Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:43 pm GMT

PDB ID	:	6FO6
EMDB ID	:	EMD-4292
Title	:	CryoEM structure of bovine cytochrome bc1 in complex with the anti-malarial inhibitor SCR0911
Authors	:	Johnson, R.M.; Amporndanai, K.; O'Neill, P.M.; Fishwick, C.W.G.; Jamson, A.H.; Rawson, S.D.; Hasnain, S.S.; Antonyuk, S.V.; Muench, S.P.
Deposited on	:	2018-02-06
Resolution	:	4.10 Å(reported)

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

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

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

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

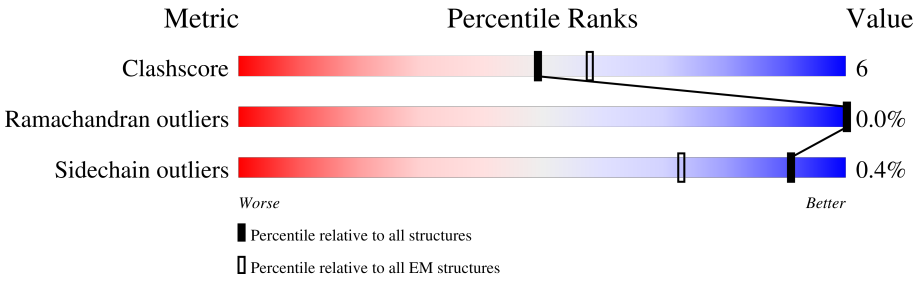
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	E	274	57% 54% 10% 35%
1	R	274	58% 53% 12% 35%
2	A	480	68% 83% 9% 8%
2	N	480	71% 83% 10% 8%
3	B	453	79% 83% 8% 9%
3	O	453	77% 82% 9% 9%
4	C	379	43% 85% 12% ••
4	P	379	44% 86% 11% ••

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Mol	Chain	Length	Quality of chain
5	D	325	59% 65% 8% 27%
5	Q	325	54% 66% 7% 27%
6	F	111	57% 80% 8% 12%
6	S	111	59% 78% 10% 12%
7	G	82	65% 79% 9% 12%
7	T	82	65% 76% 12% 12%
8	H	91	71% 67% 29%
8	U	91	71% 67% 29%
9	J	64	86% 88% 9%
9	W	64	88% 84% 5% 11%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 30720 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	178	Total	C	N	O	S	0	0
			1361	862	227	264	8		
1	R	178	Total	C	N	O	S	0	0
			1350	856	225	261	8		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	444	Total	C	N	O	S	0	0
			3439	2148	607	664	20		
2	N	444	Total	C	N	O	S	0	0
			3439	2148	607	664	20		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	414	Total	C	N	O	S	0	0
			3113	1955	551	600	7		
3	O	411	Total	C	N	O	S	0	0
			3095	1944	548	596	7		

- Molecule 4 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	370	Total	C	N	O	S	0	0
			2936	1973	456	489	18		
4	P	370	Total	C	N	O	S	0	0
			2936	1973	456	489	18		

- Molecule 5 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	237	Total	C	N	O	S	0	0
			1887	1206	325	341	15		
5	Q	237	Total	C	N	O	S	0	0
			1887	1206	325	341	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	98	Total	C	N	O	S	0	0
			860	547	154	157	2		
6	S	98	Total	C	N	O	S	0	0
			860	547	154	157	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	conflict	UNP P00129
S	56	ASP	ASN	conflict	UNP P00129

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	72	Total	C	N	O	S	0	0
			612	400	115	96	1		
7	T	72	Total	C	N	O	S	0	0
			612	400	115	96	1		

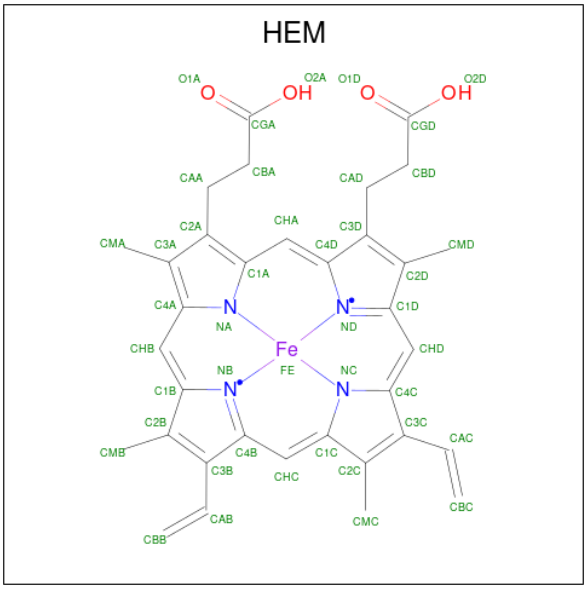
- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total	C	N	O	S	0	0
			529	321	96	107	5		
8	U	65	Total	C	N	O	S	0	0
			529	321	96	107	5		

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

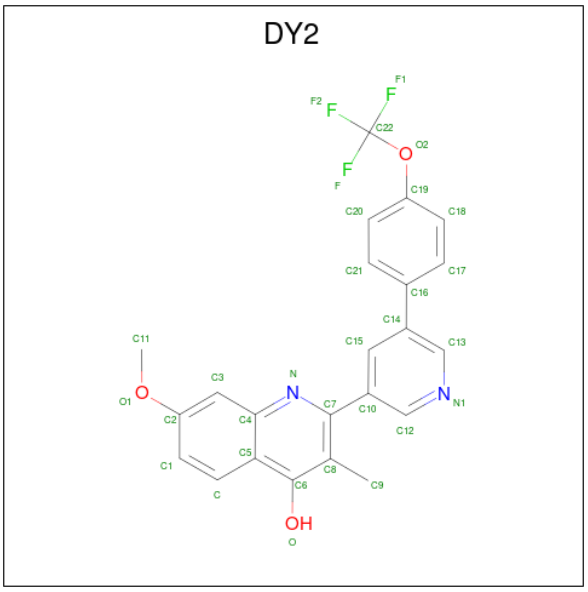
Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	58	Total	C	N	O	0	0
			482	317	83	82		
9	W	57	Total	C	N	O	0	0
			473	312	82	79		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



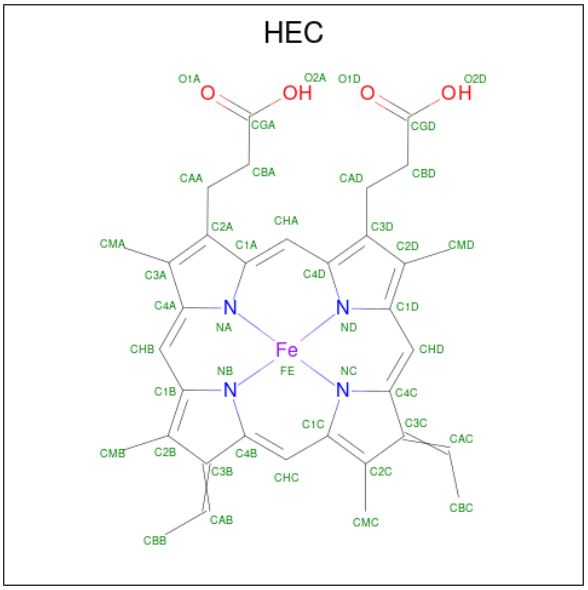
Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
10	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
10	P	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
10	P	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 11 is 7-methoxy-3-methyl-2-[5-[4-(trifluoromethyloxy)phenyl]pyridin-3-yl]quinolin-4-ol (three-letter code: DY2) (formula: $C_{23}H_{17}F_3N_2O_3$).



Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	F	N	O	0
			31	23	3	2	3	
11	P	1	Total	C	F	N	O	0
			31	23	3	2	3	

- Molecule 12 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



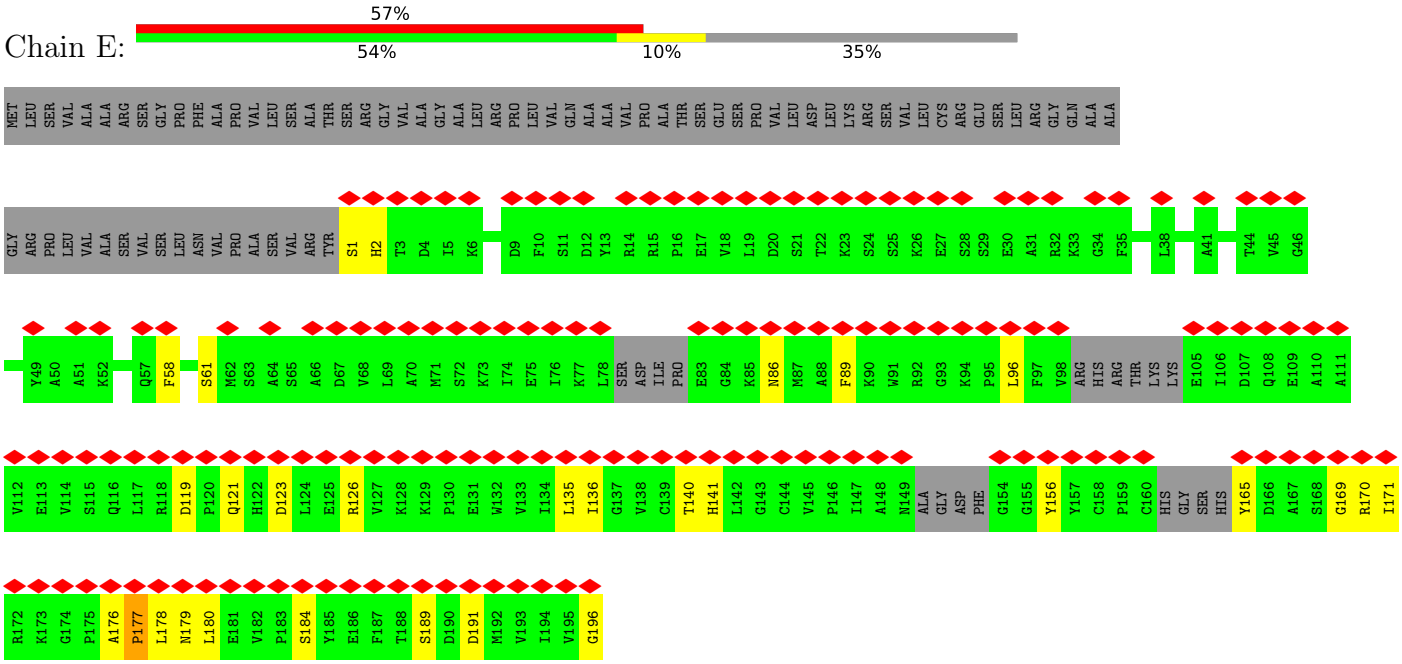
Mol	Chain	Residues	Atoms					AltConf
12	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots (i)

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

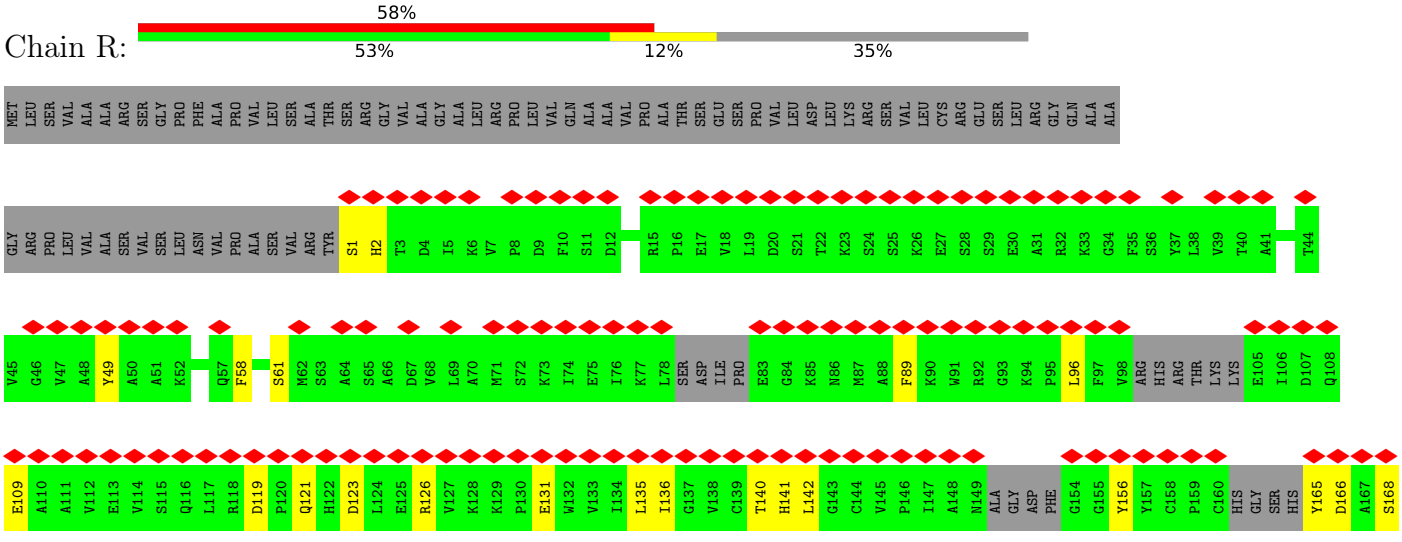
• Molecule 1: Cytochrome b-c1 complex subunit Rieske, mitochondrial

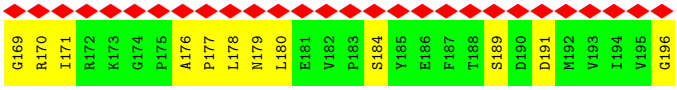
Chain E:



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

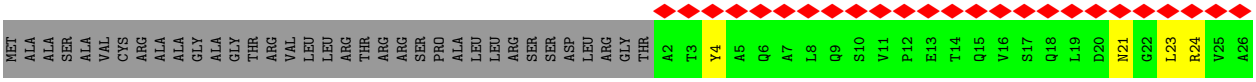
Chain R:

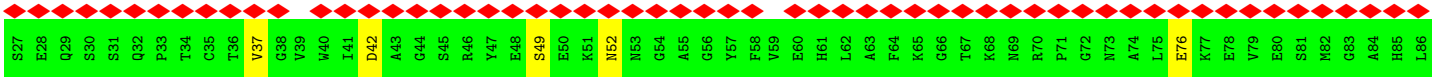


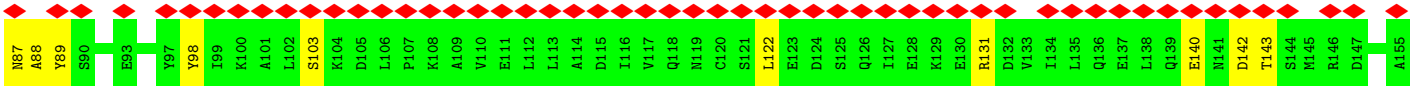


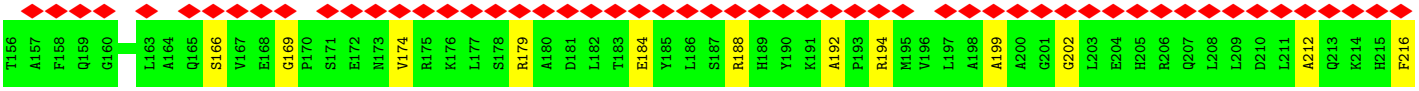
• Molecule 2: Cytochrome b-c1 complex subunit 1, mitochondrial

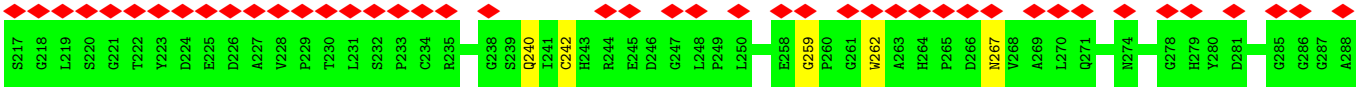
Chain A:

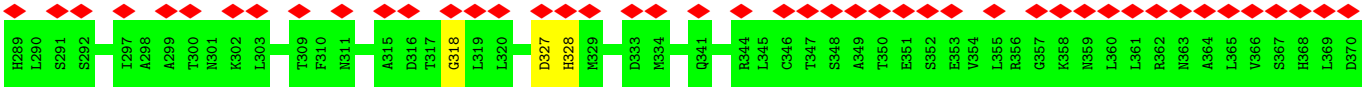


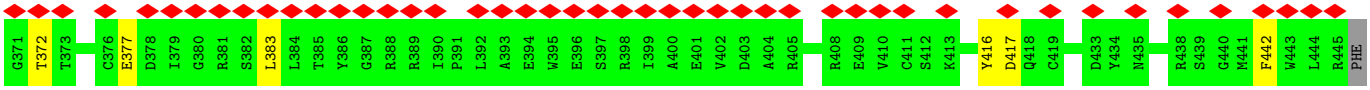






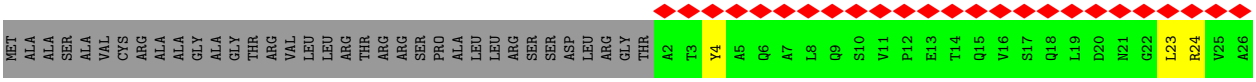


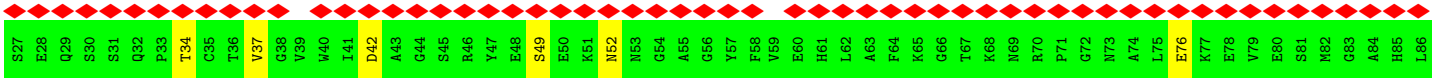


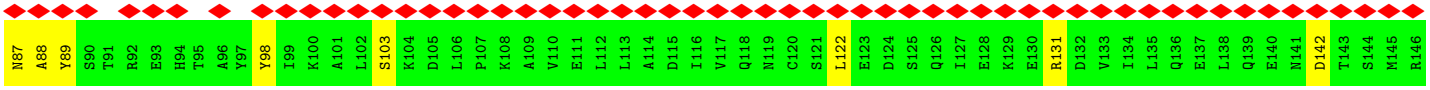


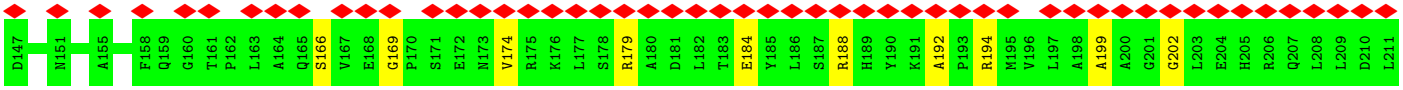
• Molecule 2: Cytochrome b-c1 complex subunit 1, mitochondrial

