:37:SER:O	2.15	0.46
17:i:36:ALA:CB	17:i:73:PRO:HB2	2.46	0.46
1:1:101:PHE:CZ	1:1:253:GLN:HB2	2.51	0.46
1:1:228:VAL:HB	1:1:229:PRO:CD	2.45	0.46
3:3:101:ARG:NH1	3:3:101:ARG:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:337:ARG:H	3:3:337:ARG:HD2	1.80	0.46
3:3:722:THR:CG2	3:3:755:LYS:HB3	2.45	0.46
4:4:44:MET:HA	4:4:44:MET:CE	2.46	0.46
6:6:163:TYR:HD1	6:6:168:GLU:O	1.99	0.46
8:8:33:LEU:HD11	8:8:161:TYR:HB2	1.98	0.46
9:A:29:GLN:HB3	10:B:12:GLU:O	2.16	0.46
11:C:245:PHE:CG	12:D:17:LEU:HD13	2.50	0.46
17:I:70:LEU:HB3	52:I:1016:HOH:O	2.16	0.46
19:K:15:ARG:CG	9:a:408:ARG:CZ	2.83	0.46
9:a:111:GLU:HG3	9:a:215:HIS:CE1	2.50	0.46
14:f:12:TRP:O	14:f:16:ILE:N	2.36	0.46
34:m:1523:UNK:C	34:m:1525:UNK:N	2.72	0.46
3:3:476:ILE:O	3:3:480:LEU:HG	2.16	0.45
5:5:195:LEU:HD22	5:5:195:LEU:N	2.30	0.45
9:A:15:GLN:HE21	10:B:12:GLU:HB2	1.81	0.45
10:B:257:LEU:O	10:B:323:GLY:HA3	2.15	0.45
12:D:43:MET:HE2	12:D:91:PHE:CE2	2.51	0.45
15:G:40:ARG:NH2	48:G:2004:CDL:HB31	2.32	0.45
20:L:431:LEU:HD21	20:L:450:TRP:HB2	1.99	0.45
20:L:449:MET:HE3	30:V:40:TRP:HB3	1.98	0.45
32:X:37:LEU:HA	32:X:37:LEU:HD23	1.83	0.45
33:Y:57:ILE:C	33:Y:57:ILE:HD12	2.41	0.45
9:a:354:VAL:HG21	9:a:404:ALA:HA	1.96	0.45
16:h:41:ASP:O	16:h:45:SER:HB2	2.15	0.45
1:1:53:VAL:HG23	1:1:231:MET:CE	2.45	0.45
5:5:15:TYR:OH	5:5:33:ARG:HD3	2.15	0.45
6:6:89:ALA:N	6:6:90:PRO:HD2	2.31	0.45
8:8:34:LYS:HB3	8:8:35:PRO:HD2	1.97	0.45
28:T:19:PHE:CD1	28:T:19:PHE:C	2.94	0.45
9:a:281:ASP:C	9:a:281:ASP:OD1	2.58	0.45
17:i:36:ALA:HB3	17:i:73:PRO:CG	2.46	0.45
4:4:200:ARG:O	4:4:204:TYR:CD1	2.70	0.45
5:5:47:ASN:ND2	5:5:76:SER:HA	2.31	0.45
6:6:155:GLN:C	6:6:157:LYS:N	2.75	0.45
9:A:85:HIS:O	9:A:99:ILE:HA	2.16	0.45
11:C:193:ALA:O	11:C:196:HIS:HB3	2.16	0.45
21:M:60:GLU:CD	21:M:61:VAL:H	2.24	0.45
23:O:33:LEU:HD13	23:O:41:LYS:HG3	1.97	0.45
9:a:307:PHE:CD1	9:a:307:PHE:C	2.95	0.45
12:d:144:ARG:HG3	12:d:147:LEU:HD12	1.98	0.45
19:k:24:TRP:O	19:k:25:GLY:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1:440:FMN:H1'1	39:1:440:FMN:H9	1.62	0.45
3:3:2:VAL:HG13	3:3:89:ASP:CA	2.47	0.45
3:3:55:PRO:CG	3:3:73:ILE:HA	2.45	0.45
4:4:142:ALA:HB1	4:4:145:PRO:HD2	1.99	0.45
6:6:145:GLU:HG2	8:8:31:VAL:HG21	1.98	0.45
8:8:125:GLU:O	8:8:128:ASP:HB2	2.16	0.45
17:I:76:VAL:HG13	17:I:76:VAL:O	2.16	0.45
21:M:76:ILE:O	21:M:79:PRO:HD2	2.16	0.45
24:P:70:VAL:HG12	24:P:71:VAL:N	2.31	0.45
25:Q:98:HIS:ND1	25:Q:98:HIS:N	2.64	0.45
29:U:2:GLU:CG	29:U:3:ASN:H	2.30	0.45
3:3:200:LEU:HD12	3:3:200:LEU:HA	1.80	0.45
3:3:469:ARG:HG2	3:3:754:PRO:HG3	1.97	0.45
3:3:588:SER:C	3:3:589:HIS:ND1	2.75	0.45
3:3:616:ASN:HB3	3:3:620:ARG:H	1.81	0.45
6:6:84:LEU:HD11	6:6:89:ALA:HA	1.98	0.45
17:I:36:ALA:CB	17:I:73:PRO:HB2	2.46	0.45
21:M:41:ILE:O	21:M:45:MET:HG2	2.16	0.45
1:1:45:LEU:HD12	1:1:163:PHE:HD2	1.81	0.45
3:3:417:VAL:CG1	3:3:443:ARG:HB3	2.46	0.45
4:4:350:ARG:NE	4:4:403:VAL:HG23	2.32	0.45
5:5:75:VAL:HG12	5:5:76:SER:N	2.31	0.45
5:5:161:GLU:CG	5:5:163:ARG:NH2	2.79	0.45
20:L:240:HIS:O	20:L:243:VAL:HG22	2.16	0.45
23:O:79:LYS:NZ	30:V:15:ASN:HD21	2.15	0.45
1:1:397:ARG:O	1:1:397:ARG:HG2	2.16	0.45
3:3:305:ARG:NH2	3:3:609:GLU:CD	2.74	0.45
3:3:541:ALA:O	3:3:545:GLU:HG3	2.15	0.45
4:4:105:LEU:HD13	4:4:309:ILE:CD1	2.44	0.45
4:4:158:ASP:OD1	8:8:34:LYS:HE3	2.17	0.45
5:5:72:TYR:HB2	5:5:90:VAL:HG13	1.98	0.45
6:6:125:GLN:O	6:6:126:ASN:CB	2.64	0.45
11:c:217:LYS:HG3	15:g:7:LEU:HD13	1.98	0.45
15:g:71:ARG:NH1	15:g:72:LYS:HD2	2.32	0.45
19:k:23:LEU:N	19:k:23:LEU:HD23	2.32	0.45
21:M:58:ALA:O	21:M:60:GLU:HG3	2.16	0.45
21:M:162:SER:HB2	21:M:198:GLU:HB2	1.99	0.45
33:Y:17:CYS:SG	44:Y:500:HEM:C3C	3.10	0.45
52:c:3113:HOH:O	14:f:20:TYR:HE1	1.98	0.45
18:j:16:ARG:O	18:j:19:THR:HG22	2.17	0.45
3:3:115:HIS:HB3	4:4:321:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:101:VAL:HG11	4:4:175:ILE:HD12	1.98	0.45
4:4:314:ARG:NH2	8:8:108:CYS:O	2.50	0.45
10:B:327:ILE:HG21	17:I:55:LEU:HD11	1.98	0.45
23:O:33:LEU:HD22	23:O:37:GLN:HB3	1.97	0.45
1:1:358:PRO:CD	3:3:107:MET:HE1	2.46	0.45
3:3:29:ASP:OD2	5:5:186:GLY:HA3	2.17	0.45
3:3:694:LEU:HD23	3:3:760:LEU:HB3	1.98	0.45
4:4:221:VAL:HG12	4:4:388:GLU:OE1	2.17	0.45
10:B:28:ARG:HH21	10:B:390:GLY:HA3	1.81	0.45
18:J:16:ARG:NH1	18:J:16:ARG:HG3	2.32	0.45
20:L:51:ASP:O	20:L:55:ASN:HB2	2.17	0.45
20:L:306:THR:HB	20:L:359:ALA:O	2.15	0.45
25:Q:31:TYR:HE1	25:Q:98:HIS:CE1	2.34	0.45
33:Y:25:LYS:HE2	12:d:145:GLU:OE1	2.17	0.45
10:b:71:LEU:CD2	17:i:68:VAL:HG21	2.43	0.45
11:c:327:ALA:HA	15:g:51:PRO:HB3	1.98	0.45
4:4:101:VAL:CG1	4:4:175:ILE:HD12	2.47	0.44
5:5:103:THR:HG22	5:5:127:GLU:O	2.17	0.44
16:H:31:VAL:O	16:H:35:GLU:HG3	2.18	0.44
20:L:131:PRO:HB2	21:M:159:VAL:HA	1.99	0.44
20:L:158:ILE:O	20:L:162:ILE:HG13	2.17	0.44
1:1:68:ALA:HB1	40:1:441:NAI:H51A	1.98	0.44
1:1:149:ILE:HD13	1:1:171:LEU:CB	2.37	0.44
3:3:13:VAL:HG21	3:3:17:THR:HG21	1.99	0.44
3:3:20:MET:HB3	3:3:20:MET:HE2	1.69	0.44
3:3:497:TRP:O	3:3:500:ALA:HB3	2.17	0.44
4:4:185:GLU:O	4:4:189:GLU:HG2	2.17	0.44
4:4:190:LEU:HG	4:4:194:LEU:HD22	1.98	0.44
4:4:253:PRO:HB2	4:4:258:GLU:HG3	1.99	0.44
4:4:263:ASP:HB2	4:4:285:GLU:OE1	2.16	0.44
13:E:145:VAL:HG23	11:c:141:TRP:CH2	2.52	0.44
15:G:40:ARG:CZ	48:G:2004:CDL:HB31	2.47	0.44
24:P:78:HIS:CE1	28:T:12:LEU:HD22	2.52	0.44
11:c:213:SER:OG	11:c:217:LYS:NZ	2.42	0.44
1:1:414:LEU:HD13	1:1:421:TYR:CE2	2.53	0.44
2:2:87:SER:HB3	2:2:128:CYS:HB3	2.00	0.44
3:3:36:GLU:HG3	3:3:37:LYS:N	2.32	0.44
4:4:339:LYS:HA	4:4:359:SER:O	2.17	0.44
5:5:111:ALA:O	5:5:115:GLU:HG3	2.17	0.44
5:5:119:TYR:O	5:5:122:PHE:O	2.35	0.44
6:6:84:LEU:HD12	6:6:124:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:145:GLU:HG2	8:8:31:VAL:CG2	2.47	0.44
9:A:39:VAL:HG11	9:A:195:MET:HE3	1.98	0.44
11:C:304:ILE:HB	11:C:305:PRO:HD3	1.99	0.44
18:J:8:ARG:HA	18:J:8:ARG:HD2	1.76	0.44
26:R:42:ARG:HG3	26:R:42:ARG:NH1	2.32	0.44
29:U:30:ILE:HG13	29:U:31:LEU:N	2.33	0.44
13:e:112:VAL:CG2	13:e:172:ARG:NH2	2.80	0.44
1:1:408:TRP:HB2	1:1:409:PRO:HD2	1.99	0.44
3:3:36:GLU:HB3	3:3:39:LEU:HD12	1.99	0.44
3:3:736:VAL:HG11	3:3:760:LEU:HD22	1.98	0.44
9:A:354:VAL:HG21	9:A:404:ALA:HA	1.98	0.44
13:E:95:PRO:HG2	13:E:145:VAL:HG22	1.98	0.44
22:N:41:THR:O	22:N:45:ILE:HG13	2.18	0.44
22:N:63:ARG:HA	22:N:67:PHE:CD2	2.53	0.44
25:Q:33:ILE:HG22	25:Q:34:LEU:HD12	1.98	0.44
26:R:3:ALA:O	26:R:4:ALA:HB2	2.17	0.44
33:Y:72:LYS:HE2	52:Y:273:HOH:O	2.17	0.44
9:a:19:LEU:HD22	9:a:213:GLN:HG3	1.99	0.44
11:c:13:ILE:O	11:c:13:ILE:HG22	2.17	0.44
13:e:75:GLU:HG2	13:e:194:ILE:HG12	2.00	0.44
1:1:102:LYS:HE3	1:1:103:ASP:CG	2.42	0.44
1:1:391:LEU:HB2	1:1:392:PRO:HD3	2.00	0.44
2:2:123:GLU:O	2:2:124:CYS:C	2.61	0.44
4:4:213:ILE:O	4:4:214:PHE:C	2.60	0.44
4:4:363:SER:CB	5:5:174:LEU:H	2.25	0.44
49:L:516:HEA:HHC	49:L:516:HEA:O11	2.17	0.44
22:N:183:GLU:O	26:R:42:ARG:NH2	2.50	0.44
10:b:34:VAL:C	10:b:35:ILE:HD12	2.41	0.44
46:c:3002:UQ1:HM31	52:c:3116:HOH:O	2.17	0.44
1:1:42:LYS:HG3	1:1:163:PHE:CD1	2.53	0.44
1:1:97:GLU:HB2	40:1:441:NAI:C4N	2.27	0.44
2:2:26:ALA:O	2:2:30:LEU:HG	2.18	0.44
4:4:47:LEU:HD13	4:4:52:VAL:HA	1.98	0.44
6:6:145:GLU:HA	6:6:148:ILE:HD13	1.99	0.44
7:7:70:ALA:HA	7:7:83:GLY:O	2.17	0.44
7:7:74:PRO:HG2	7:7:77:ALA:HB2	1.99	0.44
15:G:38:LEU:HB3	15:G:42:ARG:NH1	2.32	0.44
20:L:32:ALA:HB3	31:W:36:PRO:HG2	1.98	0.44
11:c:270:PRO:HG2	11:c:278:TYR:CG	2.53	0.44
12:d:44:ASP:OD1	12:d:93:LYS:HE2	2.18	0.44
17:i:62:ARG:HB3	17:i:63:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:184:GLU:OE1	1:1:186:THR:CG2	2.52	0.44
2:2:31:LEU:HD22	2:2:49:ILE:HD12	1.99	0.44
2:2:45:ARG:O	2:2:49:ILE:HG13	2.18	0.44
5:5:39:ALA:HA	5:5:107:LEU:HD13	1.99	0.44
6:6:25:GLU:HA	6:6:28:VAL:HG23	1.98	0.44
11:C:197:LEU:HD21	44:C:502:HEM:HMA1	2.00	0.44
52:D:4077:HOH:O	14:F:71:ARG:HD3	2.18	0.44
21:M:63:THR:HA	21:M:66:THR:HG22	2.00	0.44
21:M:122:MET:HB2	21:M:208:PRO:CD	2.47	0.44
28:T:61:GLU:OE1	28:T:64:ARG:NH1	2.51	0.44
13:e:112:VAL:HG22	13:e:172:ARG:NH2	2.33	0.44
14:f:110:LYS:HG3	14:f:110:LYS:O	2.17	0.44
3:3:317:LEU:HD22	3:3:317:LEU:N	2.32	0.44
3:3:753:VAL:HA	3:3:754:PRO:HD2	1.84	0.44
4:4:333:GLU:CD	5:5:189:ARG:HH11	2.25	0.44
5:5:144:HIS:O	5:5:147:ARG:HG2	2.17	0.44
6:6:81:ALA:CB	6:6:108:MET:HE2	2.48	0.44
6:6:132:PRO:HB3	6:6:174:ALA:HB1	2.00	0.44
8:8:103:LEU:HA	8:8:103:LEU:HD23	1.78	0.44
9:A:27:SER:HA	9:A:199:ALA:O	2.18	0.44
17:I:36:ALA:CB	17:I:73:PRO:CD	2.95	0.44
29:U:36:MET:O	29:U:40:LEU:HG	2.18	0.44
12:d:42:SER:HB3	12:d:94:PRO:HD2	2.00	0.44
1:1:260:ARG:HA	1:1:261:PRO:HD2	1.75	0.44
2:2:125:LEU:HD12	2:2:133:VAL:HG12	2.00	0.44
3:3:587:LEU:O	3:3:604:ALA:HB3	2.17	0.44
3:3:646:GLU:C	3:3:648:LEU:H	2.26	0.44
7:7:13:TRP:O	7:7:17:LEU:HG	2.16	0.44
11:C:92:ILE:O	11:C:96:MET:HG2	2.17	0.44
21:M:98:LYS:HE3	21:M:98:LYS:HB2	1.80	0.44
9:a:433:ASP:OD2	9:a:435:ASN:HB2	2.17	0.44
1:1:171:LEU:HD12	1:1:171:LEU:HA	1.73	0.43
1:1:397:ARG:O	3:3:46:ARG:HD3	2.18	0.43
3:3:152:PRO:HG3	4:4:305:PRO:O	2.18	0.43
3:3:368:HIS:CE1	3:3:563:ALA:HA	2.53	0.43
44:C:501:HEM:HBC2	44:C:501:HEM:HMC1	2.00	0.43
16:H:51:GLU:HG3	16:H:52:GLU:N	2.32	0.43
21:M:59:GLN:CA	21:M:62:GLU:HB2	2.46	0.43
9:a:416:TYR:HB3	18:j:15:ARG:NH2	2.33	0.43
11:c:369:ALA:O	11:c:373:GLU:HG3	2.18	0.43
17:i:36:ALA:CB	17:i:73:PRO:HD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:32:LEU:O	19:k:33:VAL:C	2.61	0.43
3:3:514:ASP:OD1	3:3:516:VAL:HB	2.17	0.43
5:5:138:PRO:HA	6:6:87:LYS:HD2	2.00	0.43
6:6:36:LEU:HD22	6:6:77:VAL:CG2	2.46	0.43
6:6:155:GLN:C	6:6:157:LYS:H	2.26	0.43
9:A:240:GLN:NE2	52:A:4184:HOH:O	2.51	0.43
9:A:307:PHE:CD1	9:A:307:PHE:C	2.96	0.43
20:L:379:TYR:CE2	20:L:383:MET:HE2	2.52	0.43
22:N:137:LEU:HD12	22:N:137:LEU:HA	1.69	0.43
26:R:54:ARG:N	26:R:54:ARG:CD	2.80	0.43
1:1:299:PRO:HG3	1:1:341:MET:HE1	2.00	0.43
2:2:122:VAL:CG1	2:2:123:GLU:H	2.31	0.43
3:3:222:PHE:CD1	3:3:411:LEU:HD11	2.52	0.43
3:3:344:TYR:CD2	3:3:568:TYR:CE1	3.07	0.43
3:3:505:LEU:HD21	3:3:507:LEU:CD2	2.48	0.43
4:4:260:TYR:HE2	4:4:293:ALA:HB2	1.82	0.43
6:6:31:GLY:C	6:6:33:SER:N	2.73	0.43
13:E:75:GLU:HG2	13:E:194:ILE:HG12	2.00	0.43
20:L:377:PHE:CD2	49:L:516:HEA:HAD1	2.54	0.43
21:M:121:TYR:C	21:M:138:VAL:HG23	2.42	0.43
28:T:68:ILE:HG13	28:T:69:PHE:N	2.33	0.43
31:W:35:ALA:HB3	31:W:36:PRO:HD3	1.99	0.43
9:a:224:ASP:OD1	9:a:227:ALA:HB2	2.18	0.43
9:a:267:ASN:O	9:a:271:GLN:HG2	2.19	0.43
1:1:361:GLU:H	1:1:361:GLU:HG2	1.53	0.43
3:3:9:ARG:HD2	3:3:26:ALA:O	2.19	0.43
3:3:49:LEU:HA	3:3:80:ALA:O	2.18	0.43
3:3:173:PHE:HB3	3:3:296:PHE:CE2	2.54	0.43
3:3:223:SER:O	3:3:226:ILE:HG12	2.19	0.43
3:3:716:LEU:HD21	3:3:758:LEU:HB3	1.99	0.43
4:4:200:ARG:HA	4:4:200:ARG:HD2	1.86	0.43
8:8:73:ALA:HB3	8:8:87:TYR:CZ	2.53	0.43
9:A:383:LEU:O	9:A:387:GLY:HA2	2.18	0.43
21:M:1:MET:SD	21:M:133:LEU:HD13	2.58	0.43
33:Y:61[A]:GLU:HG3	52:Y:280:HOH:O	2.17	0.43
52:Y:350:HOH:O	12:d:106:ASN:CB	2.11	0.43
9:a:15:GLN:O	9:a:26:ALA:HA	2.18	0.43
10:b:314:ALA:HA	17:i:63:PRO:HD3	2.00	0.43
14:f:77:LYS:HA	14:f:80:TRP:CE2	2.53	0.43
1:1:180:TYR:N	1:1:351:GLU:OE1	2.47	0.43
3:3:125:GLY:HA2	3:3:245:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:300:TRP:N	3:3:705:VAL:HG21	2.33	0.43
3:3:305:ARG:NH2	3:3:609:GLU:OE1	2.51	0.43
3:3:719:HIS:CD2	3:3:755:LYS:HG2	2.54	0.43
4:4:257:TYR:C	4:4:259:THR:N	2.72	0.43
9:A:381:ARG:HG2	52:A:4120:HOH:O	2.19	0.43
19:K:15:ARG:HG3	9:a:408:ARG:NH1	2.14	0.43
22:N:19:THR:CG2	22:N:53:THR:OG1	2.66	0.43
23:O:40:LEU:HD22	23:O:59:LEU:CD1	2.47	0.43
29:U:3:ASN:ND2	29:U:5:VAL:HG13	2.33	0.43
33:Y:25:LYS:CE	12:d:145:GLU:OE1	2.66	0.43
11:c:269:LYS:HA	11:c:270:PRO:HD3	1.83	0.43
2:2:81:GLN:HB3	2:2:122:VAL:CG2	2.43	0.43
3:3:504:VAL:HG12	3:3:505:LEU:N	2.34	0.43
4:4:257:TYR:O	4:4:259:THR:N	2.51	0.43
6:6:46:CYS:HB3	6:6:108:MET:HE2	2.00	0.43
6:6:163:TYR:CD2	8:8:152:ARG:NH1	2.85	0.43
8:8:101:CYS:SG	8:8:103:LEU:HB2	2.58	0.43
10:B:230:LEU:HB3	10:B:233:SER:OG	2.17	0.43
15:G:48:VAL:O	15:G:51:PRO:HD2	2.18	0.43
19:K:20:THR:HG23	19:K:24:TRP:HD1	1.83	0.43
21:M:86:MET:HE3	21:M:86:MET:HB2	1.80	0.43
22:N:80:ARG:HG2	22:N:233:PHE:CE1	2.54	0.43
28:T:26:MET:N	28:T:26:MET:SD	2.91	0.43
33:Y:72:LYS:HG2	52:Y:273:HOH:O	2.17	0.43
1:1:314:GLU:HA	1:1:317:GLN:HB3	1.99	0.43
2:2:33:ARG:O	2:2:34:VAL:C	2.61	0.43
3:3:343:LEU:CD1	3:3:360:LEU:HD23	2.49	0.43
3:3:550:LEU:CD2	3:3:684:ARG:HH21	2.31	0.43
3:3:594:ALA:O	3:3:598:ALA:HB3	2.19	0.43
4:4:241:ALA:O	4:4:270:GLY:HA2	2.18	0.43
8:8:71:GLU:HA	8:8:72:PRO:HD3	1.80	0.43
15:G:50:PRO:HB2	15:G:51:PRO:HD3	2.01	0.43
20:L:240:HIS:NE2	20:L:244:TYR:CE2	2.81	0.43
21:M:162:SER:HB3	21:M:197:SER:C	2.44	0.43
23:O:24:LEU:HA	23:O:25:PRO:HD2	1.93	0.43
27:S:57:ARG:HB3	27:S:57:ARG:NH1	2.31	0.43
33:Y:25:LYS:CE	12:d:145:GLU:OE2	2.46	0.43
9:a:288:ALA:HB2	9:a:300:THR:HG22	2.01	0.43
10:b:345:LYS:O	10:b:349:GLN:HG3	2.19	0.43
1:1:401:PRO:HG2	39:1:440:FMN:C8M	2.49	0.43
5:5:25:LEU:N	5:5:25:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:178:ASP:HA	5:5:179:PRO:HD2	1.84	0.43
6:6:76:ASP:O	6:6:77:VAL:CB	2.65	0.43
9:A:61:HIS:CE1	9:A:137:GLU:OE1	2.72	0.43
18:J:25:VAL:HG12	19:k:30:VAL:HG12	2.01	0.43
22:N:148:HIS:CE1	22:N:152:MET:HE3	2.54	0.43
28:T:21:ILE:O	28:T:25:PHE:HD2	2.02	0.43
30:V:9:PHE:CD1	30:V:9:PHE:C	2.97	0.43
30:V:44:PRO:HA	30:V:47:ARG:NH1	2.34	0.43
9:a:286:GLY:HA3	9:a:290:LEU:CD2	2.47	0.43
14:f:58:ARG:HD3	52:f:2031:HOH:O	2.18	0.43
3:3:254:THR:HG23	3:3:255:THR:N	2.34	0.43
3:3:585:MET:HG3	3:3:598:ALA:CB	2.48	0.43
5:5:178:ASP:OD1	5:5:179:PRO:HD2	2.19	0.43
6:6:174:ALA:O	6:6:175:ALA:HB2	2.19	0.43
10:B:181:TYR:CD2	10:b:248:ASN:HA	2.54	0.43
12:D:97:ASN:HB2	12:D:98:PRO:HD2	2.01	0.43
20:L:273:MET:HG3	20:L:319:LYS:NZ	2.30	0.43
21:M:52:HIS:CD2	24:P:40:ASP:HB2	2.54	0.43
22:N:60:ASP:O	22:N:64:GLU:HG3	2.19	0.43
26:R:78:LEU:HA	26:R:78:LEU:HD12	1.75	0.43
31:W:41:ARG:HD2	32:X:40:TYR:CZ	2.54	0.43
33:Y:14:CYS:CB	44:Y:500:HEM:HAB	2.47	0.43
11:c:12:LYS:HE2	11:c:16:ASN:HB2	1.99	0.43
12:d:43:MET:HE2	12:d:91:PHE:CE2	2.53	0.43
1:1:45:LEU:HD12	1:1:163:PHE:CD2	2.54	0.43
2:2:15:PHE:HE1	2:2:23:ARG:HB3	1.84	0.43
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.59	0.43
3:3:186:ARG:HD2	3:3:231:PRO:HD3	1.99	0.43
3:3:194:VAL:HB	3:3:195:PRO:CD	2.44	0.43
3:3:225:ASN:HD21	3:3:289:TRP:HB3	1.84	0.43
3:3:483:ASP:O	3:3:484:LYS:HG2	2.19	0.43
3:3:672:ALA:O	3:3:673:MET:HB2	2.19	0.43
10:B:307:PHE:CD1	10:B:307:PHE:C	2.96	0.43
12:D:47:ALA:HA	12:D:90:TYR:HA	2.01	0.43
13:E:112:VAL:HG22	13:E:172:ARG:NH2	2.34	0.43
10:b:246:GLU:O	10:b:427:SER:HA	2.19	0.43
10:b:257:LEU:O	10:b:323:GLY:HA3	2.19	0.43
2:2:26:ALA:C	2:2:29:PRO:HG2	2.43	0.42
3:3:225:ASN:O	3:3:229:ILE:HG13	2.19	0.42
4:4:338:PRO:HG2	5:5:193:ARG:HD3	2.01	0.42
10:B:71:LEU:CD2	17:I:68:VAL:HG21	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:106:PRO:HB2	20:L:107:PRO:HD3	2.01	0.42
20:L:356:ILE:HD13	20:L:356:ILE:HA	1.90	0.42
26:R:5:LYS:CD	26:R:6:GLY:N	2.81	0.42
13:e:117:LEU:HD13	13:e:170:ARG:HD2	2.00	0.42
3:3:258:LEU:HD11	3:3:703:GLN:NE2	2.34	0.42
3:3:326:PHE:CE2	3:3:330:LYS:HE3	2.55	0.42
3:3:403:THR:HG22	3:3:404:GLU:OE2	2.19	0.42
3:3:513:GLN:NE2	3:3:769:LEU:HD21	2.34	0.42
3:3:689:LYS:H	3:3:689:LYS:HG2	1.44	0.42
4:4:159:LEU:O	4:4:162:TRP:HB2	2.19	0.42
5:5:74:LEU:O	5:5:87:ARG:HA	2.19	0.42
5:5:77:LEU:HA	5:5:78:PRO:HD3	1.61	0.42
6:6:140:CYS:SG	6:6:140:CYS:O	2.77	0.42
7:7:17:LEU:HD22	7:7:54:ILE:HD11	2.00	0.42
9:A:79:VAL:HA	9:A:82:MET:HE3	2.01	0.42
20:L:70:VAL:HG11	20:L:246:LEU:HD22	1.99	0.42
20:L:247:ILE:HB	49:L:516:HEA:HBC1	2.01	0.42
21:M:100:MET:HE3	21:M:157:GLU:HG3	2.01	0.42
10:b:102:ARG:HH22	10:b:161:GLU:CD	2.27	0.42
1:1:67:GLY:HA2	1:1:324:GLY:O	2.20	0.42
3:3:118:ASP:O	3:3:119:CYS:C	2.62	0.42
4:4:304:ASP:HA	4:4:305:PRO:HD2	1.87	0.42
9:A:111:GLU:HG3	9:A:215:HIS:CE1	2.54	0.42
10:B:181:TYR:CE1	10:B:182:ARG:HG2	2.54	0.42
10:B:361:LYS:HE2	10:B:402:ILE:O	2.18	0.42
16:H:19:THR:O	16:H:23:GLN:HG3	2.19	0.42
22:N:19:THR:HG22	22:N:53:THR:OG1	2.18	0.42
24:P:27:TRP:CH2	25:Q:86:GLY:HA2	2.54	0.42
29:U:11:LEU:HD23	29:U:11:LEU:C	2.43	0.42
9:a:3:THR:OG1	9:a:6:GLN:HG3	2.19	0.42
1:1:135:ARG:C	1:1:137:GLU:H	2.26	0.42
1:1:291:ILE:HA	1:1:292:PRO:HD2	1.84	0.42
3:3:206:GLY:O	3:3:209:THR:CG2	2.67	0.42
3:3:329:LEU:HD21	3:3:644:LEU:HD12	2.01	0.42
4:4:339:LYS:HG2	4:4:360:ASP:HA	2.01	0.42
9:A:267:ASN:O	9:A:271:GLN:HG2	2.20	0.42
16:H:31:VAL:CG2	16:H:32:LYS:N	2.82	0.42
20:L:173:PRO:HA	20:L:174:PRO:HD3	1.96	0.42
20:L:462:LEU:O	20:L:466:MET:HG3	2.20	0.42
23:O:37:GLN:O	23:O:41:LYS:HG2	2.18	0.42
10:b:28:ARG:NH1	10:b:28:ARG:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:228:GLY:O	10:b:231:GLY:HA2	2.19	0.42
11:c:67:THR:HB	12:d:115:TYR:OH	2.20	0.42
2:2:101:THR:HG22	7:7:108:ILE:CD1	2.46	0.42
3:3:258:LEU:HD23	3:3:258:LEU:HA	1.89	0.42
3:3:717:TRP:CD1	3:3:748:VAL:HB	2.54	0.42
4:4:317:LEU:HD12	4:4:317:LEU:HA	1.91	0.42
7:7:96:HIS:O	7:7:103:LEU:HD12	2.19	0.42
8:8:100:PHE:CD1	8:8:100:PHE:N	2.87	0.42
17:I:77:ARG:O	17:I:78:TYR:HB2	2.19	0.42
19:K:20:THR:HG23	19:K:24:TRP:CD1	2.54	0.42
49:L:515:HEA:HHC	49:L:515:HEA:H122	2.02	0.42
21:M:3:TYR:CD1	21:M:3:TYR:N	2.87	0.42
