Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 01:46 PM EST

PDB ID	:	8D4T
EMDB ID	:	EMD-27196
Title	:	Mammalian CIV with GDN bound
Authors	:	Di Trani, J.; Rubinstein, J.
Deposited on	:	2022-06-02
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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

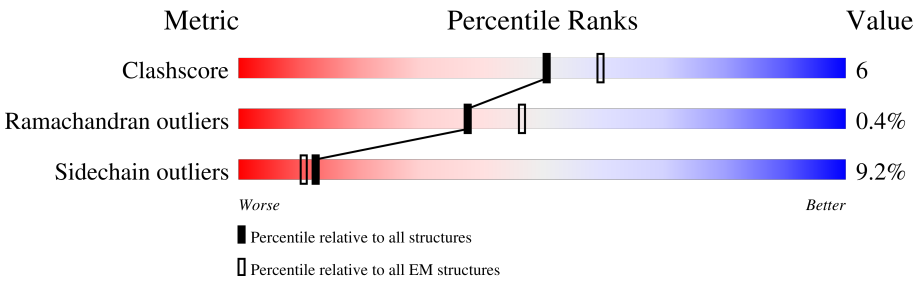
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 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)
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	N	513	81% 18% •
2	O	227	5% 69% 26% •
3	P	258	• 91% 8% •
4	Q	137	• 82% 17% •
5	R	102	• 75% 23% •
6	S	91	• 81% 16% •
7	T	72	17% 76% 21% •
8	U	78	12% 77% 19% •

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Mol	Chain	Length	Quality of chain
9	V	70	77% 17% 6%
10	W	55	93% 5%
11	X	47	87% 11%
12	Y	46	67% 28%
13	M	43	28% 88% 12%

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
17	HEA	N	604	X	-	-	-
17	HEA	N	605	X	-	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 28177 atoms, of which 13913 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	N	512	7982	2676	3977	620	674	35	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	O	227	3657	1185	1833	281	340	18	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	P	258	4117	1406	2017	333	349	12	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	Q	137	2264	744	1123	187	206	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	R	102	1641	527	816	138	158	2	0	0

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	S	91	1381	436	681	124	135	5	0	0

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	T	72	1164	387	569	113	94	1	0	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	U	78	1263	411	610	119	118	5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	V	70	1172	378	592	104	94	4	0	0

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	W	55	866	280	432	72	79	3	0	0

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	X	47	726	242	354	63	65	2	0	0

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	Y	46	760	254	380	64	60	2	0	0

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	M	43	681	222	346	55	56	2	0	0

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
14	N	1	1	1	0
			Total	Cu	
14	O	2	2	2	0

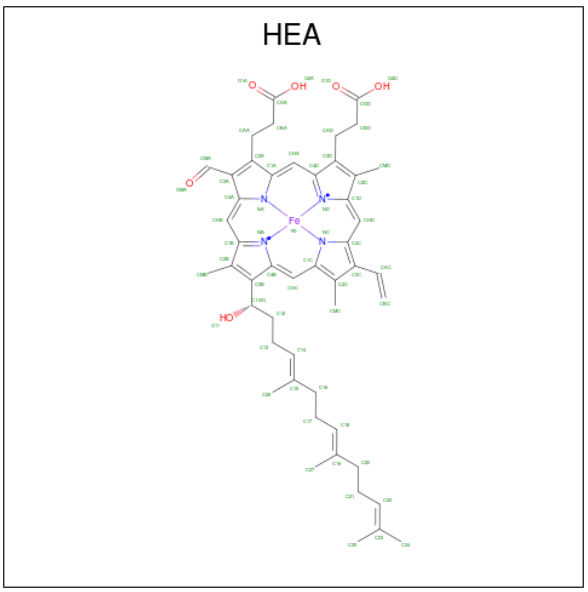
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
15	N	1	1	1	0

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
16	N	1	1	1	0

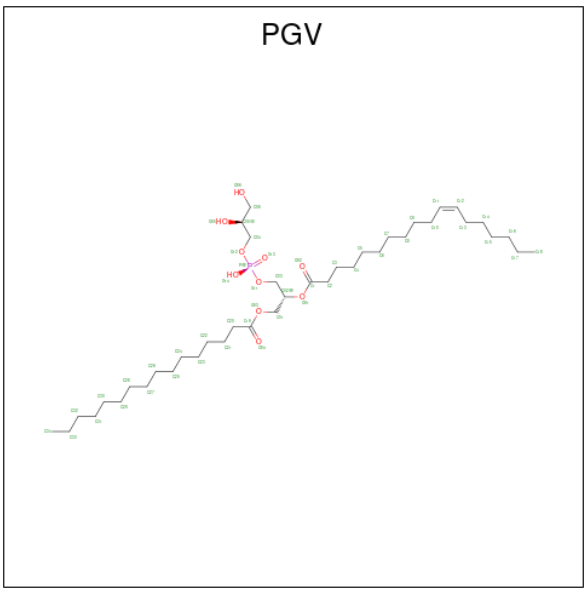
- Molecule 17 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
17	N	1	228	98	2	108	8	12	0
			Total	C	Fe	H	N	O	
17	N	1	228	98	2	108	8	12	0

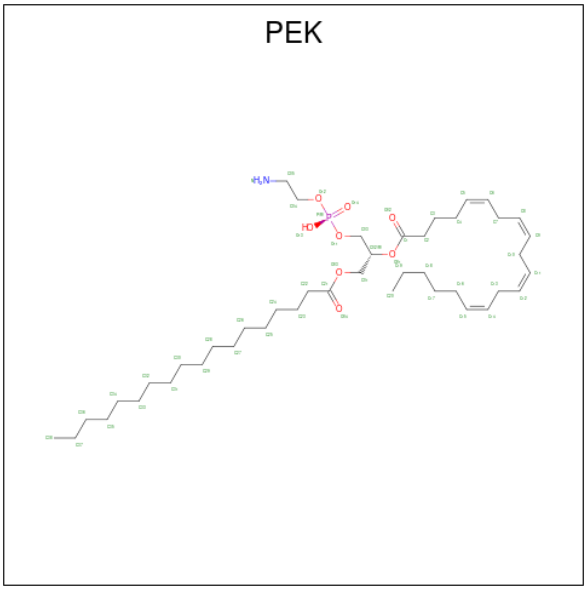
- Molecule 18 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE

(three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



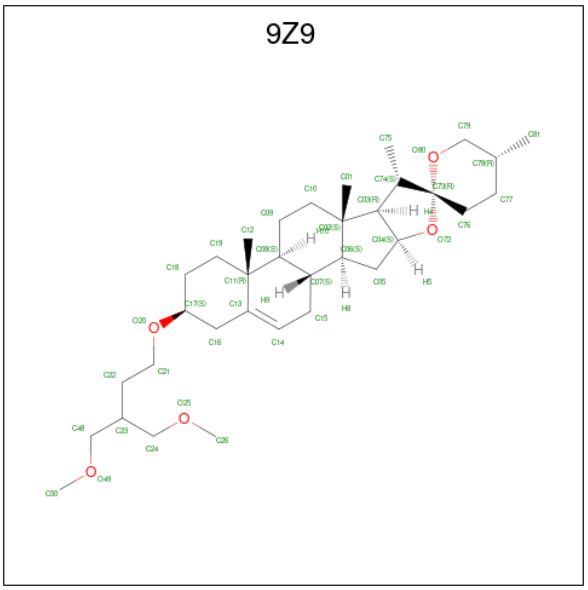
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	N	1	51	40	10	1	0
			Total	C	O	P	
18	P	1	51	40	10	1	0

- Molecule 19 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
19	P	1	128	43	75	1	8	1	0

- Molecule 20 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: $C_{34}H_{56}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	P	1	39	34	5	0

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

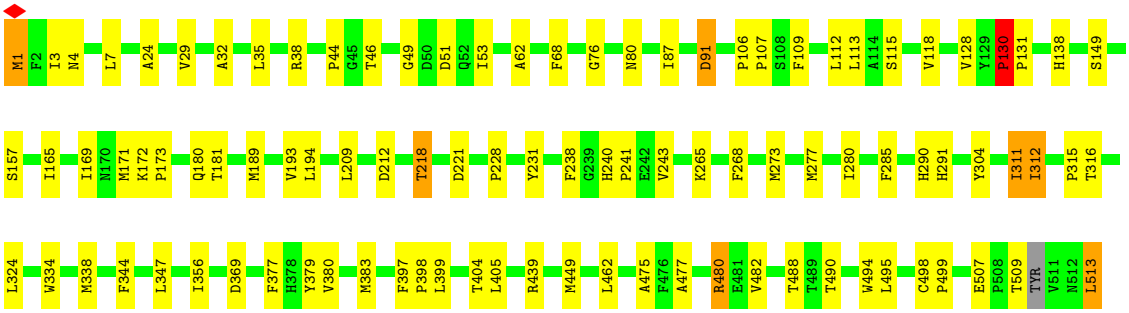
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
21	S	1	1	1	0

3 Residue-property plots (i)

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

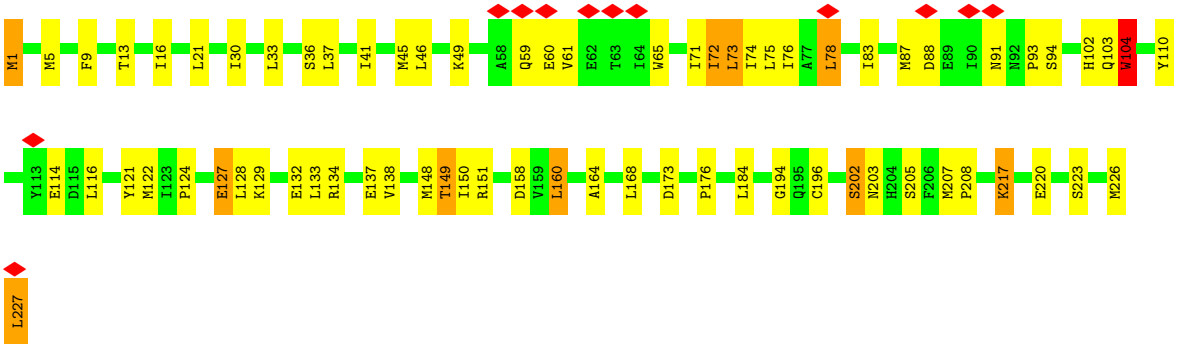
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



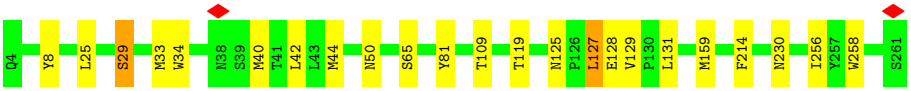
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



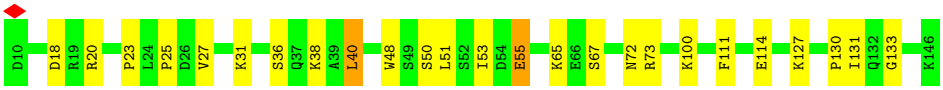
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



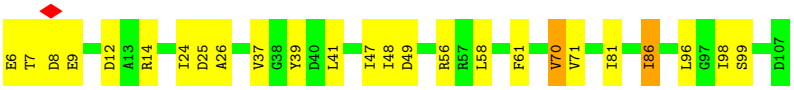
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q:



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

Chain R:

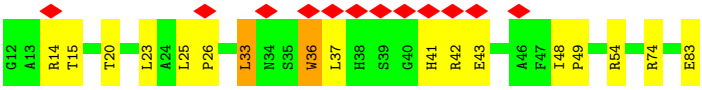


• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:

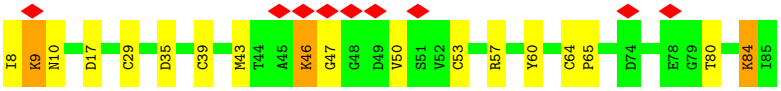
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



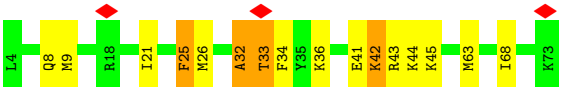
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



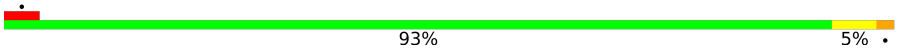
• Molecule 9: Cytochrome c oxidase subunit 6C