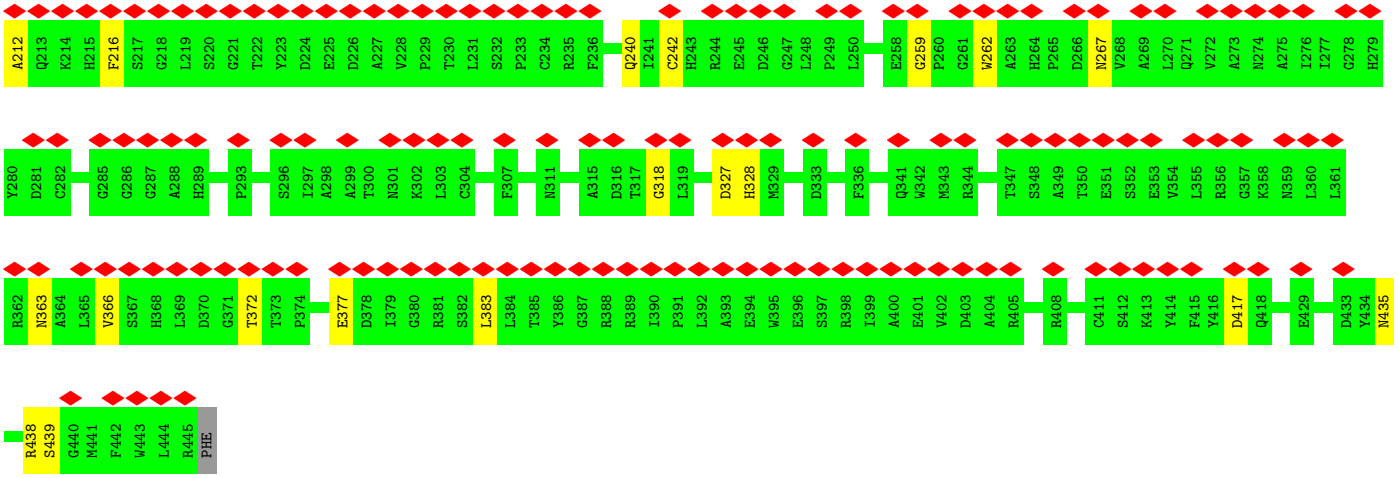
Chain N:





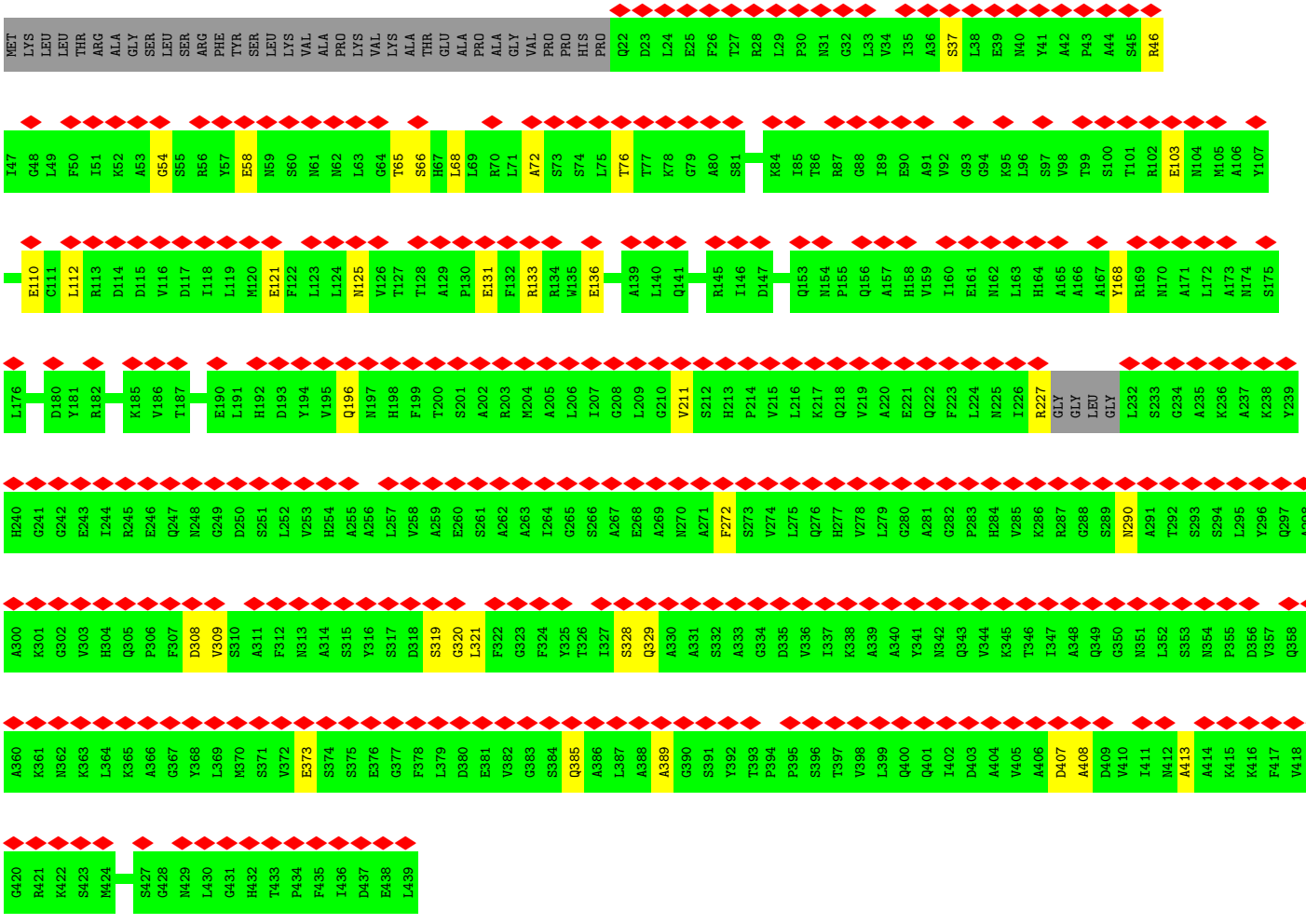






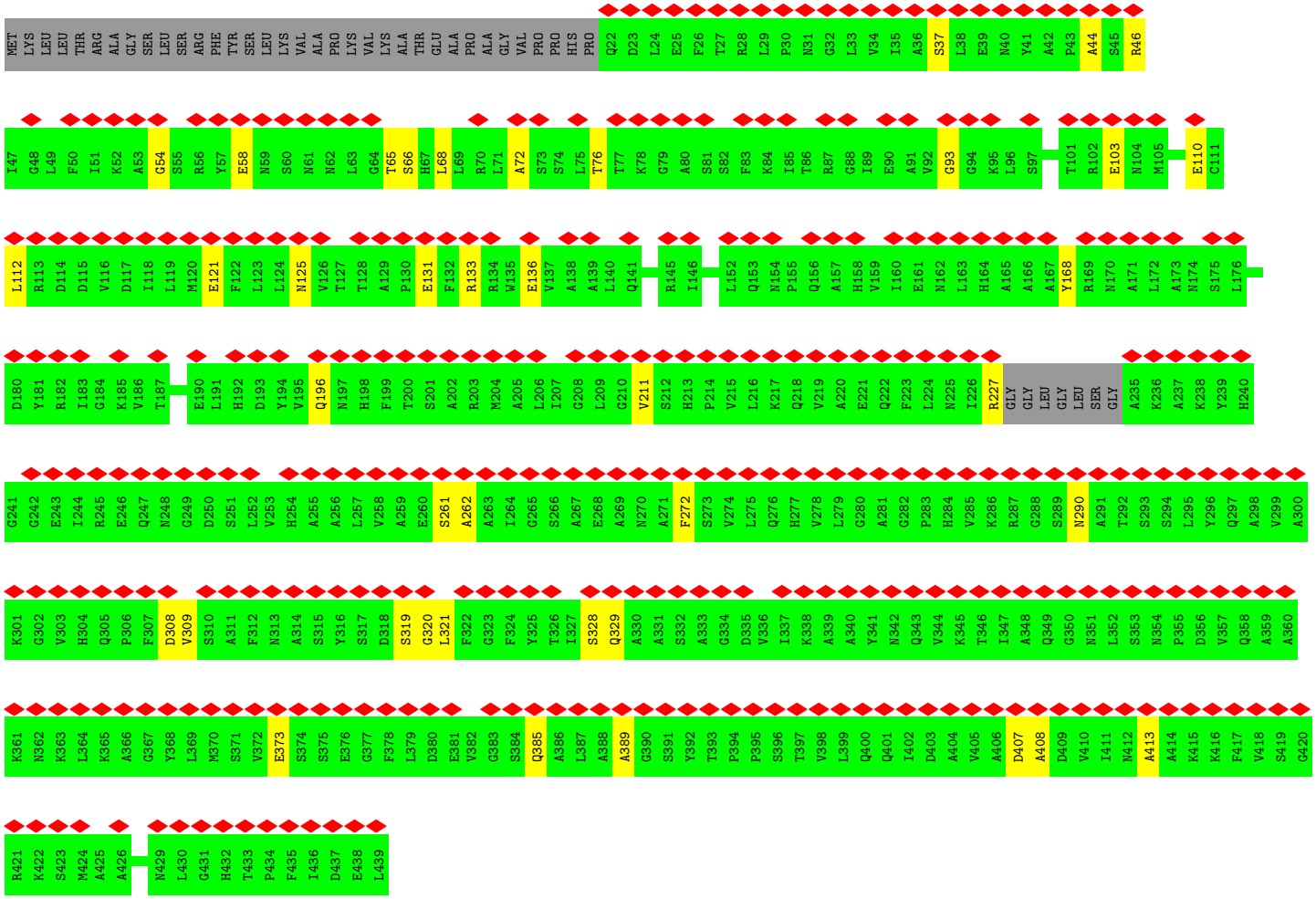
• Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



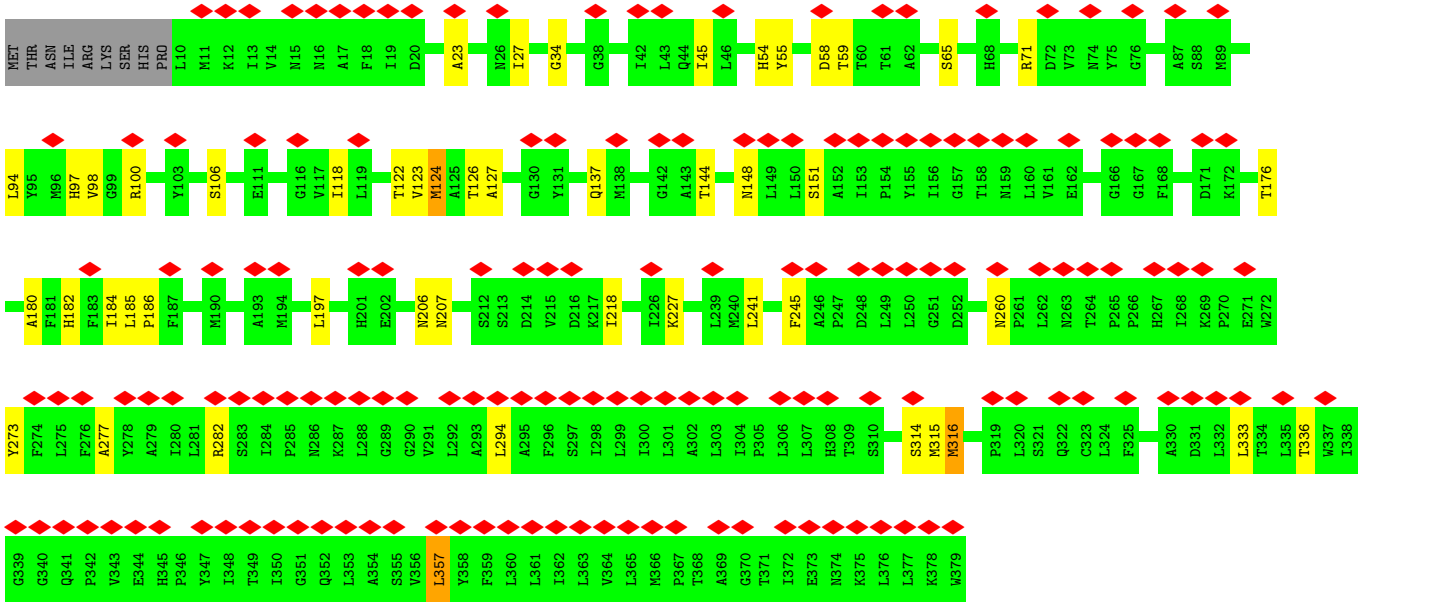
• Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain O:



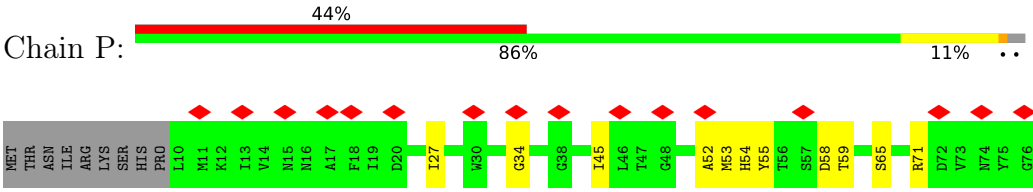
• Molecule 4: Cytochrome b

Chain C:



• Molecule 4: Cytochrome b

Chain P:

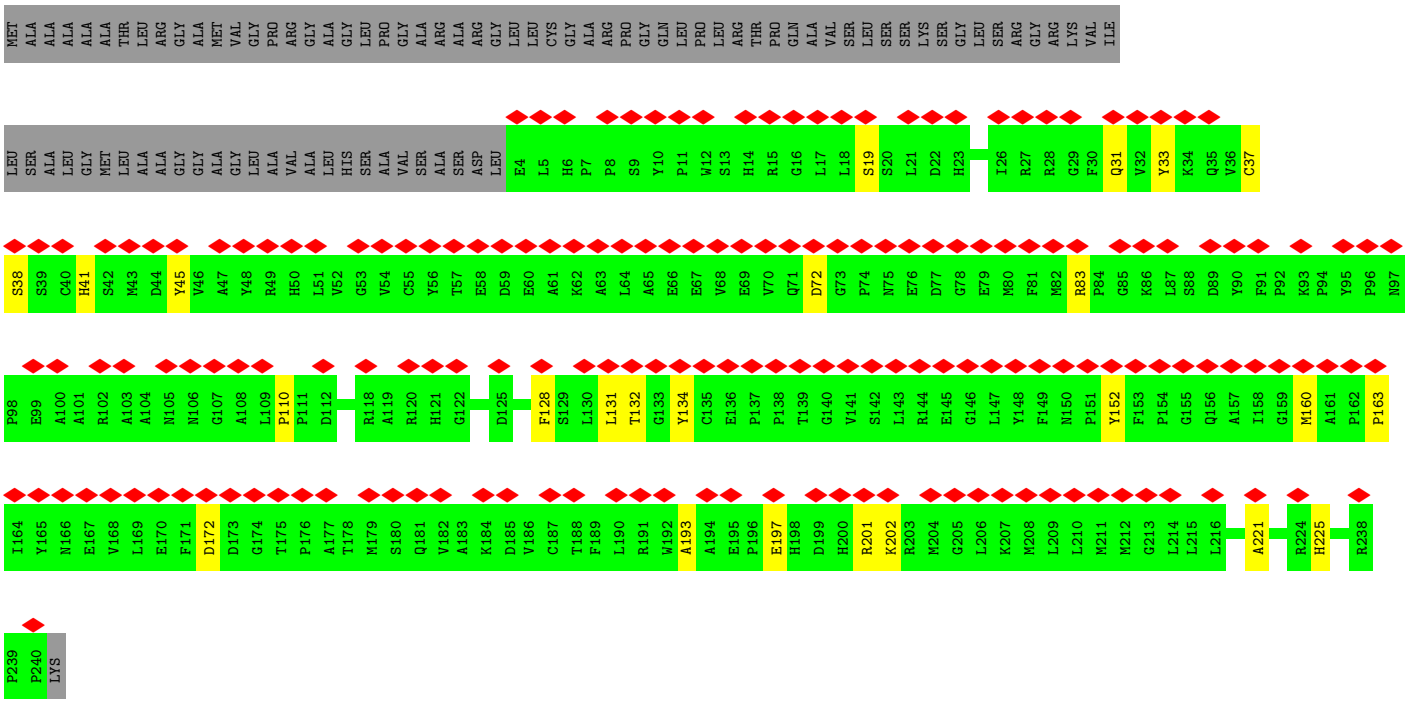


• Molecule 5: Cytochrome c1, heme protein, mitochondrial

Chain D:

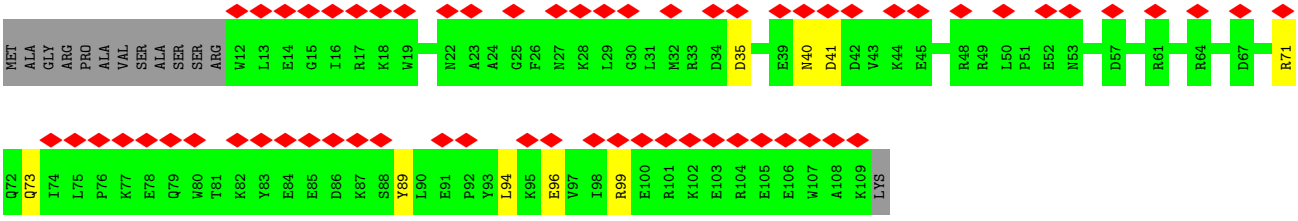
• Molecule 5: Cytochrome c1, heme protein, mitochondrial

Chain Q:



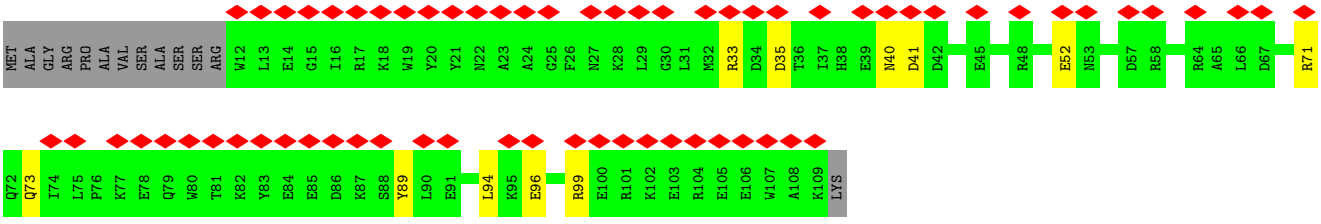
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:



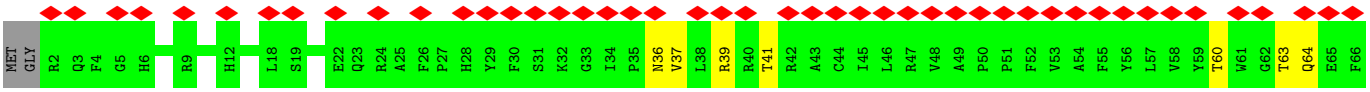
• Molecule 6: Cytochrome b-c1 complex subunit 7