22:N:110:PRO:HB3	27:S:30:TRP:CD2	2.54	0.42
25:Q:74:LEU:HA	25:Q:74:LEU:HD23	1.87	0.42
9:a:156:THR:HA	13:e:7:VAL:HG21	2.01	0.42
1:1:6:LEU:HD12	1:1:240:GLN:HG3	2.01	0.42
1:1:437:TRP:O	1:1:437:TRP:HD1	2.03	0.42
3:3:163:HIS:C	3:3:164:VAL:HG13	2.45	0.42
3:3:473:GLU:H	3:3:473:GLU:HG2	1.67	0.42
3:3:681:LYS:O	3:3:682:GLU:HB3	2.20	0.42
6:6:163:TYR:OH	6:6:169:ARG:NH2	2.52	0.42
9:A:381:ARG:HG2	9:A:381:ARG:HH11	1.84	0.42
11:C:68:HIS:HE1	52:C:2049:HOH:O	2.01	0.42
20:L:495:LEU:HD23	20:L:495:LEU:HA	1.68	0.42
17:i:64:LEU:CD1	17:i:78:TYR:C	2.93	0.42
19:k:24:TRP:CE3	19:k:24:TRP:HA	2.55	0.42
35:n:823:UNK:C	35:n:825:UNK:N	2.77	0.42
3:3:5:LYS:HB2	3:3:10:ILE:HG13	2.01	0.42
3:3:155:THR:HB	4:4:322:GLU:OE1	2.19	0.42
3:3:586:HIS:NE2	3:3:604:ALA:HB2	2.34	0.42
4:4:350:ARG:HE	4:4:403:VAL:HG23	1.85	0.42
8:8:170:LEU:HD23	8:8:170:LEU:HA	1.88	0.42
20:L:498:CYS:HA	20:L:499:PRO:HA	1.78	0.42
25:Q:53:THR:HG22	25:Q:54:ASN:OD1	2.19	0.42
16:h:23:GLN:O	16:h:26:GLN:HG2	2.20	0.42
1:1:390:LEU:HD23	1:1:390:LEU:HA	1.84	0.42
3:3:20:MET:HG3	3:3:82:SER:OG	2.20	0.42
4:4:88:LEU:HD23	4:4:88:LEU:HA	1.95	0.42
4:4:213:ILE:HG22	4:4:217:ARG:CG	2.49	0.42
4:4:306:ASN:HA	4:4:307:PRO:HD3	1.81	0.42
6:6:163:TYR:HD1	6:6:169:ARG:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:270:PRO:HG2	11:C:278:TYR:CG	2.54	0.42
44:C:501:HEM:O2D	44:C:501:HEM:O2A	2.37	0.42
17:I:64:LEU:CD1	17:I:78:TYR:C	2.92	0.42
30:V:13:TYR:O	30:V:14:GLY:C	2.63	0.42
1:1:110:VAL:N	1:1:111:PRO:CD	2.82	0.42
1:1:408:TRP:CB	1:1:409:PRO:CD	2.98	0.42
3:3:370:ASP:OD2	3:3:558:TRP:CD1	2.73	0.42
3:3:497:TRP:O	3:3:528:LYS:HE3	2.20	0.42
4:4:52:VAL:HG23	4:4:388:GLU:O	2.20	0.42
4:4:72:HIS:O	4:4:73:ARG:HD3	2.19	0.42
5:5:116:ARG:CG	5:5:129:HIS:CE1	3.02	0.42
6:6:143:ARG:HG2	6:6:145:GLU:OE1	2.20	0.42
8:8:46:HIS:HB3	8:8:47:PRO:HD2	2.01	0.42
9:A:11:VAL:HA	9:A:12:PRO:HD3	1.93	0.42
9:A:78:GLU:OE2	9:A:108:LYS:HD2	2.20	0.42
9:A:405:ARG:O	9:A:409:GLU:HG3	2.20	0.42
13:E:188:THR:C	13:E:189:SER:O	2.60	0.42
13:E:189:SER:O	13:E:190:ASP:C	2.63	0.42
24:P:21:LYS:O	24:P:57:ARG:NH1	2.53	0.42
27:S:24:ASN:HD22	27:S:25:GLN:N	2.18	0.42
28:T:21:ILE:HA	28:T:21:ILE:HD12	1.81	0.42
9:a:280:TYR:HA	9:a:284:TYR:CE2	2.54	0.42
35:n:916:UNK:C	35:n:1203:UNK:CA	2.98	0.42
2:2:28:MET:HB3	2:2:28:MET:HE2	1.75	0.42
2:2:30:LEU:O	2:2:34:VAL:HG23	2.20	0.42
3:3:116:PRO:HG3	3:3:180:ARG:HG2	2.02	0.42
3:3:157:PHE:CZ	3:3:159:PHE:HB2	2.55	0.42
3:3:368:HIS:HE2	3:3:554:LYS:HG2	1.85	0.42
3:3:563:ALA:HB3	3:3:580:LYS:HE3	2.01	0.42
3:3:743:VAL:HG12	3:3:744:GLU:N	2.34	0.42
4:4:66:PHE:CG	4:4:85:MET:HE3	2.55	0.42
8:8:81:VAL:HG11	8:8:87:TYR:CD2	2.54	0.42
9:A:158:PHE:O	9:A:164:ALA:HB2	2.20	0.42
10:B:95:LYS:HB2	17:I:32:ALA:CB	2.41	0.42
12:D:91:PHE:HA	12:D:92:PRO:HD3	1.93	0.42
23:O:86:MET:O	30:V:25:CYS:HB2	2.20	0.42
26:R:42:ARG:NH1	26:R:74:ARG:NH2	2.68	0.42
10:b:307:PHE:CD1	10:b:307:PHE:C	2.98	0.42
14:f:12:TRP:O	14:f:15:GLY:N	2.53	0.42
1:1:65:ARG:HG3	1:1:65:ARG:HH11	1.85	0.41
2:2:59:GLU:O	2:2:63:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:249:MET:HE3	3:3:268:ASP:CB	2.48	0.41
3:3:651:ARG:HD2	3:3:651:ARG:C	2.44	0.41
4:4:296:ARG:O	4:4:298:GLU:HG3	2.20	0.41
9:A:281:ASP:C	9:A:281:ASP:OD1	2.63	0.41
9:A:347:THR:HA	19:k:16:ASN:HD22	1.85	0.41
11:C:269:LYS:HA	11:C:270:PRO:HD3	1.82	0.41
17:I:62:ARG:HB3	17:I:63:PRO:HD2	2.02	0.41
20:L:311:ILE:HD13	20:L:311:ILE:HG21	1.75	0.41
20:L:474:GLU:HG3	20:L:475:ALA:N	2.34	0.41
27:S:57:ARG:HA	27:S:60:TYR:CD2	2.55	0.41
11:c:68:HIS:HE1	52:c:3053:HOH:O	2.03	0.41
1:1:427:GLU:OE1	1:1:429:ARG:HD3	2.20	0.41
3:3:229:ILE:HD13	3:3:229:ILE:HG21	1.85	0.41
3:3:317:LEU:HD22	3:3:317:LEU:H	1.85	0.41
3:3:469:ARG:HD2	3:3:757:HIS:HE1	1.85	0.41
4:4:53:LEU:N	4:4:53:LEU:CD2	2.83	0.41
4:4:169:HIS:O	4:4:170:HIS:C	2.63	0.41
7:7:16:LEU:HD13	7:7:20:MET:HG3	2.03	0.41
12:D:43:MET:HE2	12:D:91:PHE:HE2	1.85	0.41
20:L:199:LEU:HD12	20:L:199:LEU:HA	1.91	0.41
22:N:146:TRP:CE2	26:R:17:ARG:HB2	2.56	0.41
23:O:127:LYS:O	23:O:130:PRO:HD3	2.20	0.41
28:T:35:TYR:O	28:T:39:VAL:HB	2.19	0.41
29:U:5:VAL:O	29:U:9:GLN:HG3	2.21	0.41
9:a:85:HIS:O	9:a:99:ILE:HA	2.21	0.41
10:b:212:SER:OG	10:b:215:VAL:HG23	2.21	0.41
13:e:95:PRO:HG2	13:e:145:VAL:HG22	2.02	0.41
2:2:87:SER:CB	2:2:128:CYS:HB3	2.50	0.41
2:2:112:THR:HG21	2:2:116:LEU:HD23	2.03	0.41
2:2:145:VAL:HG12	2:2:150:LEU:HB2	2.03	0.41
2:2:163:LEU:HA	2:2:166:ILE:HD11	2.00	0.41
5:5:67:ARG:HB3	5:5:96:GLU:HB2	2.02	0.41
8:8:96:LEU:CD2	8:8:129:LEU:HD13	2.45	0.41
16:H:23:GLN:O	16:H:26:GLN:HG2	2.20	0.41
21:M:164:ALA:HB2	21:M:171:LYS:HD3	2.03	0.41
22:N:224:LYS:NZ	22:N:226:HIS:HE2	2.18	0.41
23:O:126:MET:HG3	23:O:128:VAL:HG23	2.01	0.41
23:O:130:PRO:O	23:O:136:ALA:HB2	2.20	0.41
29:U:12:PHE:O	29:U:23:LYS:HE2	2.21	0.41
9:a:189:HIS:ND1	9:a:194:ARG:NH2	2.68	0.41
11:c:19:ILE:HD13	11:c:19:ILE:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:109:ASP:O	1:1:110:VAL:CG1	2.69	0.41
1:1:309:THR:HA	1:1:310:PRO:HD3	1.92	0.41
1:1:357:THR:N	1:1:358:PRO:CD	2.80	0.41
3:3:373:GLY:O	3:3:374:ARG:C	2.63	0.41
3:3:683:LEU:N	3:3:683:LEU:HD23	2.35	0.41
4:4:128:SER:OG	4:4:350:ARG:NH1	2.47	0.41
4:4:233:GLY:CA	5:5:48:PHE:HE1	2.33	0.41
4:4:279:ARG:O	4:4:283:MET:HG3	2.20	0.41
4:4:379:GLN:O	4:4:382:PRO:HD2	2.21	0.41
5:5:82:ASP:O	5:5:83:GLY:C	2.63	0.41
7:7:59:LEU:HB2	7:7:68:LEU:HB3	2.02	0.41
7:7:65:GLU:HA	7:7:66:PRO:HD3	1.73	0.41
8:8:162:VAL:HA	8:8:176:PRO:O	2.21	0.41
10:B:46:ARG:O	10:B:47:ILE:HD13	2.21	0.41
10:B:249:GLY:O	10:B:250:ASP:C	2.64	0.41
12:D:229:VAL:CG2	15:G:20:PRO:HD3	2.49	0.41
18:J:29:LEU:HD11	19:k:34:SER:HB2	2.02	0.41
21:M:193:TYR:N	21:M:193:TYR:CD1	2.88	0.41
22:N:182:TYR:O	26:R:72:ASN:HB2	2.21	0.41
23:O:137:LYS:O	23:O:145:TRP:HE3	2.03	0.41
24:P:93:LEU:HD23	24:P:93:LEU:HA	1.88	0.41
18:j:14:PHE:HA	18:j:20:PHE:HD1	1.85	0.41
34:m:119:UNK:C	34:m:122:UNK:N	2.83	0.41
1:1:95:GLU:OE2	1:1:102:LYS:HD3	2.20	0.41
1:1:287:ILE:HG22	1:1:302:PHE:HB2	2.03	0.41
2:2:33:ARG:NH2	2:2:37:GLU:CG	2.83	0.41
4:4:184:GLU:CD	4:4:184:GLU:H	2.28	0.41
4:4:290:ILE:O	4:4:294:LEU:HB2	2.20	0.41
6:6:44:ALA:O	6:6:46:CYS:N	2.53	0.41
8:8:153:THR:HG22	8:8:155:LYS:N	2.36	0.41
14:F:63:LYS:HG3	52:F:4045:HOH:O	2.20	0.41
20:L:298:ASP:HB2	20:L:301:THR:CG2	2.49	0.41
20:L:314:ILE:HB	20:L:315:PRO:CD	2.50	0.41
24:P:104:LEU:HA	24:P:104:LEU:HD23	1.87	0.41
33:Y:72:LYS:HD3	33:Y:78:THR:CG2	2.48	0.41
18:j:2:ALA:HA	18:j:3:PRO:HD3	1.82	0.41
19:k:20:THR:HG23	19:k:24:TRP:HD1	1.85	0.41
1:1:402:LEU:HD23	1:1:402:LEU:C	2.46	0.41
2:2:154:LEU:O	2:2:158:ARG:HB2	2.21	0.41
3:3:408:ILE:O	3:3:408:ILE:HG23	2.21	0.41
3:3:464:ILE:H	3:3:464:ILE:HG12	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:84:ARG:O	6:6:83:ARG:NH2	2.54	0.41
4:4:221:VAL:HG23	4:4:272:VAL:CG1	2.50	0.41
6:6:143:ARG:CG	6:6:144:PRO:HD2	2.50	0.41
8:8:48:ASN:HB2	8:8:50:LEU:CD2	2.50	0.41
18:J:21:ALA:CB	19:k:24:TRP:CZ3	3.03	0.41
20:L:354:THR:HG21	20:L:376:HIS:HA	2.03	0.41
20:L:501:PRO:O	20:L:502:TYR:C	2.63	0.41
22:N:146:TRP:NE1	26:R:17:ARG:HB2	2.35	0.41
25:Q:16:LEU:O	25:Q:20:VAL:HG13	2.21	0.41
9:a:86:LEU:HD13	9:a:99:ILE:CG1	2.50	0.41
11:c:320:LEU:HG	52:c:3113:HOH:O	2.19	0.41
15:g:50:PRO:HB2	15:g:51:PRO:HD3	2.03	0.41
3:3:169:PRO:HA	3:3:175:ILE:HA	2.03	0.41
3:3:261:VAL:HG12	3:3:406:ALA:HB1	2.02	0.41
3:3:272:GLY:HA2	3:3:628:PRO:O	2.20	0.41
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.80	0.41
3:3:473:GLU:O	3:3:477:LEU:CD1	2.69	0.41
4:4:163:VAL:HG13	4:4:164:THR:HG23	2.02	0.41
6:6:145:GLU:CD	6:6:145:GLU:H	2.28	0.41
7:7:55:MET:HE2	7:7:55:MET:HB3	1.90	0.41
7:7:75:ARG:HE	7:7:76:HIS:CE1	2.39	0.41
14:F:77:LYS:HA	14:F:80:TRP:CE2	2.55	0.41
17:I:36:ALA:HB3	17:I:73:PRO:HB2	2.02	0.41
18:J:25:VAL:CG1	19:k:30:VAL:HG12	2.50	0.41
20:L:442:ASP:OD2	21:M:134:ARG:NH2	2.54	0.41
26:R:77:PRO:HA	26:R:82:TYR:HA	2.02	0.41
30:V:24:PHE:CE1	30:V:28:VAL:HG21	2.56	0.41
32:X:19:LEU:HD23	32:X:19:LEU:C	2.45	0.41
11:c:223:TYR:HB3	12:d:227:TRP:CZ2	2.56	0.41
14:f:14:GLU:N	52:f:2070:HOH:O	2.53	0.41
16:h:31:VAL:CG2	16:h:32:LYS:N	2.84	0.41
1:1:102:LYS:HD3	1:1:102:LYS:H	1.84	0.41
1:1:287:ILE:HG13	1:1:330:LEU:HB3	2.03	0.41
3:3:91:MET:HE3	3:3:93:VAL:HG22	2.03	0.41
3:3:259:CYS:CB	3:3:260:PRO:CD	2.98	0.41
3:3:285:VAL:HG13	3:3:286:ASN:H	1.86	0.41
3:3:651:ARG:NH1	3:3:653:PRO:HA	2.36	0.41
8:8:144:LYS:HB2	8:8:145:PRO:CD	2.50	0.41
9:A:430:GLN:O	9:A:430:GLN:HG2	2.21	0.41
11:C:111:GLU:H	11:C:111:GLU:CD	2.28	0.41
12:D:237:TYR:HB2	14:F:60:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:29:LEU:HD11	19:k:34:SER:CB	2.51	0.41
20:L:398:PRO:HB3	20:L:482:VAL:HG21	2.03	0.41
20:L:430:PHE:O	20:L:431:LEU:C	2.64	0.41
24:P:86:ILE:HD13	24:P:86:ILE:HA	1.88	0.41
11:c:162:GLU:OE2	11:c:168:PHE:CD1	2.73	0.41
1:1:65:ARG:HA	1:1:65:ARG:HD3	1.76	0.41
1:1:184:GLU:HG2	39:1:440:FMN:HM82	2.03	0.41
1:1:202:LYS:N	1:1:203:PRO:CD	2.84	0.41
3:3:5:LYS:HA	3:3:10:ILE:HA	2.03	0.41
3:3:87:VAL:HG23	3:3:87:VAL:O	2.21	0.41
3:3:205:ARG:HH11	3:3:205:ARG:CG	2.33	0.41
3:3:249:MET:HE1	3:3:275:LEU:HB3	2.02	0.41
3:3:436:GLN:HE21	3:3:436:GLN:HB3	1.65	0.41
3:3:501:LYS:H	3:3:501:LYS:CD	2.21	0.41
3:3:627:ALA:HA	3:3:628:PRO:HD3	1.82	0.41
3:3:707:LYS:C	3:3:709:GLN:N	2.78	0.41
4:4:30:VAL:CG1	4:4:31:GLY:N	2.83	0.41
4:4:48:SER:H	4:4:53:LEU:HD23	1.85	0.41
4:4:318:GLU:OE2	7:7:75:ARG:NH2	2.54	0.41
5:5:52:ILE:HG23	5:5:52:ILE:O	2.20	0.41
5:5:116:ARG:HG3	5:5:129:HIS:CE1	2.56	0.41
6:6:107:SER:HB2	6:6:133:VAL:HG11	2.03	0.41
6:6:163:TYR:HB3	6:6:168:GLU:O	2.21	0.41
7:7:68:LEU:HD13	7:7:69:LEU:N	2.36	0.41
7:7:75:ARG:HE	7:7:76:HIS:CD2	2.39	0.41
8:8:33:LEU:HD22	8:8:37:PHE:CD2	2.55	0.41
9:A:280:TYR:HA	9:A:284:TYR:CE2	2.56	0.41
16:H:51:GLU:HG3	16:H:52:GLU:H	1.86	0.41
18:J:29:LEU:CG	19:k:34:SER:CB	2.93	0.41
20:L:168:ILE:CG2	20:L:189:MET:HG3	2.51	0.41
20:L:264:LYS:NZ	21:M:56:MET:HE2	2.35	0.41
22:N:228:THR:O	22:N:232:HIS:HD2	2.04	0.41
27:S:20:PHE:N	27:S:21:PRO:HD3	2.35	0.41
27:S:58:ARG:HD2	27:S:58:ARG:HA	1.74	0.41
29:U:31:LEU:HA	29:U:31:LEU:HD23	1.83	0.41
36:o:1215:UNK:C	36:o:1217:UNK:N	2.83	0.41
1:1:141:ALA:O	1:1:145:LEU:HB2	2.21	0.41
2:2:24:ARG:HG2	2:2:53:VAL:HG11	2.03	0.41
3:3:504:VAL:CG1	3:3:505:LEU:N	2.84	0.41
3:3:652:PRO:HA	3:3:653:PRO:HD3	1.82	0.41
4:4:289:ILE:O	4:4:290:ILE:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:311:PRO:HD3	4:4:330:HIS:CE1	2.56	0.41
4:4:329:LYS:O	4:4:333:GLU:O	2.39	0.41
6:6:147:LEU:O	6:6:151:VAL:HG13	2.21	0.41
13:E:84:GLY:N	13:E:100:HIS:O	2.54	0.41
20:L:276:ALA:O	20:L:280:ILE:HG13	2.21	0.41
21:M:146:MET:SD	21:M:189:PRO:HB3	2.60	0.41
22:N:6:HIS:CD2	22:N:8:TYR:HB2	2.55	0.41
25:Q:49:VAL:O	25:Q:91:LEU:HD12	2.21	0.41
25:Q:86:GLY:O	25:Q:87:THR:O	2.37	0.41
33:Y:68:LEU:HD21	44:Y:500:HEM:HMB2	2.02	0.41
39:1:440:FMN:HM71	39:1:440:FMN:HM83	1.81	0.40
3:3:156:ARG:HH11	3:3:156:ARG:CG	2.28	0.40
3:3:478:LEU:HD12	3:3:520:ARG:CZ	2.52	0.40
4:4:241:ALA:CB	4:4:278:VAL:HG21	2.51	0.40
5:5:75:VAL:HG22	5:5:87:ARG:HG3	2.03	0.40
9:A:264:HIS:ND1	9:A:265:PRO:HD2	2.36	0.40
14:F:101:ARG:O	14:F:105:GLU:HG3	2.21	0.40
22:N:42:LEU:HD12	22:N:42:LEU:HA	1.66	0.40
11:c:104:TYR:CD1	11:c:208:PRO:HA	2.56	0.40
1:1:180:TYR:OH	40:1:441:NAI:H5N	2.21	0.40
3:3:299:GLU:O	3:3:303:GLN:HG3	2.21	0.40
3:3:550:LEU:N	3:3:550:LEU:CD1	2.83	0.40
4:4:196:VAL:O	4:4:200:ARG:HB2	2.21	0.40
4:4:404:MET:HA	4:4:407:VAL:HG12	2.02	0.40
5:5:49:LEU:HD23	5:5:111:ALA:HB2	2.02	0.40
5:5:161:GLU:HG3	5:5:163:ARG:HH22	1.84	0.40
7:7:73:SER:HA	7:7:74:PRO:HD2	1.90	0.40
8:8:44:THR:OG1	8:8:52:LYS:HD2	2.21	0.40
9:A:163:LEU:HD23	9:A:163:LEU:HA	1.92	0.40
18:J:25:VAL:HG12	19:k:30:VAL:HG11	2.03	0.40
27:S:65:PRO:HG2	27:S:68:TRP:CG	2.55	0.40
29:U:3:ASN:C	29:U:3:ASN:ND2	2.77	0.40
32:X:35:TYR:HD2	32:X:36:HIS:CE1	2.39	0.40
33:Y:16:GLN:HB3	12:d:148:TYR:HE2	1.74	0.40
44:c:501:HEM:HMC1	44:c:501:HEM:HBC2	2.02	0.40
18:j:16:ARG:NH1	18:j:16:ARG:HG3	2.36	0.40
1:1:89:LEU:O	1:1:130:GLY:HA2	2.21	0.40
1:1:117:GLY:O	1:1:120:LEU:HB2	2.21	0.40
1:1:196:ARG:HG2	2:2:63:VAL:HA	2.04	0.40
1:1:273:ARG:O	1:1:277:TYR:HB2	2.21	0.40
3:3:372:GLN:HB2	3:3:570:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:689:LYS:HD2	3:3:772:GLU:CG	2.51	0.40
4:4:327:HIS:CE1	8:8:107:ALA:O	2.74	0.40
8:8:99:ILE:HA	8:8:99:ILE:HD12	1.84	0.40
10:B:102:ARG:HH22	10:B:161:GLU:CD	2.28	0.40
12:D:223:LYS:C	12:D:223:LYS:HD3	2.47	0.40
13:E:117:LEU:HD13	13:E:170:ARG:HD2	2.03	0.40
23:O:11:TYR:CD1	23:O:11:TYR:C	2.99	0.40
23:O:102:TYR:HD2	32:X:35:TYR:HE1	1.68	0.40
25:Q:91:LEU:HD12	25:Q:91:LEU:HA	1.89	0.40
9:a:19:LEU:CD2	9:a:213:GLN:HG3	2.51	0.40
9:a:429:GLU:OE2	15:g:7:LEU:HB2	2.21	0.40
17:i:62:ARG:HB2	17:i:78:TYR:CG	2.56	0.40
1:1:429:ARG:HA	1:1:430:PRO:HD2	1.92	0.40
2:2:163:LEU:HA	2:2:166:ILE:CD1	2.52	0.40
3:3:469:ARG:HG2	3:3:754:PRO:CG	2.52	0.40
4:4:64:THR:HB	4:4:66:PHE:CE1	2.57	0.40
4:4:224:ILE:HA	4:4:225:PRO:HD2	1.87	0.40
4:4:348:SER:C	4:4:350:ARG:N	2.80	0.40
5:5:2:ARG:HB2	5:5:84:ASP:OD2	2.21	0.40
6:6:16:ARG:NH1	6:6:17:GLU:OE2	2.54	0.40
8:8:177:THR:C	8:8:179:GLY:N	2.79	0.40
9:A:288:ALA:HB2	9:A:300:THR:HG22	2.02	0.40
10:B:254:HIS:O	10:B:426:ALA:HA	2.21	0.40
17:I:62:ARG:NH2	52:I:1591:HOH:O	2.54	0.40
20:L:23:GLY:HA3	20:L:73:ILE:HG13	2.03	0.40
21:M:168:LEU:HD13	21:M:184:LEU:HG	2.03	0.40
24:P:79:LYS:H	24:P:79:LYS:HD3	1.87	0.40
25:Q:10:GLU:HG2	25:Q:25:ARG:HH22	1.86	0.40
25:Q:77:GLY:O	25:Q:90:LYS:NZ	2.54	0.40
26:R:15:THR:O	26:R:19:LEU:HG	2.22	0.40
27:S:84:LYS:HD2	27:S:84:LYS:HA	1.83	0.40
11:c:12:LYS:HG3	11:c:13:ILE:N	2.37	0.40
11:c:233:LEU:HD11	12:d:219:VAL:HG21	2.03	0.40
11:c:237:LEU:HD13	12:d:212:MET:HG3	2.03	0.40
17:i:70:LEU:HB3	52:i:1017:HOH:O	2.22	0.40
1:1:436:LEU:HD23	2:2:90:LEU:HA	2.03	0.40
3:3:274:LEU:HA	3:3:274:LEU:HD12	1.82	0.40
3:3:688:ARG:CB	3:3:770:ARG:HD3	2.51	0.40
4:4:230:ILE:O	4:4:230:ILE:CG2	2.67	0.40
5:5:103:THR:HG21	5:5:128:GLY:C	2.46	0.40
6:6:115:GLY:HA3	6:6:125:GLN:CD	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:108:CYS:HA	8:8:109:PRO:HD2	1.78	0.40
16:H:41:ASP:O	16:H:45:SER:CB	2.70	0.40
20:L:34:SER:HB3	20:L:61:HIS:CE1	2.57	0.40
20:L:461:SER:O	20:L:465:VAL:HG13	2.21	0.40
22:N:40:MET:O	22:N:41:THR:C	2.62	0.40
9:a:192:ALA:HB3	9:a:193:PRO:HD3	2.02	0.40
15:g:45:ILE:HG22	15:g:46:LEU:N	2.37	0.40
15:g:71:ARG:NH1	15:g:72:LYS:HZ2	2.17	0.40
34:m:419:UNK:C	34:m:421:UNK:N	2.85	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	1	435/438 (99%)	380 (87%)	48 (11%)	7 (2%)	7	38
2	2	177/181 (98%)	151 (85%)	22 (12%)	4 (2%)	5	28
3	3	748/783 (96%)	624 (83%)	101 (14%)	23 (3%)	3	22
4	4	374/409 (91%)	331 (88%)	34 (9%)	9 (2%)	4	27
5	5	194/207 (94%)	166 (86%)	24 (12%)	4 (2%)	5	30
6	6	140/181 (77%)	114 (81%)	21 (15%)	5 (4%)	2	20
7	7	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	16	54
8	8	152/182 (84%)	129 (85%)	22 (14%)	1 (1%)	18	56
9	A	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	24	63
9	a	441/446 (99%)	424 (96%)	16 (4%)	1 (0%)	43	78
10	B	418/439 (95%)	409 (98%)	8 (2%)	1 (0%)	43	78
10	b	420/439 (96%)	406 (97%)	12 (3%)	2 (0%)	24	63
11	C	363/379 (96%)	354 (98%)	6 (2%)	3 (1%)	16	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	c	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	9	40
12	D	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
12	d	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
13	E	194/196 (99%)	183 (94%)	7 (4%)	4 (2%)	5	30
13	e	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	24	63
14	F	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
14	f	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
15	G	73/81 (90%)	72 (99%)	1 (1%)	0	100	100
15	g	74/81 (91%)	69 (93%)	4 (5%)	1 (1%)	9	40
16	H	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
16	h	64/78 (82%)	62 (97%)	1 (2%)	1 (2%)	7	38
17	I	38/65 (58%)	36 (95%)	1 (3%)	1 (3%)	4	25
17	i	38/65 (58%)	36 (95%)	1 (3%)	1 (3%)	4	25
18	J	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	36
18	j	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	36
19	K	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	1	16
19	k	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0	7
20	L	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	54
21	M	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
22	N	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
23	O	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
24	P	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
25	Q	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	17
26	R	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	13
27	S	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9	40
28	T	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
29	U	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	2	20
30	V	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
31	W	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
32	X	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
33	Y	109/104 (105%)	106 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8228/8726 (94%)	7616 (93%)	511 (6%)	101 (1%)	13 44

