Full wwPDB EM Validation Report (i)

Nov 2, 2022 – 09:21 AM EDT

PDB ID	:	5TV4
EMDB ID	:	EMD-8469
Title	:	3D cryo-EM reconstruction of nucleotide-free MsbA in lipid nanodisc
Authors	:	Mi, W.; Walz, T.; Liao, M.
Deposited on	:	2016-11-08
Resolution	:	4.20 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 (i)) were used in the production of this report:

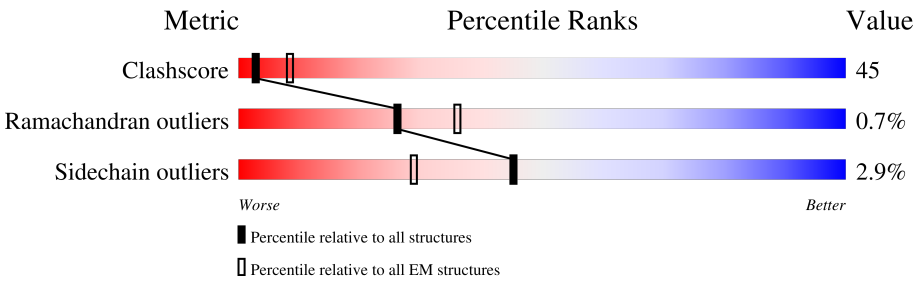
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 4.20 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	A	605	23% 60% 33% • 6%
1	B	605	21% 62% 31% • 6%
2	C	7	14% 100%

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
2	PA1	C	2	X	-	X	-
2	KDO	C	3	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GMH	C	4	-	-	X	-
2	KDO	C	7	-	-	X	-
3	PO4	A	608	-	-	X	-
3	PO4	B	601	-	-	X	-
4	FTT	B	604	-	-	X	-
4	FTT	B	606	-	-	X	-
4	FTT	B	607	-	-	X	-
6	DAO	B	605	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6548 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 Lipid A export ATP-binding/permease protein MsbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	570	3205	1990	614	592	9	0	0
1	B	570	3180	1955	618	600	7	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P60753
A	-21	GLY	-	expression tag	UNP P60753
A	-20	HIS	-	expression tag	UNP P60753
A	-19	HIS	-	expression tag	UNP P60753
A	-18	HIS	-	expression tag	UNP P60753
A	-17	HIS	-	expression tag	UNP P60753
A	-16	HIS	-	expression tag	UNP P60753
A	-15	HIS	-	expression tag	UNP P60753
A	-14	HIS	-	expression tag	UNP P60753
A	-13	HIS	-	expression tag	UNP P60753
A	-12	HIS	-	expression tag	UNP P60753
A	-11	HIS	-	expression tag	UNP P60753
A	-10	SER	-	expression tag	UNP P60753
A	-9	SER	-	expression tag	UNP P60753
A	-8	GLY	-	expression tag	UNP P60753
A	-7	HIS	-	expression tag	UNP P60753
A	-6	ILE	-	expression tag	UNP P60753
A	-5	ASP	-	expression tag	UNP P60753
A	-4	ASP	-	expression tag	UNP P60753
A	-3	ASP	-	expression tag	UNP P60753
A	-2	ASP	-	expression tag	UNP P60753
A	-1	LYS	-	expression tag	UNP P60753
A	0	HIS	-	expression tag	UNP P60753
B	-22	MET	-	initiating methionine	UNP P60753
B	-21	GLY	-	expression tag	UNP P60753
B	-20	HIS	-	expression tag	UNP P60753