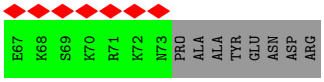
Chain S:



• Molecule 7: Cytochrome b-c1 complex subunit 8

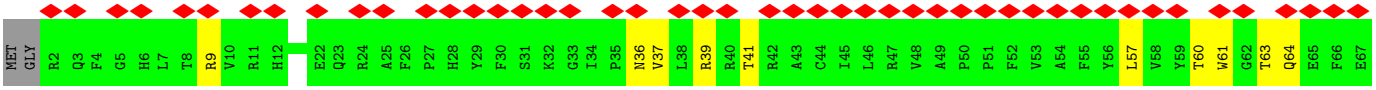
Chain G:

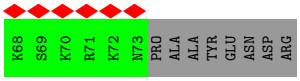




• Molecule 7: Cytochrome b-c1 complex subunit 8

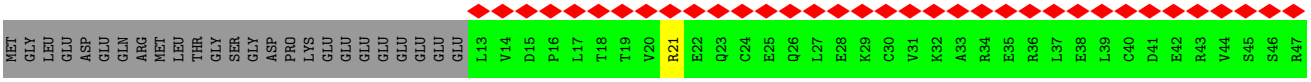
Chain T:

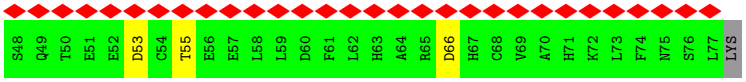




• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

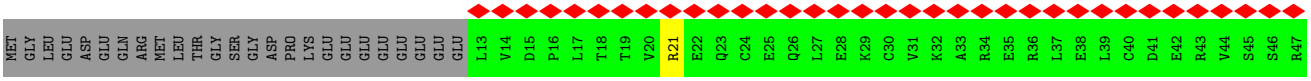
Chain H:

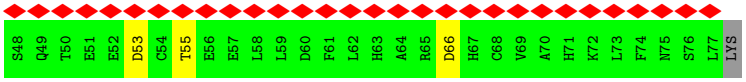




• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

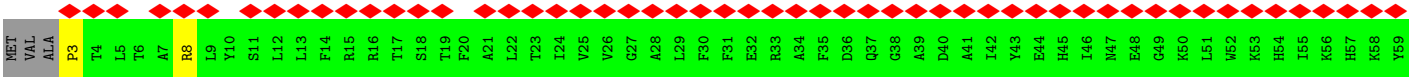
Chain U:





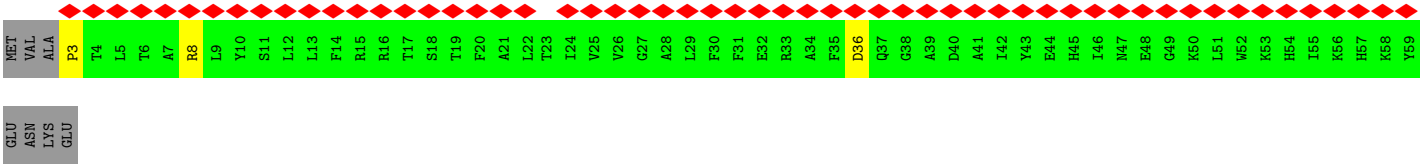
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain J:



• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain W:


MET VAL ALA P3 T4 L5 T6 A7 R8 L9 Y10 S11 L12 L13 F14 R15 R16 T17 S18 T19 F20 A21 L22 T23 I24 V25 V26 G27 A28 L29 F30 F31 E32 R33 A34 F35 D36 Q37 G38 A39 D40 A41 I42 Y43 E44 H45 I46 N47 E48 G49 K50 L51 W52 K53 H54 I55 K56 H57 K58 Y59
GLU ASN LYS GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	114130	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	85	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	79000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.510	Depositor
Minimum map value	-0.297	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.173	Depositor
Map size (Å)	213.40001, 213.40001, 213.40001	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DY2, HEC, HEM

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	E	0.39	0/1386	0.51	0/1873
1	R	0.39	0/1375	0.51	0/1860
2	A	0.48	0/3511	0.57	0/4766
2	N	0.48	0/3511	0.57	0/4766
3	B	0.43	0/3168	0.54	0/4296
3	O	0.43	0/3150	0.54	0/4272
4	C	0.62	0/3031	0.61	5/4150 (0.1%)
4	P	0.62	0/3031	0.61	5/4150 (0.1%)
5	D	0.48	0/1946	0.56	0/2643
5	Q	0.48	0/1946	0.56	0/2643
6	F	0.49	0/879	0.58	0/1180
6	S	0.49	0/879	0.58	1/1180 (0.1%)
7	G	0.50	0/632	0.62	0/854
7	T	0.50	0/632	0.62	0/854
8	H	0.29	0/534	0.48	0/718
8	U	0.29	0/534	0.48	0/718
9	J	0.41	0/495	0.50	0/667
9	W	0.41	0/486	0.50	0/655
All	All	0.49	0/31126	0.56	11/42245 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	316	MET	CG-SD-CE	7.35	111.96	100.20
4	C	316	MET	CG-SD-CE	7.34	111.94	100.20
4	C	124	MET	CG-SD-CE	6.62	110.79	100.20
4	P	124	MET	CG-SD-CE	6.62	110.79	100.20
4	C	357	LEU	CB-CG-CD1	5.95	121.11	111.00
4	P	357	LEU	CB-CG-CD1	5.92	121.07	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	124	MET	CB-CG-SD	5.16	127.88	112.40
4	P	124	MET	CB-CG-SD	5.16	127.87	112.40
4	P	357	LEU	CB-CG-CD2	5.07	119.62	111.00
4	C	357	LEU	CB-CG-CD2	5.07	119.61	111.00
6	S	33	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1361	0	1339	44	0
1	R	1350	0	1320	71	0
2	A	3439	0	3337	28	0
2	N	3439	0	3337	30	0
3	B	3113	0	3094	25	0
3	O	3095	0	3075	31	0
4	C	2936	0	2996	35	0
4	P	2936	0	2996	33	0
5	D	1887	0	1834	19	0
5	Q	1887	0	1834	19	0
6	F	860	0	849	4	0
6	S	860	0	849	5	0
7	G	612	0	618	11	0
7	T	612	0	618	14	0
8	H	529	0	511	3	0
8	U	529	0	511	3	0
9	J	482	0	483	1	0
9	W	473	0	477	2	0
10	C	86	0	60	15	0
10	P	86	0	60	17	0
11	C	31	0	0	0	0
11	P	31	0	0	0	0
12	D	43	0	32	10	0
12	Q	43	0	32	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30720	0	30262	373	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 6.