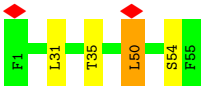
Chain V:



• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



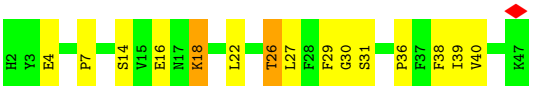


• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:

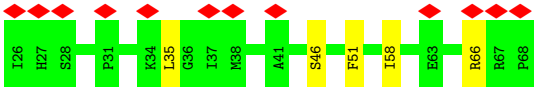
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



• Molecule 13: Cytochrome c oxidase subunit 8A, mitochondrial

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4161	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 ($e^-/Å^2$)	42.7	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.611	Depositor
Minimum map value	-5.291	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.239	Depositor
Recommended contour level	1.07	Depositor
Map size (Å)	263.68, 263.68, 263.68	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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: PEK, NA, 9Z9, FME, PGV, CU, MG, ZN, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	N	0.59	1/4132 (0.0%)	0.78	5/5646 (0.1%)
2	O	0.60	0/1860	0.90	2/2534 (0.1%)
3	P	0.55	0/2186	0.69	0/2990
4	Q	0.60	1/1175 (0.1%)	0.89	3/1588 (0.2%)
5	R	0.60	0/843	0.89	2/1146 (0.2%)
6	S	0.64	1/716 (0.1%)	0.94	1/973 (0.1%)
7	T	0.54	0/621	0.85	0/848
8	U	0.60	0/673	0.92	1/910 (0.1%)
9	V	0.60	0/593	0.85	0/785
10	W	0.53	0/443	0.70	0/598
11	X	0.64	0/385	0.91	0/527
12	Y	0.80	0/393	1.00	2/526 (0.4%)
13	M	0.30	0/345	0.59	0/470
All	All	0.59	3/14365 (0.0%)	0.82	16/19541 (0.1%)

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	N	0	2
4	Q	0	1
11	X	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	51	SER	CA-CB	-6.37	1.43	1.52
4	Q	67	SER	CA-CB	-5.15	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	157	SER	CA-CB	-5.13	1.45	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	72	ASN	CB-CA-C	-7.57	95.26	110.40
1	N	130	PRO	CB-CA-C	-7.56	93.10	112.00
1	N	130	PRO	N-CA-CB	-6.94	94.96	102.60
5	R	61	PHE	CB-CA-C	-6.74	96.92	110.40
1	N	480	ARG	CB-CA-C	-5.94	98.51	110.40
1	N	439	ARG	CB-CA-C	5.94	122.28	110.40
2	O	103	GLN	CA-C-N	-5.83	104.38	117.20
12	Y	7	PRO	N-CD-CG	-5.69	94.67	103.20
8	U	53	CYS	CB-CA-C	-5.48	99.45	110.40
4	Q	133	GLY	N-CA-C	5.45	126.71	113.10
5	R	39	TYR	CB-CA-C	-5.36	99.67	110.40
12	Y	7	PRO	N-CA-CB	-5.36	96.70	102.60
4	Q	55	GLU	CB-CA-C	5.33	121.06	110.40
2	O	104	TRP	N-CA-C	5.28	125.25	111.00
1	N	268	PHE	CB-CA-C	-5.22	99.95	110.40
6	S	93	PRO	CB-CA-C	-5.13	99.18	112.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain
4	Q	27	VAL	Mainchain
11	X	45	VAL	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4005	3977	3978	56	0
2	O	1824	1833	1833	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2100	2017	2018	12	0
4	Q	1141	1123	1123	12	0
5	R	825	816	816	8	0
6	S	700	681	681	4	0
7	T	595	569	569	5	0
8	U	653	610	610	8	0
9	V	580	592	592	9	0
10	W	434	432	432	3	0
11	X	372	354	354	1	0
12	Y	380	380	380	27	0
13	M	335	346	346	19	0
14	N	1	0	0	0	0
14	O	2	0	0	0	0
15	N	1	0	0	0	0
16	N	1	0	0	0	0
17	N	120	108	108	3	0
18	N	51	0	76	1	0
18	P	51	0	76	1	0
19	P	53	75	77	6	0
20	P	39	0	0	2	0
21	S	1	0	0	0	0
All	All	14264	13913	14069	167	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 (167) 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)
12:Y:38:PHE:CZ	13:M:58:ILE:HD11	1.54	1.41
12:Y:38:PHE:CE2	13:M:58:ILE:HD11	1.86	1.11
12:Y:18:LYS:NZ	13:M:35:LEU:HD21	1.72	1.04
12:Y:38:PHE:CZ	13:M:58:ILE:CD1	2.45	0.99
12:Y:18:LYS:HZ2	13:M:35:LEU:HD21	1.31	0.90
4:Q:40:LEU:HD11	4:Q:55:GLU:HB3	1.57	0.85
12:Y:30:GLY:CA	13:M:51:PHE:CE1	2.65	0.79
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.69	0.73
12:Y:30:GLY:HA2	13:M:51:PHE:CE1	2.23	0.73
12:Y:38:PHE:CE1	13:M:58:ILE:HD11	2.20	0.72
12:Y:18:LYS:HZ1	13:M:35:LEU:HD21	1.53	0.72
12:Y:38:PHE:CE2	13:M:58:ILE:CD1	2.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:85:CYS:SG	6:S:87:THR:HG23	2.31	0.71
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.70	0.71
1:N:1:FME:HCN	1:N:4:ASN:H	1.54	0.70
1:N:193:VAL:HG11	20:P:303:9Z9:O72	1.92	0.70
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.27	0.70
12:Y:30:GLY:CA	13:M:51:PHE:HE1	2.07	0.67
12:Y:18:LYS:NZ	13:M:35:LEU:CD2	2.53	0.67
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.77	0.65
19:P:301:PEK:H32	19:P:301:PEK:H72	1.78	0.65
12:Y:38:PHE:CE1	13:M:58:ILE:CD1	2.78	0.64
1:N:130:PRO:HG3	1:N:209:LEU:HD13	1.80	0.62
1:N:449:MET:SD	2:O:5:MET:HG2	2.40	0.62
9:V:32:ALA:O	9:V:34:PHE:N	2.32	0.61
1:N:53:ILE:HD11	12:Y:40:VAL:HA	1.83	0.61
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.66	0.60
2:O:116:LEU:HD13	2:O:227:LEU:HD23	1.84	0.60
19:P:301:PEK:O14	19:P:301:PEK:H052	2.02	0.60
2:O:116:LEU:HD11	2:O:226:MET:HB3	1.84	0.59
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.83	0.59
12:Y:30:GLY:HA3	13:M:51:PHE:HE1	1.68	0.59
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.02	0.58
2:O:116:LEU:HD21	2:O:223:SER:HA	1.85	0.58
2:O:124:PRO:HB2	2:O:127:GLU:HG3	1.85	0.58
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.87	0.57
12:Y:30:GLY:HA3	13:M:51:PHE:CE1	2.40	0.57
9:V:32:ALA:C	9:V:34:PHE:N	2.59	0.56
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.40	0.56
12:Y:18:LYS:HZ1	13:M:35:LEU:CD2	2.17	0.56
12:Y:18:LYS:HZ2	13:M:35:LEU:CD2	2.12	0.55
18:N:606:PGV:H91	3:P:50:ASN:OD1	2.06	0.54
5:R:81:ILE:HG23	9:V:9:MET:HG2	1.90	0.53
1:N:404:THR:HG22	1:N:482:VAL:HG22	1.89	0.53
17:N:604:HEA:HBC1	17:N:604:HEA:HMC1	1.90	0.53
2:O:150:ILE:HD12	2:O:184:LEU:HD22	1.91	0.53
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.40	0.52
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.42	0.52
1:N:488:THR:HB	1:N:495:LEU:HD13	1.92	0.52
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.91	0.51
3:P:81:TYR:OH	20:P:303:9Z9:C48	2.59	0.51
2:O:83:ILE:O	2:O:87:MET:HG3	2.12	0.50
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:22:LEU:HD21	13:M:46:SER:OG	2.11	0.50
1:N:87:ILE:O	1:N:173:PRO:HD3	2.11	0.50
2:O:102:HIS:O	2:O:104:TRP:N	2.45	0.50
3:P:34:TRP:CD1	3:P:40:MET:HG2	2.47	0.49
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.00	0.49
1:N:379:TYR:O	1:N:383:MET:HB2	2.12	0.49
1:N:51:ASP:HB3	2:O:202:SER:O	2.11	0.49
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.94	0.49
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.95	0.48
1:N:311:ILE:O	1:N:315:PRO:HD2	2.13	0.48
2:O:71:ILE:HA	2:O:74:ILE:HD12	1.95	0.48
8:U:84:LYS:HB3	8:U:84:LYS:HE3	1.40	0.48
9:V:32:ALA:O	9:V:33:THR:C	2.51	0.48
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.96	0.48
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.13	0.48
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.95	0.47
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.96	0.47
2:O:30:ILE:HD13	2:O:76:ILE:HG12	1.97	0.47
2:O:73:LEU:HD12	2:O:73:LEU:HA	1.76	0.47
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.49	0.47
2:O:104:TRP:HA	2:O:207:MET:SD	2.54	0.47
3:P:25:LEU:O	3:P:29:SER:HB2	2.15	0.47
10:W:50:LEU:HD22	10:W:50:LEU:O	2.14	0.47
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.97	0.47
1:N:509:THR:HG22	6:S:57:ILE:HB	1.97	0.47
9:V:42:LYS:HB3	9:V:42:LYS:HE2	1.43	0.46
1:N:347:LEU:HD13	1:N:383:MET:SD	2.54	0.46
3:P:127:LEU:HD12	3:P:131:LEU:HD22	1.98	0.46
6:S:76:LYS:HE2	6:S:76:LYS:HB3	1.61	0.46
12:Y:27:LEU:O	12:Y:31:SER:HB3	2.16	0.46
2:O:1:FME:SD	2:O:133:LEU:CD1	3.04	0.46
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.83	0.46
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.51	0.46
6:S:48:LEU:HD12	6:S:90:LYS:HB3	1.97	0.46
1:N:480:ARG:HE	1:N:480:ARG:HB2	1.61	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.98	0.46
2:O:91:ASN:HB3	2:O:149:THR:HG21	1.98	0.46
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.52	0.45
19:P:301:PEK:H32	19:P:301:PEK:H12	1.98	0.45
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.81	0.45
8:U:46:LYS:HB3	8:U:46:LYS:HE3	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:40:LEU:HD13	4:Q:40:LEU:HA	1.64	0.45
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.99	0.45
1:N:49:GLY:HA3	13:M:66:ARG:NH2	2.32	0.45
1:N:131:PRO:HG2	2:O:176:PRO:HG3	1.99	0.45
1:N:62:ALA:HB2	17:N:604:HEA:HBD1	1.99	0.45
7:T:33:LEU:HD22	7:T:33:LEU:HA	1.70	0.45
7:T:36:TRP:HA	7:T:36:TRP:CE3	2.51	0.45
5:R:48:ILE:HG13	5:R:71:VAL:HG21	1.99	0.45
7:T:20:THR:O	7:T:25:LEU:HG	2.17	0.44
7:T:23:LEU:C	7:T:26:PRO:HD2	2.37	0.44
1:N:344:PHE:C	1:N:344:PHE:CD1	2.91	0.44
2:O:78:LEU:HD12	2:O:78:LEU:HA	1.82	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.44
2:O:220:GLU:O	2:O:223:SER:HB2	2.18	0.44
2:O:1:FME:SD	2:O:133:LEU:HD13	2.58	0.43
1:N:131:PRO:HD2	2:O:160:LEU:HG	1.99	0.43
1:N:35:LEU:HD11	1:N:462:LEU:HD13	2.00	0.43
1:N:118:VAL:HA	10:W:54:SER:HA	2.00	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.18	0.43
1:N:324:LEU:HD13	2:O:41:ILE:HG22	2.01	0.43
5:R:86:ILE:HA	5:R:86:ILE:HD13	1.65	0.43
2:O:121:TYR:O	2:O:138:VAL:HA	2.19	0.43
19:P:301:PEK:O14	19:P:301:PEK:C05	2.60	0.43
8:U:8:ILE:HD12	8:U:8:ILE:HA	1.98	0.43
1:N:29:VAL:HG13	12:Y:36:PRO:HG3	2.01	0.42
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.18	0.42
1:N:477:ALA:HB1	12:Y:18:LYS:HB3	2.01	0.42
8:U:46:LYS:O	8:U:47:GLY:C	2.56	0.42
9:V:32:ALA:C	9:V:34:PHE:H	2.22	0.42
1:N:165:ILE:O	1:N:169:ILE:HG12	2.19	0.42
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.55	0.42
4:Q:131:ILE:HD12	4:Q:131:ILE:N	2.34	0.42
1:N:76:GLY:O	1:N:80:ASN:HB2	2.19	0.42
9:V:63:MET:HB3	9:V:68:ILE:CD1	2.45	0.42
12:Y:18:LYS:H	12:Y:18:LYS:HG3	1.63	0.42
1:N:24:ALA:HB1	12:Y:29:PHE:HE2	1.84	0.42
1:N:113:LEU:HD22	12:Y:39:ILE:HD11	2.01	0.42
1:N:243:VAL:HB	17:N:605:HEA:CAC	2.50	0.42
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.00	0.42
1:N:513:LEU:HD22	1:N:513:LEU:HA	1.89	0.42
2:O:72:ILE:H	2:O:72:ILE:HG13	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:68:PHE:CE2	1:N:112:LEU:HD13	2.52	0.41
1:N:112:LEU:C	1:N:112:LEU:HD23	2.40	0.41
1:N:130:PRO:HD2	1:N:231:TYR:CG	2.55	0.41
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.50	0.41
2:O:93:PRO:HG3	2:O:151:ARG:NH2	2.35	0.41
5:R:56:ARG:C	5:R:58:LEU:N	2.73	0.41
5:R:96:LEU:HB2	5:R:98:ILE:HG13	2.01	0.41
1:N:3:ILE:HG23	1:N:7:LEU:HD22	2.02	0.41
7:T:49:PRO:HD2	8:U:80:THR:HG22	2.03	0.41
8:U:9:LYS:HE2	8:U:9:LYS:HB2	1.74	0.41
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.98	0.41
19:P:301:PEK:C10	19:P:301:PEK:H161	2.51	0.41
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.02	0.41
1:N:312:ILE:O	1:N:315:PRO:HG2	2.21	0.41
4:Q:18:ASP:OD1	4:Q:65:LYS:HB3	2.20	0.41
3:P:125:ASN:HB3	3:P:128:GLU:HB2	2.02	0.41
3:P:128:GLU:HB3	3:P:129:VAL:H	1.78	0.41
4:Q:73:ARG:HE	4:Q:73:ARG:HB2	1.45	0.41
1:N:130:PRO:HD2	1:N:231:TYR:CD1	2.56	0.41
1:N:218:THR:HG22	1:N:221:ASP:HB3	2.02	0.41
19:P:301:PEK:H011	19:P:301:PEK:H31	2.03	0.41
1:N:128:VAL:O	1:N:128:VAL:HG12	2.21	0.40
3:P:65:SER:HB2	18:P:302:PGV:H041	2.03	0.40
9:V:25:PHE:HD1	9:V:25:PHE:HA	1.75	0.40
8:U:9:LYS:HB3	8:U:10:ASN:H	1.81	0.40
12:Y:22:LEU:O	12:Y:26:THR:HB	2.21	0.40
2:O:13:THR:HB	2:O:168:LEU:HD23	2.03	0.40
1:N:498:CYS:HA	1:N:499:PRO:HA	1.94	0.40
3:P:40:MET:O	3:P:44:MET:HG2	2.21	0.40
11:X:44:PRO:HB3	11:X:48:VAL:HB	2.04	0.40
1:N:277:MET:HE2	1:N:277:MET:HB2	1.92	0.40
1:N:397:PHE:HB3	1:N:398:PRO:HD3	2.04	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	N	508/513 (99%)	492 (97%)	15 (3%)	1 (0%)	47	79
2	O	225/227 (99%)	208 (92%)	16 (7%)	1 (0%)	34	69
3	P	256/258 (99%)	250 (98%)	6 (2%)	0	100	100
4	Q	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
5	R	100/102 (98%)	97 (97%)	2 (2%)	1 (1%)	15	49
6	S	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
7	T	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
8	U	76/78 (97%)	70 (92%)	6 (8%)	0	100	100
9	V	68/70 (97%)	66 (97%)	0	2 (3%)	4	24
10	W	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
11	X	45/47 (96%)	43 (96%)	0	2 (4%)	2	15
12	Y	44/46 (96%)	44 (100%)	0	0	100	100
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	1710/1739 (98%)	1642 (96%)	61 (4%)	7 (0%)	38	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	V	32	ALA
9	V	33	THR
2	O	104	TRP
5	R	26	ALA
11	X	27	ALA
1	N	91	ASP
11	X	45	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	424/425 (100%)	399 (94%)	25 (6%)	19	50
2	O	210/210 (100%)	182 (87%)	28 (13%)	4	16
3	P	223/223 (100%)	213 (96%)	10 (4%)	27	60
4	Q	121/121 (100%)	112 (93%)	9 (7%)	13	42
5	R	89/89 (100%)	77 (86%)	12 (14%)	4	16
6	S	77/77 (100%)	66 (86%)	11 (14%)	3	14
7	T	62/62 (100%)	50 (81%)	12 (19%)	1	6
8	U	70/70 (100%)	59 (84%)	11 (16%)	2	11
9	V	56/56 (100%)	46 (82%)	10 (18%)	2	8
10	W	46/46 (100%)	44 (96%)	2 (4%)	29	62
11	X	38/38 (100%)	36 (95%)	2 (5%)	22	54
12	Y	39/39 (100%)	34 (87%)	5 (13%)	4	18
13	M	37/37 (100%)	37 (100%)	0	100	100
All	All	1492/1493 (100%)	1355 (91%)	137 (9%)	13	33