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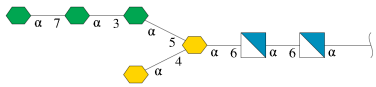
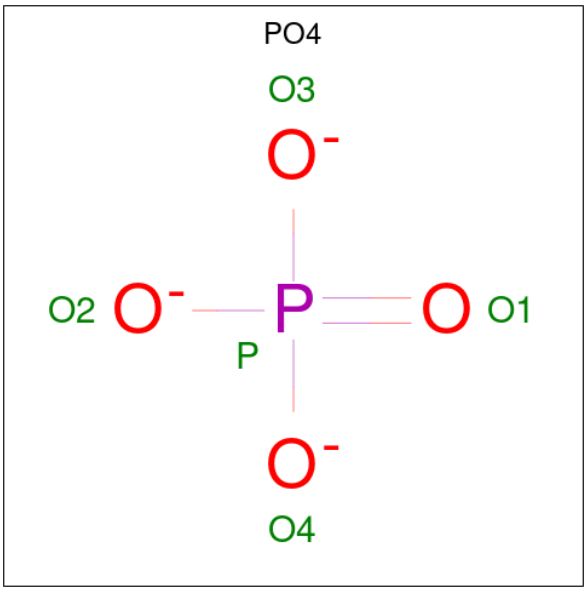
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	HIS	-	expression tag	UNP P60753
B	-18	HIS	-	expression tag	UNP P60753
B	-17	HIS	-	expression tag	UNP P60753
B	-16	HIS	-	expression tag	UNP P60753
B	-15	HIS	-	expression tag	UNP P60753
B	-14	HIS	-	expression tag	UNP P60753
B	-13	HIS	-	expression tag	UNP P60753
B	-12	HIS	-	expression tag	UNP P60753
B	-11	HIS	-	expression tag	UNP P60753
B	-10	SER	-	expression tag	UNP P60753
B	-9	SER	-	expression tag	UNP P60753
B	-8	GLY	-	expression tag	UNP P60753
B	-7	HIS	-	expression tag	UNP P60753
B	-6	ILE	-	expression tag	UNP P60753
B	-5	ASP	-	expression tag	UNP P60753
B	-4	ASP	-	expression tag	UNP P60753
B	-3	ASP	-	expression tag	UNP P60753
B	-2	ASP	-	expression tag	UNP P60753
B	-1	LYS	-	expression tag	UNP P60753
B	0	HIS	-	expression tag	UNP P60753

- Molecule 2 is an oligosaccharide called L-glycero-alpha-D-manno-heptopyranose-(1-7)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose.



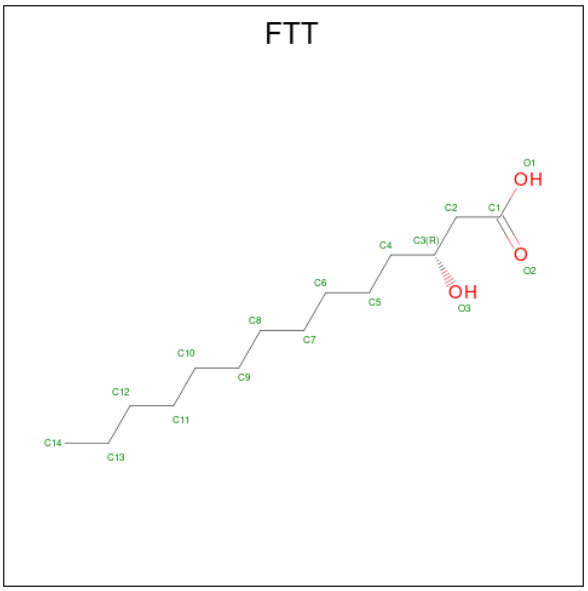
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	7	91	49	2	40	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



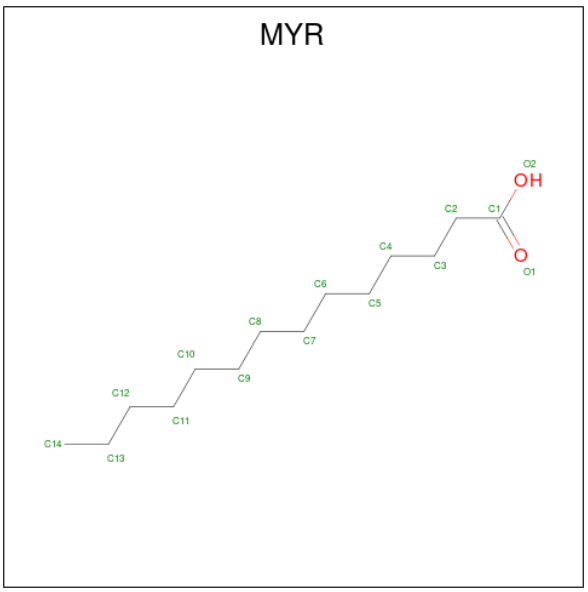
Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
3	A	1	12	9	3	0
			Total	O	P	
3	A	1	12	9	3	0
			Total	O	P	
3	A	1	12	9	3	0
			Total	O	P	
3	B	1	4	3	1	0

- Molecule 4 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: $C_{14}H_{28}O_3$).