All (373) 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)
2:A:417:ASP:OD1	2:A:442:PHE:HB3	1.25	1.25
7:T:60:THR:O	7:T:63:THR:HG22	1.41	1.17
7:G:60:THR:O	7:G:63:THR:HG22	1.41	1.17
1:R:171:ILE:HG22	1:R:179:ASN:OD1	1.46	1.14
1:E:171:ILE:HG22	1:E:179:ASN:OD1	1.50	1.10
1:R:171:ILE:CD1	1:R:176:ALA:HB3	1.82	1.08
1:R:171:ILE:HD12	1:R:176:ALA:HB3	1.30	1.07
1:R:121:GLN:HG3	1:R:126:ARG:NH2	1.80	0.96
1:R:121:GLN:CG	1:R:126:ARG:NH2	2.31	0.94
1:E:126:ARG:NH2	1:E:179:ASN:HD22	1.69	0.91
1:E:171:ILE:HD12	1:E:176:ALA:HB3	1.52	0.90
2:A:417:ASP:OD1	2:A:442:PHE:CB	2.17	0.89
3:B:58:GLU:OE2	3:B:65:THR:HG22	1.73	0.88
3:O:58:GLU:OE2	3:O:65:THR:HG22	1.73	0.88
1:R:121:GLN:O	1:R:170:ARG:NH1	2.07	0.87
1:R:165:TYR:HE1	1:R:171:ILE:HD12	1.40	0.86
7:G:60:THR:O	7:G:63:THR:CG2	2.23	0.86
1:E:171:ILE:CD1	1:E:176:ALA:HB3	2.07	0.85
1:R:156:TYR:HE2	1:R:180:LEU:HD11	1.42	0.85
1:R:171:ILE:HD12	1:R:176:ALA:CB	2.06	0.85
1:E:165:TYR:HE1	1:E:171:ILE:HD12	1.42	0.84
1:R:156:TYR:CE2	1:R:180:LEU:HD11	2.13	0.84
7:T:60:THR:O	7:T:63:THR:CG2	2.23	0.83
7:T:60:THR:C	7:T:63:THR:HG22	1.99	0.82
1:E:170:ARG:HA	1:E:179:ASN:HB3	1.59	0.82
7:G:60:THR:C	7:G:63:THR:HG22	1.99	0.81
1:R:156:TYR:HE2	1:R:180:LEU:CD1	1.95	0.80
4:P:71:ARG:NH1	5:Q:45:TYR:O	2.15	0.80
1:E:119:ASP:HB3	1:E:179:ASN:ND2	2.01	0.76
5:Q:41:HIS:NE2	12:Q:501:HEC:NB	2.33	0.76
4:C:71:ARG:NH1	5:D:45:TYR:O	2.18	0.76
1:R:121:GLN:HB2	1:R:126:ARG:NH2	2.02	0.75
3:B:58:GLU:OE2	3:B:65:THR:CG2	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:41:HIS:NE2	12:D:501:HEC:NB	2.34	0.75
4:P:137:GLN:OE1	4:P:260:ASN:N	2.20	0.75
4:C:137:GLN:OE1	4:C:260:ASN:N	2.20	0.74
4:P:182:HIS:NE2	10:P:501:HEM:NC	2.35	0.74
1:R:126:ARG:NH2	1:R:179:ASN:HD22	1.86	0.74
2:A:24:ARG:NH1	2:A:383:LEU:O	2.22	0.73
2:N:24:ARG:NH1	2:N:383:LEU:O	2.21	0.73
3:O:58:GLU:OE2	3:O:65:THR:CG2	2.35	0.73
3:O:121:GLU:O	3:O:125:ASN:ND2	2.22	0.73
1:R:119:ASP:HB3	1:R:179:ASN:ND2	2.04	0.73
3:B:121:GLU:O	3:B:125:ASN:ND2	2.22	0.72
2:N:131:ARG:NH1	2:N:174:VAL:O	2.22	0.72
2:A:131:ARG:NH1	2:A:174:VAL:O	2.22	0.72
3:O:65:THR:HG23	3:O:66:SER:N	2.05	0.72
1:R:140:THR:HG21	1:R:178:LEU:HB3	1.71	0.71
1:R:121:GLN:HG3	1:R:126:ARG:HH22	1.54	0.71
1:R:121:GLN:CB	1:R:126:ARG:NH2	2.53	0.71
3:B:65:THR:HG23	3:B:66:SER:N	2.05	0.71
1:R:165:TYR:HE1	1:R:171:ILE:CD1	2.03	0.71
10:C:501:HEM:HBB2	10:C:501:HEM:HHC	1.73	0.71
1:E:126:ARG:HH21	1:E:179:ASN:HD22	1.37	0.70
1:E:165:TYR:CE1	1:E:171:ILE:HB	2.27	0.70
10:P:501:HEM:HHC	10:P:501:HEM:HBB2	1.74	0.70
9:J:3:PRO:O	9:J:8:ARG:NH1	2.25	0.70
3:B:58:GLU:CD	3:B:65:THR:HG22	2.13	0.69
9:W:3:PRO:O	9:W:8:ARG:NH1	2.25	0.69
2:A:259:GLY:N	2:A:318:GLY:O	2.26	0.69
1:R:109:GLU:OE1	1:R:168:SER:OG	2.09	0.69
3:O:58:GLU:CD	3:O:65:THR:HG22	2.12	0.69
3:B:196:GLN:O	3:B:227:ARG:NH2	2.26	0.68
1:R:171:ILE:HD11	1:R:176:ALA:HB3	1.75	0.68
2:N:122:LEU:O	2:N:179:ARG:NH1	2.26	0.68
2:N:259:GLY:N	2:N:318:GLY:O	2.26	0.68
2:A:122:LEU:O	2:A:179:ARG:NH1	2.26	0.68
3:O:196:GLN:O	3:O:227:ARG:NH2	2.26	0.67
10:C:502:HEM:HBB2	10:C:502:HEM:HMB2	1.75	0.67
4:C:55:TYR:HA	4:C:65:SER:OG	1.95	0.67
4:P:55:TYR:HA	4:P:65:SER:OG	1.95	0.66
5:Q:152:TYR:OH	8:U:66:ASP:OD2	2.14	0.66
4:C:182:HIS:NE2	10:C:501:HEM:NC	2.42	0.66
5:D:134:TYR:OH	5:D:160:MET:O	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:60:THR:HA	7:T:63:THR:HG22	1.78	0.66
7:G:60:THR:HA	7:G:63:THR:HG22	1.78	0.65
7:G:60:THR:CA	7:G:63:THR:HG22	2.26	0.65
3:O:385:GLN:O	3:O:389:ALA:N	2.29	0.65
1:E:121:GLN:HG3	1:E:126:ARG:NH2	2.11	0.65
1:R:165:TYR:CE1	1:R:171:ILE:HD12	2.29	0.65
3:B:385:GLN:O	3:B:389:ALA:N	2.29	0.65
1:E:165:TYR:HE1	1:E:171:ILE:CD1	2.08	0.65
1:R:171:ILE:CG2	1:R:179:ASN:OD1	2.36	0.65
7:T:60:THR:CA	7:T:63:THR:HG22	2.26	0.64
10:P:501:HEM:HMC2	10:P:501:HEM:HBC2	1.79	0.64
10:P:502:HEM:HMC2	10:P:502:HEM:HBC2	1.80	0.64
4:C:277:ALA:HB1	4:C:294:LEU:HD11	1.80	0.64
1:R:119:ASP:HB3	1:R:179:ASN:HD21	1.61	0.63
1:R:165:TYR:CE1	1:R:171:ILE:HB	2.34	0.63
1:E:156:TYR:HE2	1:E:180:LEU:CD1	2.10	0.63
4:C:54:HIS:O	4:C:65:SER:OG	2.17	0.63
7:G:36:ASN:OD1	7:G:39:ARG:NH2	2.31	0.63
7:T:60:THR:HA	7:T:63:THR:CG2	2.29	0.63
4:P:54:HIS:O	4:P:65:SER:OG	2.17	0.63
7:T:36:ASN:OD1	7:T:39:ARG:NH2	2.31	0.63
1:E:165:TYR:CD1	1:E:171:ILE:HA	2.34	0.63
12:D:501:HEC:HMB1	12:D:501:HEC:HBB2	1.80	0.63
5:Q:134:TYR:OH	5:Q:160:MET:O	2.08	0.63
12:Q:501:HEC:HMB1	12:Q:501:HEC:HBB2	1.79	0.63
7:G:60:THR:HA	7:G:63:THR:CG2	2.29	0.63
2:N:34:THR:HG1	3:O:373:GLU:CD	2.02	0.63
4:P:277:ALA:HB1	4:P:294:LEU:HD11	1.80	0.63
2:A:87:ASN:ND2	2:A:98:TYR:OH	2.32	0.62
1:R:121:GLN:HB2	1:R:126:ARG:HH21	1.63	0.62
4:P:106:SER:HB3	10:P:502:HEM:HBD2	1.82	0.62
6:S:71:ARG:NH1	6:S:73:GLN:OE1	2.33	0.62
2:N:87:ASN:ND2	2:N:98:TYR:OH	2.32	0.62
2:A:262:TRP:O	2:A:267:ASN:ND2	2.33	0.62
4:C:106:SER:HB3	10:C:502:HEM:HBD2	1.82	0.62
1:E:119:ASP:HB3	1:E:179:ASN:CG	2.21	0.62
10:C:502:HEM:HBC2	10:C:502:HEM:HMC2	1.80	0.62
6:F:71:ARG:NH1	6:F:73:GLN:OE1	2.33	0.62
2:N:262:TRP:O	2:N:267:ASN:ND2	2.33	0.61
1:R:165:TYR:CD1	1:R:171:ILE:HA	2.35	0.61
2:A:49:SER:N	2:A:52:ASN:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:170:ARG:HA	1:R:179:ASN:HB3	1.81	0.61
7:T:60:THR:HG23	7:T:61:TRP:N	2.16	0.61
2:N:49:SER:N	2:N:52:ASN:OD1	2.33	0.61
4:P:241:LEU:O	4:P:245:PHE:N	2.34	0.61
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.16	0.61
4:C:241:LEU:O	4:C:245:PHE:N	2.34	0.60
1:E:156:TYR:CE2	1:E:180:LEU:HD11	2.37	0.60
5:Q:132:THR:O	8:U:21:ARG:NH2	2.34	0.60
6:S:35:ASP:OD1	6:S:89:TYR:OH	2.16	0.60
1:E:89:PHE:O	1:E:96:LEU:N	2.35	0.60
1:R:89:PHE:O	1:R:96:LEU:N	2.35	0.60
1:R:141:HIS:HB2	1:R:177:PRO:HD3	1.84	0.60
10:P:502:HEM:HMB1	10:P:502:HEM:HBB2	1.84	0.60
1:R:165:TYR:CE1	1:R:171:ILE:CG1	2.85	0.59
1:R:156:TYR:CE2	1:R:180:LEU:CD1	2.78	0.59
1:R:165:TYR:OH	1:R:176:ALA:HB1	2.02	0.59
10:P:501:HEM:O1D	10:P:501:HEM:HBA2	2.03	0.59
3:B:65:THR:CG2	3:B:66:SER:N	2.66	0.58
3:O:65:THR:CG2	3:O:66:SER:N	2.66	0.58
2:N:34:THR:OG1	3:O:373:GLU:CD	2.40	0.58
12:Q:501:HEC:HBD1	12:Q:501:HEC:HHA	1.86	0.58
4:P:100:ARG:HH22	10:P:502:HEM:HBD1	1.69	0.58
5:D:152:TYR:OH	8:H:66:ASP:OD2	2.21	0.58
4:C:100:ARG:HH22	10:C:502:HEM:HBD1	1.68	0.57
5:D:19:SER:O	5:D:202:LYS:NZ	2.37	0.57
12:D:501:HEC:HBD1	12:D:501:HEC:HHA	1.86	0.57
1:E:86:ASN:ND2	1:E:156:TYR:OH	2.36	0.57
1:R:119:ASP:CG	1:R:178:LEU:HD12	2.25	0.57
1:E:1:SER:OG	1:E:2:HIS:N	2.38	0.56
2:A:76:GLU:OE2	3:B:290:ASN:N	2.37	0.56
1:R:165:TYR:HE1	1:R:171:ILE:CG1	2.17	0.56
5:Q:19:SER:O	5:Q:202:LYS:NZ	2.37	0.56
2:N:76:GLU:OE2	3:O:290:ASN:N	2.38	0.56
1:E:165:TYR:CE1	1:E:171:ILE:HD12	2.33	0.56
2:A:212:ALA:O	2:A:216:PHE:N	2.39	0.56
1:E:140:THR:HG22	1:E:177:PRO:HG2	1.88	0.56
2:N:212:ALA:O	2:N:216:PHE:N	2.39	0.56
10:C:501:HEM:O1D	10:C:501:HEM:HBA2	2.05	0.55
7:T:57:LEU:O	7:T:60:THR:HG22	2.06	0.55
1:R:1:SER:OG	1:R:2:HIS:N	2.38	0.55
1:E:140:THR:HG21	1:E:178:LEU:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:TYR:CE1	1:E:171:ILE:CG1	2.90	0.55
5:Q:163:PRO:CG	12:Q:501:HEC:HAB	2.37	0.55
4:C:176:THR:HG22	4:P:52:ALA:O	2.07	0.55
10:C:501:HEM:HBC2	10:C:501:HEM:HMC2	1.88	0.55
5:D:163:PRO:CG	12:D:501:HEC:HAB	2.37	0.55
1:R:121:GLN:HG3	1:R:126:ARG:CZ	2.37	0.55
4:C:277:ALA:HB1	4:C:294:LEU:CD1	2.37	0.54
2:N:184:GLU:OE2	2:N:188:ARG:NH2	2.39	0.54
4:P:277:ALA:HB1	4:P:294:LEU:CD1	2.37	0.54
4:P:123:VAL:O	4:P:126:THR:N	2.40	0.54
1:E:165:TYR:CE1	1:E:171:ILE:CB	2.91	0.54
2:A:184:GLU:OE2	2:A:188:ARG:NH2	2.39	0.54
1:E:156:TYR:CE2	1:E:180:LEU:CD1	2.90	0.54
5:D:31:GLN:NE2	5:D:172:ASP:OD2	2.41	0.53
1:R:119:ASP:HB3	1:R:179:ASN:CG	2.28	0.53
1:R:189:SER:OG	1:R:191:ASP:OD1	2.21	0.53
4:C:333:LEU:O	4:C:336:THR:OG1	2.27	0.53
7:G:63:THR:HG23	7:G:64:GLN:N	2.24	0.53
4:C:71:ARG:NH2	5:D:193:ALA:O	2.42	0.53
4:C:123:VAL:O	4:C:126:THR:N	2.40	0.53
5:Q:31:GLN:NE2	5:Q:172:ASP:OD2	2.41	0.53
1:E:119:ASP:HB3	1:E:179:ASN:HD21	1.69	0.53
1:R:140:THR:HG22	1:R:177:PRO:HG2	1.91	0.53
2:N:23:LEU:HB2	2:N:192:ALA:HB1	1.91	0.53
2:A:23:LEU:HB2	2:A:192:ALA:HB1	1.91	0.52
4:C:186:PRO:HG2	10:C:501:HEM:HMC1	1.91	0.52
1:R:171:ILE:HD13	1:R:176:ALA:O	2.09	0.52
4:P:333:LEU:O	4:P:336:THR:OG1	2.26	0.52
2:N:42:ASP:O	2:N:194:ARG:NH2	2.43	0.52
7:T:63:THR:HG23	7:T:64:GLN:N	2.24	0.52
2:N:37:VAL:HG23	2:N:199:ALA:HB2	1.92	0.52
3:B:308:ASP:OD1	3:B:309:VAL:N	2.43	0.52
5:D:37:CYS:SG	12:D:501:HEC:HBB3	2.50	0.52
2:A:42:ASP:O	2:A:194:ARG:NH2	2.43	0.51
1:E:156:TYR:HE2	1:E:180:LEU:HD11	1.71	0.51
2:A:240:GLN:NE2	2:A:242:CYS:SG	2.83	0.51
1:R:135:LEU:HD11	1:R:168:SER:O	2.10	0.51
2:A:37:VAL:HG23	2:A:199:ALA:HB2	1.92	0.51
1:R:140:THR:CG2	1:R:178:LEU:HB3	2.39	0.51
3:O:308:ASP:OD1	3:O:309:VAL:N	2.43	0.51
5:Q:37:CYS:SG	12:Q:501:HEC:HBB3	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:144:THR:O	4:C:148:ASN:ND2	2.44	0.51
5:D:132:THR:O	8:H:21:ARG:NH2	2.44	0.51
1:E:165:TYR:HE1	1:E:171:ILE:CG1	2.22	0.51
1:R:140:THR:HG21	1:R:178:LEU:CB	2.39	0.51
2:N:240:GLN:NE2	2:N:242:CYS:SG	2.83	0.51
4:P:71:ARG:NH2	5:Q:193:ALA:O	2.43	0.51
1:R:49:TYR:OH	9:W:36:ASP:OD1	2.26	0.51
1:R:135:LEU:HD13	1:R:180:LEU:HD12	1.93	0.51
1:R:165:TYR:CE1	1:R:171:ILE:CB	2.94	0.51
4:P:144:THR:O	4:P:148:ASN:ND2	2.44	0.50
4:C:34:GLY:HA3	10:C:502:HEM:HBA2	1.94	0.50
2:A:87:ASN:OD1	2:A:88:ALA:N	2.44	0.50
2:N:4:TYR:CE1	3:O:112:LEU:HD22	2.46	0.50
4:P:97:HIS:NE2	10:P:502:HEM:ND	2.59	0.50
4:C:97:HIS:NE2	10:C:502:HEM:ND	2.60	0.50
2:A:372:THR:OG1	3:B:373:GLU:OE2	2.22	0.49
1:R:140:THR:HG22	1:R:140:THR:O	2.11	0.49
3:O:54:GLY:N	3:O:103:GLU:O	2.44	0.49
2:A:327:ASP:OD1	2:A:328:HIS:N	2.46	0.49
1:E:123:ASP:HA	1:E:170:ARG:HH12	1.77	0.49
1:E:135:LEU:CD1	1:E:169:GLY:HA3	2.43	0.49
1:R:141:HIS:HB2	1:R:177:PRO:CD	2.42	0.49
3:O:46:ARG:NH1	3:O:110:GLU:OE2	2.45	0.49
2:N:366:VAL:HG11	3:O:44:ALA:HB2	1.95	0.49
2:N:435:ASN:O	2:N:439:SER:OG	2.24	0.49
10:P:501:HEM:HBC2	10:P:501:HEM:CMC	2.43	0.49
1:E:140:THR:HG22	1:E:140:THR:O	2.11	0.48
2:N:87:ASN:OD1	2:N:88:ALA:N	2.44	0.48
3:B:46:ARG:NH1	3:B:110:GLU:OE2	2.45	0.48
4:C:176:THR:CG2	4:P:52:ALA:O	2.61	0.48
1:R:140:THR:CB	1:R:178:LEU:HB3	2.43	0.48
1:R:171:ILE:CD1	1:R:176:ALA:CB	2.72	0.48
2:N:372:THR:HG23	3:O:373:GLU:OE2	2.13	0.48
2:A:142:ASP:OD1	2:A:142:ASP:O	2.31	0.48
3:B:168:TYR:OH	3:B:320:GLY:O	2.31	0.48
1:E:189:SER:OG	1:E:191:ASP:OD1	2.21	0.48
2:A:416:TYR:CE2	2:A:417:ASP:OD2	2.67	0.48
1:R:165:TYR:HD1	1:R:171:ILE:HA	1.78	0.48
2:N:34:THR:OG1	3:O:373:GLU:OE1	2.26	0.48
4:C:314:SER:OG	4:C:315:MET:N	2.45	0.48
2:N:327:ASP:OD1	2:N:328:HIS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:168:TYR:OH	3:O:320:GLY:O	2.31	0.48
4:P:58:ASP:OD1	4:P:59:THR:N	2.47	0.48
1:R:123:ASP:OD1	1:R:168:SER:HB3	2.14	0.48
1:R:165:TYR:CE1	1:R:171:ILE:HG13	2.49	0.48
1:E:141:HIS:HB2	1:E:176:ALA:HA	1.95	0.48
3:B:131:GLU:OE1	3:B:133:ARG:NE	2.47	0.48
3:O:131:GLU:OE1	3:O:133:ARG:NE	2.47	0.48
1:R:119:ASP:CG	1:R:178:LEU:CD1	2.83	0.48
1:E:165:TYR:HD1	1:E:171:ILE:HA	1.76	0.47
3:B:272:PHE:CD1	3:B:413:ALA:HB1	2.49	0.47
4:P:314:SER:OG	4:P:315:MET:N	2.45	0.47
5:Q:33:TYR:O	5:Q:38:SER:N	2.46	0.47
7:T:60:THR:CG2	7:T:61:TRP:N	2.77	0.47
1:R:119:ASP:HB3	1:R:179:ASN:OD1	2.14	0.47
3:O:272:PHE:CD1	3:O:413:ALA:HB1	2.49	0.47
5:Q:41:HIS:NE2	12:Q:501:HEC:NC	2.63	0.47
4:C:58:ASP:OD1	4:C:59:THR:N	2.47	0.47
2:N:89:TYR:OH	2:N:377:GLU:OE1	2.22	0.47
4:P:27:ILE:O	4:P:227:LYS:NZ	2.48	0.47
1:R:126:ARG:HE	1:R:170:ARG:HG2	1.79	0.47
4:P:94:LEU:O	4:P:97:HIS:N	2.48	0.47
3:B:54:GLY:N	3:B:103:GLU:O	2.44	0.47
10:C:501:HEM:HBC2	10:C:501:HEM:CMC	2.45	0.47
6:S:52:GLU:OE1	7:T:9:ARG:NH1	2.48	0.46
4:C:27:ILE:O	4:C:227:LYS:NZ	2.48	0.46
4:C:94:LEU:O	4:C:97:HIS:N	2.48	0.46
4:P:206:ASN:OD1	4:P:207:ASN:N	2.45	0.46
6:F:40:ASN:OD1	6:F:41:ASP:N	2.47	0.46
3:O:272:PHE:CE1	3:O:413:ALA:HB1	2.51	0.46
5:Q:110:PRO:HG3	12:Q:501:HEC:HMD3	1.97	0.46
1:R:165:TYR:CD1	1:R:171:ILE:HG13	2.50	0.46
1:R:178:LEU:HG	1:R:179:ASN:N	2.30	0.46
4:C:206:ASN:OD1	4:C:207:ASN:N	2.45	0.46
3:O:76:THR:OG1	3:O:136:GLU:OE2	2.33	0.46
1:E:119:ASP:HB3	1:E:179:ASN:OD1	2.15	0.45
3:B:272:PHE:CE1	3:B:413:ALA:HB1	2.51	0.45
1:R:1:SER:OG	2:N:142:ASP:OD1	2.27	0.45
8:U:53:ASP:OD2	8:U:55:THR:OG1	2.33	0.45
3:B:328:SER:OG	3:B:329:GLN:N	2.50	0.45
5:D:41:HIS:NE2	12:D:501:HEC:NC	2.65	0.45
2:A:140:GLU:O	2:A:143:THR:OG1	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:328:SER:OG	3:O:329:GLN:N	2.50	0.45
4:P:127:ALA:HB1	4:P:273:TYR:OH	2.17	0.45
4:C:127:ALA:HB1	4:C:273:TYR:OH	2.17	0.45
2:N:327:ASP:OD1	2:N:328:HIS:ND1	2.50	0.45
3:B:68:LEU:O	3:B:72:ALA:N	2.50	0.45
1:R:135:LEU:CD1	1:R:169:GLY:HA3	2.47	0.44
2:N:166:SER:OG	2:N:169:GLY:N	2.47	0.44
1:E:58:PHE:O	1:E:61:SER:HB3	2.18	0.44
3:O:37:SER:OG	3:O:211:VAL:O	2.35	0.44
2:A:327:ASP:OD1	2:A:328:HIS:ND1	2.50	0.44
4:C:180:ALA:O	4:C:184:ILE:HG22	2.18	0.44
1:R:156:TYR:CD2	1:R:180:LEU:HD11	2.52	0.44
3:O:68:LEU:O	3:O:72:ALA:N	2.50	0.44
3:B:76:THR:OG1	3:B:136:GLU:OE2	2.33	0.44
5:D:72:ASP:OD2	5:D:83:ARG:NH2	2.50	0.44
5:Q:221:ALA:O	5:Q:225:HIS:N	2.51	0.44
1:E:123:ASP:CA	1:E:170:ARG:HH12	2.31	0.44
8:H:53:ASP:OD2	8:H:55:THR:OG1	2.33	0.44
4:P:186:PRO:HG2	10:P:501:HEM:HMC1	1.99	0.44
3:B:37:SER:OG	3:B:211:VAL:O	2.35	0.44
3:B:65:THR:CG2	3:B:66:SER:H	2.30	0.44
3:B:319:SER:OG	3:B:320:GLY:N	2.51	0.44
4:C:282:ARG:NH1	1:R:142:LEU:HD22	2.33	0.44
1:R:166:ASP:OD1	1:R:170:ARG:N	2.51	0.44
5:Q:72:ASP:OD2	5:Q:83:ARG:NH2	2.50	0.44
5:Q:197:GLU:O	5:Q:201:ARG:N	2.50	0.44
1:E:121:GLN:CG	1:E:126:ARG:NH2	2.78	0.44
2:A:103:SER:HB2	2:A:202:GLY:O	2.18	0.44
4:C:148:ASN:O	4:C:151:SER:HB3	2.18	0.44
5:D:131:LEU:HD11	12:D:501:HEC:HMB1	2.00	0.44
4:C:197:LEU:HD21	10:C:502:HEM:HMA3	2.00	0.44
1:R:58:PHE:O	1:R:61:SER:HB3	2.18	0.44
1:R:119:ASP:OD2	1:R:179:ASN:ND2	2.51	0.44
1:R:121:GLN:HB2	1:R:126:ARG:CZ	2.48	0.43
2:N:103:SER:HB2	2:N:202:GLY:O	2.18	0.43
3:O:319:SER:OG	3:O:320:GLY:N	2.51	0.43
4:C:45:ILE:HA	10:C:501:HEM:HMC3	1.99	0.43
4:P:127:ALA:HB2	10:P:501:HEM:HMB3	2.01	0.43
5:D:221:ALA:O	5:D:225:HIS:N	2.51	0.43
1:R:121:GLN:CB	1:R:126:ARG:CZ	2.96	0.43
4:P:94:LEU:O	4:P:98:VAL:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:148:ASN:O	4:P:151:SER:HB3	2.18	0.43
4:P:45:ILE:HA	10:P:501:HEM:HMC3	1.99	0.43
5:D:163:PRO:HG3	12:D:501:HEC:HAB	2.00	0.43
4:P:180:ALA:O	4:P:184:ILE:HG22	2.18	0.43
2:N:363:ASN:ND2	3:O:93:GLY:O	2.52	0.43
3:O:65:THR:CG2	3:O:66:SER:H	2.30	0.43
6:S:40:ASN:OD1	6:S:41:ASP:N	2.47	0.43
6:S:96:GLU:OE2	6:S:99:ARG:NH2	2.50	0.43
4:P:184:ILE:HG23	4:P:185:LEU:N	2.33	0.43
4:P:197:LEU:HD21	10:P:502:HEM:HMA3	2.01	0.43
4:P:34:GLY:HA3	10:P:502:HEM:HBA2	2.01	0.42
10:P:502:HEM:HBB2	10:P:502:HEM:CMB	2.48	0.42
5:Q:163:PRO:HG3	12:Q:501:HEC:HAB	1.99	0.42
2:A:4:TYR:CE1	3:B:112:LEU:HD22	2.54	0.42
7:T:63:THR:CG2	7:T:64:GLN:N	2.82	0.42
7:G:63:THR:CG2	7:G:64:GLN:N	2.82	0.42
1:E:171:ILE:HD12	1:E:176:ALA:CB	2.35	0.42
4:C:184:ILE:HG23	4:C:185:LEU:N	2.34	0.42
5:D:33:TYR:O	5:D:38:SER:N	2.46	0.42
1:E:165:TYR:CD1	1:E:171:ILE:HG13	2.55	0.42
6:F:96:GLU:OE2	6:F:99:ARG:NH2	2.50	0.42
4:C:23:ALA:O	4:C:218:ILE:N	2.50	0.42
5:D:197:GLU:O	5:D:201:ARG:N	2.50	0.42
2:A:166:SER:OG	2:A:169:GLY:N	2.47	0.42
1:R:141:HIS:N	1:R:177:PRO:HD2	2.35	0.42
3:O:407:ASP:OD1	3:O:408:ALA:N	2.52	0.42
3:B:407:ASP:OD1	3:B:408:ALA:N	2.52	0.41
4:C:176:THR:HB	4:P:53:MET:O	2.20	0.41
12:D:501:HEC:HMC1	12:D:501:HEC:HBC3	2.01	0.41
7:G:37:VAL:O	7:G:41:THR:N	2.53	0.41
1:E:165:TYR:HB3	1:E:170:ARG:O	2.20	0.41
10:C:502:HEM:HBB2	10:C:502:HEM:CMB	2.48	0.41
1:R:141:HIS:CB	1:R:177:PRO:HD3	2.50	0.41
7:T:37:VAL:O	7:T:41:THR:N	2.53	0.41
1:E:165:TYR:CD1	1:E:171:ILE:CB	3.04	0.41
1:R:184:SER:O	1:R:196:GLY:N	2.51	0.41
10:P:502:HEM:HBC2	10:P:502:HEM:CMC	2.47	0.41
5:D:130:LEU:O	5:D:150:ASN:ND2	2.45	0.41
1:E:184:SER:O	1:E:196:GLY:N	2.51	0.41
4:C:118:ILE:O	4:C:122:THR:OG1	2.32	0.41
5:Q:131:LEU:HD11	12:Q:501:HEC:HMB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:89:TYR:OH	2:A:377:GLU:OE1	2.22	0.41
2:N:417:ASP:OD1	2:N:438:ARG:NH2	2.48	0.41
1:E:140:THR:CG2	1:E:177:PRO:HG2	2.50	0.41
1:E:123:ASP:HA	1:E:170:ARG:NH1	2.35	0.40
5:D:110:PRO:HG3	12:D:501:HEC:HMD3	2.02	0.40
7:G:60:THR:HA	7:G:63:THR:HG21	2.02	0.40
12:Q:501:HEC:HBC3	12:Q:501:HEC:HMC1	2.02	0.40
3:O:261:SER:OG	3:O:262:ALA:N	2.54	0.40
2:A:21:ASN:O	2:A:192:ALA:HB3	2.22	0.40
4:C:94:LEU:O	4:C:98:VAL:N	2.46	0.40
1:R:131:GLU:OE1	1:R:131:GLU:N	2.52	0.40
5:Q:128:PHE:O	5:Q:132:THR:OG1	2.15	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	E	168/274 (61%)	155 (92%)	12 (7%)	1 (1%)	25 63
1	R	168/274 (61%)	156 (93%)	12 (7%)	0	100 100
2	A	442/480 (92%)	423 (96%)	19 (4%)	0	100 100
2	N	442/480 (92%)	423 (96%)	19 (4%)	0	100 100
3	B	410/453 (90%)	385 (94%)	25 (6%)	0	100 100
3	O	407/453 (90%)	382 (94%)	25 (6%)	0	100 100
4	C	368/379 (97%)	345 (94%)	23 (6%)	0	100 100
4	P	368/379 (97%)	344 (94%)	24 (6%)	0	100 100
5	D	235/325 (72%)	226 (96%)	9 (4%)	0	100 100
5	Q	235/325 (72%)	226 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	96/111 (86%)	93 (97%)	3 (3%)	0	100	100
6	S	96/111 (86%)	93 (97%)	3 (3%)	0	100	100
7	G	70/82 (85%)	67 (96%)	3 (4%)	0	100	100
7	T	70/82 (85%)	66 (94%)	4 (6%)	0	100	100
8	H	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
8	U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
9	J	56/64 (88%)	54 (96%)	2 (4%)	0	100	100
9	W	55/64 (86%)	54 (98%)	1 (2%)	0	100	100
All	All	3812/4518 (84%)	3616 (95%)	195 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	177	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	150/228 (66%)	149 (99%)	1 (1%)	84	90
1	R	147/228 (64%)	146 (99%)	1 (1%)	84	90
2	A	368/394 (93%)	368 (100%)	0	100	100
2	N	368/394 (93%)	368 (100%)	0	100	100
3	B	326/355 (92%)	325 (100%)	1 (0%)	92	95
3	O	324/355 (91%)	323 (100%)	1 (0%)	92	95
4	C	318/327 (97%)	315 (99%)	3 (1%)	78	87
4	P	318/327 (97%)	315 (99%)	3 (1%)	78	87
5	D	202/257 (79%)	202 (100%)	0	100	100
5	Q	202/257 (79%)	202 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	90/99 (91%)	89 (99%)	1 (1%)	73 84
6	S	90/99 (91%)	89 (99%)	1 (1%)	73 84
7	G	65/72 (90%)	65 (100%)	0	100 100
7	T	65/72 (90%)	65 (100%)	0	100 100
8	H	62/85 (73%)	62 (100%)	0	100 100
8	U	62/85 (73%)	62 (100%)	0	100 100
9	J	49/54 (91%)	49 (100%)	0	100 100
9	W	48/54 (89%)	48 (100%)	0	100 100
All	All	3254/3742 (87%)	3242 (100%)	12 (0%)	91 94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	136	ILE
3	B	321	LEU
4	C	124	MET
4	C	316	MET
4	C	357	LEU
6	F	94	LEU
1	R	136	ILE
3	O	321	LEU
4	P	124	MET
4	P	316	MET
4	P	357	LEU
6	S	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	179	ASN
3	B	125	ASN
1	R	179	ASN
3	O	125	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	DY2	P	503	-	34,34,34	1.23	2 (5%)	50,50,50	1.29	6 (12%)
10	HEM	P	502	4	41,50,50	1.54	4 (9%)	45,82,82	1.24	5 (11%)
10	HEM	C	501	4	41,50,50	1.63	5 (12%)	45,82,82	1.35	7 (15%)
10	HEM	C	502	4	41,50,50	1.54	4 (9%)	45,82,82	1.28	5 (11%)
12	HEC	Q	501	5	32,50,50	2.27	3 (9%)	24,82,82	1.41	3 (12%)
10	HEM	P	501	4	41,50,50	1.68	4 (9%)	45,82,82	1.42	8 (17%)
12	HEC	D	501	5	32,50,50	2.27	3 (9%)	24,82,82	1.41	3 (12%)
11	DY2	C	503	-	34,34,34	1.22	2 (5%)	50,50,50	1.32	7 (14%)

