Full wwPDB EM Validation Report

Oct 26, 2026 – 02:41 PM EDT

PDB ID	:	9OCV / pdb_00009ocv
EMDB ID	:	EMD-70333
Title	:	Cryo-EM structure of the CIII2CIV1 respiratory supercomplex from Bacillus subtilis
Authors	:	Zheng, W.; Gu, M.; Zong, Y.; Zhu, J.; Zhang, K.
Deposited on	:	2025-04-25
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

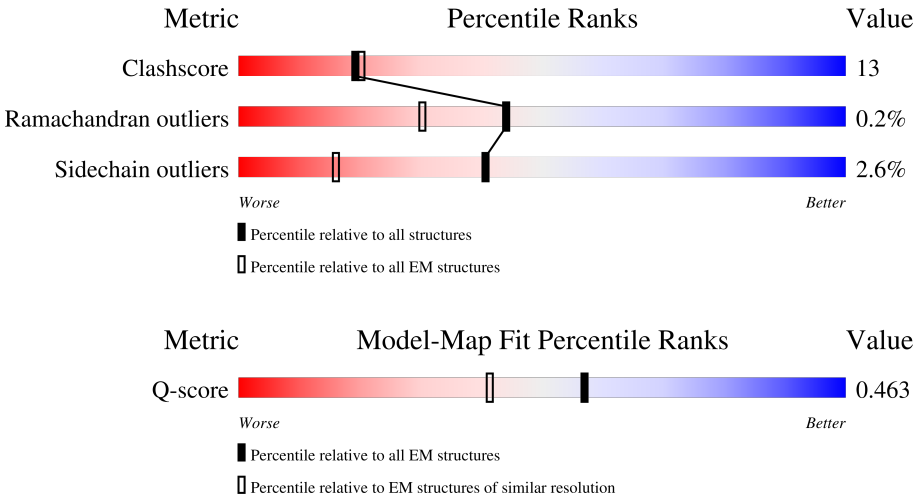
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



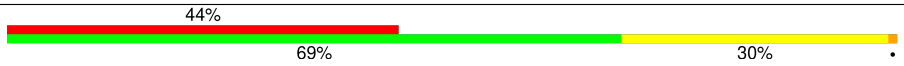
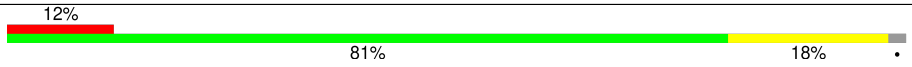
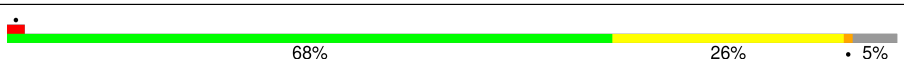
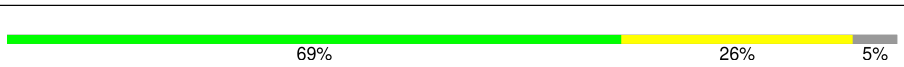
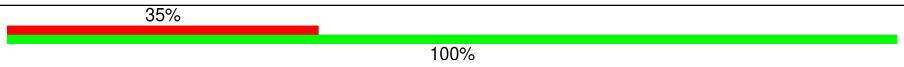
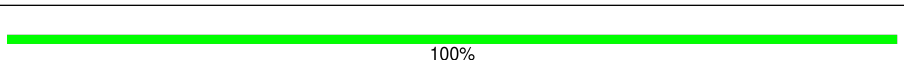
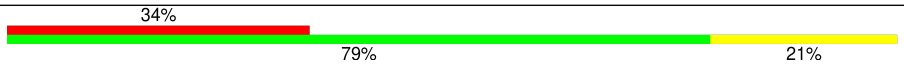
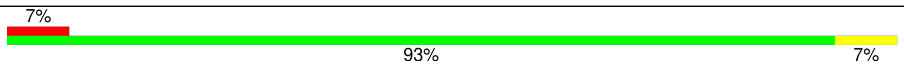
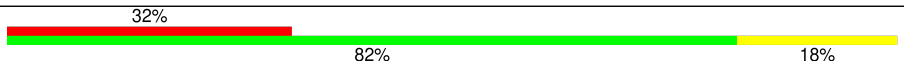
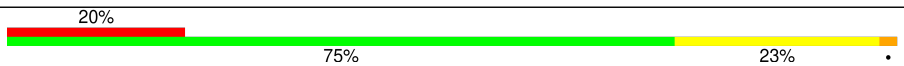
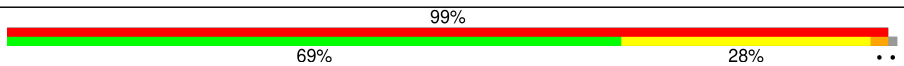
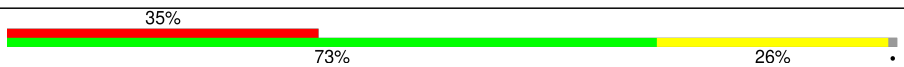
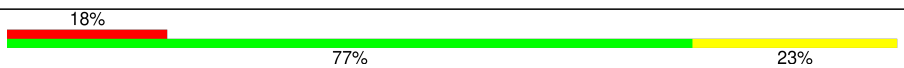
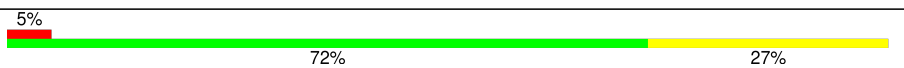
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	A	167	71% 68% 29%
1	a	167	68% 68% 25% 5%
2	B	224	62% 37%
2	b	224	69% 29%

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Mol	Chain	Length	Quality of chain
3	C	255	
3	c	255	
4	D	57	
4	d	57	
5	E	81	
5	e	81	
6	F	23	
6	f	23	
7	G	29	
7	g	29	
8	H	44	
8	h	44	
9	I	120	
9	i	120	
10	J	120	
11	K	110	
12	L	207	
13	M	622	
14	N	356	

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
15	FES	A	201	-	-	X	-
18	HEC	B	305	X	-	-	-
18	HEC	C	301	X	-	-	-
18	HEC	J	201	X	-	-	-
18	HEC	N	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEC	b	304	X	-	-	-
18	HEC	c	302	X	-	-	-
23	HAS	M	701	X	-	-	-
23	HAS	M	702	X	-	-	-

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 27762 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 Menaquinol:cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	163	Total	C	N	O	S	0	0
			1290	825	216	239	10		
1	a	158	Total	C	N	O	S	0	0
			1255	804	208	234	9		

- Molecule 2 is a protein called Menaquinol:cytochrome c reductase cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1804	1207	292	293	12		
2	b	224	Total	C	N	O	S	0	0
			1804	1207	292	293	12		

- Molecule 3 is a protein called Menaquinol:cytochrome c reductase cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	255	Total	C	N	O	S	0	0
			1986	1293	325	357	11		
3	c	255	Total	C	N	O	S	0	0
			1985	1292	325	357	11		

- Molecule 4 is a protein called YqgW.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	56	Total	C	N	O	S	0	0
			433	297	68	66	2		
4	d	56	Total	C	N	O	S	0	0
			433	297	68	66	2		

- Molecule 5 is a protein called YqgY.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	77	Total	C	N	O	S	0	0
			645	447	91	101	6		
5	e	77	Total	C	N	O	S	0	0
			645	447	91	101	6		

- Molecule 6 is a protein called QcrF.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	23	Total	C	N	O	0	0
			114	69	23	22		
6	f	23	Total	C	N	O	0	0
			114	69	23	22		

- Molecule 7 is a protein called QcrG.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	29	Total	C	N	O	S	0	0
			221	147	32	39	3		
7	g	29	Total	C	N	O	S	0	0
			221	147	32	39	3		

- Molecule 8 is a protein called Uncharacterized membrane protein YqzM.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	44	Total	C	N	O	S	0	0
			342	223	55	62	2		
8	h	44	Total	C	N	O	S	0	0
			342	223	55	62	2		

- Molecule 9 is a protein called YlbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	119	Total	C	N	O	S	0	0
			941	603	153	181	4		
9	i	119	Total	C	N	O	S	0	0
			941	603	153	181	4		

- Molecule 10 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	120	Total	C	N	O	S	0	0
			895	567	147	176	5		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 4B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	110	Total	C	N	O	S	0	0
			894	604	141	144	5		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	207	Total	C	N	O	S	0	0
			1647	1104	251	282	10		

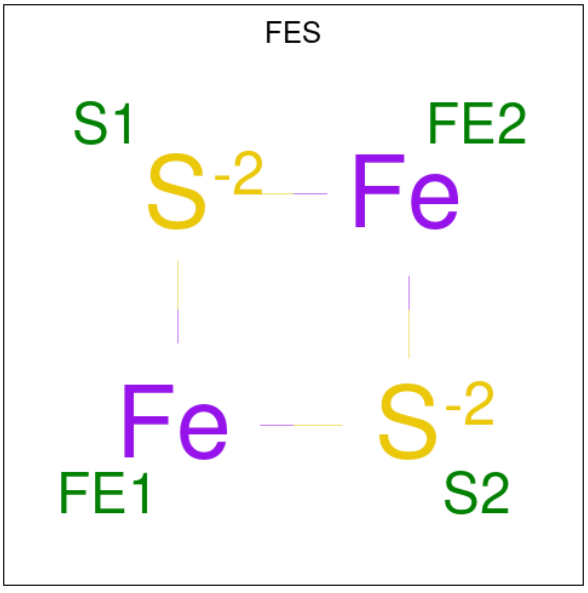
- Molecule 13 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	603	Total	C	N	O	S	0	0
			4748	3206	745	771	26		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 2.

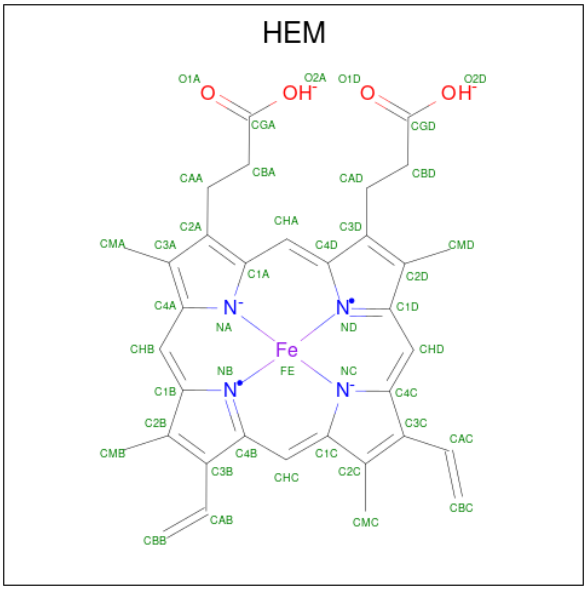
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	335	Total	C	N	O	S	0	0
			2649	1704	437	496	12		

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



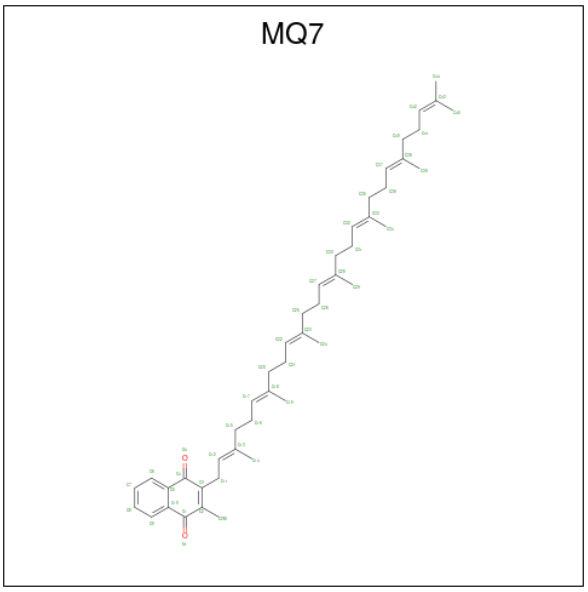
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total Fe S 4 2 2	0
15	a	1	Total Fe S 4 2 2	0

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



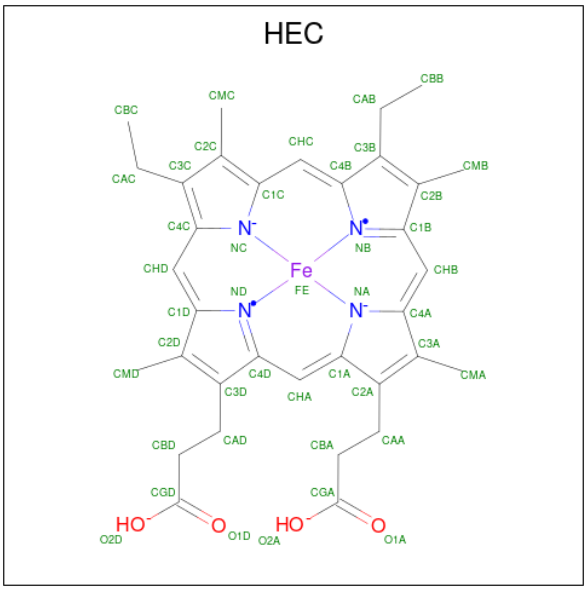
Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total C Fe N O 43 34 1 4 4	0
16	B	1	Total C Fe N O 43 34 1 4 4	0
16	b	1	Total C Fe N O 43 34 1 4 4	0
16	b	1	Total C Fe N O 43 34 1 4 4	0

- Molecule 17 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



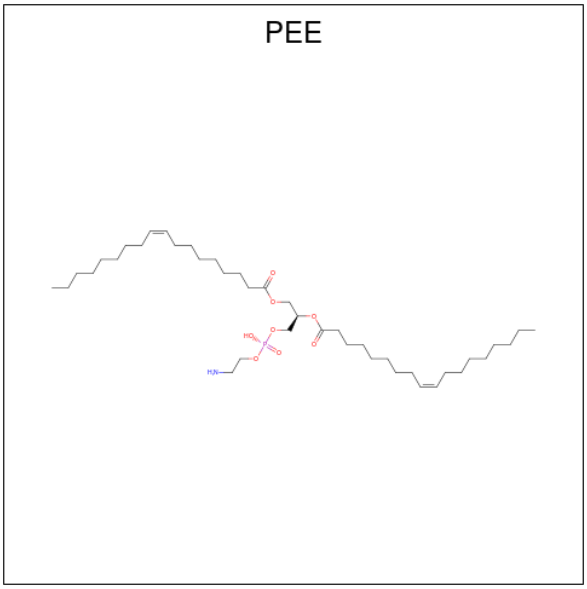
Mol	Chain	Residues	Atoms	AltConf
17	B	1	Total C O 48 46 2	0
17	B	1	Total C O 48 46 2	0
17	b	1	Total C O 48 46 2	0
17	c	1	Total C O 48 46 2	0

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



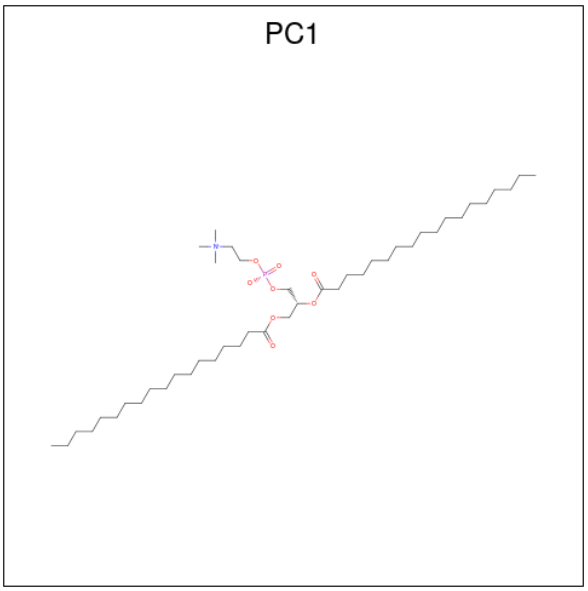
Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	c	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 19 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



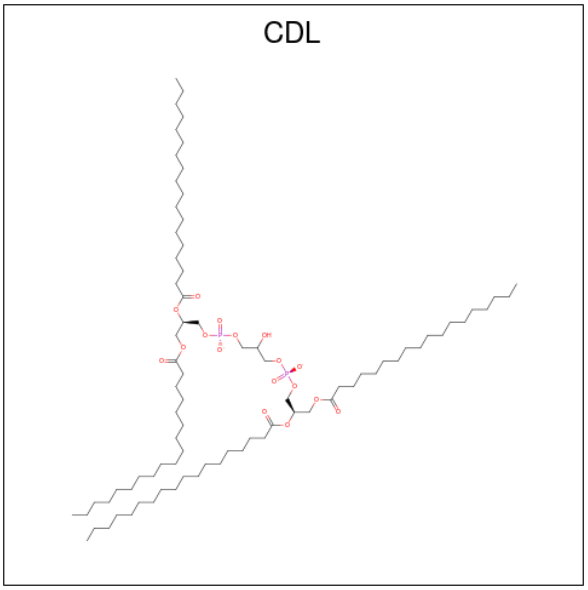
Mol	Chain	Residues	Atoms					AltConf
19	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
19	J	1	Total	C	N	O	P	0
			40	30	1	8	1	
19	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
19	c	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 20 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
20	C	1	Total	C	N	O	P	0
			48	38	1	8	1	
20	c	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 21 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



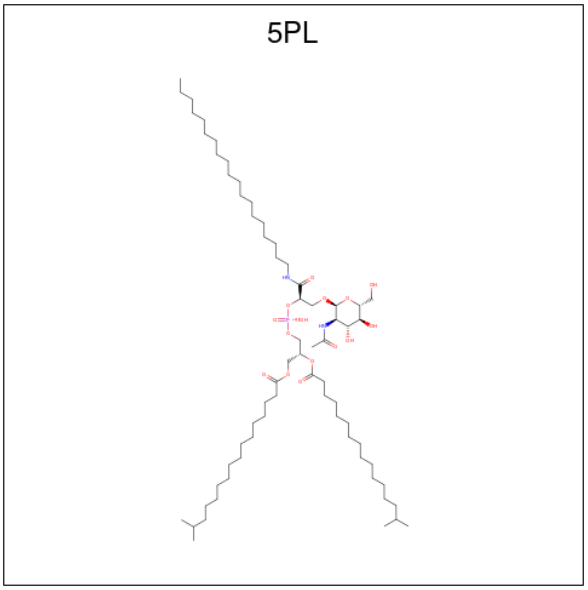
Mol	Chain	Residues	Atoms				AltConf
21	J	1	Total	C	O	P	0
			100	81	17	2	
21	K	1	Total	C	O	P	0
			100	81	17	2	

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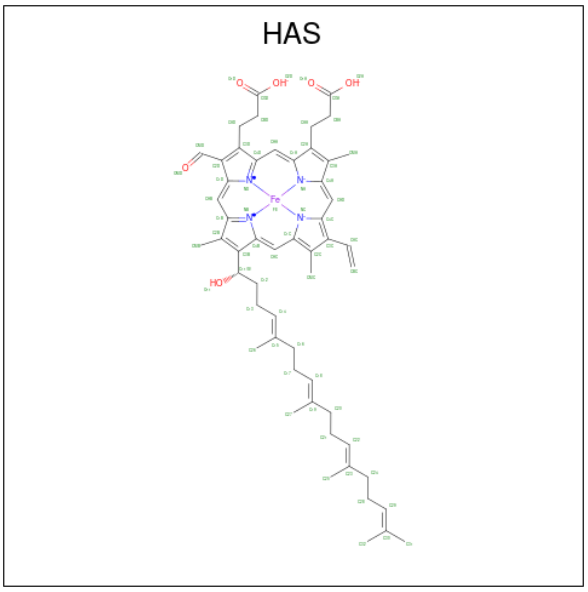
Mol	Chain	Residues	Atoms				AltConf
21	L	1	Total	C	O	P	0
			98	79	17	2	

- Molecule 22 is (1R,4S,6R)-6-({[2-(ACETYLAMINO)-2-DEOXY-ALPHA-D-GLUCOPYRANOSYL]OXY}METHYL)-4-HYDROXY-1-{[(15-METHYLHEXADECANOYL)OXY]METHYL}-4-OXIDO-7-OXO-3,5-DIOXA-8-AZA-4-PHOSPHAHEPTACOS-1-YL 15-METHYLHEXADECANOATE (CCD ID: 5PL) (formula: $C_{67}H_{129}N_2O_{15}P$).



Mol	Chain	Residues	Atoms					AltConf
22	L	1	Total	C	N	O	P	0
			85	67	2	15	1	

- Molecule 23 is HEME-AS (CCD ID: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
23	M	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
23	M	1	Total	C	Fe	N	O	0
			65	54	1	4	6	

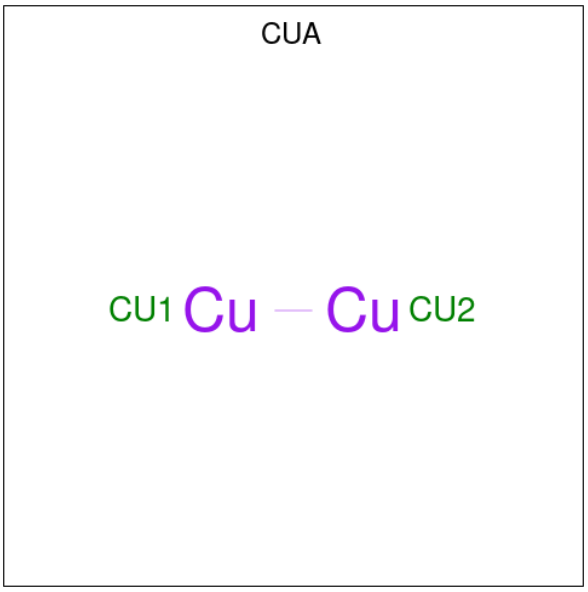
- Molecule 24 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
24	M	1	Total	Cu	0
			1	1	

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	M	1	Total	Mg	0
			1	1	

- Molecule 26 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



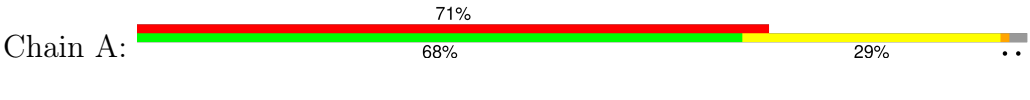
Mol	Chain	Residues	Atoms		AltConf
26	N	1	Total	Cu	0
			2	2	

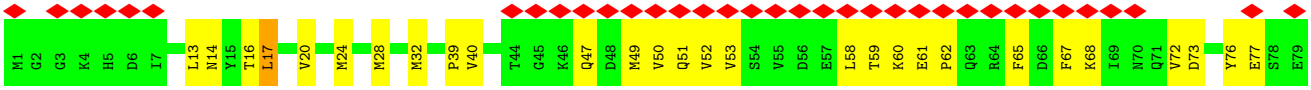
3 Residue-property plots (i)

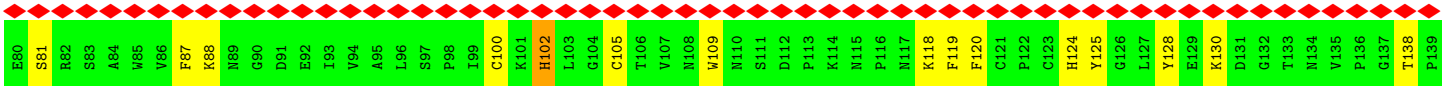
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

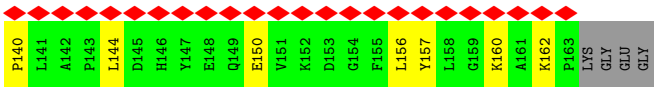
• Molecule 1: Menaquinol:cytochrome c reductase iron-sulfur subunit

Chain A:





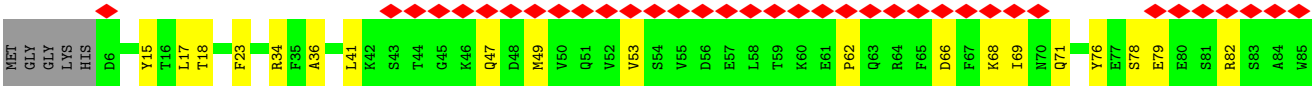


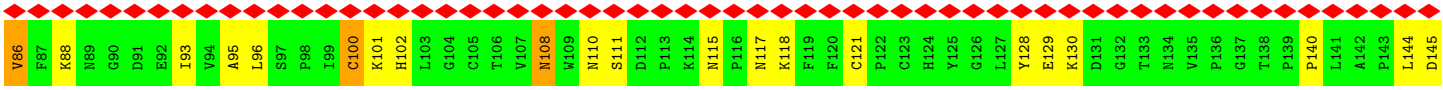


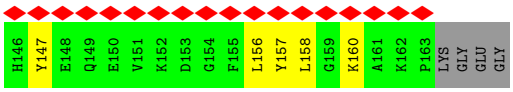
• Molecule 1: Menaquinol:cytochrome c reductase iron-sulfur subunit

Chain a:





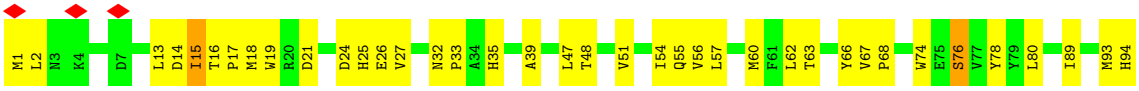


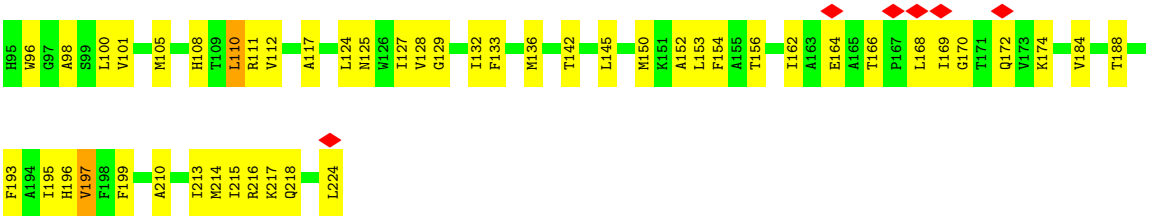


• Molecule 2: Menaquinol:cytochrome c reductase cytochrome b subunit

Chain B:



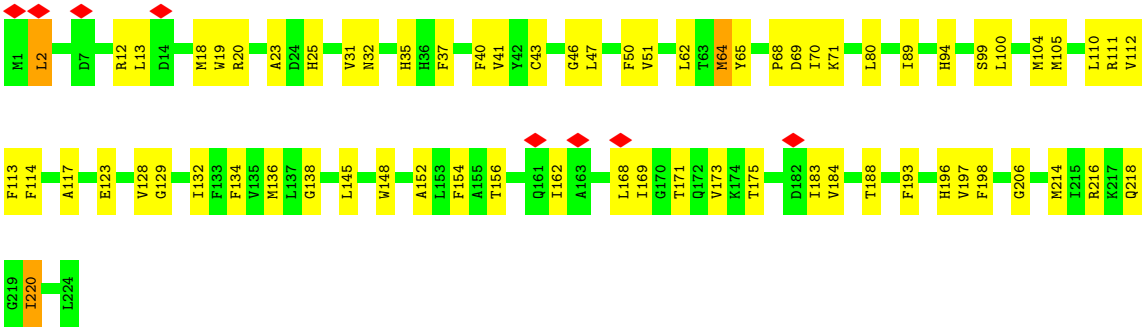




• Molecule 2: Menaquinol:cytochrome c reductase cytochrome b subunit

Chain b:

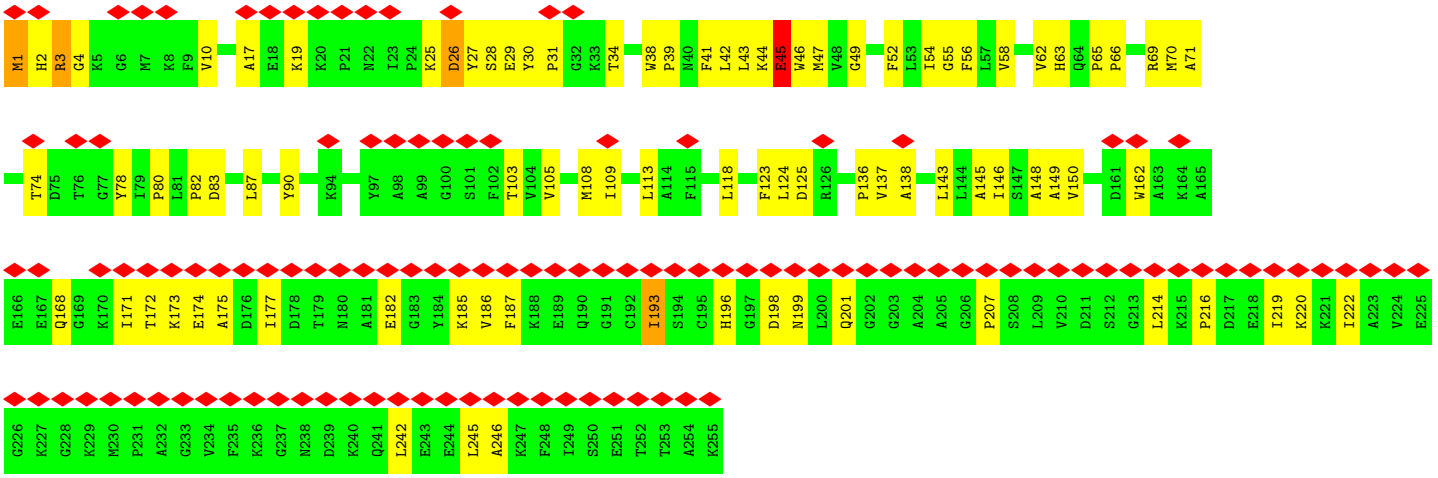




• Molecule 3: Menaquinol:cytochrome c reductase cytochrome c subunit

Chain C:

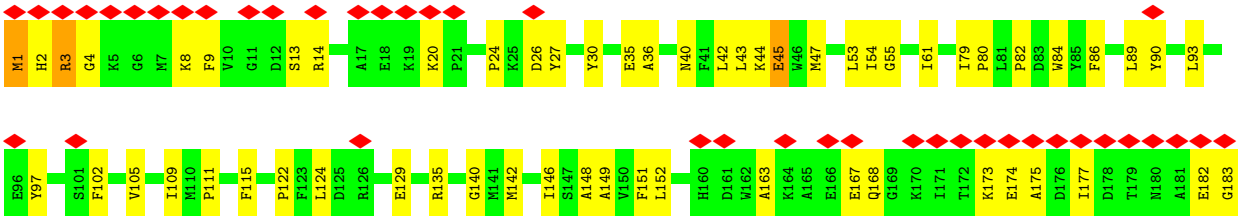


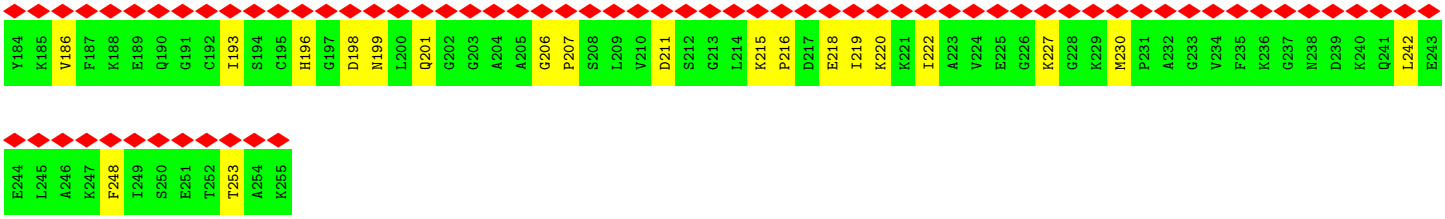


• Molecule 3: Menaquinol:cytochrome c reductase cytochrome c subunit

Chain c:



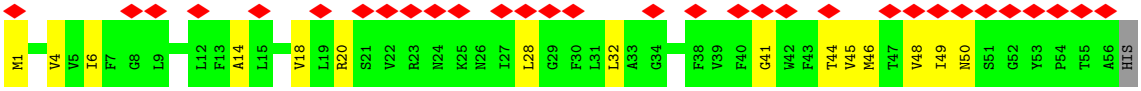




• Molecule 4: YqgW

Chain D:

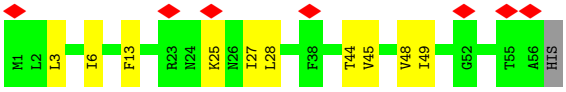




• Molecule 4: YqgW

Chain d:

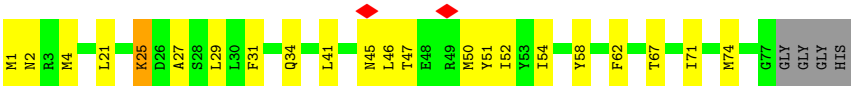




• Molecule 5: YqgY

Chain E:

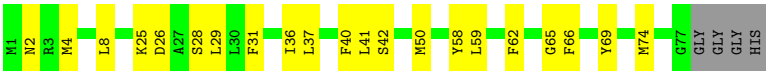




• Molecule 5: YqgY

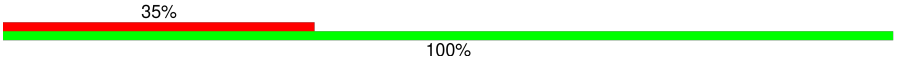
Chain e:

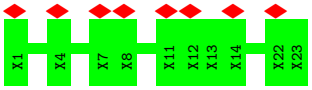




• Molecule 6: QcrF

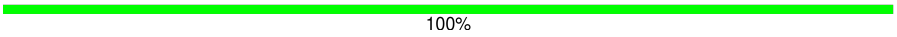
Chain F:





• Molecule 6: QcrF

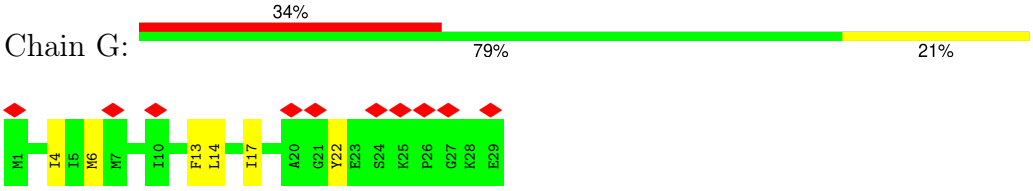
Chain f:



There are no outlier residues recorded for this chain.