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
2	2	108	PRO
3	3	6	VAL
3	3	117	LEU
3	3	216	PHE
3	3	367	PRO
3	3	509	ALA
4	4	212	PRO
4	4	255	SER
5	5	81	LYS
7	7	87	PRO
9	A	224	ASP
11	C	16	ASN
11	C	17	ALA
17	I	41	PRO
18	J	61	ASN
20	L	328	HIS
20	L	508	PRO
25	Q	2	SER
25	Q	87	THR
25	Q	95	GLN
26	R	4	ALA
26	R	9	GLY
27	S	46	LYS
29	U	2	GLU
9	a	224	ASP
11	c	17	ALA
15	g	72	LYS
17	i	41	PRO
18	j	61	ASN
1	1	360	ARG
2	2	86	LEU
2	2	124	CYS
3	3	31	PRO
3	3	32	LEU
3	3	125	GLY
3	3	164	VAL

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Mol	Chain	Res	Type
3	3	263	CYS
3	3	453	PRO
3	3	554	LYS
4	4	51	GLU
4	4	258	GLU
5	5	83	GLY
6	6	45	CYS
8	8	152	ARG
10	B	171	ALA
13	E	112	VAL
26	R	5	LYS
10	b	171	ALA
10	b	231	GLY
11	c	16	ASN
16	h	48	SER
1	1	71	PRO
2	2	76	GLY
3	3	28	TYR
3	3	271	SER
3	3	285	VAL
3	3	365	LYS
3	3	374	ARG
3	3	690	GLY
4	4	214	PHE
4	4	389	GLN
6	6	98	GLN
6	6	126	ASN
21	M	104	TRP
26	R	61	SER
13	e	189	SER
19	k	33	VAL
1	1	313	TYR
3	3	682	GLU
3	3	730	GLU
4	4	268	GLU
4	4	270	GLY
6	6	77	VAL
20	L	51	ASP
3	3	203	ILE
3	3	455	ARG
5	5	127	GLU
9	A	228	VAL

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Mol	Chain	Res	Type
11	C	18	PHE
13	E	189	SER
13	E	191	ASP
21	M	103	GLN
29	U	3	ASN
11	c	11	MET
19	k	34	SER
1	1	311	MET
4	4	390	VAL
6	6	20	LEU
20	L	91	ASP
21	M	158	ASP
26	R	49	PRO
11	c	18	PHE
1	1	202	LYS
5	5	52	ILE
13	E	82	PRO
1	1	3	GLY
11	c	13	ILE
25	Q	15	GLY
3	3	626	PRO
19	K	33	VAL

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	1	355/356 (100%)	316 (89%)	39 (11%)	6 20
2	2	150/152 (99%)	129 (86%)	21 (14%)	3 13
3	3	607/628 (97%)	553 (91%)	54 (9%)	9 28
4	4	326/355 (92%)	287 (88%)	39 (12%)	5 17
5	5	167/175 (95%)	151 (90%)	16 (10%)	8 25
6	6	117/149 (78%)	104 (89%)	13 (11%)	6 20
7	7	104/106 (98%)	99 (95%)	5 (5%)	23 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	8	126/150 (84%)	110 (87%)	16 (13%)	4	16
9	A	364/370 (98%)	358 (98%)	6 (2%)	55	70
9	a	364/370 (98%)	359 (99%)	5 (1%)	59	72
10	B	332/343 (97%)	332 (100%)	0	100	100
10	b	332/343 (97%)	330 (99%)	2 (1%)	78	83
11	C	312/327 (95%)	311 (100%)	1 (0%)	86	86
11	c	316/327 (97%)	313 (99%)	3 (1%)	70	79
12	D	206/206 (100%)	202 (98%)	4 (2%)	50	67
12	d	206/206 (100%)	202 (98%)	4 (2%)	50	67
13	E	168/168 (100%)	166 (99%)	2 (1%)	63	75
13	e	168/168 (100%)	164 (98%)	4 (2%)	43	64
14	F	90/98 (92%)	87 (97%)	3 (3%)	33	55
14	f	90/98 (92%)	87 (97%)	3 (3%)	33	55
15	G	66/71 (93%)	65 (98%)	1 (2%)	57	72
15	g	66/71 (93%)	64 (97%)	2 (3%)	36	57
16	H	63/74 (85%)	61 (97%)	2 (3%)	34	56
16	h	63/74 (85%)	62 (98%)	1 (2%)	55	70
17	I	28/51 (55%)	26 (93%)	2 (7%)	13	35
17	i	28/51 (55%)	25 (89%)	3 (11%)	6	21
18	J	51/52 (98%)	49 (96%)	2 (4%)	28	49
18	j	51/52 (98%)	49 (96%)	2 (4%)	28	49
19	K	15/46 (33%)	11 (73%)	4 (27%)	0	3
19	k	15/46 (33%)	10 (67%)	5 (33%)	0	2
20	L	427/427 (100%)	387 (91%)	40 (9%)	8	26
21	M	211/211 (100%)	191 (90%)	20 (10%)	8	25
22	N	226/226 (100%)	199 (88%)	27 (12%)	5	18
23	O	128/129 (99%)	118 (92%)	10 (8%)	11	32
24	P	95/95 (100%)	89 (94%)	6 (6%)	16	37
25	Q	81/81 (100%)	73 (90%)	8 (10%)	7	24
26	R	68/68 (100%)	52 (76%)	16 (24%)	1	5
27	S	67/75 (89%)	58 (87%)	9 (13%)	4	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	T	58/58 (100%)	51 (88%)	7 (12%)	5	17
29	U	47/50 (94%)	41 (87%)	6 (13%)	4	15
30	V	39/46 (85%)	36 (92%)	3 (8%)	12	32
31	W	40/40 (100%)	37 (92%)	3 (8%)	12	33
32	X	37/38 (97%)	34 (92%)	3 (8%)	11	31
33	Y	91/84 (108%)	91 (100%)	0	100	100
All	All	6961/7311 (95%)	6539 (94%)	422 (6%)	19	38

All (422) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	6	LEU
1	1	9	LEU
1	1	10	ASP
1	1	16	THR
1	1	29	LEU
1	1	49	THR
1	1	96	SER
1	1	102	LYS
1	1	104	ARG
1	1	114	LEU
1	1	128	THR
1	1	134	VAL
1	1	144	ARG
1	1	145	LEU
1	1	147	GLN
1	1	155	ARG
1	1	171	LEU
1	1	201	LEU
1	1	228	VAL
1	1	243	THR
1	1	253	GLN
1	1	255	SER
1	1	270	THR
1	1	287	ILE
1	1	290	ILE
1	1	323	LEU
1	1	329	ILE
1	1	337	MET
1	1	342	TRP

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Mol	Chain	Res	Type
1	1	363	VAL
1	1	368	VAL
1	1	370	LEU
1	1	374	ILE
1	1	397	ARG
1	1	398	SER
1	1	414	LEU
1	1	419	ASP
1	1	431	VAL
1	1	437	TRP
2	2	5	ASP
2	2	7	LYS
2	2	14	THR
2	2	33	ARG
2	2	35	GLN
2	2	46	ILE
2	2	56	THR
2	2	80	LEU
2	2	85	THR
2	2	106	ILE
2	2	110	GLU
2	2	114	ASP
2	2	119	VAL
2	2	128	CYS
2	2	150	LEU
2	2	153	LEU
2	2	163	LEU
2	2	172	CYS
2	2	176	VAL
2	2	178	GLU
2	2	179	VAL
3	3	20	MET
3	3	32	LEU
3	3	42	ILE
3	3	46	ARG
3	3	54	LEU
3	3	101	ARG
3	3	107	MET
3	3	117	LEU
3	3	124	LYS
3	3	133	ARG
3	3	142	LYS

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Mol	Chain	Res	Type
3	3	156	ARG
3	3	188	VAL
3	3	192	GLU
3	3	207	VAL
3	3	209	THR
3	3	218	LEU
3	3	232	VAL
3	3	261	VAL
3	3	265	ILE
3	3	275	LEU
3	3	282	VAL
3	3	284	GLU
3	3	290	ILE
3	3	303	GLN
3	3	305	ARG
3	3	317	LEU
3	3	337	ARG
3	3	381	LEU
3	3	408	ILE
3	3	417	VAL
3	3	440	ARG
3	3	450	LEU
3	3	460	LYS
3	3	464	ILE
3	3	473	GLU
3	3	492	LYS
3	3	507	LEU
3	3	512	LEU
3	3	515	THR
3	3	542	ARG
3	3	550	LEU
3	3	585	MET
3	3	617	LEU
3	3	655	ARG
3	3	676	LEU
3	3	683	LEU
3	3	684	ARG
3	3	716	LEU
3	3	747	VAL
3	3	761	SER
3	3	771	VAL
3	3	776	LEU

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Mol	Chain	Res	Type
3	3	777	VAL
4	4	41	LEU
4	4	44	MET
4	4	59	ILE
4	4	74	THR
4	4	76	LEU
4	4	79	ILE
4	4	99	LEU
4	4	105	LEU
4	4	109	VAL
4	4	116	ILE
4	4	120	LEU
4	4	123	LEU
4	4	138	LEU
4	4	152	GLU
4	4	156	ILE
4	4	163	VAL
4	4	166	GLN
4	4	168	PHE
4	4	170	HIS
4	4	182	LEU
4	4	193	LEU
4	4	194	LEU
4	4	199	HIS
4	4	201	ILE
4	4	221	VAL
4	4	234	LEU
4	4	239	LEU
4	4	262	PHE
4	4	272	VAL
4	4	294	LEU
4	4	314	ARG
4	4	316	LEU
4	4	319	THR
4	4	363	SER
4	4	367	ARG
4	4	371	ARG
4	4	385	CYS
4	4	396	ILE
4	4	407	VAL
5	5	1	MET
5	5	5	ARG

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Mol	Chain	Res	Type
5	5	25	LEU
5	5	27	VAL
5	5	32	GLU
5	5	47	ASN
5	5	84	ASP
5	5	90	VAL
5	5	91	ARG
5	5	100	ARG
5	5	103	THR
5	5	135	ILE
5	5	146	LEU
5	5	154	GLU
5	5	157	THR
5	5	175	THR
6	6	19	ILE
6	6	20	LEU
6	6	32	ARG
6	6	40	THR
6	6	45	CYS
6	6	78	MET
6	6	83	ARG
6	6	84	LEU
6	6	121	TYR
6	6	131	VAL
6	6	147	LEU
6	6	153	GLN
6	6	158	VAL
7	7	43	ARG
7	7	63	LEU
7	7	82	ILE
7	7	93	LEU
7	7	120	ASP
8	8	26	TYR
8	8	33	LEU
8	8	36	ARG
8	8	42	VAL
8	8	70	VAL
8	8	97	ARG
8	8	99	ILE
8	8	130	VAL
8	8	133	LYS
8	8	137	LEU

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Mol	Chain	Res	Type
8	8	138	VAL
8	8	139	ASP
8	8	157	VAL
8	8	158	LYS
8	8	159	VAL
8	8	163	VAL
9	A	51	LYS
9	A	149	VAL
9	A	203	LEU
9	A	245	GLU
9	A	281	ASP
9	A	308	GLN
11	C	222	PRO
12	D	17	LEU
12	D	43	MET
12	D	76	GLU
12	D	144	ARG
13	E	17	GLU
13	E	80	ASP
14	F	33	ARG
14	F	78	GLU
14	F	95	LYS
15	G	45	ILE
16	H	47	ARG
16	H	51	GLU
17	I	42	VAL
17	I	70	LEU
18	J	8	ARG
18	J	16	ARG
19	K	20	THR
19	K	23	LEU
19	K	27	VAL
19	K	36	THR
20	L	18	LEU
20	L	35	LEU
20	L	92	MET
20	L	96	ARG
20	L	105	LEU
20	L	115	SER
20	L	136	LEU
20	L	138	HIS
20	L	150	LEU

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Mol	Chain	Res	Type
20	L	158	ILE
20	L	159	LEU
20	L	187	SER
20	L	188	VAL
20	L	189	MET
20	L	194	LEU
20	L	199	LEU
20	L	213	ARG
20	L	241	PRO
20	L	273	MET
20	L	295	VAL
20	L	301	THR
20	L	306	THR
20	L	318	VAL
20	L	324	LEU
20	L	347	LEU
20	L	353	LEU
20	L	354	THR
20	L	365	ILE
20	L	369	ASP
20	L	373	VAL
20	L	383	MET
20	L	417	MET
20	L	444	PRO
20	L	465	VAL
20	L	467	LEU
20	L	474	GLU
20	L	492	LEU
20	L	508	PRO
20	L	509	THR
20	L	512	ASN
21	M	7	LEU
21	M	16	ILE
21	M	31	VAL
21	M	33	LEU
21	M	52	HIS
21	M	60	GLU
21	M	63	THR
21	M	67	ILE
21	M	88	ASP
21	M	92	ASN
21	M	125	THR

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Mol	Chain	Res	Type
21	M	130	PRO
21	M	134	ARG
21	M	142	VAL
21	M	147	GLU
21	M	170	LEU
21	M	171	LYS
21	M	185	MET
21	M	205	SER
21	M	216	LEU
22	N	1	MET
22	N	11	VAL
22	N	13	PRO
22	N	14	SER
22	N	18	LEU
22	N	19	THR
22	N	22	LEU
22	N	26	LEU
22	N	38	ASN
22	N	39	SER
22	N	85	LEU
22	N	92	LEU
22	N	112	LEU
22	N	127	LEU
22	N	128	GLU
22	N	131	LEU
22	N	132	LEU
22	N	137	LEU
22	N	142	VAL
22	N	160	LEU
22	N	163	LEU
22	N	188	ILE
22	N	196	THR
22	N	199	VAL
22	N	213	THR
22	N	222	GLN
22	N	230	ASN
23	O	9	GLU
23	O	27	VAL
23	O	31	LYS
23	O	36	SER
23	O	40	LEU
23	O	59	LEU

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Mol	Chain	Res	Type
23	O	62	LEU
23	O	107	ILE
23	O	143	ASN
23	O	147	LYS
24	P	7	THR
24	P	29	LEU
24	P	70	VAL
24	P	79	LYS
24	P	80	GLU
24	P	90	ARG
25	Q	6	VAL
25	Q	20	VAL
25	Q	37	LYS
25	Q	52	ILE
25	Q	53	THR
25	Q	74	LEU
25	Q	95	GLN
25	Q	98	HIS
26	R	5	LYS
26	R	7	ASP
26	R	8	HIS
26	R	14	ARG
26	R	17	ARG
26	R	33	LEU
26	R	34	ASN
26	R	37	LEU
26	R	41	HIS
26	R	42	ARG
26	R	43	GLU
26	R	48	ILE
26	R	54	ARG
26	R	56	ARG
26	R	68	THR
26	R	78	LEU
27	S	19	ARG
27	S	29	CYS
27	S	41	LYS
27	S	51	SER
27	S	53	CYS
27	S	57	ARG
27	S	60	TYR
27	S	67	SER

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Mol	Chain	Res	Type
27	S	75	ARG
28	T	2	THR
28	T	4	LEU
28	T	8	GLN
28	T	22	VAL
28	T	26	MET
28	T	44	LYS
28	T	64	ARG
29	U	2	GLU
29	U	5	VAL
29	U	8	LYS
29	U	16	ASN
29	U	23	LYS
29	U	27	THR
30	V	45	VAL
30	V	48	VAL
30	V	49	THR
31	W	15	VAL
31	W	22	LEU
31	W	26	THR
32	X	13	LYS
32	X	24	LEU
32	X	42	LYS
9	a	149	VAL
9	a	203	LEU
9	a	245	GLU
9	a	281	ASP
9	a	308	GLN
10	b	35	ILE
10	b	236	LYS
11	c	12	LYS
11	c	43	LEU
11	c	222	PRO
12	d	17	LEU
12	d	35	GLN
12	d	43	MET
12	d	144	ARG
13	e	17	GLU
13	e	113	GLU
13	e	128	LYS
13	e	190	ASP
14	f	33	ARG

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Mol	Chain	Res	Type
14	f	78	GLU
14	f	95	LYS
15	g	45	ILE
15	g	73	ASN
16	h	46	SER
17	i	42	VAL
17	i	52	ARG
17	i	70	LEU
18	j	16	ARG
18	j	25	VAL
19	k	20	THR
19	k	23	LEU
19	k	27	VAL
19	k	34	SER
19	k	36	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	87	HIS
1	1	161	ASN
1	1	219	ASN
1	1	220	ASN
1	1	240	GLN
1	1	369	ASN
2	2	137	ASN
3	3	303	GLN
3	3	613	HIS
3	3	757	HIS
4	4	93	HIS
4	4	171	ASN
4	4	199	HIS
4	4	292	GLN
4	4	327	HIS
4	4	330	HIS
5	5	47	ASN
6	6	161	GLN
7	7	92	HIS
8	8	94	ASN
9	A	15	GLN
9	A	61	HIS
9	A	136	GLN

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Mol	Chain	Res	Type
9	A	165	GLN
9	A	213	GLN
9	A	271	GLN
9	A	308	GLN
9	A	339	GLN
10	B	22	GLN
10	B	343	GLN
10	B	401	GLN
10	B	412	ASN
10	B	429	ASN
11	C	68	HIS
11	C	159	ASN
11	C	312	GLN
12	D	106	ASN
12	D	121	HIS
12	D	225	HIS
13	E	116	GLN
15	G	6	HIS
15	G	73	ASN
16	H	23	GLN
16	H	71	HIS
18	J	37	GLN
18	J	57	HIS
20	L	4	ASN
20	L	11	ASN
20	L	12	HIS
20	L	55	ASN
20	L	99	ASN
20	L	170	ASN
20	L	178	GLN
20	L	256	HIS
20	L	360	ASN
20	L	368	HIS
20	L	413	HIS
20	L	512	ASN
21	M	52	HIS
21	M	102	HIS
21	M	103	GLN
21	M	195	GLN
21	M	203	ASN
22	N	3	HIS
22	N	6	HIS

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Mol	Chain	Res	Type
22	N	12	ASN
22	N	133	ASN
22	N	148	HIS
22	N	158	HIS
22	N	204	HIS
22	N	207	HIS
22	N	222	GLN
22	N	232	HIS
23	O	109	HIS
24	P	34	ASN
25	Q	66	ASN
26	R	41	HIS
26	R	51	HIS
26	R	52	HIS
27	S	23	GLN
27	S	24	ASN
27	S	25	GLN
27	S	28	ASN
27	S	32	ASN
27	S	37	HIS
29	U	3	ASN
29	U	16	ASN
29	U	21	HIS
30	V	10	HIS
30	V	15	ASN
30	V	35	GLN
30	V	41	ASN
31	W	42	HIS
32	X	39	ASN
33	Y	54	ASN
33	Y	70	ASN
9	a	53	ASN
9	a	61	HIS
9	a	136	GLN
9	a	139	GLN
9	a	165	GLN
9	a	213	GLN
9	a	271	GLN
10	b	22	GLN
10	b	305	GLN
10	b	343	GLN
10	b	401	GLN