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
11	DY2	P	503	-	-	6/15/15/15	0/4/4/4
10	HEM	P	502	4	-	3/12/54/54	-
10	HEM	C	501	4	-	4/12/54/54	-
10	HEM	C	502	4	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEC	Q	501	5	-	5/10/54/54	-
10	HEM	P	501	4	-	4/12/54/54	-
12	HEC	D	501	5	-	4/10/54/54	-
11	DY2	C	503	-	-	6/15/15/15	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Q	501	HEC	C3C-C2C	-7.03	1.33	1.40
12	D	501	HEC	C2B-C3B	-6.97	1.33	1.40
12	D	501	HEC	C3C-C2C	-6.94	1.33	1.40
12	Q	501	HEC	C2B-C3B	-6.88	1.33	1.40
10	P	501	HEM	C3C-C2C	-5.69	1.32	1.40
10	C	501	HEM	C3C-C2C	-5.59	1.32	1.40
12	Q	501	HEC	C3D-C2D	5.25	1.53	1.37
12	D	501	HEC	C3D-C2D	5.24	1.53	1.37
10	C	502	HEM	C3C-C2C	-4.94	1.33	1.40
10	P	502	HEM	C3C-C2C	-4.91	1.33	1.40
10	P	501	HEM	FE-ND	4.59	2.19	1.96
11	P	503	DY2	C5-C4	-4.50	1.35	1.42
11	C	503	DY2	C5-C4	-4.43	1.35	1.42
10	C	501	HEM	FE-ND	3.97	2.16	1.96
10	P	502	HEM	FE-ND	3.41	2.13	1.96
10	C	502	HEM	FE-ND	3.34	2.13	1.96
10	P	502	HEM	C3C-CAC	3.21	1.54	1.47
10	C	502	HEM	C3C-CAC	3.20	1.54	1.47
11	P	503	DY2	C10-C7	3.08	1.52	1.49
11	C	503	DY2	C10-C7	3.03	1.52	1.49
10	C	501	HEM	C3C-CAC	2.89	1.53	1.47
10	P	501	HEM	C3C-CAC	2.89	1.53	1.47
10	C	502	HEM	CAB-C3B	2.69	1.54	1.47
10	P	502	HEM	CAB-C3B	2.65	1.54	1.47
10	C	501	HEM	CAB-C3B	2.65	1.54	1.47
10	P	501	HEM	CAB-C3B	2.64	1.54	1.47
10	C	501	HEM	C3D-C2D	-2.08	1.32	1.36

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	501	HEM	C1B-NB-C4B	3.32	108.50	105.07
11	P	503	DY2	C8-C7-N	-3.26	120.04	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	501	HEM	C1B-NB-C4B	3.14	108.32	105.07
11	C	503	DY2	C8-C7-N	-3.12	120.18	123.23
11	C	503	DY2	C13-N1-C12	3.05	121.64	117.48
11	P	503	DY2	C13-N1-C12	3.04	121.63	117.48
10	P	501	HEM	CAD-CBD-CGD	-2.87	107.43	113.60
11	P	503	DY2	C11-O1-C2	-2.71	111.64	117.51
10	P	502	HEM	CBA-CAA-C2A	-2.69	108.02	112.62
10	C	501	HEM	C4B-CHC-C1C	2.66	126.07	122.56
10	C	502	HEM	CBA-CAA-C2A	-2.65	108.11	112.62
11	C	503	DY2	C11-O1-C2	-2.62	111.82	117.51
12	Q	501	HEC	CMB-C2B-C1B	-2.60	124.47	128.46
12	D	501	HEC	CMB-C2B-C1B	-2.60	124.47	128.46
10	C	501	HEM	CAD-CBD-CGD	-2.56	108.10	113.60
11	P	503	DY2	C7-N-C4	2.54	122.43	117.27
10	P	501	HEM	C4B-CHC-C1C	2.51	125.88	122.56
10	P	501	HEM	CHC-C4B-C3B	2.49	128.38	124.57
10	C	502	HEM	CMC-C2C-C3C	2.47	129.29	124.68
11	C	503	DY2	C-C5-C4	2.46	121.08	118.33
11	C	503	DY2	C7-N-C4	2.43	122.21	117.27
10	P	501	HEM	CMC-C2C-C3C	2.42	129.20	124.68
11	P	503	DY2	C-C5-C4	2.39	121.00	118.33
10	C	501	HEM	CHC-C4B-C3B	2.38	128.22	124.57
10	P	502	HEM	CMC-C2C-C3C	2.37	129.11	124.68
12	Q	501	HEC	C1D-C2D-C3D	-2.33	105.38	107.00
12	D	501	HEC	C1D-C2D-C3D	-2.26	105.42	107.00
10	C	501	HEM	C3B-C2B-C1B	2.26	108.16	106.49
10	C	502	HEM	CAD-CBD-CGD	-2.24	108.78	113.60
10	C	502	HEM	C1B-NB-C4B	2.24	107.38	105.07
10	P	502	HEM	CAD-CBD-CGD	-2.21	108.86	113.60
10	P	501	HEM	C3B-C2B-C1B	2.18	108.11	106.49
11	C	503	DY2	C15-C10-C12	2.17	119.26	117.11
11	C	503	DY2	C21-C16-C14	-2.15	117.63	121.36
10	C	502	HEM	CHD-C1D-C2D	2.14	128.32	124.98
10	P	502	HEM	C1B-NB-C4B	2.13	107.27	105.07
12	Q	501	HEC	CMC-C2C-C1C	-2.08	125.27	128.46
11	P	503	DY2	C15-C10-C12	2.06	119.15	117.11
10	C	501	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
12	D	501	HEC	CMC-C2C-C1C	-2.03	125.35	128.46
10	P	501	HEM	CMA-C3A-C4A	-2.02	125.36	128.46
10	P	501	HEM	C4A-C3A-C2A	2.01	108.40	107.00
10	C	501	HEM	C4A-C3A-C2A	2.01	108.39	107.00
10	P	502	HEM	CHD-C1D-C2D	2.00	128.11	124.98

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	501	HEM	C1A-C2A-CAA-CBA
11	C	503	DY2	C12-C10-C7-N
11	C	503	DY2	F-C22-O2-C19
11	C	503	DY2	F2-C22-O2-C19
11	P	503	DY2	F2-C22-O2-C19
12	D	501	HEC	C2D-C3D-CAD-CBD
12	D	501	HEC	C4D-C3D-CAD-CBD
12	Q	501	HEC	C2D-C3D-CAD-CBD
12	Q	501	HEC	C4D-C3D-CAD-CBD
11	P	503	DY2	C3-C2-O1-C11
11	C	503	DY2	C3-C2-O1-C11
11	C	503	DY2	C1-C2-O1-C11
11	P	503	DY2	C1-C2-O1-C11
11	P	503	DY2	F-C22-O2-C19
11	P	503	DY2	C12-C10-C7-N
11	C	503	DY2	F1-C22-O2-C19
11	P	503	DY2	F1-C22-O2-C19
10	C	501	HEM	C3D-CAD-CBD-CGD
10	P	501	HEM	C3D-CAD-CBD-CGD
10	C	501	HEM	C4B-C3B-CAB-CBB
10	C	501	HEM	C3A-C2A-CAA-CBA
10	P	501	HEM	C1A-C2A-CAA-CBA
10	P	501	HEM	C3A-C2A-CAA-CBA
12	Q	501	HEC	CAD-CBD-CGD-O2D
12	D	501	HEC	CAD-CBD-CGD-O2D
12	Q	501	HEC	CAD-CBD-CGD-O1D
12	D	501	HEC	CAD-CBD-CGD-O1D
10	P	502	HEM	CAA-CBA-CGA-O1A
10	C	502	HEM	CAA-CBA-CGA-O1A
10	P	501	HEM	C4B-C3B-CAB-CBB
10	C	502	HEM	CAA-CBA-CGA-O2A
10	P	502	HEM	CAA-CBA-CGA-O2A
10	P	502	HEM	C2D-C3D-CAD-CBD
12	Q	501	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

6 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	P	502	HEM	9	0

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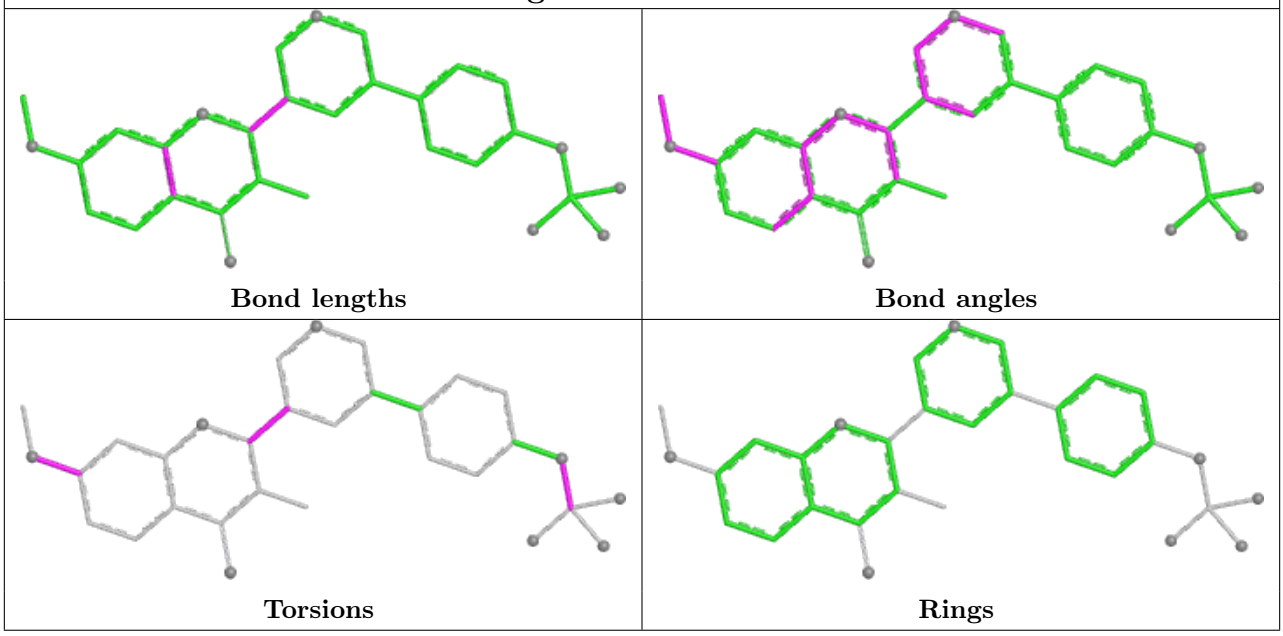
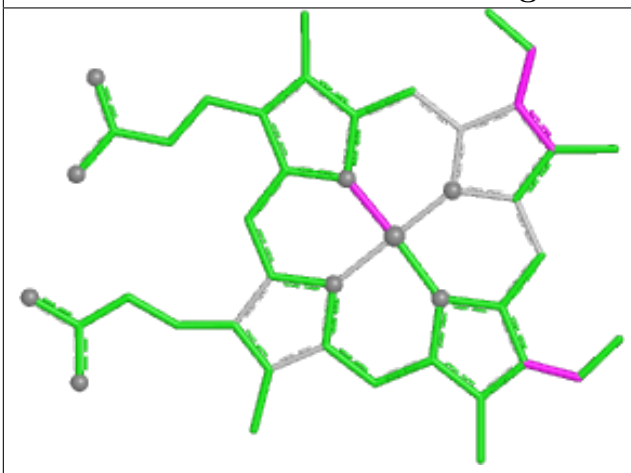
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	501	HEM	7	0
10	C	502	HEM	8	0
12	Q	501	HEC	10	0
10	P	501	HEM	8	0
12	D	501	HEC	10	0

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.