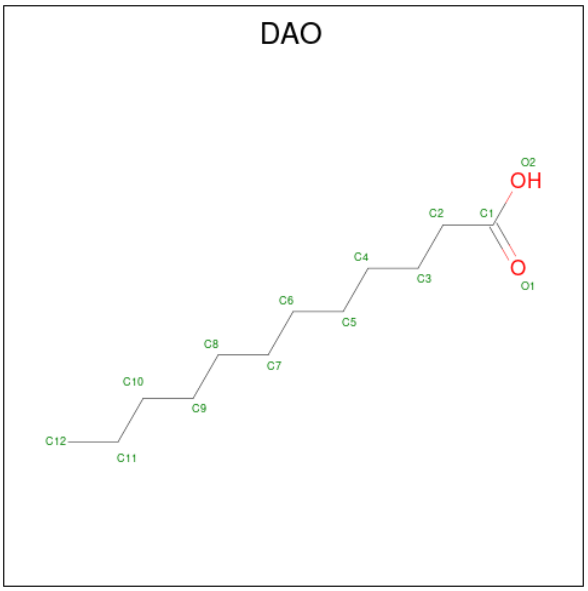
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	B	1	42	34	8	0
4	B	1	42	34	8	0
4	B	1	42	34	8	0
4	B	1	42	34	8	0

- Molecule 5 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	B	1	6	5	1	0

- Molecule 6 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



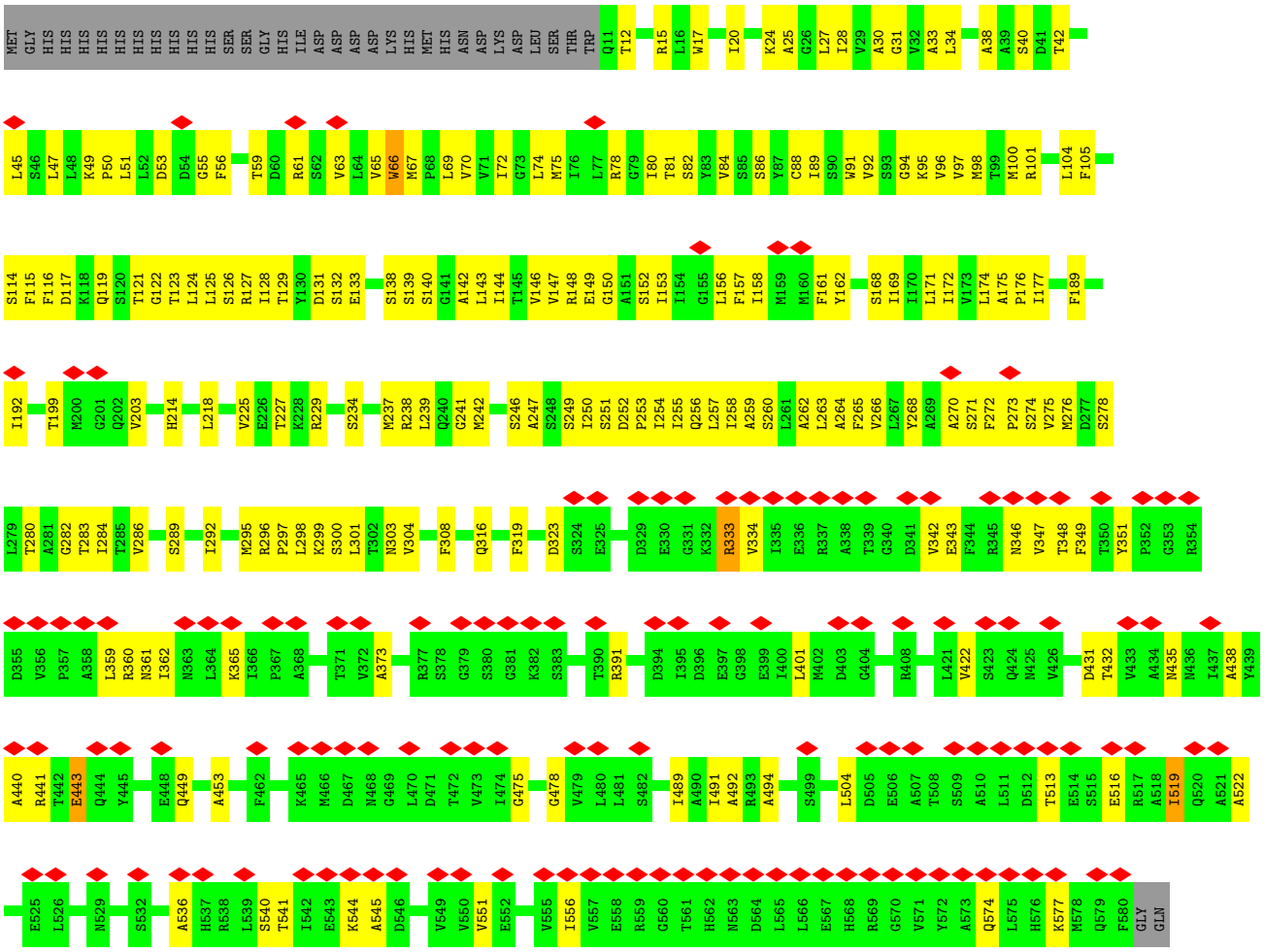
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	B	1	8	7	1	0

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.