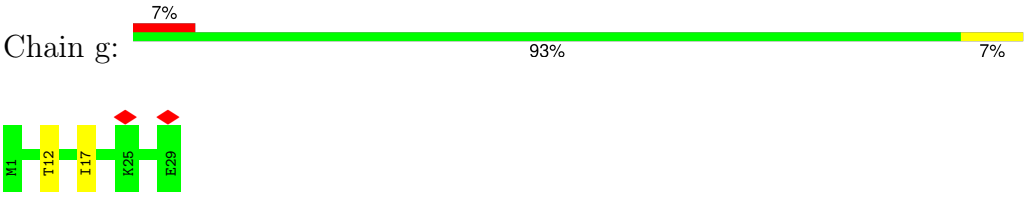
• Molecule 7: QcrG

Chain G:



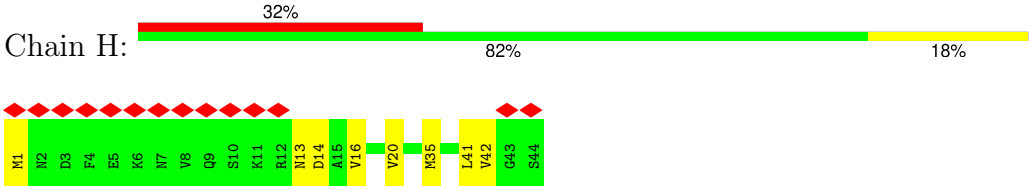
• Molecule 7: QcrG

Chain g:



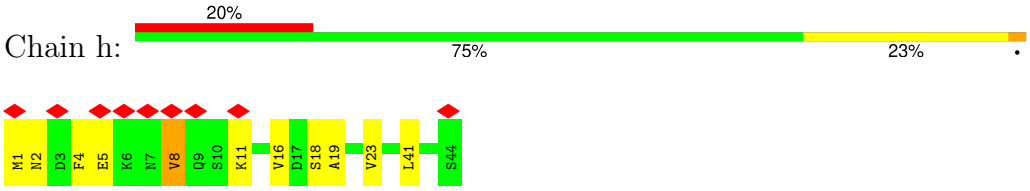
• Molecule 8: Uncharacterized membrane protein YqzM

Chain H:



• Molecule 8: Uncharacterized membrane protein YqzM

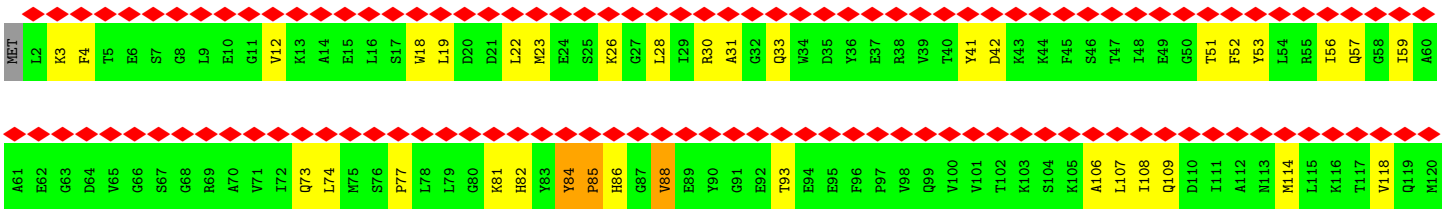
Chain h:



• Molecule 9: YlbA

Chain I:

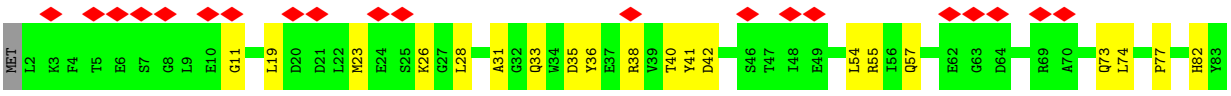


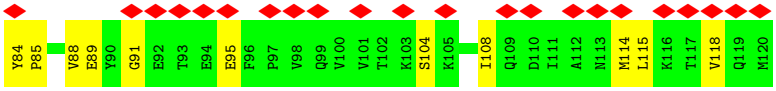


• Molecule 9: YlbA

Chain i:



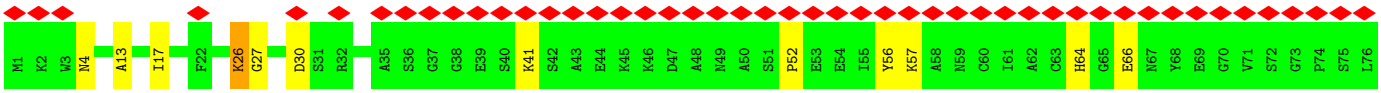


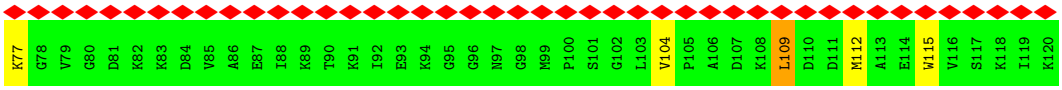


• Molecule 10: Cytochrome c-550

Chain J:



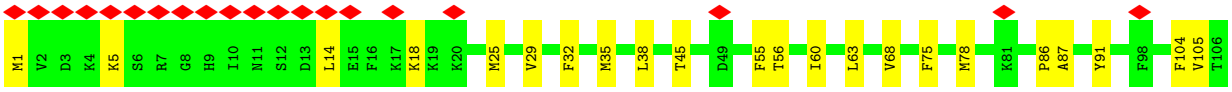




• Molecule 11: Cytochrome c oxidase subunit 4B

Chain K:



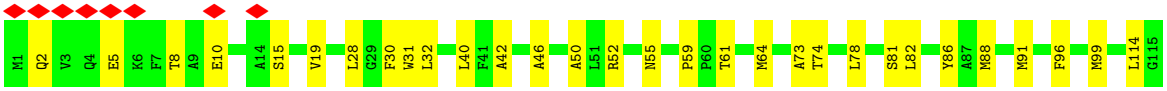


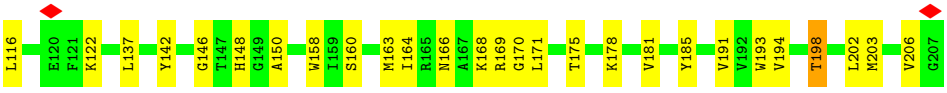


• Molecule 12: Cytochrome c oxidase subunit 3

Chain L:



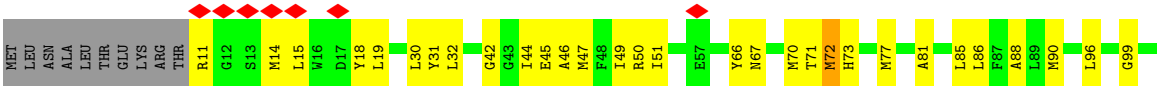


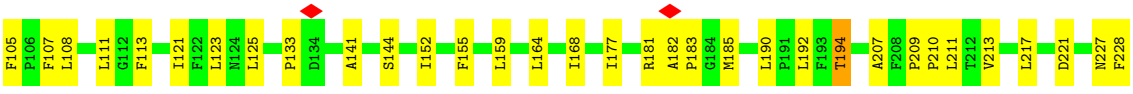


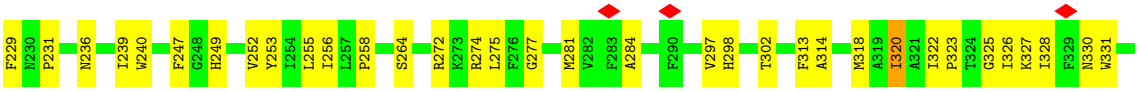
• Molecule 13: Cytochrome c oxidase subunit 1

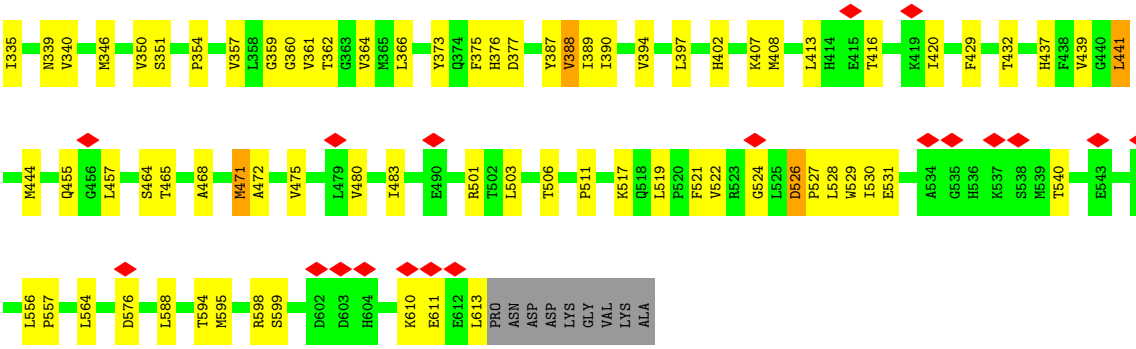
Chain M:







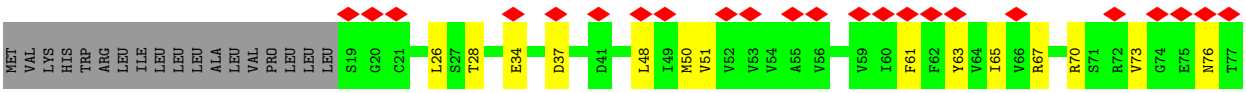


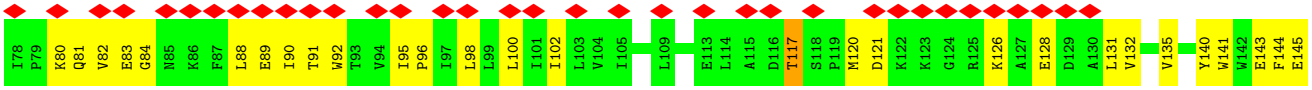


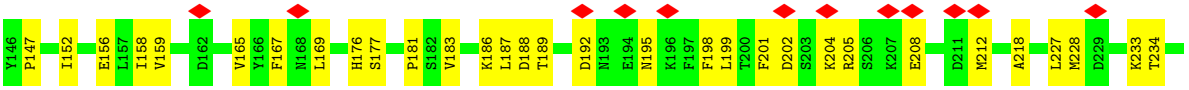
• Molecule 14: Cytochrome c oxidase subunit 2

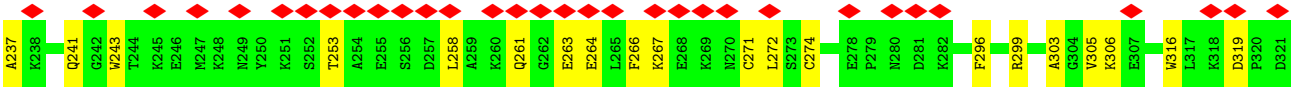
Chain N:

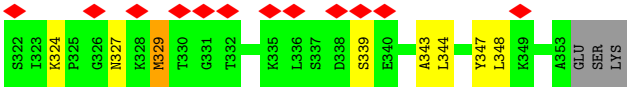












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70713	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.641	Depositor
Minimum map value	-0.412	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	297.0, 297.0, 297.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: 5PL, FES, HEM, CDL, CU, CUA, HEC, PEE, MQ7, HAS, MG, PC1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.15	0/1326	0.39	0/1796
1	a	0.14	0/1290	0.35	0/1750
2	B	0.18	0/1863	0.35	0/2533
2	b	0.18	0/1863	0.36	0/2533
3	C	0.15	0/2040	0.42	1/2759 (0.0%)
3	c	0.17	0/2039	0.41	0/2757
4	D	0.14	0/444	0.32	0/605
4	d	0.14	0/444	0.31	0/605
5	E	0.10	0/667	0.23	0/900
5	e	0.14	0/667	0.28	0/900
7	G	0.13	0/224	0.34	0/299
7	g	0.12	0/224	0.25	0/299
8	H	0.10	0/349	0.30	0/468
8	h	0.18	0/349	0.41	0/468
9	I	0.14	0/959	0.38	0/1291
9	i	0.15	0/959	0.38	0/1291
10	J	0.18	0/910	0.45	2/1221 (0.2%)
11	K	0.13	0/920	0.31	0/1243
12	L	0.13	0/1698	0.27	0/2304
13	M	0.15	0/4912	0.35	0/6695
14	N	0.15	0/2706	0.34	0/3660
All	All	0.15	0/26853	0.36	3/36377 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	26	LYS	CA-CB-CG	-8.02	98.05	114.10
10	J	26	LYS	CD-CE-NZ	5.52	129.56	111.90
3	C	45	GLU	CA-CB-CG	5.21	124.51	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	15	ILE	Peptide
9	I	84	TYR	Peptide
1	a	82	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1290	0	1254	38	0
1	a	1255	0	1217	32	0
2	B	1804	0	1813	88	0
2	b	1804	0	1813	61	0
3	C	1986	0	1999	85	0
3	c	1985	0	1993	81	0
4	D	433	0	463	9	0
4	d	433	0	463	8	0
5	E	645	0	642	18	0
5	e	645	0	642	20	0
6	F	114	0	25	0	0
6	f	114	0	26	0	0
7	G	221	0	241	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	g	221	0	241	1	0
8	H	342	0	334	6	0
8	h	342	0	334	10	0
9	I	941	0	938	30	0
9	i	941	0	938	29	0
10	J	895	0	906	12	0
11	K	894	0	923	28	0
12	L	1647	0	1645	44	0
13	M	4748	0	4773	128	0
14	N	2649	0	2679	71	0
15	A	4	0	0	2	0
15	a	4	0	0	0	0
16	B	86	0	60	11	0
16	b	86	0	60	5	0
17	B	96	0	128	11	0
17	b	48	0	64	3	0
17	c	48	0	64	6	0
18	B	43	0	30	9	0
18	C	43	0	29	2	0
18	J	43	0	30	0	0
18	N	43	0	32	4	0
18	b	43	0	31	7	0
18	c	43	0	25	7	0
19	C	42	0	54	6	0
19	J	40	0	52	4	0
19	L	51	0	78	3	0
19	c	42	0	52	3	0
20	C	48	0	73	4	0
20	c	43	0	60	1	0
21	J	100	0	154	7	0
21	K	100	0	156	7	0
21	L	98	0	149	6	0
22	L	85	0	128	11	0
23	M	130	0	124	14	0
24	M	1	0	0	0	0
25	M	1	0	0	0	0
26	N	2	0	0	0	0
All	All	27762	0	27935	704	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 13.