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	38	ARG
1	N	46	THR
1	N	91	ASP
1	N	109	PHE
1	N	115	SER
1	N	130	PRO
1	N	138	HIS
1	N	149	SER
1	N	180	GLN
1	N	189	MET
1	N	212	ASP
1	N	218	THR
1	N	228	PRO
1	N	238	PHE
1	N	241	PRO
1	N	273	MET
1	N	280	ILE
1	N	311	ILE
1	N	312	ILE
1	N	316	THR

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Mol	Chain	Res	Type
1	N	338	MET
1	N	356	ILE
1	N	369	ASP
1	N	507	GLU
1	N	513	LEU
2	O	16	ILE
2	O	33	LEU
2	O	36	SER
2	O	37	LEU
2	O	59	GLN
2	O	60	GLU
2	O	61	VAL
2	O	65	TRP
2	O	72	ILE
2	O	73	LEU
2	O	75	LEU
2	O	78	LEU
2	O	88	ASP
2	O	94	SER
2	O	104	TRP
2	O	110	TYR
2	O	114	GLU
2	O	127	GLU
2	O	129	LYS
2	O	148	MET
2	O	149	THR
2	O	158	ASP
2	O	160	LEU
2	O	173	ASP
2	O	202	SER
2	O	205	SER
2	O	217	LYS
2	O	227	LEU
3	P	29	SER
3	P	33	MET
3	P	109	THR
3	P	119	THR
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
3	P	256	ILE

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Mol	Chain	Res	Type
3	P	258	TRP
4	Q	31	LYS
4	Q	36	SER
4	Q	38	LYS
4	Q	40	LEU
4	Q	50	SER
4	Q	51	LEU
4	Q	53	ILE
4	Q	100	LYS
4	Q	114	GLU
5	R	6	GLU
5	R	7	THR
5	R	8	ASP
5	R	9	GLU
5	R	14	ARG
5	R	24	ILE
5	R	25	ASP
5	R	41	LEU
5	R	49	ASP
5	R	70	VAL
5	R	86	ILE
5	R	99	SER
6	S	42	THR
6	S	43	LYS
6	S	44	GLU
6	S	48	LEU
6	S	53	THR
6	S	55	LYS
6	S	63	GLU
6	S	76	LYS
6	S	78	GLU
6	S	80	GLN
6	S	92	VAL
7	T	14	ARG
7	T	15	THR
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
7	T	41	HIS
7	T	42	ARG
7	T	43	GLU
7	T	48	ILE

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Mol	Chain	Res	Type
7	T	54	ARG
7	T	74	ARG
7	T	83	GLU
8	U	9	LYS
8	U	17	ASP
8	U	29	CYS
8	U	35	ASP
8	U	39	CYS
8	U	43	MET
8	U	46	LYS
8	U	50	VAL
8	U	57	ARG
8	U	60	TYR
8	U	84	LYS
9	V	8	GLN
9	V	21	ILE
9	V	25	PHE
9	V	26	MET
9	V	36	LYS
9	V	41	GLU
9	V	42	LYS
9	V	43	ARG
9	V	44	LYS
9	V	45	LYS
10	W	35	THR
10	W	50	LEU
11	X	8	ASP
11	X	54	ARG
12	Y	4	GLU
12	Y	14	SER
12	Y	16	GLU
12	Y	18	LYS
12	Y	26	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	FME	N	1	1	8,9,10	0.79	0	7,9,11	1.87	2 (28%)
2	FME	O	1	2	8,9,10	0.66	0	7,9,11	1.87	2 (28%)

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
1	FME	N	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	1/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	1	FME	CA-N-CN	-4.24	116.30	122.82
2	O	1	FME	C-CA-N	3.66	116.34	109.73
2	O	1	FME	CA-N-CN	-2.97	118.26	122.82
1	N	1	FME	O-C-CA	-2.09	119.31	124.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
2	O	1	FME	O1-CN-N-CA

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	N	1	FME	1	0
2	O	1	FME	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
18	PGV	P	302	-	50,50,50	0.41	0	53,56,56	0.49	0
17	HEA	N	604	1	57,67,67	1.15	3 (5%)	61,103,103	1.34	10 (16%)
20	9Z9	P	303	3	44,44,44	0.62	1 (2%)	66,68,68	1.04	4 (6%)
17	HEA	N	605	1	57,67,67	1.95	18 (31%)	61,103,103	2.78	29 (47%)
18	PGV	N	606	-	50,50,50	1.02	3 (6%)	53,56,56	0.99	3 (5%)
19	PEK	P	301	-	52,52,52	0.37	0	55,57,57	0.88	3 (5%)

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
18	PGV	P	302	-	-	21/55/55/55	-
17	HEA	N	604	1	3/3/16/16	7/32/76/76	-
20	9Z9	P	303	3	-	8/12/100/100	0/6/6/6
17	HEA	N	605	1	2/2/16/16	8/32/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PGV	N	606	-	-	15/55/55/55	-
19	PEK	P	301	-	-	33/56/56/56	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	605	HEA	C3B-C2B	4.92	1.45	1.34
17	N	605	HEA	C3D-C2D	4.70	1.46	1.36
17	N	605	HEA	C3C-C2C	4.68	1.46	1.40
17	N	605	HEA	CHD-C1D	4.56	1.46	1.35
17	N	605	HEA	CHC-C4B	4.23	1.45	1.35
18	N	606	PGV	C12-C11	3.92	1.54	1.31
17	N	605	HEA	C1D-ND	-3.42	1.34	1.40
17	N	604	HEA	C3A-C2A	-3.21	1.35	1.40
17	N	604	HEA	C3A-CMA	-3.19	1.39	1.46
17	N	605	HEA	FE-NB	3.11	2.12	1.96
17	N	605	HEA	C3A-C2A	2.96	1.44	1.40
17	N	605	HEA	C4B-NB	-2.92	1.35	1.40
17	N	605	HEA	FE-ND	2.82	2.10	1.96
17	N	605	HEA	C4D-ND	-2.55	1.33	1.38
17	N	605	HEA	C4B-C3B	2.39	1.48	1.44
17	N	605	HEA	CAA-C2A	-2.26	1.48	1.52
17	N	604	HEA	C1C-NC	2.25	1.40	1.36
18	N	606	PGV	O03-C19	2.24	1.39	1.33
18	N	606	PGV	C01-C02	2.19	1.57	1.50
17	N	605	HEA	O2A-CGA	-2.18	1.23	1.30
17	N	605	HEA	O2D-CGD	-2.12	1.23	1.30
17	N	605	HEA	C1B-NB	-2.06	1.34	1.38
17	N	605	HEA	C1B-C2B	2.04	1.48	1.44
20	P	303	9Z9	O80-C79	-2.02	1.40	1.43
17	N	605	HEA	C1D-C2D	2.01	1.48	1.44