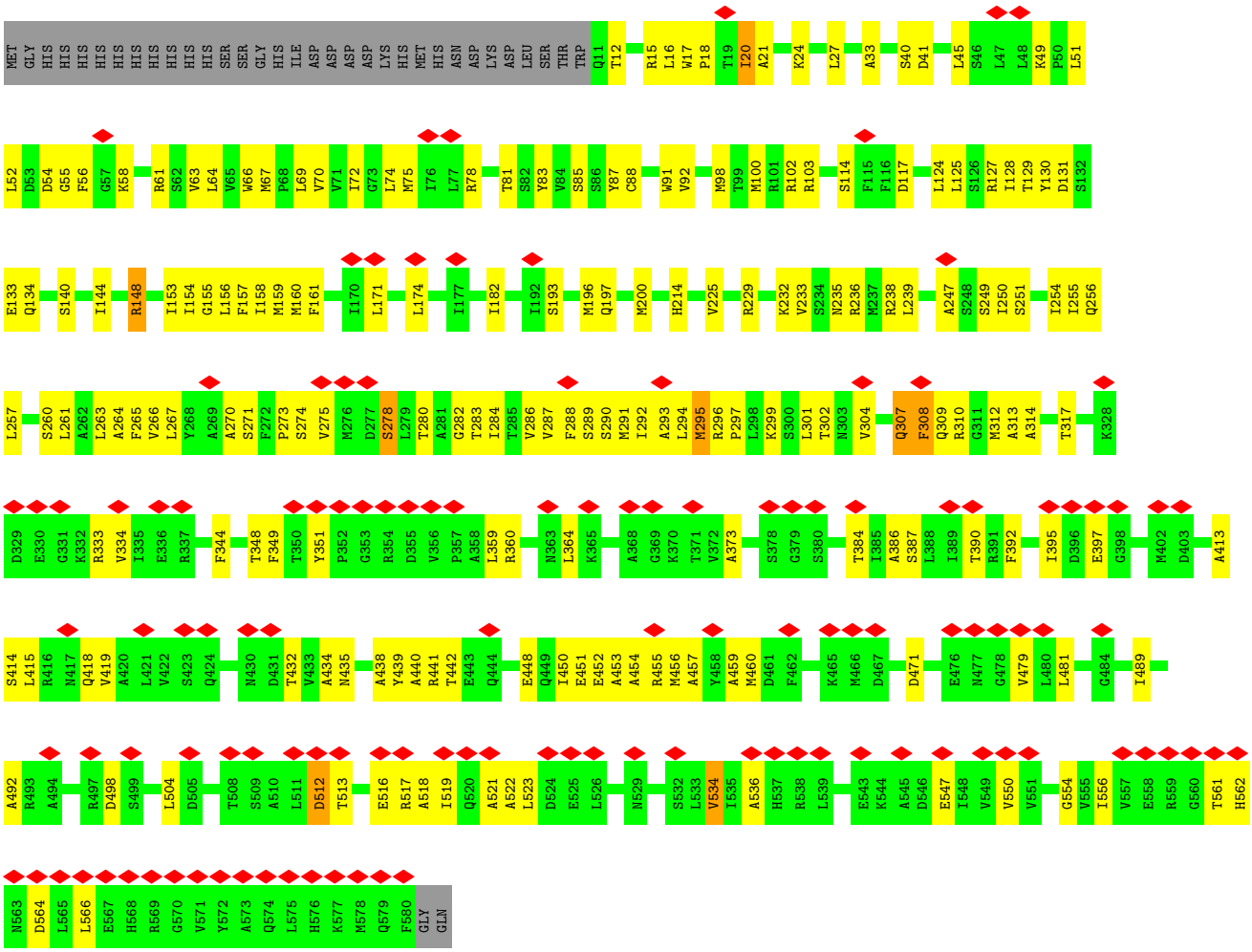
• Molecule 1: Lipid A export ATP-binding/permease protein MsbA

Chain A:



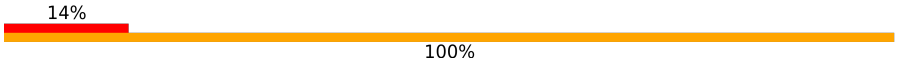
• Molecule 1: Lipid A export ATP-binding/permease protein MsbA

Chain B:



• Molecule 2: L-glycero-alpha-D-manno-heptopyranose-(1-7)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67220	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	236.16, 236.16, 236.16	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	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: FTT, MYR, KDO, PA1, DAO, GMH, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.31	0/3228	0.60	0/4455
1	B	0.34	0/3205	0.61	1/4432 (0.0%)
All	All	0.33	0/6433	0.60	1/8887 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	7
All	All	0	10

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	45	LEU	CA-CB-CG	-5.77	102.02	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	ARG	Peptide
1	A	351	TYR	Peptide
1	A	391	ARG	Peptide
1	B	20	ILE	Peptide
1	B	278	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	351	TYR	Peptide
1	B	395	ILE	Peptide
1	B	471	ASP	Peptide
1	B	498	ASP	Peptide
1	B	512	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3205	0	2134	245	0
1	B	3180	0	2031	236	0
2	C	91	0	66	36	0
3	A	12	0	0	5	0
3	B	4	0	0	2	0
4	B	42	0	53	45	0
5	B	6	0	6	0	0
6	B	8	0	10	12	0
All	All	6548	0	4300	489	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 45.

All (489) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ARG:CB	4:B:604:FTT:H41	1.26	1.61
1:B:256:GLN:HE22	4:B:607:FTT:C4	1.12	1.55
1:A:157:PHE:HD2	1:A:161:PHE:CZ	1.29	1.49
1:A:157:PHE:CD2	1:A:161:PHE:CZ	2.09	1.40
1:A:157:PHE:HD2	1:A:161:PHE:CE2	1.40	1.38
1:B:256:GLN:NE2	4:B:607:FTT:H42	1.01	1.32
1:B:295:MET:CE	1:B:299:LYS:HB2	1.63	1.28
1:B:296:ARG:HB2	4:B:604:FTT:C4	1.63	1.28
1:B:196:MET:O	1:B:200:MET:HG3	1.14	1.24
1:B:196:MET:O	1:B:200:MET:CG	1.83	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PHE:CD2	1:A:161:PHE:CE2	2.27	1.20
1:A:266:VAL:O	1:A:270:ALA:HB3	1.38	1.20
1:B:296:ARG:CB	4:B:604:FTT:C4	2.21	1.16
1:B:196:MET:C	1:B:200:MET:HE3	1.65	1.16
1:A:81:THR:O	1:A:84:VAL:HG12	1.45	1.14
1:B:296:ARG:HG2	4:B:604:FTT:C2	1.77	1.13
1:A:129:THR:O	1:A:133:GLU:CB	1.95	1.13
1:A:94:GLY:CA	1:B:238:ARG:HG3	1.79	1.13
1:B:293:ALA:HA	4:B:604:FTT:C5	1.77	1.12
1:A:153:ILE:O	1:A:157:PHE:HD1	1.31	1.12
1:A:94:GLY:HA3	1:B:238:ARG:HG3	1.23	1.11
1:B:295:MET:HE1	1:B:299:LYS:HB2	1.22	1.11
1:B:296:ARG:HB3	4:B:604:FTT:H41	1.33	1.10
1:A:301:LEU:O	1:A:304:VAL:HG12	1.52	1.09
1:B:182:ILE:HD12	1:B:302:THR:OG1	1.52	1.07
2:C:3:KDO:H5	2:C:7:KDO:H6	1.32	1.06
1:A:121:THR:O	1:A:125:LEU:CB	2.05	1.04
1:B:197:GLN:CA	1:B:200:MET:HE3	1.86	1.04
1:B:292:ILE:HG21	6:B:605:DAO:C4	1.89	1.03