All (704) 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)
1:A:105:CYS:HB2	15:A:201:FES:S2	1.98	1.02
9:I:86:HIS:HB2	3:c:1:MET:HB2	1.59	0.83
1:a:49:MET:HE2	1:a:157:TYR:HB3	1.64	0.80
3:c:105:VAL:HA	3:c:109:ILE:HB	1.63	0.80
2:B:33:PRO:HG2	5:E:4:MET:HE1	1.62	0.80
3:c:174:GLU:HA	3:c:201:GLN:HE21	1.50	0.76
13:M:357:VAL:O	13:M:361:VAL:HG23	1.87	0.75
3:c:79:ILE:H	3:c:168:GLN:HE22	1.31	0.75
7:G:14:LEU:HA	7:G:17:ILE:HD12	1.70	0.74
2:B:110:LEU:HD11	3:C:146:ILE:HD11	1.69	0.74
3:C:222:ILE:HD13	18:C:301:HEC:HAA1	1.68	0.74
9:I:4:PHE:HB2	9:I:77:PRO:HG2	1.69	0.72
13:M:231:PRO:HB3	14:N:192:ASP:HB3	1.70	0.72
2:B:184:VAL:HG13	2:B:188:THR:HG21	1.72	0.71
1:a:96:LEU:HD13	1:a:144:LEU:HD13	1.71	0.71
2:B:150:MET:HE2	3:C:69:ARG:HH12	1.54	0.70
3:C:125:ASP:HB2	19:C:302:PEE:H8	1.74	0.69
9:I:114:MET:HA	9:I:114:MET:HE3	1.75	0.69
12:L:122:LYS:HG2	21:L:302:CDL:H322	1.73	0.69
1:A:138:THR:HG22	1:A:140:PRO:HD2	1.75	0.69
2:B:19:TRP:HE1	8:H:14:ASP:HB3	1.57	0.69
2:B:166:THR:HB	2:B:170:GLY:HA2	1.74	0.69
2:B:217:LYS:HE3	17:B:304:MQ7:H212	1.75	0.68
1:A:32:MET:HE2	2:B:93:MET:HE1	1.76	0.68
2:b:220:ILE:HD12	18:b:304:HEC:HAD1	1.76	0.68
12:L:160:SER:O	12:L:164:ILE:HG12	1.94	0.68
14:N:169:LEU:HB3	14:N:189:THR:HG22	1.77	0.67
13:M:366:LEU:HD22	23:M:702:HAS:HBD2	1.77	0.67
3:c:8:LYS:HD3	3:c:9:PHE:H	1.59	0.66
2:B:48:THR:HG22	16:B:302:HEM:HBC2	1.77	0.66
13:M:105:PHE:HB2	13:M:108:LEU:HB2	1.78	0.66
9:i:82:HIS:HA	9:i:88:VAL:H	1.59	0.66
14:N:63:TYR:O	14:N:67:ARG:HB3	1.96	0.65
13:M:49:ILE:HD11	13:M:70:MET:HA	1.77	0.65
2:B:210:ALA:O	2:B:214:MET:HG3	1.97	0.65
10:J:4:ASN:HD22	19:J:203:PEE:H9	1.60	0.65
9:I:28:LEU:HB3	9:I:41:TYR:HB3	1.77	0.65
13:M:472:ALA:HA	23:M:701:HAS:H161	1.79	0.65
3:C:105:VAL:HA	3:C:109:ILE:HB	1.77	0.64
18:B:305:HEC:CAC	3:C:45:GLU:HB2	2.27	0.64
2:b:216:ARG:HG2	18:b:304:HEC:HBA2	1.80	0.64
10:J:27:GLY:HA2	10:J:30:ASP:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:184:VAL:HG13	2:b:188:THR:HG21	1.78	0.64
2:B:213:ILE:HG21	17:B:304:MQ7:H22	1.80	0.64
4:D:44:THR:O	4:D:48:VAL:HG23	1.98	0.64
13:M:190:LEU:HD22	13:M:194:THR:HG21	1.79	0.64
11:K:14:LEU:O	11:K:18:LYS:HG2	1.98	0.64
13:M:177:ILE:HD12	13:M:194:THR:HG23	1.80	0.64
14:N:183:VAL:HG12	14:N:199:LEU:HD22	1.79	0.64
2:b:154:PHE:HB3	3:c:80:PRO:HB3	1.80	0.64
13:M:325:GLY:HA2	23:M:702:HAS:H271	1.79	0.63
5:e:25:LYS:HA	5:e:28:SER:HB3	1.79	0.63
9:i:54:LEU:HD11	9:i:108:ILE:HD11	1.81	0.63
2:B:62:LEU:HD22	2:B:80:LEU:HD21	1.78	0.63
21:K:201:CDL:H601	21:K:201:CDL:H362	1.82	0.62
13:M:32:LEU:HD13	13:M:408:MET:HE1	1.81	0.62
2:b:2:LEU:HD22	8:h:16:VAL:HG13	1.82	0.62
9:i:35:ASP:HB3	9:i:38:ARG:HB2	1.80	0.62
4:D:14:ALA:O	4:D:18:VAL:HG23	1.99	0.62
2:b:18:MET:HE3	2:b:18:MET:HA	1.81	0.61
1:A:49:MET:HE3	1:A:50:VAL:H	1.63	0.61
1:a:18:THR:HG21	8:h:18:SER:HB2	1.82	0.61
18:B:305:HEC:HMC3	3:C:41:PHE:CZ	2.35	0.61
22:L:303:5PL:HAE2	13:M:168:ILE:HG12	1.83	0.61
2:b:110:LEU:HD21	3:c:146:ILE:HD11	1.81	0.61
3:c:79:ILE:H	3:c:168:GLN:NE2	1.97	0.61
1:a:49:MET:HE3	1:a:49:MET:HA	1.83	0.61
13:M:144:SER:HB3	13:M:152:ILE:HG21	1.81	0.61
9:I:23:MET:HB3	9:I:28:LEU:HB2	1.82	0.61
3:c:43:LEU:O	3:c:47:MET:HG3	2.01	0.61
13:M:42:GLY:HA3	13:M:77:MET:HG3	1.83	0.61
13:M:133:PRO:HG3	13:M:155:PHE:HB2	1.83	0.61
11:K:60:ILE:HG22	12:L:198:THR:HG23	1.83	0.60
4:d:45:VAL:O	4:d:49:ILE:HG12	2.00	0.60
1:a:100:CYS:SG	1:a:102:HIS:HB3	2.41	0.60
2:B:55:GLN:HE22	2:B:98:ALA:N	1.99	0.60
12:L:59:PRO:HG2	12:L:64:MET:HE3	1.82	0.60
1:A:39:PRO:HB2	2:b:175:THR:HG22	1.82	0.60
3:C:193:ILE:HG23	3:C:198:ASP:HA	1.82	0.60
18:b:304:HEC:C1C	3:c:45:GLU:HG3	2.32	0.60
2:B:145:LEU:HA	2:B:152:ALA:HB1	1.83	0.60
16:B:302:HEM:HHC	16:B:302:HEM:HBB2	1.84	0.60
1:a:118:LYS:HG2	1:a:129:GLU:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:364:VAL:HG11	14:N:50:MET:HE1	1.82	0.60
13:M:501:ARG:HB3	13:M:526:ASP:HB3	1.83	0.60
9:i:40:THR:HG21	9:i:55:ARG:HH21	1.66	0.60
3:c:196:HIS:HE1	18:c:302:HEC:NA	1.99	0.59
2:B:35:HIS:HE1	9:I:31:ALA:HB1	1.66	0.59
2:B:133:PHE:HB2	16:B:302:HEM:HBB1	1.84	0.59
21:J:202:CDL:H471	12:L:191:VAL:HG11	1.84	0.59
2:b:89:ILE:HG13	5:e:74:MET:HE1	1.84	0.59
14:N:344:LEU:HD12	18:N:401:HEC:HBC1	1.84	0.59
3:c:79:ILE:N	3:c:168:GLN:HE22	2.01	0.59
2:B:67:VAL:HG11	2:b:69:ASP:HB2	1.85	0.58
8:h:4:PHE:HE1	9:i:38:ARG:HE	1.49	0.58
2:B:154:PHE:HB3	3:C:80:PRO:HB3	1.84	0.58
12:L:166:ASN:HD22	12:L:169:ARG:HD3	1.68	0.58
13:M:339:ASN:HB2	14:N:73:VAL:HG11	1.85	0.58
14:N:263:GLU:HA	14:N:347:TYR:CE2	2.38	0.58
2:b:99:SER:HB3	3:c:84:TRP:HE1	1.68	0.58
2:b:145:LEU:HA	2:b:152:ALA:HB1	1.85	0.58
2:b:62:LEU:HD22	2:b:80:LEU:HD11	1.85	0.58
3:C:4:GLY:HA3	9:i:85:PRO:HD2	1.86	0.58
16:B:301:HEM:HBB2	16:B:301:HEM:HHC	1.84	0.58
14:N:187:LEU:HD13	14:N:195:ASN:HB3	1.86	0.58
14:N:296:PHE:HD2	14:N:348:LEU:HB3	1.68	0.58
13:M:346:MET:O	13:M:350:VAL:HG12	2.04	0.57
17:B:303:MQ7:H8	3:C:90:TYR:CD1	2.39	0.57
2:b:123:GLU:HG2	3:c:122:PRO:HB3	1.85	0.57
9:I:84:TYR:O	9:I:84:TYR:HD1	1.88	0.57
14:N:202:ASP:HB3	14:N:205:ARG:HB2	1.86	0.57
3:C:220:LYS:HG2	3:C:242:LEU:HG	1.86	0.57
3:C:143:LEU:HA	3:C:146:ILE:HD12	1.86	0.57
1:a:88:LYS:HG2	1:a:93:ILE:HD12	1.87	0.57
11:K:45:THR:HG22	11:K:56:THR:HG23	1.86	0.57
2:B:66:TYR:HA	2:B:76:SER:OG	2.04	0.57
2:B:169:ILE:HG23	2:B:172:GLN:HB2	1.86	0.57
1:A:72:VAL:HG12	1:A:77:GLU:HG3	1.87	0.56
13:M:86:LEU:HD22	13:M:258:PRO:HB2	1.87	0.56
13:M:47:MET:O	13:M:51:ILE:HD12	2.05	0.56
13:M:328:ILE:HA	13:M:331:TRP:HE3	1.71	0.56
2:b:19:TRP:O	2:b:23:ALA:HB3	2.03	0.56
13:M:185:MET:HE2	13:M:522:VAL:HG21	1.88	0.56
1:A:52:VAL:HB	1:A:67:PHE:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:LEU:HD22	3:C:71:ALA:HB1	1.87	0.56
11:K:68:VAL:HG22	12:L:191:VAL:HG13	1.88	0.56
13:M:361:VAL:HG13	14:N:50:MET:HG2	1.88	0.56
2:B:125:ASN:HD21	2:B:215:ILE:HG13	1.70	0.56
12:L:91:MET:HB2	12:L:99:MET:SD	2.45	0.56
2:b:35:HIS:HE1	9:i:31:ALA:HB1	1.71	0.56
2:b:50:PHE:HZ	3:c:53:LEU:HD22	1.71	0.56
9:i:35:ASP:HB3	9:i:38:ARG:CG	2.36	0.56
2:B:15:ILE:HD12	2:B:18:MET:HB2	1.88	0.55
2:B:133:PHE:HD2	16:B:302:HEM:HBB1	1.71	0.55
9:i:35:ASP:OD1	9:i:36:TYR:N	2.39	0.55
12:L:40:LEU:HB2	13:M:209:PRO:HB3	1.88	0.55
2:b:206:GLY:HA3	17:c:301:MQ7:H401	1.88	0.55
2:B:19:TRP:NE1	8:H:14:ASP:HB3	2.22	0.55
4:D:49:ILE:HG13	4:D:50:ASN:OD1	2.05	0.55
1:A:119:PHE:HE1	1:A:130:LYS:HA	1.70	0.55
2:B:33:PRO:HA	2:B:39:ALA:HB3	1.89	0.55
13:M:46:ALA:HB2	13:M:73:HIS:CE1	2.42	0.55
21:L:302:CDL:H511	21:L:302:CDL:H761	1.89	0.55
13:M:77:MET:HA	13:M:81:ALA:HB3	1.89	0.55
3:c:89:LEU:HD21	3:c:111:PRO:HG3	1.88	0.55
3:C:3:ARG:HH21	9:i:89:GLU:HG2	1.71	0.55
3:c:47:MET:HE3	5:e:8:LEU:HD11	1.88	0.55
14:N:91:THR:HG22	14:N:95:ILE:HD11	1.89	0.55
13:M:14:MET:HE2	13:M:14:MET:HA	1.88	0.54
2:b:31:VAL:HG11	2:b:220:ILE:HG21	1.89	0.54
3:c:124:LEU:HB3	19:c:303:PEE:H8	1.89	0.54
14:N:117:THR:HG22	14:N:120:MET:HG3	1.89	0.54
13:M:50:ARG:HD3	13:M:465:THR:HA	1.89	0.54
2:B:108:HIS:HD2	16:B:302:HEM:NC	2.06	0.54
2:B:213:ILE:CG2	17:B:304:MQ7:H22	2.38	0.54
13:M:389:ILE:HG21	23:M:701:HAS:CAC	2.36	0.54
2:b:46:GLY:HA3	18:b:304:HEC:CHC	2.37	0.54
3:c:207:PRO:HG3	18:c:302:HEC:O1A	2.08	0.54
9:I:77:PRO:HG3	9:I:108:ILE:HG21	1.89	0.54
21:K:201:CDL:H182	21:K:201:CDL:H572	1.90	0.54
13:M:30:LEU:HB3	13:M:113:PHE:CZ	2.42	0.54
13:M:376:HIS:CD2	13:M:377:ASP:HB2	2.43	0.54
2:b:41:VAL:HG11	7:g:17:ILE:HA	1.88	0.54
14:N:176:HIS:ND1	14:N:228:MET:HE1	2.22	0.54
13:M:331:TRP:O	13:M:335:ILE:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:266:PHE:O	14:N:271:CYS:HB2	2.07	0.54
3:c:90:TYR:CD1	17:c:301:MQ7:H8	2.42	0.54
13:M:277:GLY:O	13:M:281:MET:HG2	2.08	0.54
1:A:62:PRO:HA	1:A:87:PHE:HB3	1.90	0.54
2:B:193:PHE:O	2:B:197:VAL:HB	2.08	0.54
9:I:19:LEU:O	9:I:23:MET:HG2	2.08	0.54
19:L:301:PEE:H68	5:e:40:PHE:HZ	1.71	0.54
13:M:72:MET:HE2	13:M:133:PRO:HD2	1.90	0.54
12:L:52:ARG:HA	12:L:137:LEU:HD13	1.88	0.53
3:C:150:VAL:HG22	20:C:303:PC1:H272	1.91	0.53
3:C:216:PRO:HA	3:C:246:ALA:HB1	1.90	0.53
13:M:517:LYS:HG3	13:M:613:LEU:HD23	1.90	0.53
2:b:112:VAL:HG13	2:b:117:ALA:HB3	1.89	0.53
11:K:45:THR:HA	5:e:29:LEU:HD13	1.90	0.53
13:M:85:LEU:HB3	13:M:397:LEU:HD22	1.90	0.53
5:E:67:THR:O	5:E:71:ILE:HB	2.09	0.53
3:C:136:PRO:HD2	4:D:20:ARG:HH22	1.73	0.53
3:C:138:ALA:HB2	19:C:302:PEE:H7	1.90	0.53
13:M:211:LEU:HB2	13:M:247:PHE:CG	2.44	0.53
13:M:387:TYR:HA	13:M:429:PHE:HZ	1.74	0.53
2:B:74:TRP:HB3	3:C:70:MET:HG3	1.90	0.53
9:i:11:GLY:HA2	9:i:73:GLN:HE21	1.72	0.53
13:M:99:GLY:HA3	13:M:182:ALA:HB2	1.90	0.52
3:C:124:LEU:HD11	4:D:32:LEU:HD12	1.90	0.52
9:I:12:VAL:HG13	9:I:74:LEU:HB2	1.91	0.52
12:L:8:THR:HG23	12:L:10:GLU:H	1.75	0.52
13:M:31:TYR:HB3	13:M:88:ALA:HB2	1.91	0.52
13:M:272:ARG:HH12	14:N:76:ASN:HA	1.75	0.52
2:B:133:PHE:CD2	16:B:302:HEM:HBB1	2.45	0.52
5:E:41:LEU:HD13	5:E:54:ILE:HD13	1.92	0.52
14:N:167:PHE:HE2	14:N:199:LEU:HB2	1.74	0.52
22:L:303:5PL:OCM	22:L:303:5PL:HBI1	2.09	0.52
3:c:24:PRO:HD2	8:h:11:LYS:HA	1.92	0.52
3:c:44:LYS:HG2	5:e:4:MET:HG2	1.91	0.52
1:A:150:GLU:HB3	1:A:157:TYR:HB2	1.92	0.52
13:M:387:TYR:HA	13:M:429:PHE:CZ	2.45	0.52
2:B:14:ASP:O	2:B:17:PRO:HD2	2.10	0.52
11:K:35:MET:HE2	12:L:78:LEU:HD11	1.91	0.52
13:M:44:ILE:HG12	23:M:701:HAS:H22	1.92	0.52
1:A:17:LEU:HD13	3:C:42:LEU:HB3	1.91	0.52
1:A:73:ASP:HB2	2:b:183:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:TRP:HD1	20:C:303:PC1:H153	1.75	0.52
9:i:33:GLN:HG3	9:i:40:THR:HB	1.90	0.52
2:B:218:GLN:HB3	3:c:13:SER:HB2	1.92	0.52
11:K:104:PHE:HE2	13:M:239:ILE:HG23	1.75	0.52
13:M:362:THR:HG21	13:M:437:HIS:NE2	2.25	0.52
2:B:13:LEU:HD21	2:b:214:MET:HG2	1.91	0.52
13:M:107:PHE:CE2	13:M:557:PRO:HD3	2.45	0.51
13:M:388:VAL:HG11	23:M:702:HAS:C2C	2.40	0.51
2:B:47:LEU:O	2:B:51:VAL:HG23	2.11	0.51
1:a:76:TYR:HE2	1:a:78:SER:HB3	1.75	0.51
2:b:105:MET:HE1	2:b:136:MET:HE3	1.92	0.51
3:c:54:ILE:HG12	5:e:62:PHE:CE2	2.46	0.51
2:B:150:MET:HE2	3:C:69:ARG:NH1	2.24	0.51
1:A:59:THR:HG23	1:A:61:GLU:H	1.75	0.51
1:A:68:LYS:HD2	1:A:81:SER:HA	1.93	0.51
12:L:88:MET:HE2	12:L:88:MET:HA	1.92	0.51
14:N:316:TRP:CZ2	14:N:329:MET:HG2	2.45	0.51
3:C:42:LEU:O	3:C:46:TRP:HB2	2.11	0.51
22:L:303:5PL:HAK2	13:M:164:LEU:HD11	1.92	0.51
13:M:297:VAL:HB	13:M:313:PHE:CG	2.45	0.51
2:b:47:LEU:O	2:b:51:VAL:HG23	2.11	0.51
2:B:145:LEU:HB2	2:B:156:THR:OG1	2.10	0.51
5:E:47:THR:HG23	5:E:50:MET:H	1.75	0.51
21:J:202:CDL:HA61	12:L:203:MET:SD	2.51	0.51
14:N:98:LEU:O	14:N:102:ILE:HG23	2.11	0.51
1:A:16:THR:HG21	5:E:52:ILE:HG12	1.93	0.51
3:C:3:ARG:NH2	9:i:89:GLU:HG2	2.26	0.51
3:C:118:LEU:HB2	19:C:302:PEE:H61	1.93	0.51
13:M:335:ILE:HG23	13:M:340:VAL:HG11	1.92	0.51
1:A:52:VAL:HG13	1:A:53:VAL:H	1.75	0.51
2:b:105:MET:HE2	16:b:302:HEM:HAB	1.93	0.51
2:b:214:MET:O	2:b:218:GLN:HG2	2.10	0.51
2:b:43:CYS:HB3	18:b:304:HEC:HMC2	1.93	0.51
2:B:63:THR:HG21	2:b:198:PHE:HE2	1.75	0.50
1:a:88:LYS:HA	1:a:93:ILE:HA	1.92	0.50
3:c:207:PRO:HG3	18:c:302:HEC:CGA	2.40	0.50
13:M:416:THR:O	13:M:420:ILE:HG23	2.11	0.50
17:b:303:MQ7:H17	17:b:303:MQ7:C22	2.41	0.50
9:i:84:TYR:HB3	9:i:85:PRO:HD3	1.93	0.50
18:B:305:HEC:HMC3	3:C:41:PHE:CE2	2.46	0.50
3:C:26:ASP:CG	3:C:29:GLU:HG3	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:444:MET:HB2	13:M:457:LEU:HD13	1.93	0.50
14:N:61:PHE:O	14:N:65:ILE:HG12	2.12	0.50
12:L:158:TRP:HH2	12:L:181:VAL:HG12	1.76	0.50
9:i:28:LEU:HB3	9:i:41:TYR:HB3	1.92	0.50
9:i:42:ASP:HA	9:i:54:LEU:O	2.11	0.50
2:B:164:GLU:HB2	2:B:174:LYS:HD3	1.94	0.50
1:A:20:VAL:O	1:A:24:MET:HG3	2.12	0.50
9:I:85:PRO:HG3	3:c:9:PHE:CZ	2.46	0.50
14:N:89:GLU:HA	14:N:92:TRP:CE2	2.47	0.50
1:a:110:ASN:ND2	1:a:117:ASN:H	2.09	0.50
3:c:173:LYS:HG3	3:c:175:ALA:H	1.75	0.50
4:d:44:THR:O	4:d:48:VAL:HG13	2.12	0.50
1:A:124:HIS:HE1	15:A:201:FES:S2	2.18	0.50
2:B:25:HIS:CE1	3:c:14:ARG:HH22	2.30	0.50
11:K:32:PHE:HB2	11:K:75:PHE:HZ	1.76	0.50
1:A:51:GLN:HB3	1:A:157:TYR:HE1	1.76	0.50
9:I:59:ILE:HG22	9:I:73:GLN:HB3	1.92	0.50
13:M:284:ALA:HB2	13:M:326:ILE:HD11	1.94	0.50
11:K:108:ILE:HD11	13:M:239:ILE:HG13	1.94	0.50
1:a:36:ALA:HA	2:b:64:MET:HE1	1.94	0.50
2:B:108:HIS:HE1	2:B:111:ARG:HH21	1.59	0.49
3:C:214:LEU:HB2	3:C:219:ILE:HD11	1.94	0.49
13:M:323:PRO:O	13:M:326:ILE:HG12	2.12	0.49
2:B:16:THR:HB	2:B:17:PRO:HD3	1.93	0.49
1:A:128:TYR:HD2	1:A:144:LEU:HD22	1.77	0.49
3:C:1:MET:HG3	2:b:25:HIS:HA	1.95	0.49
1:a:86:VAL:HG13	1:a:95:ALA:HB2	1.94	0.49
17:B:304:MQ7:H6	3:c:1:MET:N	2.28	0.49
3:C:207:PRO:HG3	18:C:301:HEC:HAD2	1.93	0.49
2:B:128:VAL:O	2:B:132:ILE:HG13	2.12	0.49
13:M:314:ALA:O	13:M:318:MET:HG2	2.12	0.49
9:i:77:PRO:HG2	9:i:108:ILE:HD12	1.95	0.49
9:i:114:MET:HE3	9:i:118:VAL:HB	1.95	0.49
3:c:55:GLY:HA2	5:e:31:PHE:CZ	2.47	0.49
2:b:169:ILE:HG12	2:b:173:VAL:HG23	1.95	0.49
9:i:35:ASP:HB3	9:i:38:ARG:HG3	1.95	0.49
14:N:141:TRP:CD1	18:N:401:HEC:HAA1	2.48	0.49
14:N:177:SER:HA	14:N:188:ASP:HA	1.95	0.49
2:b:50:PHE:HE2	3:c:53:LEU:HB2	1.78	0.49
3:c:105:VAL:HG12	3:c:109:ILE:HD12	1.95	0.49
3:c:183:GLY:HA3	3:c:248:PHE:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:30:ARG:O	9:I:33:GLN:HG3	2.13	0.49
12:L:61:THR:HG23	12:L:137:LEU:HD21	1.95	0.49
13:M:439:VAL:HG13	13:M:457:LEU:HD22	1.94	0.49
17:b:303:MQ7:H17	17:b:303:MQ7:H22	1.95	0.49
9:I:18:TRP:NE1	9:I:118:VAL:HG21	2.28	0.49
9:I:42:ASP:OD1	9:I:53:TYR:HB3	2.12	0.49
18:B:305:HEC:HBD2	3:C:46:TRP:HE1	1.78	0.48
10:J:13:ALA:HB2	19:J:203:PEE:H65	1.95	0.48
13:M:249:HIS:O	13:M:252:VAL:HG22	2.13	0.48
14:N:296:PHE:CD2	14:N:348:LEU:HB3	2.48	0.48
2:B:24:ASP:OD1	3:C:25:LYS:HB2	2.13	0.48
22:L:303:5PL:HAZ1	22:L:303:5PL:HBD1	1.94	0.48
14:N:319:ASP:OD1	14:N:319:ASP:O	2.31	0.48
3:C:177:ILE:HB	3:C:199:ASN:HB3	1.96	0.48
9:I:84:TYR:O	9:I:84:TYR:CD1	2.66	0.48
13:M:556:LEU:HD22	13:M:594:THR:HG23	1.95	0.48
1:A:28:MET:HE2	2:B:54:ILE:HG13	1.94	0.48
8:H:13:ASN:HB3	8:H:16:VAL:HB	1.95	0.48
13:M:67:ASN:HA	13:M:70:MET:HE2	1.95	0.48
13:M:471:MET:CE	23:M:701:HAS:H11	2.44	0.48
9:i:55:ARG:HH11	9:i:88:VAL:HG21	1.78	0.48
16:B:302:HEM:HBB2	16:B:302:HEM:CHC	2.43	0.48
3:C:174:GLU:HA	3:C:201:GLN:HE21	1.77	0.48
11:K:29:VAL:HG21	19:L:301:PEE:H7	1.95	0.48
13:M:253:TYR:HA	13:M:256:ILE:HG22	1.95	0.48
3:c:211:ASP:HA	3:c:253:THR:HG22	1.95	0.48
11:K:55:PHE:HA	5:e:69:TYR:OH	2.13	0.48
12:L:73:ALA:HB2	12:L:116:LEU:HD23	1.95	0.48
13:M:302:THR:HG22	13:M:373:TYR:HA	1.95	0.48
2:B:96:TRP:HZ2	3:C:63:HIS:CD2	2.31	0.48
2:B:142:THR:OG1	2:B:196:HIS:HB2	2.13	0.48
2:B:214:MET:SD	17:B:304:MQ7:H312	2.53	0.48
3:C:124:LEU:HB3	19:C:302:PEE:H1	1.96	0.48
3:C:148:ALA:HB2	4:D:6:ILE:HG21	1.95	0.48
13:M:359:GLY:HA3	13:M:388:VAL:HG23	1.96	0.48
13:M:375:PHE:HE1	13:M:441:LEU:HD11	1.78	0.48
1:A:53:VAL:HG11	1:A:65:PHE:CD2	2.48	0.48
2:B:108:HIS:HD2	16:B:302:HEM:C1C	2.32	0.48
5:E:2:ASN:HD21	5:E:45:ASN:HA	1.77	0.48
2:b:20:ARG:NH2	3:c:24:PRO:HA	2.29	0.48
1:A:40:VAL:HG12	2:b:175:THR:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:146:GLY:HA3	21:L:302:CDL:H191	1.95	0.48
12:L:148:HIS:NE2	12:L:193:TRP:HB2	2.28	0.48
1:A:100:CYS:SG	1:A:102:HIS:HB3	2.54	0.47
18:B:305:HEC:C1D	3:C:45:GLU:OE2	2.58	0.47
13:M:503:LEU:HD11	13:M:527:PRO:HG2	1.96	0.47
14:N:34:GLU:HA	14:N:37:ASP:HB2	1.96	0.47
2:B:94:HIS:CD2	16:B:301:HEM:ND	2.82	0.47
13:M:506:THR:HG22	13:M:528:LEU:HD13	1.97	0.47
14:N:233:LYS:HB2	14:N:233:LYS:HE3	1.62	0.47
1:a:23:PHE:CD2	5:e:59:LEU:HD22	2.49	0.47
2:B:1:MET:HE3	2:B:1:MET:HB2	1.76	0.47
2:B:25:HIS:HD2	2:B:26:GLU:N	2.13	0.47
2:B:124:LEU:HD21	17:B:304:MQ7:H311	1.95	0.47
13:M:121:ILE:O	13:M:125:LEU:HB2	2.14	0.47
1:a:147:TYR:HD2	1:a:158:LEU:HB3	1.79	0.47
3:c:163:ALA:O	3:c:167:GLU:HG3	2.14	0.47
23:M:701:HAS:H212	23:M:701:HAS:H18	1.61	0.47
2:b:12:ARG:C	2:b:13:LEU:HD23	2.40	0.47
2:b:100:LEU:O	2:b:104:MET:HG2	2.15	0.47
9:I:26:LYS:HB3	9:I:107:LEU:HD11	1.96	0.47
21:J:202:CDL:H812	21:J:202:CDL:H661	1.97	0.47
1:a:47:GLN:HB3	1:a:160:LYS:HZ2	1.80	0.47
1:A:109:TRP:HB2	1:A:119:PHE:CE2	2.49	0.47
5:E:2:ASN:ND2	5:E:45:ASN:HA	2.29	0.47
13:M:77:MET:HE3	23:M:701:HAS:HMC2	1.97	0.47
2:b:138:GLY:HA3	17:c:301:MQ7:H243	1.97	0.47
3:c:61:ILE:HD11	5:e:66:PHE:HD1	1.80	0.47
2:B:217:LYS:HZ2	17:B:304:MQ7:C19	2.26	0.47
21:J:202:CDL:H552	21:J:202:CDL:H512	1.97	0.47
12:L:30:PHE:CZ	12:L:185:TYR:HB2	2.50	0.47
12:L:150:ALA:HB1	22:L:303:5PL:H71C	1.96	0.47
13:M:390:ILE:HA	13:M:394:VAL:HB	1.97	0.47
2:b:162:ILE:HD11	3:c:93:LEU:HD11	1.97	0.47
2:b:193:PHE:O	2:b:197:VAL:HB	2.14	0.47
2:B:25:HIS:C	2:B:25:HIS:CD2	2.93	0.47
2:B:27:VAL:O	3:C:34:THR:HG23	2.15	0.47
21:K:201:CDL:H162	5:e:50:MET:HE1	1.97	0.47
1:a:147:TYR:CD2	1:a:158:LEU:HB3	2.50	0.47
2:B:2:LEU:HD12	2:B:2:LEU:HA	1.79	0.46
9:I:56:ILE:HG22	9:I:77:PRO:HB3	1.97	0.46
11:K:38:LEU:HD22	11:K:63:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:14:MET:SD	13:M:18:TYR:HD2	2.37	0.46
13:M:526:ASP:HB2	13:M:529:TRP:HB3	1.97	0.46
1:a:69:ILE:HD12	1:a:71:GLN:HB3	1.97	0.46
19:J:203:PEE:H49	19:J:203:PEE:H8	1.31	0.46
11:K:14:LEU:HG	11:K:18:LYS:HE2	1.98	0.46
14:N:26:LEU:O	14:N:181:PRO:HB2	2.15	0.46
1:a:68:LYS:HB3	1:a:79:GLU:HG3	1.96	0.46
3:c:220:LYS:HG2	3:c:242:LEU:HG	1.96	0.46
3:C:43:LEU:O	3:C:47:MET:HG2	2.15	0.46
9:I:85:PRO:HG2	3:c:4:GLY:HA3	1.97	0.46
12:L:202:LEU:O	12:L:206:VAL:HG13	2.15	0.46
13:M:15:LEU:HD12	13:M:19:LEU:HG	1.97	0.46
3:c:152:LEU:HD21	4:d:3:LEU:HD22	1.97	0.46
2:B:54:ILE:HG21	3:C:56:PHE:HE2	1.79	0.46
18:B:305:HEC:CAC	3:C:45:GLU:OE1	2.59	0.46
4:D:45:VAL:O	4:D:49:ILE:HG23	2.16	0.46
14:N:82:VAL:HG12	14:N:84:GLY:H	1.79	0.46
14:N:140:TYR:HB3	14:N:324:LYS:HE2	1.97	0.46
1:a:17:LEU:HD11	3:c:42:LEU:HG	1.97	0.46
9:i:35:ASP:HB3	9:i:38:ARG:CB	2.43	0.46
1:A:58:LEU:HD11	1:A:88:LYS:HB3	1.97	0.46
13:M:441:LEU:O	14:N:28:THR:HG22	2.15	0.46
1:a:101:LYS:HE3	1:a:145:ASP:H	1.81	0.46
3:C:54:ILE:HG12	5:E:62:PHE:CD2	2.51	0.46
21:K:201:CDL:H742	21:K:201:CDL:H171	1.98	0.46
2:B:216:ARG:HD2	17:B:304:MQ7:C1	2.45	0.46
3:C:44:LYS:HD3	5:E:1:MET:HE2	1.97	0.46
13:M:181:ARG:HD3	13:M:190:LEU:HD21	1.98	0.46
2:b:110:LEU:HD22	2:b:114:PHE:CE2	2.51	0.46
11:K:108:ILE:HG13	13:M:236:ASN:HD22	1.81	0.46
13:M:47:MET:HE1	13:M:468:ALA:HB1	1.97	0.46
18:b:304:HEC:C1C	3:c:45:GLU:CG	2.93	0.46
18:B:305:HEC:HHC	3:C:41:PHE:HE2	1.81	0.46
12:L:55:ASN:HB3	12:L:137:LEU:HD23	1.97	0.46
13:M:213:VAL:O	13:M:217:LEU:HG	2.16	0.46
1:a:156:LEU:HD12	1:a:157:TYR:H	1.80	0.46
3:c:148:ALA:HB2	4:d:6:ILE:HG21	1.97	0.46
1:A:118:LYS:HA	1:A:118:LYS:HD3	1.81	0.45
2:B:15:ILE:O	2:B:15:ILE:HG13	2.15	0.45
10:J:57:LYS:HE3	10:J:66:GLU:HG2	1.97	0.45
14:N:159:VAL:HG21	14:N:201:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:86:PHE:CE1	17:c:301:MQ7:H152	2.51	0.45
3:c:206:GLY:HA2	18:c:302:HEC:C3A	2.46	0.45
2:B:136:MET:HE2	2:B:136:MET:HB2	1.90	0.45
13:M:209:PRO:HB2	13:M:210:PRO:HD3	1.98	0.45
17:c:301:MQ7:H412	17:c:301:MQ7:H391	1.70	0.45
9:i:40:THR:HG23	9:i:57:GLN:HG2	1.98	0.45
2:B:111:ARG:HG2	2:B:112:VAL:H	1.80	0.45
10:J:56:TYR:OH	10:J:64:HIS:HB2	2.17	0.45
2:B:35:HIS:CE1	9:I:31:ALA:HB1	2.50	0.45
3:C:55:GLY:HA2	5:E:31:PHE:CZ	2.51	0.45
12:L:142:TYR:HD2	21:L:302:CDL:H161	1.81	0.45
14:N:135:VAL:HG22	14:N:144:PHE:HD1	1.80	0.45
3:c:26:ASP:OD2	8:h:4:PHE:HB3	2.16	0.45
2:B:89:ILE:HG12	5:E:74:MET:HE1	1.97	0.45
2:B:112:VAL:HA	2:B:117:ALA:HB3	1.98	0.45
20:C:303:PC1:H282	20:C:303:PC1:H361	1.98	0.45
13:M:253:TYR:OH	13:M:320:ILE:HG21	2.17	0.45
2:b:111:ARG:HH22	16:b:302:HEM:HBD1	1.80	0.45
12:L:30:PHE:CG	12:L:181:VAL:HG13	2.51	0.45
14:N:329:MET:HE1	18:N:401:HEC:C1C	2.46	0.45
3:C:27:TYR:HD1	3:C:30:TYR:CE2	2.35	0.45
9:I:81:LYS:HG2	9:I:82:HIS:H	1.81	0.45
21:K:201:CDL:H822	5:e:58:TYR:HB2	1.98	0.45
14:N:95:ILE:HB	14:N:96:PRO:HD3	1.99	0.45
14:N:135:VAL:HB	14:N:169:LEU:HD23	1.98	0.45
14:N:183:VAL:HG21	14:N:201:PHE:CE2	2.52	0.45
2:B:112:VAL:HG13	2:B:117:ALA:HB3	1.99	0.45
10:J:104:VAL:HG11	10:J:112:MET:HE1	1.99	0.45
23:M:702:HAS:H242	23:M:702:HAS:H211	1.67	0.45
2:b:196:HIS:HE1	16:b:301:HEM:C4C	2.26	0.45
3:c:26:ASP:OD1	3:c:26:ASP:O	2.35	0.45
3:c:222:ILE:HG12	3:c:227:LYS:HB2	1.99	0.45
11:K:86:PRO:HB3	12:L:31:TRP:CG	2.51	0.45
14:N:80:LYS:HE2	14:N:80:LYS:HB2	1.72	0.45
5:e:65:GLY:O	5:e:69:TYR:HD1	2.00	0.45
3:C:10:VAL:N	3:C:17:ALA:HB2	2.32	0.45
13:M:45:GLU:HB3	13:M:73:HIS:HB2	1.98	0.45
14:N:145:GLU:HG3	14:N:152:ILE:HG12	1.99	0.45
14:N:227:LEU:HB3	14:N:305:VAL:HG21	1.99	0.45
3:c:142:MET:SD	19:c:303:PEE:H58	2.57	0.45
3:c:177:ILE:HB	3:c:199:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:GLY:HA3	16:B:302:HEM:C2B	2.53	0.44
2:B:224:LEU:HB3	7:G:22:TYR:HD1	1.80	0.44
3:C:26:ASP:OD1	3:C:29:GLU:HG3	2.17	0.44
22:L:303:5PL:HAU2	22:L:303:5PL:HBZ2	1.98	0.44
13:M:564:LEU:HD23	13:M:564:LEU:HA	1.85	0.44
14:N:88:LEU:HD23	14:N:88:LEU:HA	1.84	0.44
2:B:56:VAL:O	2:B:60:MET:HG3	2.17	0.44
5:E:34:GLN:NE2	5:E:58:TYR:HE1	2.15	0.44
11:K:108:ILE:HG12	12:L:50:ALA:HB1	1.98	0.44
3:c:20:LYS:H	3:c:20:LYS:HD2	1.82	0.44
3:c:215:LYS:HB2	3:c:218:GLU:HG3	1.99	0.44
2:B:47:LEU:HD21	3:C:49:GLY:HA2	1.99	0.44
3:C:109:ILE:O	3:C:113:LEU:HB2	2.17	0.44
14:N:89:GLU:HA	14:N:92:TRP:NE1	2.33	0.44
8:H:41:LEU:HD23	8:H:42:VAL:HG23	1.99	0.44
3:c:149:ALA:HB1	20:c:304:PC1:H2B1	2.00	0.44
8:h:8:VAL:HG23	8:h:11:LYS:HZ2	1.81	0.44
3:C:196:HIS:CE1	3:C:207:PRO:HD2	2.53	0.44
11:K:32:PHE:CD2	12:L:82:LEU:HD22	2.53	0.44
13:M:407:LYS:HA	13:M:407:LYS:HD3	1.61	0.44
1:a:34:ARG:HA	1:a:34:ARG:HD2	1.84	0.44
1:a:115:ASN:HB3	1:a:118:LYS:HD2	2.00	0.44
3:C:82:PRO:HG2	3:C:87:LEU:HD23	1.99	0.44
11:K:86:PRO:HB3	12:L:31:TRP:CD2	2.53	0.44
13:M:11:ARG:HA	13:M:11:ARG:HD3	1.76	0.44
2:b:129:GLY:HA3	16:b:302:HEM:C3C	2.52	0.44
13:M:67:ASN:O	13:M:71:THR:HG22	2.18	0.44
8:h:1:MET:HE1	9:i:91:GLY:HA2	1.98	0.44
2:B:26:GLU:HB3	3:C:34:THR:HG21	2.00	0.44
2:b:136:MET:HE2	2:b:136:MET:HB2	1.90	0.44
1:A:60:LYS:HZ2	1:A:88:LYS:HE2	1.83	0.43
2:B:105:MET:HE3	2:B:133:PHE:CG	2.53	0.43
3:C:65:PRO:HA	3:C:66:PRO:HD3	1.93	0.43
3:C:173:LYS:HG3	3:C:175:ALA:H	1.82	0.43
13:M:217:LEU:HD22	13:M:228:PHE:CE2	2.53	0.43
14:N:267:LYS:HE3	14:N:267:LYS:HB3	1.77	0.43
3:c:196:HIS:CE1	18:c:302:HEC:C1A	3.01	0.43
9:i:19:LEU:HD21	9:i:74:LEU:HD21	1.99	0.43
2:B:110:LEU:HD13	2:B:110:LEU:HA	1.69	0.43
11:K:5:LYS:HE3	11:K:5:LYS:HB3	1.84	0.43
13:M:183:PRO:HD3	13:M:519:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:113:PHE:HZ	19:c:303:PEE:H49	1.83	0.43
11:K:35:MET:HE1	11:K:75:PHE:CE2	2.54	0.43
19:L:301:PEE:H81	5:e:36:ILE:HD11	2.00	0.43
13:M:141:ALA:HB2	13:M:240:TRP:HB3	2.00	0.43
13:M:610:LYS:HA	13:M:613:LEU:HD13	1.99	0.43
14:N:48:LEU:O	14:N:51:VAL:HG12	2.18	0.43
14:N:263:GLU:HA	14:N:347:TYR:HE2	1.81	0.43
2:b:128:VAL:O	2:b:132:ILE:HG13	2.18	0.43
3:c:193:ILE:HG23	3:c:198:ASP:HA	2.00	0.43
9:i:41:TYR:O	9:i:55:ARG:HA	2.19	0.43
1:A:119:PHE:CE1	1:A:130:LYS:HA	2.51	0.43
2:B:32:ASN:HA	3:C:41:PHE:HE1	1.82	0.43
2:B:111:ARG:O	2:B:112:VAL:HB	2.19	0.43
2:B:166:THR:HG23	3:C:108:MET:HE1	2.00	0.43
13:M:207:ALA:C	13:M:210:PRO:HD2	2.43	0.43
1:a:41:LEU:HB3	8:h:41:LEU:HD11	1.99	0.43
5:E:46:LEU:HB2	5:E:51:TYR:CE1	2.53	0.43
14:N:237:ALA:O	14:N:241:GLN:HG2	2.18	0.43
4:d:27:ILE:HG13	4:d:28:LEU:N	2.33	0.43
12:L:150:ALA:HA	21:L:302:CDL:H432	2.00	0.43
14:N:261:GLN:HA	14:N:264:GLU:HG2	2.00	0.43
2:b:50:PHE:CE2	3:c:53:LEU:HB2	2.54	0.43
2:B:195:ILE:HA	2:B:199:PHE:HD2	1.83	0.43
5:E:25:LYS:HD2	5:E:25:LYS:HA	1.52	0.43
10:J:77:LYS:HB2	10:J:77:LYS:HE3	1.92	0.43
11:K:78:MET:HE2	11:K:78:MET:HB3	1.82	0.43
14:N:329:MET:HE1	18:N:401:HEC:NC	2.33	0.43
5:e:37:LEU:O	5:e:41:LEU:HB2	2.19	0.43
5:E:4:MET:HE2	5:E:4:MET:HA	2.01	0.43
13:M:256:ILE:HB	23:M:702:HAS:HBC1	2.00	0.43
3:c:26:ASP:O	3:c:27:TYR:HB2	2.19	0.43
2:B:100:LEU:HD12	3:C:52:PHE:HZ	1.82	0.43
3:C:69:ARG:HG3	3:C:69:ARG:HH11	1.84	0.43
3:C:145:ALA:HB1	19:C:302:PEE:H67	2.00	0.43
13:M:192:LEU:HD23	13:M:264:SER:HB3	2.00	0.43
13:M:521:PHE:HB3	13:M:540:THR:HB	1.99	0.43
14:N:165:VAL:HG12	14:N:199:LEU:O	2.18	0.43
2:b:145:LEU:HD12	2:b:156:THR:HG21	1.99	0.43
3:C:31:PRO:HG3	9:I:88:VAL:CG2	2.49	0.43
9:I:106:ALA:O	9:I:109:GLN:HG2	2.19	0.43
11:K:91:TYR:CE2	21:K:201:CDL:H341	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:96:PHE:CE2	12:L:170:GLY:HA2	2.53	0.43
22:L:303:5PL:HBJ1	13:M:111:LEU:HD21	2.00	0.43
14:N:272:LEU:HD23	14:N:272:LEU:HA	1.89	0.43
2:b:134:PHE:CZ	3:c:115:PHE:HB3	2.54	0.43
1:A:162:LYS:HE3	1:A:162:LYS:HB3	1.89	0.42
3:C:78:TYR:HA	3:C:168:GLN:NE2	2.34	0.42
3:C:182:GLU:HA	3:C:185:LYS:HD2	2.01	0.42
5:E:21:LEU:HD23	7:G:6:MET:HE2	2.00	0.42
9:I:51:THR:HG23	9:I:82:HIS:HB3	2.00	0.42
11:K:1:MET:HE3	11:K:1:MET:HB3	1.89	0.42
13:M:327:LYS:HE2	13:M:327:LYS:HB3	1.91	0.42
13:M:475:VAL:HG11	23:M:701:HAS:H261	2.01	0.42
13:M:524:GLY:HA3	13:M:530:ILE:HG13	2.01	0.42
9:I:3:LYS:HB2	9:I:3:LYS:HE2	1.79	0.42
11:K:78:MET:HE1	11:K:87:ALA:HA	2.01	0.42
22:L:303:5PL:HBA2	13:M:599:SER:HB2	2.00	0.42
14:N:186:LYS:HB3	14:N:186:LYS:HE3	1.73	0.42
4:d:25:LYS:HD2	4:d:25:LYS:N	2.33	0.42
3:C:26:ASP:O	3:C:27:TYR:HB2	2.19	0.42
7:G:13:PHE:O	7:G:17:ILE:HG13	2.19	0.42
11:K:56:THR:O	11:K:60:ILE:HG12	2.19	0.42
14:N:324:LYS:HB2	14:N:327:ASN:HD22	1.84	0.42
1:a:62:PRO:HD3	1:a:130:LYS:HE3	2.02	0.42
2:b:110:LEU:HD23	3:c:142:MET:HE3	2.00	0.42
1:A:53:VAL:HG11	1:A:65:PHE:CE2	2.54	0.42
1:A:120:PHE:CE1	1:A:125:TYR:HA	2.54	0.42
3:C:145:ALA:HB2	19:C:302:PEE:H32	2.01	0.42
9:I:85:PRO:HB3	3:c:2:HIS:H	1.83	0.42
21:L:302:CDL:H712	21:L:302:CDL:HB61	1.85	0.42
14:N:177:SER:HB3	14:N:218:ALA:H	1.84	0.42
1:a:47:GLN:NE2	1:a:69:ILE:HB	2.35	0.42
3:c:54:ILE:HG23	5:e:62:PHE:CE1	2.55	0.42
2:B:57:LEU:HD23	2:B:57:LEU:HA	1.87	0.42
12:L:114:LEU:HD12	12:L:114:LEU:HA	1.82	0.42
14:N:126:LYS:HG3	14:N:128:GLU:HB2	2.02	0.42
14:N:156:GLU:HB2	14:N:299:ARG:HD3	2.02	0.42
18:b:304:HEC:CHC	3:c:45:GLU:HG3	2.48	0.42
18:B:305:HEC:HMC1	18:B:305:HEC:CBC	2.50	0.42
3:C:26:ASP:C	3:C:28:SER:H	2.27	0.42
22:L:303:5PL:HAV2	13:M:595:MET:HE3	2.02	0.42
13:M:275:LEU:HD21	13:M:281:MET:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:519:LEU:HD23	13:M:519:LEU:HA	1.82	0.42
14:N:96:PRO:O	14:N:100:LEU:HD23	2.19	0.42
1:a:110:ASN:HD22	1:a:117:ASN:H	1.67	0.42
17:b:303:MQ7:H412	17:b:303:MQ7:H391	1.75	0.42
3:c:140:GLY:HA3	4:d:13:PHE:CE2	2.55	0.42
2:B:19:TRP:HH2	3:C:38:TRP:CE2	2.38	0.42
10:J:41:LYS:HA	10:J:41:LYS:HD3	1.78	0.42
12:L:28:LEU:O	12:L:32:LEU:HG	2.19	0.42
12:L:158:TRP:CH2	12:L:181:VAL:HG12	2.52	0.42
13:M:361:VAL:HG13	14:N:50:MET:CG	2.48	0.42
14:N:258:LEU:HG	14:N:343:ALA:HA	2.00	0.42
1:a:128:TYR:CZ	1:a:140:PRO:HB3	2.54	0.42
1:A:156:LEU:HD12	1:A:157:TYR:N	2.34	0.42
3:C:58:VAL:HG11	5:E:31:PHE:HE1	1.84	0.42
12:L:168:LYS:HA	12:L:168:LYS:HD2	1.90	0.42
14:N:141:TRP:CZ3	14:N:143:GLU:HB2	2.55	0.42
2:b:37:PHE:O	2:b:40:PHE:HD1	2.02	0.42
1:A:14:ASN:OD1	3:C:39:PRO:HG3	2.19	0.42
4:D:1:MET:O	4:D:4:VAL:HG12	2.20	0.42
13:M:527:PRO:O	13:M:531:GLU:HG2	2.19	0.42
1:A:52:VAL:HG13	1:A:53:VAL:N	2.35	0.42
4:D:41:GLY:O	4:D:45:VAL:HG22	2.19	0.42
3:C:62:VAL:HG21	5:E:27:ALA:HB2	2.01	0.41
3:C:219:ILE:HA	3:C:222:ILE:HD12	2.02	0.41
10:J:109:LEU:O	10:J:112:MET:HG3	2.19	0.41
13:M:86:LEU:O	13:M:90:MET:HG3	2.20	0.41
13:M:298:HIS:CD2	13:M:298:HIS:C	2.98	0.41
3:c:82:PRO:HB2	3:c:86:PHE:HB2	2.01	0.41
1:A:47:GLN:HE22	1:A:160:LYS:HD3	1.85	0.41
21:J:202:CDL:H262	21:J:202:CDL:H451	2.02	0.41
13:M:72:MET:HE1	13:M:123:LEU:HG	2.03	0.41
3:c:129:GLU:O	3:c:135:ARG:HD3	2.20	0.41
9:i:23:MET:HG3	9:i:41:TYR:CD2	2.55	0.41
2:B:166:THR:HA	3:C:108:MET:CE	2.50	0.41
9:I:18:TRP:HE1	9:I:118:VAL:HG21	1.84	0.41
10:J:13:ALA:O	10:J:17:ILE:HG12	2.20	0.41
11:K:108:ILE:HG23	11:K:109:TRP:CD1	2.56	0.41
12:L:2:GLN:HG2	12:L:5:GLU:HA	2.02	0.41
13:M:339:ASN:HD21	14:N:70:ARG:HD3	1.86	0.41
13:M:360:GLY:HA3	23:M:702:HAS:H162	2.03	0.41
13:M:611:GLU:OE2	13:M:611:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:115:LEU:HD23	9:i:115:LEU:HA	1.84	0.41
12:L:15:SER:O	12:L:19:VAL:HG23	2.21	0.41
3:c:2:HIS:ND1	3:c:3:ARG:HG2	2.35	0.41
3:c:27:TYR:HE2	3:c:40:ASN:OD1	2.04	0.41
3:c:182:GLU:O	3:c:186:VAL:HG23	2.20	0.41
3:c:196:HIS:HE1	18:c:302:HEC:C1A	2.33	0.41
3:C:182:GLU:O	3:C:186:VAL:HG23	2.20	0.41
13:M:351:SER:O	13:M:354:PRO:HD2	2.19	0.41
13:M:402:HIS:CD2	13:M:413:LEU:HD13	2.55	0.41
14:N:132:VAL:O	14:N:147:PRO:HD2	2.19	0.41
13:M:123:LEU:HD12	13:M:123:LEU:HA	1.91	0.41
14:N:131:LEU:HB3	14:N:165:VAL:HG23	2.02	0.41
2:b:71:LYS:HA	2:b:71:LYS:HD3	1.83	0.41
2:B:127:ILE:HD11	3:C:123:PHE:HE2	1.86	0.41
17:c:301:MQ7:H361	17:c:301:MQ7:H341	1.81	0.41
5:e:2:ASN:O	5:e:42:SER:HB2	2.21	0.41
9:i:104:SER:O	9:i:108:ILE:HG12	2.20	0.41
2:B:2:LEU:HD23	8:H:20:VAL:HG23	2.02	0.41
3:C:149:ALA:HB1	20:C:303:PC1:H2B1	2.02	0.41
11:K:25:MET:HE2	12:L:86:TYR:CD1	2.55	0.41
12:L:163:MET:HE3	12:L:163:MET:HB3	1.94	0.41
22:L:303:5PL:HAR2	13:M:598:ARG:HH22	1.86	0.41
13:M:483:ILE:HD13	13:M:483:ILE:HA	1.93	0.41
13:M:556:LEU:N	13:M:557:PRO:HD2	2.36	0.41
14:N:90:ILE:HD12	14:N:90:ILE:HA	1.93	0.41
2:B:68:PRO:HD2	2:b:68:PRO:HD2	2.03	0.41
2:B:127:ILE:HD11	3:C:123:PHE:CE2	2.55	0.41
17:B:303:MQ7:O1	3:C:82:PRO:HB3	2.20	0.41
3:C:187:PHE:N	3:C:245:LEU:HD21	2.36	0.41
10:J:26:LYS:HE2	21:J:202:CDL:H721	0.94	0.41
21:K:201:CDL:H871	5:e:58:TYR:CE1	2.56	0.41
13:M:221:ASP:OD1	13:M:228:PHE:HB2	2.21	0.41
13:M:322:ILE:O	13:M:326:ILE:HG23	2.21	0.41
14:N:81:GLN:H	14:N:81:GLN:HG2	1.72	0.41
14:N:158:ILE:HD13	14:N:243:TRP:CZ2	2.56	0.41
1:a:108:ASN:HB2	1:a:111:SER:HB3	2.03	0.41
2:b:32:ASN:HD21	3:c:35:GLU:HB2	1.86	0.41
2:b:65:TYR:HB2	2:b:80:LEU:HD12	2.03	0.41
3:c:151:PHE:CE2	4:d:3:LEU:HB2	2.55	0.41
8:h:19:ALA:O	8:h:23:VAL:HG23	2.21	0.41
9:I:52:PHE:CE2	9:I:81:LYS:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:85:PRO:HD2	3:c:3:ARG:O	2.21	0.41
13:M:49:ILE:CG2	23:M:701:HAS:HMD	2.50	0.41
3:c:54:ILE:HG12	5:e:62:PHE:CD2	2.55	0.41
3:c:97:TYR:HA	3:c:102:PHE:HE1	1.85	0.41
2:B:55:GLN:NE2	2:B:98:ALA:N	2.68	0.40
2:B:78:TYR:CE1	3:C:171:ILE:HG21	2.56	0.40
2:B:110:LEU:HB3	7:G:17:ILE:HD13	2.03	0.40
13:M:327:LYS:HE2	13:M:331:TRP:CH2	2.56	0.40
13:M:432:THR:HA	13:M:464:SER:HA	2.03	0.40
8:h:2:ASN:HD22	8:h:5:GLU:HG3	1.85	0.40
18:B:305:HEC:HBD2	3:C:46:TRP:NE1	2.36	0.40
3:C:25:LYS:HG3	3:C:26:ASP:H	1.85	0.40
13:M:96:LEU:HD11	13:M:511:PRO:HG2	2.03	0.40
13:M:274:ARG:HH11	14:N:83:GLU:HA	1.87	0.40
14:N:204:LYS:O	14:N:208:GLU:HG3	2.22	0.40
14:N:212:MET:O	14:N:212:MET:HG3	2.21	0.40
17:B:303:MQ7:H311	17:B:303:MQ7:H352	1.92	0.40
8:H:1:MET:HG2	9:I:3:LYS:HE3	2.02	0.40
13:M:229:PHE:CZ	13:M:240:TRP:HB2	2.56	0.40
13:M:588:LEU:HD23	13:M:588:LEU:HA	1.92	0.40
14:N:303:ALA:HB1	14:N:324:LYS:HD2	2.03	0.40
1:a:49:MET:HE1	1:a:158:LEU:C	2.46	0.40
1:a:76:TYR:CE2	1:a:78:SER:HB3	2.56	0.40
2:b:70:ILE:HG22	2:b:148:TRP:CE2	2.55	0.40
3:c:206:GLY:HA2	18:c:302:HEC:C2A	2.51	0.40
3:c:216:PRO:HA	3:c:219:ILE:HD12	2.03	0.40
9:i:26:LYS:HD3	9:i:26:LYS:HA	1.82	0.40
1:A:73:ASP:HB3	2:b:183:ILE:HD13	2.03	0.40
1:A:76:TYR:CD2	2:b:70:ILE:HD11	2.57	0.40
3:C:2:HIS:O	3:C:4:GLY:N	2.54	0.40
19:J:203:PEE:H23	1:a:15:TYR:HB3	2.03	0.40
12:L:74:THR:HA	12:L:193:TRP:HE1	1.86	0.40
12:L:171:LEU:HD23	12:L:171:LEU:HA	1.87	0.40
12:L:178:LYS:HE3	22:L:303:5PL:HAX2	2.04	0.40
13:M:255:LEU:HD23	13:M:255:LEU:HA	1.89	0.40
3:c:30:TYR:CE2	3:c:36:ALA:HB2	2.56	0.40
3:c:218:GLU:O	3:c:222:ILE:HG13	2.22	0.40
10:J:52:PRO:HB2	10:J:115:TRP:CZ3	2.56	0.40
21:J:202:CDL:H401	12:L:42:ALA:HA	2.03	0.40
11:K:104:PHE:CB	12:L:46:ALA:HB1	2.51	0.40
13:M:49:ILE:HG23	13:M:66:TYR:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:330:ASN:HD22	13:M:330:ASN:HA	1.72	0.40
13:M:362:THR:HG21	13:M:437:HIS:CD2	2.56	0.40
14:N:306:LYS:HB3	14:N:306:LYS:HE3	1.77	0.40
2:b:94:HIS:CE1	16:b:301:HEM:ND	2.90	0.40
3:c:142:MET:O	3:c:146:ILE:HG12	2.22	0.40
3:c:196:HIS:CD2	3:c:207:PRO:O	2.75	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	A	161/167 (96%)	146 (91%)	15 (9%)	0	100	100
1	a	156/167 (93%)	145 (93%)	11 (7%)	0	100	100
2	B	222/224 (99%)	208 (94%)	13 (6%)	1 (0%)	24	57
2	b	222/224 (99%)	219 (99%)	2 (1%)	1 (0%)	24	57
3	C	253/255 (99%)	239 (94%)	13 (5%)	1 (0%)	30	61
3	c	253/255 (99%)	238 (94%)	14 (6%)	1 (0%)	30	61
4	D	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
4	d	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
5	E	75/81 (93%)	75 (100%)	0	0	100	100
5	e	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
7	G	27/29 (93%)	22 (82%)	5 (18%)	0	100	100
7	g	27/29 (93%)	27 (100%)	0	0	100	100
8	H	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
8	h	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
9	I	117/120 (98%)	111 (95%)	5 (4%)	1 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	i	117/120 (98%)	108 (92%)	9 (8%)	0	100 100
10	J	118/120 (98%)	112 (95%)	5 (4%)	1 (1%)	16 47
11	K	108/110 (98%)	105 (97%)	3 (3%)	0	100 100
12	L	205/207 (99%)	201 (98%)	4 (2%)	0	100 100
13	M	601/622 (97%)	582 (97%)	19 (3%)	0	100 100
14	N	333/356 (94%)	316 (95%)	17 (5%)	0	100 100
All	All	3262/3369 (97%)	3111 (95%)	145 (4%)	6 (0%)	44 73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	3	ARG
3	c	3	ARG
9	I	85	PRO
2	B	168	LEU
10	J	109	LEU
2	b	168	LEU