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	605	HEA	C3D-C4D-ND	7.43	117.55	110.36
17	N	605	HEA	C3B-C4B-NB	6.11	117.08	109.84
17	N	605	HEA	CBA-CAA-C2A	-5.89	102.69	112.60
17	N	605	HEA	C2D-C1D-ND	5.62	116.50	109.84
17	N	605	HEA	C1D-C2D-C3D	-5.05	101.65	106.96
17	N	605	HEA	C2B-C1B-NB	4.97	115.84	109.88
17	N	605	HEA	CMC-C2C-C3C	4.95	133.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	303	9Z9	O80-C73-C76	4.64	115.08	110.77
18	N	606	PGV	C01-O03-C19	-4.22	101.51	117.12
19	P	301	PEK	O13-P-O12	4.01	126.39	107.75
17	N	605	HEA	C3C-C4C-NC	4.00	114.38	109.21
17	N	605	HEA	OMA-CMA-C3A	-3.77	116.69	124.91
19	P	301	PEK	O12-P-O14	-3.57	95.10	109.07
17	N	605	HEA	C4B-C3B-C2B	-3.55	101.35	107.41
17	N	605	HEA	CMB-C2B-C1B	3.49	130.35	125.04
17	N	605	HEA	C27-C19-C20	3.27	120.77	115.27
17	N	605	HEA	CHA-C4D-C3D	-3.23	120.09	124.84
17	N	605	HEA	CAA-CBA-CGA	-3.21	104.76	113.76
17	N	605	HEA	CHB-C1B-NB	-3.16	121.00	124.43
17	N	605	HEA	C13-C14-C15	-3.15	120.06	127.66
17	N	605	HEA	C4D-C3D-C2D	-3.10	102.38	106.90
20	P	303	9Z9	C77-C78-C79	3.07	112.83	108.56
17	N	605	HEA	C1D-ND-C4D	-3.06	101.91	105.07
17	N	605	HEA	C26-C15-C16	2.99	120.30	115.27
17	N	604	HEA	C27-C19-C18	-2.98	116.02	123.68
17	N	605	HEA	CAD-CBD-CGD	-2.91	107.35	113.60
17	N	605	HEA	C4B-NB-C1B	-2.82	102.17	105.07
17	N	604	HEA	C17-C18-C19	-2.72	121.10	127.66
17	N	605	HEA	C1B-C2B-C3B	-2.70	103.57	106.80
17	N	605	HEA	CAD-C3D-C2D	2.61	132.75	127.88
17	N	604	HEA	CMC-C2C-C3C	2.61	129.56	124.68
17	N	604	HEA	C20-C19-C18	2.50	126.18	121.12
17	N	605	HEA	C25-C23-C24	2.47	120.06	114.60
20	P	303	9Z9	C79-O80-C73	2.37	118.21	113.72
19	P	301	PEK	O13-P-O11	-2.31	96.99	107.75
18	N	606	PGV	C3-C2-C1	-2.30	105.25	113.62
17	N	605	HEA	CHC-C4B-NB	-2.29	121.55	124.38
17	N	605	HEA	CMB-C2B-C3B	-2.23	126.08	130.34
17	N	604	HEA	C26-C15-C14	-2.23	117.96	123.68
17	N	604	HEA	C13-C14-C15	-2.17	122.43	127.66
17	N	604	HEA	C2D-C1D-ND	2.14	112.37	109.84
17	N	604	HEA	C21-C20-C19	-2.12	106.01	112.98
18	N	606	PGV	C22-C21-C20	2.11	120.78	113.19
17	N	604	HEA	CMC-C2C-C1C	-2.08	125.26	128.46
17	N	604	HEA	C16-C15-C14	2.07	125.30	121.12
17	N	605	HEA	CMC-C2C-C1C	-2.04	125.33	128.46
17	N	605	HEA	O1A-CGA-CBA	-2.04	116.53	123.08
20	P	303	9Z9	O80-C73-O72	-2.01	104.17	109.78
17	N	605	HEA	CHD-C1D-C2D	-2.00	121.19	126.72

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	N	604	HEA	NA
17	N	604	HEA	NB
17	N	604	HEA	ND
17	N	605	HEA	ND
17	N	605	HEA	NB

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	P	302	PGV	C04-O12-P-O14
19	P	301	PEK	C04-O12-P-O14
19	P	301	PEK	C2-C1-O01-C02
19	P	301	PEK	C5-C6-C7-C8
19	P	301	PEK	C12-C13-C14-C15
20	P	303	9Z9	C22-C21-O20-C17
20	P	303	9Z9	C48-C23-C24-O25
20	P	303	9Z9	C24-C23-C48-O49
19	P	301	PEK	O02-C1-O01-C02
19	P	301	PEK	C13-C14-C15-C16
18	P	302	PGV	C28-C29-C30-C31
19	P	301	PEK	C22-C21-O03-C01
18	P	302	PGV	O12-C04-C05-O05
19	P	301	PEK	O04-C21-O03-C01
18	N	606	PGV	C19-C20-C21-C22
18	N	606	PGV	C15-C16-C17-C18
18	N	606	PGV	C5-C6-C7-C8
18	P	302	PGV	C22-C23-C24-C25
18	N	606	PGV	C6-C7-C8-C9
18	P	302	PGV	C7-C8-C9-C10
18	P	302	PGV	C13-C14-C15-C16
18	N	606	PGV	C29-C30-C31-C32
18	P	302	PGV	C10-C11-C12-C13
19	P	301	PEK	C10-C11-C12-C13
18	P	302	PGV	C14-C15-C16-C17
19	P	301	PEK	C23-C24-C25-C26
18	N	606	PGV	C7-C8-C9-C10
18	P	302	PGV	C25-C26-C27-C28
18	P	302	PGV	C30-C31-C32-C33
20	P	303	9Z9	C21-C22-C23-C24
17	N	604	HEA	C21-C22-C23-C25
20	P	303	9Z9	O20-C21-C22-C23
20	P	303	9Z9	C22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
20	P	303	9Z9	C22-C23-C48-O49
18	P	302	PGV	C12-C13-C14-C15
18	N	606	PGV	C23-C24-C25-C26
18	P	302	PGV	C19-C20-C21-C22
19	P	301	PEK	C4-C5-C6-C7
19	P	301	PEK	C04-O12-P-O11
19	P	301	PEK	O03-C01-C02-C03
19	P	301	PEK	C21-C22-C23-C24
18	N	606	PGV	C30-C31-C32-C33
18	P	302	PGV	C11-C10-C9-C8
19	P	301	PEK	C17-C18-C19-C20
18	P	302	PGV	C15-C16-C17-C18
19	P	301	PEK	C30-C31-C32-C33
20	P	303	9Z9	C23-C24-O25-C26
18	N	606	PGV	C31-C32-C33-C34
19	P	301	PEK	C7-C8-C9-C10
18	P	302	PGV	C04-O12-P-O11
19	P	301	PEK	C26-C27-C28-C29
17	N	604	HEA	C15-C16-C17-C18
18	N	606	PGV	C25-C26-C27-C28
18	P	302	PGV	C02-C03-O11-P
19	P	301	PEK	C31-C32-C33-C34
19	P	301	PEK	O03-C01-C02-O01
18	N	606	PGV	C20-C21-C22-C23
18	P	302	PGV	C04-O12-P-O13
19	P	301	PEK	C03-O11-P-O13
19	P	301	PEK	C03-O11-P-O14
19	P	301	PEK	C04-O12-P-O13
17	N	605	HEA	C2D-C3D-CAD-CBD
19	P	301	PEK	C05-C04-O12-P
18	P	302	PGV	C29-C30-C31-C32
17	N	605	HEA	C4D-C3D-CAD-CBD
18	N	606	PGV	C26-C27-C28-C29
17	N	604	HEA	C21-C22-C23-C24
19	P	301	PEK	C29-C30-C31-C32
17	N	605	HEA	C11-C12-C13-C14
19	P	301	PEK	C03-O11-P-O12
19	P	301	PEK	C34-C35-C36-C37
18	N	606	PGV	C9-C10-C11-C12
18	P	302	PGV	C20-C19-O03-C01
17	N	605	HEA	CAD-CBD-CGD-O2D
18	P	302	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
17	N	605	HEA	CAD-CBD-CGD-O1D
19	P	301	PEK	C3-C4-C5-C6
18	P	302	PGV	O12-C04-C05-C06
17	N	605	HEA	CAA-CBA-CGA-O2A
17	N	604	HEA	CAD-CBD-CGD-O1D
17	N	605	HEA	C26-C15-C16-C17
18	N	606	PGV	C11-C12-C13-C14
17	N	605	HEA	CAA-CBA-CGA-O1A
18	N	606	PGV	C4-C5-C6-C7
19	P	301	PEK	C25-C26-C27-C28
17	N	604	HEA	CAA-CBA-CGA-O1A
17	N	604	HEA	CAD-CBD-CGD-O2D
19	P	301	PEK	O12-C04-C05-N
19	P	301	PEK	C16-C17-C18-C19
19	P	301	PEK	C01-C02-O01-C1
17	N	604	HEA	CAA-CBA-CGA-O2A
19	P	301	PEK	C2-C3-C4-C5

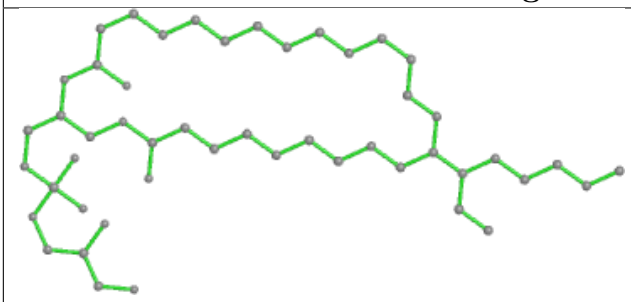
There are no ring outliers.

6 monomers are involved in 13 short contacts:

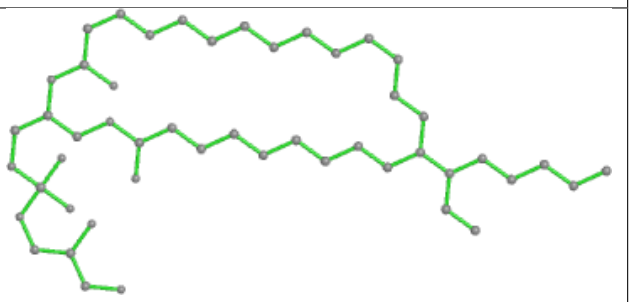
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	P	302	PGV	1	0
17	N	604	HEA	2	0
20	P	303	9Z9	2	0
17	N	605	HEA	1	0
18	N	606	PGV	1	0
19	P	301	PEK	6	0