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Mol	Chain	Res	Type
10	b	412	ASN
10	b	429	ASN
11	c	68	HIS
11	c	159	ASN
12	d	106	ASN
12	d	121	HIS
12	d	225	HIS
13	e	149	ASN
14	f	73	GLN
15	g	28	HIS
16	h	23	GLN
17	i	71	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 12 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
38	SF4	3	784	3	0,12,12	-	-	-		
44	HEM	c	502	11	50,50,50	1.80	12 (24%)	66,82,82	1.43	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
42	FES	3	787	3	0,4,4	-	-	-		
44	HEM	C	501	11	50,50,50	1.74	8 (16%)	66,82,82	1.62	17 (25%)
49	HEA	L	515	20	66,67,67	1.10	3 (4%)	78,103,103	1.39	11 (14%)
48	CDL	g	3004	-	48,48,99	1.14	4 (8%)	54,60,111	1.10	2 (3%)
38	SF4	8	184	8	0,12,12	-	-	-		
49	HEA	L	516	20	66,67,67	1.21	7 (10%)	78,103,103	1.35	12 (15%)
38	SF4	8	183	8	0,12,12	-	-	-		
48	CDL	G	2003	-	49,49,99	1.09	3 (6%)	55,61,111	1.07	4 (7%)
48	CDL	G	2004	-	43,43,99	1.12	2 (4%)	49,55,111	1.20	4 (8%)
47	HEC	d	501	12	50,50,50	1.10	3 (6%)	68,82,82	1.26	6 (8%)
46	UQ1	c	3002	-	14,14,18	2.05	8 (57%)	18,20,25	0.40	0
39	FMN	1	440	-	33,33,33	1.24	2 (6%)	48,50,50	1.84	12 (25%)
48	CDL	d	3003	-	49,49,99	1.08	5 (10%)	55,61,111	1.14	4 (7%)
44	HEM	C	502	11	50,50,50	1.59	8 (16%)	66,82,82	1.49	12 (18%)
38	SF4	1	439	1	0,12,12	-	-	-		
44	HEM	Y	500	33	50,50,50	1.66	11 (22%)	66,82,82	1.51	8 (12%)
40	NAI	1	441	-	45,48,48	3.80	31 (68%)	60,73,73	1.78	13 (21%)
38	SF4	3	785	3	0,12,12	-	-	-		
42	FES	E	501	13	0,4,4	-	-	-		
46	UQ1	C	2002	-	14,14,18	2.25	8 (57%)	18,20,25	0.53	0
45	SMA	C	2001	-	38,38,38	1.41	7 (18%)	48,52,52	1.09	4 (8%)
42	FES	e	501	13	0,4,4	-	-	-		
42	FES	2	182	2	0,4,4	-	-	-		
47	HEC	D	501	12	50,50,50	1.01	2 (4%)	68,82,82	1.27	7 (10%)
44	HEM	c	501	11	50,50,50	1.62	6 (12%)	66,82,82	1.27	8 (12%)
38	SF4	6	182	6	0,12,12	-	-	-		
38	SF4	3	786	3	0,12,12	-	-	-		
45	SMA	c	3001	-	38,38,38	1.55	9 (23%)	48,52,52	1.12	4 (8%)

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
38	SF4	3	784	3	-	-	0/6/5/5
44	HEM	c	502	11	-	4/14/54/54	-
44	HEM	C	501	11	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	HEA	L	515	20	-	8/36/76/76	-
42	FES	3	787	3	-	-	0/1/1/1
48	CDL	g	3004	-	-	21/57/57/110	-
38	SF4	8	184	8	-	-	0/6/5/5
49	HEA	L	516	20	-	7/36/76/76	-
38	SF4	8	183	8	-	-	0/6/5/5
48	CDL	G	2003	-	-	26/58/58/110	-
48	CDL	G	2004	-	-	34/52/52/110	-
47	HEC	d	501	12	1/1/3/7	8/14/54/54	-
46	UQ1	c	3002	-	-	2/4/28/33	0/1/1/1
39	FMN	1	440	-	-	6/18/18/18	0/3/3/3
48	CDL	d	3003	-	-	37/58/58/110	-
44	HEM	C	502	11	-	4/14/54/54	-
38	SF4	1	439	1	-	-	0/6/5/5
44	HEM	Y	500	33	-	4/14/54/54	-
40	NAI	1	441	-	-	7/29/72/72	0/5/5/5
38	SF4	3	785	3	-	-	0/6/5/5
42	FES	E	501	13	-	-	0/1/1/1
46	UQ1	C	2002	-	-	0/4/28/33	0/1/1/1
45	SMA	C	2001	-	-	2/34/34/34	0/2/2/2
42	FES	2	182	2	-	-	0/1/1/1
47	HEC	D	501	12	1/1/3/7	7/14/54/54	-
42	FES	e	501	13	-	-	0/1/1/1
44	HEM	c	501	11	-	4/14/54/54	-
38	SF4	6	182	6	-	-	0/6/5/5
38	SF4	3	786	3	-	-	0/6/5/5
45	SMA	c	3001	-	-	2/34/34/34	0/2/2/2

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	441	NAI	C2A-N1A	11.40	1.55	1.33
40	1	441	NAI	C5A-N7A	7.21	1.52	1.39
40	1	441	NAI	C8A-N9A	7.06	1.50	1.37
40	1	441	NAI	C3D-C4D	-5.77	1.38	1.53
40	1	441	NAI	C2B-C3B	-5.61	1.38	1.53
44	c	502	HEM	CBB-CAB	5.40	1.57	1.30
40	1	441	NAI	C6A-N6A	5.32	1.47	1.34
44	c	501	HEM	CBB-CAB	5.30	1.56	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	441	NAI	C3B-C4B	-5.26	1.39	1.53
40	1	441	NAI	C2D-C1D	-5.08	1.37	1.53
40	1	441	NAI	C5A-C6A	5.03	1.55	1.41
44	C	501	HEM	CBB-CAB	4.89	1.54	1.30
44	C	501	HEM	CBC-CAC	4.79	1.54	1.30
44	C	502	HEM	CBB-CAB	4.74	1.53	1.30
44	C	502	HEM	CBC-CAC	4.67	1.53	1.30
40	1	441	NAI	C2B-C1B	-4.58	1.38	1.53
44	c	502	HEM	CBC-CAC	4.48	1.52	1.30
40	1	441	NAI	C7N-N7N	4.47	1.45	1.33
44	c	501	HEM	CBC-CAC	4.37	1.52	1.30
39	1	440	FMN	C4A-N5	4.19	1.38	1.30
40	1	441	NAI	PA-O1A	4.16	1.65	1.50
40	1	441	NAI	C6A-N1A	-4.11	1.23	1.35
44	c	501	HEM	CAB-C3B	-4.10	1.36	1.47
44	C	501	HEM	CAC-C3C	-4.09	1.36	1.47
40	1	441	NAI	PN-O2N	4.05	1.65	1.50
40	1	441	NAI	C7N-C3N	3.94	1.57	1.48
40	1	441	NAI	C4A-N9A	3.89	1.46	1.37
44	Y	500	HEM	C3B-C2B	3.83	1.45	1.37
44	c	501	HEM	CAC-C3C	-3.73	1.37	1.47
49	L	516	HEA	CMA-C3A	-3.72	1.37	1.45
44	C	502	HEM	CAC-C3C	-3.71	1.37	1.47
44	Y	500	HEM	CAC-C3C	-3.71	1.37	1.47
44	c	502	HEM	CAB-C3B	-3.66	1.37	1.47
47	d	501	HEC	C4B-C3B	3.65	1.51	1.45
45	c	3001	SMA	C6-C5	3.64	1.45	1.38
44	c	502	HEM	CAC-C3C	-3.64	1.37	1.47
40	1	441	NAI	C4N-C5N	3.60	1.58	1.48
44	Y	500	HEM	C1B-NB	-3.52	1.34	1.40
44	C	501	HEM	CAB-C3B	-3.42	1.38	1.47
44	C	501	HEM	C4D-C3D	3.34	1.50	1.45
45	C	2001	SMA	C4A-C5	3.28	1.46	1.40
45	c	3001	SMA	O1-C2	3.27	1.40	1.36
40	1	441	NAI	C2D-C3D	-3.25	1.44	1.53
40	1	441	NAI	O4D-C4D	-3.23	1.37	1.45
46	C	2002	UQ1	O3-C3	3.20	1.44	1.36
44	Y	500	HEM	C3B-C4B	-3.17	1.38	1.44
45	c	3001	SMA	C6-C7	3.13	1.44	1.38
46	C	2002	UQ1	C3-C4	3.03	1.57	1.48
40	1	441	NAI	O4B-C4B	-3.02	1.38	1.45
46	C	2002	UQ1	C2-C1	3.01	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	2001	SMA	C6-C7	3.01	1.44	1.38
46	C	2002	UQ1	C7-C6	2.98	1.57	1.50
46	c	3002	UQ1	C7-C6	2.98	1.57	1.50
45	C	2001	SMA	C7-C8	2.95	1.44	1.40
46	C	2002	UQ1	O2-C2	2.91	1.44	1.36
45	c	3001	SMA	C4A-C5	2.90	1.45	1.40
45	C	2001	SMA	C6-C5	2.89	1.44	1.38
44	Y	500	HEM	C3C-C4C	2.89	1.51	1.46
49	L	516	HEA	FE-NA	2.88	2.04	1.95
46	C	2002	UQ1	CM5-C5	2.86	1.56	1.50
44	C	502	HEM	FE-NB	2.84	2.03	1.94
39	1	440	FMN	C9A-N10	-2.82	1.36	1.41
44	c	502	HEM	CMC-C2C	2.81	1.56	1.50
46	c	3002	UQ1	CM5-C5	2.80	1.56	1.50
44	Y	500	HEM	C4C-NC	-2.77	1.34	1.39
49	L	515	HEA	CMA-C3A	-2.72	1.39	1.45
44	Y	500	HEM	CHB-C4A	-2.72	1.33	1.39
45	c	3001	SMA	C20-C19	2.68	1.35	1.33
45	c	3001	SMA	C7-C8	2.67	1.43	1.40
44	c	501	HEM	C4D-C3D	2.66	1.49	1.45
49	L	516	HEA	C1D-C2D	2.65	1.49	1.44
49	L	516	HEA	C1D-ND	-2.65	1.35	1.40
40	1	441	NAI	C1D-N1N	-2.64	1.38	1.46
49	L	515	HEA	C1A-C2A	-2.62	1.40	1.45
48	G	2004	CDL	O1-C1	2.61	1.51	1.43
46	c	3002	UQ1	C2-C1	2.60	1.56	1.48
49	L	516	HEA	C3A-C2A	-2.60	1.31	1.36
40	1	441	NAI	O3B-C3B	-2.57	1.36	1.43
46	c	3002	UQ1	O2-C2	2.55	1.43	1.36
44	c	502	HEM	C1B-C2B	2.53	1.49	1.44
46	c	3002	UQ1	O3-C3	2.53	1.43	1.36
40	1	441	NAI	O4D-C1D	-2.52	1.36	1.42
44	C	502	HEM	C3B-C4B	2.48	1.49	1.44
45	c	3001	SMA	C3-C2	2.48	1.39	1.34
46	c	3002	UQ1	C6-C1	2.48	1.56	1.47
40	1	441	NAI	PN-O1N	-2.47	1.43	1.55
48	g	3004	CDL	O1-C1	2.47	1.50	1.43
44	C	501	HEM	C1A-C2A	2.45	1.49	1.44
44	c	502	HEM	CHC-C1C	-2.45	1.33	1.38
48	g	3004	CDL	OA8-CA6	-2.44	1.39	1.45
44	C	502	HEM	C1D-C2D	2.43	1.49	1.44
44	C	501	HEM	C4C-NC	-2.43	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	441	NAI	PN-O5D	2.42	1.69	1.59
44	c	502	HEM	C3C-C2C	2.42	1.42	1.37
46	C	2002	UQ1	C6-C1	2.40	1.55	1.47
40	1	441	NAI	O4B-C1B	-2.39	1.36	1.42
44	c	502	HEM	C4A-C3A	2.39	1.48	1.43
44	c	502	HEM	C1A-C2A	2.38	1.49	1.44
49	L	515	HEA	C3A-C4A	-2.37	1.41	1.46
46	c	3002	UQ1	C3-C4	2.37	1.55	1.48
46	c	3002	UQ1	C5-C4	2.36	1.55	1.47
49	L	516	HEA	CMD-C2D	2.34	1.55	1.50
48	g	3004	CDL	OB8-CB6	-2.33	1.39	1.45
45	C	2001	SMA	C3-C2	2.32	1.39	1.34
46	C	2002	UQ1	C5-C4	2.32	1.55	1.47
48	g	3004	CDL	CA3-CA4	2.31	1.57	1.50
44	c	501	HEM	C4A-C3A	2.31	1.48	1.43
44	C	502	HEM	C4D-C3D	2.30	1.49	1.45
44	Y	500	HEM	C1D-C2D	2.30	1.49	1.44
45	C	2001	SMA	C20-C19	2.29	1.35	1.33
44	c	502	HEM	C1D-C2D	2.28	1.49	1.44
40	1	441	NAI	C4A-N3A	2.28	1.38	1.34
48	d	3003	CDL	O1-C1	2.27	1.50	1.43
48	G	2003	CDL	O1-C1	2.25	1.50	1.43
40	1	441	NAI	O2B-C2B	-2.25	1.37	1.43
40	1	441	NAI	PA-O2A	-2.20	1.45	1.55
47	D	501	HEC	C4C-C3C	2.20	1.49	1.44
44	Y	500	HEM	CHD-C4C	-2.19	1.34	1.38
44	c	502	HEM	FE-NC	2.19	2.02	1.95
44	Y	500	HEM	C3C-C2C	2.19	1.41	1.37
45	C	2001	SMA	O1-C2	2.15	1.39	1.36
45	c	3001	SMA	C4A-C4	2.14	1.52	1.46
40	1	441	NAI	C4N-C3N	2.13	1.54	1.49
40	1	441	NAI	C8A-N7A	2.13	1.35	1.31
44	C	501	HEM	C1C-C2C	2.12	1.49	1.45
45	c	3001	SMA	C8-C8A	2.10	1.42	1.39
47	d	501	HEC	C1C-C2C	2.08	1.48	1.43
48	G	2003	CDL	CA3-CA4	2.07	1.57	1.50
48	G	2004	CDL	OA8-CA6	-2.06	1.40	1.45
49	L	516	HEA	FE-NC	2.05	2.02	1.95
48	d	3003	CDL	CB3-CB4	2.05	1.57	1.50
48	d	3003	CDL	OA8-CA6	-2.05	1.40	1.45
48	d	3003	CDL	OB8-CB6	-2.05	1.40	1.45
47	d	501	HEC	C1C-NC	-2.03	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	Y	500	HEM	C4D-C3D	2.02	1.48	1.45
44	C	502	HEM	FE-ND	2.02	2.01	1.94
48	d	3003	CDL	OB2-CB2	-2.01	1.37	1.44
47	D	501	HEC	C1A-C2A	2.01	1.48	1.45
48	G	2003	CDL	OB8-CB6	-2.00	1.40	1.45

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	1	440	FMN	C5'-C4'-C3'	-5.12	102.31	112.20
39	1	440	FMN	O2'-C2'-C3'	5.10	121.51	109.10
40	1	441	NAI	N3A-C2A-N1A	-4.74	121.19	128.60
45	c	3001	SMA	C9-C10-C11	-4.72	105.90	114.52
44	C	502	HEM	C4B-C3B-C2B	-4.69	103.39	107.11
40	1	441	NAI	C5A-C4A-N3A	-4.59	120.77	126.75
44	Y	500	HEM	C4C-C3C-C2C	-4.48	103.07	106.75
48	G	2004	CDL	CB4-OB6-CB5	-4.32	109.85	117.90
44	C	501	HEM	C2D-C1D-ND	4.29	115.02	109.88
45	C	2001	SMA	C9-C10-C11	-4.26	106.74	114.52
44	Y	500	HEM	C3B-C2B-C1B	-4.25	103.33	106.49
47	D	501	HEC	CAB-C3B-C4B	-4.03	119.58	124.81
49	L	515	HEA	C17-C18-C19	-3.98	118.07	127.66
44	c	502	HEM	CHC-C1C-NC	-3.91	120.21	124.44
44	C	502	HEM	CHD-C1D-ND	-3.89	120.19	124.42
40	1	441	NAI	C4D-O4D-C1D	-3.85	100.98	109.47
48	d	3003	CDL	CB4-OB6-CB5	-3.83	110.77	117.90
47	d	501	HEC	CAC-C3C-C2C	3.80	132.94	126.86
48	g	3004	CDL	CA4-OA6-CA5	-3.79	110.84	117.90
44	C	502	HEM	CHC-C4B-NB	-3.65	120.45	124.42
40	1	441	NAI	N9A-C8A-N7A	-3.60	108.99	113.91
44	C	501	HEM	CHD-C1D-ND	-3.60	120.51	124.42
47	D	501	HEC	CAC-C3C-C2C	3.58	132.60	126.86
48	G	2003	CDL	CA4-OA6-CA5	-3.56	111.26	117.90
44	c	501	HEM	CHC-C1C-NC	-3.50	120.65	124.44
39	1	440	FMN	C1'-C2'-C3'	-3.45	100.13	109.79
47	d	501	HEC	CHC-C4B-NB	-3.43	120.14	124.37
44	C	501	HEM	C4A-C3A-C2A	-3.37	102.89	106.83
44	C	502	HEM	C1B-NB-C4B	-3.36	101.60	105.07
44	c	502	HEM	C4A-NA-C1A	-3.29	102.13	105.35
49	L	516	HEA	CHA-C1A-NA	-3.21	120.96	124.44
49	L	515	HEA	C13-C14-C15	-3.19	119.98	127.66
40	1	441	NAI	C5A-N7A-C8A	3.18	108.03	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	440	FMN	C4'-C3'-C2'	3.17	119.96	113.36
44	C	501	HEM	C4D-ND-C1D	-3.17	101.80	105.07
40	1	441	NAI	C2A-N3A-C4A	3.17	119.24	111.75
39	1	440	FMN	O4-C4-C4A	-3.14	118.28	126.60
44	Y	500	HEM	CAD-CBD-CGD	3.13	120.33	113.60
44	Y	500	HEM	C2B-C1B-NB	3.12	113.54	109.84
44	c	502	HEM	C2A-C1A-NA	3.08	113.59	110.15
44	c	501	HEM	C4C-NC-C1C	-3.07	102.34	105.35
44	Y	500	HEM	CBD-CAD-C3D	-3.07	104.11	112.63
44	C	501	HEM	CMA-C3A-C4A	3.06	130.03	125.37
40	1	441	NAI	O4D-C1D-N1N	3.05	114.02	108.06
40	1	441	NAI	C5A-C4A-N9A	3.04	109.32	105.78
44	c	502	HEM	CHD-C4C-NC	-3.03	121.16	124.44
44	C	502	HEM	CBD-CAD-C3D	-3.01	104.26	112.63
48	g	3004	CDL	CB4-OB6-CB5	-3.00	110.42	117.79
39	1	440	FMN	C4-N3-C2	-2.92	120.24	125.64
44	C	501	HEM	C4B-C3B-C2B	-2.91	104.81	107.11
48	d	3003	CDL	CA6-CA4-CA3	-2.91	104.92	111.79
44	C	501	HEM	CHD-C4C-C3C	-2.88	120.34	125.26
44	c	502	HEM	C4C-NC-C1C	-2.88	102.53	105.35
44	C	501	HEM	C1D-C2D-C3D	-2.85	103.96	106.96
40	1	441	NAI	O5B-C5B-C4B	2.85	118.80	108.99
40	1	441	NAI	C3N-C7N-N7N	2.83	122.70	117.67
45	c	3001	SMA	C4A-C4-C3	-2.83	114.62	118.79
49	L	515	HEA	C1B-C2B-C3B	2.80	110.16	106.80
48	G	2004	CDL	CA6-CA4-CA3	-2.72	105.34	111.79
49	L	516	HEA	C4A-C3A-C2A	2.71	108.98	106.75
44	c	501	HEM	C4A-NA-C1A	-2.70	102.70	105.35
48	G	2003	CDL	CB4-OB6-CB5	-2.70	111.14	117.79
45	C	2001	SMA	C4A-C4-C3	-2.65	114.89	118.79
44	C	502	HEM	C4D-ND-C1D	-2.65	102.34	105.07
44	Y	500	HEM	CBC-CAC-C3C	2.63	140.73	127.62
48	d	3003	CDL	CA4-OA6-CA5	-2.58	111.43	117.79
44	C	502	HEM	CHB-C1B-NB	-2.58	121.20	124.37
44	C	502	HEM	C2D-C1D-ND	2.57	112.97	109.88
44	c	502	HEM	CMD-C2D-C1D	2.57	128.96	125.04
44	c	502	HEM	CMA-C3A-C4A	-2.56	121.47	125.37
49	L	516	HEA	CMD-C2D-C1D	2.56	128.94	125.04
47	d	501	HEC	CAB-C3B-C2B	2.49	131.79	127.53
47	D	501	HEC	CAC-C3C-C4C	-2.49	121.46	124.92
39	1	440	FMN	O2-C2-N1	-2.45	117.77	121.83
39	1	440	FMN	C10-C4A-N5	-2.44	119.68	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	L	515	HEA	C3C-C4C-NC	2.43	111.74	110.25
49	L	515	HEA	C17-C16-C15	-2.41	105.06	112.98
49	L	516	HEA	C1D-C2D-C3D	-2.40	104.44	106.96
44	C	502	HEM	C2B-C1B-NB	2.39	112.68	109.84
49	L	516	HEA	CAA-C2A-C1A	2.39	129.40	124.89
44	C	501	HEM	C3C-C2C-C1C	-2.39	104.80	107.08
40	1	441	NAI	C4A-C5A-N7A	-2.38	107.72	110.62
44	C	501	HEM	C3A-C4A-NA	2.38	113.70	110.08
48	G	2003	CDL	CB6-CB4-CB3	-2.37	106.19	111.79
49	L	515	HEA	C20-C19-C18	2.36	125.89	121.12
49	L	515	HEA	C16-C17-C18	-2.34	104.19	111.88
49	L	515	HEA	CAD-C3D-C4D	2.33	128.73	124.66
49	L	516	HEA	C25-C23-C24	2.32	119.73	114.60
47	d	501	HEC	CAC-C3C-C4C	-2.31	121.71	124.92
47	D	501	HEC	CAB-C3B-C2B	2.31	131.47	127.53
39	1	440	FMN	C4A-C4-N3	2.30	119.02	113.19
49	L	516	HEA	CMB-C2B-C3B	-2.29	125.98	130.34
49	L	516	HEA	C13-C14-C15	-2.28	122.17	127.66
44	c	502	HEM	CMA-C3A-C2A	2.28	130.53	125.61
44	C	501	HEM	CHA-C4D-ND	-2.27	121.57	124.37
45	c	3001	SMA	O1-C2-C9	-2.26	105.80	110.58
39	1	440	FMN	C1'-N10-C9A	-2.25	116.77	120.51
44	c	501	HEM	CMD-C2D-C1D	2.24	128.45	125.04
44	c	501	HEM	CAD-C3D-C4D	2.22	128.53	124.66
47	d	501	HEC	C1D-ND-C4D	-2.21	102.79	105.07
44	c	501	HEM	CHD-C4C-NC	-2.20	122.06	124.44
48	d	3003	CDL	CB6-OB8-CB7	-2.20	111.57	117.10
48	G	2004	CDL	CA4-OA6-CA5	-2.20	112.38	117.79
49	L	516	HEA	C26-C15-C16	2.20	118.97	115.27
44	C	501	HEM	C1A-C2A-C3A	2.19	110.34	106.89
40	1	441	NAI	C6A-C5A-C4A	2.19	120.12	117.18
44	C	502	HEM	CHA-C4D-ND	-2.18	121.68	124.37
44	C	501	HEM	CMC-C2C-C1C	2.17	128.54	124.71
49	L	515	HEA	C12-C13-C14	-2.16	106.54	112.23
44	C	502	HEM	CHB-C4A-C3A	-2.15	121.18	127.24
44	C	501	HEM	C3B-C2B-C1B	2.14	108.08	106.49
47	D	501	HEC	C3A-C4A-NA	2.14	113.63	109.69
49	L	515	HEA	C4B-C3B-C2B	-2.13	103.78	107.41
49	L	516	HEA	C3C-C4C-NC	2.12	111.56	110.25
39	1	440	FMN	C4A-C10-N10	2.12	119.58	116.48
49	L	516	HEA	C3A-C2A-C1A	-2.10	105.07	107.08
44	c	501	HEM	CAC-C3C-C4C	-2.10	119.82	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	Y	500	HEM	C1D-C2D-C3D	-2.10	104.75	106.96
44	C	501	HEM	CHD-C4C-NC	2.10	126.71	124.44
39	1	440	FMN	O5'-C5'-C4'	2.10	114.96	109.36
48	G	2003	CDL	CA6-OA8-CA7	-2.09	111.85	117.10
44	c	502	HEM	CAD-C3D-C4D	2.09	128.31	124.66
48	G	2004	CDL	CB6-CB4-CB3	-2.09	106.85	111.79
47	D	501	HEC	C2B-C1B-NB	2.08	112.38	109.88
44	C	502	HEM	CMA-C3A-C2A	2.08	130.11	125.61
45	c	3001	SMA	C9-C2-C3	2.07	130.11	127.07
44	c	502	HEM	C1A-C2A-C3A	-2.07	103.63	106.89
47	d	501	HEC	CHC-C4B-C3B	2.06	129.20	125.33
49	L	515	HEA	C27-C19-C18	-2.06	118.39	123.68
45	C	2001	SMA	C9-C2-C3	2.05	130.08	127.07
45	C	2001	SMA	O1-C2-C9	-2.05	106.23	110.58
49	L	516	HEA	CBD-CAD-C3D	2.05	118.32	112.63
44	Y	500	HEM	O2A-CGA-CBA	2.04	120.57	114.03
40	1	441	NAI	O7N-C7N-N7N	-2.03	118.13	122.88
44	C	501	HEM	CAA-C2A-C3A	-2.01	122.46	127.07
44	c	501	HEM	C4A-C3A-C2A	-2.01	104.48	106.83
47	D	501	HEC	CMB-C2B-C1B	2.01	128.10	125.04
44	C	501	HEM	CHC-C4B-NB	-2.00	122.24	124.42

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
47	D	501	HEC	NA
47	d	501	HEC	NA

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	1	440	FMN	N10-C1'-C2'-O2'
39	1	440	FMN	N10-C1'-C2'-C3'
39	1	440	FMN	C1'-C2'-C3'-O3'
39	1	440	FMN	C1'-C2'-C3'-C4'
40	1	441	NAI	O4B-C4B-C5B-O5B
40	1	441	NAI	C3B-C4B-C5B-O5B
40	1	441	NAI	C5D-O5D-PN-O3
45	C	2001	SMA	C3-C2-C9-C10
45	C	2001	SMA	O1-C2-C9-C10
45	c	3001	SMA	C3-C2-C9-C10
45	c	3001	SMA	O1-C2-C9-C10