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	A	142/144 (99%)	139 (98%)	3 (2%)	47 71
1	a	139/144 (96%)	133 (96%)	6 (4%)	26 57
2	B	188/188 (100%)	182 (97%)	6 (3%)	34 64
2	b	188/188 (100%)	184 (98%)	4 (2%)	47 71
3	C	205/205 (100%)	195 (95%)	10 (5%)	22 53
3	c	205/205 (100%)	202 (98%)	3 (2%)	57 75
4	D	45/46 (98%)	43 (96%)	2 (4%)	25 56
4	d	45/46 (98%)	45 (100%)	0	100 100
5	E	66/67 (98%)	64 (97%)	2 (3%)	36 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	66/67 (98%)	65 (98%)	1 (2%)	57	75
7	G	25/25 (100%)	24 (96%)	1 (4%)	28	60
7	g	25/25 (100%)	24 (96%)	1 (4%)	28	60
8	H	37/37 (100%)	36 (97%)	1 (3%)	39	67
8	h	37/37 (100%)	36 (97%)	1 (3%)	39	67
9	I	100/101 (99%)	96 (96%)	4 (4%)	28	60
9	i	100/101 (99%)	99 (99%)	1 (1%)	68	79
10	J	96/96 (100%)	96 (100%)	0	100	100
11	K	94/94 (100%)	92 (98%)	2 (2%)	47	71
12	L	173/173 (100%)	169 (98%)	4 (2%)	44	70
13	M	490/506 (97%)	478 (98%)	12 (2%)	43	69
14	N	291/311 (94%)	283 (97%)	8 (3%)	39	67
All	All	2757/2806 (98%)	2685 (97%)	72 (3%)	41	68

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	17	LEU
1	A	102	HIS
2	B	21	ASP
2	B	76	SER
2	B	101	VAL
2	B	110	LEU
2	B	162	ILE
2	B	197	VAL
3	C	1	MET
3	C	19	LYS
3	C	26	ASP
3	C	45	GLU
3	C	74	THR
3	C	83	ASP
3	C	103	THR
3	C	137	VAL
3	C	172	THR
3	C	193	ILE
4	D	28	LEU
4	D	46	MET

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Mol	Chain	Res	Type
5	E	25	LYS
5	E	29	LEU
7	G	4	ILE
8	H	35	MET
9	I	22	LEU
9	I	57	GLN
9	I	88	VAL
9	I	93	THR
11	K	105	VAL
11	K	107	ILE
12	L	81	SER
12	L	175	THR
12	L	194	VAL
12	L	198	THR
13	M	72	MET
13	M	159	LEU
13	M	194	THR
13	M	227	ASN
13	M	320	ILE
13	M	388	VAL
13	M	441	LEU
13	M	455	GLN
13	M	471	MET
13	M	480	VAL
13	M	526	ASP
13	M	576	ASP
14	N	117	THR
14	N	121	ASP
14	N	198	PHE
14	N	234	THR
14	N	253	THR
14	N	274	CYS
14	N	329	MET
14	N	339	SER
1	a	53	VAL
1	a	66	ASP
1	a	86	VAL
1	a	100	CYS
1	a	108	ASN
1	a	121	CYS
2	b	2	LEU
2	b	64	MET

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Mol	Chain	Res	Type
2	b	171	THR
2	b	220	ILE
3	c	1	MET
3	c	45	GLU
3	c	230	MET
5	e	26	ASP
7	g	12	THR
8	h	8	VAL
9	i	95	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	HIS
2	B	35	HIS
3	C	190	GLN
5	E	34	GLN
8	H	13	ASN
8	H	40	HIS
9	I	33	GLN
9	I	86	HIS
9	I	113	ASN
10	J	64	HIS
11	K	83	HIS
12	L	53	ASN
12	L	166	ASN
13	M	64	GLN
13	M	67	ASN
13	M	330	ASN
14	N	241	GLN
14	N	261	GLN
14	N	327	ASN
1	a	11	GLN
1	a	47	GLN
1	a	110	ASN
1	a	146	HIS
2	b	32	ASN
2	b	35	HIS
2	b	55	GLN
2	b	72	ASN
2	b	81	GLN
2	b	94	HIS

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Mol	Chain	Res	Type
2	b	180	HIS
3	c	168	GLN
3	c	196	HIS
3	c	199	ASN
8	h	2	ASN
8	h	9	GLN
9	i	57	GLN
9	i	73	GLN

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 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
17	MQ7	c	301	-	49,49,49	0.39	0	61,63,63	0.49	1 (1%)
19	PEE	L	301	-	50,50,50	0.31	0	53,55,55	0.40	0
22	5PL	L	303	-	84,85,85	0.25	0	95,101,101	0.57	1 (1%)
20	PC1	C	303	-	47,47,53	0.52	0	53,55,61	0.49	1 (1%)
21	CDL	K	201	-	99,99,99	0.28	0	105,111,111	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	PC1	c	304	-	42,42,53	0.55	0	48,50,61	0.50	1 (2%)
21	CDL	J	202	-	99,99,99	0.31	0	105,111,111	0.56	2 (1%)
26	CUA	N	402	14	0,1,1	-	-	-		
17	MQ7	B	303	-	49,49,49	0.42	0	61,63,63	0.67	2 (3%)
17	MQ7	b	303	-	49,49,49	0.38	0	61,63,63	0.70	2 (3%)
15	FES	a	201	1	0,4,4	-	-	-		
16	HEM	B	302	2	50,50,50	1.59	10 (20%)	67,82,82	1.58	12 (17%)
19	PEE	J	203	-	39,39,50	0.32	0	42,44,55	0.51	1 (2%)
16	HEM	B	301	2	50,50,50	1.58	8 (16%)	67,82,82	1.67	12 (17%)
16	HEM	b	302	2	50,50,50	1.59	8 (16%)	67,82,82	1.56	12 (17%)
19	PEE	C	302	-	41,41,50	0.33	0	44,46,55	0.38	0
18	HEC	N	401	14	50,50,50	3.00	28 (56%)	68,82,82	2.30	27 (39%)
18	HEC	J	201	10	50,50,50	3.10	30 (60%)	68,82,82	2.29	27 (39%)
23	HAS	M	702	13	72,72,72	2.40	28 (38%)	87,109,109	2.44	32 (36%)
23	HAS	M	701	13	72,72,72	2.47	27 (37%)	87,109,109	2.21	35 (40%)
17	MQ7	B	304	-	49,49,49	0.37	0	61,63,63	0.54	1 (1%)
18	HEC	C	301	3	50,50,50	3.04	30 (60%)	68,82,82	2.29	27 (39%)
15	FES	A	201	1	0,4,4	-	-	-		
18	HEC	c	302	-	50,50,50	2.95	26 (52%)	68,82,82	2.50	25 (36%)
18	HEC	B	305	2,3	50,50,50	3.10	28 (56%)	68,82,82	2.58	30 (44%)
16	HEM	b	301	2	50,50,50	1.58	8 (16%)	67,82,82	1.64	12 (17%)
21	CDL	L	302	-	97,97,99	0.27	0	103,109,111	0.43	0
19	PEE	c	303	-	41,41,50	0.33	0	44,46,55	0.42	0
18	HEC	b	304	2	50,50,50	3.06	29 (58%)	68,82,82	2.31	27 (39%)

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
17	MQ7	c	301	-	-	7/41/61/61	0/2/2/2
19	PEE	L	301	-	-	8/54/54/54	-
22	5PL	L	303	-	-	21/87/107/107	0/1/1/1
20	PC1	C	303	-	-	14/51/51/57	-
21	CDL	K	201	-	-	11/110/110/110	-
20	PC1	c	304	-	-	12/46/46/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CDL	J	202	-	-	21/110/110/110	-
17	MQ7	B	303	-	-	9/41/61/61	0/2/2/2
17	MQ7	b	303	-	-	8/41/61/61	0/2/2/2
15	FES	a	201	1	-	-	0/1/1/1
16	HEM	B	302	2	-	6/14/54/54	-
19	PEE	J	203	-	-	8/43/43/54	-
16	HEM	B	301	2	-	7/14/54/54	-
16	HEM	b	302	2	-	6/14/54/54	-
19	PEE	C	302	-	-	2/45/45/54	-
18	HEC	N	401	14	1/1/3/7	7/14/54/54	-
18	HEC	J	201	10	1/1/3/7	12/14/54/54	-
23	HAS	M	702	13	1/1/8/18	14/42/82/82	-
23	HAS	M	701	13	1/1/8/18	13/42/82/82	-
17	MQ7	B	304	-	-	14/41/61/61	0/2/2/2
18	HEC	C	301	3	1/1/3/7	7/14/54/54	-
15	FES	A	201	1	-	-	0/1/1/1
18	HEC	c	302	-	1/1/3/7	10/14/54/54	-
18	HEC	B	305	2,3	1/1/3/7	8/14/54/54	-
16	HEM	b	301	2	-	7/14/54/54	-
21	CDL	L	302	-	-	22/108/108/110	-
19	PEE	c	303	-	-	8/45/45/54	-
18	HEC	b	304	2	1/1/3/7	9/14/54/54	-

All (260) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	M	701	HAS	C3B-C2B	5.95	1.48	1.34
18	B	305	HEC	CHD-C4C	5.72	1.52	1.39
18	J	201	HEC	C3B-C2B	5.69	1.49	1.36
18	C	301	HEC	C2A-C3A	5.68	1.49	1.36
18	b	304	HEC	C2A-C3A	5.64	1.48	1.36
18	b	304	HEC	C3D-C2D	5.62	1.48	1.36
18	N	401	HEC	C3B-C2B	5.58	1.48	1.36
18	b	304	HEC	C3B-C2B	5.56	1.48	1.36
18	C	301	HEC	C3B-C2B	5.55	1.48	1.36
23	M	702	HAS	C3B-C2B	5.55	1.47	1.34
18	J	201	HEC	C2A-C3A	5.54	1.48	1.36
18	J	201	HEC	C3D-C2D	5.50	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	304	HEC	CHB-C4A	5.46	1.49	1.38
18	B	305	HEC	CHD-C1D	5.46	1.49	1.38
18	J	201	HEC	CHB-C4A	5.44	1.49	1.38
18	b	304	HEC	CHA-C1A	5.39	1.48	1.38
18	B	305	HEC	C2A-C3A	5.38	1.48	1.36
18	J	201	HEC	CHA-C1A	5.36	1.48	1.38
16	B	301	HEM	FE-NB	5.36	2.11	1.94
18	B	305	HEC	C3D-C2D	5.35	1.48	1.36
16	b	301	HEM	FE-NB	5.31	2.11	1.94
18	B	305	HEC	C3B-C2B	5.30	1.48	1.36
18	C	301	HEC	C3D-C2D	5.30	1.48	1.36
18	C	301	HEC	CHA-C1A	5.29	1.48	1.38
18	C	301	HEC	CHB-C4A	5.28	1.48	1.38
18	J	201	HEC	CHC-C4B	5.28	1.49	1.38
18	J	201	HEC	CHD-C1D	5.27	1.49	1.38
18	c	302	HEC	C2A-C3A	5.27	1.48	1.36
18	N	401	HEC	CHB-C4A	5.26	1.48	1.38
18	N	401	HEC	CHC-C4B	5.26	1.49	1.38
18	b	304	HEC	CHD-C1D	5.24	1.49	1.38
18	c	302	HEC	FE-ND	5.24	2.11	1.94
18	c	302	HEC	C3B-C2B	5.23	1.48	1.36
18	c	302	HEC	FE-NB	5.21	2.11	1.94
18	N	401	HEC	C2A-C3A	5.21	1.48	1.36
23	M	702	HAS	FE-NB	5.19	2.10	1.94
23	M	702	HAS	C2A-C3A	5.17	1.47	1.36
18	N	401	HEC	C3D-C2D	5.17	1.47	1.36
16	b	302	HEM	FE-NB	5.12	2.10	1.94
18	C	301	HEC	CHC-C4B	5.10	1.48	1.38
23	M	701	HAS	CHC-C4B	5.10	1.48	1.38
23	M	701	HAS	CHA-C1A	5.10	1.48	1.38
18	N	401	HEC	CHA-C1A	5.09	1.48	1.38
18	c	302	HEC	CHB-C4A	5.09	1.48	1.38
18	B	305	HEC	FE-NB	5.09	2.10	1.94
16	B	302	HEM	FE-NB	5.09	2.10	1.94
23	M	702	HAS	FE-ND	5.05	2.10	1.94
18	B	305	HEC	FE-ND	5.05	2.10	1.94
18	C	301	HEC	CHD-C1D	5.03	1.48	1.38
23	M	701	HAS	C2A-C3A	5.03	1.47	1.36
18	B	305	HEC	FE-NC	5.01	2.11	1.95
18	c	302	HEC	CHA-C1A	5.00	1.48	1.38
18	B	305	HEC	CHA-C1A	4.97	1.48	1.38
18	c	302	HEC	C3D-C2D	4.95	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	M	702	HAS	CHD-C4A	4.91	1.48	1.38
18	b	304	HEC	CHC-C4B	4.88	1.48	1.38
18	B	305	HEC	CHB-C4A	4.87	1.47	1.38
23	M	701	HAS	CHB-C1D	4.86	1.48	1.38
18	C	301	HEC	FE-ND	4.85	2.09	1.94
18	C	301	HEC	FE-NB	4.81	2.09	1.94
23	M	701	HAS	FE-NB	4.79	2.09	1.94
18	N	401	HEC	CHD-C1D	4.78	1.48	1.38
23	M	702	HAS	CHA-C1A	4.74	1.47	1.38
23	M	701	HAS	FE-ND	4.74	2.09	1.94
18	c	302	HEC	FE-NC	4.74	2.10	1.95
23	M	702	HAS	FE-NA	4.70	2.10	1.95
18	c	302	HEC	FE-NA	4.68	2.10	1.95
23	M	702	HAS	CHB-C1D	4.68	1.47	1.38
18	N	401	HEC	FE-ND	4.66	2.09	1.94
18	J	201	HEC	FE-ND	4.66	2.09	1.94
23	M	702	HAS	FE-NC	4.63	2.10	1.95
18	c	302	HEC	CHC-C4B	4.62	1.47	1.38
18	J	201	HEC	FE-NB	4.61	2.09	1.94
18	N	401	HEC	FE-NB	4.61	2.09	1.94
18	B	305	HEC	FE-NA	4.59	2.10	1.95
18	B	305	HEC	CHC-C4B	4.59	1.47	1.38
23	M	701	HAS	CHD-C4A	4.59	1.47	1.38
18	B	305	HEC	C4C-C3C	4.58	1.53	1.44
18	c	302	HEC	CHD-C1D	4.56	1.47	1.38
18	b	304	HEC	FE-ND	4.52	2.08	1.94
18	b	304	HEC	CHA-C4D	4.50	1.49	1.39
18	b	304	HEC	FE-NB	4.48	2.08	1.94
23	M	701	HAS	C2D-C3D	4.48	1.47	1.37
23	M	702	HAS	CHC-C4B	4.45	1.47	1.38
18	J	201	HEC	CHB-C1B	4.43	1.49	1.39
18	C	301	HEC	FE-NC	4.42	2.09	1.95
18	b	304	HEC	CHD-C4C	4.39	1.49	1.39
18	C	301	HEC	FE-NA	4.37	2.09	1.95
23	M	701	HAS	FE-NA	4.37	2.09	1.95
18	N	401	HEC	FE-NC	4.34	2.09	1.95
23	M	701	HAS	FE-NC	4.31	2.09	1.95
18	J	201	HEC	CHC-C1C	4.31	1.49	1.39
18	N	401	HEC	FE-NA	4.30	2.09	1.95
23	M	701	HAS	CHC-C1C	4.29	1.49	1.39
18	J	201	HEC	CHD-C4C	4.27	1.49	1.39
16	b	301	HEM	FE-NC	4.24	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	401	HEC	CHC-C1C	4.24	1.48	1.39
18	J	201	HEC	CHA-C4D	4.23	1.48	1.39
18	J	201	HEC	FE-NC	4.21	2.09	1.95
18	N	401	HEC	CHD-C4C	4.20	1.48	1.39
18	C	301	HEC	CHB-C1B	4.19	1.48	1.39
16	b	302	HEM	FE-NC	4.16	2.08	1.95
23	M	702	HAS	C2D-C3D	4.16	1.46	1.37
18	J	201	HEC	FE-NA	4.15	2.08	1.95
18	C	301	HEC	CHC-C1C	4.11	1.48	1.39
18	N	401	HEC	CHA-C4D	4.11	1.48	1.39
18	C	301	HEC	CHA-C4D	4.10	1.48	1.39
18	C	301	HEC	CHD-C4C	4.10	1.48	1.39
23	M	701	HAS	CHA-C4D	4.09	1.48	1.39
16	B	301	HEM	FE-NC	4.08	2.08	1.95
18	N	401	HEC	CHB-C1B	4.08	1.48	1.39
23	M	701	HAS	CHB-C1B	4.07	1.48	1.39
18	b	304	HEC	C3C-C2C	4.06	1.49	1.38
18	B	305	HEC	CHA-C4D	4.03	1.48	1.39
18	b	304	HEC	CHB-C1B	4.02	1.48	1.39
18	c	302	HEC	CHB-C1B	3.97	1.48	1.39
16	B	302	HEM	FE-NC	3.94	2.08	1.95
18	c	302	HEC	CHA-C4D	3.93	1.48	1.39
18	B	305	HEC	CHC-C1C	3.92	1.48	1.39
18	b	304	HEC	FE-NA	3.90	2.08	1.95
18	b	304	HEC	FE-NC	3.90	2.08	1.95
18	J	201	HEC	C3C-C2C	3.89	1.49	1.38
18	B	305	HEC	CHB-C1B	3.84	1.47	1.39
18	c	302	HEC	CHC-C1C	3.84	1.48	1.39
23	M	702	HAS	CHD-C4C	3.84	1.48	1.39
18	B	305	HEC	C3C-C2C	3.83	1.48	1.38
18	c	302	HEC	CHD-C4C	3.80	1.47	1.39
18	b	304	HEC	CHC-C1C	3.77	1.47	1.39
23	M	702	HAS	CHB-C1B	3.76	1.47	1.39
18	C	301	HEC	C3C-C2C	3.73	1.48	1.38
23	M	702	HAS	CHA-C4D	3.67	1.47	1.39
16	b	302	HEM	C1B-NB	-3.59	1.34	1.40
23	M	702	HAS	CHC-C1C	3.59	1.47	1.39
18	c	302	HEC	C3C-C2C	3.57	1.48	1.38
16	B	302	HEM	C4D-ND	-3.56	1.34	1.40
23	M	701	HAS	CHD-C4C	3.55	1.47	1.39
18	b	304	HEC	C4B-NB	-3.49	1.34	1.40
18	N	401	HEC	C3C-C2C	3.48	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	302	HEM	C1B-NB	-3.41	1.34	1.40
18	N	401	HEC	C1D-ND	-3.30	1.34	1.40
16	B	301	HEM	C1B-NB	-3.29	1.34	1.40
16	b	301	HEM	C1B-NB	-3.26	1.34	1.40
16	B	301	HEM	C4D-ND	-3.23	1.34	1.40
16	b	301	HEM	C4D-ND	-3.22	1.34	1.40
16	b	302	HEM	C4D-ND	-3.21	1.34	1.40
23	M	701	HAS	C4B-NB	-3.19	1.34	1.40
18	B	305	HEC	C1D-ND	-3.19	1.34	1.40
23	M	701	HAS	C1C-C2C	3.17	1.50	1.43
18	J	201	HEC	C4B-NB	-3.16	1.34	1.40
18	J	201	HEC	C1D-ND	-3.13	1.34	1.40
18	B	305	HEC	C4B-NB	-3.11	1.34	1.40
18	N	401	HEC	C4B-NB	-3.11	1.34	1.40
18	b	304	HEC	C1D-ND	-3.07	1.34	1.40
23	M	701	HAS	C1D-ND	-3.01	1.35	1.40
18	c	302	HEC	C4D-C3D	2.96	1.50	1.45
18	C	301	HEC	C4B-NB	-2.93	1.35	1.40
18	C	301	HEC	C1D-ND	-2.88	1.35	1.40
23	M	702	HAS	C1D-ND	-2.84	1.35	1.40
18	c	302	HEC	C1D-ND	-2.83	1.35	1.40
18	b	304	HEC	C1A-NA	-2.82	1.34	1.39
18	C	301	HEC	C1C-C2C	2.79	1.49	1.43
18	J	201	HEC	C4D-C3D	2.77	1.49	1.45
23	M	702	HAS	C4B-NB	-2.77	1.35	1.40
18	b	304	HEC	C4C-C3C	2.77	1.50	1.44
18	c	302	HEC	C1C-C2C	2.75	1.49	1.43
18	J	201	HEC	C1C-C2C	2.74	1.49	1.43
16	B	302	HEM	FE-ND	-2.74	1.86	1.94
18	c	302	HEC	C4B-NB	-2.72	1.35	1.40
23	M	701	HAS	C11-C3B	-2.71	1.48	1.51
16	b	302	HEM	C1C-C2C	-2.68	1.40	1.45
18	b	304	HEC	C4D-C3D	2.66	1.49	1.45
23	M	701	HAS	C4A-NA	-2.64	1.34	1.39
23	M	701	HAS	C4C-NC	-2.63	1.34	1.39
18	J	201	HEC	C1A-NA	-2.63	1.34	1.39
18	b	304	HEC	C4A-NA	-2.61	1.34	1.39
16	b	302	HEM	FE-ND	-2.58	1.87	1.94
18	N	401	HEC	C1C-C2C	2.58	1.49	1.43
18	N	401	HEC	C1A-NA	-2.56	1.34	1.39
18	J	201	HEC	C1B-C2B	2.55	1.49	1.44
18	N	401	HEC	C4A-NA	-2.53	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	c	302	HEC	C1B-C2B	2.52	1.49	1.44
23	M	701	HAS	C4D-C3D	2.52	1.49	1.45
18	J	201	HEC	C4A-NA	-2.52	1.34	1.39
18	C	301	HEC	C1A-NA	-2.52	1.34	1.39
18	B	305	HEC	C4D-C3D	2.51	1.49	1.45
18	J	201	HEC	C4C-NC	-2.51	1.34	1.39
18	b	304	HEC	C1C-NC	-2.51	1.34	1.39
18	C	301	HEC	C4D-C3D	2.50	1.49	1.45
16	B	302	HEM	C1C-C2C	-2.50	1.40	1.45
23	M	701	HAS	C4B-C3B	2.46	1.49	1.44
18	N	401	HEC	C4D-C3D	2.46	1.49	1.45
18	C	301	HEC	C1B-C2B	2.45	1.49	1.44
23	M	701	HAS	C1A-NA	-2.45	1.35	1.39
16	B	301	HEM	FE-ND	-2.45	1.87	1.94
16	b	301	HEM	C1C-C2C	-2.43	1.40	1.45
18	b	304	HEC	C4C-NC	-2.42	1.35	1.39
23	M	702	HAS	C1C-C2C	2.41	1.48	1.43
18	B	305	HEC	C1B-C2B	2.41	1.49	1.44
18	C	301	HEC	C4C-NC	-2.39	1.35	1.39
23	M	701	HAS	C1A-C2A	2.39	1.49	1.45
16	b	301	HEM	FE-ND	-2.38	1.87	1.94
18	c	302	HEC	C4C-NC	-2.38	1.35	1.39
23	M	702	HAS	C1A-NA	-2.37	1.35	1.39
23	M	702	HAS	C4B-C3B	2.37	1.48	1.44
18	N	401	HEC	C4C-NC	-2.37	1.35	1.39
18	B	305	HEC	C4A-NA	-2.37	1.35	1.39
18	N	401	HEC	C4C-C3C	2.37	1.49	1.44
23	M	702	HAS	C4D-C3D	2.36	1.49	1.45
18	J	201	HEC	C1D-C2D	2.33	1.49	1.44
18	C	301	HEC	C4A-NA	-2.33	1.35	1.39
16	B	301	HEM	C1C-C2C	-2.32	1.40	1.45
18	B	305	HEC	C1A-NA	-2.32	1.35	1.39
18	J	201	HEC	C1A-C2A	2.31	1.49	1.45
18	b	304	HEC	C1B-C2B	2.31	1.49	1.44
18	C	301	HEC	C1D-C2D	2.29	1.49	1.44
18	N	401	HEC	C1B-C2B	2.28	1.49	1.44
18	J	201	HEC	C1C-NC	-2.27	1.35	1.39
18	B	305	HEC	C1A-C2A	2.26	1.49	1.45
23	M	702	HAS	C4A-NA	-2.25	1.35	1.39
23	M	702	HAS	C11-C3B	-2.25	1.48	1.51
18	C	301	HEC	C4B-C3B	2.25	1.48	1.45
16	B	302	HEM	C1D-ND	-2.24	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	M	702	HAS	C4C-NC	-2.24	1.35	1.39
18	B	305	HEC	C1D-C2D	2.24	1.49	1.44
16	b	302	HEM	C1D-ND	-2.23	1.34	1.38
18	c	302	HEC	C4A-NA	-2.23	1.35	1.39
16	B	301	HEM	C3B-C4B	2.22	1.49	1.44
18	J	201	HEC	C4B-C3B	2.20	1.48	1.45
16	b	301	HEM	C3C-C4C	-2.18	1.42	1.46
23	M	701	HAS	C1C-NC	-2.18	1.35	1.39
23	M	702	HAS	C1B-C2B	2.17	1.48	1.44
23	M	701	HAS	C1B-C2B	2.16	1.48	1.44
18	C	301	HEC	C4A-C3A	2.15	1.49	1.45
18	N	401	HEC	C4B-C3B	2.15	1.48	1.45
16	B	302	HEM	C3B-C4B	2.14	1.49	1.44
16	B	301	HEM	C3C-C4C	-2.14	1.42	1.46
18	N	401	HEC	C1C-NC	-2.13	1.35	1.39
18	C	301	HEC	C1C-NC	-2.12	1.35	1.39
18	b	304	HEC	C1C-C2C	2.12	1.48	1.43
18	J	201	HEC	C4C-C3C	2.11	1.48	1.44
18	B	305	HEC	C4B-C3B	2.10	1.48	1.45
18	C	301	HEC	C1A-C2A	2.10	1.48	1.45
16	b	302	HEM	C4B-NB	-2.09	1.34	1.38
18	N	401	HEC	C1D-C2D	2.08	1.48	1.44
18	b	304	HEC	C1D-C2D	2.08	1.48	1.44
18	C	301	HEC	C4C-C3C	2.07	1.48	1.44
18	c	302	HEC	C4B-C3B	2.06	1.48	1.45
23	M	702	HAS	C4A-C3A	2.06	1.49	1.45
16	b	301	HEM	C1D-ND	-2.05	1.34	1.38
18	b	304	HEC	C4D-ND	-2.04	1.34	1.38
16	B	302	HEM	C3C-C4C	-2.04	1.42	1.46
16	B	302	HEM	C4B-NB	-2.04	1.34	1.38
23	M	702	HAS	C1C-NC	-2.04	1.35	1.39
18	J	201	HEC	C4A-C3A	2.03	1.49	1.45
18	B	305	HEC	C4D-ND	-2.03	1.34	1.38
18	c	302	HEC	C1D-C2D	2.03	1.48	1.44
18	B	305	HEC	C1C-C2C	2.03	1.47	1.43
23	M	702	HAS	C3C-C4C	2.02	1.48	1.42
18	b	304	HEC	C1A-C2A	2.01	1.48	1.45
18	c	302	HEC	C1A-NA	-2.01	1.35	1.39