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

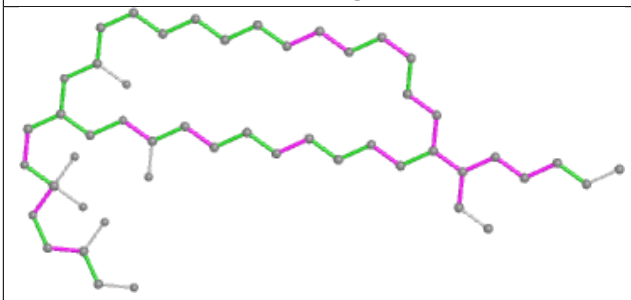
Ligand PGV P 302



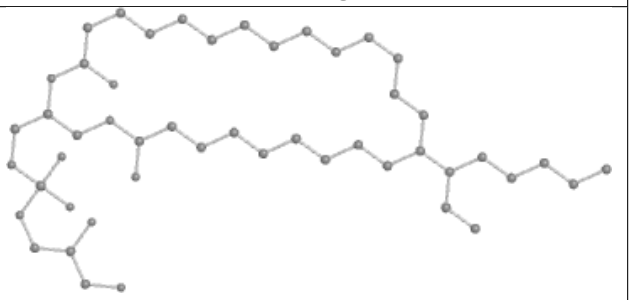
Bond lengths



Bond angles

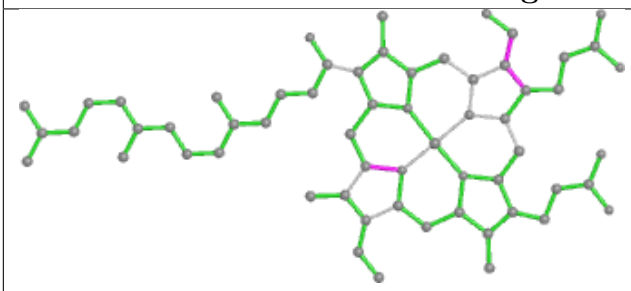


Torsions

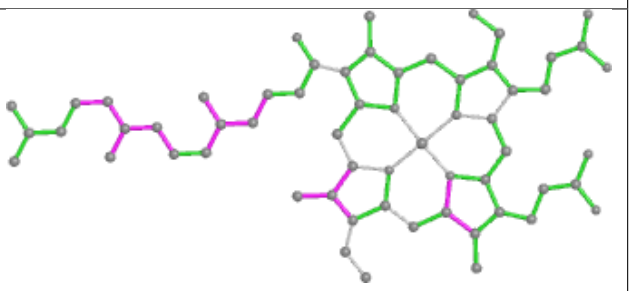


Rings

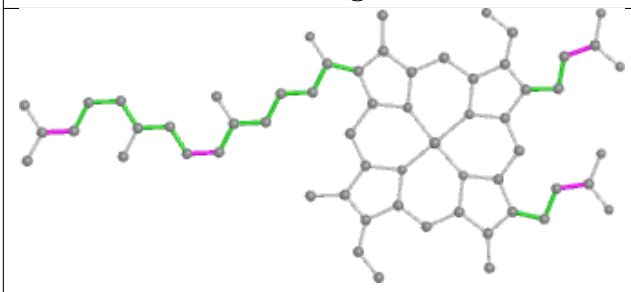
Ligand HEA N 604



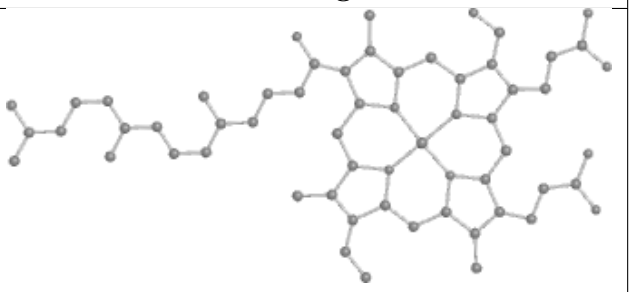
Bond lengths



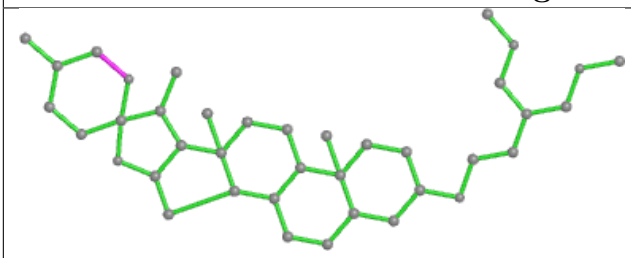
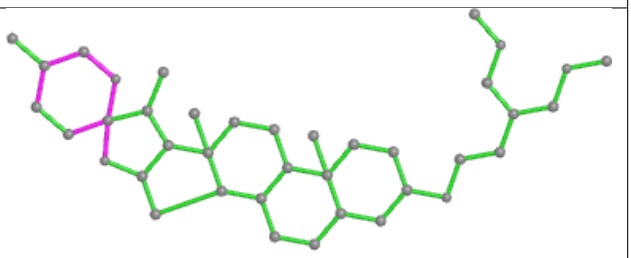
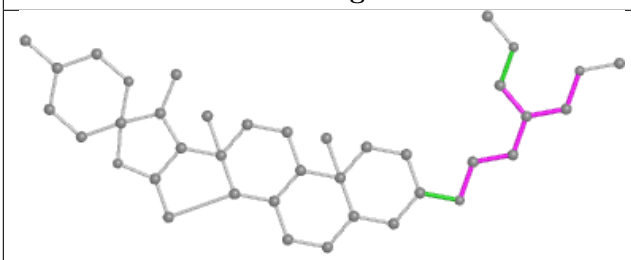
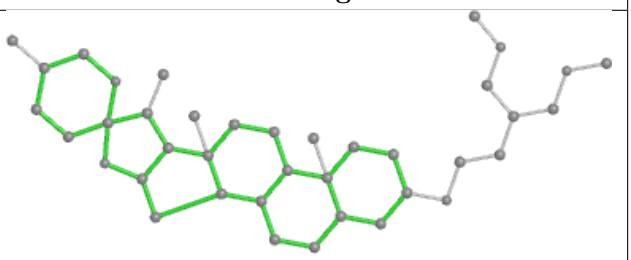
Bond angles

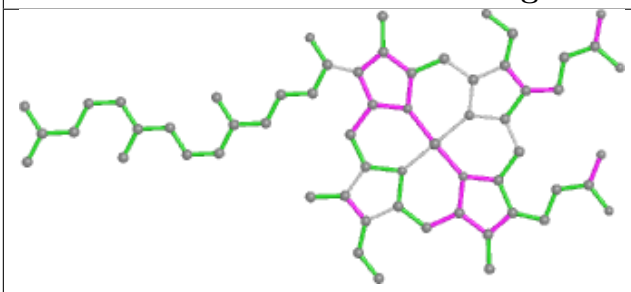
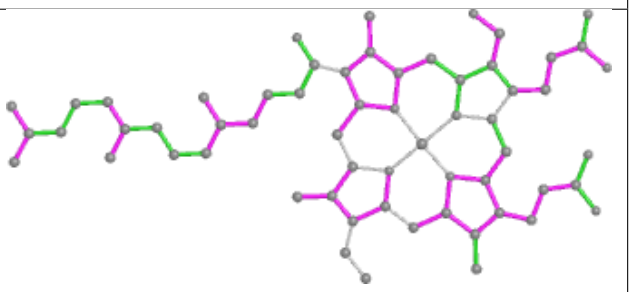
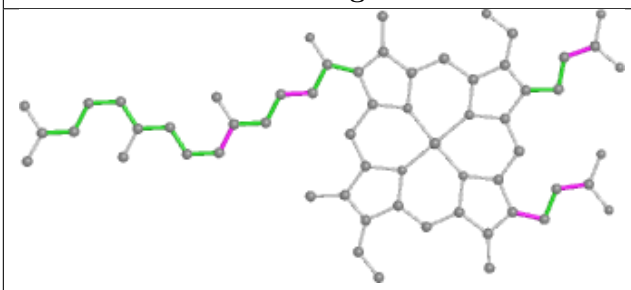
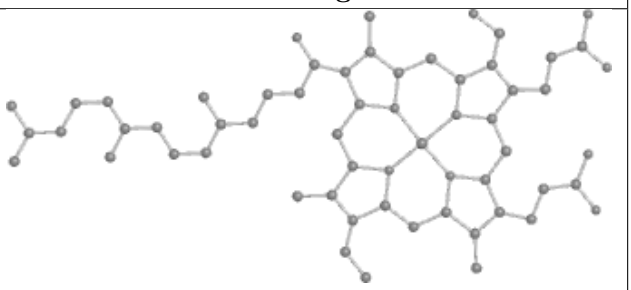


Torsions

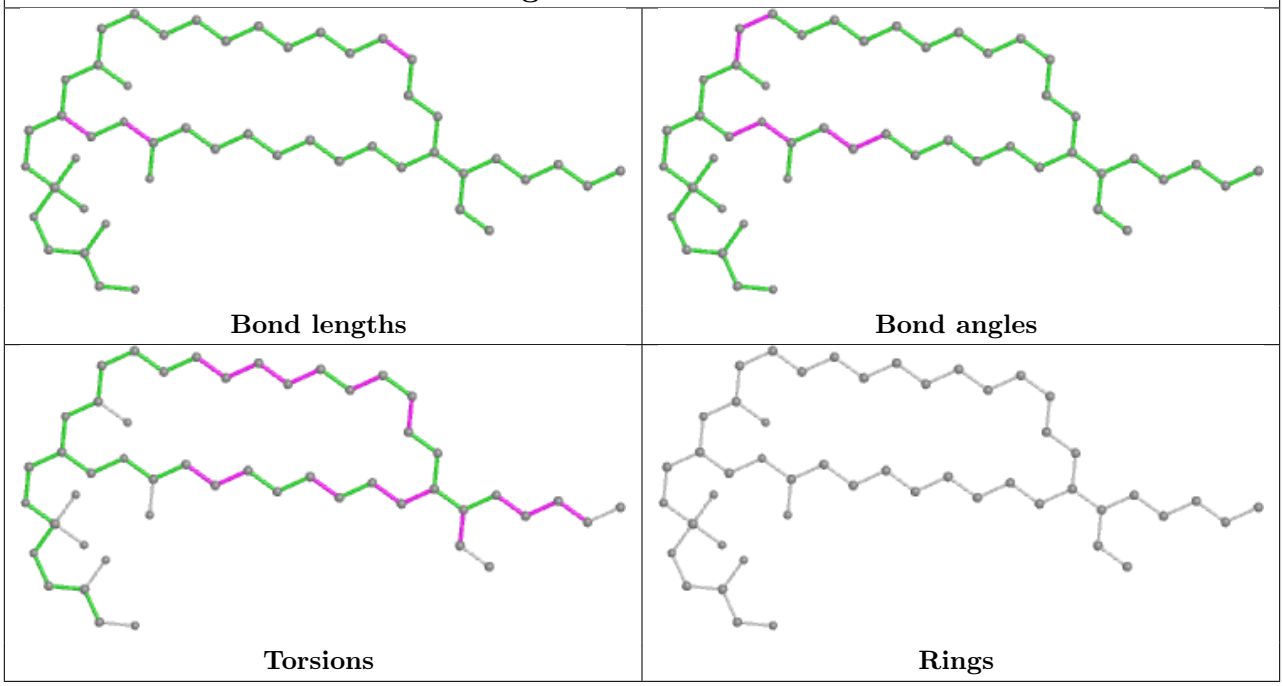


Rings

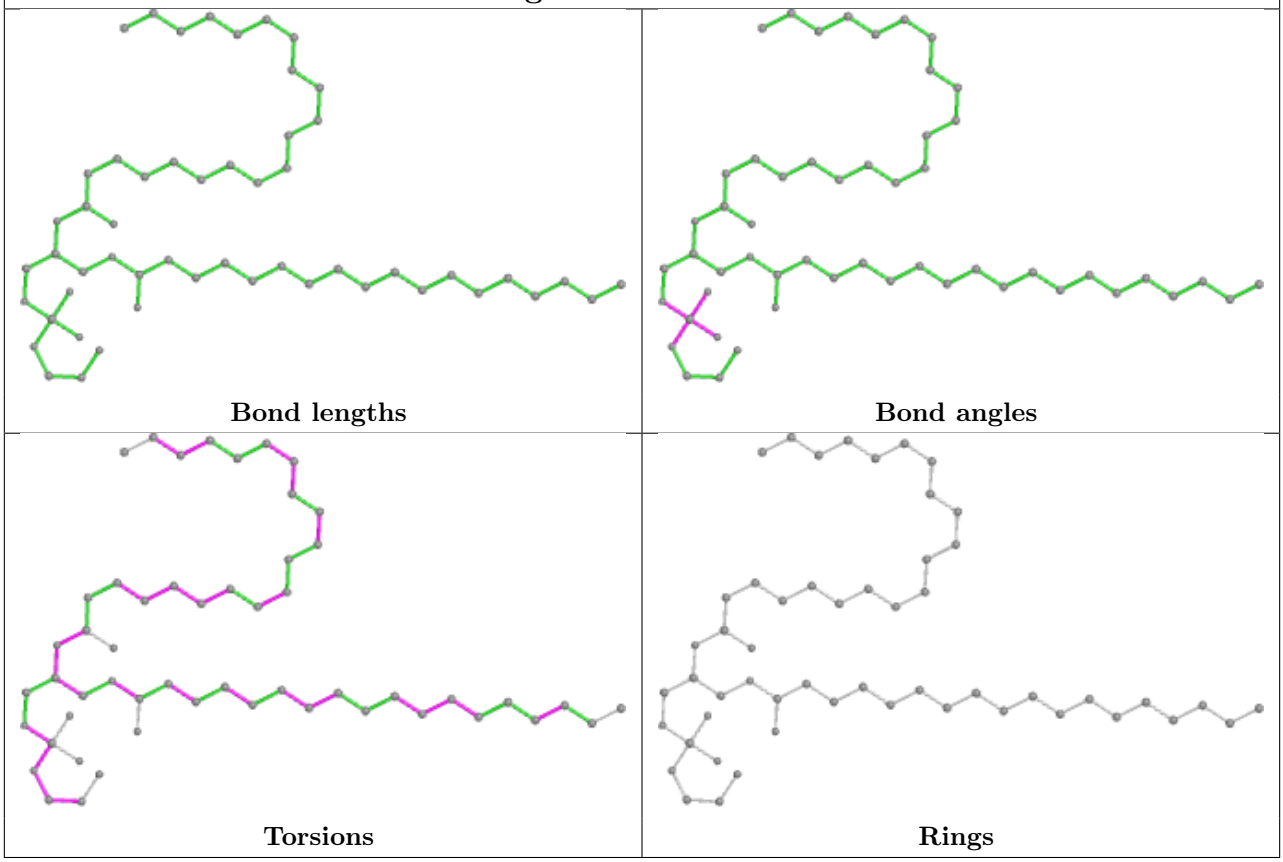
Ligand 9Z9 P 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA N 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV N 606