1:B:292:ILE:HD11	4:B:606:FTT:H92	1.37	1.03
1:B:297:PRO:O	1:B:301:LEU:HG	1.57	1.03
1:B:196:MET:O	1:B:200:MET:HE3	1.59	1.02
1:A:161:PHE:CD1	1:A:168:SER:CB	2.43	1.02
1:B:295:MET:HE1	1:B:299:LYS:CB	1.90	1.02
1:B:292:ILE:HG21	6:B:605:DAO:H41	1.36	1.02
1:B:292:ILE:CG2	6:B:605:DAO:H31	1.90	1.01
1:B:292:ILE:HG21	6:B:605:DAO:C3	1.91	1.01
1:B:196:MET:C	1:B:200:MET:CE	2.28	1.00
1:B:434:ALA:O	1:B:438:ALA:HB3	1.61	1.00
1:A:157:PHE:CD2	1:A:161:PHE:HZ	1.77	1.00
1:B:197:GLN:HA	1:B:200:MET:HE3	1.39	1.00
1:A:153:ILE:O	1:A:157:PHE:CD1	2.16	0.99
2:C:3:KDO:C5	2:C:7:KDO:H6	1.94	0.98
1:A:257:LEU:HD12	1:B:75:MET:HB3	1.45	0.97
1:B:197:GLN:N	1:B:200:MET:HE3	1.78	0.97
1:A:161:PHE:CE1	1:A:168:SER:CB	2.48	0.97
2:C:3:KDO:C3	2:C:4:GMH:H72	1.95	0.96
1:B:296:ARG:CG	4:B:604:FTT:H22	1.93	0.96
1:B:295:MET:HE3	1:B:299:LYS:HB2	1.45	0.96
1:B:296:ARG:HG2	4:B:604:FTT:H22	0.96	0.95
1:A:42:THR:HG23	1:A:156:LEU:HD23	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3:KDO:O5	2:C:7:KDO:O8	1.85	0.95
1:A:256:GLN:OE1	1:B:78:ARG:NH2	2.01	0.94
1:A:158:ILE:O	1:A:162:TYR:CB	2.15	0.93
2:C:3:KDO:H32	2:C:4:GMH:H72	1.48	0.93
2:C:6:GMH:O3	2:C:7:KDO:O1B	1.85	0.93
2:C:4:GMH:O7	2:C:7:KDO:O1A	1.85	0.91
1:A:257:LEU:HD11	1:B:75:MET:C	1.90	0.91
1:A:255:ILE:O	1:A:258:ILE:HG13	1.69	0.90
1:A:257:LEU:CD1	1:B:75:MET:HB3	2.01	0.90
1:B:197:GLN:HA	1:B:200:MET:CE	2.01	0.90
1:A:296:ARG:HD2	4:B:606:FTT:O2	1.71	0.89
1:B:256:GLN:NE2	4:B:607:FTT:C4	1.90	0.89
1:B:307:GLN:O	1:B:309:GLN:N	2.05	0.88
1:B:289:SER:O	1:B:293:ALA:HB3	1.74	0.86
1:B:454:ALA:HA	1:B:459:ALA:HB3	1.55	0.86
1:A:94:GLY:HA3	1:B:238:ARG:CG	1.96	0.85
1:B:452:GLU:O	1:B:456:MET:N	2.08	0.85
2:C:4:GMH:O2	2:C:7:KDO:H7	1.76	0.85
1:A:89:ILE:O	1:A:92:VAL:HG12	1.77	0.85
1:A:92:VAL:HG22	1:A:96:VAL:CG2	2.06	0.85
1:A:125:LEU:O	1:A:128:ILE:HG12	1.76	0.84
1:A:148:ARG:C	1:A:149:GLU:CA	2.46	0.83
1:A:161:PHE:HD1	1:A:168:SER:CB	1.92	0.83
1:B:196:MET:O	1:B:200:MET:CE	2.27	0.83
1:B:307:GLN:C	1:B:309:GLN:H	1.81	0.82
1:B:373:ALA:HB1	1:B:536:ALA:HB2	1.61	0.82
3:A:608:PO4:O3	2:C:1:PA1:N2	2.13	0.82
1:A:250:ILE:HG22	1:B:83:TYR:CE1	2.14	0.82
1:A:257:LEU:CD1	1:B:75:MET:O	2.28	0.81
1:A:157:PHE:HB3	1:A:161:PHE:CE2	2.16	0.81
1:A:257:LEU:HD11	1:B:75:MET:O	1.80	0.81
1:B:292:ILE:CD1	4:B:606:FTT:H92	2.10	0.81
1:A:42:THR:CG2	1:A:156:LEU:HD23	2.10	0.81
1:A:349:PHE:N	1:A:359:LEU:O	2.10	0.81
1:A:519:ILE:O	1:A:522:ALA:N	2.13	0.80
2:C:4:GMH:O2	2:C:5:GMH:O5	1.98	0.80
1:A:63:VAL:O	1:A:66:TRP:CD1	2.35	0.79
1:B:304:VAL:O	1:B:307:GLN:HG2	1.82	0.79