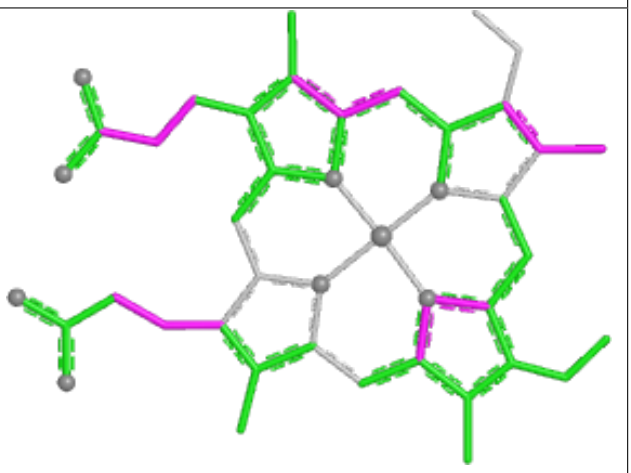
Ligand DY2 P 503



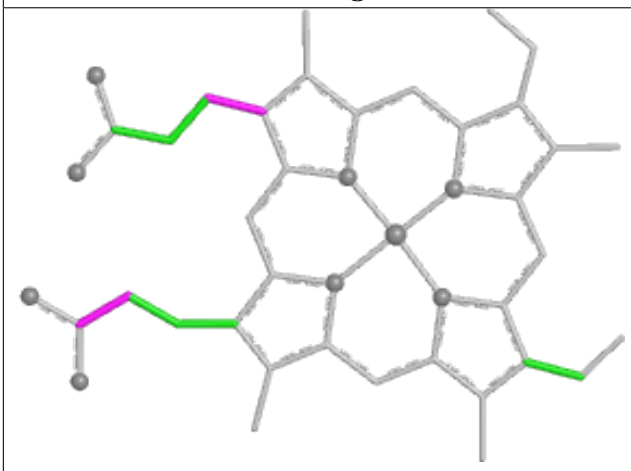
Ligand HEM P 502



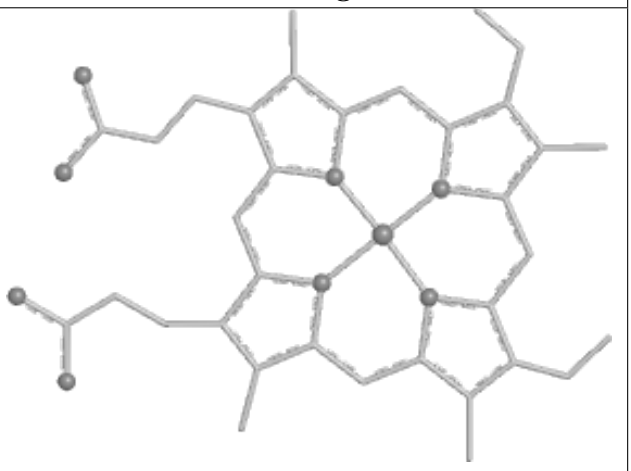
Bond lengths



Bond angles

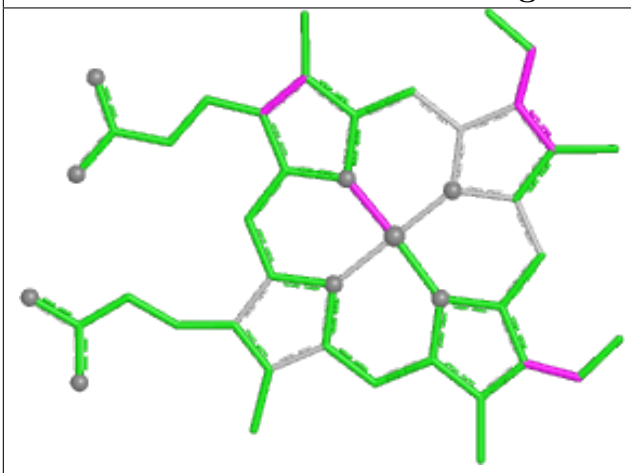


Torsions

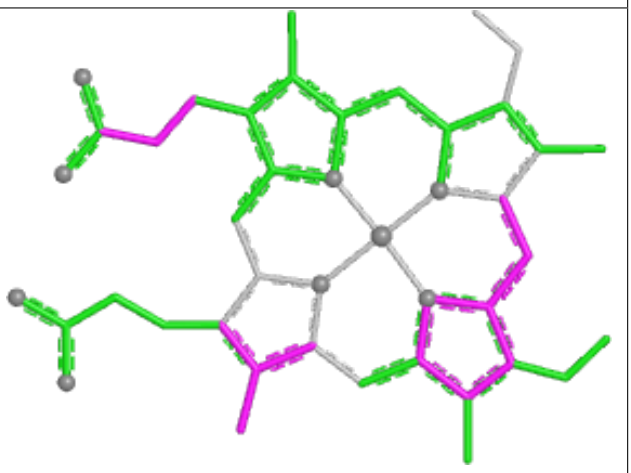


Rings

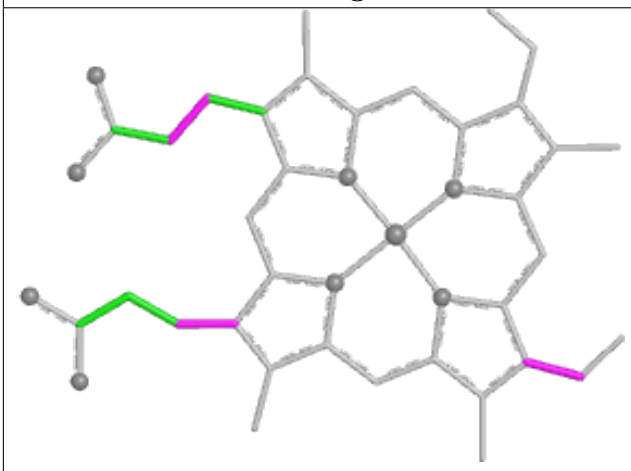
Ligand HEM C 501



Bond lengths



Bond angles



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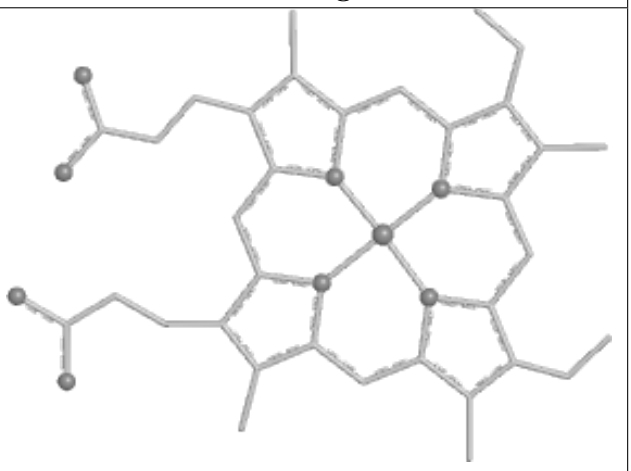
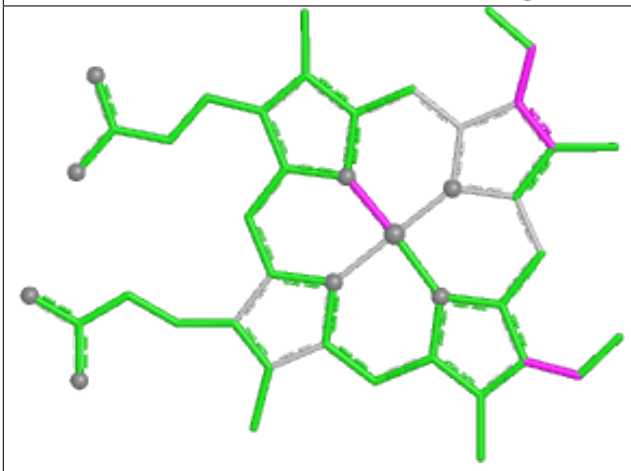
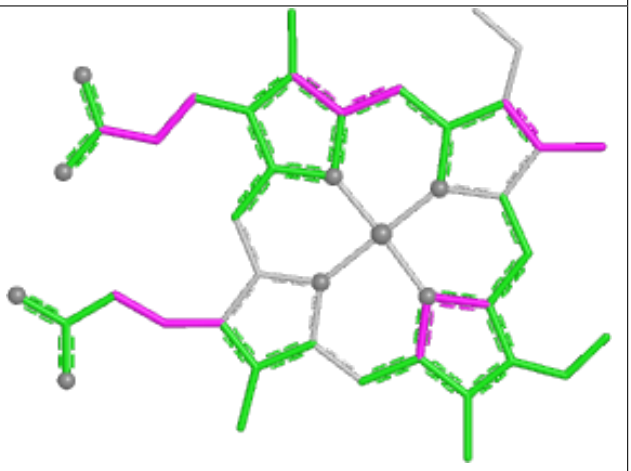


Rings

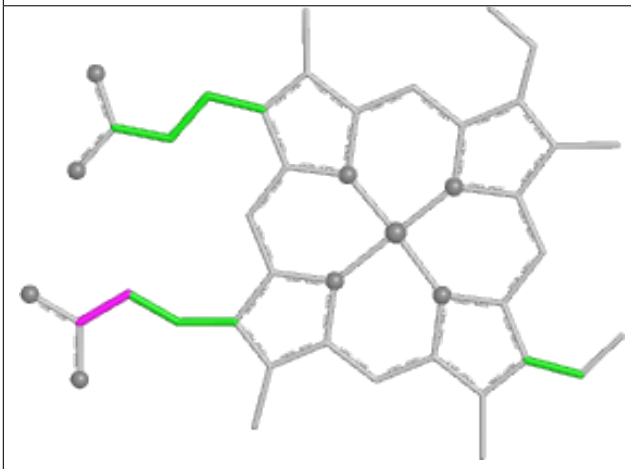
Ligand HEM C 502



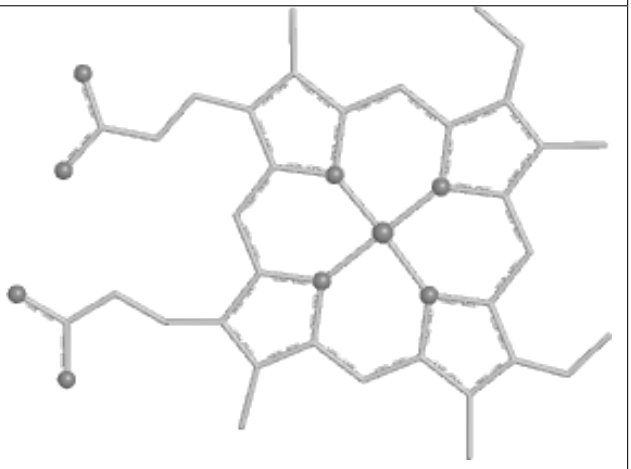
Bond lengths



Bond angles

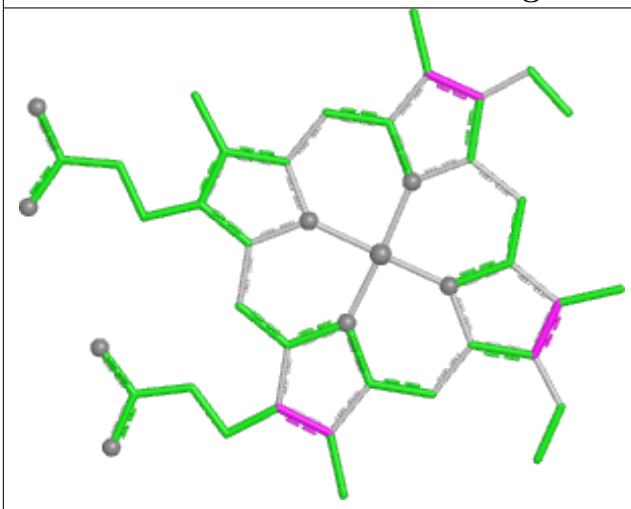


Torsions

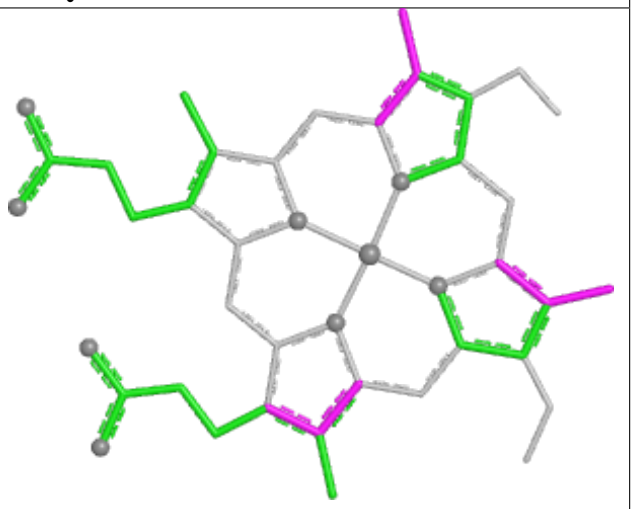


Rings

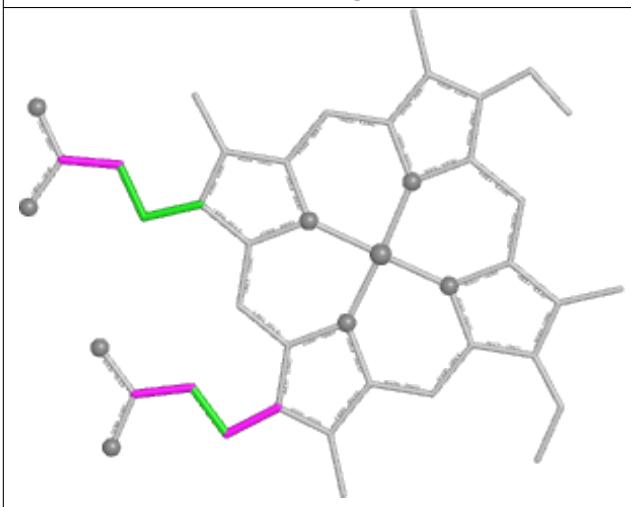
Ligand HEC Q 501



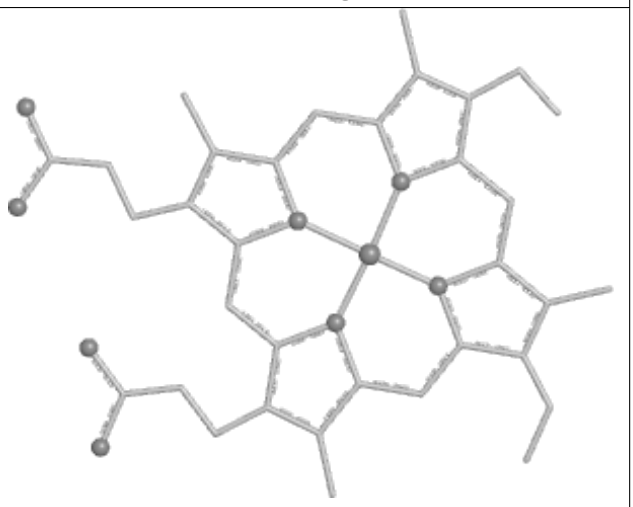
Bond lengths



Bond angles

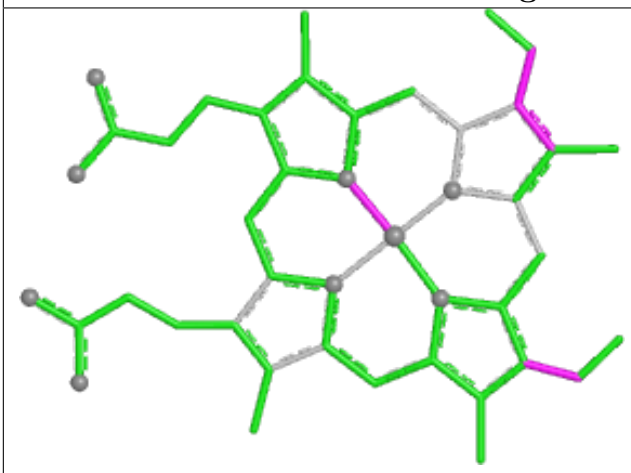


Torsions

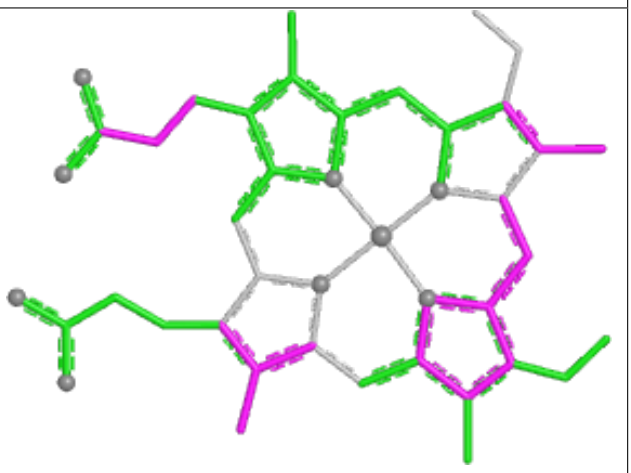


Rings

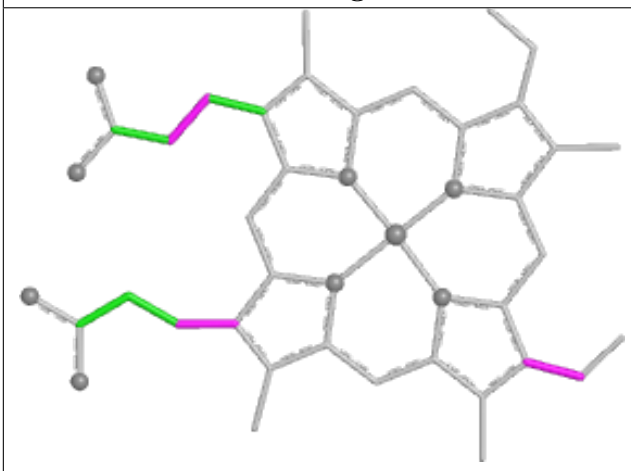
Ligand HEM P 501



Bond lengths



Bond angles



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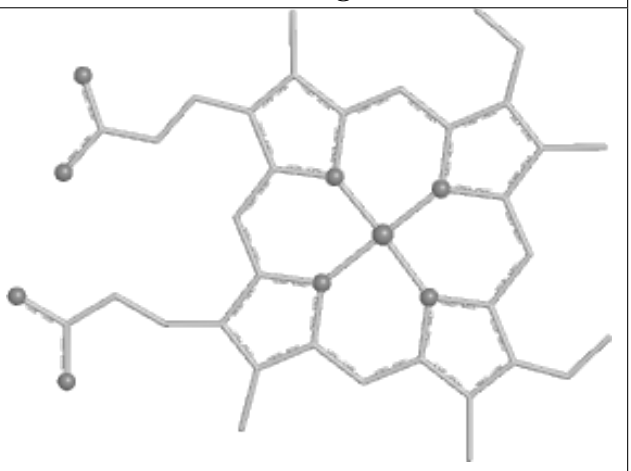
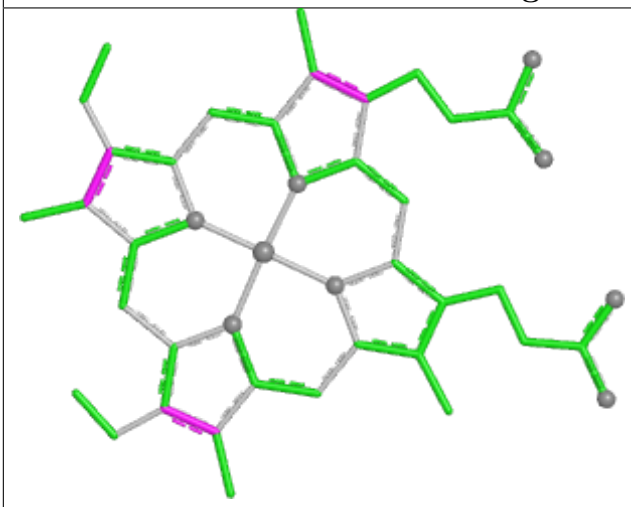


Rings

Ligand HEC D 501



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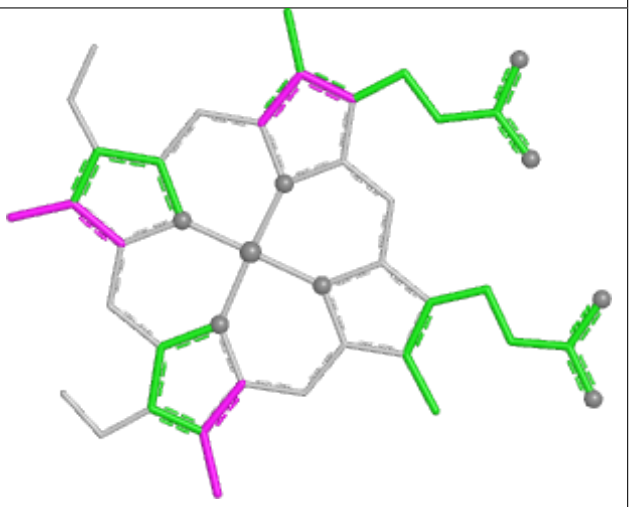
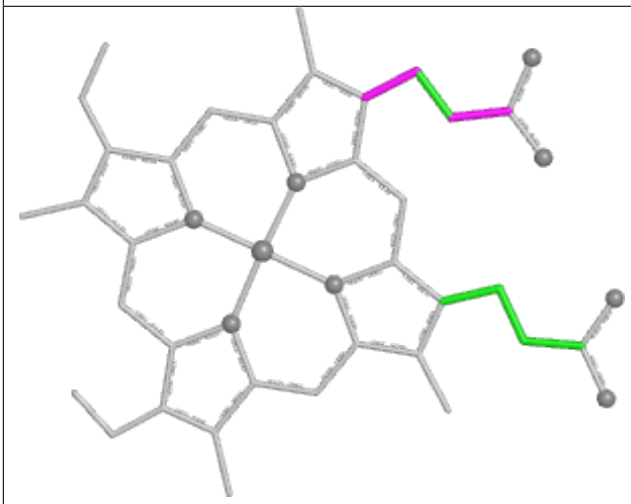