Ligand PEK P 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

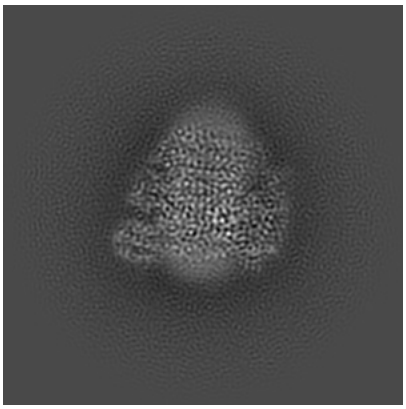
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-27196. These allow visual inspection of the internal detail of the map and identification of artifacts.

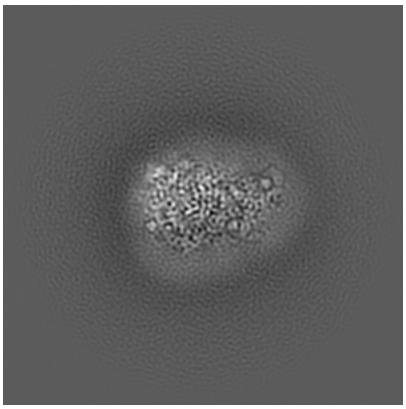
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

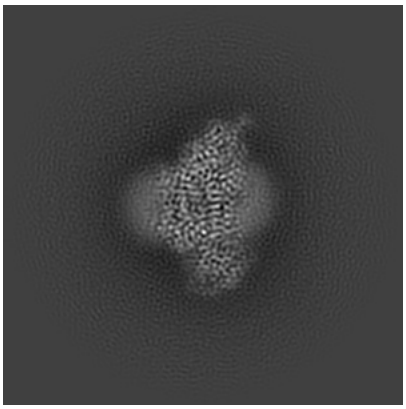
6.1.1 Primary map



X

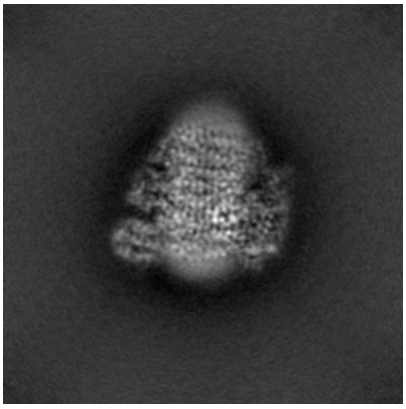


Y

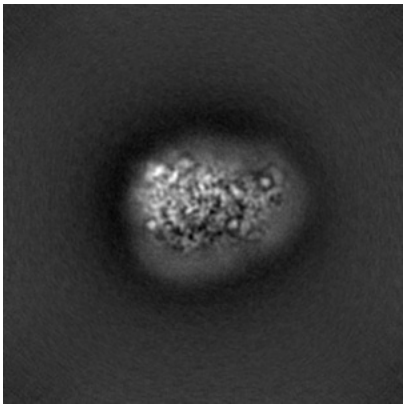


Z

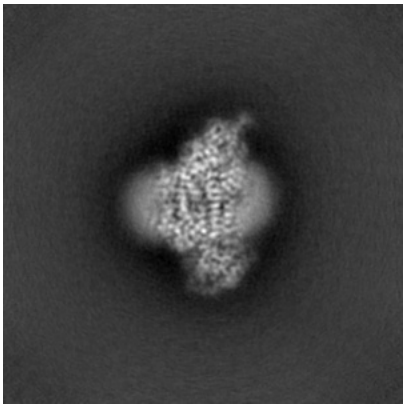
6.1.2 Raw map



X



Y

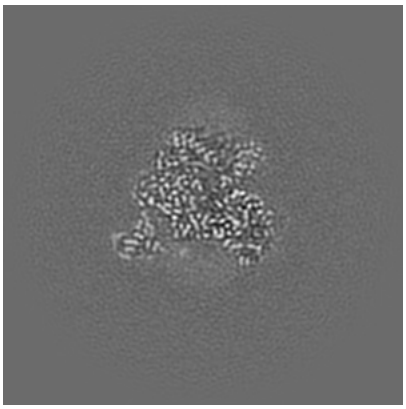


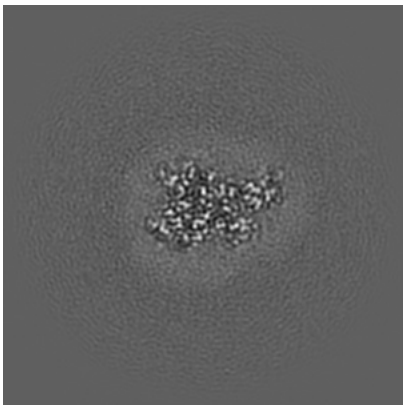
Z

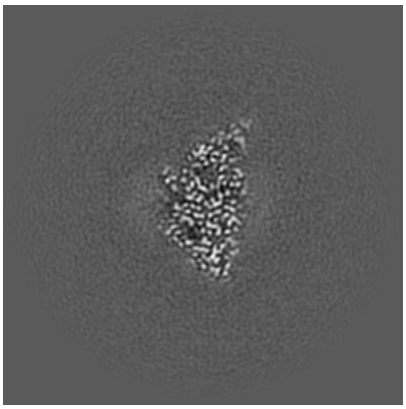
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

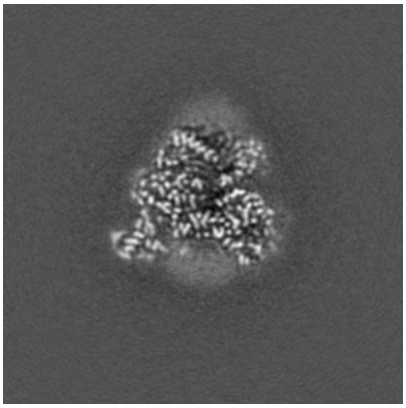
6.2.1 Primary map

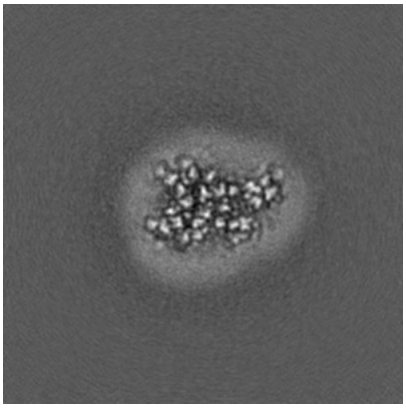

X Index: 128

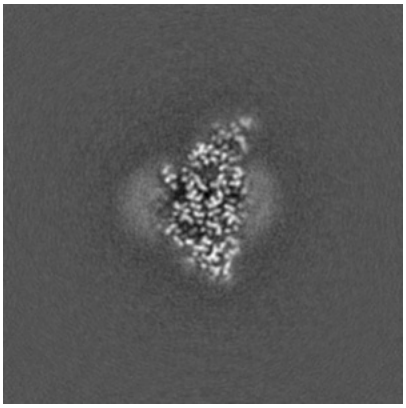

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

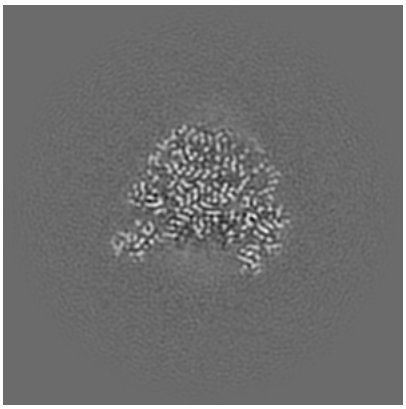

Y Index: 128

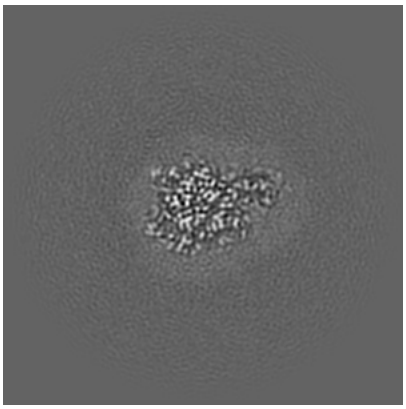

Z Index: 128

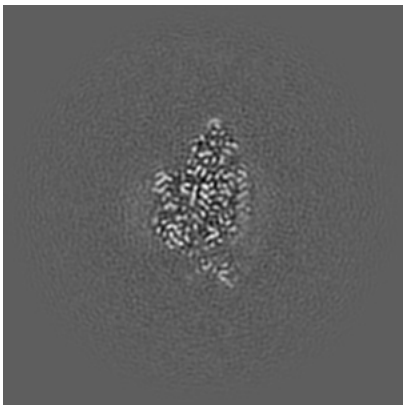
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

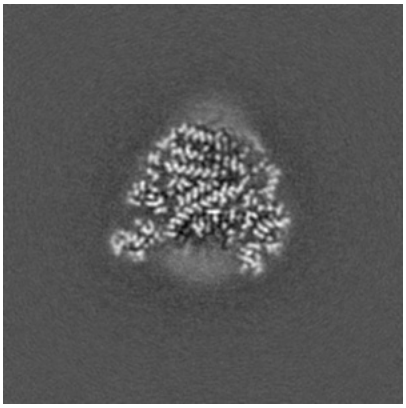
6.3.1 Primary map

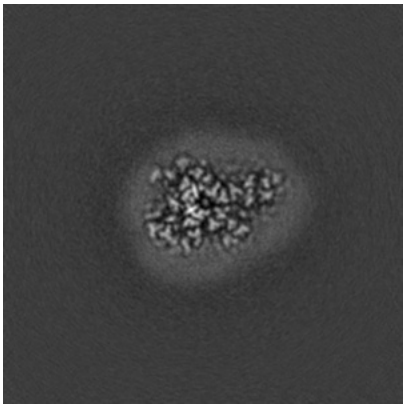

X Index: 135

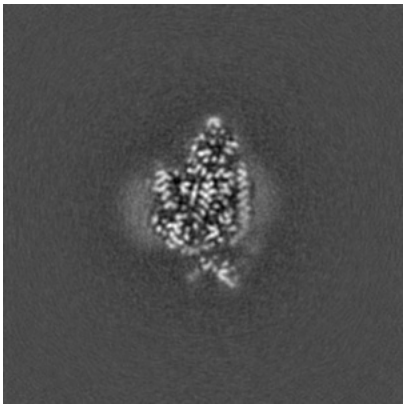

Y Index: 140


Z Index: 117

6.3.2 Raw map


X Index: 135


Y Index: 136


Z Index: 117

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 1.07. 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.