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Mol	Chain	Res	Type	Atoms
48	G	2003	CDL	OA7-CA5-OA6-CA4
48	G	2003	CDL	C11-CA5-OA6-CA4
48	G	2003	CDL	CB2-OB2-PB2-OB3
48	G	2003	CDL	OB5-CB3-CB4-OB6
48	G	2004	CDL	CA2-C1-CB2-OB2
48	G	2004	CDL	CA2-OA2-PA1-OA3
48	G	2004	CDL	CA2-OA2-PA1-OA4
48	G	2004	CDL	CA3-OA5-PA1-OA3
48	G	2004	CDL	CA3-OA5-PA1-OA4
48	G	2004	CDL	OA7-CA5-OA6-CA4
48	G	2004	CDL	CB3-OB5-PB2-OB3
48	G	2004	CDL	CB3-OB5-PB2-OB4
48	G	2004	CDL	C51-CB5-OB6-CB4
48	d	3003	CDL	CA2-OA2-PA1-OA3
48	d	3003	CDL	CA2-OA2-PA1-OA4
48	d	3003	CDL	CA2-OA2-PA1-OA5
48	d	3003	CDL	CA3-OA5-PA1-OA2
48	d	3003	CDL	CA3-OA5-PA1-OA3
48	d	3003	CDL	CA3-OA5-PA1-OA4
48	d	3003	CDL	OA6-CA4-CA6-OA8
48	d	3003	CDL	CB2-OB2-PB2-OB3
48	d	3003	CDL	CB2-OB2-PB2-OB4
48	d	3003	CDL	CB2-OB2-PB2-OB5
48	d	3003	CDL	CB3-OB5-PB2-OB3
48	g	3004	CDL	CB2-C1-CA2-OA2
48	g	3004	CDL	CA2-OA2-PA1-OA3
48	g	3004	CDL	CA2-OA2-PA1-OA4
49	L	515	HEA	C2A-C3A-CMA-OMA
49	L	515	HEA	C4A-C3A-CMA-OMA
49	L	515	HEA	C12-C11-C3B-C2B
49	L	516	HEA	C2A-C3A-CMA-OMA
49	L	516	HEA	C4A-C3A-CMA-OMA
48	d	3003	CDL	C51-CB5-OB6-CB4
48	g	3004	CDL	C11-CA5-OA6-CA4
48	G	2003	CDL	C31-CA7-OA8-CA6
48	d	3003	CDL	C71-CB7-OB8-CB6
48	d	3003	CDL	OB7-CB5-OB6-CB4
48	g	3004	CDL	OA7-CA5-OA6-CA4
47	d	501	HEC	C4C-C3C-CAC-CBC
48	G	2004	CDL	OB7-CB5-OB6-CB4
48	g	3004	CDL	C71-CB7-OB8-CB6
48	G	2004	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
48	G	2003	CDL	OA9-CA7-OA8-CA6
48	G	2003	CDL	C71-CB7-OB8-CB6
48	d	3003	CDL	OB9-CB7-OB8-CB6
48	g	3004	CDL	OB9-CB7-OB8-CB6
48	G	2004	CDL	O1-C1-CB2-OB2
48	g	3004	CDL	O1-C1-CA2-OA2
48	G	2003	CDL	OB9-CB7-OB8-CB6
39	1	440	FMN	O2'-C2'-C3'-C4'
49	L	515	HEA	C15-C16-C17-C18
48	d	3003	CDL	CA2-C1-CB2-OB2
48	d	3003	CDL	O1-C1-CB2-OB2
48	g	3004	CDL	C51-CB5-OB6-CB4
47	d	501	HEC	C2C-C3C-CAC-CBC
39	1	440	FMN	O2'-C2'-C3'-O3'
48	d	3003	CDL	CA7-C31-C32-C33
48	d	3003	CDL	CA5-C11-C12-C13
48	G	2003	CDL	O1-C1-CA2-OA2
48	G	2003	CDL	CB2-OB2-PB2-OB5
48	G	2004	CDL	CA2-OA2-PA1-OA5
48	G	2004	CDL	CA3-OA5-PA1-OA2
48	G	2004	CDL	CB2-OB2-PB2-OB5
48	G	2004	CDL	CB3-OB5-PB2-OB2
48	g	3004	CDL	CA2-OA2-PA1-OA5
48	G	2003	CDL	CB2-C1-CA2-OA2
48	g	3004	CDL	OB7-CB5-OB6-CB4
47	D	501	HEC	C4C-C3C-CAC-CBC
48	g	3004	CDL	C71-C72-C73-C74
48	g	3004	CDL	CB7-C71-C72-C73
48	d	3003	CDL	C37-C38-C39-C40
48	G	2003	CDL	C51-CB5-OB6-CB4
48	G	2004	CDL	C33-C34-C35-C36
48	d	3003	CDL	C31-C32-C33-C34
48	d	3003	CDL	C38-C39-C40-C41
48	G	2004	CDL	O1-C1-CA2-OA2
48	d	3003	CDL	C36-C37-C38-C39
48	G	2003	CDL	OB7-CB5-OB6-CB4
48	d	3003	CDL	C33-C34-C35-C36
48	g	3004	CDL	C53-C54-C55-C56
44	Y	500	HEM	C2B-C3B-CAB-CBB
48	G	2004	CDL	C31-C32-C33-C34
48	d	3003	CDL	CB3-OB5-PB2-OB2
48	G	2004	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
48	G	2004	CDL	C31-CA7-OA8-CA6
47	D	501	HEC	C2C-C3C-CAC-CBC
48	G	2003	CDL	CB3-CB4-CB6-OB8
48	d	3003	CDL	CA3-CA4-CA6-OA8
48	g	3004	CDL	CB3-CB4-CB6-OB8
48	G	2003	CDL	C73-C74-C75-C76
48	d	3003	CDL	C32-C33-C34-C35
48	G	2004	CDL	OA6-CA4-CA6-OA8
48	G	2004	CDL	OA9-CA7-OA8-CA6
48	g	3004	CDL	C54-C55-C56-C57
48	d	3003	CDL	C39-C40-C41-C42
48	G	2003	CDL	OB5-CB3-CB4-CB6
48	d	3003	CDL	OA5-CA3-CA4-CA6
48	d	3003	CDL	C35-C36-C37-C38
48	G	2004	CDL	CA3-CA4-CA6-OA8
48	g	3004	CDL	OA5-CA3-CA4-OA6
48	G	2004	CDL	CB2-C1-CA2-OA2
48	g	3004	CDL	OA5-CA3-CA4-CA6
48	G	2004	CDL	C71-CB7-OB8-CB6
48	G	2004	CDL	CB3-CB4-CB6-OB8
48	G	2004	CDL	OA5-CA3-CA4-OA6
48	d	3003	CDL	OA5-CA3-CA4-OA6
44	Y	500	HEM	C4B-C3B-CAB-CBB
47	d	501	HEC	C4B-C3B-CAB-CBB
48	G	2003	CDL	OB6-CB4-CB6-OB8
48	G	2003	CDL	C72-C73-C74-C75
48	d	3003	CDL	C34-C35-C36-C37
40	1	441	NAI	C5D-O5D-PN-O1N
48	G	2003	CDL	CB2-OB2-PB2-OB4
48	G	2004	CDL	CB2-OB2-PB2-OB3
48	G	2003	CDL	C71-C72-C73-C74
48	G	2003	CDL	CB7-C71-C72-C73
48	g	3004	CDL	OB6-CB4-CB6-OB8
48	G	2004	CDL	OB5-CB3-CB4-CB6
40	1	441	NAI	O4D-C1D-N1N-C2N
44	C	501	HEM	CAD-CBD-CGD-O1D
44	c	502	HEM	CAA-CBA-CGA-O1A
44	c	501	HEM	CAD-CBD-CGD-O1D
44	C	502	HEM	CAA-CBA-CGA-O2A
44	c	502	HEM	CAA-CBA-CGA-O2A
48	g	3004	CDL	C52-C53-C54-C55
44	C	502	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
49	L	516	HEA	CAD-CBD-CGD-O2D
48	d	3003	CDL	C11-C12-C13-C14
44	c	501	HEM	CAD-CBD-CGD-O2D
49	L	516	HEA	CAD-CBD-CGD-O1D
47	d	501	HEC	C2B-C3B-CAB-CBB
48	G	2003	CDL	OA5-CA3-CA4-OA6
44	C	501	HEM	CAA-CBA-CGA-O1A
44	C	501	HEM	CAD-CBD-CGD-O2D
46	c	3002	UQ1	C4-C3-O3-CM3
48	G	2003	CDL	C78-C79-C80-C81
48	G	2004	CDL	OB9-CB7-OB8-CB6
44	C	501	HEM	CAA-CBA-CGA-O2A
44	Y	500	HEM	CAA-CBA-CGA-O2A
48	G	2003	CDL	C76-C77-C78-C79
48	G	2004	CDL	C12-C11-CA5-OA6
44	Y	500	HEM	CAA-CBA-CGA-O1A
47	D	501	HEC	CAD-CBD-CGD-O1D
49	L	515	HEA	CAD-CBD-CGD-O2D
44	c	502	HEM	CAD-CBD-CGD-O2D
47	D	501	HEC	CAA-CBA-CGA-O2A
48	d	3003	CDL	C32-C31-CA7-OA8
44	c	501	HEM	CAA-CBA-CGA-O2A
47	d	501	HEC	CAD-CBD-CGD-O1D
44	c	501	HEM	CAA-CBA-CGA-O1A
44	c	502	HEM	CAD-CBD-CGD-O1D
49	L	516	HEA	CAA-CBA-CGA-O2A
47	d	501	HEC	CAA-CBA-CGA-O2A
48	G	2003	CDL	OA5-CA3-CA4-CA6
47	D	501	HEC	CAA-CBA-CGA-O1A
49	L	515	HEA	CAD-CBD-CGD-O1D
48	G	2003	CDL	C51-C52-C53-C54
47	d	501	HEC	CAD-CBD-CGD-O2D
49	L	516	HEA	CAA-CBA-CGA-O1A
48	G	2004	CDL	C32-C31-CA7-OA8
46	c	3002	UQ1	C2-C3-O3-CM3
44	C	502	HEM	CAD-CBD-CGD-O2D
47	D	501	HEC	CAD-CBD-CGD-O2D
47	D	501	HEC	C4B-C3B-CAB-CBB
40	1	441	NAI	C5B-O5B-PA-O1A
40	1	441	NAI	C2N-C3N-C7N-N7N
48	g	3004	CDL	CB2-OB2-PB2-OB3
48	d	3003	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
47	d	501	HEC	CAA-CBA-CGA-O1A
48	G	2004	CDL	C32-C31-CA7-OA9
48	d	3003	CDL	C32-C31-CA7-OA9
49	L	515	HEA	CAA-CBA-CGA-O2A
44	C	502	HEM	CAD-CBD-CGD-O1D
48	d	3003	CDL	OA9-CA7-OA8-CA6
49	L	516	HEA	C26-C15-C16-C17
49	L	515	HEA	O11-C11-C3B-C2B

There are no ring outliers.

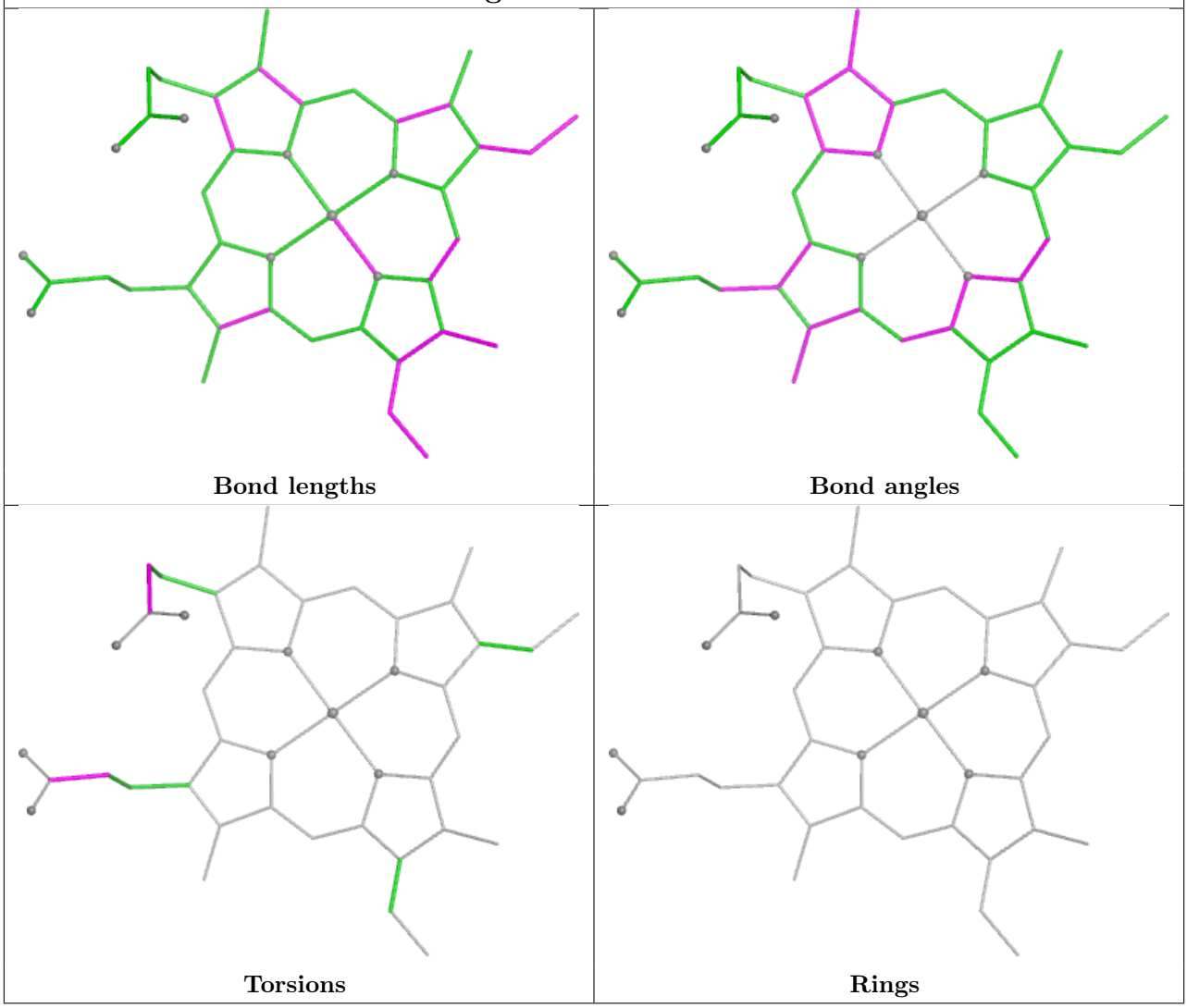
21 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	3	784	SF4	1	0
44	c	502	HEM	2	0
42	3	787	FES	1	0
44	C	501	HEM	2	0
49	L	515	HEA	1	0
49	L	516	HEA	3	0
38	8	183	SF4	2	0
48	G	2004	CDL	5	0
47	d	501	HEC	4	0
46	c	3002	UQ1	5	0
39	1	440	FMN	7	0
44	C	502	HEM	3	0
44	Y	500	HEM	7	0
40	1	441	NAI	5	0
38	3	785	SF4	1	0
46	C	2002	UQ1	2	0
45	C	2001	SMA	1	0
44	c	501	HEM	1	0
38	6	182	SF4	1	0
38	3	786	SF4	1	0
45	c	3001	SMA	1	0

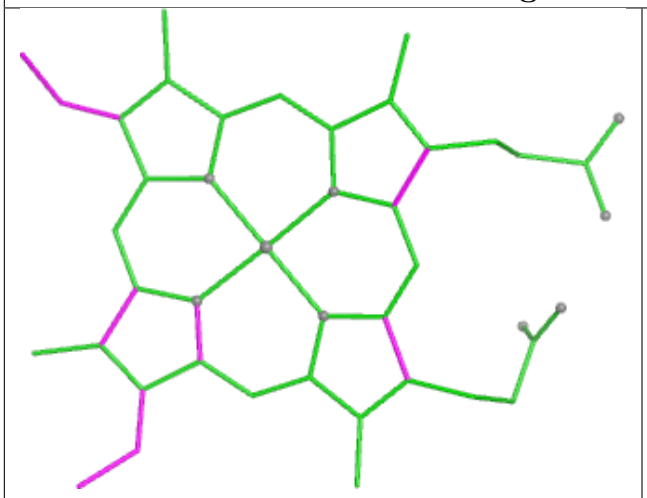
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

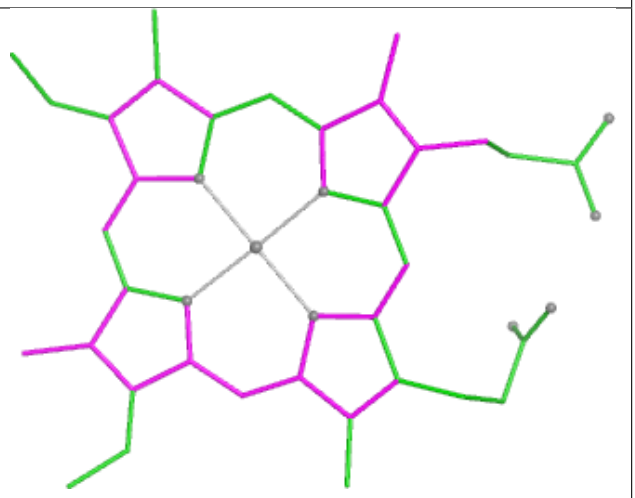
Ligand HEM c 502



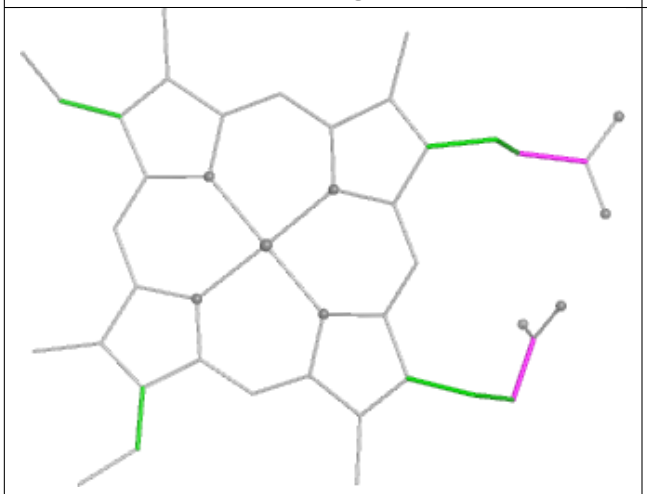
Ligand HEM C 501



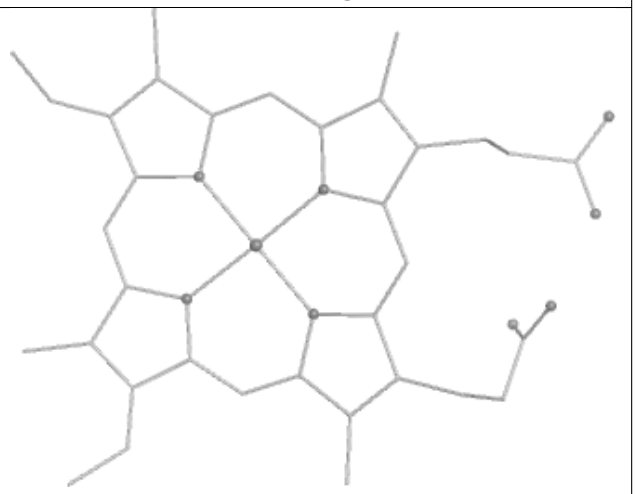
Bond lengths



Bond angles

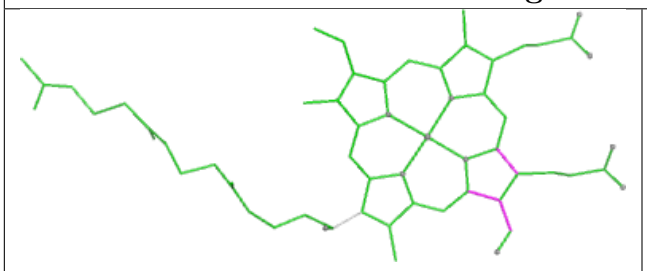


Torsions



Rings

Ligand HEA L 515



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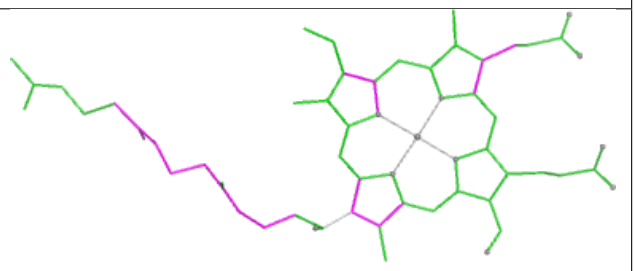

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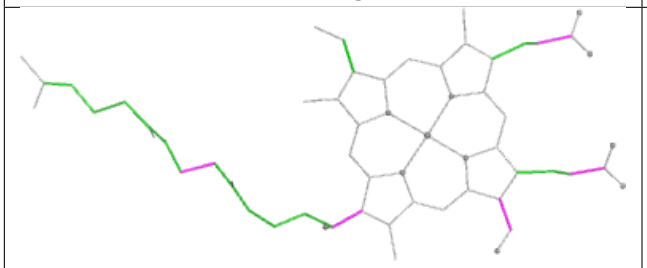

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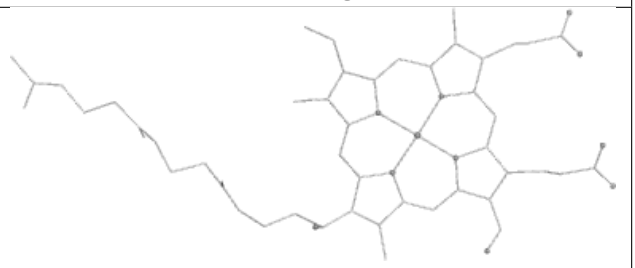
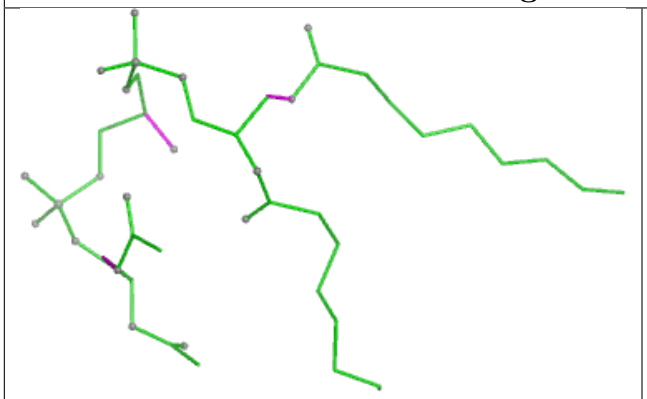
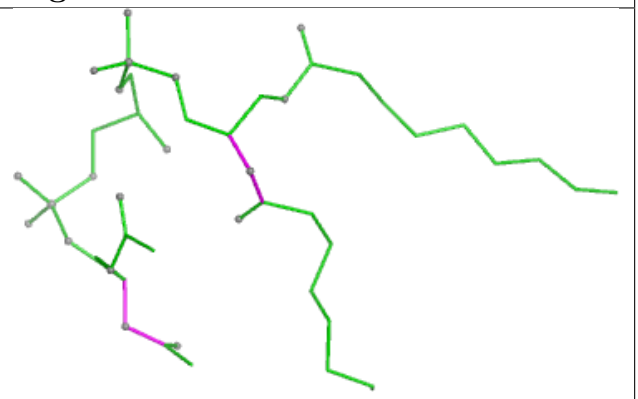


Rings

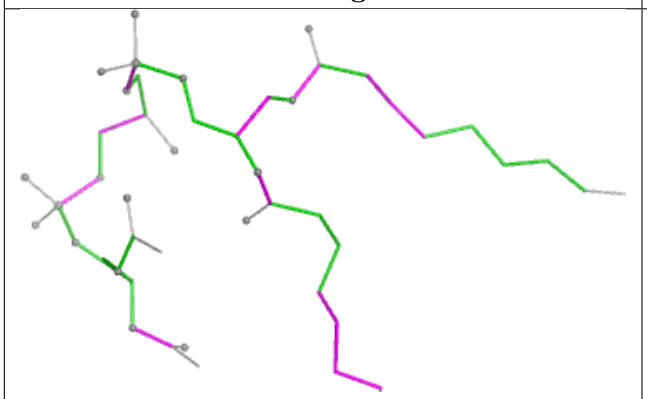
Ligand CDL g 3004



Bond lengths



Bond angles



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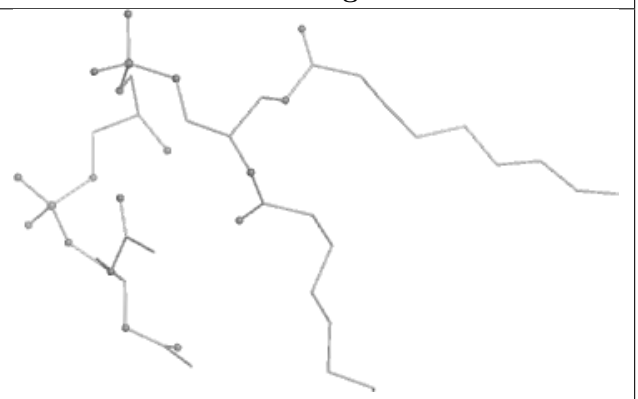
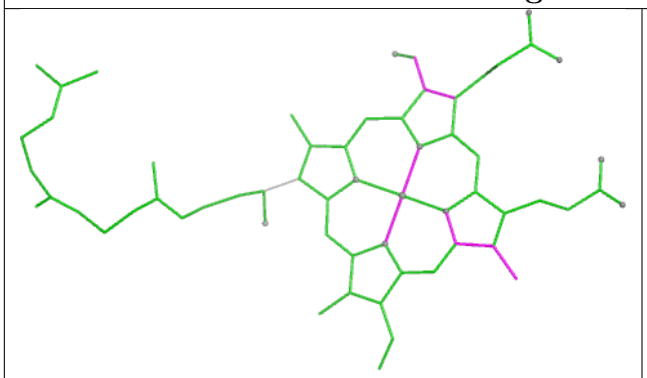


Rings

Ligand HEA L 516



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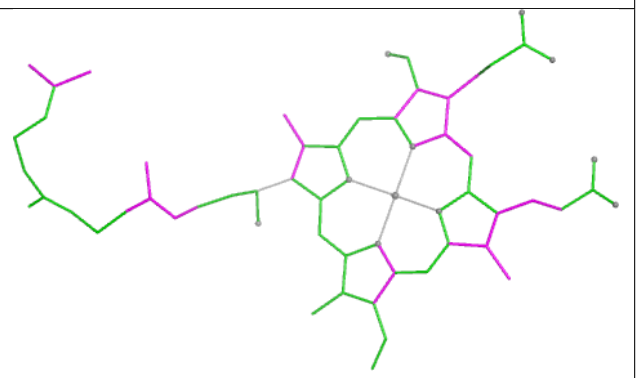