All (290) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M	702	HAS	C2D-C3D-C4D	-7.74	100.83	106.43
23	M	701	HAS	C2D-C3D-C4D	-7.20	101.22	106.43
18	b	304	HEC	C1B-C2B-C3B	-6.03	100.64	106.98
23	M	702	HAS	C2A-C1A-NA	5.94	116.05	110.32
18	B	305	HEC	C1B-C2B-C3B	-5.93	100.74	106.98
18	N	401	HEC	C1B-C2B-C3B	-5.86	100.82	106.98
23	M	702	HAS	C3D-C4D-ND	5.80	115.95	110.35
18	c	302	HEC	C1B-C2B-C3B	-5.70	100.99	106.98
23	M	702	HAS	C3C-C2C-C1C	-5.55	100.63	107.17
18	C	301	HEC	C1B-C2B-C3B	-5.53	101.17	106.98
18	J	201	HEC	C1B-C2B-C3B	-5.52	101.17	106.98
18	c	302	HEC	C1C-C2C-C3C	-5.48	100.54	106.82
18	B	305	HEC	CBC-CAC-C3C	5.46	127.22	112.42
18	B	305	HEC	C2B-C1B-NB	5.38	116.12	109.90
18	c	302	HEC	C2B-C1B-NB	5.33	116.06	109.90
18	c	302	HEC	C2A-C1A-NA	5.18	115.32	110.32
18	b	304	HEC	C1C-C2C-C3C	-5.13	100.94	106.82
23	M	702	HAS	C3B-C4B-NB	5.12	115.73	109.84
18	c	302	HEC	C2D-C1D-ND	5.11	115.71	109.84
23	M	701	HAS	C3C-C2C-C1C	-5.04	101.23	107.17
18	C	301	HEC	C1C-C2C-C3C	-5.04	101.04	106.82
18	B	305	HEC	C2A-C1A-NA	5.03	115.18	110.32
16	b	301	HEM	CHC-C4B-NB	5.01	129.81	124.42
18	J	201	HEC	C1C-C2C-C3C	-4.97	101.13	106.82
18	b	304	HEC	CMC-C2C-C3C	4.93	136.07	125.62
23	M	701	HAS	C3C-C4C-NC	4.92	113.94	109.80
18	c	302	HEC	C3D-C4D-ND	4.89	115.08	110.35
23	M	702	HAS	C2B-C1B-NB	4.80	115.46	109.90
18	B	305	HEC	C2D-C1D-ND	4.69	115.23	109.84
18	B	305	HEC	CHD-C4C-NC	-4.67	115.38	123.86
23	M	702	HAS	C3C-C4C-NC	4.67	113.73	109.80
16	B	301	HEM	CHD-C1D-ND	4.67	129.45	124.42
16	b	302	HEM	CHC-C4B-NB	4.64	129.42	124.42
18	C	301	HEC	CBB-CAB-C3B	4.63	124.96	112.42
18	c	302	HEC	CBB-CAB-C3B	4.62	124.95	112.42
18	J	201	HEC	CBB-CAB-C3B	4.62	124.94	112.42
18	C	301	HEC	C2B-C1B-NB	4.62	115.24	109.90
18	N	401	HEC	C2B-C1B-NB	4.59	115.21	109.90
18	B	305	HEC	CAC-C3C-C4C	4.59	131.22	124.91
18	J	201	HEC	CBC-CAC-C3C	4.54	124.72	112.42
18	C	301	HEC	CBC-CAC-C3C	4.54	124.71	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c	302	HEC	CBC-CAC-C3C	4.53	124.70	112.42
18	N	401	HEC	C1C-C2C-C3C	-4.52	101.64	106.82
23	M	701	HAS	C3D-C4D-ND	4.52	114.72	110.35
18	b	304	HEC	C2B-C1B-NB	4.51	115.12	109.90
16	B	301	HEM	CHC-C4B-NB	4.44	129.20	124.42
18	B	305	HEC	C1D-C2D-C3D	-4.43	102.32	106.98
18	B	305	HEC	CBB-CAB-C3B	4.43	124.42	112.42
18	B	305	HEC	C3D-C4D-ND	4.39	114.60	110.35
18	C	301	HEC	C3D-C4D-ND	4.35	114.56	110.35
18	N	401	HEC	CBC-CAC-C3C	4.32	124.12	112.42
23	M	701	HAS	C2A-C1A-NA	4.31	114.48	110.32
18	N	401	HEC	CBB-CAB-C3B	4.30	124.08	112.42
18	C	301	HEC	C2A-C1A-NA	4.30	114.47	110.32
23	M	701	HAS	C2B-C1B-NB	4.25	114.81	109.90
18	N	401	HEC	C2A-C1A-NA	4.21	114.39	110.32
16	B	302	HEM	C1B-NB-C4B	4.21	110.19	105.21
18	N	401	HEC	C2D-C1D-ND	4.18	114.65	109.84
16	b	301	HEM	CHD-C1D-ND	4.07	128.80	124.42
18	B	305	HEC	C1C-C2C-C3C	-4.07	102.16	106.82
18	J	201	HEC	CHA-C4D-ND	-4.06	120.05	124.42
18	J	201	HEC	C2B-C1B-NB	4.05	114.59	109.90
18	C	301	HEC	C2D-C1D-ND	4.02	114.46	109.84
18	N	401	HEC	C1D-C2D-C3D	-4.00	102.78	106.98
23	M	702	HAS	C2C-C1C-NC	3.99	116.53	110.14
18	B	305	HEC	CHD-C1D-ND	-3.93	119.51	124.37
18	J	201	HEC	C3D-C4D-ND	3.93	114.15	110.35
18	b	304	HEC	CHB-C1B-NB	-3.93	120.20	124.42
18	N	401	HEC	C3D-C4D-ND	3.91	114.13	110.35
18	b	304	HEC	CBC-CAC-C3C	3.91	123.01	112.42
16	b	301	HEM	CHA-C4D-ND	3.90	129.19	124.37
16	b	302	HEM	CHD-C1D-ND	3.87	128.58	124.42
18	J	201	HEC	C2A-C1A-NA	3.86	114.05	110.32
18	b	304	HEC	C1D-C2D-C3D	-3.84	102.94	106.98
23	M	701	HAS	C1B-C2B-C3B	-3.84	102.35	106.80
18	c	302	HEC	C2C-C1C-NC	3.83	116.29	110.14
18	c	302	HEC	CAD-C3D-C4D	3.83	131.37	124.70
23	M	702	HAS	C17-C18-C19	-3.83	118.86	127.62
18	b	304	HEC	CBB-CAB-C3B	3.82	122.79	112.42
18	C	301	HEC	C1D-C2D-C3D	-3.80	102.98	106.98
18	c	302	HEC	C3B-C4B-NB	3.78	114.31	110.17
18	N	401	HEC	CAC-C3C-C4C	3.77	130.10	124.91
18	c	302	HEC	C1D-C2D-C3D	-3.76	103.02	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M	701	HAS	C3B-C4B-NB	3.76	114.16	109.84
16	B	301	HEM	CHA-C4D-ND	3.74	128.99	124.37
16	b	301	HEM	CHB-C1B-NB	3.64	128.87	124.37
18	b	304	HEC	C2C-C1C-NC	3.62	115.95	110.14
23	M	701	HAS	C12-C11-C3B	-3.62	106.47	112.12
18	c	302	HEC	C3C-C4C-NC	3.61	114.16	110.15
16	B	301	HEM	CHB-C1B-NB	3.61	128.83	124.37
18	B	305	HEC	C3B-C4B-NB	3.60	114.12	110.17
18	b	304	HEC	C2D-C1D-ND	3.58	113.95	109.84
16	B	302	HEM	CHD-C1D-ND	3.57	128.26	124.42
18	J	201	HEC	CHB-C1B-NB	-3.53	120.62	124.42
23	M	702	HAS	C1A-C2A-C3A	-3.53	102.47	107.11
18	J	201	HEC	CHA-C1A-NA	-3.51	120.63	124.45
18	J	201	HEC	C2D-C1D-ND	3.50	113.86	109.84
16	B	302	HEM	C3B-C4B-NB	-3.48	106.97	109.47
23	M	702	HAS	C27-C19-C20	3.46	121.23	115.23
18	J	201	HEC	C1D-C2D-C3D	-3.45	103.36	106.98
18	B	305	HEC	C1A-C2A-C3A	-3.43	102.59	107.11
18	N	401	HEC	CHB-C4A-NA	-3.42	120.73	124.45
17	B	303	MQ7	C11-C3-C2	-3.39	119.07	124.89
23	M	702	HAS	C1B-C2B-C3B	-3.39	102.87	106.80
18	c	302	HEC	C1A-C2A-C3A	-3.39	102.65	107.11
18	b	304	HEC	CHA-C4D-ND	-3.37	120.79	124.42
23	M	702	HAS	C13-C14-C15	-3.36	119.93	127.62
16	b	302	HEM	C1B-NB-C4B	3.36	109.18	105.21
18	B	305	HEC	CMC-C2C-C3C	3.36	132.74	125.62
17	b	303	MQ7	C11-C3-C2	-3.35	119.15	124.89
18	b	304	HEC	C2A-C1A-NA	3.31	113.52	110.32
18	b	304	HEC	CHB-C4A-NA	-3.30	120.86	124.45
23	M	701	HAS	CMC-C2C-C1C	3.30	130.44	125.42
18	J	201	HEC	C1A-C2A-C3A	-3.28	102.79	107.11
16	b	302	HEM	CHA-C4D-ND	3.24	128.38	124.37
18	C	301	HEC	C4A-C3A-C2A	-3.24	102.16	106.97
23	M	701	HAS	C1A-C2A-C3A	-3.22	102.87	107.11
16	b	302	HEM	CHB-C1B-NB	3.22	128.34	124.37
18	B	305	HEC	C2C-C1C-NC	3.22	115.30	110.14
18	J	201	HEC	CHB-C4A-NA	-3.21	120.96	124.45
16	B	301	HEM	C1B-NB-C4B	3.21	109.01	105.21
18	b	304	HEC	C3D-C4D-ND	3.20	113.45	110.35
22	L	303	5PL	OCK-CBU-CBV	3.18	118.37	111.48
23	M	702	HAS	C3A-C4A-NA	3.17	115.50	109.64
18	C	301	HEC	C2C-C1C-NC	3.14	115.18	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M	702	HAS	CAD-C3D-C4D	3.11	130.12	124.70
23	M	702	HAS	C21-C22-C23	-3.09	120.55	127.62
23	M	701	HAS	C3A-C4A-NA	3.09	115.35	109.64
16	B	302	HEM	CHC-C4B-NB	3.08	127.74	124.42
18	N	401	HEC	CHB-C1B-NB	-3.08	121.11	124.42
18	J	201	HEC	CAD-C3D-C4D	3.08	130.07	124.70
18	N	401	HEC	C1A-C2A-C3A	-3.08	103.05	107.11
18	B	305	HEC	C3A-C4A-NA	3.07	115.31	109.64
16	B	302	HEM	CHB-C1B-NB	3.06	128.15	124.37
18	c	302	HEC	C4D-C3D-C2D	-3.02	102.49	106.89
23	M	702	HAS	C4A-C3A-C2A	-3.01	102.50	106.97
18	J	201	HEC	C4D-C3D-C2D	-3.01	102.51	106.89
23	M	701	HAS	C26-C15-C16	3.00	120.43	115.23
23	M	702	HAS	C4B-C3B-C2B	-2.98	102.43	107.44
18	B	305	HEC	CHA-C4D-ND	-2.97	121.23	124.42
16	b	301	HEM	C1B-NB-C4B	2.96	108.72	105.21
18	c	302	HEC	CMC-C2C-C3C	2.94	131.86	125.62
18	N	401	HEC	CHD-C1D-ND	-2.94	120.73	124.37
18	C	301	HEC	C1A-C2A-C3A	-2.93	103.25	107.11
18	B	305	HEC	C4A-C3A-C2A	-2.93	102.63	106.97
18	C	301	HEC	CHA-C4D-ND	-2.93	121.27	124.42
16	B	302	HEM	CHA-C4D-ND	2.92	127.98	124.37
23	M	701	HAS	C4A-C3A-C2A	-2.91	102.65	106.97
23	M	701	HAS	OMD-CMD-C2D	-2.90	119.07	125.62
18	c	302	HEC	C3A-C4A-NA	2.89	114.99	109.64
18	b	304	HEC	C1A-C2A-C3A	-2.89	103.30	107.11
18	C	301	HEC	CMC-C2C-C3C	2.89	131.75	125.62
18	J	201	HEC	CMC-C2C-C3C	2.89	131.75	125.62
18	C	301	HEC	CHB-C4A-NA	-2.88	121.32	124.45
18	b	304	HEC	C4A-C3A-C2A	-2.88	102.70	106.97
23	M	702	HAS	C25-C23-C24	2.87	120.22	115.23
16	B	301	HEM	CHD-C1D-C2D	-2.86	120.51	125.03
18	J	201	HEC	C2C-C1C-NC	2.86	114.72	110.14
16	B	302	HEM	C1C-CHC-C4B	-2.85	119.96	126.02
18	N	401	HEC	CHA-C4D-ND	-2.85	121.36	124.42
23	M	701	HAS	CAA-CBA-CGA	-2.83	106.15	113.67
16	B	301	HEM	C3B-C4B-NB	-2.83	107.44	109.47
23	M	701	HAS	CHB-C1B-NB	-2.83	121.38	124.42
18	N	401	HEC	C4A-C3A-C2A	-2.82	102.79	106.97
18	C	301	HEC	C4D-C3D-C2D	-2.82	102.79	106.89
23	M	701	HAS	CAD-CBD-CGD	-2.81	106.21	113.67
18	C	301	HEC	C3B-C4B-NB	2.80	113.24	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M	702	HAS	C32-C30-C31	2.78	120.98	114.59
18	N	401	HEC	C2C-C1C-NC	2.78	114.59	110.14
18	J	201	HEC	CHD-C1D-ND	-2.77	120.94	124.37
23	M	701	HAS	CHA-C1A-NA	-2.77	121.44	124.45
16	B	302	HEM	C4D-ND-C1D	2.76	108.48	105.21
18	C	301	HEC	C3A-C4A-NA	2.76	114.74	109.64
18	c	302	HEC	C4A-C3A-C2A	-2.75	102.89	106.97
23	M	701	HAS	CAD-C3D-C4D	2.73	129.45	124.70
23	M	701	HAS	C2C-C1C-NC	2.72	114.51	110.14
18	b	304	HEC	CHA-C1A-NA	-2.71	121.50	124.45
18	C	301	HEC	CHB-C1B-NB	-2.71	121.51	124.42
16	B	301	HEM	CHD-C4C-NC	2.71	127.40	124.45
16	b	301	HEM	CHD-C4C-NC	2.71	127.40	124.45
18	C	301	HEC	C3C-C4C-NC	2.70	113.15	110.15
23	M	702	HAS	CAA-CBA-CGA	-2.69	106.53	113.67
23	M	701	HAS	C21-C22-C23	-2.69	121.47	127.62
18	B	305	HEC	C4D-C3D-C2D	-2.69	102.98	106.89
18	N	401	HEC	C4D-C3D-C2D	-2.69	102.98	106.89
23	M	702	HAS	OMD-CMD-C2D	-2.66	119.61	125.62
23	M	701	HAS	C13-C14-C15	-2.66	121.54	127.62
23	M	702	HAS	CAD-CBD-CGD	-2.65	106.64	113.67
16	b	302	HEM	C3B-C4B-NB	-2.63	107.58	109.47
23	M	702	HAS	CHA-C1A-C2A	-2.62	120.72	124.86
18	J	201	HEC	C4A-C3A-C2A	-2.60	103.12	106.97
23	M	701	HAS	C27-C19-C20	2.60	119.74	115.23
18	b	304	HEC	C4D-C3D-C2D	-2.60	103.11	106.89
18	c	302	HEC	CAC-C3C-C2C	2.59	130.99	126.89
18	N	401	HEC	CAD-C3D-C4D	2.56	129.16	124.70
16	B	302	HEM	C1A-CHA-C4D	-2.55	120.26	126.25
18	B	305	HEC	CHB-C1B-NB	-2.54	121.69	124.42
16	b	301	HEM	CHA-C4D-C3D	-2.51	120.61	125.23
18	C	301	HEC	CAC-C3C-C2C	2.50	130.85	126.89
18	N	401	HEC	C3A-C4A-NA	2.49	114.25	109.64
18	B	305	HEC	CHD-C4C-C3C	2.48	130.74	125.30
18	N	401	HEC	CMA-C3A-C4A	2.47	129.07	124.73
17	B	304	MQ7	C11-C3-C2	-2.46	120.68	124.89
18	J	201	HEC	CAC-C3C-C2C	2.45	130.77	126.89
23	M	701	HAS	C4B-C3B-C2B	-2.45	103.31	107.44
23	M	702	HAS	CMB-C2B-C1B	2.45	128.86	125.03
18	C	301	HEC	CHA-C1A-NA	-2.44	121.80	124.45
18	b	304	HEC	CHD-C1D-ND	-2.43	121.36	124.37
18	C	301	HEC	CAD-C3D-C4D	2.43	128.93	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M	702	HAS	CHC-C1C-C2C	-2.42	120.41	127.43
23	M	702	HAS	CHA-C4D-C3D	-2.42	121.25	124.77
18	c	302	HEC	CMD-C2D-C1D	2.40	128.79	125.03
20	C	303	PC1	O12-P-O14	2.40	123.61	112.44
18	N	401	HEC	CMD-C2D-C1D	2.38	128.76	125.03
17	c	301	MQ7	C11-C3-C2	-2.38	120.80	124.89
21	J	202	CDL	C72-C71-CB7	-2.37	105.00	113.69
18	B	305	HEC	CHA-C1A-NA	-2.37	121.87	124.45
20	c	304	PC1	O12-P-O14	2.37	123.47	112.44
21	J	202	CDL	OB6-CB5-C51	2.37	116.61	111.48
23	M	701	HAS	C17-C18-C19	-2.37	122.21	127.62
18	b	304	HEC	CAA-CBA-CGA	-2.36	107.41	113.67
16	b	301	HEM	C3B-C4B-NB	-2.34	107.78	109.47
18	b	304	HEC	C3B-C4B-NB	2.34	112.74	110.17
17	B	303	MQ7	C11-C3-C4	2.34	121.05	118.58
16	B	301	HEM	C1A-CHA-C4D	-2.34	120.74	126.25
18	b	304	HEC	CHC-C1C-C2C	-2.34	120.63	127.43
16	b	301	HEM	C4C-CHD-C1D	-2.34	121.05	126.02
23	M	702	HAS	CMC-C2C-C3C	2.33	132.03	126.55
18	J	201	HEC	CHC-C4B-NB	-2.32	121.49	124.37
18	b	304	HEC	CHD-C4C-NC	-2.32	119.65	123.86
16	b	302	HEM	C4D-ND-C1D	2.32	107.96	105.21
23	M	701	HAS	C32-C30-C31	2.32	119.92	114.59
18	b	304	HEC	CMB-C2B-C3B	2.32	132.41	126.15
16	b	302	HEM	C4A-CHB-C1B	-2.31	120.81	126.25
16	B	302	HEM	C4C-CHD-C1D	-2.30	121.13	126.02
16	b	301	HEM	CHD-C1D-C2D	-2.30	121.40	125.03
16	b	302	HEM	C4C-CHD-C1D	-2.27	121.19	126.02
18	N	401	HEC	CMB-C2B-C3B	2.27	132.29	126.15
23	M	701	HAS	C25-C23-C24	2.27	119.16	115.23
18	J	201	HEC	C3B-C4B-NB	2.26	112.65	110.17
18	N	401	HEC	CMC-C2C-C1C	2.26	128.85	125.42
16	B	301	HEM	CHA-C4D-C3D	-2.25	121.09	125.23
23	M	702	HAS	C13-C12-C11	-2.25	110.81	114.39
16	b	302	HEM	C1A-CHA-C4D	-2.24	120.98	126.25
23	M	701	HAS	CHA-C4D-ND	-2.24	122.02	124.42
18	c	302	HEC	CHA-C1A-C2A	-2.24	121.33	124.86
18	c	302	HEC	CHA-C4D-ND	-2.23	122.03	124.42
16	b	301	HEM	CHB-C1B-C2B	-2.22	120.63	126.95
18	B	305	HEC	CAA-CBA-CGA	-2.22	107.77	113.67
18	N	401	HEC	CHA-C1A-NA	-2.22	122.04	124.45
18	C	301	HEC	CHD-C1D-ND	-2.22	121.62	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	302	HEM	C4A-CHB-C1B	-2.21	121.05	126.25
23	M	702	HAS	C28-C29-C30	-2.21	120.28	127.64
18	C	301	HEC	CMD-C2D-C1D	2.21	128.48	125.03
18	J	201	HEC	C3A-C4A-NA	2.20	113.71	109.64
23	M	701	HAS	CAA-C2A-C1A	2.20	129.32	124.85
23	M	701	HAS	CHC-C4B-NB	-2.19	121.66	124.37
18	J	201	HEC	C3C-C4C-NC	2.18	112.57	110.15
18	B	305	HEC	CHC-C4B-NB	-2.18	121.67	124.37
18	b	304	HEC	CHC-C4B-NB	-2.18	121.67	124.37
18	B	305	HEC	CMB-C2B-C3B	2.18	132.03	126.15
18	b	304	HEC	C3A-C4A-NA	2.17	113.65	109.64
18	N	401	HEC	C3B-C4B-NB	2.17	112.55	110.17
18	B	305	HEC	CAC-C3C-C2C	-2.15	123.49	126.89
18	B	305	HEC	CHB-C4A-NA	-2.14	122.12	124.45
18	c	302	HEC	CHC-C1C-C2C	-2.14	121.22	127.43
18	J	201	HEC	CMD-C2D-C1D	2.13	128.37	125.03
18	c	302	HEC	CHB-C1B-C2B	-2.13	121.66	125.03
16	b	301	HEM	C1A-CHA-C4D	-2.13	121.24	126.25
18	N	401	HEC	CBD-CAD-C3D	-2.13	106.65	112.53
23	M	701	HAS	CMB-C2B-C1B	2.13	128.36	125.03
23	M	701	HAS	CHD-C4A-NA	-2.12	122.14	124.45
23	M	701	HAS	C28-C29-C30	-2.12	120.59	127.64
18	B	305	HEC	CMD-C2D-C1D	2.11	128.34	125.03
16	B	301	HEM	CHB-C1B-C2B	-2.10	120.97	126.95
18	J	201	HEC	CMA-C3A-C4A	2.10	128.43	124.73
23	M	701	HAS	CHC-C1C-NC	-2.10	120.06	123.86
16	b	302	HEM	CHD-C1D-C2D	-2.08	121.74	125.03
23	M	702	HAS	CHB-C1B-C2B	-2.08	121.74	125.03
19	J	203	PEE	O2-C2-C1	2.08	115.80	108.34
16	B	301	HEM	CHA-C1A-NA	2.07	127.61	123.86
18	B	305	HEC	CHC-C1C-C2C	-2.07	121.43	127.43
16	B	302	HEM	C2A-C1A-NA	-2.06	107.86	110.15
16	b	302	HEM	O2A-CGA-CBA	2.06	120.52	114.00
18	C	301	HEC	CHC-C4B-NB	-2.06	121.81	124.37
18	C	301	HEC	CMB-C2B-C3B	2.05	131.70	126.15
18	c	302	HEC	CBD-CAD-C3D	2.05	118.20	112.53
18	b	304	HEC	CAD-C3D-C4D	2.03	128.24	124.70
23	M	702	HAS	CAA-C2A-C3A	2.02	131.66	127.87
17	b	303	MQ7	C11-C3-C4	2.01	120.69	118.58

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	B	305	HEC	NA
18	C	301	HEC	NA
18	J	201	HEC	NA
18	N	401	HEC	NA
18	b	304	HEC	NA
18	c	302	HEC	NA
23	M	701	HAS	NA
23	M	702	HAS	NA

All (271) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	301	HEM	C2C-C3C-CAC-CBC
16	B	301	HEM	C4C-C3C-CAC-CBC
16	b	301	HEM	C2C-C3C-CAC-CBC
16	b	301	HEM	C4C-C3C-CAC-CBC
17	B	303	MQ7	C12-C11-C3-C2
17	B	303	MQ7	C12-C11-C3-C4
17	B	304	MQ7	C13-C15-C16-C17
19	J	203	PEE	C1-O3P-P-O1P
19	J	203	PEE	C1-O3P-P-O4P
19	J	203	PEE	O5-C30-O3-C3
19	J	203	PEE	C31-C30-O3-C3
20	C	303	PC1	C11-O13-P-O12
20	C	303	PC1	C11-O13-P-O14
20	C	303	PC1	C11-O13-P-O11
20	C	303	PC1	C1-O11-P-O12
20	C	303	PC1	C1-O11-P-O13
20	C	303	PC1	O13-C11-C12-N
20	C	303	PC1	O22-C21-O21-C2
20	C	303	PC1	C22-C21-O21-C2
21	J	202	CDL	CB3-OB5-PB2-OB3
21	J	202	CDL	CB4-CB3-OB5-PB2
21	J	202	CDL	OB7-CB5-OB6-CB4
21	J	202	CDL	C51-CB5-OB6-CB4
21	J	202	CDL	OB9-CB7-OB8-CB6
21	K	201	CDL	C1-CA2-OA2-PA1
21	K	201	CDL	OA9-CA7-OA8-CA6
21	K	201	CDL	C31-CA7-OA8-CA6
21	L	302	CDL	C1-CA2-OA2-PA1
21	L	302	CDL	OA9-CA7-OA8-CA6
21	L	302	CDL	C31-CA7-OA8-CA6
21	L	302	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
21	L	302	CDL	CB3-OB5-PB2-OB2
21	L	302	CDL	OB9-CB7-OB8-CB6
21	L	302	CDL	C71-CB7-OB8-CB6
22	L	303	5PL	CAW-OCJ-PCR-OCM
22	L	303	5PL	OCG-CAN-CAP-OCH
22	L	303	5PL	OCG-CAN-CAP-NCB
22	L	303	5PL	CBV-CBU-OCK-CBH
22	L	303	5PL	OCN-CBU-OCK-CBH
22	L	303	5PL	C1-C2-N2-CAQ
23	M	701	HAS	C1D-C2D-CMD-OMD
23	M	701	HAS	C3D-C2D-CMD-OMD
23	M	701	HAS	C11-C12-C13-C14
23	M	702	HAS	C1A-C2A-CAA-CBA
23	M	702	HAS	C3A-C2A-CAA-CBA
23	M	702	HAS	C1D-C2D-CMD-OMD
23	M	702	HAS	C3D-C2D-CMD-OMD
18	N	401	HEC	C2C-C3C-CAC-CBC
18	B	305	HEC	C4B-C3B-CAB-CBB
18	C	301	HEC	C4B-C3B-CAB-CBB
18	J	201	HEC	C4B-C3B-CAB-CBB
18	N	401	HEC	C4B-C3B-CAB-CBB
18	c	302	HEC	C4B-C3B-CAB-CBB
21	J	202	CDL	C71-CB7-OB8-CB6
18	C	301	HEC	C4C-C3C-CAC-CBC
18	J	201	HEC	C4C-C3C-CAC-CBC
18	N	401	HEC	C4C-C3C-CAC-CBC
18	b	304	HEC	C4C-C3C-CAC-CBC
18	c	302	HEC	C4C-C3C-CAC-CBC
18	b	304	HEC	C4B-C3B-CAB-CBB
18	B	305	HEC	C2B-C3B-CAB-CBB
18	C	301	HEC	C2B-C3B-CAB-CBB
18	J	201	HEC	C2B-C3B-CAB-CBB
18	N	401	HEC	C2B-C3B-CAB-CBB
18	b	304	HEC	C2B-C3B-CAB-CBB
18	c	302	HEC	C2B-C3B-CAB-CBB
18	B	305	HEC	C4C-C3C-CAC-CBC
18	B	305	HEC	C2C-C3C-CAC-CBC
18	C	301	HEC	C2C-C3C-CAC-CBC
18	J	201	HEC	C2C-C3C-CAC-CBC
18	b	304	HEC	C2C-C3C-CAC-CBC
18	c	302	HEC	C2C-C3C-CAC-CBC
17	B	304	MQ7	C19-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
17	b	303	MQ7	C39-C38-C40-C41
23	M	701	HAS	C26-C15-C16-C17
17	B	304	MQ7	C17-C18-C20-C21
23	M	701	HAS	C14-C15-C16-C17
17	B	304	MQ7	C39-C38-C40-C41
17	b	303	MQ7	C24-C23-C25-C26
17	c	301	MQ7	C34-C33-C35-C36
17	c	301	MQ7	C39-C38-C40-C41
17	B	304	MQ7	C37-C38-C40-C41
17	b	303	MQ7	C22-C23-C25-C26
17	c	301	MQ7	C32-C33-C35-C36
17	c	301	MQ7	C37-C38-C40-C41
17	B	303	MQ7	C33-C35-C36-C37
17	c	301	MQ7	C28-C30-C31-C32
23	M	702	HAS	C15-C16-C17-C18
23	M	702	HAS	C23-C24-C28-C29
18	J	201	HEC	C2A-CAA-CBA-CGA
18	N	401	HEC	C2A-CAA-CBA-CGA
18	c	302	HEC	C2A-CAA-CBA-CGA
18	c	302	HEC	C3D-CAD-CBD-CGD
17	B	303	MQ7	C39-C38-C40-C41
17	B	303	MQ7	C37-C38-C40-C41
17	b	303	MQ7	C37-C38-C40-C41
21	L	302	CDL	OB6-CB4-CB6-OB8
16	b	301	HEM	C2A-CAA-CBA-CGA
18	b	304	HEC	C3D-CAD-CBD-CGD
20	c	304	PC1	C22-C21-O21-C2
20	c	304	PC1	O22-C21-O21-C2
20	c	304	PC1	C32-C31-O31-C3
20	c	304	PC1	O32-C31-O31-C3
21	L	302	CDL	CA5-C11-C12-C13
22	L	303	5PL	CAM-CAN-OCG-PCR
18	J	201	HEC	C2D-C3D-CAD-CBD
18	J	201	HEC	C4D-C3D-CAD-CBD
21	L	302	CDL	CB3-CB4-CB6-OB8
19	c	303	PEE	C33-C34-C35-C36
21	K	201	CDL	CA4-CA3-OA5-PA1
20	C	303	PC1	C32-C33-C34-C35
20	C	303	PC1	C2B-C2C-C2D-C2E
20	c	304	PC1	C33-C34-C35-C36
18	B	305	HEC	C1A-C2A-CAA-CBA
22	L	303	5PL	CAN-CAM-O1-C1

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Mol	Chain	Res	Type	Atoms
16	b	302	HEM	C2C-C3C-CAC-CBC
17	B	304	MQ7	C38-C40-C41-C42
22	L	303	5PL	CBU-CBV-CBW-CBX
22	L	303	5PL	CBH-CAW-OCJ-PCR
21	J	202	CDL	C17-C18-C19-C20
21	J	202	CDL	C14-C15-C16-C17
21	K	201	CDL	C12-C13-C14-C15
20	c	304	PC1	C24-C25-C26-C27
23	M	702	HAS	C14-C15-C16-C17
18	B	305	HEC	C3A-C2A-CAA-CBA
23	M	702	HAS	C26-C15-C16-C17
21	K	201	CDL	C52-C51-CB5-OB6
19	J	203	PEE	C31-C32-C33-C34
23	M	701	HAS	C23-C24-C28-C29
17	B	304	MQ7	C25-C26-C27-C28
17	b	303	MQ7	C19-C18-C20-C21
20	C	303	PC1	C38-C39-C3A-C3B
19	c	303	PEE	C18-C19-C20-C21
21	J	202	CDL	C19-C20-C21-C22
16	B	301	HEM	C2A-CAA-CBA-CGA
18	C	301	HEC	C3D-CAD-CBD-CGD
21	L	302	CDL	OB5-CB3-CB4-CB6
22	L	303	5PL	OCJ-CAW-CBH-CBI
20	c	304	PC1	C26-C27-C28-C29
22	L	303	5PL	CAM-CAN-CAP-OCH
21	L	302	CDL	C71-C72-C73-C74
22	L	303	5PL	CAU-CAV-CBJ-C18
22	L	303	5PL	CAM-CAN-CAP-NCB
19	c	303	PEE	C32-C33-C34-C35
21	J	202	CDL	C52-C53-C54-C55
19	L	301	PEE	C36-C37-C38-C39
17	b	303	MQ7	C12-C11-C3-C2
16	B	302	HEM	C2C-C3C-CAC-CBC
16	b	301	HEM	C2B-C3B-CAB-CBB
16	b	302	HEM	C2B-C3B-CAB-CBB
22	L	303	5PL	OCJ-CAW-CBH-OCK
23	M	701	HAS	C19-C20-C21-C22
16	B	302	HEM	C4B-C3B-CAB-CBB
17	b	303	MQ7	C17-C18-C20-C21
17	b	303	MQ7	C12-C11-C3-C4
19	L	301	PEE	C5-C4-O4P-P
19	L	301	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
19	c	303	PEE	O2-C2-C3-O3
22	L	303	5PL	CBV-CBW-CBX-CBY
20	c	304	PC1	O13-C11-C12-N
17	B	303	MQ7	C24-C23-C25-C26
18	J	201	HEC	C3D-CAD-CBD-CGD
17	B	303	MQ7	C14-C13-C15-C16
21	J	202	CDL	C82-C83-C84-C85
19	C	302	PEE	C16-C17-C18-C19
21	J	202	CDL	C39-C40-C41-C42
19	J	203	PEE	C2-C1-O3P-P
16	B	302	HEM	C2A-CAA-CBA-CGA
19	J	203	PEE	C1-O3P-P-O2P
19	L	301	PEE	C4-O4P-P-O1P
19	c	303	PEE	C1-O3P-P-O1P
21	J	202	CDL	CA2-OA2-PA1-OA3
21	K	201	CDL	CA2-OA2-PA1-OA3
21	L	302	CDL	CA3-OA5-PA1-OA3
21	L	302	CDL	CB3-OB5-PB2-OB3
22	L	303	5PL	CAW-OCJ-PCR-OCG
21	L	302	CDL	C51-C52-C53-C54
20	C	303	PC1	C1-C2-O21-C21
19	L	301	PEE	C18-C19-C20-C21
21	L	302	CDL	C54-C55-C56-C57
18	b	304	HEC	C2D-C3D-CAD-CBD
21	J	202	CDL	C1-CB2-OB2-PB2
17	B	303	MQ7	C12-C13-C15-C16
17	B	303	MQ7	C22-C23-C25-C26
19	J	203	PEE	C18-C19-C20-C21
17	c	301	MQ7	C13-C15-C16-C17
16	b	301	HEM	C4B-C3B-CAB-CBB
16	b	302	HEM	C4C-C3C-CAC-CBC
18	c	302	HEC	CAA-CBA-CGA-O2A
19	c	303	PEE	C16-C17-C18-C19
18	c	302	HEC	CAA-CBA-CGA-O1A
22	L	303	5PL	C3-C2-N2-CAQ
21	L	302	CDL	C78-C79-C80-C81
17	B	304	MQ7	C34-C33-C35-C36
18	N	401	HEC	CAD-CBD-CGD-O2D
21	J	202	CDL	OB5-CB3-CB4-OB6
16	b	301	HEM	CAD-CBD-CGD-O2D
18	b	304	HEC	CAA-CBA-CGA-O2A
17	B	304	MQ7	C29-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
21	J	202	CDL	OA6-CA4-CA6-OA8
16	B	301	HEM	CAD-CBD-CGD-O1D
18	N	401	HEC	CAD-CBD-CGD-O1D
23	M	702	HAS	CAD-CBD-CGD-O1D
20	c	304	PC1	C37-C38-C39-C3A
16	B	301	HEM	CAD-CBD-CGD-O2D
21	L	302	CDL	C17-C18-C19-C20
17	B	304	MQ7	C24-C23-C25-C26
16	b	301	HEM	CAD-CBD-CGD-O1D
17	B	304	MQ7	C35-C36-C37-C38
18	b	304	HEC	CAA-CBA-CGA-O1A
21	K	201	CDL	C84-C85-C86-C87
23	M	702	HAS	CAD-CBD-CGD-O2D
22	L	303	5PL	C19-C18-CBJ-CAV
16	B	301	HEM	CAA-CBA-CGA-O1A
21	J	202	CDL	CA5-C11-C12-C13
20	c	304	PC1	C34-C35-C36-C37
21	L	302	CDL	OB5-CB3-CB4-OB6
18	c	302	HEC	CAD-CBD-CGD-O1D
21	K	201	CDL	C52-C51-CB5-OB7
20	C	303	PC1	C34-C35-C36-C37
18	J	201	HEC	CAD-CBD-CGD-O2D
19	c	303	PEE	C10-C11-C12-C13
23	M	702	HAS	CAA-CBA-CGA-O2A
18	B	305	HEC	CAA-CBA-CGA-O2A
18	c	302	HEC	CAD-CBD-CGD-O2D
17	B	304	MQ7	C27-C28-C30-C31
17	c	301	MQ7	C40-C41-C42-C43
21	J	202	CDL	C18-C19-C20-C21
16	B	302	HEM	CAD-CBD-CGD-O2D
16	B	302	HEM	CAD-CBD-CGD-O1D
20	c	304	PC1	C35-C36-C37-C38
23	M	701	HAS	CAA-CBA-CGA-O1A
21	J	202	CDL	CA6-CA4-OA6-CA5
18	C	301	HEC	CAA-CBA-CGA-O2A
22	L	303	5PL	CAZ-CBA-CBB-CBC
23	M	701	HAS	CAA-CBA-CGA-O2A
19	L	301	PEE	C1-C2-C3-O3
16	B	302	HEM	C4C-C3C-CAC-CBC
16	b	302	HEM	C4B-C3B-CAB-CBB
23	M	701	HAS	CAD-CBD-CGD-O1D
23	M	702	HAS	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	B	305	HEC	CAA-CBA-CGA-O1A
18	J	201	HEC	CAD-CBD-CGD-O1D
16	B	301	HEM	CAA-CBA-CGA-O2A
21	L	302	CDL	C12-C11-CA5-OA6
18	C	301	HEC	CAA-CBA-CGA-O1A
23	M	702	HAS	C3B-C11-C12-C13
23	M	701	HAS	C18-C19-C20-C21
18	J	201	HEC	CAA-CBA-CGA-O2A
23	M	701	HAS	C27-C19-C20-C21
23	M	702	HAS	C27-C19-C20-C21
21	K	201	CDL	C78-C79-C80-C81
20	c	304	PC1	C27-C28-C29-C2A
19	c	303	PEE	C1-C2-C3-O3
17	B	304	MQ7	C14-C13-C15-C16
21	J	202	CDL	OB6-CB4-CB6-OB8
21	K	201	CDL	OB6-CB4-CB6-OB8
21	J	202	CDL	CA4-CA6-OA8-CA7
19	L	301	PEE	O3-C30-C31-C32
20	C	303	PC1	C22-C23-C24-C25
23	M	701	HAS	CAD-CBD-CGD-O2D
22	L	303	5PL	CBA-CBB-CBC-CBD
18	b	304	HEC	C4D-C3D-CAD-CBD
18	J	201	HEC	CAA-CBA-CGA-O1A
21	L	302	CDL	C52-C51-CB5-OB6
21	L	302	CDL	C12-C11-CA5-OA7
16	b	302	HEM	CAD-CBD-CGD-O2D
19	L	301	PEE	O5-C30-C31-C32
17	B	304	MQ7	C32-C33-C35-C36
16	b	302	HEM	CAD-CBD-CGD-O1D
19	C	302	PEE	C31-C32-C33-C34

There are no ring outliers.