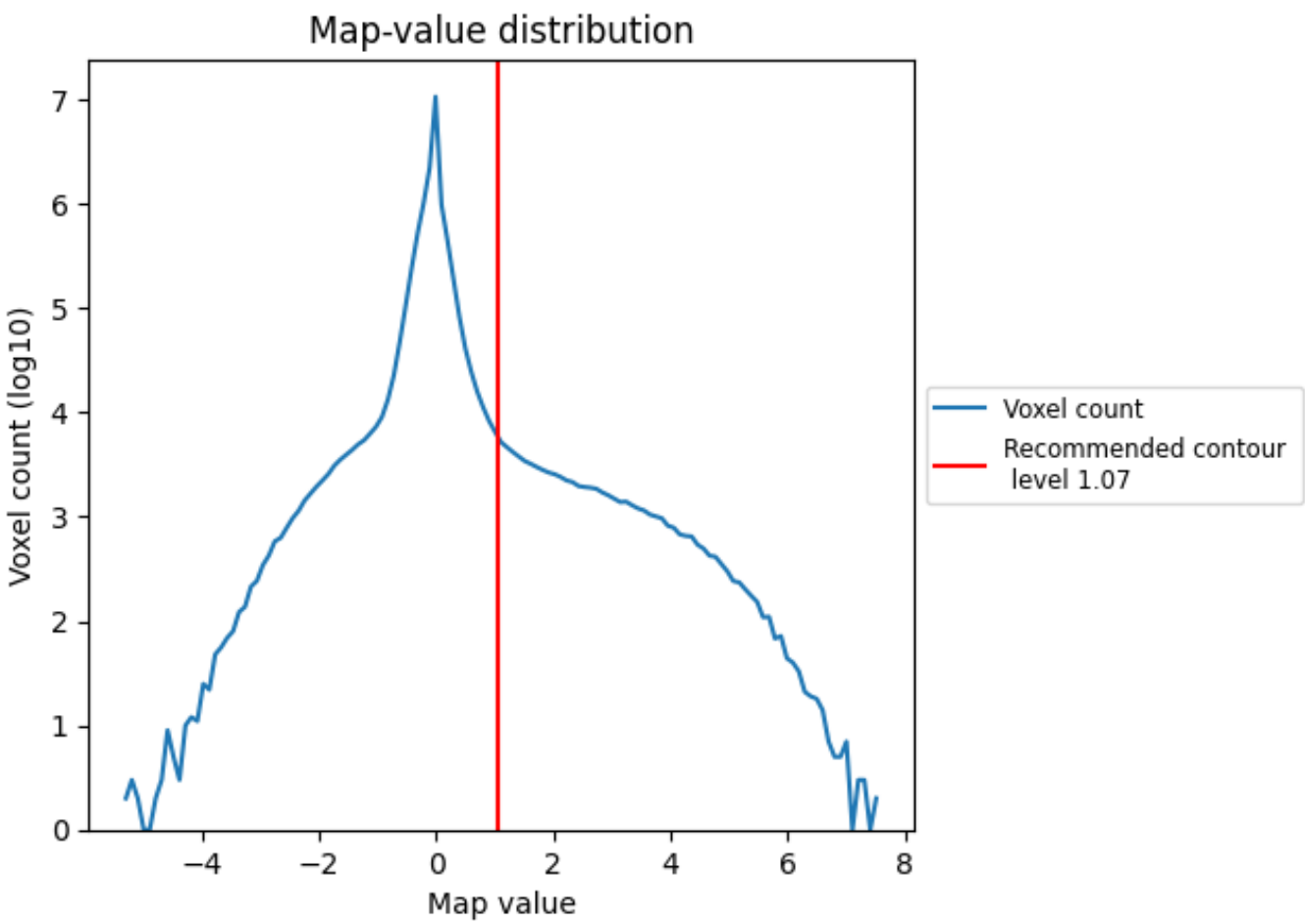
6.5 Mask visualisation (i)

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

7 Map analysis (i)

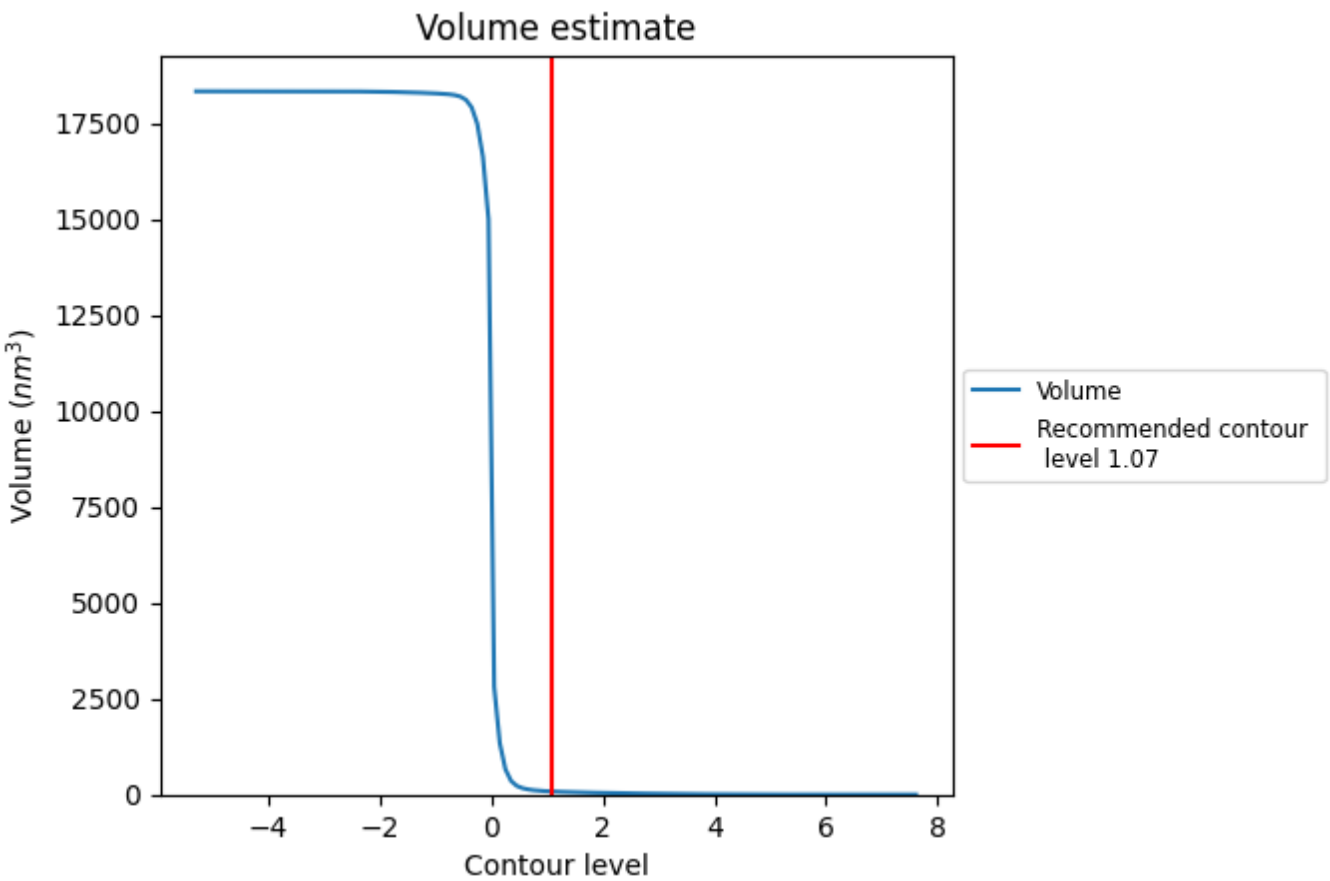
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

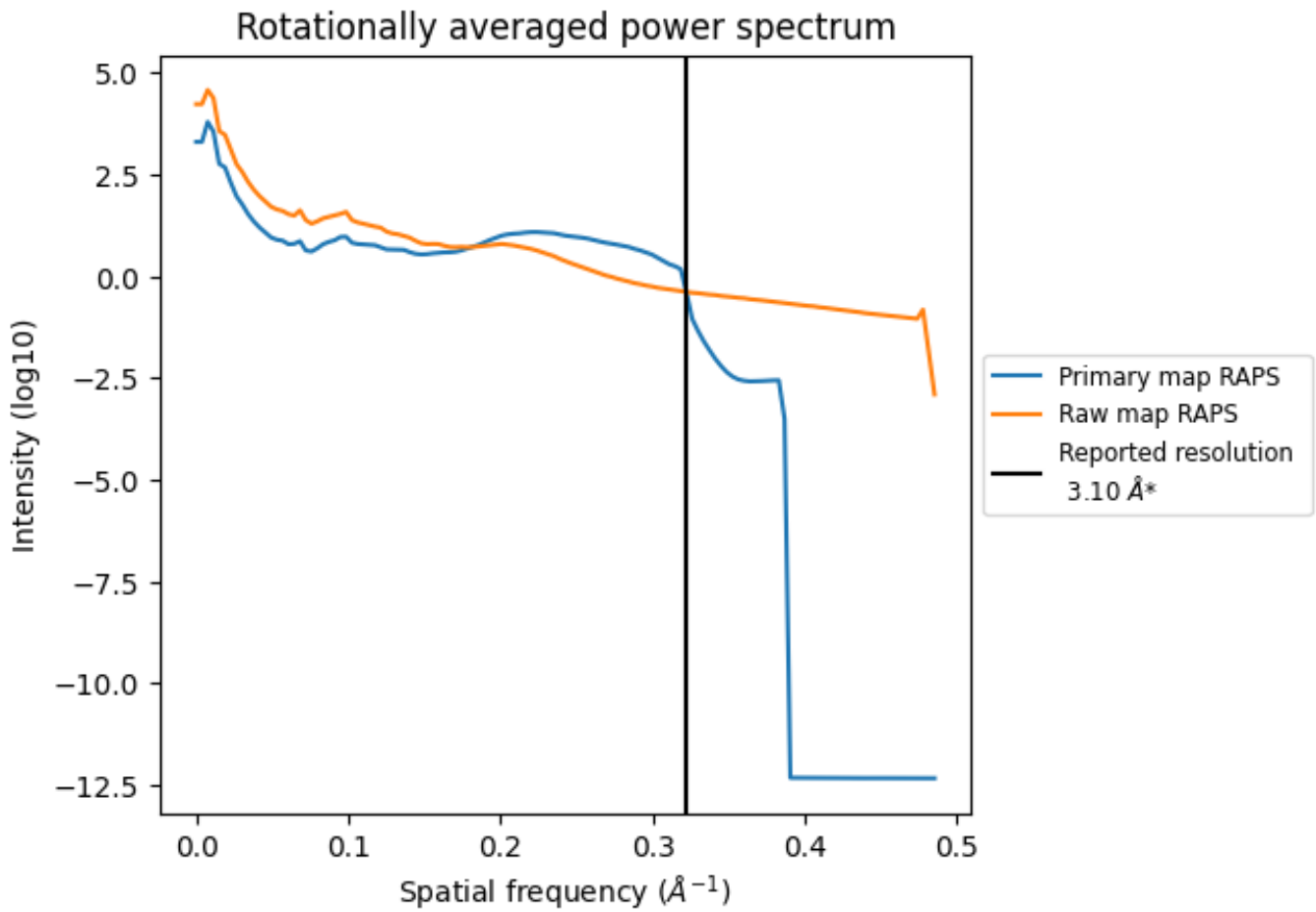
7.2 Volume estimate (i)



The volume at the recommended contour level is 81 nm^3; this corresponds to an approximate mass of 73 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)