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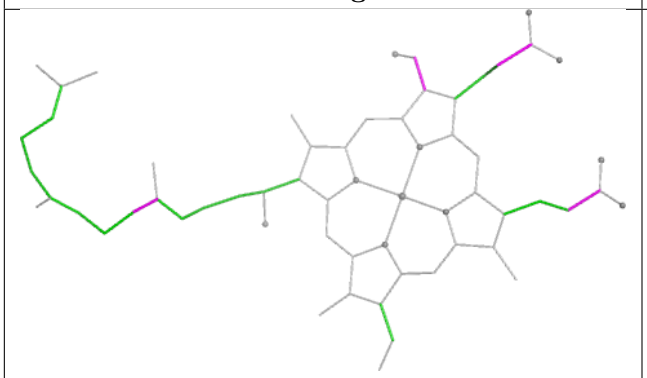
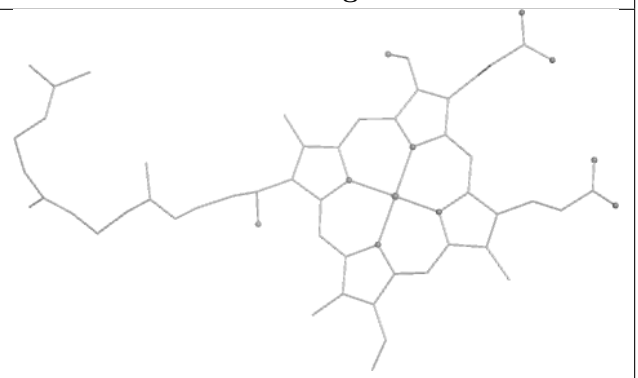
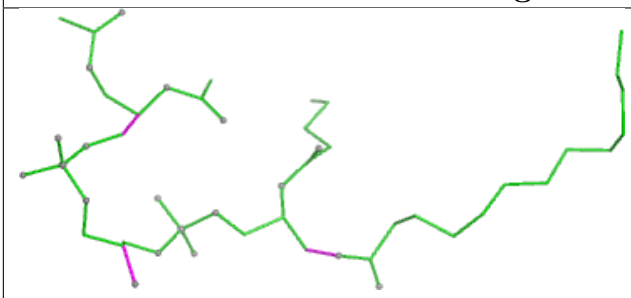
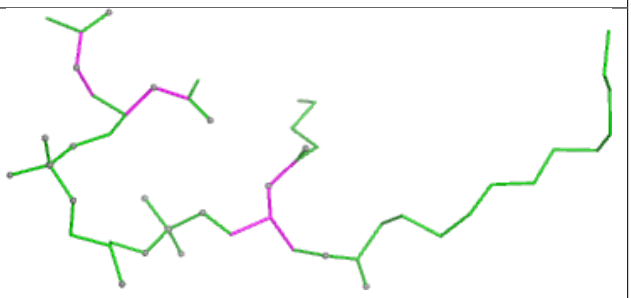
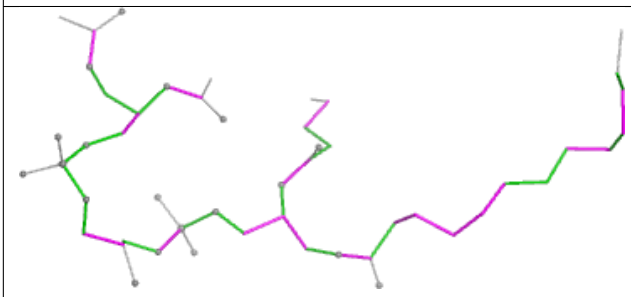
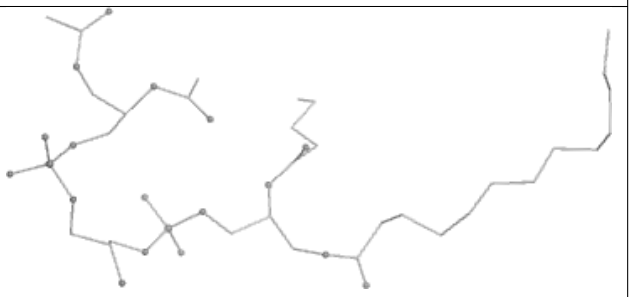


Torsions



Rings

Ligand CDL G 2003	
 Bond lengths	 Bond angles
 Torsions	 Rings

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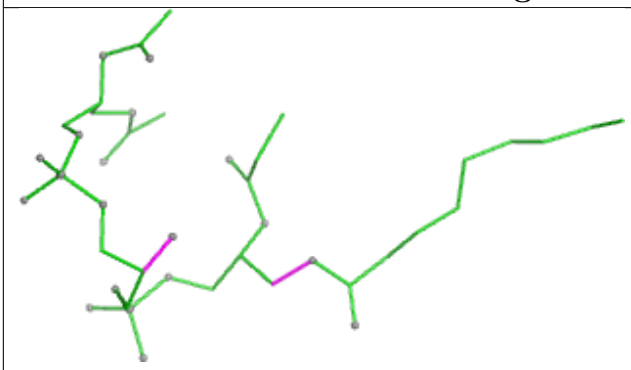
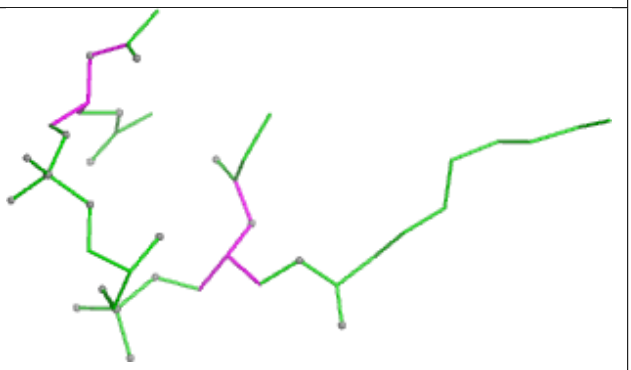
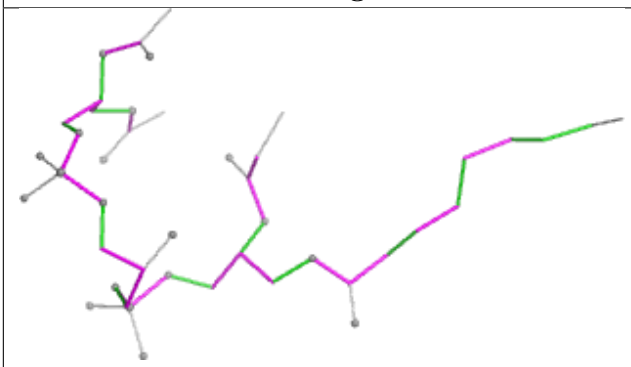
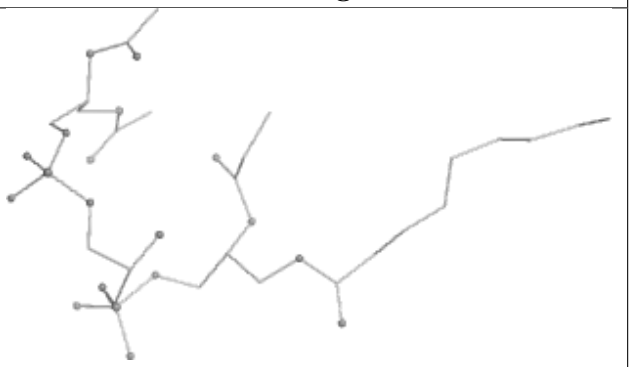
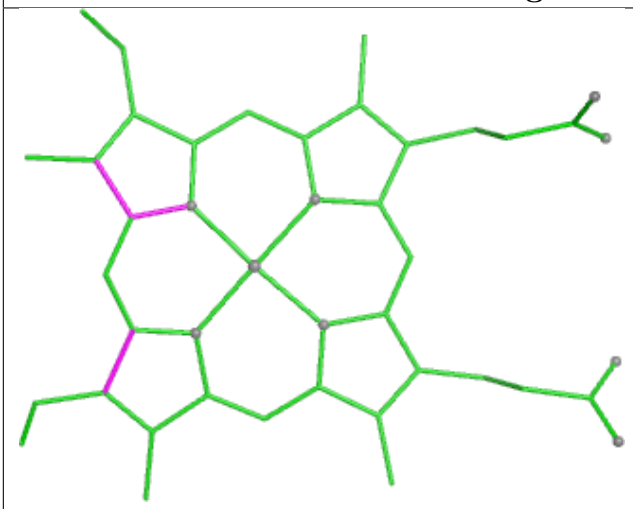
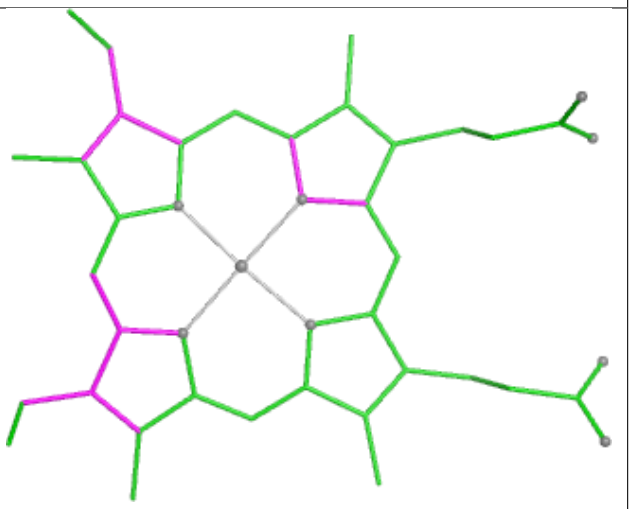
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEC d 501



Bond lengths



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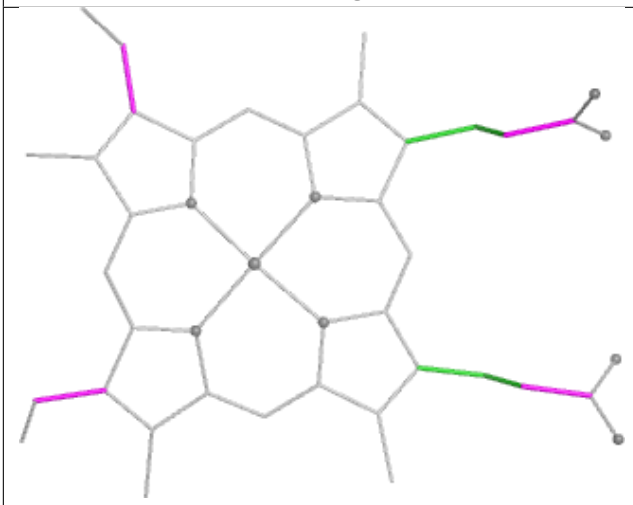
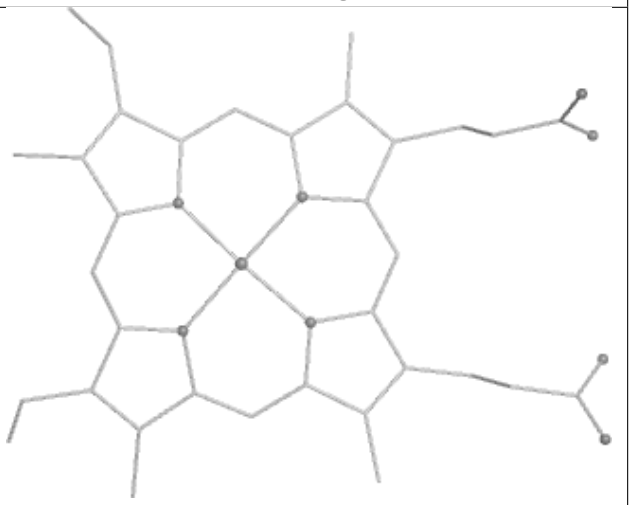
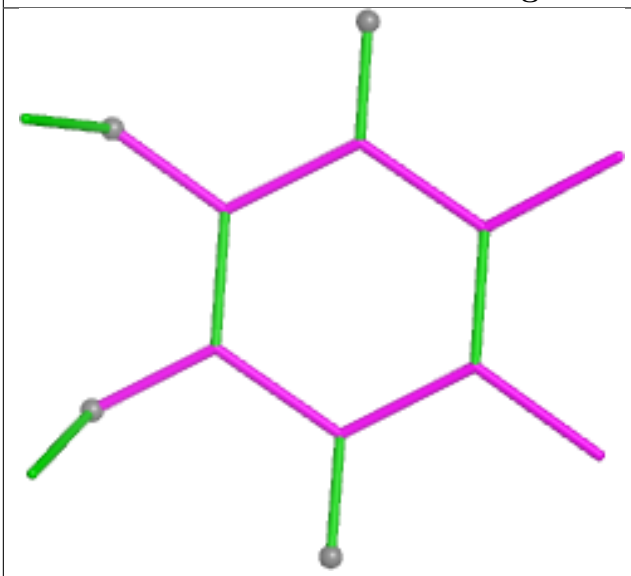


Torsions



Rings

Ligand UQ1 c 3002



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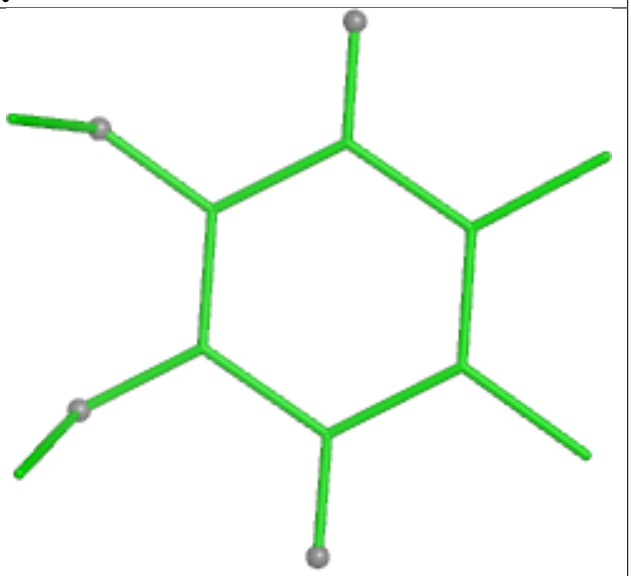
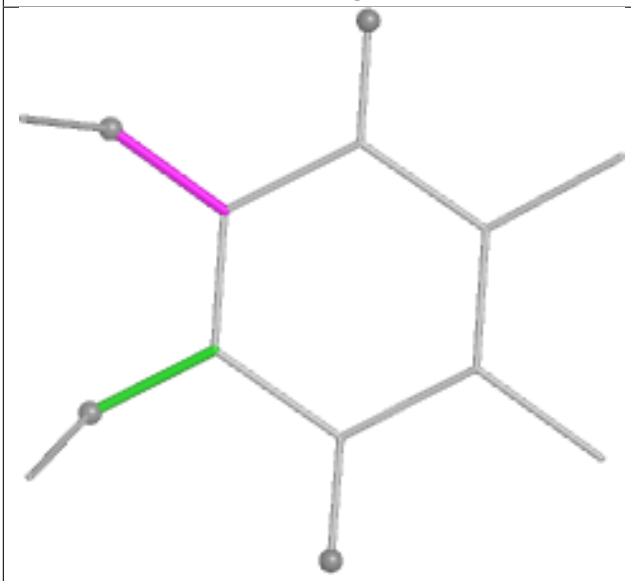


Bond angles



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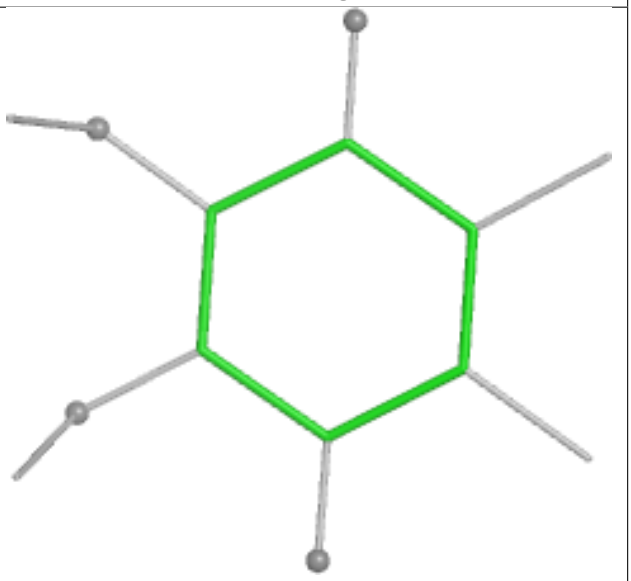
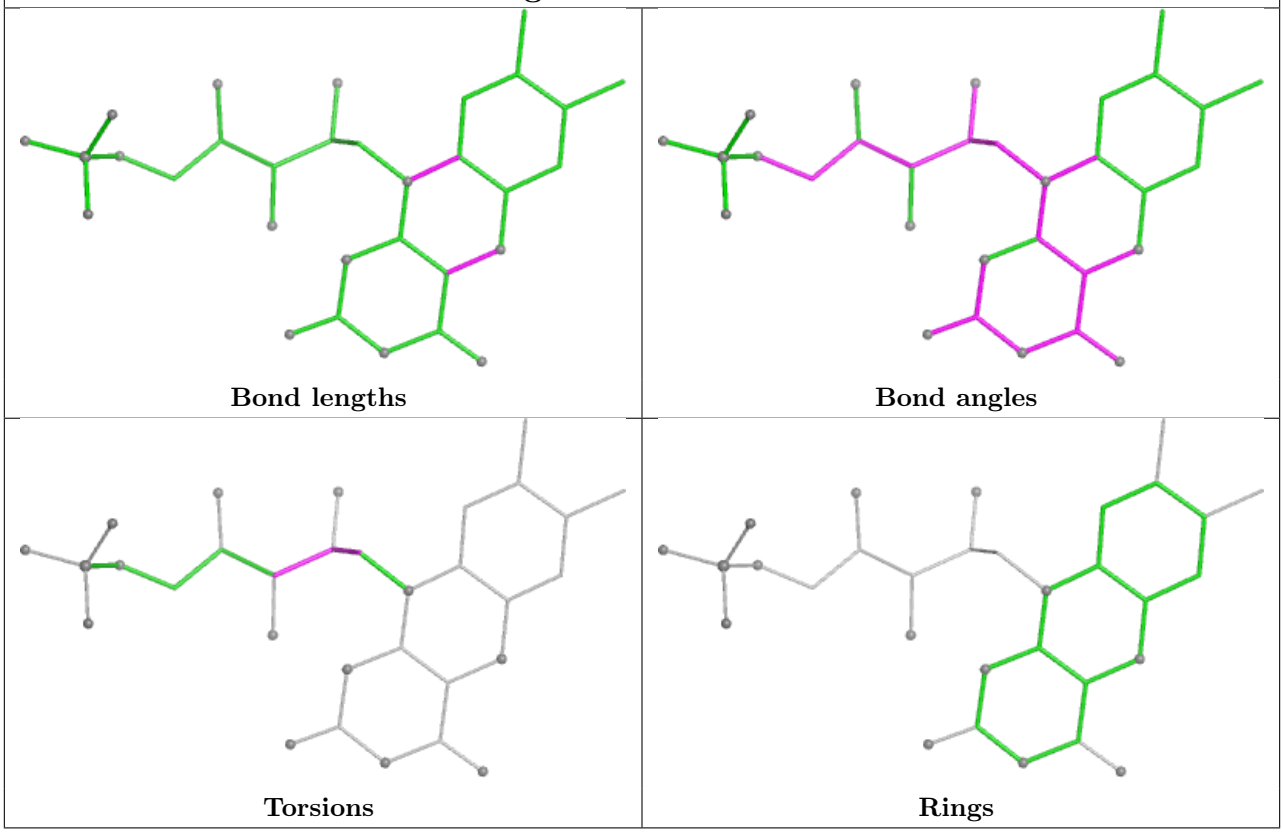
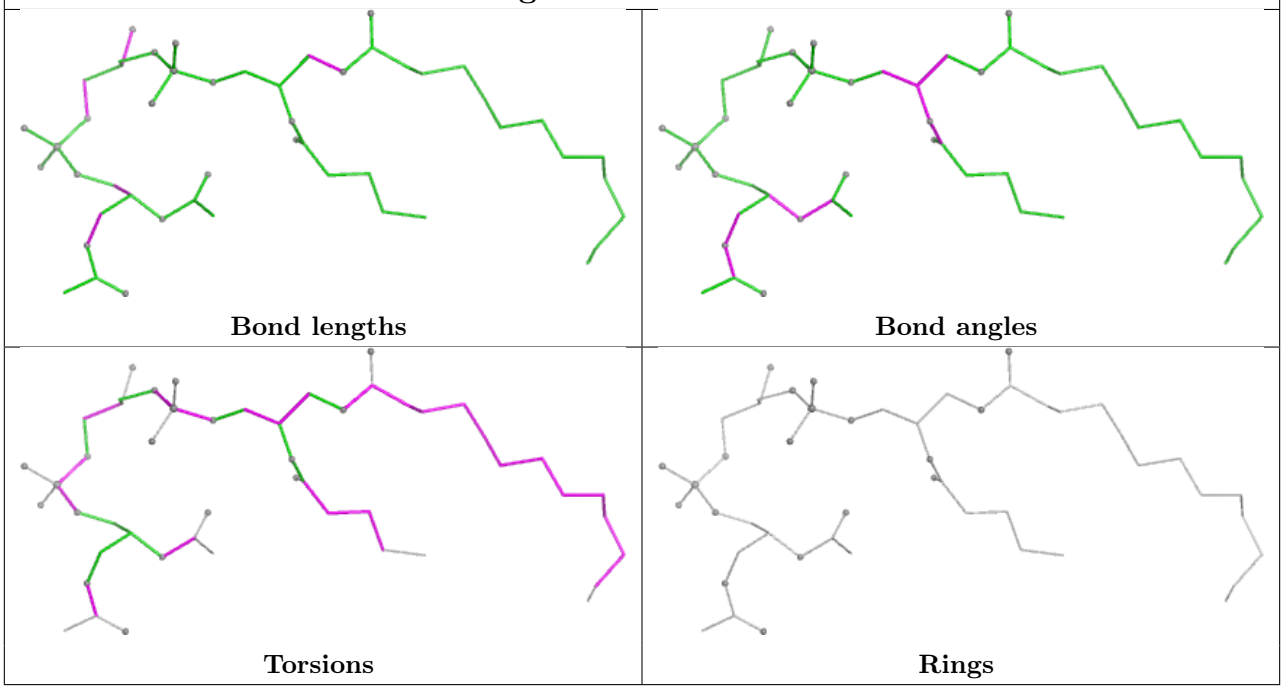


Rings

Ligand FMN 1 440



Ligand CDL d 3003



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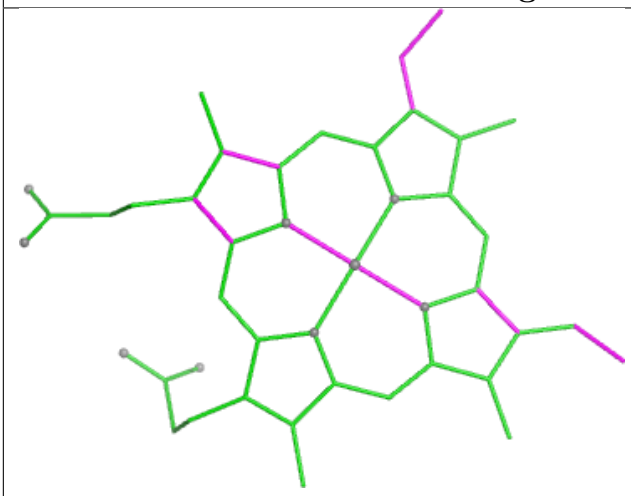

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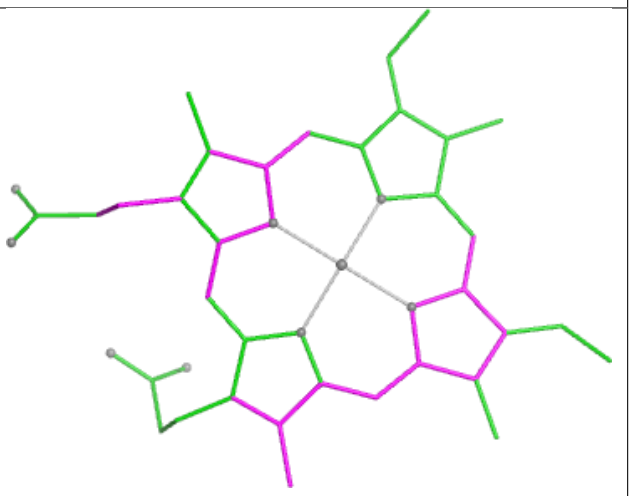
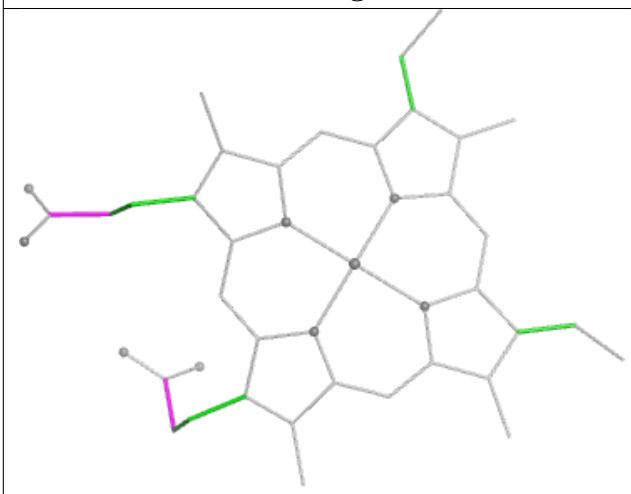


Bond angles



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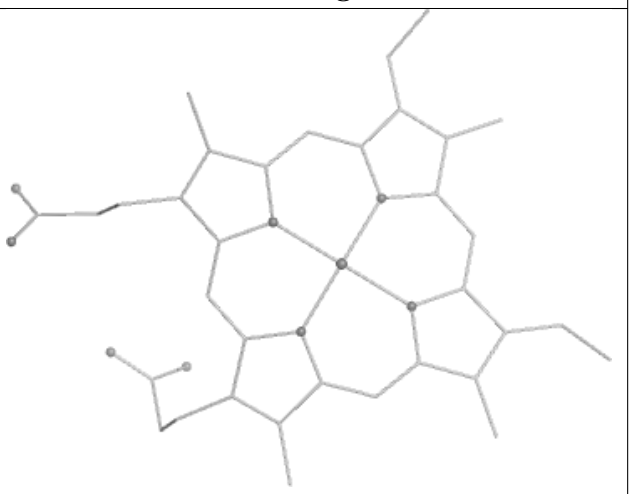

Rings

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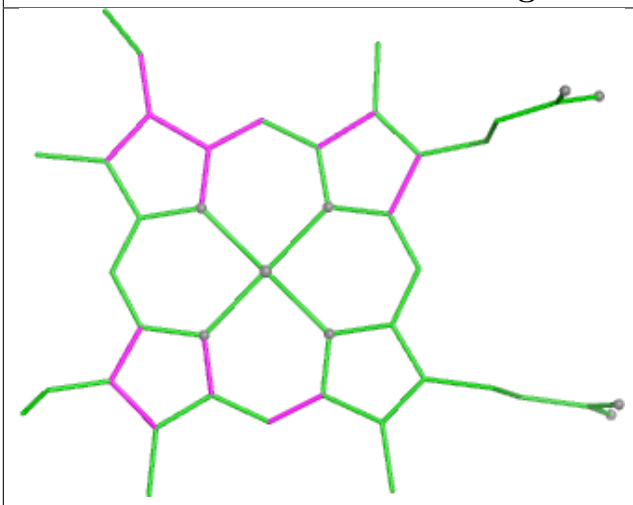