26 monomers are involved in 133 short contacts:

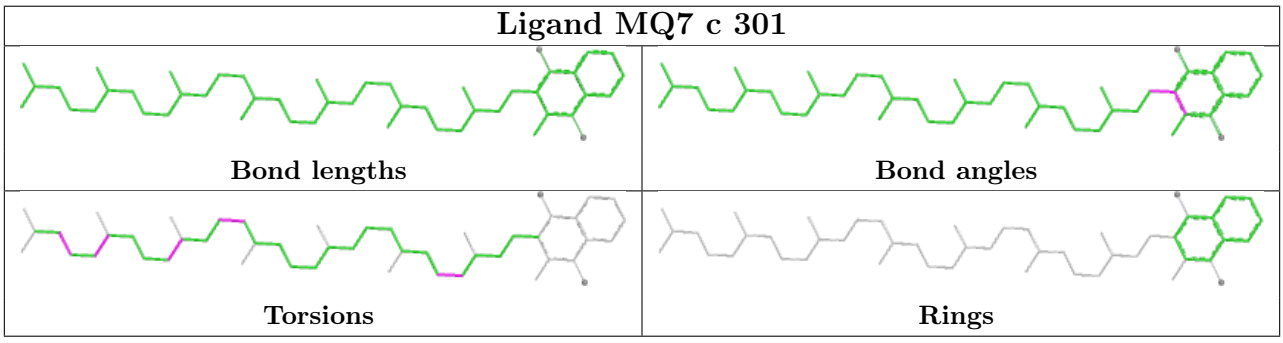
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	c	301	MQ7	6	0
19	L	301	PEE	3	0
22	L	303	5PL	11	0
20	C	303	PC1	4	0
21	K	201	CDL	7	0
20	c	304	PC1	1	0
21	J	202	CDL	7	0

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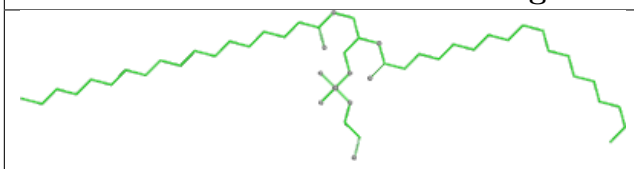
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	303	MQ7	3	0
17	b	303	MQ7	3	0
16	B	302	HEM	9	0
19	J	203	PEE	4	0
16	B	301	HEM	2	0
16	b	302	HEM	3	0
19	C	302	PEE	6	0
18	N	401	HEC	4	0
23	M	702	HAS	6	0
23	M	701	HAS	8	0
17	B	304	MQ7	8	0
18	C	301	HEC	2	0
15	A	201	FES	2	0
18	c	302	HEC	7	0
18	B	305	HEC	9	0
16	b	301	HEM	2	0
21	L	302	CDL	6	0
19	c	303	PEE	3	0
18	b	304	HEC	7	0

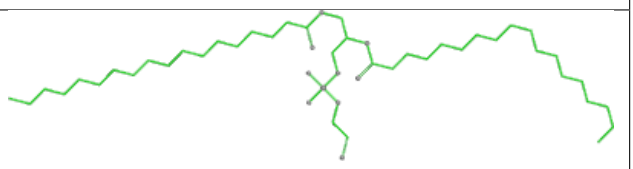
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



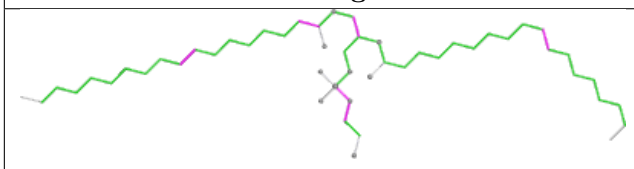
Ligand PEE L 301



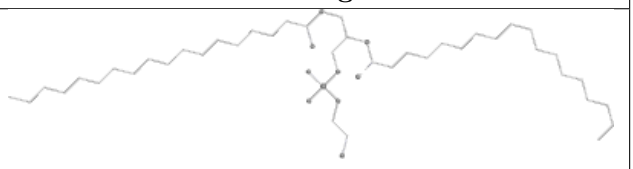
Bond lengths



Bond angles

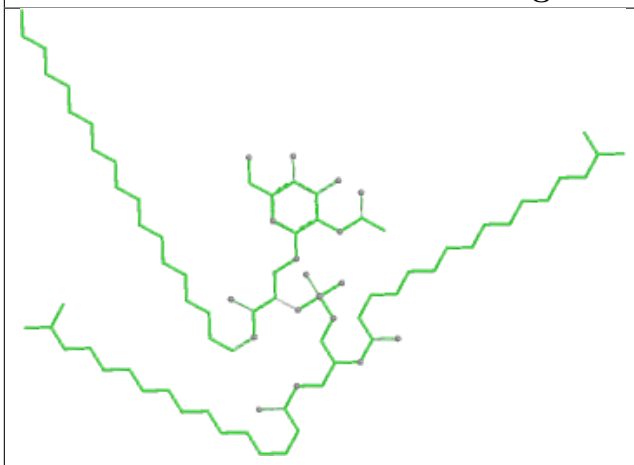


Torsions

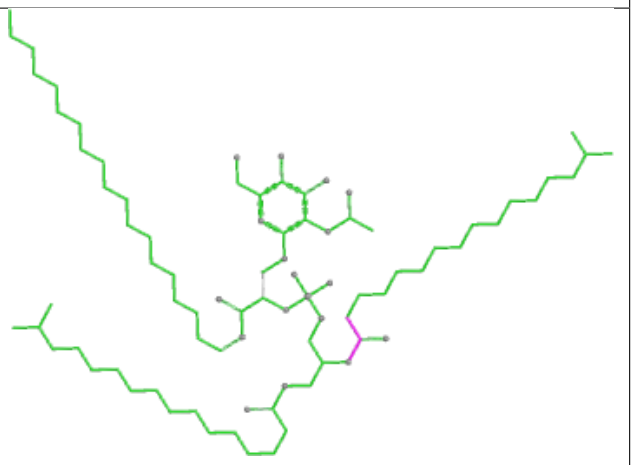


Rings

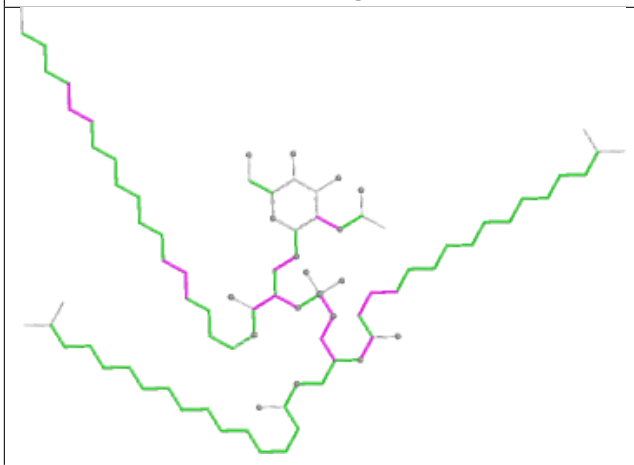
Ligand 5PL L 303



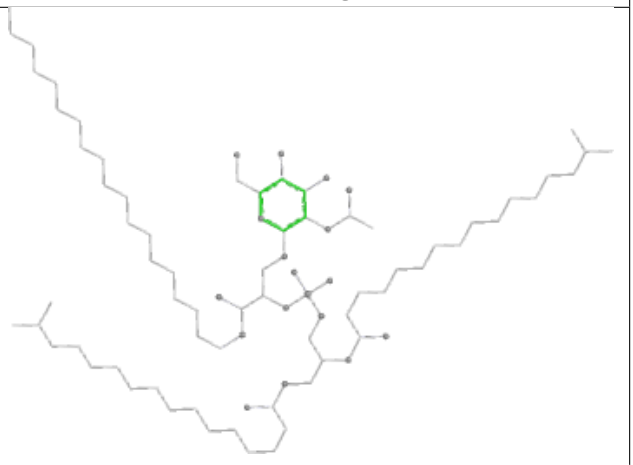
Bond lengths



Bond angles

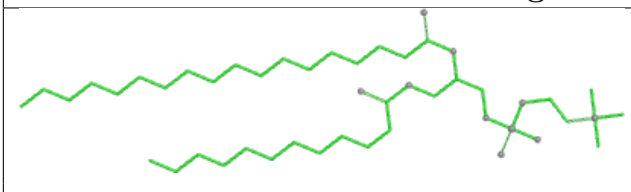


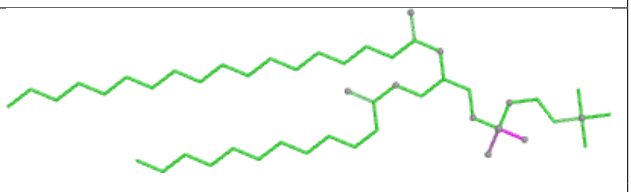
Torsions

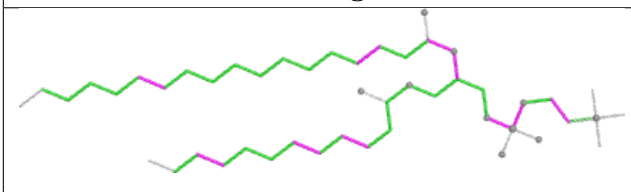


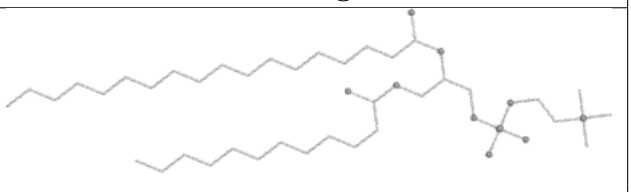
Rings

Ligand PC1 C 303

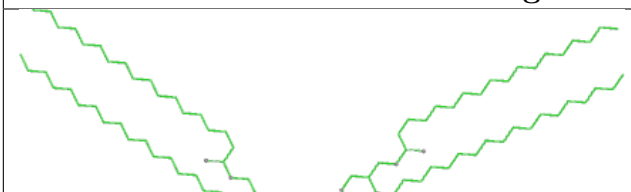

Bond lengths

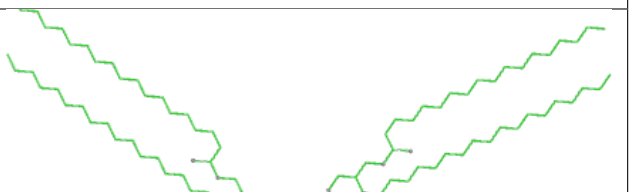

Bond angles


Torsions


Rings

Ligand CDL K 201

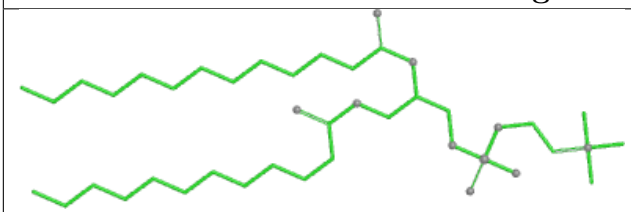

Bond lengths

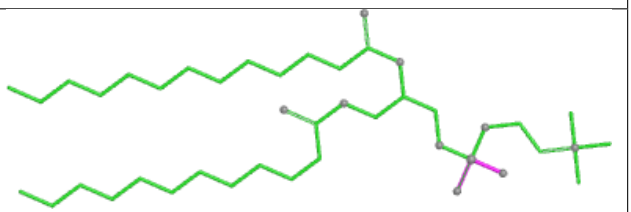

Bond angles

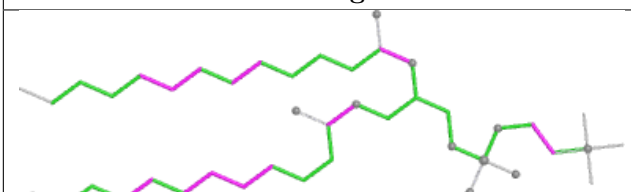

Torsions

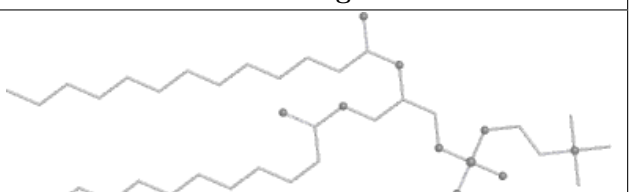

Rings

Ligand PC1 c 304

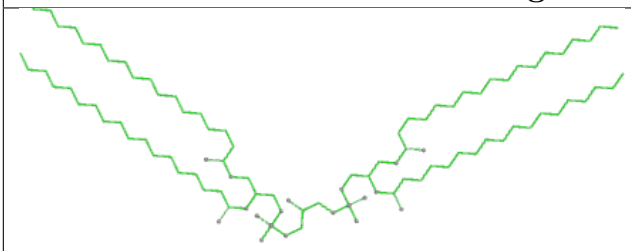

Bond lengths


Bond angles

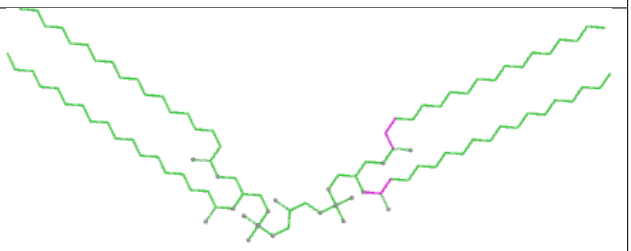

Torsions


Rings

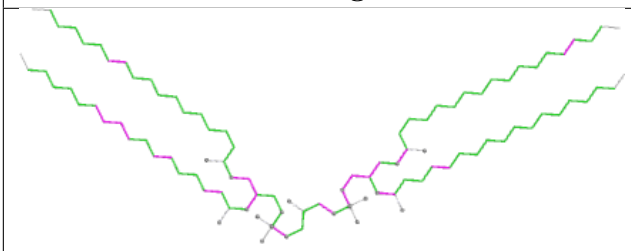
Ligand CDL J 202



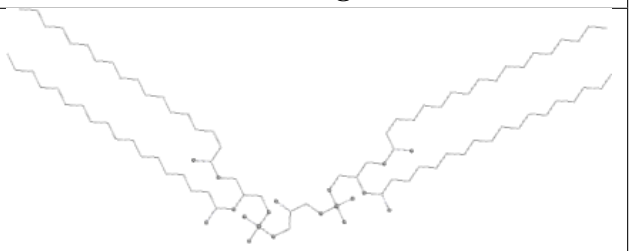
Bond lengths



Bond angles



Torsions



Rings

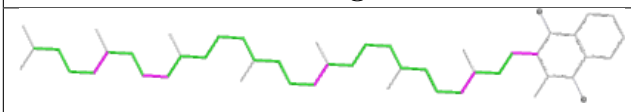
Ligand MQ7 B 303



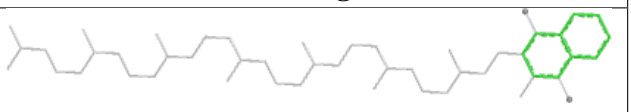
Bond lengths



Bond angles

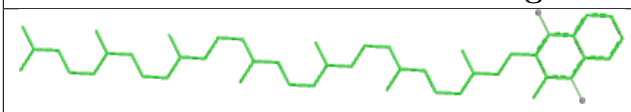


Torsions



Rings

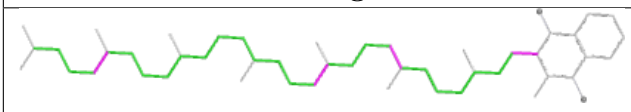
Ligand MQ7 b 303



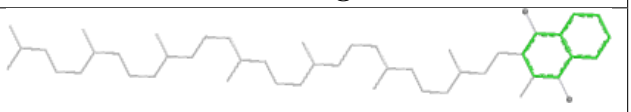
Bond lengths



Bond angles

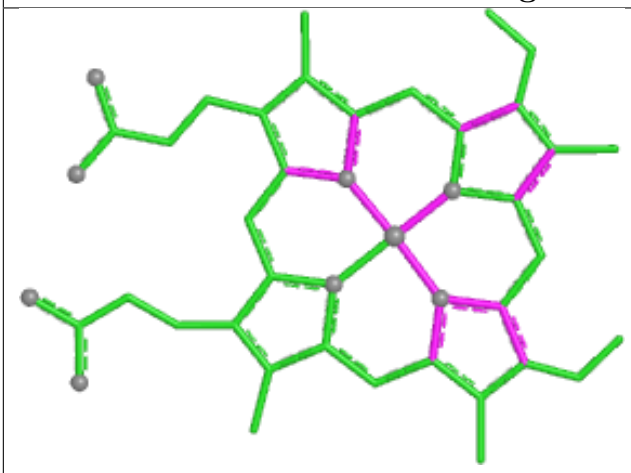


Torsions

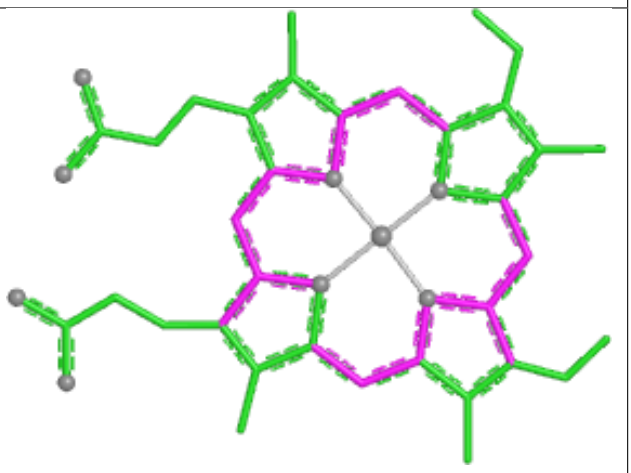


Rings

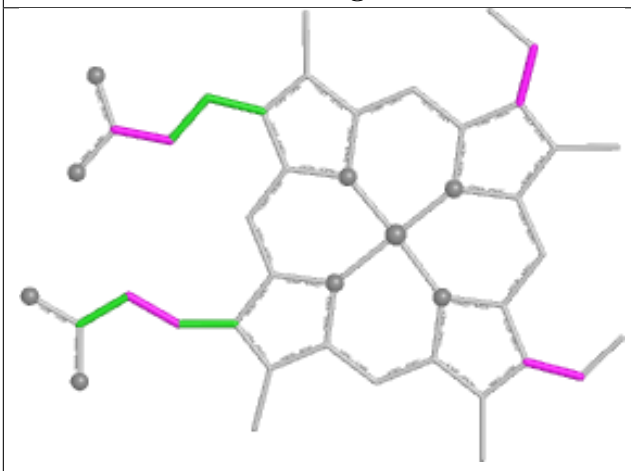
Ligand HEM B 302



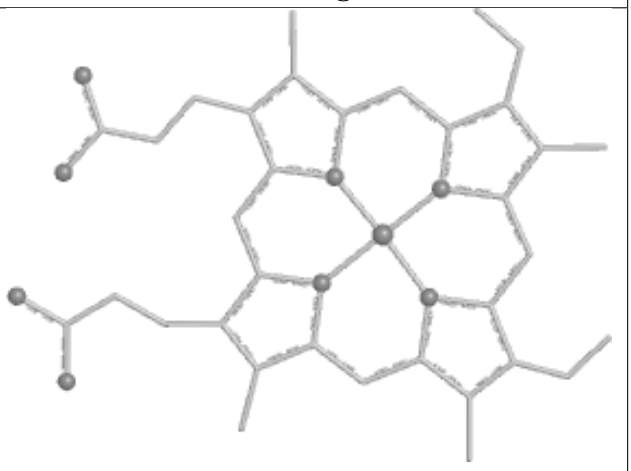
Bond lengths



Bond angles

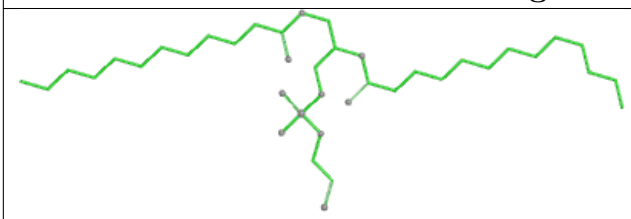


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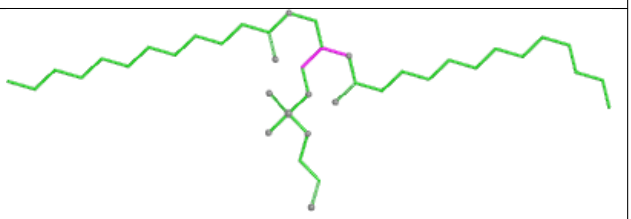


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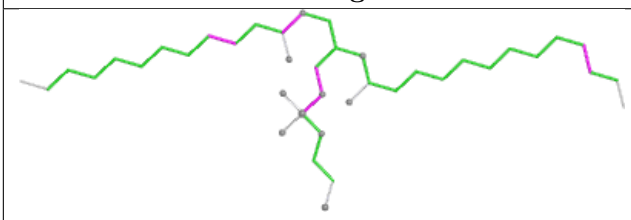
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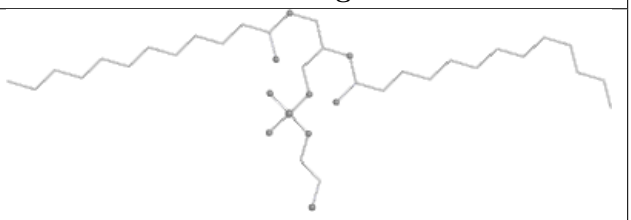
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Bond angles

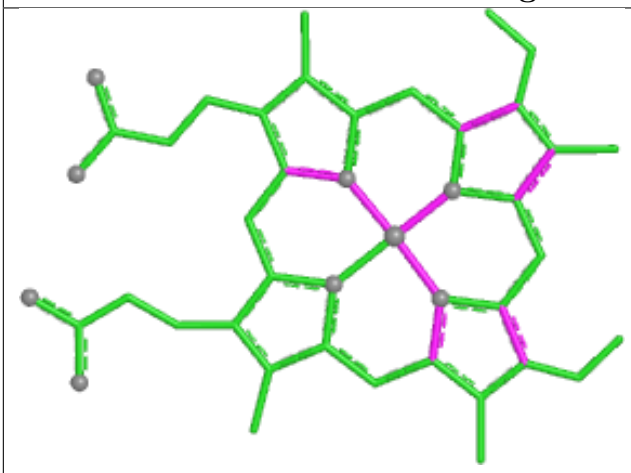


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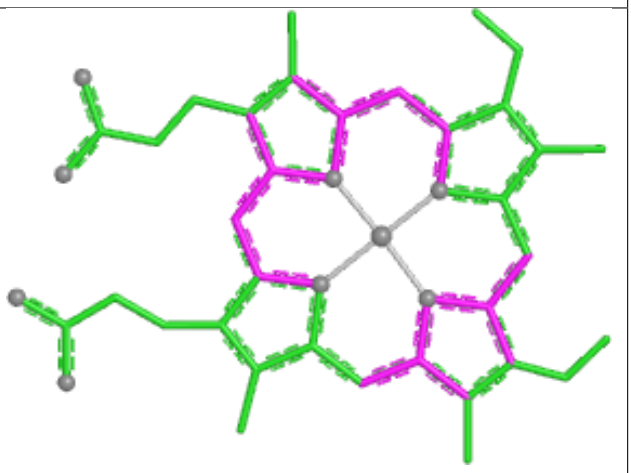


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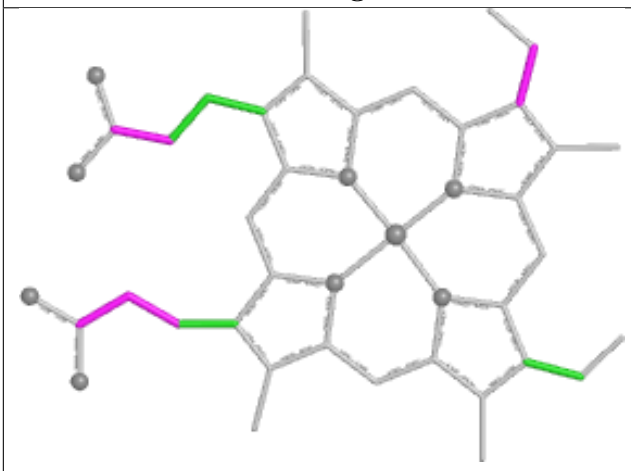
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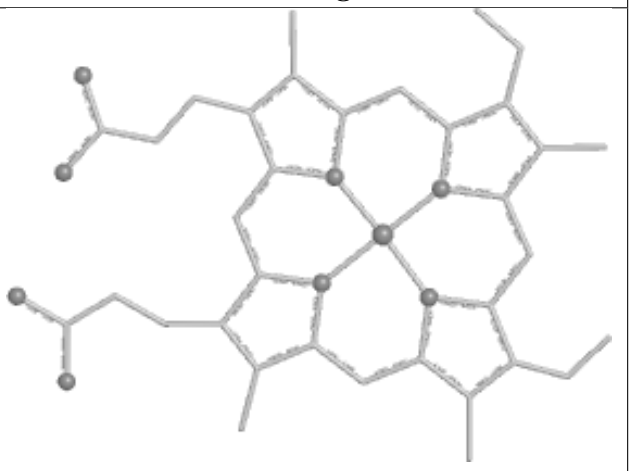
Bond lengths



Bond angles

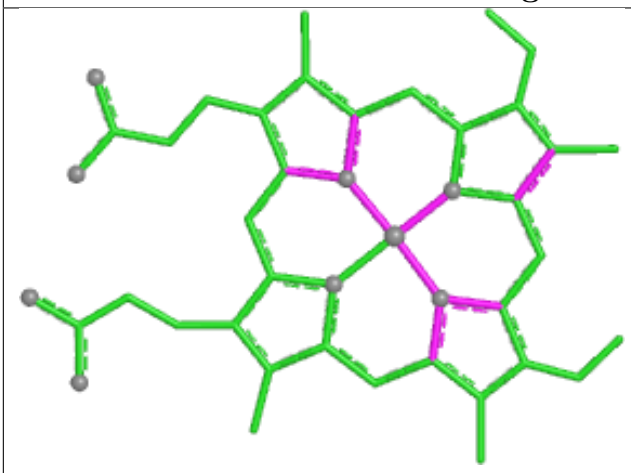


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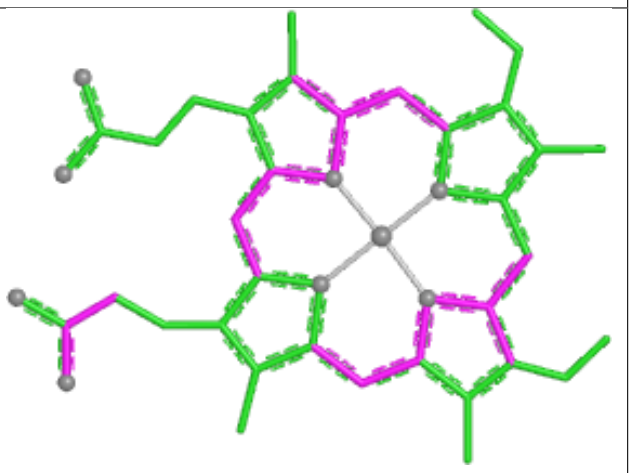


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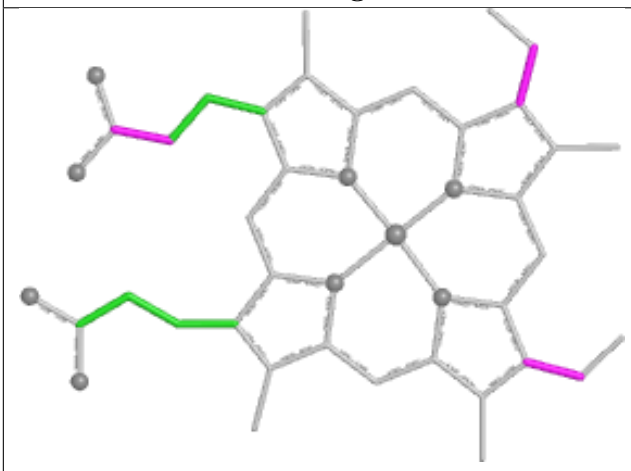
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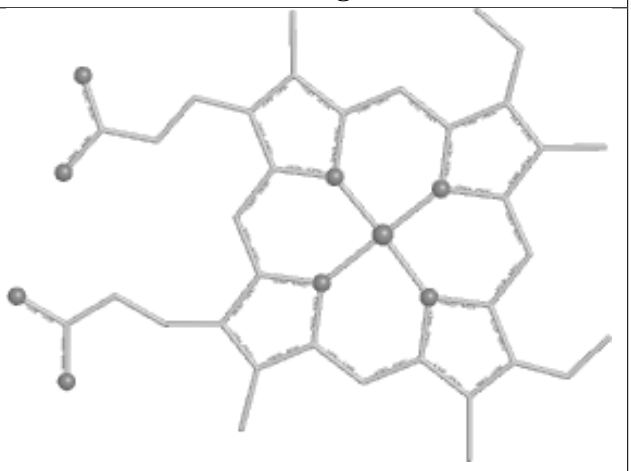
Bond lengths



Bond angles

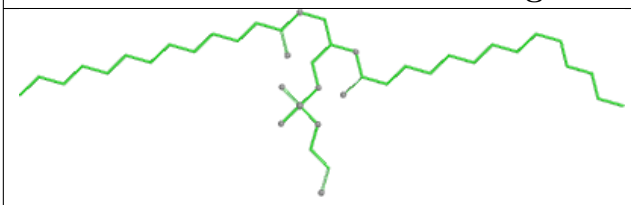


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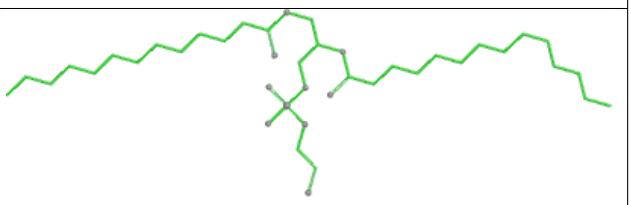


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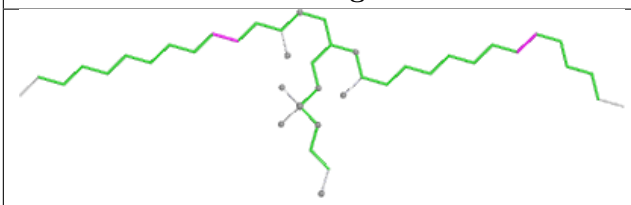
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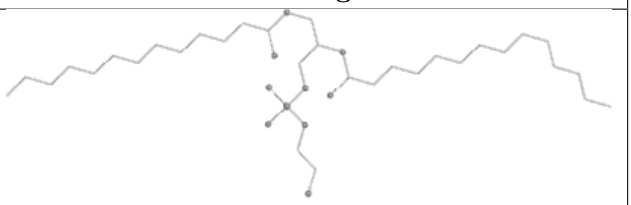
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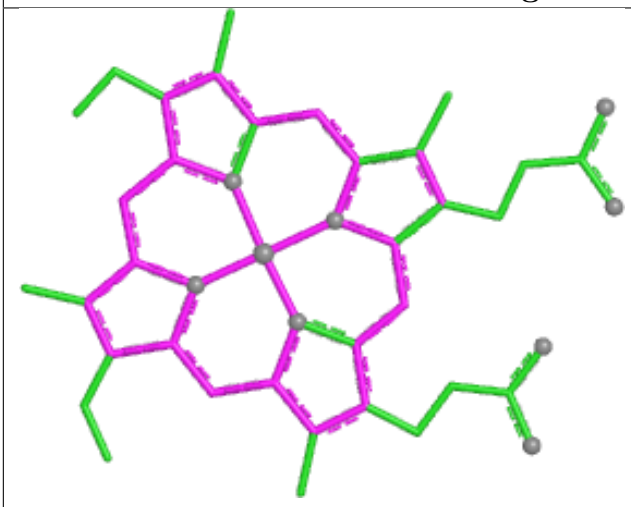


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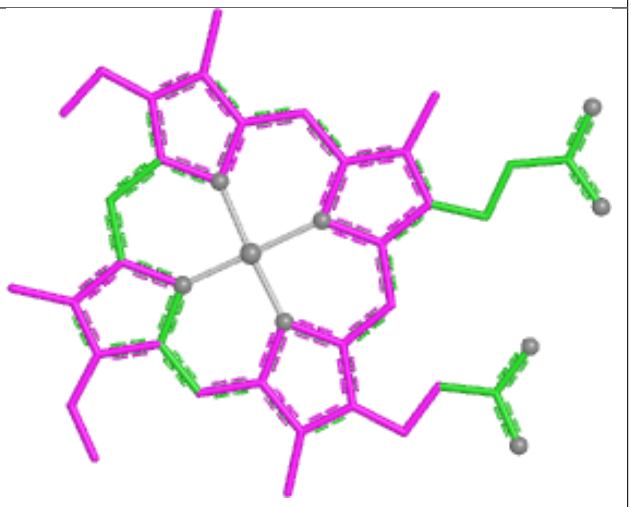


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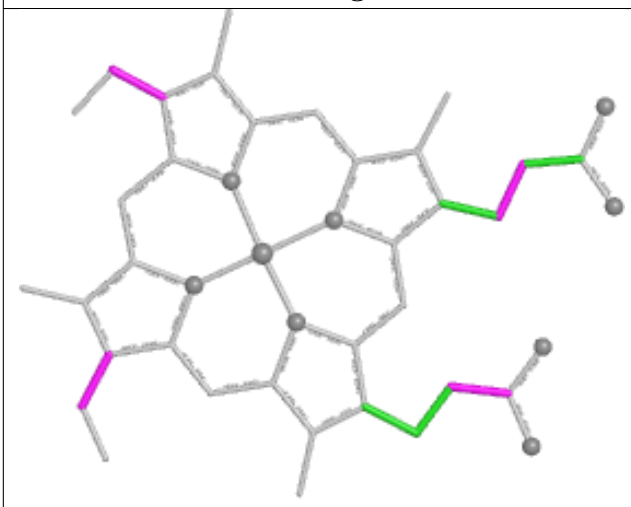
Ligand HEC N 401



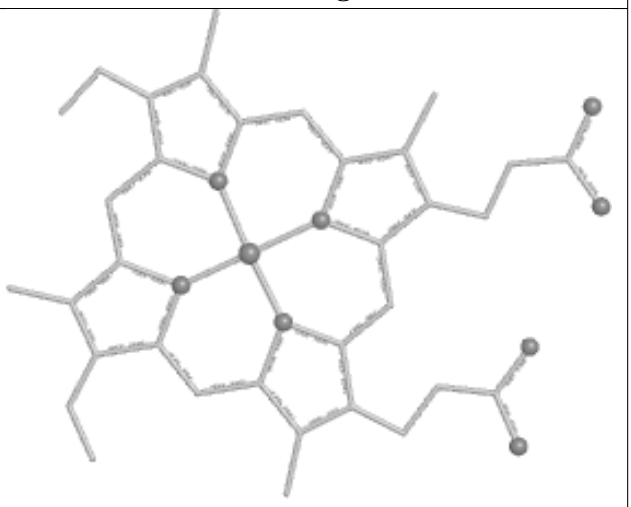
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Bond angles

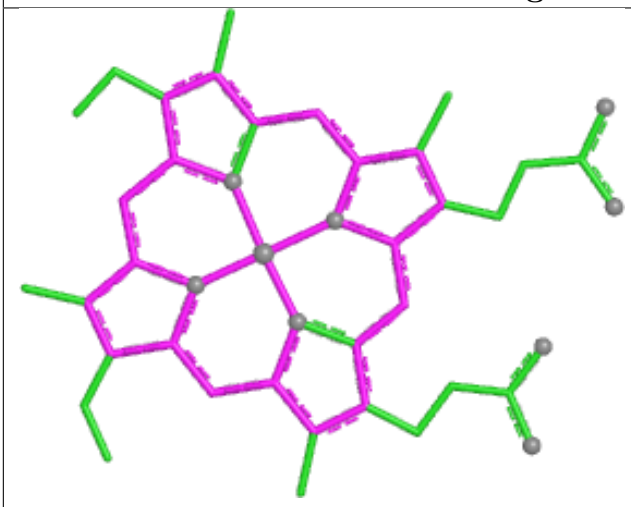


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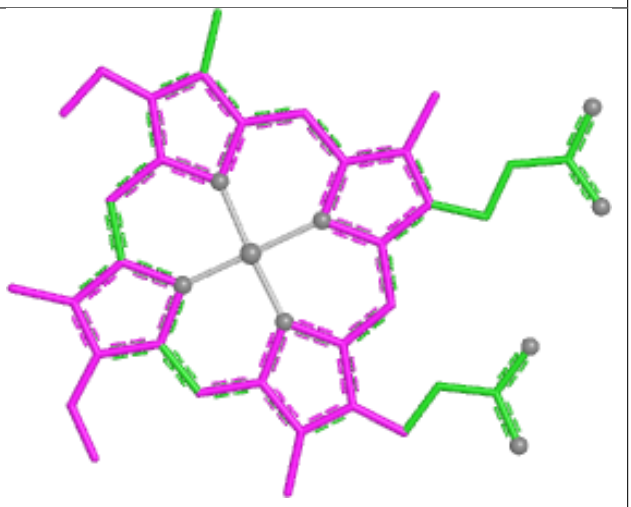


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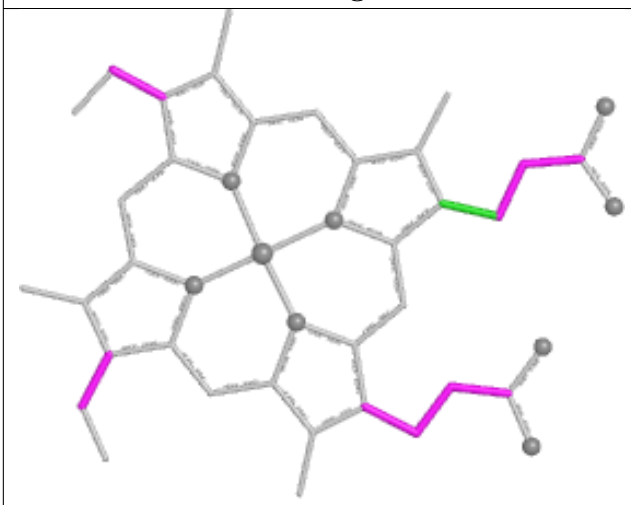
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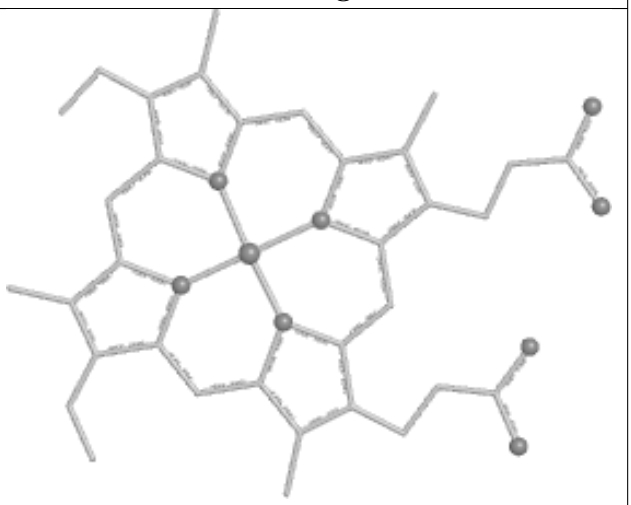
Bond lengths