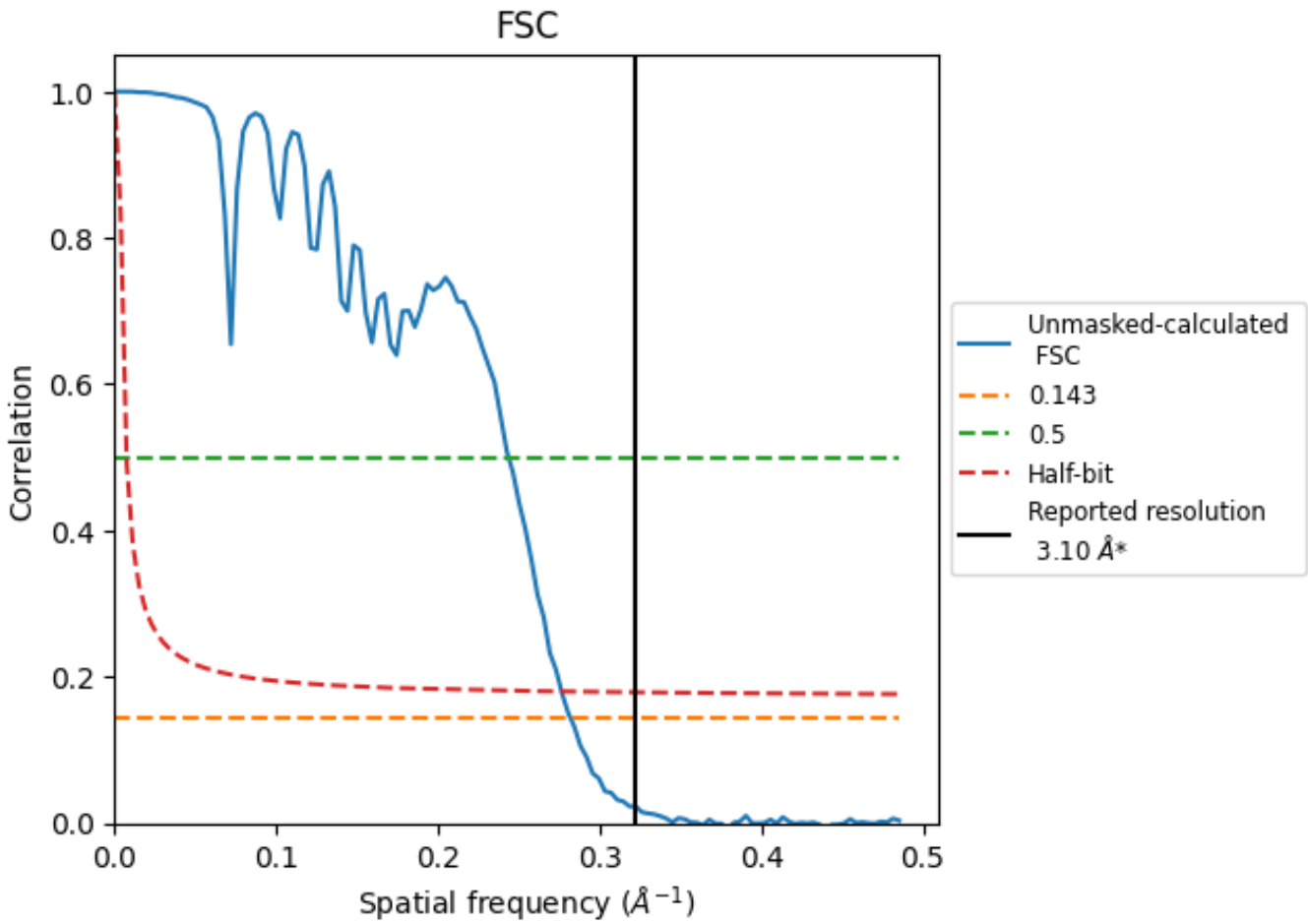


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



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

8.2 Resolution estimates (i)

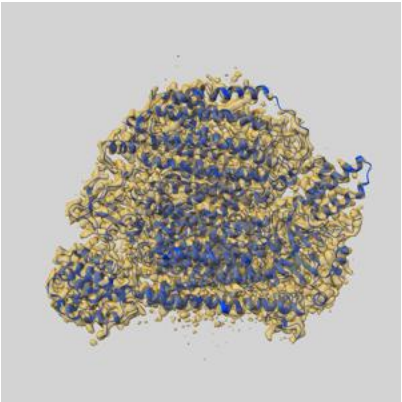
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.10	3.62

*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 3.54 differs from the reported value 3.1 by more than 10 %

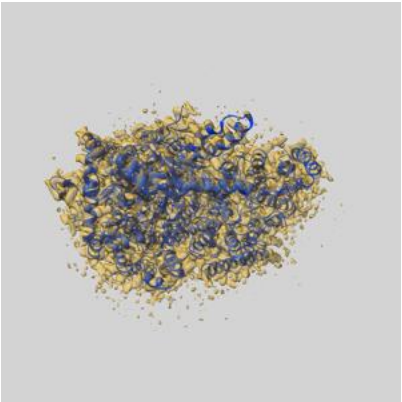
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-27196 and PDB model 8D4T. Per-residue inclusion information can be found in section 3 on page 9.

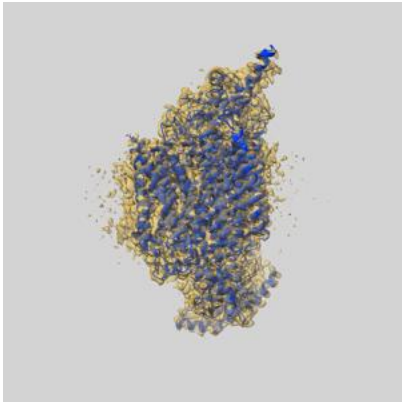
9.1 Map-model overlay (i)



X



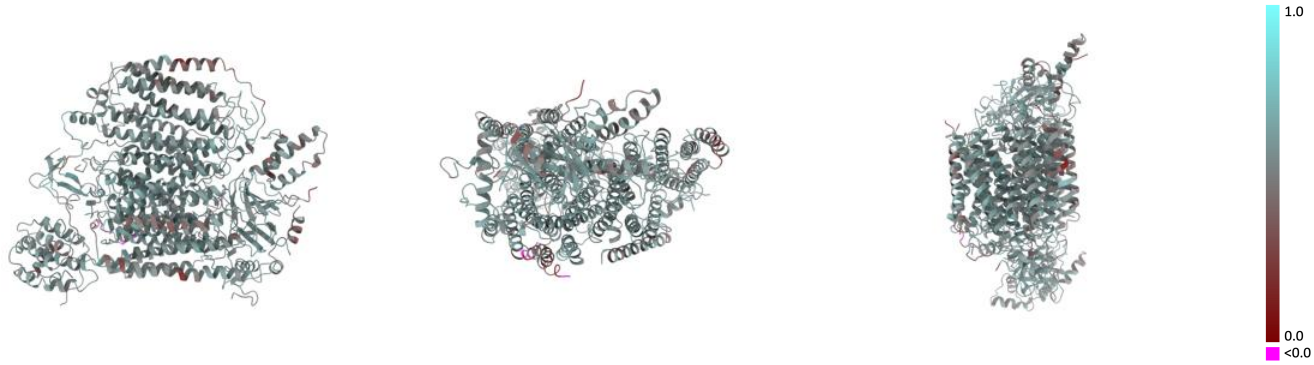
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.07 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.

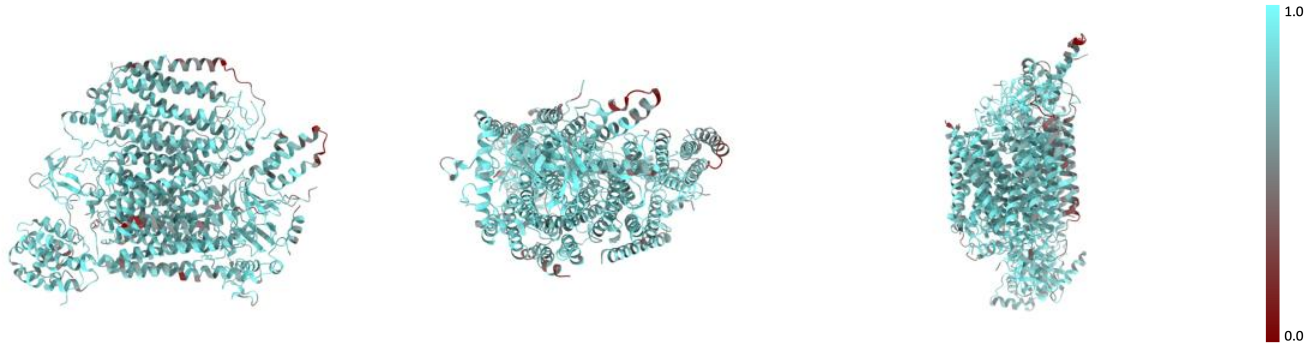
9.2 Q-score mapped to coordinate model (i)



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.

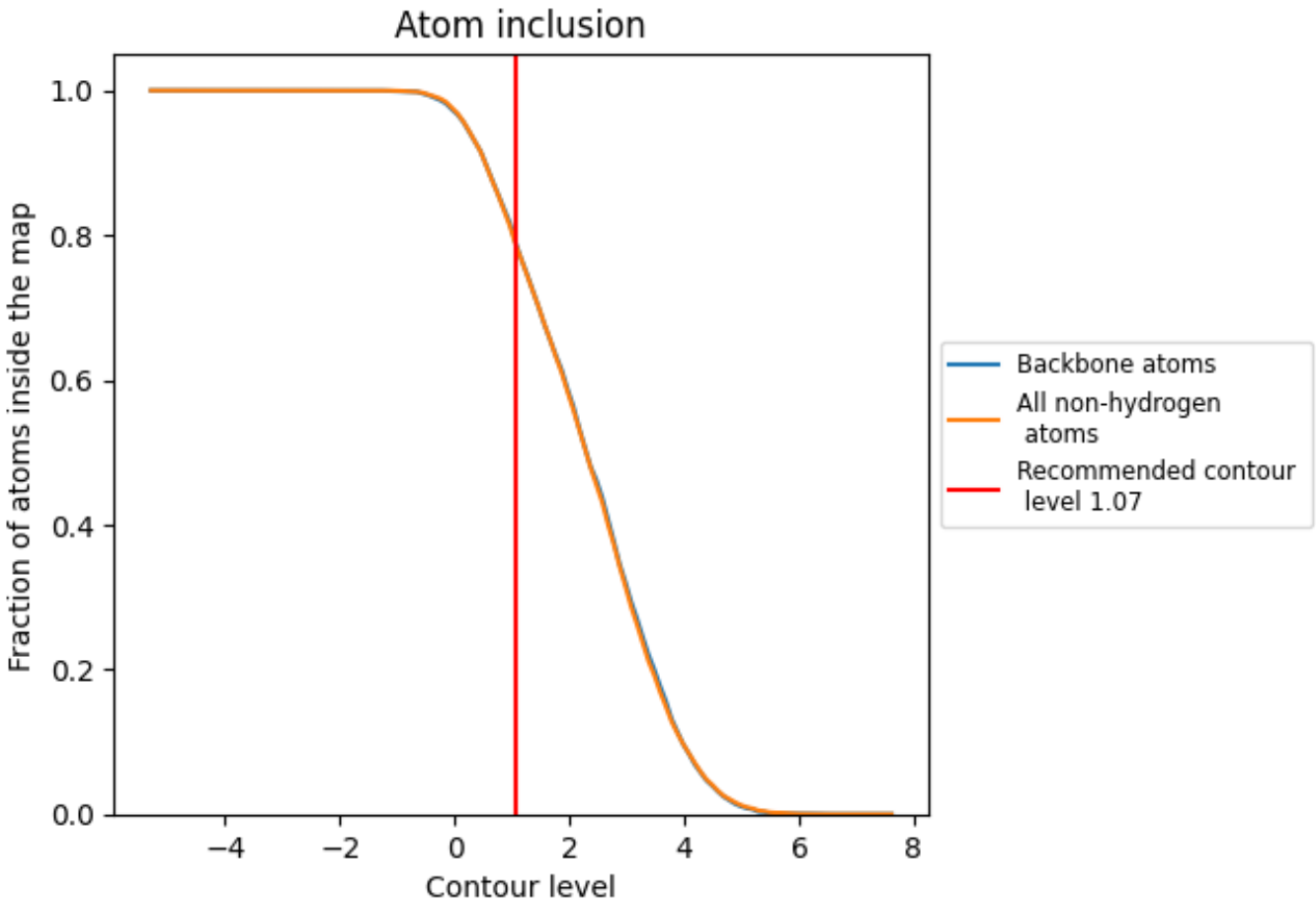
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.07).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7852	0.5450
M	0.5684	0.2740
N	0.8532	0.5790
O	0.7820	0.5460
P	0.8023	0.5530
Q	0.7853	0.5260
R	0.7801	0.5360
S	0.7736	0.5560
T	0.6788	0.5180
U	0.6957	0.5160
V	0.7509	0.5090
W	0.7300	0.5060
X	0.8292	0.5620
Y	0.8503	0.5850