Bond angles



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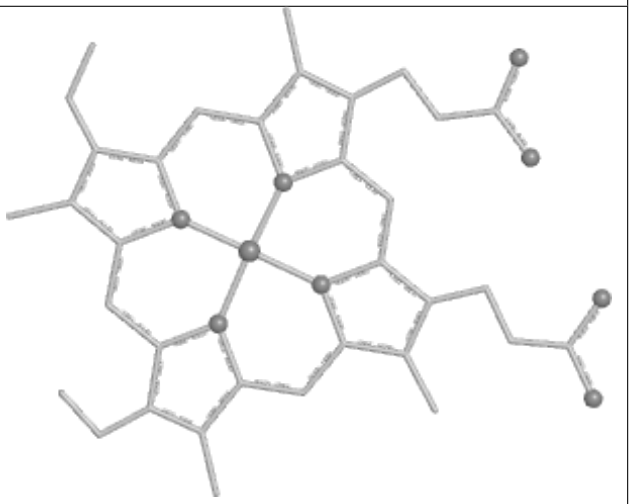
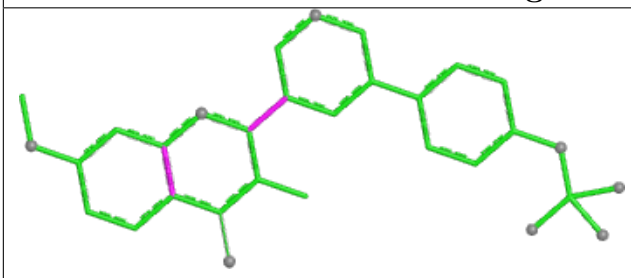
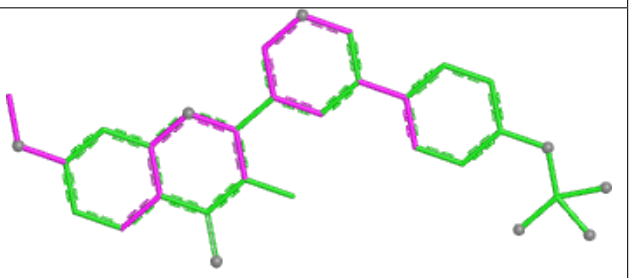


Rings

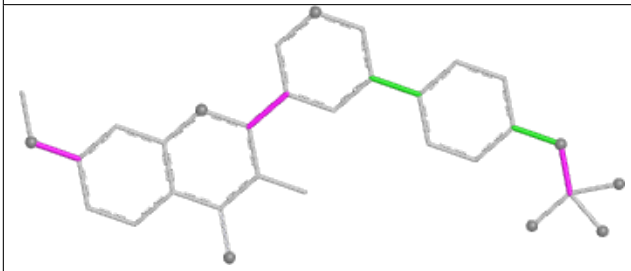
Ligand DY2 C 503



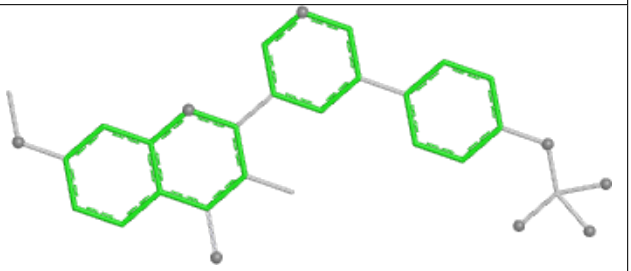
Bond lengths



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.

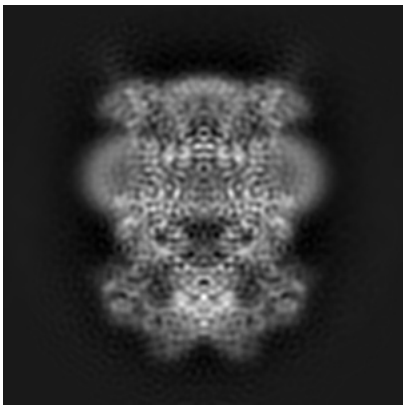
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4292. These allow visual inspection of the internal detail of the map and identification of artifacts.

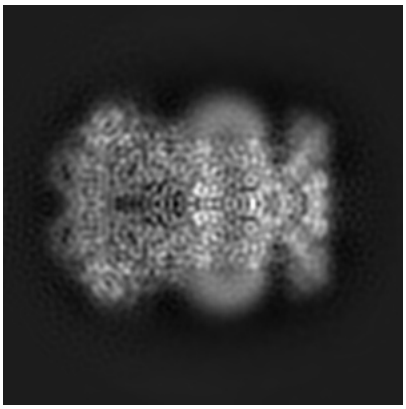
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

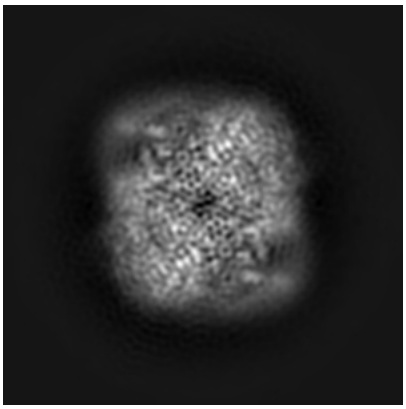
6.1.1 Primary map



X



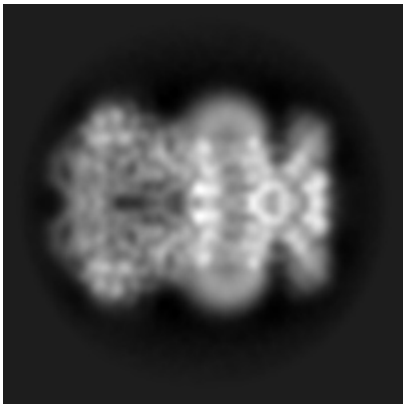
Y



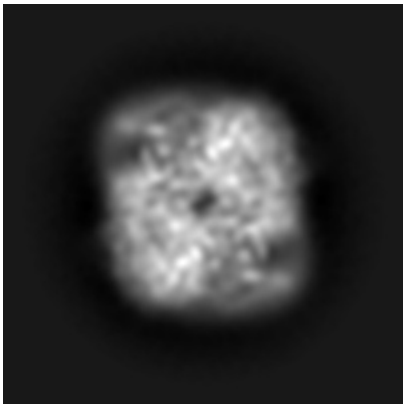
Z

6.1.2 Raw map

X



Y

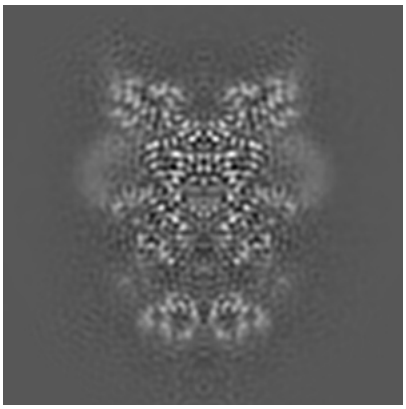


Z

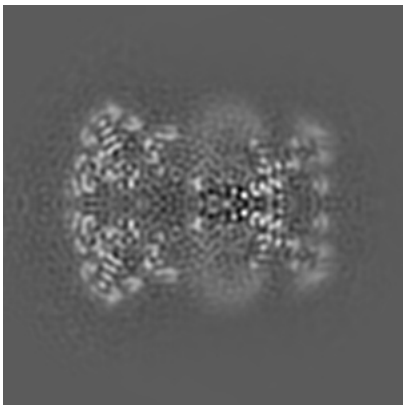
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

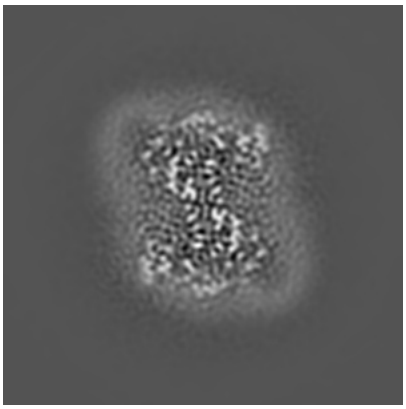
6.2.1 Primary map



X Index: 100

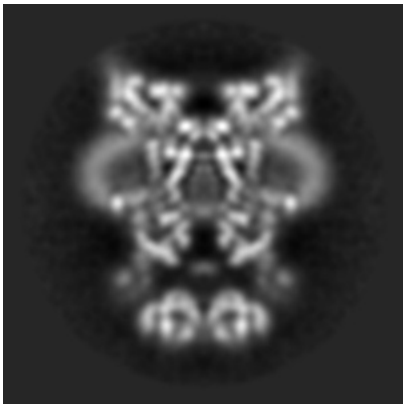


Y Index: 100

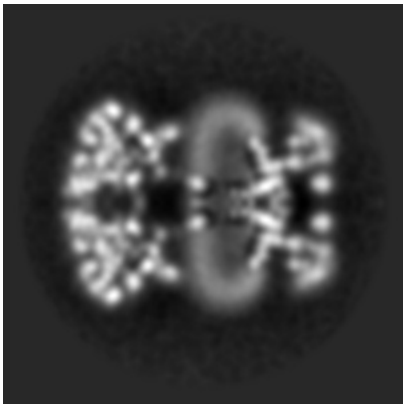


Z Index: 100

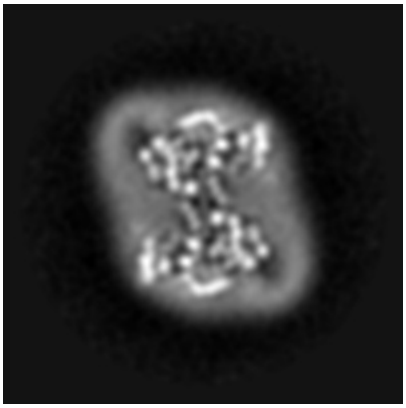
6.2.2 Raw map



X Index: 100



Y Index: 100

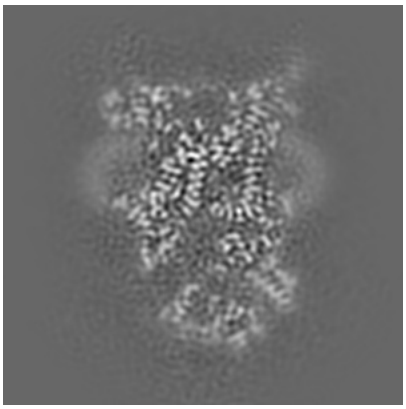


Z Index: 100

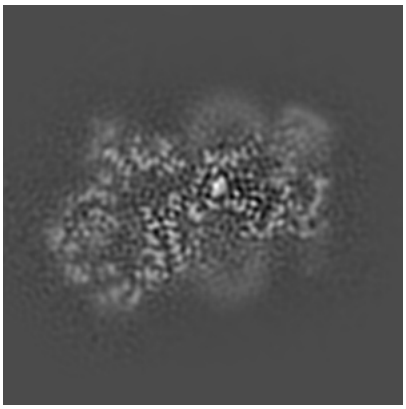
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

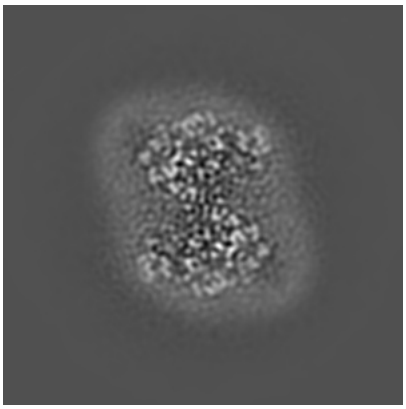
6.3.1 Primary map



X Index: 105



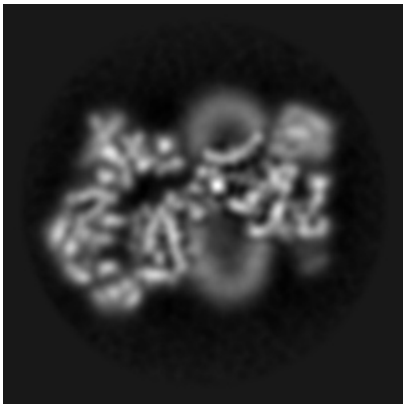
Y Index: 87



Z Index: 101

6.3.2 Raw map

X Index: 93



Y Index: 88

Z Index: 49

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

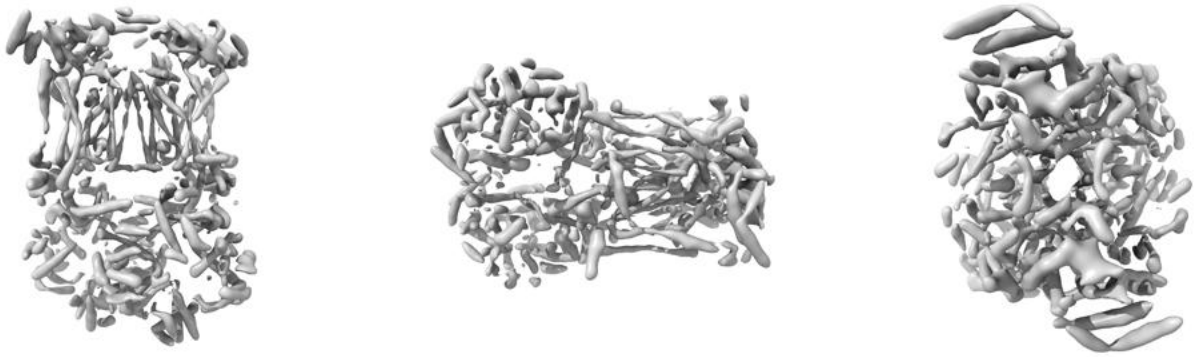
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.173. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

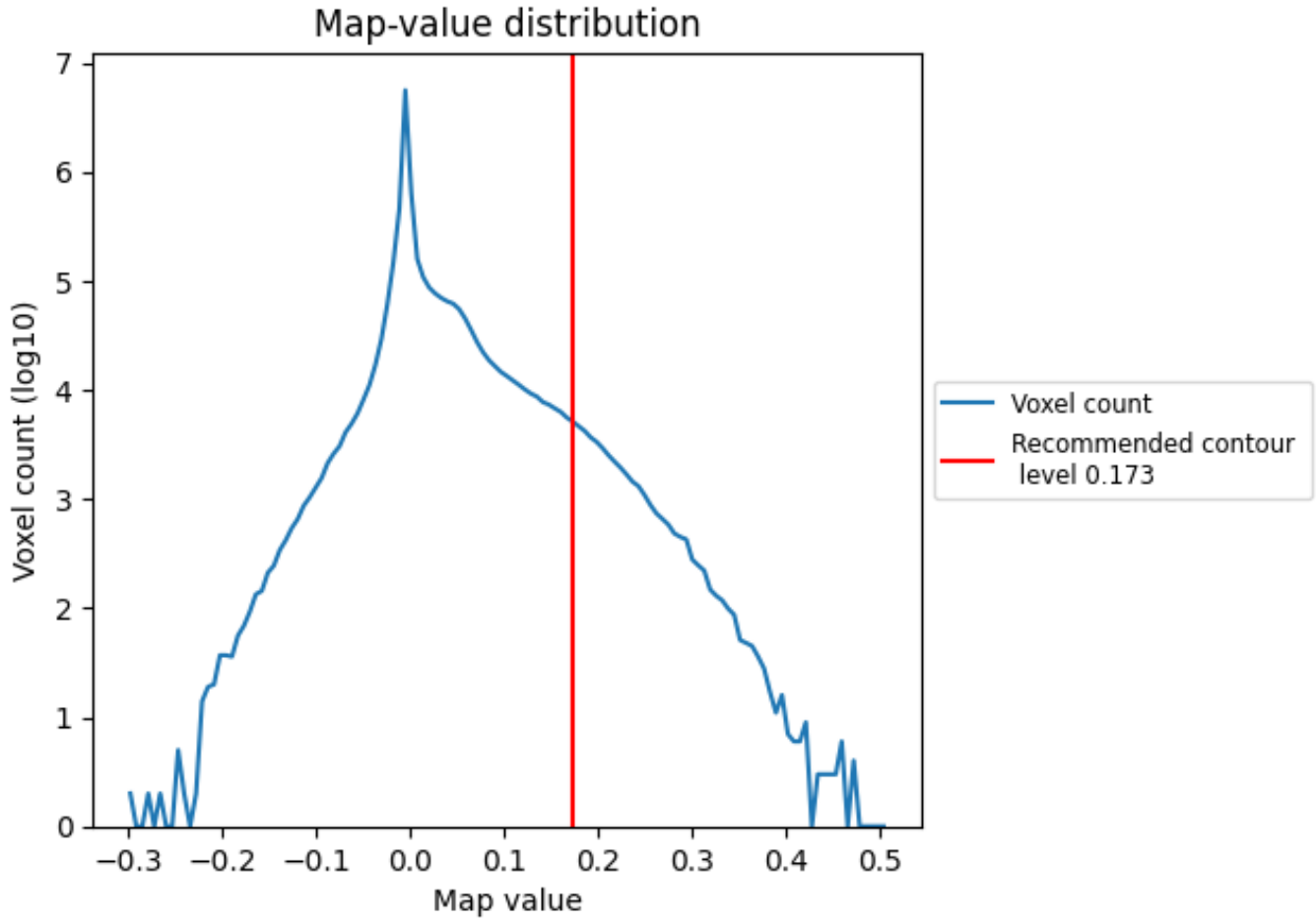
6.5 Mask visualisation (i)