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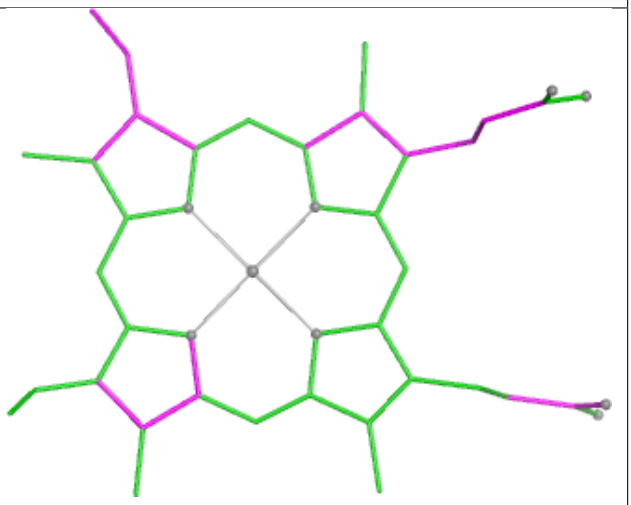

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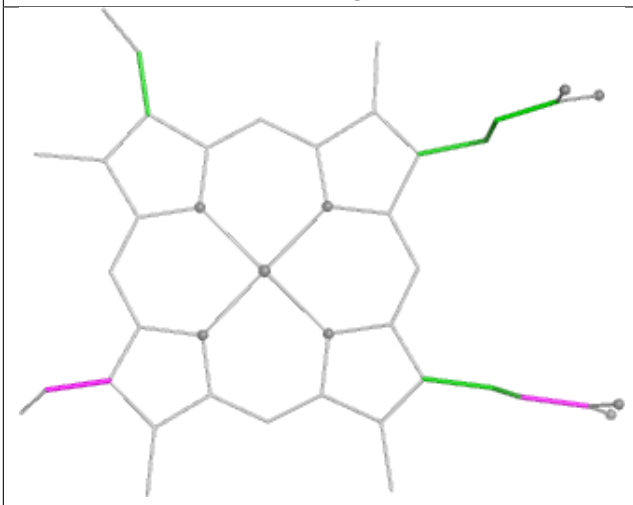

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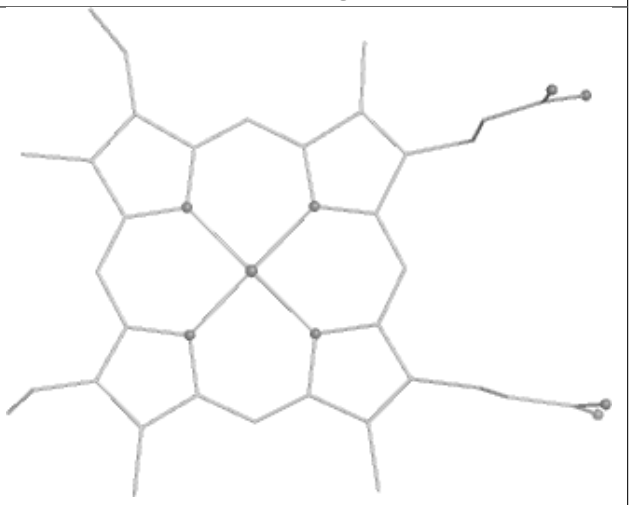
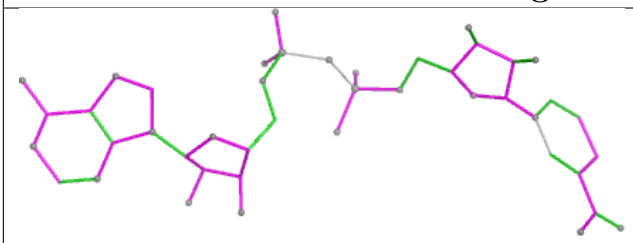


Rings

Ligand NAI 1 441



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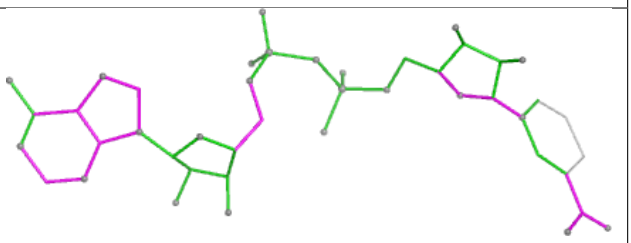
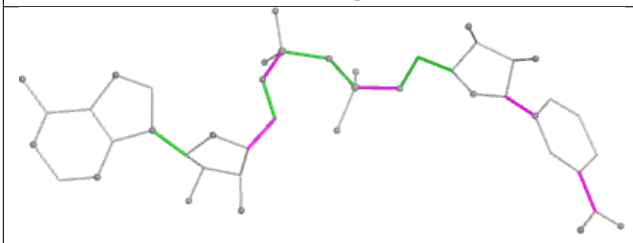
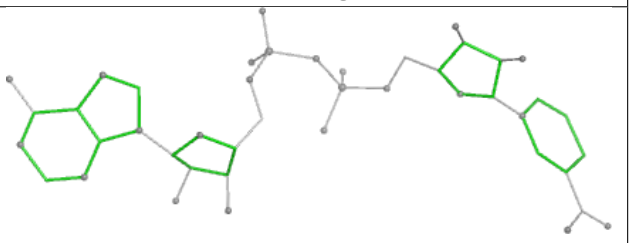


Bond angles

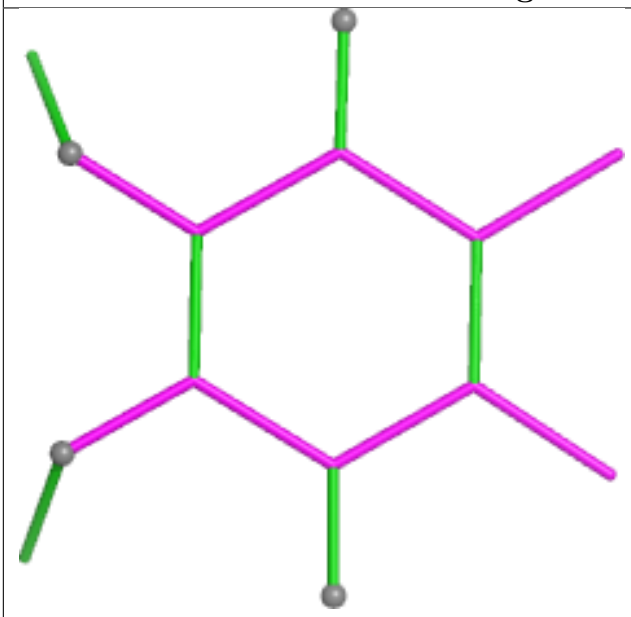


Torsions

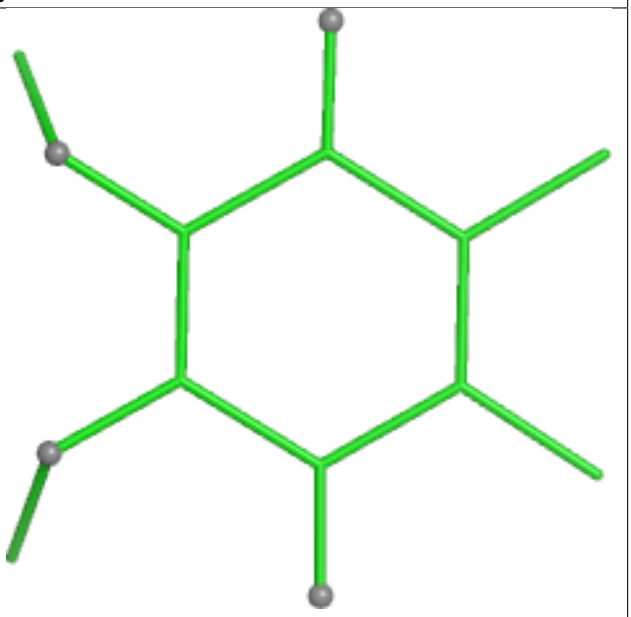


Rings

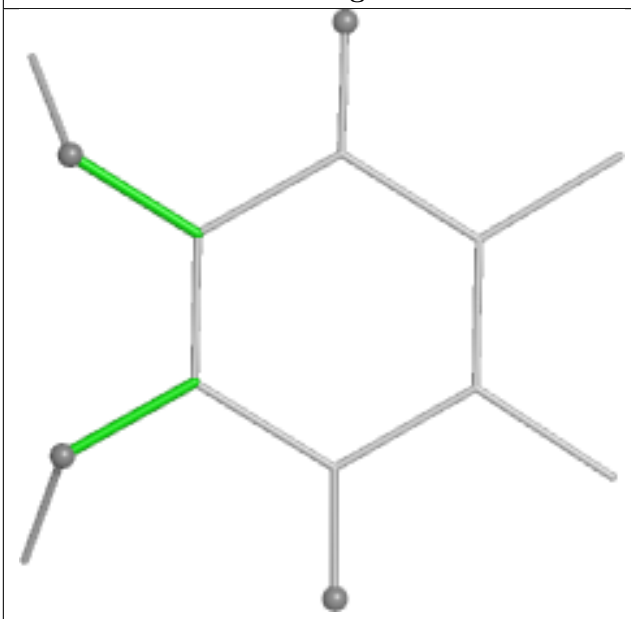
Ligand UQ1 C 2002



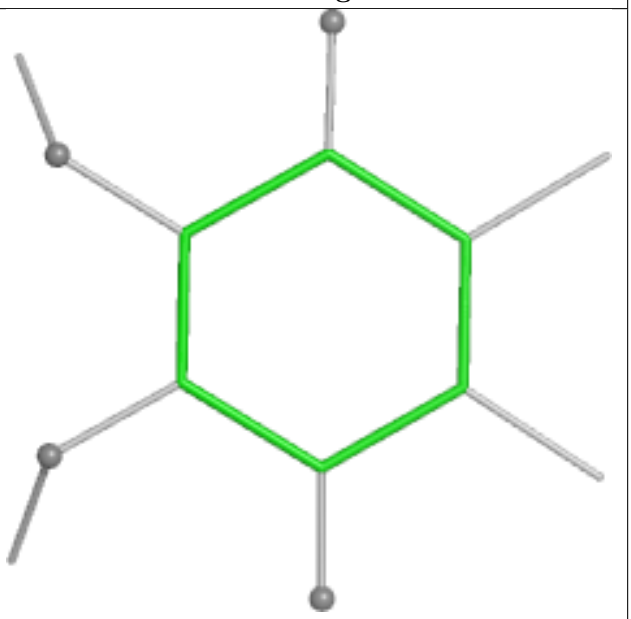
Bond lengths



Bond angles



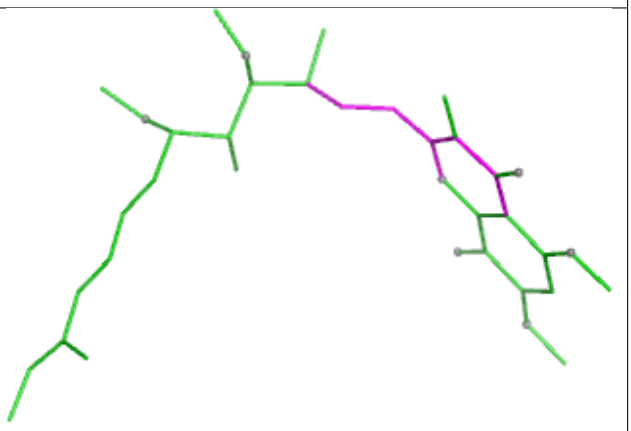
Torsions



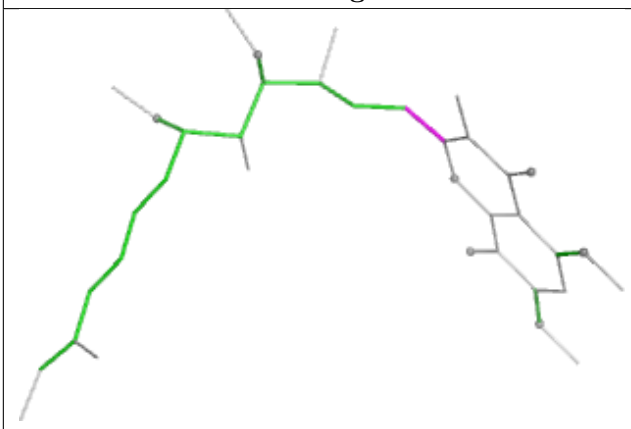
Rings

Ligand SMA C 2001

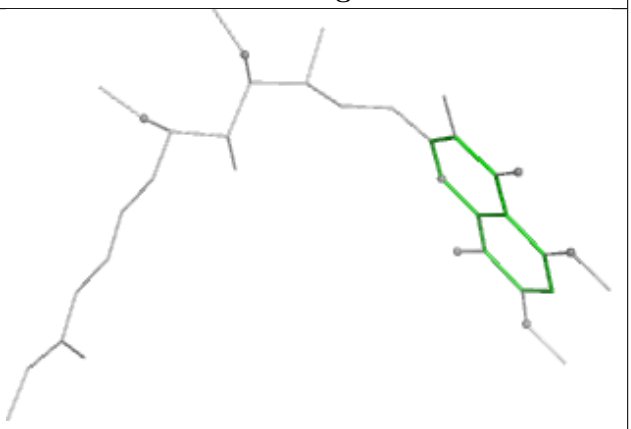
Bond lengths



Bond angles

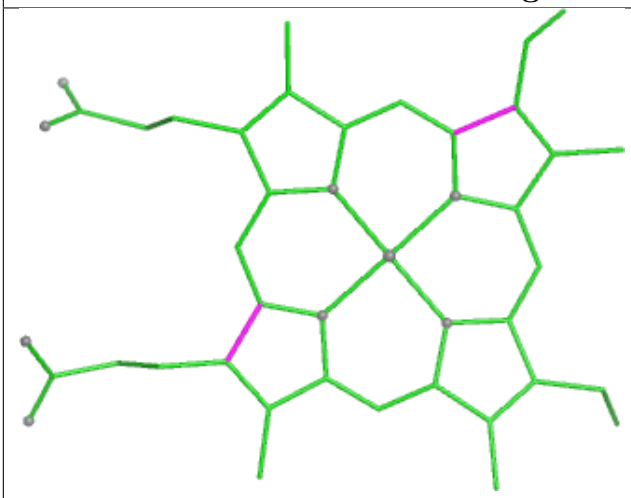


Torsions

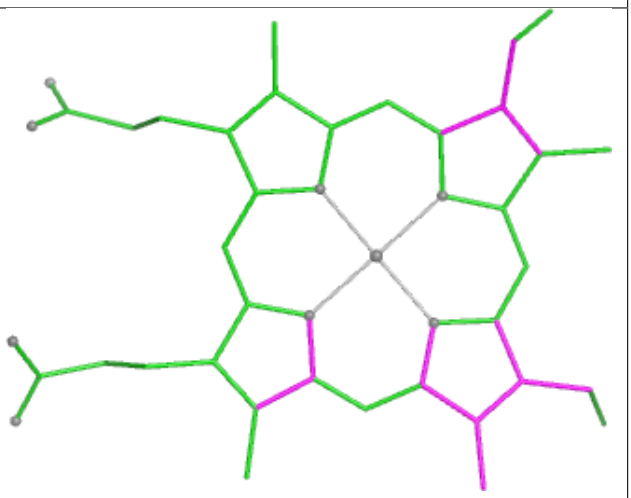


Rings

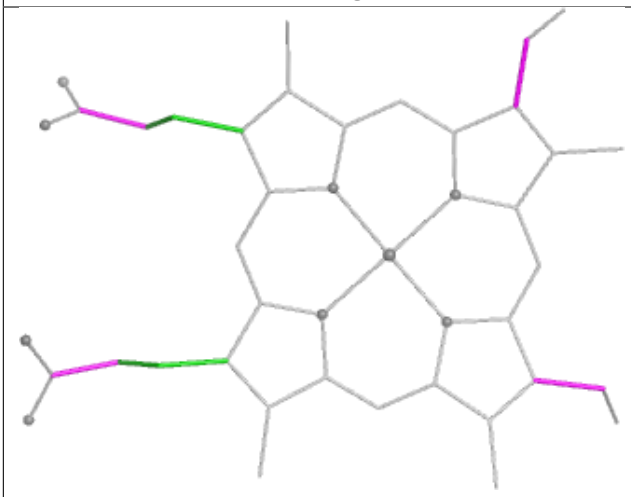
Ligand HEC D 501



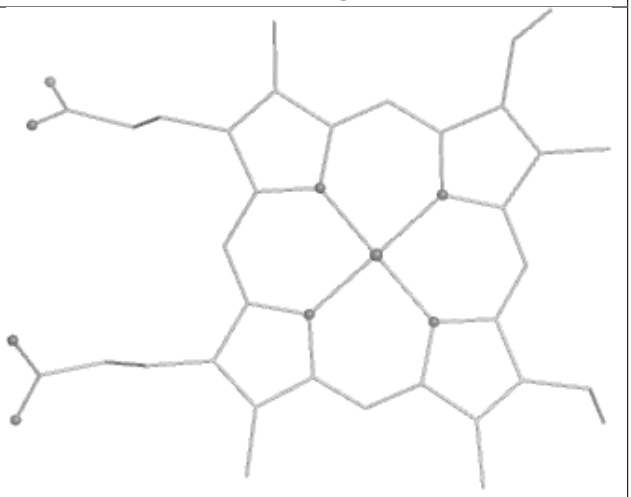
Bond lengths



Bond angles

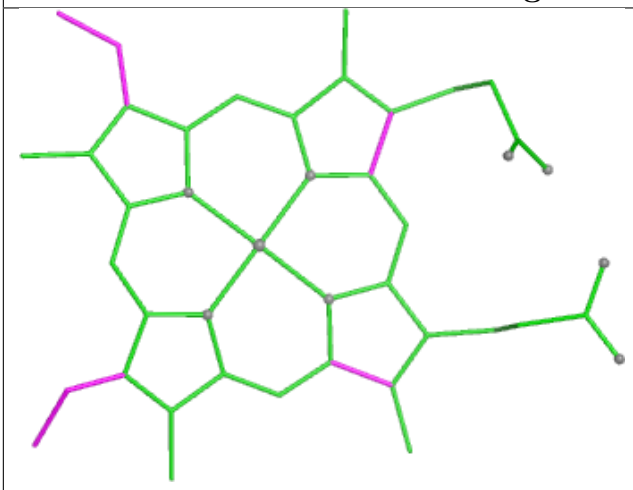


Torsions

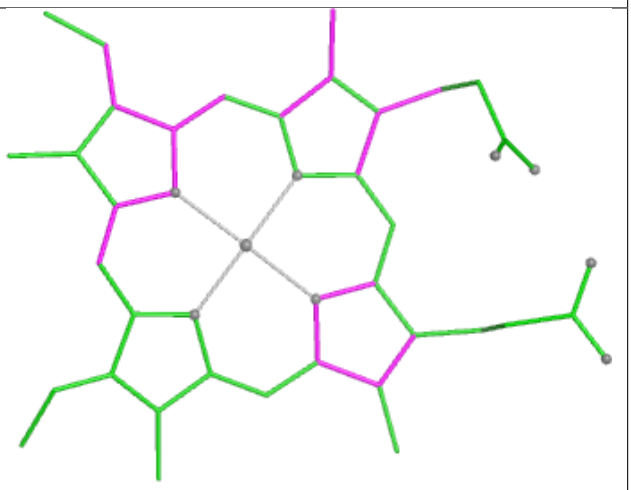


Rings

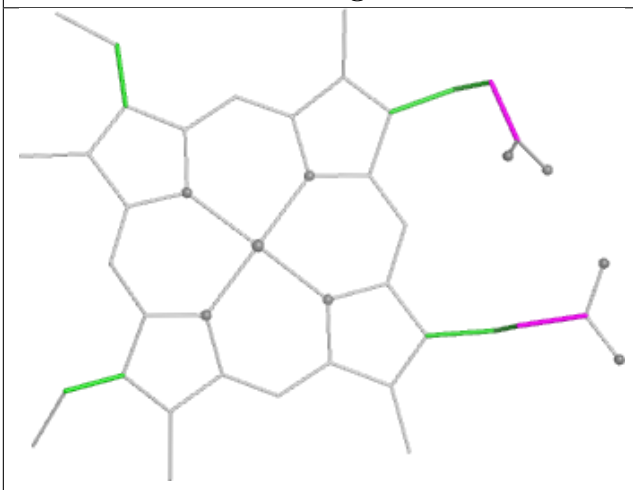
Ligand HEM c 501



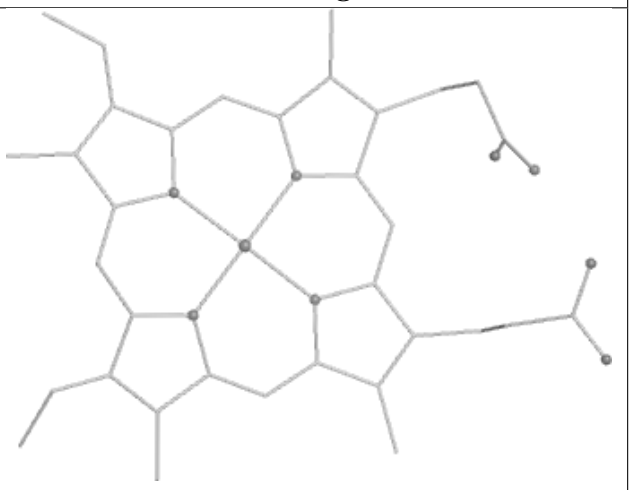
Bond lengths



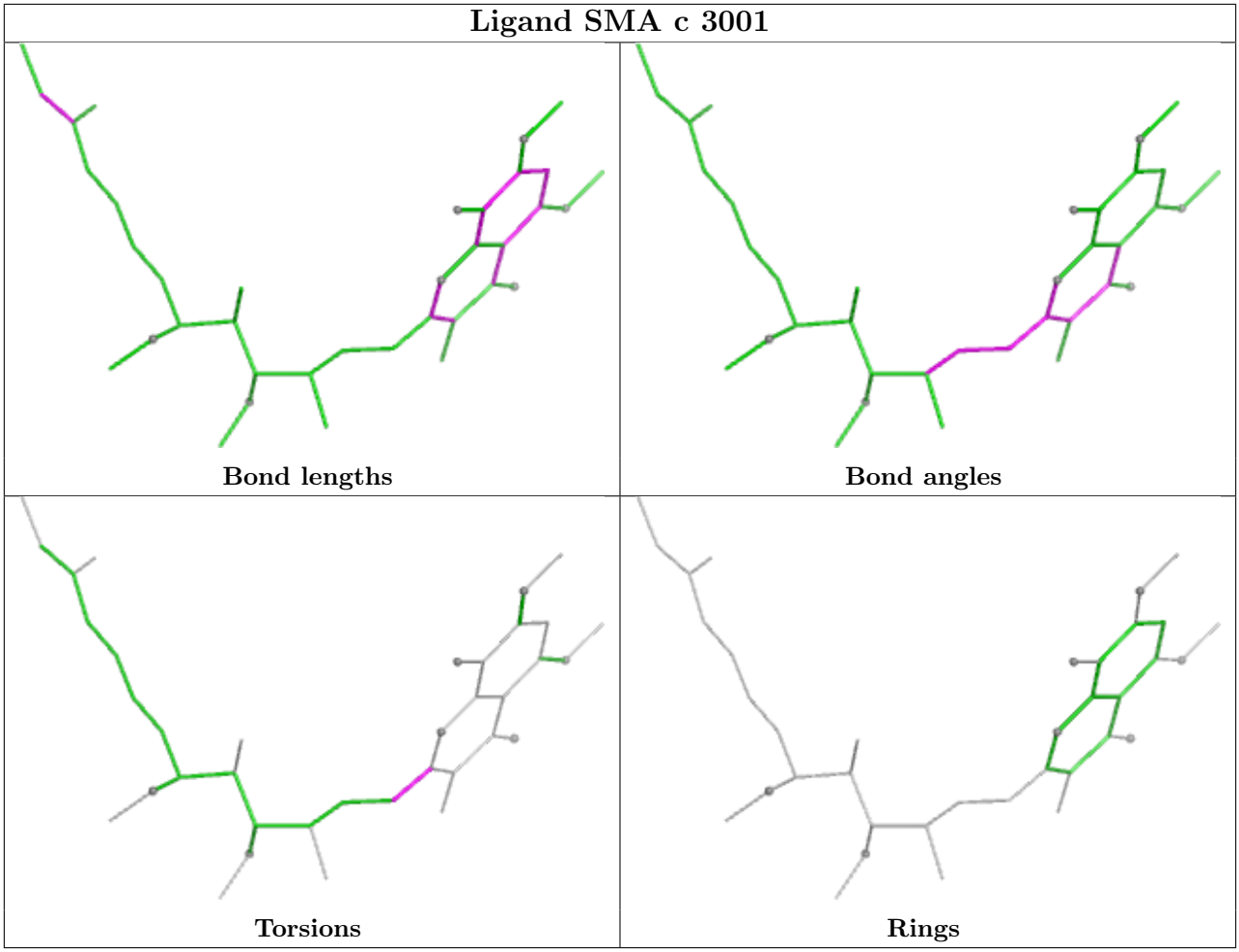
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	m	20
35	n	16
36	o	16
37	p	10
29	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	m	428:UNK	C	495:UNK	N	56.90
1	n	1024:UNK	C	1050:UNK	N	55.04
1	o	366:UNK	C	395:UNK	N	50.88
1	m	1417:UNK	C	1501:UNK	N	47.70
1	o	665:UNK	C	700:UNK	N	47.65
1	o	524:UNK	C	601:UNK	N	47.16
1	m	1326:UNK	C	1401:UNK	N	46.61
1	o	428:UNK	C	501:UNK	N	46.47
1	p	725:UNK	C	797:UNK	N	45.46
1	n	1328:UNK	C	1399:UNK	N	43.88
1	n	829:UNK	C	899:UNK	N	43.18
1	o	1222:UNK	C	1295:UNK	N	42.97
1	n	520:UNK	C	601:UNK	N	42.94
1	p	824:UNK	C	900:UNK	N	41.53
1	o	923:UNK	C	1001:UNK	N	41.07
1	p	524:UNK	C	603:UNK	N	40.88
1	m	1022:UNK	C	1050:UNK	N	40.59
1	m	520:UNK	C	601:UNK	N	40.17
1	n	228:UNK	C	301:UNK	N	39.55
1	m	922:UNK	C	1003:UNK	N	39.30
1	o	1059:UNK	C	1096:UNK	N	38.87
1	p	624:UNK	C	702:UNK	N	37.28
1	o	226:UNK	C	301:UNK	N	37.24
1	m	229:UNK	C	301:UNK	N	36.09
1	o	1022:UNK	C	1050:UNK	N	35.98
1	n	923:UNK	C	1002:UNK	N	34.04
1	m	360:UNK	C	401:UNK	N	33.91
1	o	723:UNK	C	801:UNK	N	33.47
1	n	1065:UNK	C	1100:UNK	N	30.93
1	o	121:UNK	C	202:UNK	N	29.63
1	n	123:UNK	C	201:UNK	N	28.64
1	m	1061:UNK	C	1101:UNK	N	28.15
1	n	424:UNK	C	495:UNK	N	16.18
1	m	824:UNK	C	901:UNK	N	15.99
1	n	367:UNK	C	398:UNK	N	15.97
1	m	666:UNK	C	704:UNK	N	15.22
1	n	1121:UNK	C	1200:UNK	N	14.33
1	m	732:UNK	C	802:UNK	N	14.14
1	o	823:UNK	C	903:UNK	N	13.62
1	n	734:UNK	C	800:UNK	N	12.90
1	p	919:UNK	C	997:UNK	N	12.22
1	p	125:UNK	C	202:UNK	N	11.40
1	n	1222:UNK	C	1300:UNK	N	11.26