Bond angles

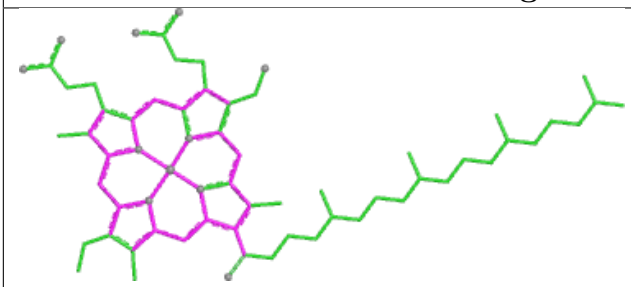


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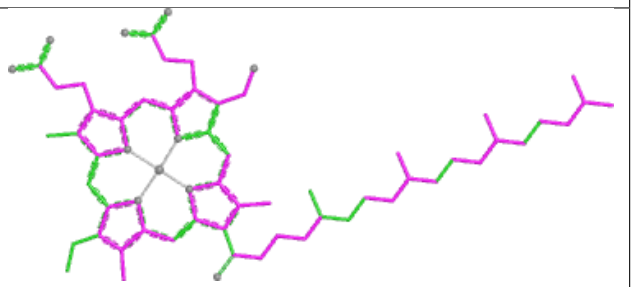


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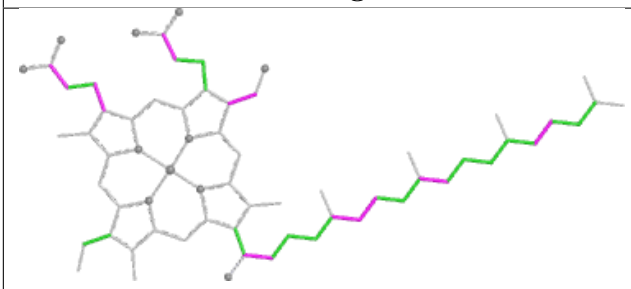
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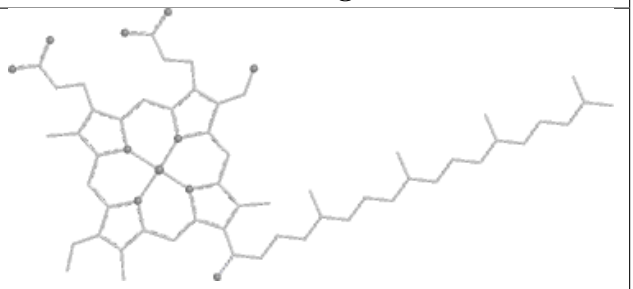
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Bond angles

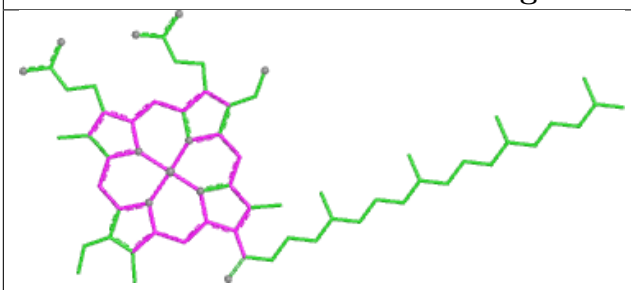


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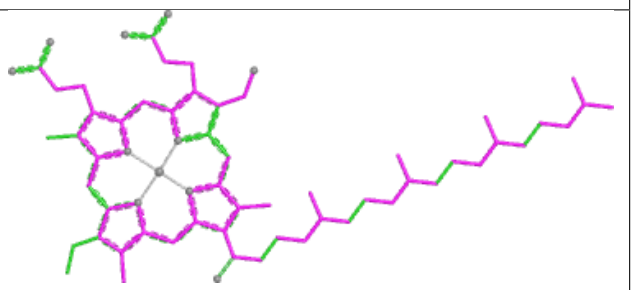


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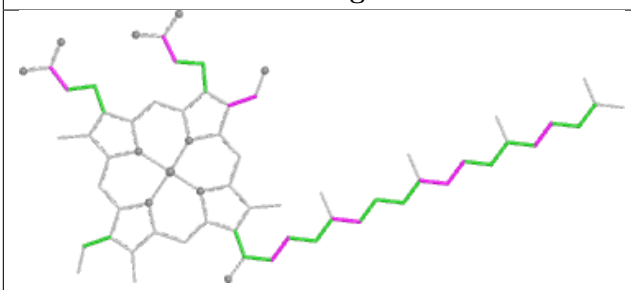
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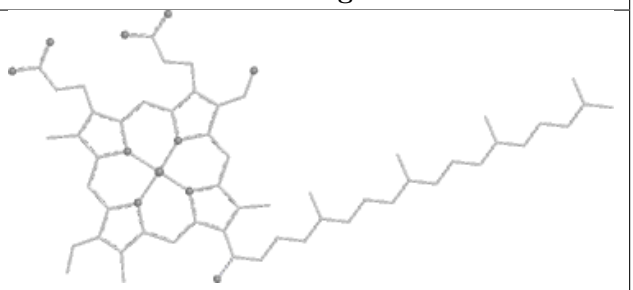
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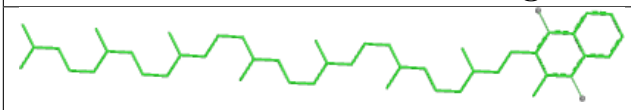


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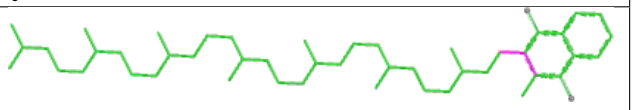


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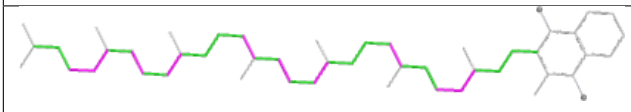
Ligand MQ7 B 304



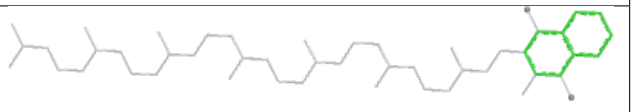
Bond lengths



Bond angles

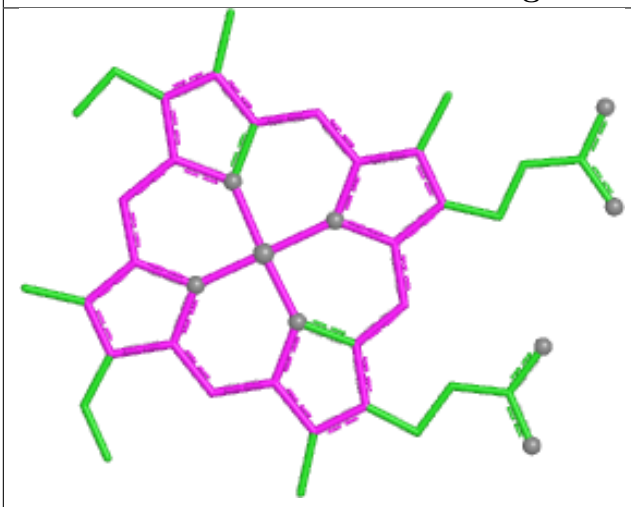


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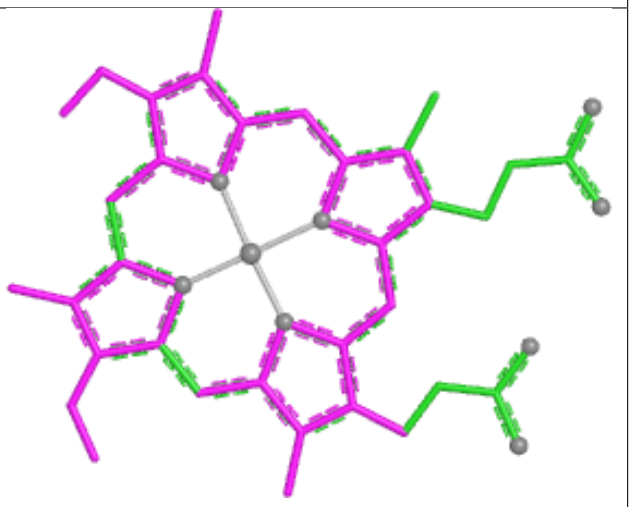


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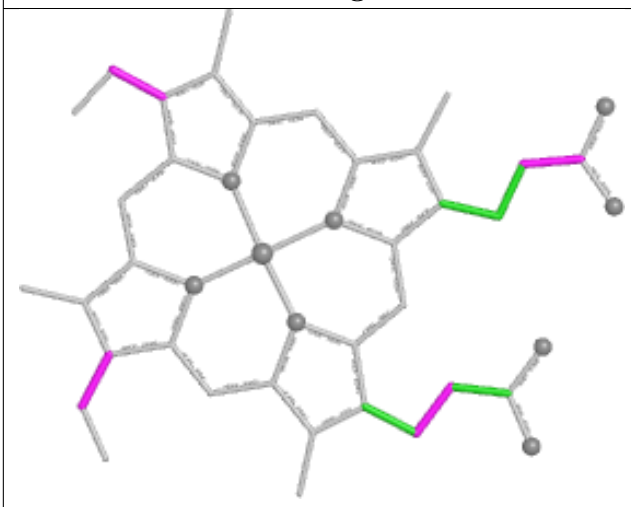
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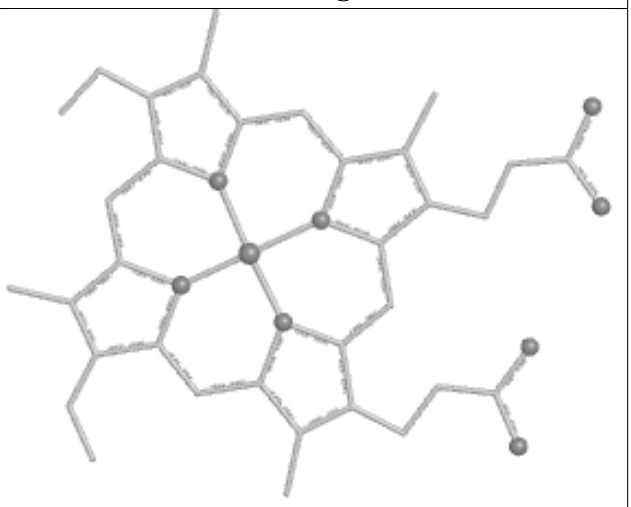
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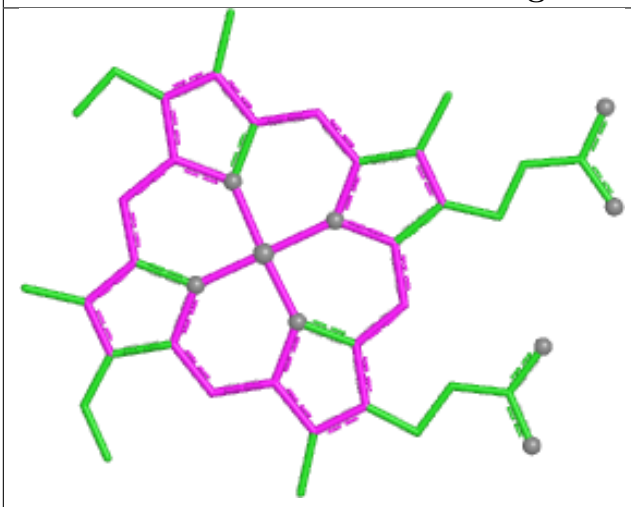


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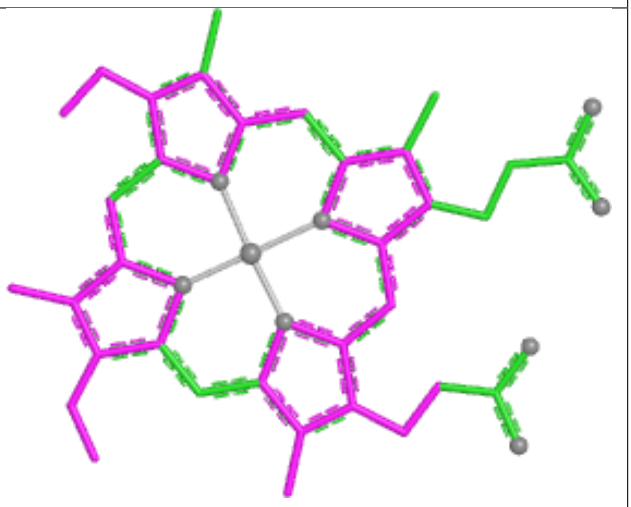


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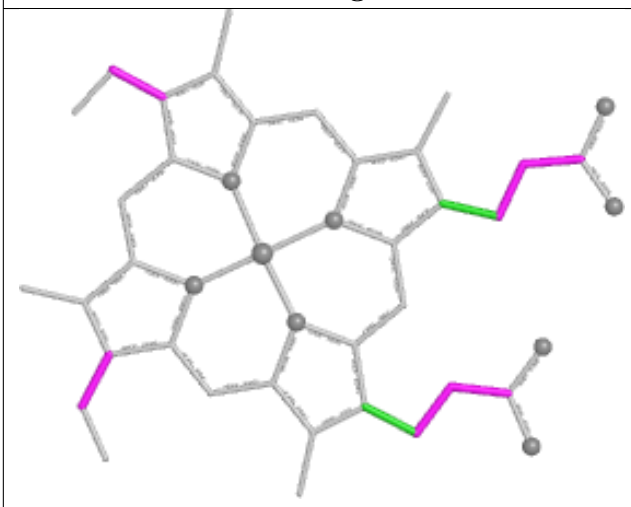
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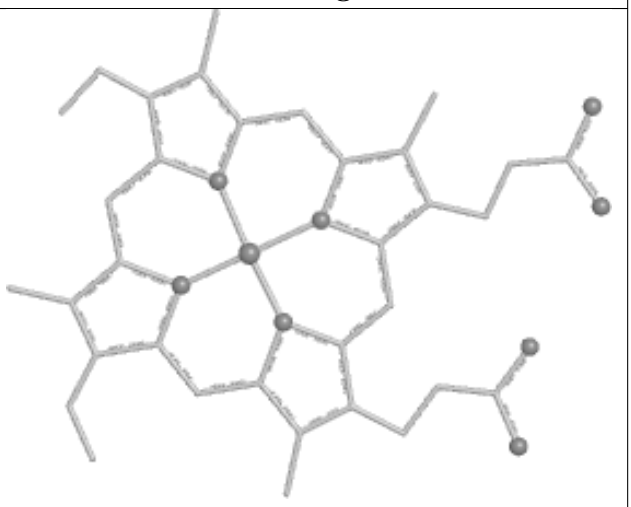
Bond lengths



Bond angles

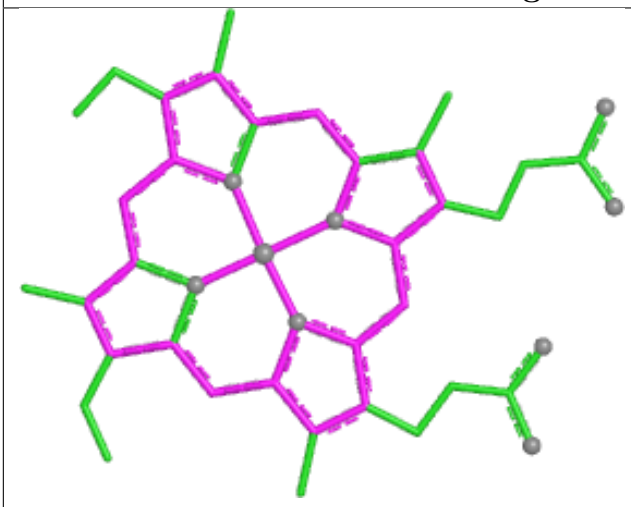


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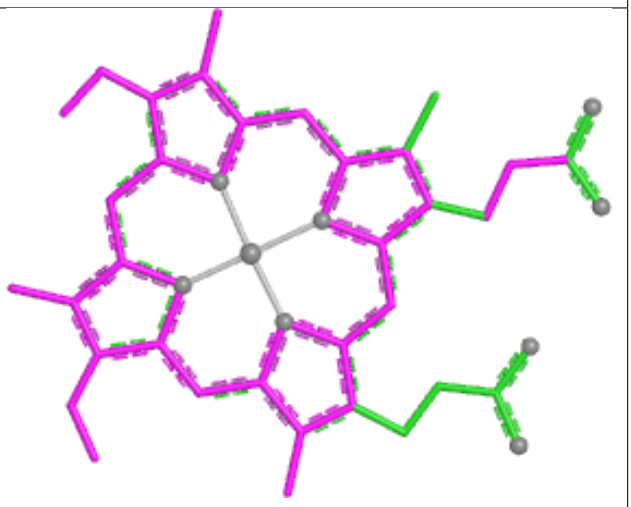


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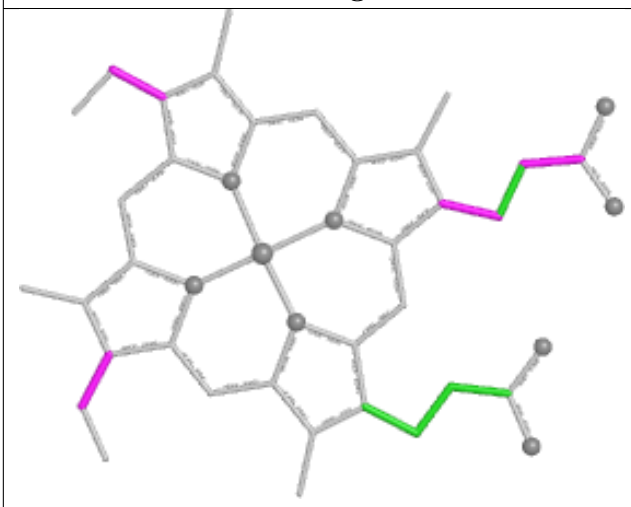
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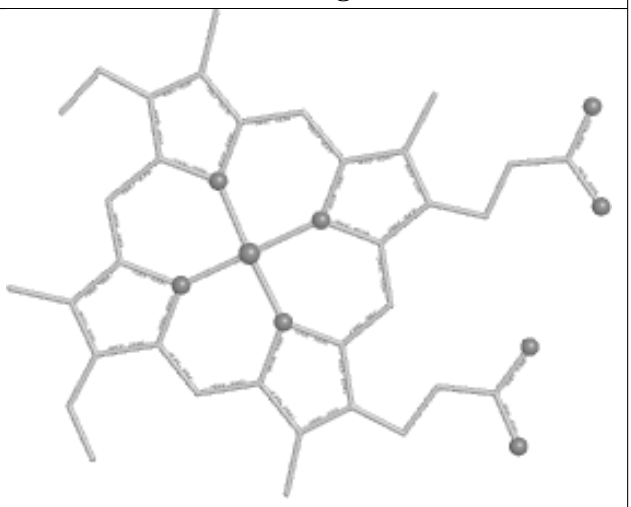
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Bond angles

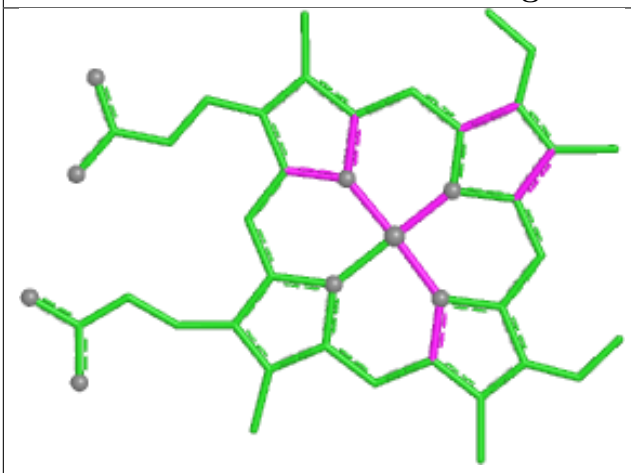


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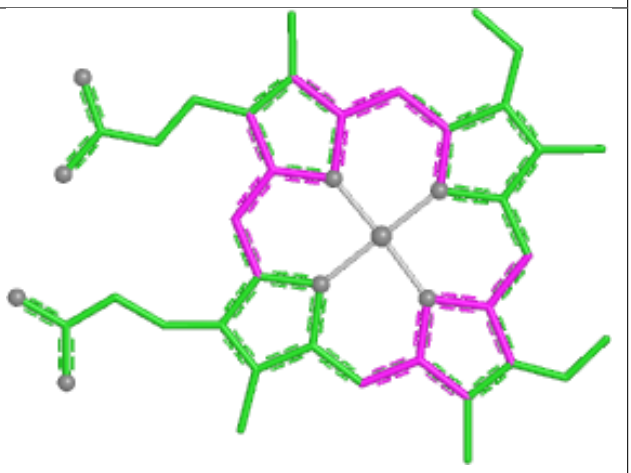


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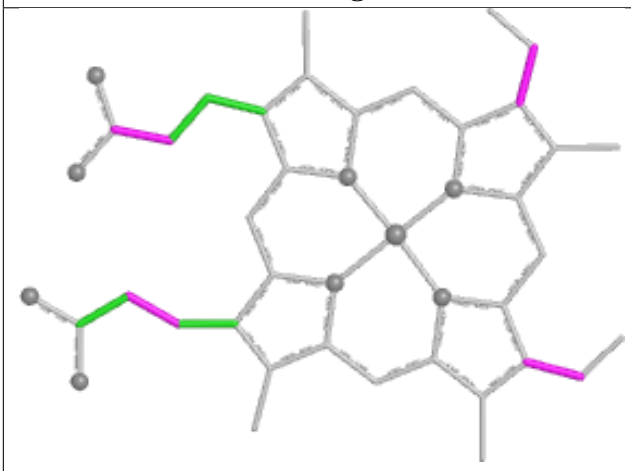
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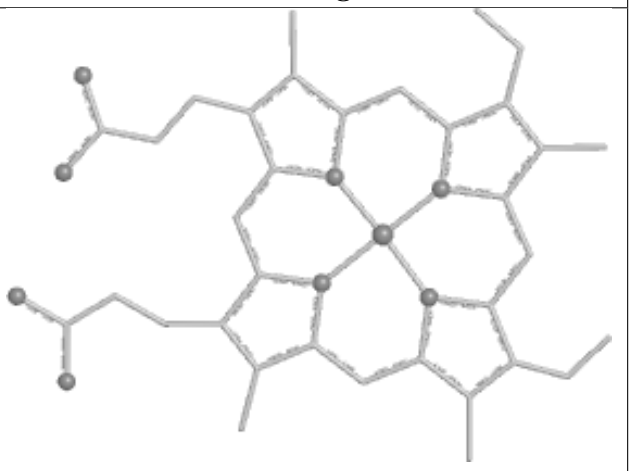
Bond lengths



Bond angles

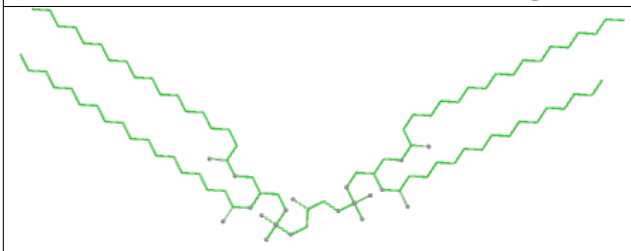


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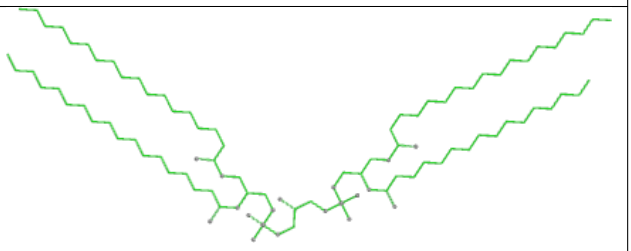


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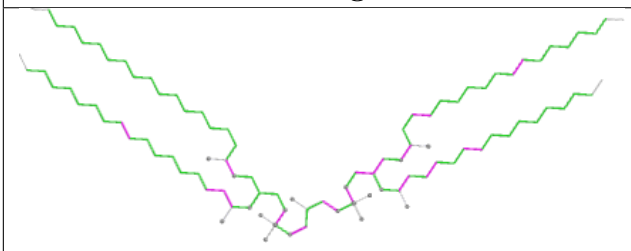
Ligand CDL L 302



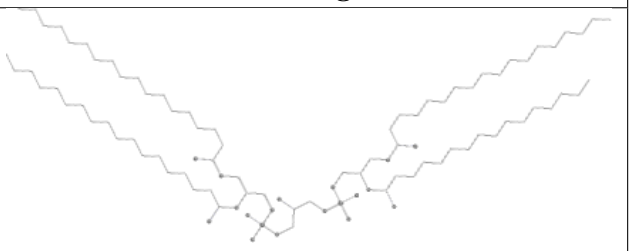
Bond lengths



Bond angles

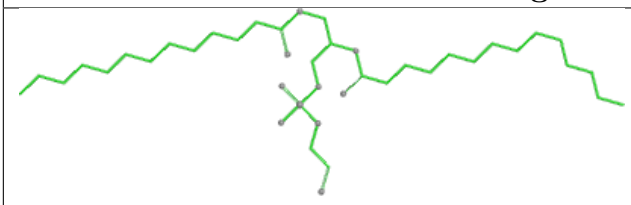


Torsions

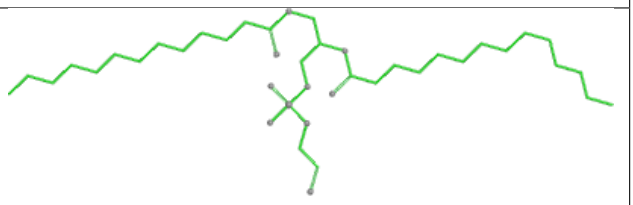


Rings

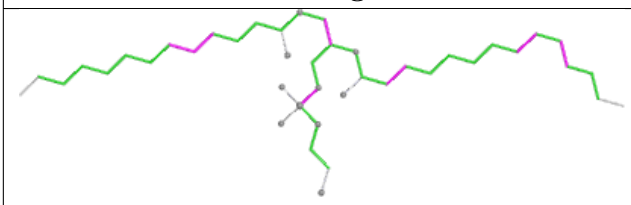
Ligand PEE c 303



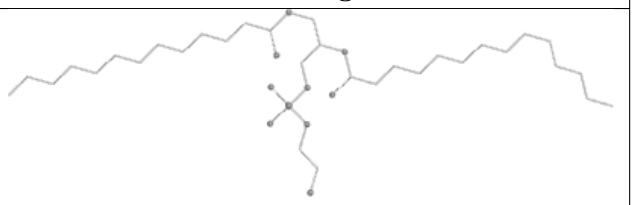
Bond lengths



Bond angles

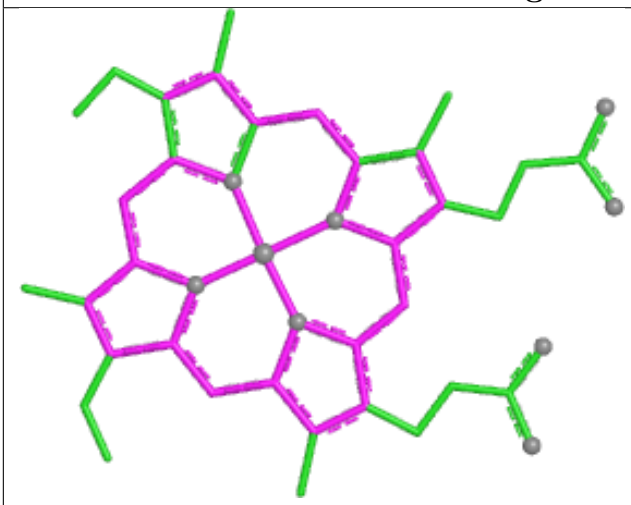


Torsions

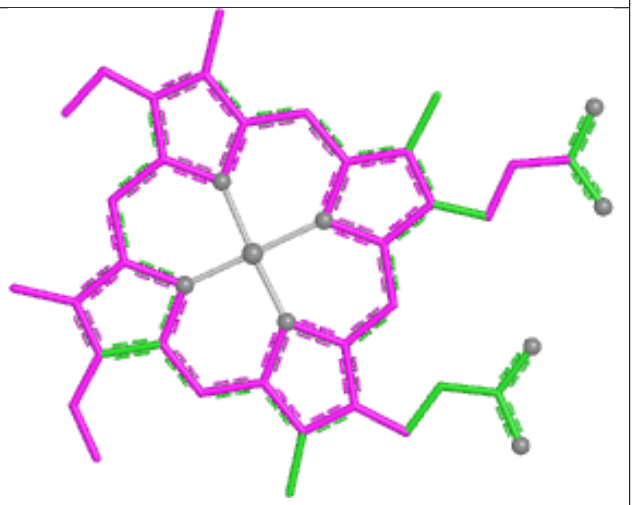


Rings

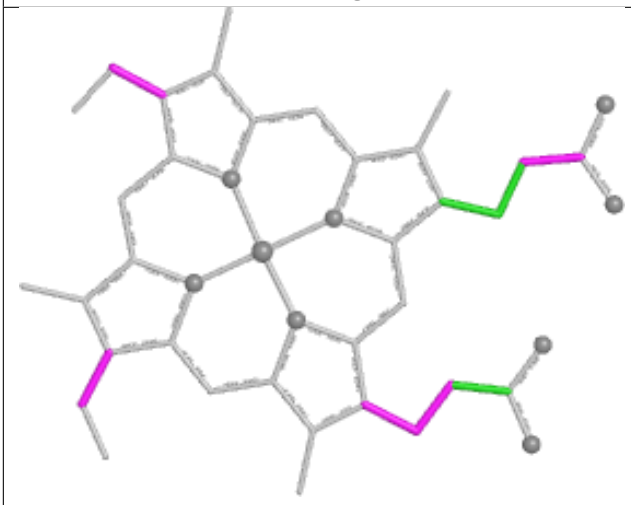
Ligand HEC b 304



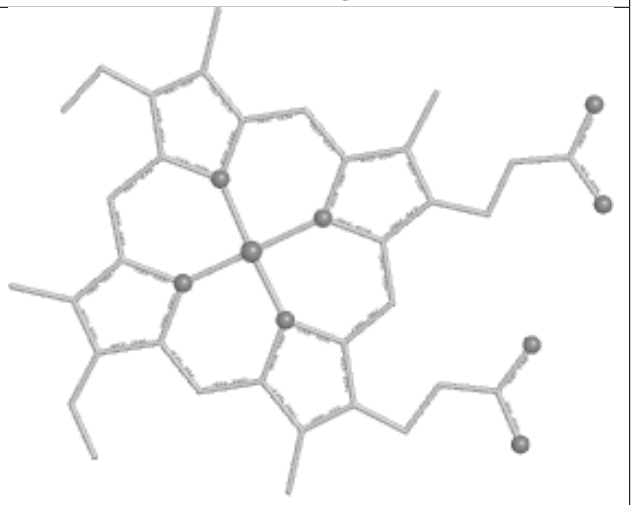
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

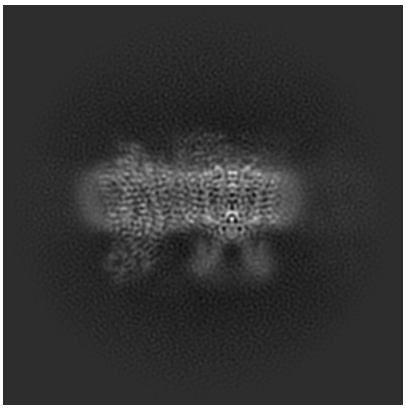
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70333. These allow visual inspection of the internal detail of the map and identification of artifacts.