1:A:225:VAL:O	1:A:229:ARG:CB	2.31	0.78
1:B:49:LYS:O	1:B:52:LEU:N	2.17	0.78
1:B:263:LEU:HD22	4:B:607:FTT:C9	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ILE:CD1	1:B:302:THR:OG1	2.30	0.78
1:A:66:TRP:HD1	1:A:67:MET:N	1.82	0.78
1:A:234:SER:O	1:A:237:MET:N	2.16	0.78
1:B:296:ARG:HB2	4:B:604:FTT:H41	0.78	0.78
1:A:260:SER:HB3	1:B:72:ILE:HD13	1.65	0.77
1:B:197:GLN:N	1:B:200:MET:CE	2.45	0.77
2:C:3:KDO:H31	2:C:4:GMH:O5	1.85	0.77
1:A:66:TRP:CD1	1:A:67:MET:N	2.54	0.76
1:A:157:PHE:CE2	1:A:161:PHE:HZ	2.02	0.76
1:A:115:PHE:O	1:A:119:GLN:CG	2.34	0.75
1:B:263:LEU:HD12	1:B:291:MET:CB	2.15	0.75
1:A:61:ARG:O	1:A:65:VAL:CB	2.35	0.75
1:A:304:VAL:O	1:A:308:PHE:HB2	1.88	0.74
1:B:290:SER:O	1:B:294:LEU:CB	2.35	0.74
1:B:288:PHE:CE1	4:B:606:FTT:C14	2.70	0.74
1:A:42:THR:OG1	1:A:156:LEU:HD23	1.87	0.73
6:B:605:DAO:C1	2:C:2:PA1:HN21	2.01	0.73
1:A:92:VAL:HG22	1:A:96:VAL:HG23	1.70	0.73
3:A:608:PO4:O4	2:C:1:PA1:H3	1.86	0.73
1:A:92:VAL:HG22	1:A:96:VAL:HG21	1.69	0.73
1:B:434:ALA:O	1:B:438:ALA:CB	2.36	0.73
1:A:42:THR:CB	1:A:156:LEU:HD23	2.19	0.73
1:A:144:ILE:O	1:A:148:ARG:HB3	1.88	0.73
1:B:292:ILE:HD11	4:B:606:FTT:C9	2.14	0.73
1:A:168:SER:O	1:A:171:LEU:N	2.21	0.72
1:A:20:ILE:HD12	1:A:96:VAL:HG13	1.70	0.72
1:A:283:THR:O	1:A:286:VAL:HG22	1.88	0.72
1:A:252:ASP:HA	1:A:255:ILE:CG2	2.18	0.72
1:A:274:SER:CA	1:A:278:SER:CB	2.68	0.72
1:A:66:TRP:HD1	1:A:67:MET:H	1.37	0.72
1:A:144:ILE:O	1:A:148:ARG:CB	2.37	0.72
1:B:414:SER:O	1:B:418:GLN:CB	2.37	0.72
1:B:288:PHE:CE1	4:B:606:FTT:H142	2.25	0.71
1:B:266:VAL:O	1:B:270:ALA:N	2.16	0.71
1:A:161:PHE:HE1	1:A:168:SER:CB	2.02	0.71
1:A:274:SER:HA	1:A:278:SER:CB	2.20	0.71
1:B:415:LEU:O	1:B:419:VAL:N	2.24	0.71
1:B:292:ILE:CG2	6:B:605:DAO:C3	2.56	0.70
1:A:252:ASP:N	1:A:253:PRO:CD	2.55	0.70
3:A:609:PO4:O3	2:C:6:GMH:O6	2.09	0.70
1:B:454:ALA:O	1:B:460:MET:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:605:DAO:O1	2:C:2:PA1:N2	2.17	0.70
1:B:263:LEU:HB3	4:B:607:FTT:C9	2.21	0.70
2:C:3:KDO:O1B	2:C:3:KDO:H7	1.92	0.70
1:A:42:THR:OG1	1:A:156:LEU:CD2	2.39	0.70
1:A:274:SER:HA	1:A:278:SER:H	1.56	0.70
1:A:301:LEU:O	1:A:304:VAL:CG1	2.35	0.70
1:A:252:ASP:O	1:A:256:GLN:NE2	2.18	0.70
1:A:254:ILE:HG13	1:A:255:ILE:H	1.57	0.70
1:B:448:GLU:O	1:B:452:GLU:CB	2.39	0.69
1:B:438:ALA:O	1:B:442:THR:CB	2.40	0.69
1:B:197:GLN:CA	1:B:200:MET:CE	2.62	0.69
1:A:116:PHE:HA	1:A:119:GLN:HB2	1.74	0.69
2:C:3:KDO:O7	2:C:7:KDO:O8	2.06	0.69
1:A:80:ILE:HG23	1:A:81:THR:N	2.08	0.69
1:A:94:GLY:HA2	1:B:238:ARG:HG3	1.74	0.69
1:A:249:SER:O	1:A:253:PRO:HG2	1.92	0.68