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	m	613:UNK	C	650:UNK	N	11.20
1	o	1122:UNK	C	1200:UNK	N	11.16
1	o	1320:UNK	C	1401:UNK	N	11.09
1	p	423:UNK	C	494:UNK	N	10.86
1	n	663:UNK	C	704:UNK	N	10.34
1	o	615:UNK	C	650:UNK	N	10.27
1	m	1123:UNK	C	1195:UNK	N	9.82
1	m	127:UNK	C	201:UNK	N	9.74
1	p	324:UNK	C	397:UNK	N	9.72
1	n	615:UNK	C	650:UNK	N	9.60
1	m	1218:UNK	C	1298:UNK	N	9.44
1	p	223:UNK	C	295:UNK	N	8.96
1	m	311:UNK	C	350:UNK	N	6.99
1	o	313:UNK	C	350:UNK	N	6.87
1	p	1021:UNK	C	1098:UNK	N	6.64
1	n	313:UNK	C	350:UNK	N	5.71
1	m	1597:UNK	C	1601:UNK	N	4.80
1	m	1543:UNK	C	1545:UNK	N	4.39
1	U	56:PRO	C	57:HIS	N	3.69
1	m	1564:UNK	C	1566:UNK	N	3.11

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1876. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map

X

Y

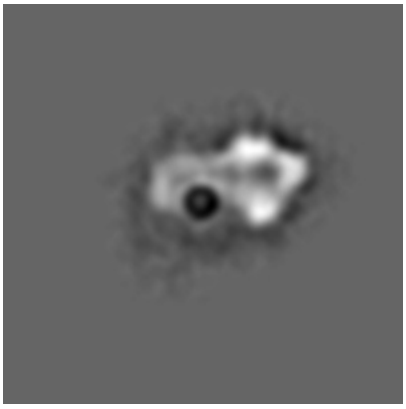
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 56



Y Index: 56

Z Index: 56

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: 67

Y Index: 37

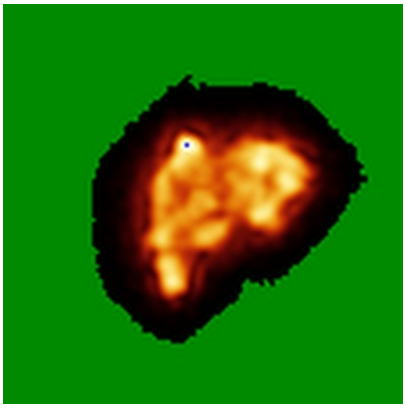
Z Index: 45

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

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



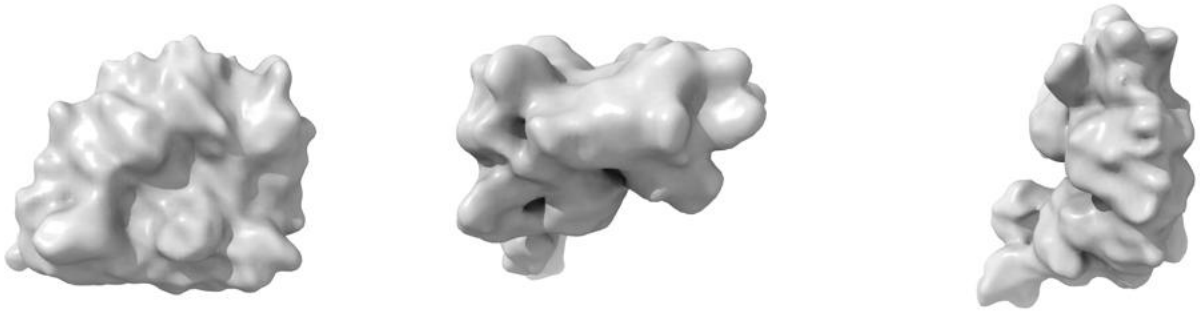
Y

Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

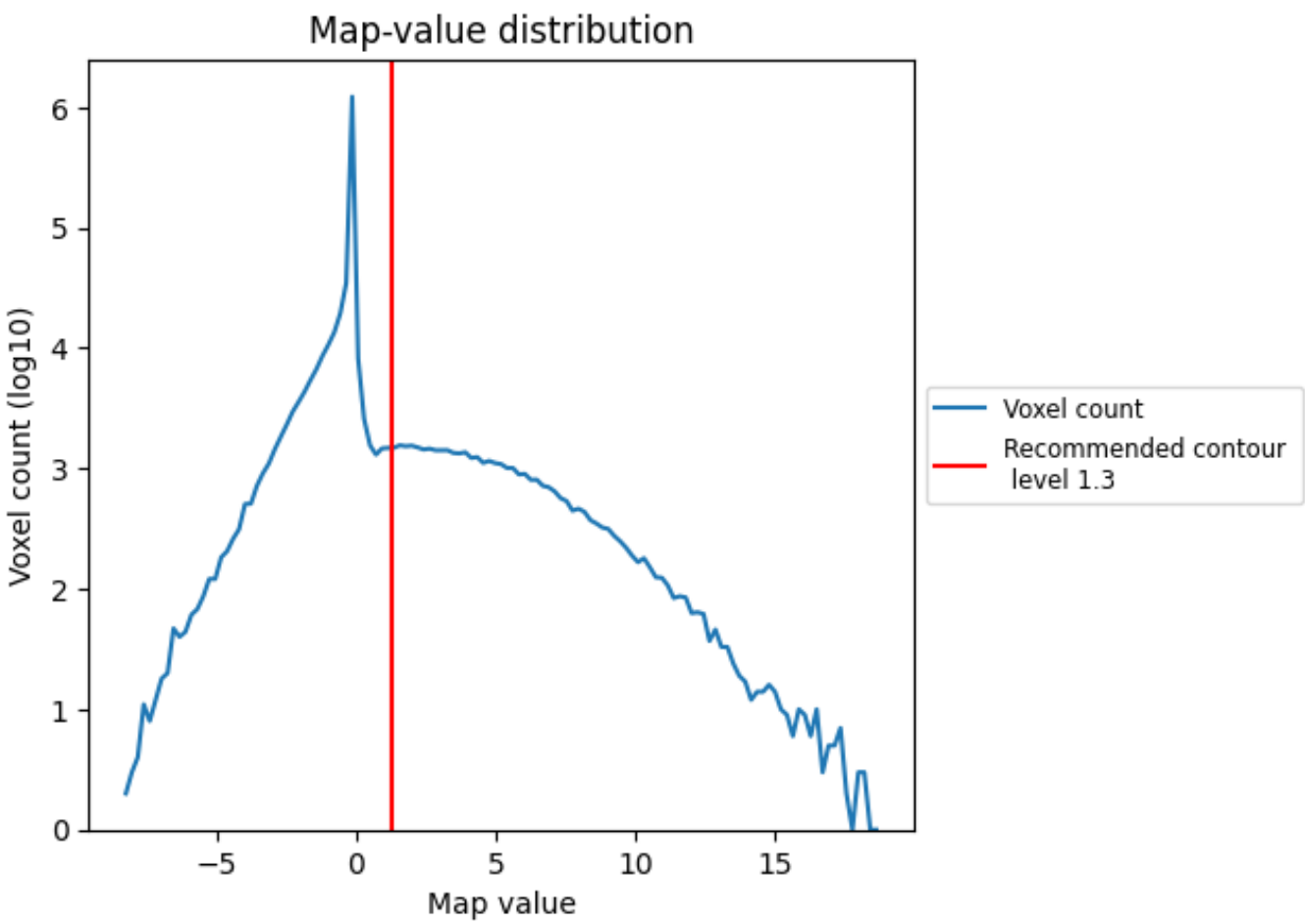
6.6 Mask visualisation (i)

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

7 Map analysis (i)

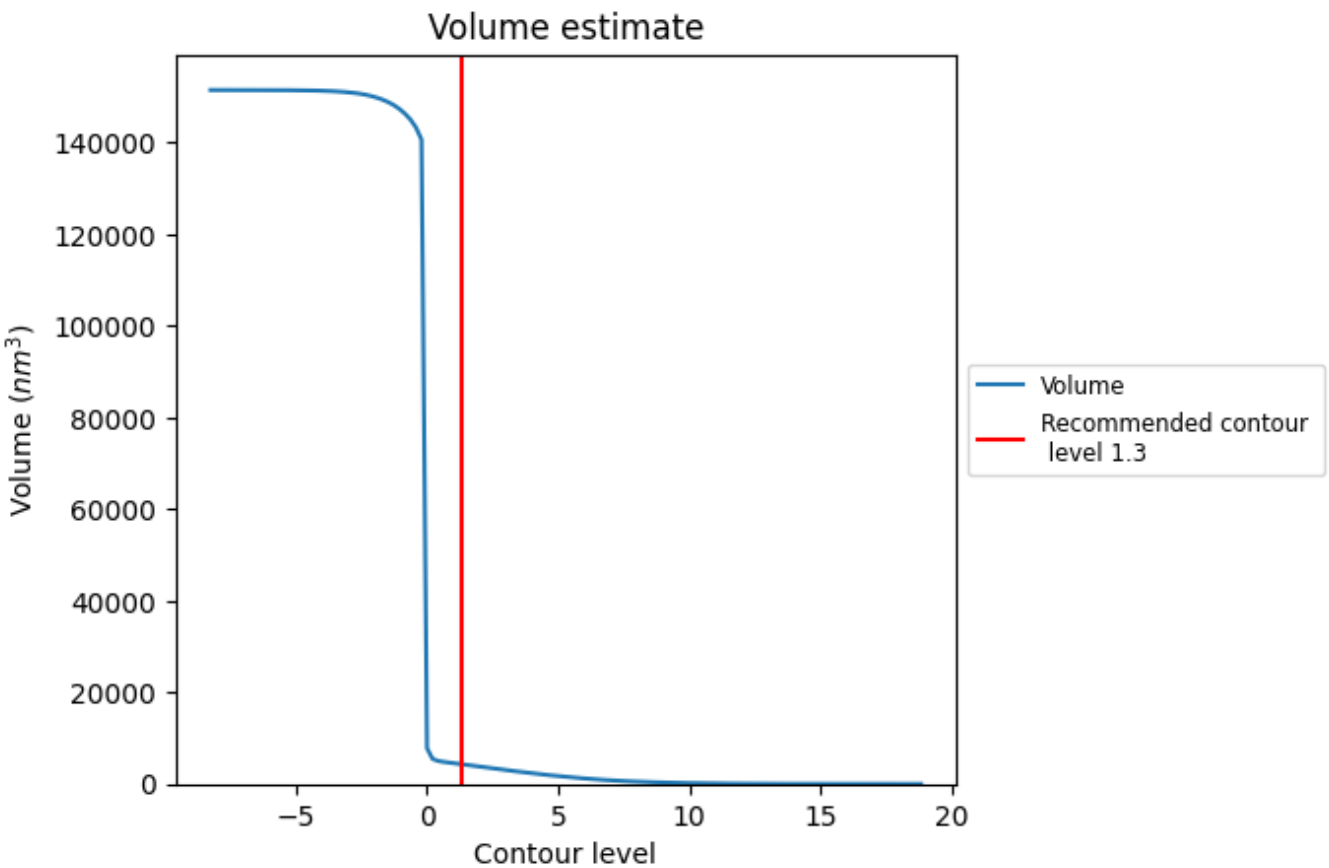
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

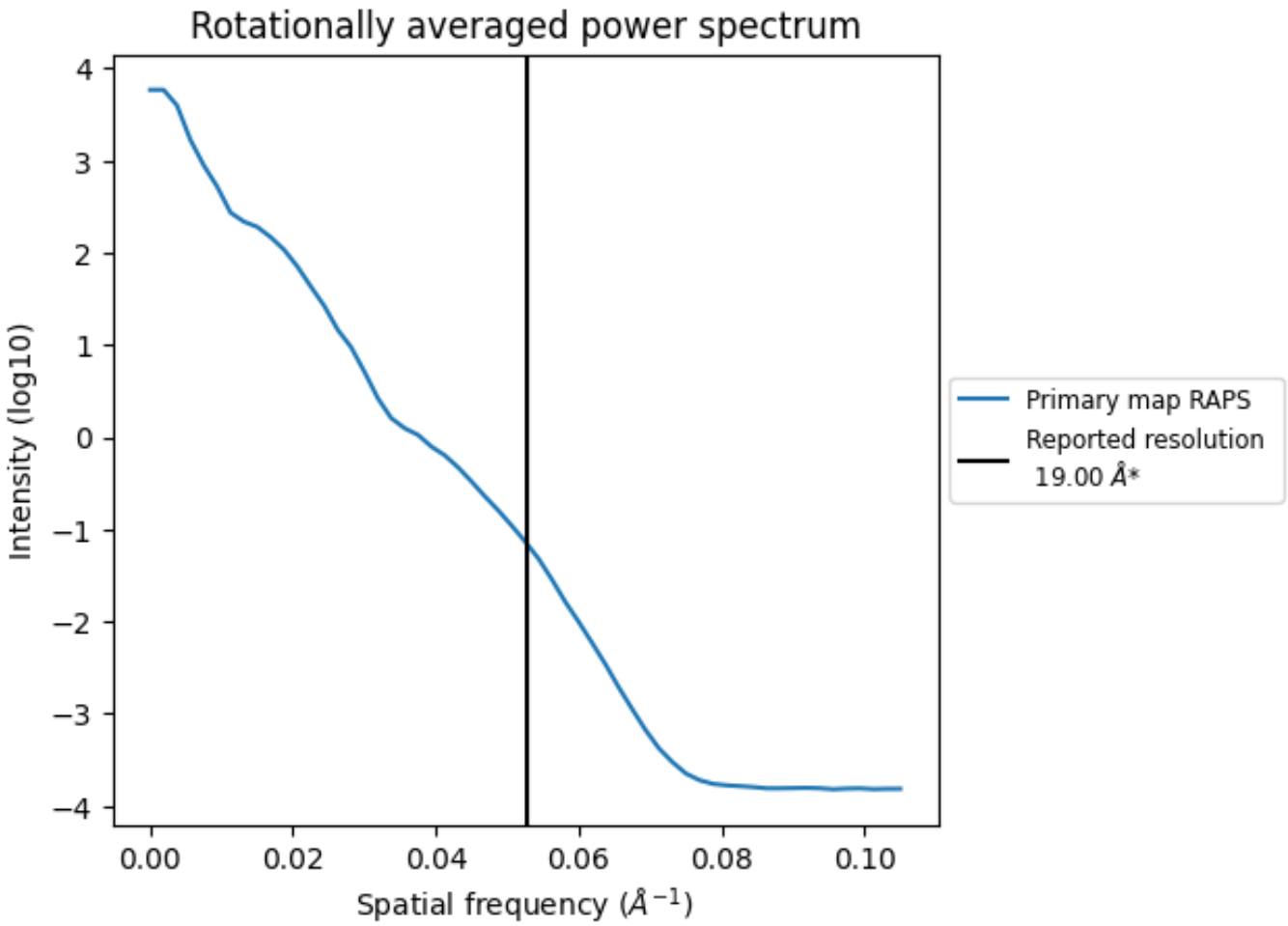
7.2 Volume estimate (i)



The volume at the recommended contour level is 4344 nm^3; this corresponds to an approximate mass of 3924 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 0.053 Å^{-1}

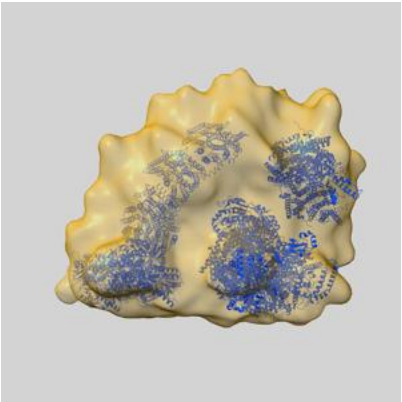
8 Fourier-Shell correlation (i)

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

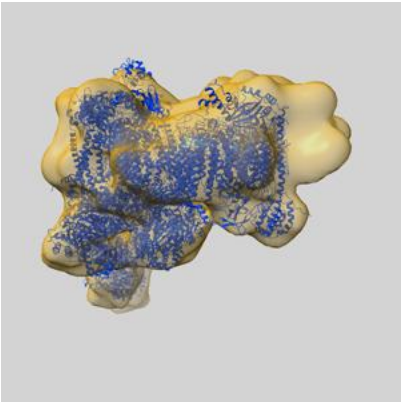
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1876 and PDB model 2YBB. Per-residue inclusion information can be found in section 3 on page 20.

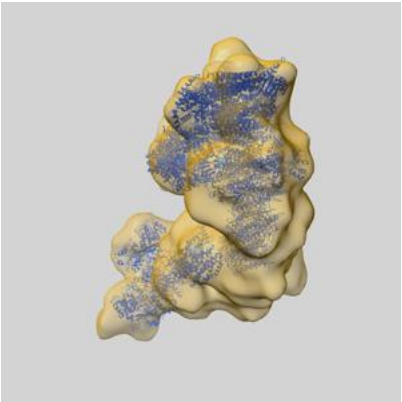
9.1 Map-model overlay (i)



X



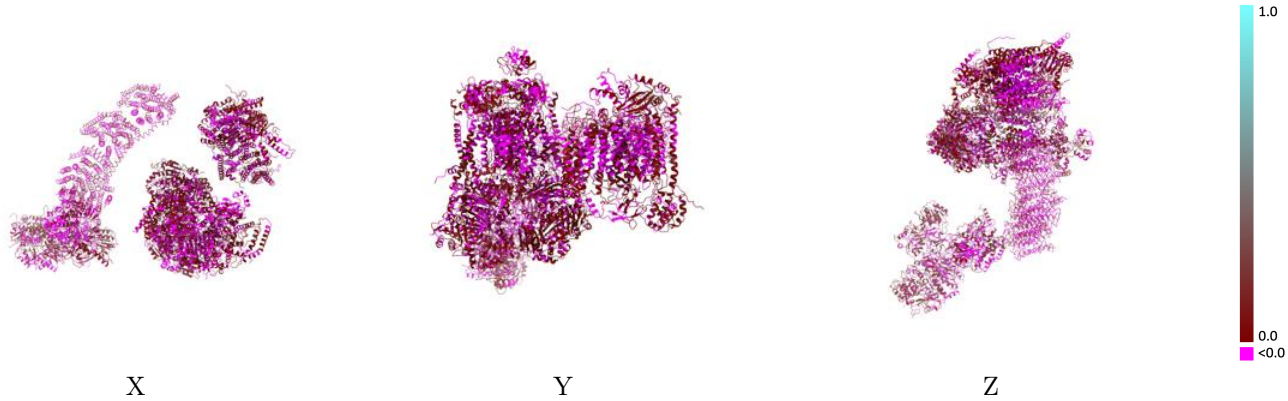
Y



Z

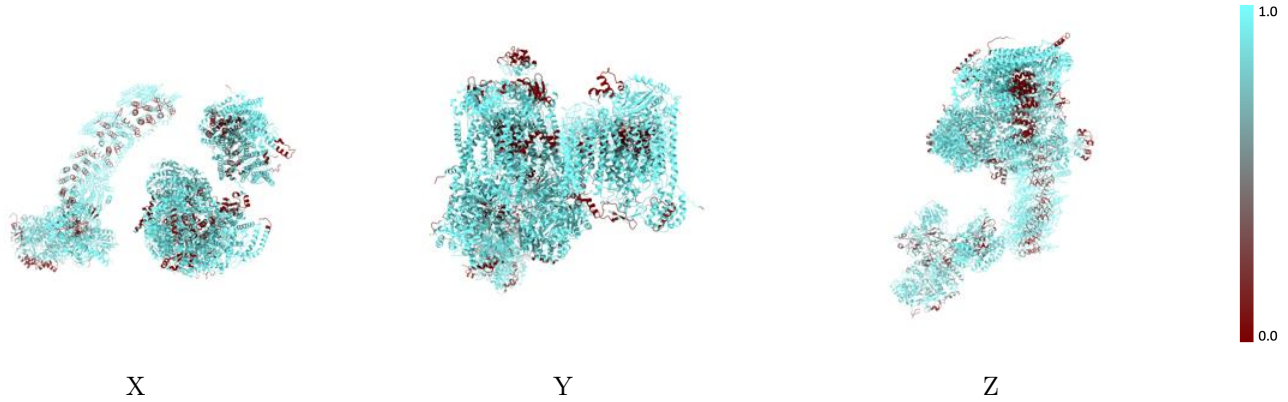
The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



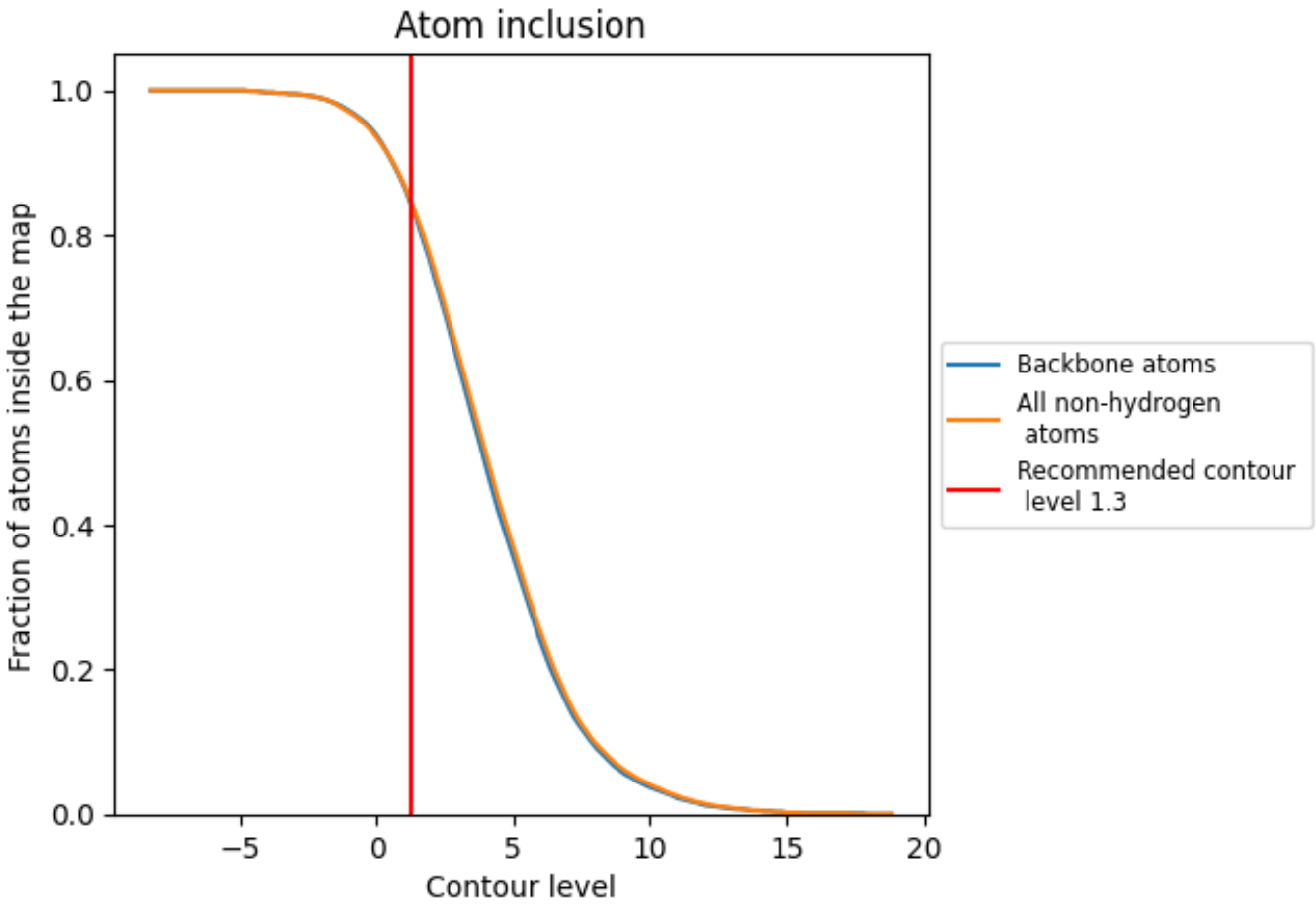
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.3).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.0170
1	0.8930	0.0350
2	0.7620	0.0130
3	0.8340	0.0270
4	0.7930	-0.0220
5	0.8620	-0.0010
6	0.9050	0.0170
7	0.6070	-0.0040
8	0.9860	0.0240
A	0.9030	0.0290
B	0.8770	0.0320
C	0.8100	0.0030
D	0.9790	0.0410
E	0.6420	-0.0200
F	0.9990	0.0630
G	0.9840	0.0320
H	0.8670	0.0440
I	0.8380	0.0050
J	0.9430	0.0100
K	0.6000	-0.0350
L	0.7930	-0.0120
M	1.0000	0.0490
N	0.9200	0.0280
O	0.8660	0.0450
P	0.8330	0.0410
Q	0.4720	-0.0070
R	0.8910	0.0240
S	0.5920	-0.0160
T	0.9810	0.0360
U	0.8390	0.0360
V	0.7330	0.0010
W	0.8630	0.0270
X	0.6390	-0.0240
Y	0.4550	0.0100
a	0.9850	0.0300

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Chain	Atom inclusion	Q-score
b	0.9430	0.0450
c	0.8190	-0.0010
d	0.9330	0.0440
e	0.6120	-0.0070
f	0.6280	0.0300
g	0.8820	0.0310
h	0.9720	0.0510
i	0.9350	-0.0200
j	0.8400	0.0400
k	1.0000	0.1370
m	0.7620	-0.0190
n	0.7310	-0.0200
o	0.7370	-0.0140
p	0.8050	0.0010