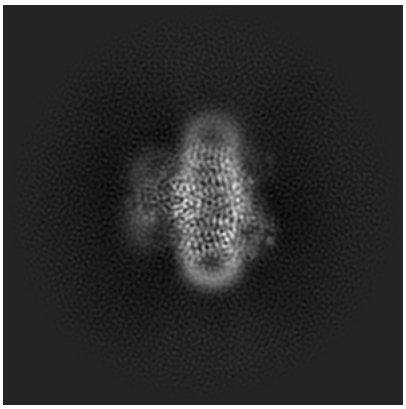
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

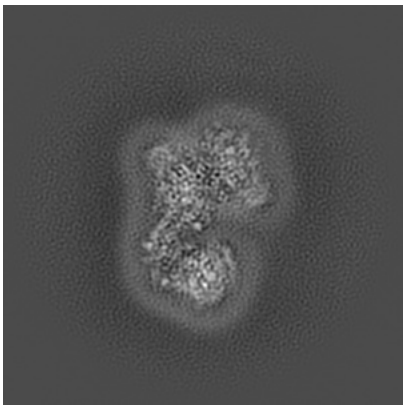
6.1.1 Primary map



X

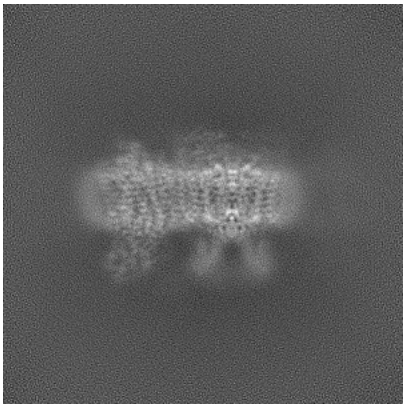


Y

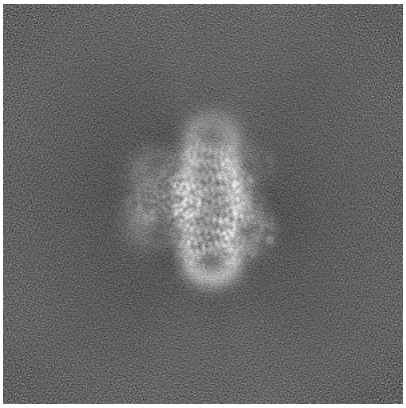


Z

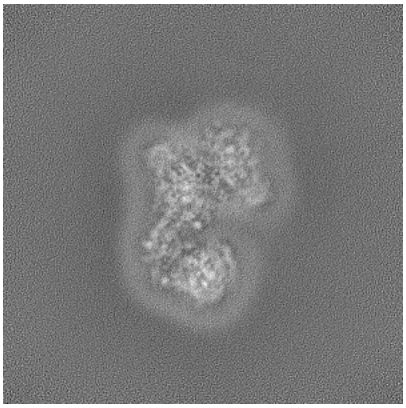
6.1.2 Raw map



X



Y

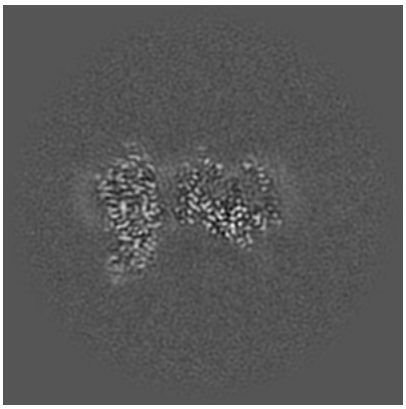


Z

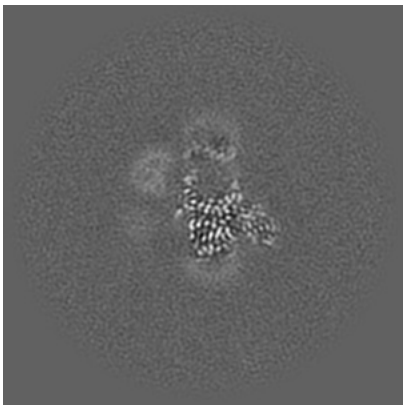
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

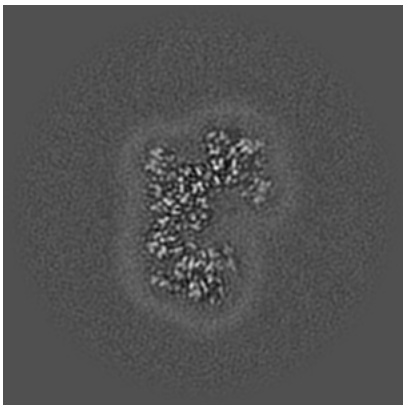
6.2.1 Primary map



X Index: 180

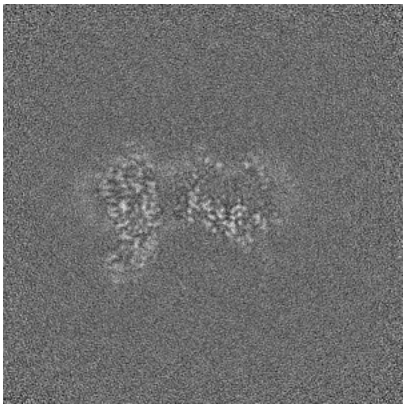


Y Index: 180

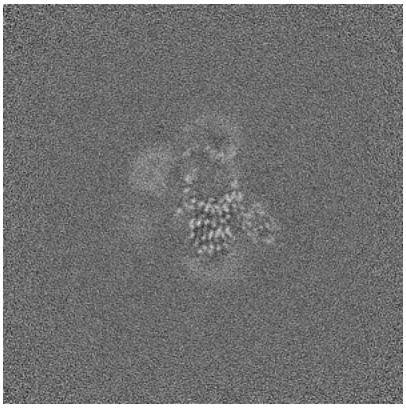


Z Index: 180

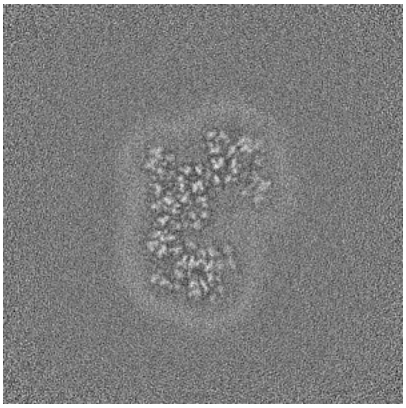
6.2.2 Raw map



X Index: 180



Y Index: 180

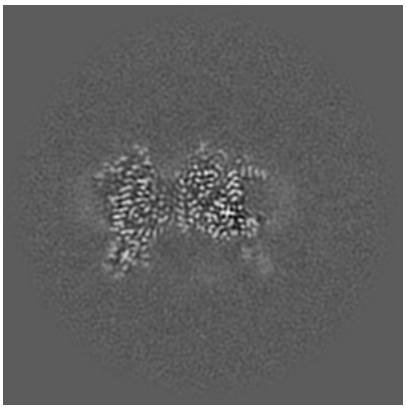


Z Index: 180

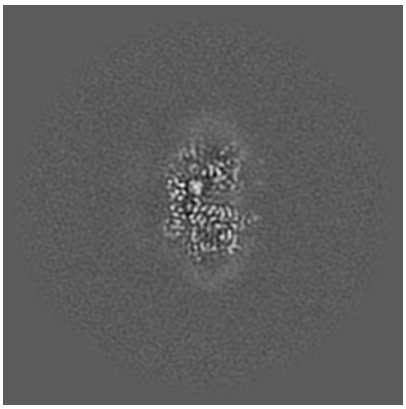
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

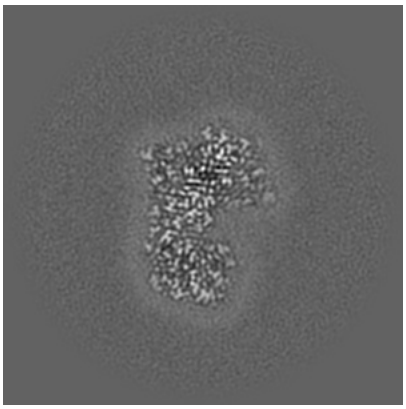
6.3.1 Primary map



X Index: 172

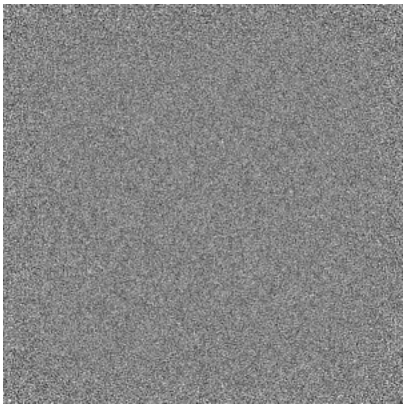


Y Index: 209

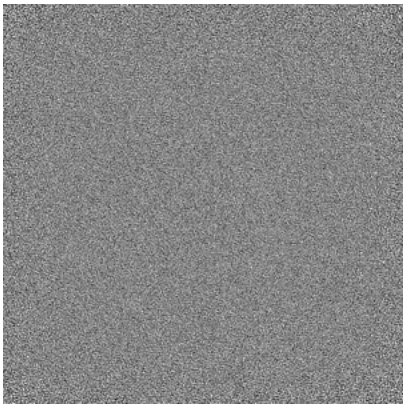


Z Index: 170

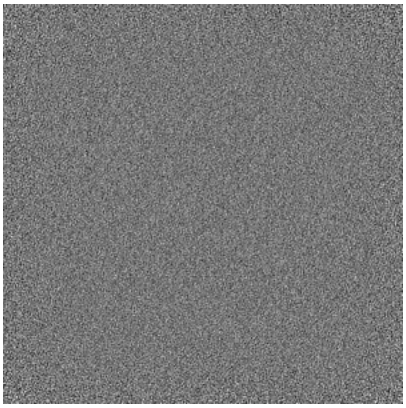
6.3.2 Raw map



X Index: 0



Y Index: 0

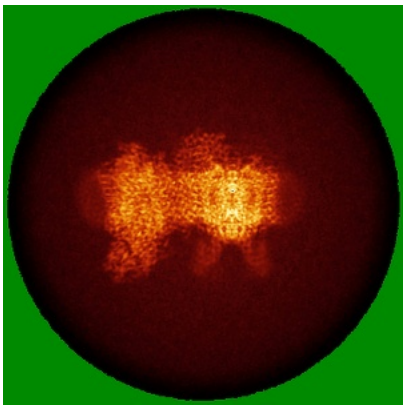


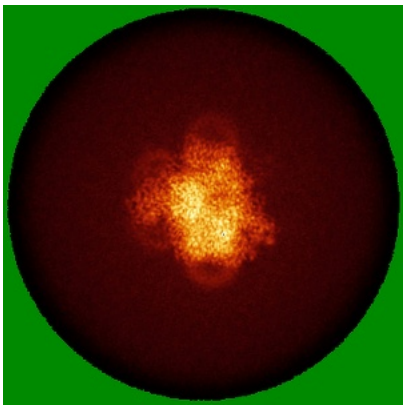
Z Index: 0

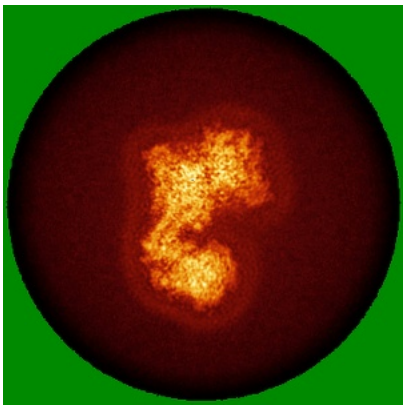
The images above show the largest variance slices of the map in three orthogonal directions.

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

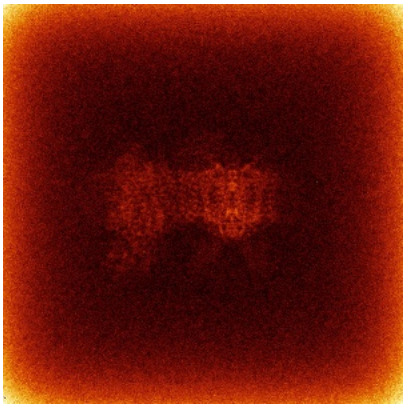
6.4.1 Primary map

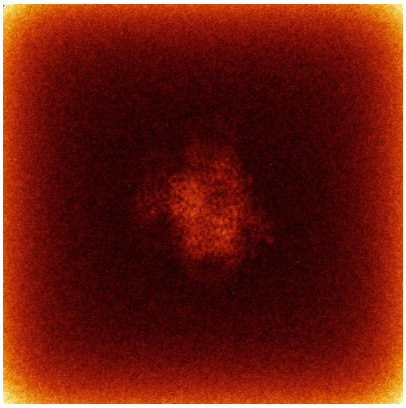

X

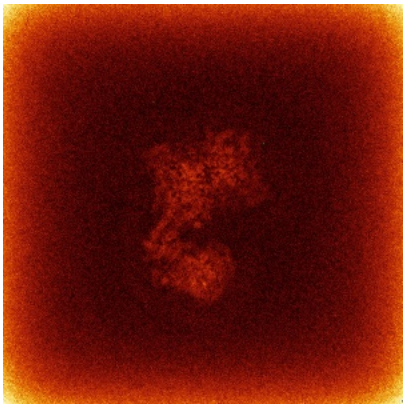

Y


Z

6.4.2 Raw map


X

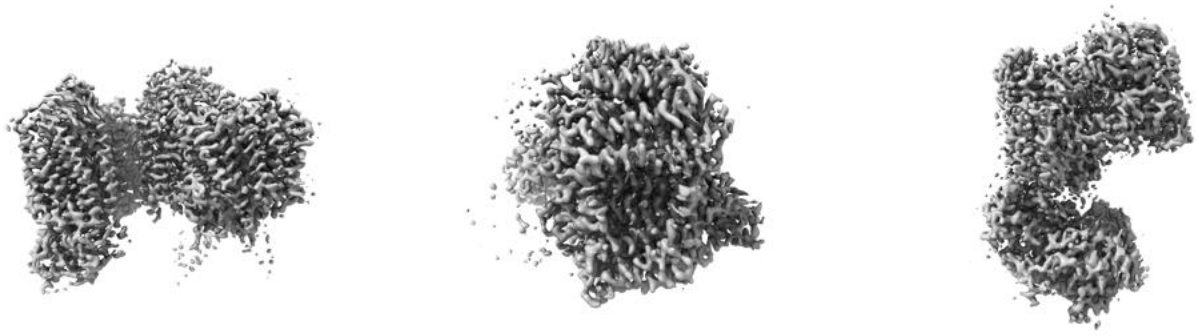

Y


Z

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

6.5 Orthogonal surface views (i)

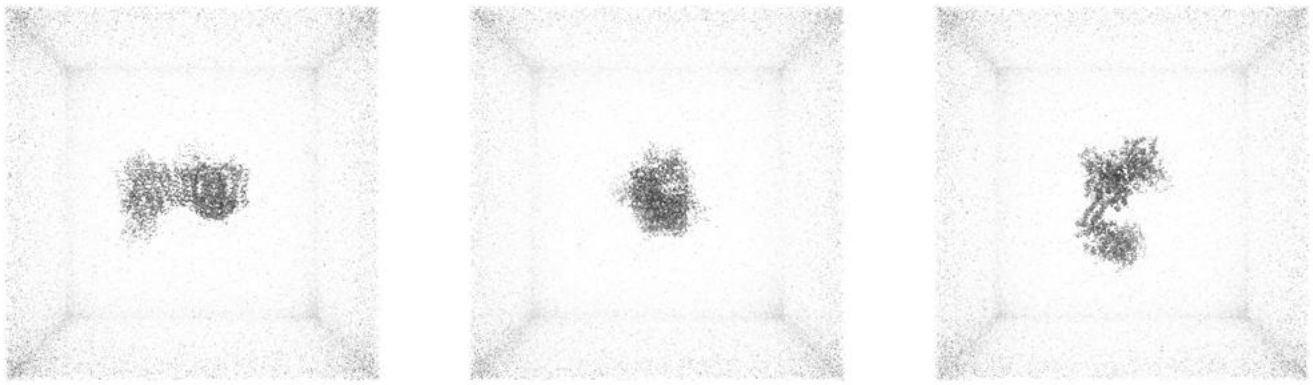
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

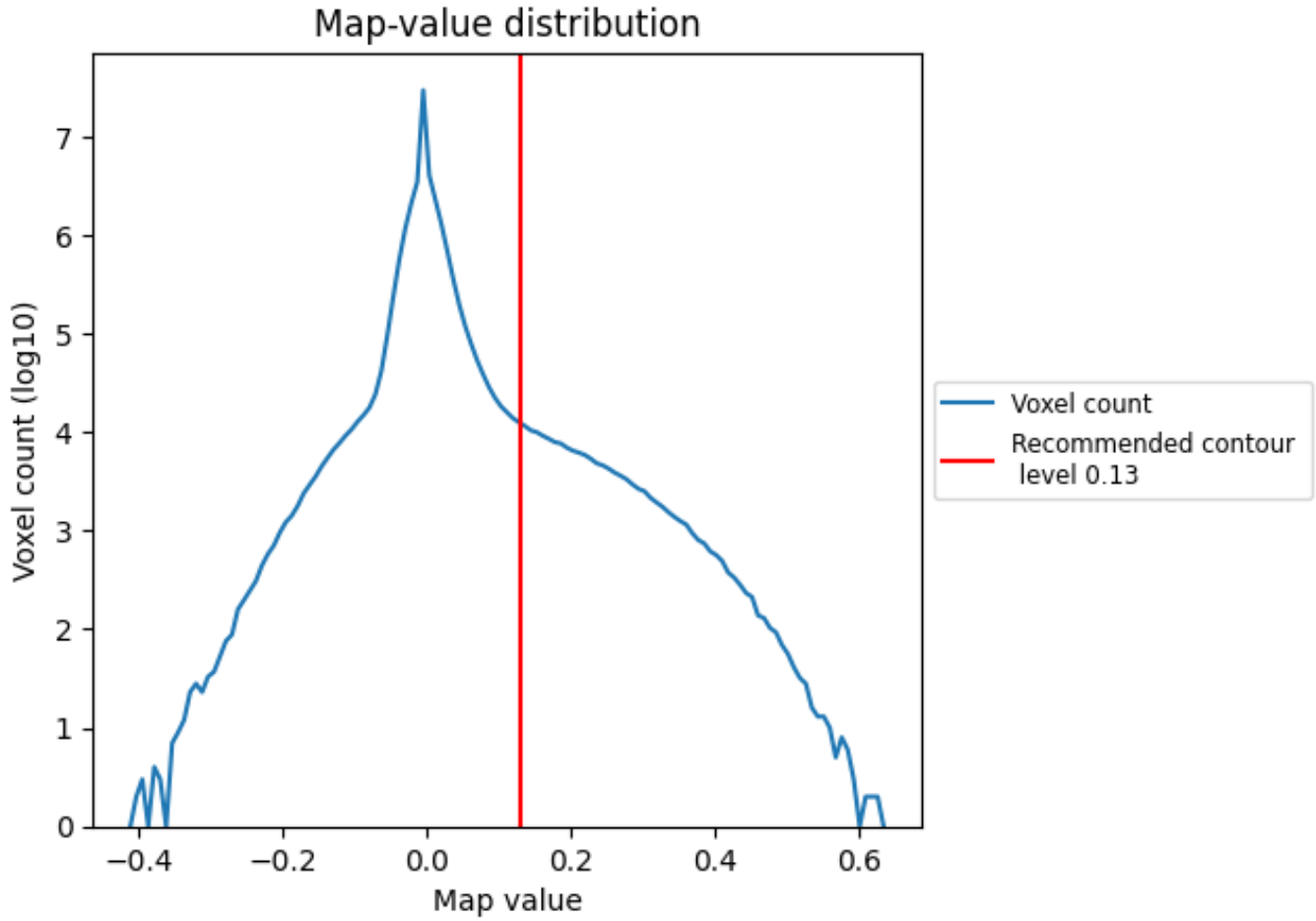
6.6 Mask visualisation (i)

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

7 Map analysis

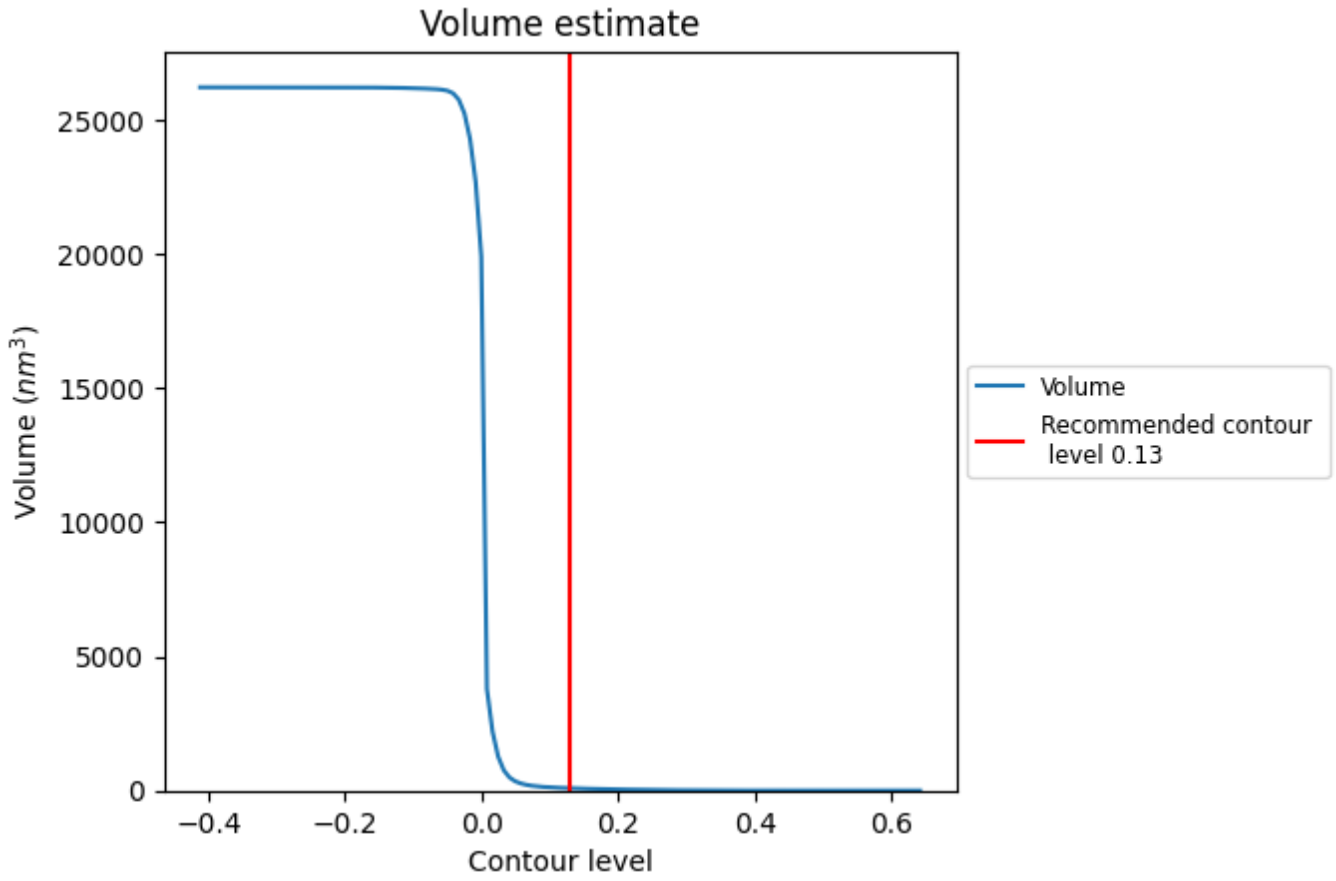
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

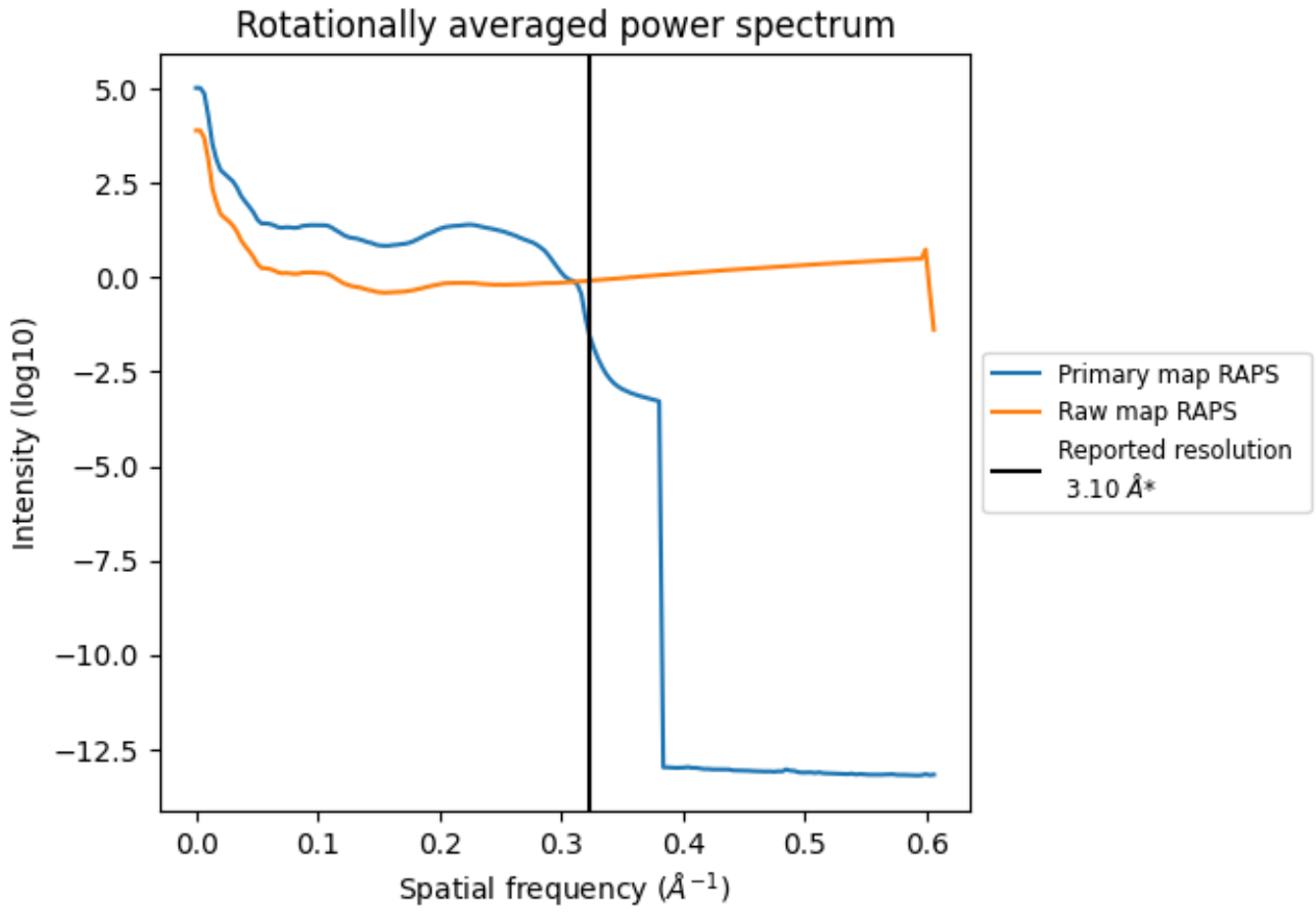
7.2 Volume estimate



The volume at the recommended contour level is 87 nm^3; this corresponds to an approximate mass of 78 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)

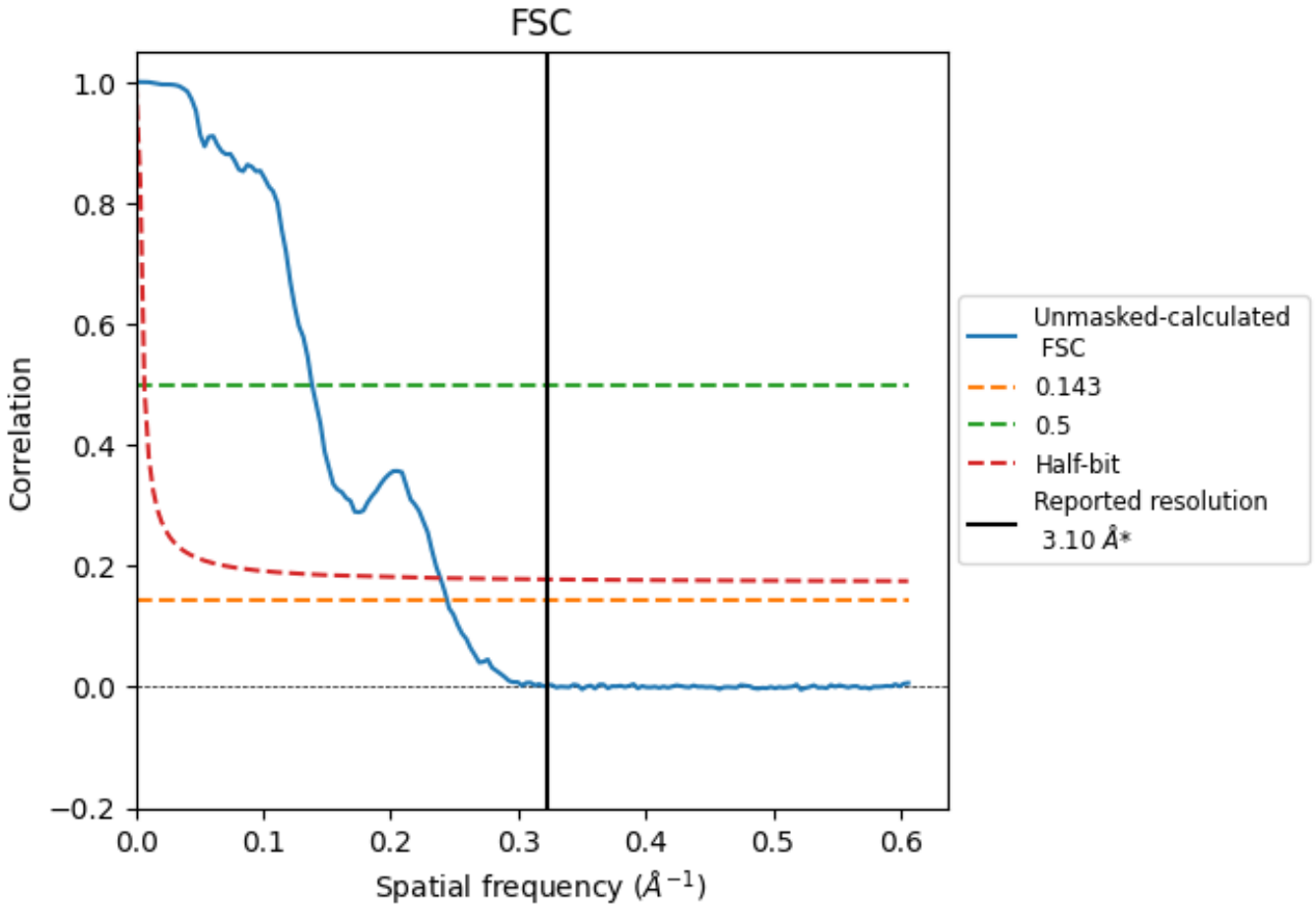


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

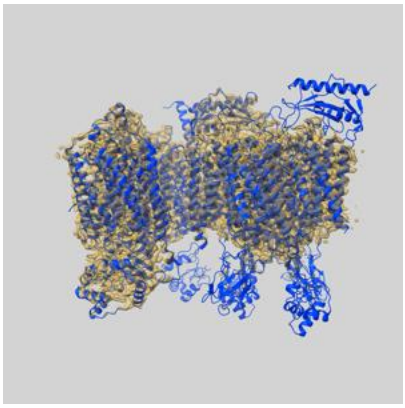
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.10	7.24	4.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.10 differs from the reported value 3.1 by more than 10 %

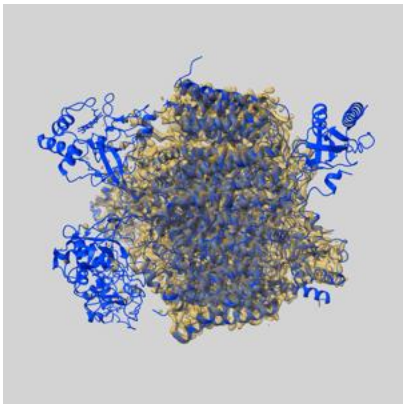
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70333 and PDB model 9OCV. Per-residue inclusion information can be found in section 3 on page 15.

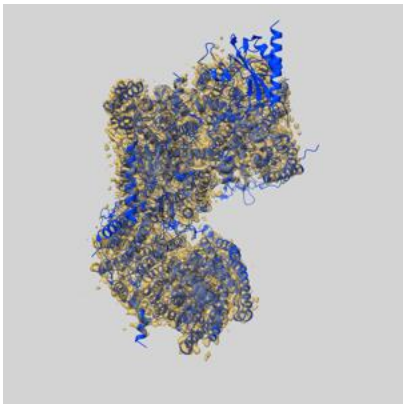
9.1 Map-model overlay



X



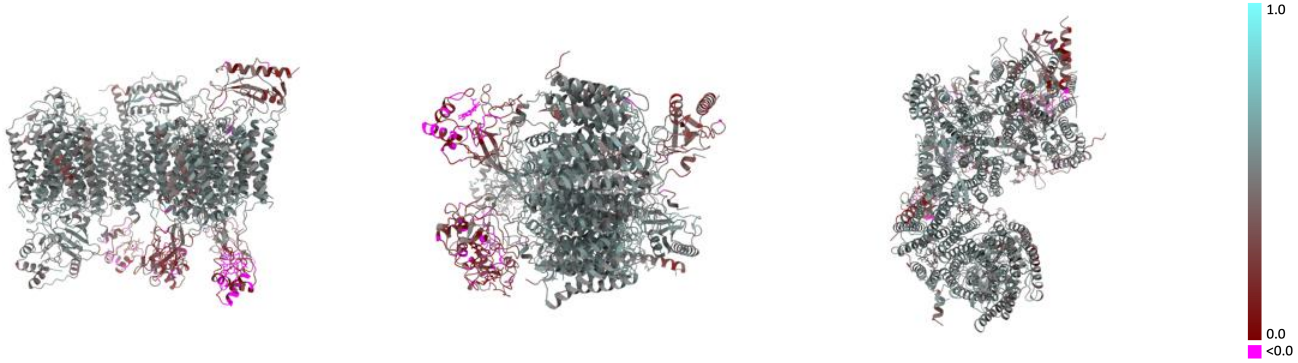
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

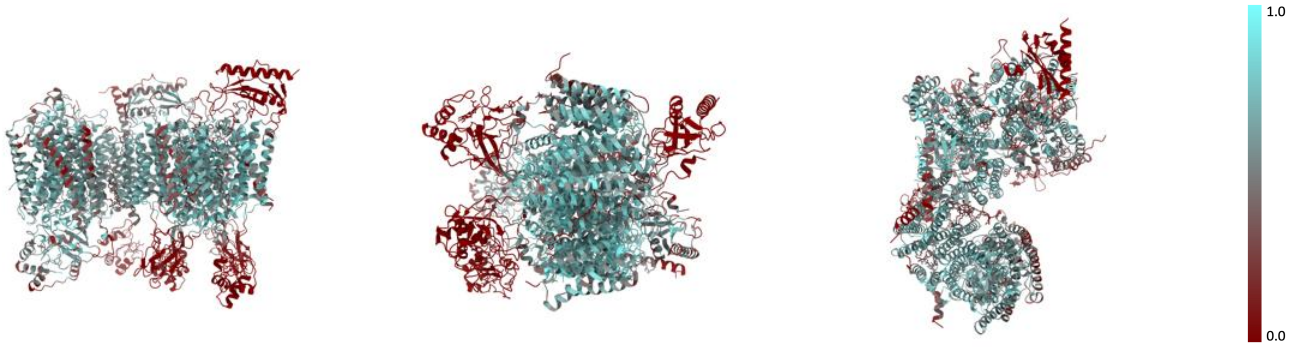
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

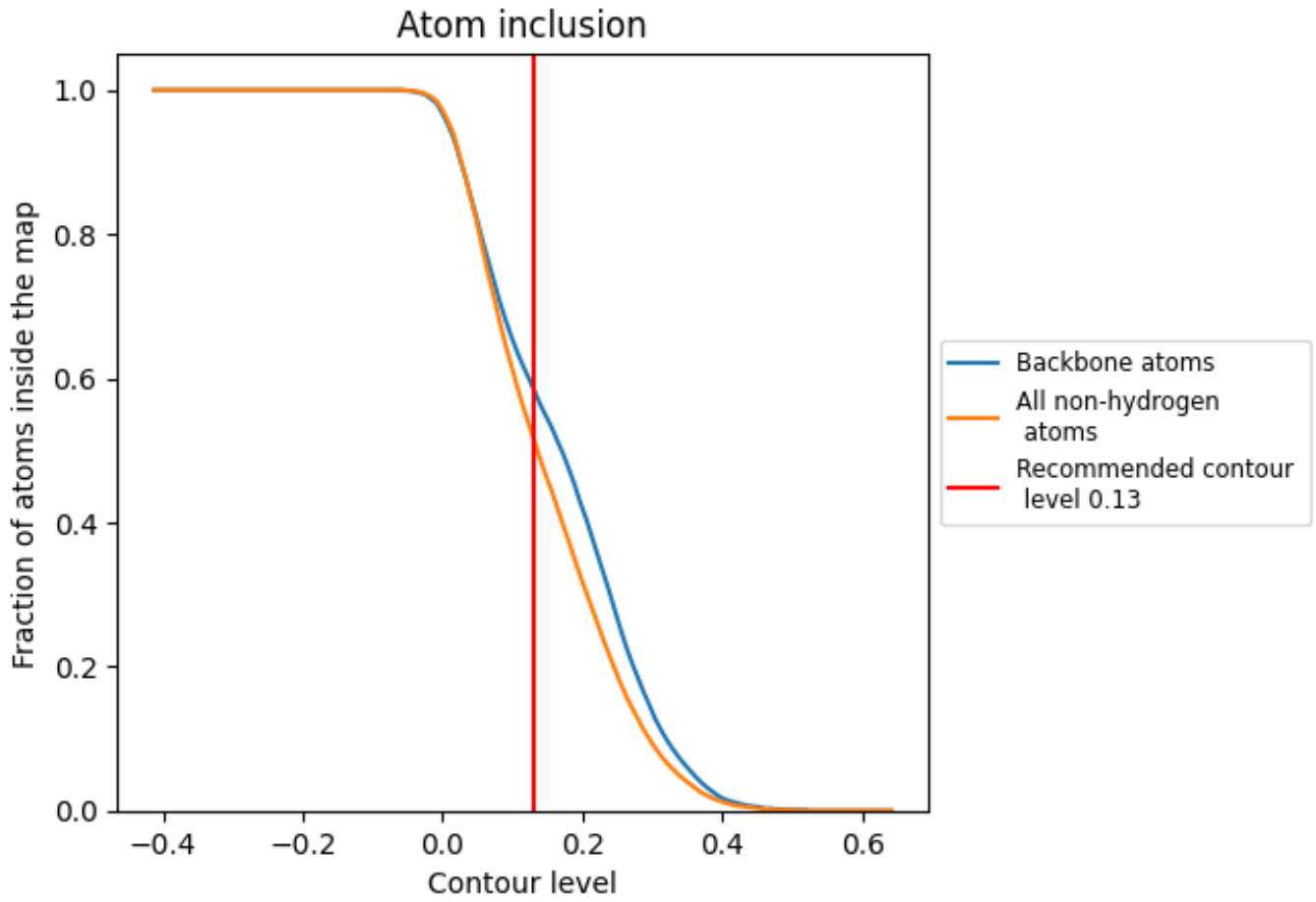
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5160	0.4630
A	0.2100	0.3540
B	0.6870	0.5230
C	0.3870	0.3590
D	0.3780	0.4420
E	0.7050	0.5270
F	0.5440	0.4960
G	0.4730	0.4530
H	0.4470	0.4680
I	0.0000	0.3250
J	0.1780	0.2830
K	0.5770	0.5040
L	0.6300	0.5180
M	0.6620	0.5200
N	0.5100	0.4890
a	0.2220	0.3490
b	0.7550	0.5420
c	0.4210	0.4020
d	0.5920	0.5050
e	0.7960	0.5570
f	0.8070	0.5340
g	0.6960	0.5340
h	0.6060	0.4950
i	0.4840	0.5160