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

7 Map analysis

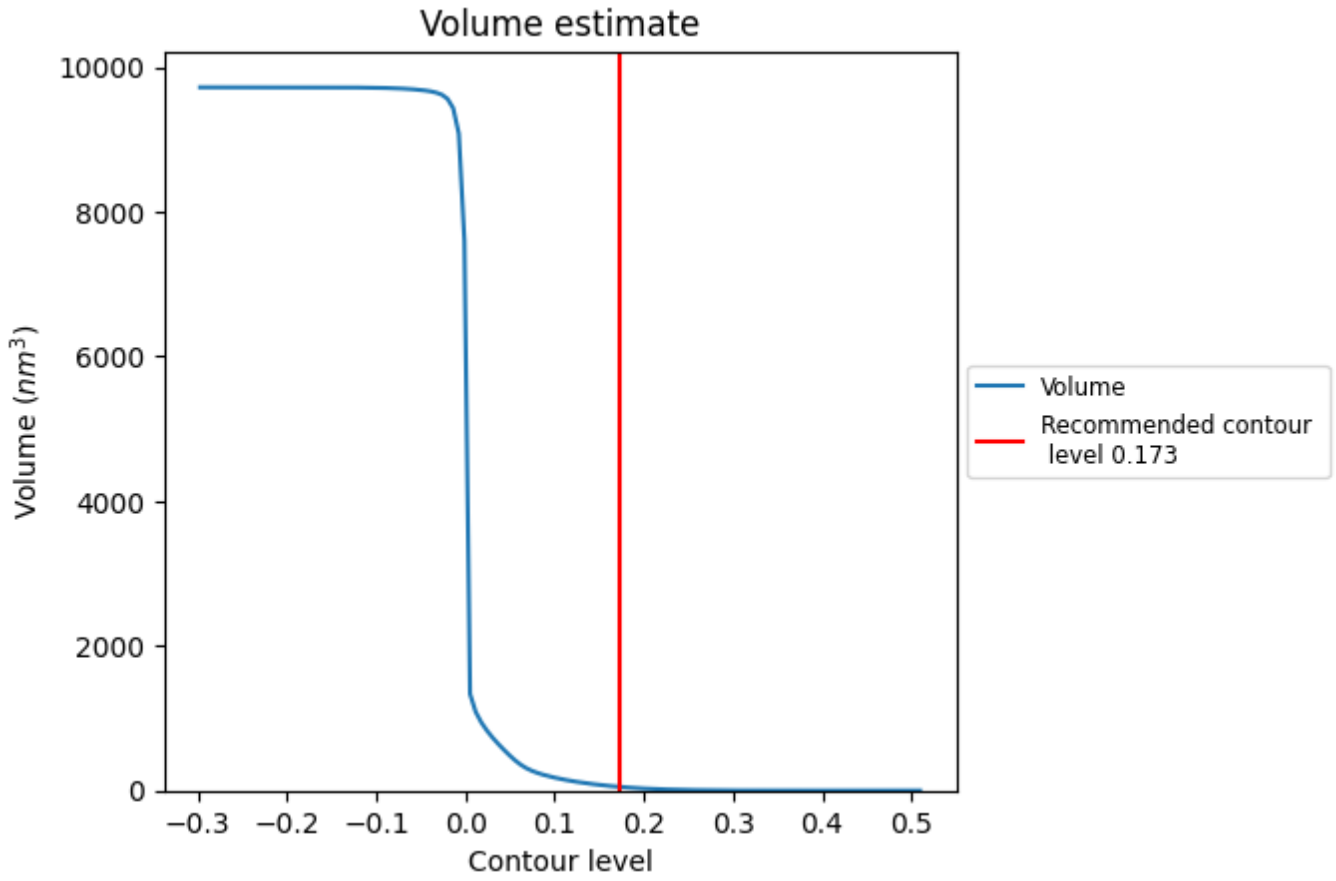
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

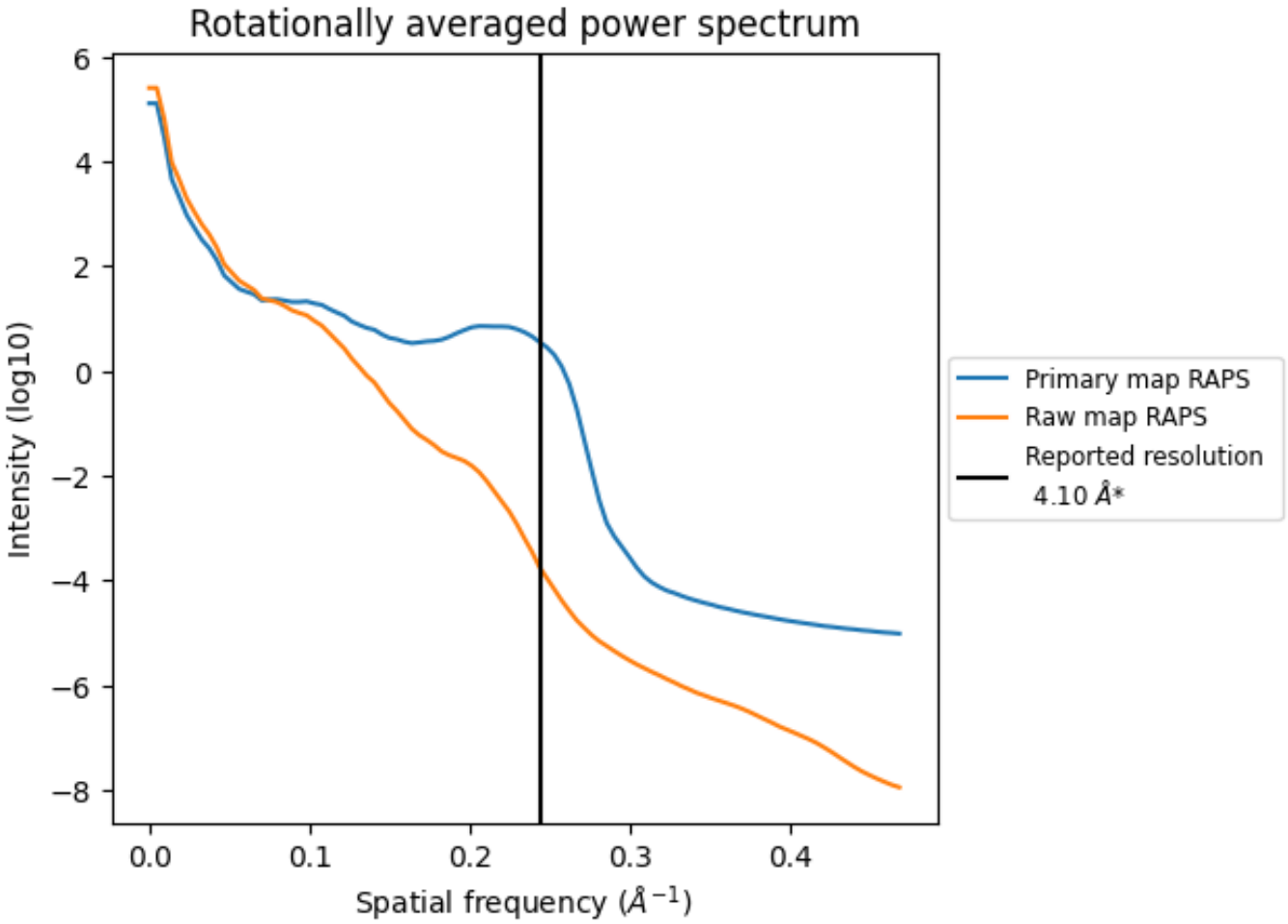
7.2 Volume estimate



The volume at the recommended contour level is 51 nm^3; this corresponds to an approximate mass of 46 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)

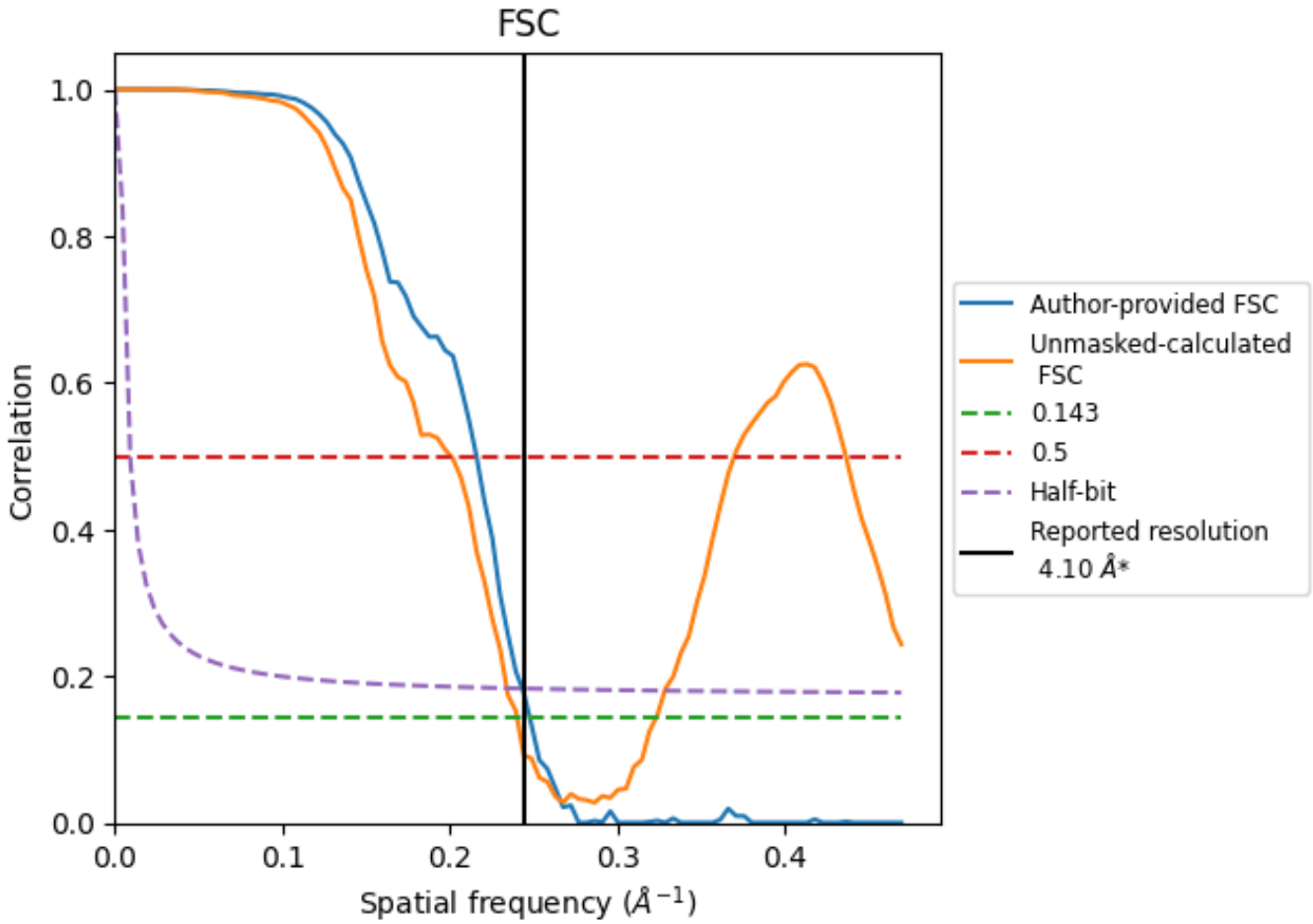


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

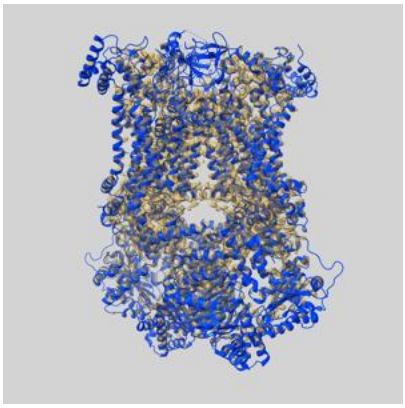
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.04	4.63	4.11
Unmasked-calculated*	4.16	4.99	4.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

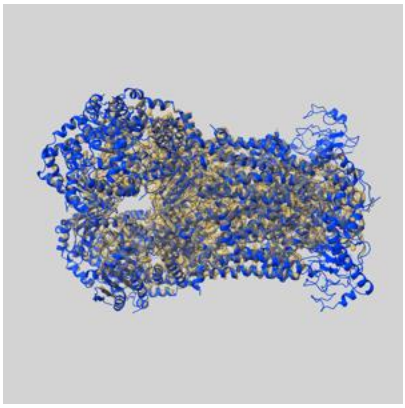
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4292 and PDB model 6FO6. Per-residue inclusion information can be found in section 3 on page 8.

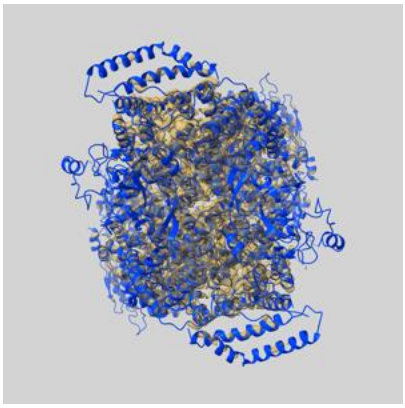
9.1 Map-model overlay



X



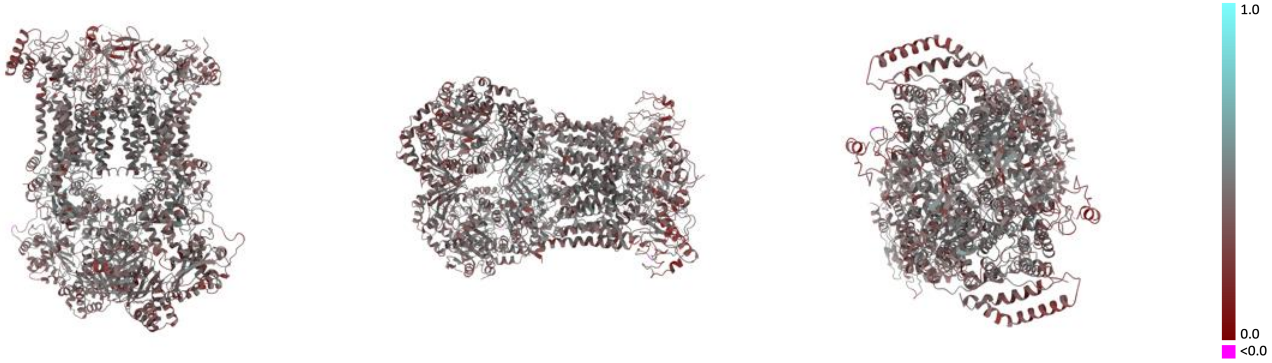
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.173 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.

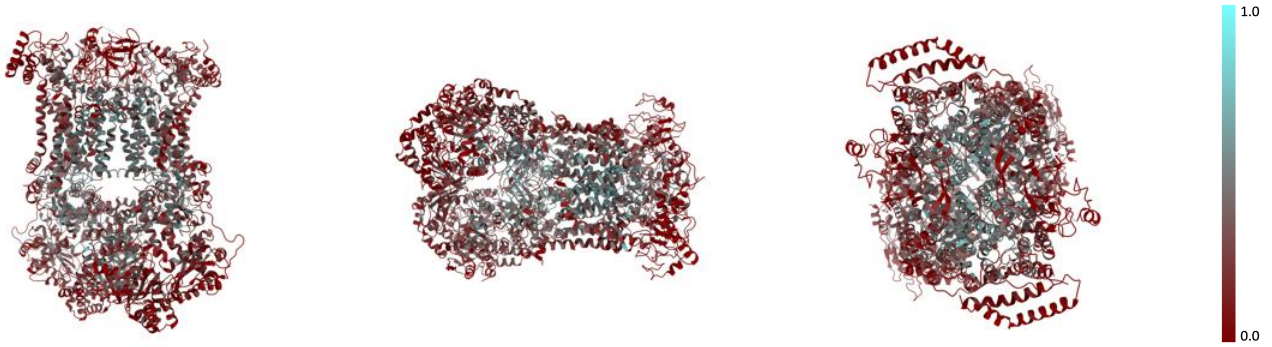
9.2 Q-score mapped to coordinate model (i)



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.

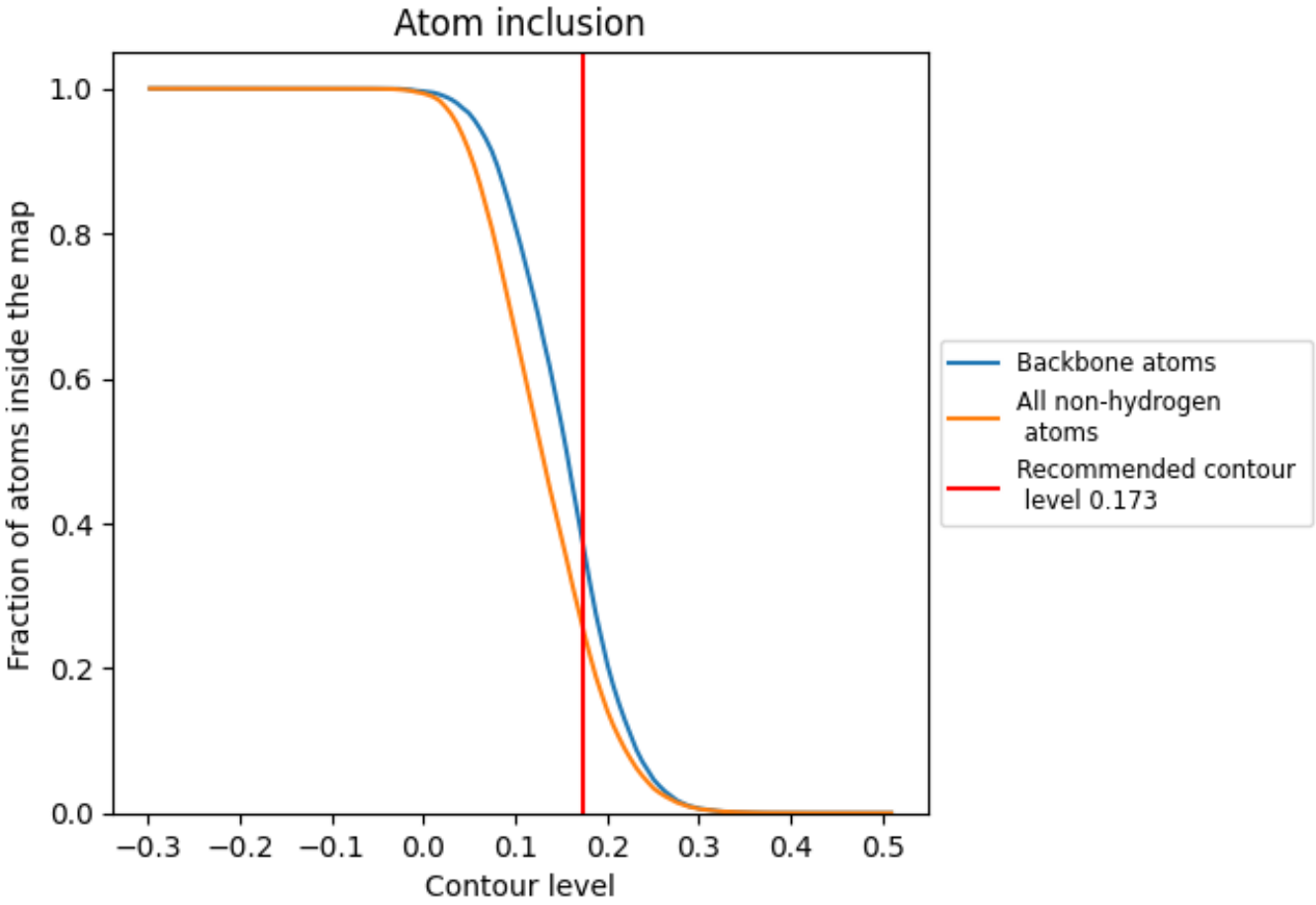
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.173).

9.4 Atom inclusion (i)



At the recommended contour level, 38% of all backbone atoms, 26% 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 (0.173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2603	0.4050
A	0.2563	0.4090
B	0.2001	0.4050
C	0.4346	0.4370
D	0.2524	0.4070
E	0.1226	0.3630
F	0.3478	0.4140
G	0.2615	0.4120
H	0.0193	0.3120
J	0.1617	0.3790
N	0.2486	0.4050
O	0.1986	0.4000
P	0.4309	0.4400
Q	0.2641	0.4050
R	0.1108	0.3650
S	0.3237	0.4150
T	0.2632	0.4070
U	0.0193	0.3090
W	0.1475	0.3910