1:A:257:LEU:CD1	1:B:75:MET:CB	2.71	0.68
1:B:196:MET:O	1:B:200:MET:CB	2.41	0.68
1:A:127:ARG:O	1:A:131:ASP:N	2.22	0.68
1:A:251:SER:O	1:A:254:ILE:HG13	1.94	0.68
1:A:169:ILE:HA	1:A:172:ILE:HG12	1.76	0.68
1:A:257:LEU:HD11	1:B:75:MET:CB	2.24	0.68
1:B:282:GLY:O	1:B:286:VAL:HG23	1.94	0.67
1:A:252:ASP:HA	1:A:255:ILE:HG22	1.76	0.67
1:B:256:GLN:NE2	4:B:607:FTT:C3	2.56	0.67
1:B:158:ILE:O	1:B:161:PHE:HB2	1.94	0.67
1:A:12:THR:O	1:A:15:ARG:N	2.27	0.67
1:A:124:LEU:C	1:A:124:LEU:HD23	2.15	0.67
1:A:91:TRP:CD1	1:A:95:LYS:HG3	2.29	0.67
1:A:116:PHE:HD2	1:B:214:HIS:CE1	2.14	0.66
1:B:292:ILE:CG2	6:B:605:DAO:H41	2.21	0.66
1:B:81:THR:O	1:B:85:SER:HB2	1.96	0.66
1:B:263:LEU:HD13	4:B:607:FTT:C9	2.25	0.66
1:B:439:TYR:O	1:B:441:ARG:N	2.28	0.66
4:B:606:FTT:O3	4:B:607:FTT:O3	2.06	0.66
1:A:115:PHE:O	1:A:119:GLN:HG2	1.95	0.66
1:A:157:PHE:CD2	1:A:161:PHE:HE2	2.10	0.66
1:A:373:ALA:HB1	1:A:536:ALA:HB2	1.78	0.66
1:A:94:GLY:CA	1:B:238:ARG:CG	2.54	0.66
1:A:268:TYR:O	1:A:271:SER:N	2.29	0.65
1:A:273:PRO:C	1:A:278:SER:CB	2.65	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:O	1:A:127:ARG:HG3	1.96	0.65
1:A:255:ILE:O	1:A:258:ILE:CG1	2.45	0.65
1:A:251:SER:O	1:A:255:ILE:HG22	1.96	0.65
1:A:259:ALA:O	1:A:262:ALA:N	2.30	0.65
1:A:263:LEU:O	1:A:266:VAL:N	2.29	0.65
1:A:266:VAL:O	1:A:270:ALA:CB	2.30	0.65
1:A:123:THR:HG23	1:A:124:LEU:N	2.11	0.65
1:B:114:SER:O	1:B:117:ASP:N	2.30	0.64
1:A:81:THR:OG1	1:A:82:SER:N	2.29	0.64
1:A:157:PHE:HB3	1:A:161:PHE:CD2	2.32	0.64
1:B:127:ARG:O	1:B:131:ASP:CB	2.46	0.63
1:A:296:ARG:CD	4:B:606:FTT:O2	2.46	0.63
1:B:296:ARG:CG	4:B:604:FTT:H41	2.20	0.63
1:B:263:LEU:CD1	1:B:291:MET:CB	2.76	0.63
2:C:3:KDO:O5	2:C:7:KDO:H6	1.97	0.63
1:B:296:ARG:HB3	4:B:604:FTT:C4	2.11	0.62
1:B:271:SER:O	1:B:275:VAL:N	2.32	0.62
1:B:288:PHE:HE1	4:B:606:FTT:H142	1.62	0.62
1:B:307:GLN:O	1:B:310:ARG:N	2.30	0.62
1:A:259:ALA:O	1:A:262:ALA:HB3	2.00	0.62
1:B:562:HIS:O	1:B:566:LEU:CB	2.48	0.62
1:A:115:PHE:O	1:A:119:GLN:HG3	1.99	0.61
1:A:242:MET:O	1:A:246:SER:CB	2.48	0.61
1:B:51:LEU:O	1:B:55:GLY:N	2.34	0.61
1:B:292:ILE:HG22	6:B:605:DAO:H31	1.78	0.61
1:B:296:ARG:HB3	1:B:297:PRO:HD3	1.82	0.61
2:C:7:KDO:O7	2:C:7:KDO:O5	2.09	0.61
2:C:2:PA1:H61	2:C:3:KDO:O1A	2.00	0.61
1:B:293:ALA:HB2	6:B:605:DAO:C7	2.31	0.60
1:B:518:ALA:O	1:B:522:ALA:HB3	2.02	0.60
1:A:78:ARG:O	1:A:81:THR:OG1	2.18	0.60
1:A:257:LEU:HD13	1:B:75:MET:O	2.00	0.60
1:B:81:THR:O	1:B:85:SER:CB	2.49	0.60
1:A:273:PRO:O	1:A:278:SER:N	2.34	0.60
1:A:189:PHE:O	1:A:192:ILE:N	2.34	0.60
1:B:41:ASP:CB	4:B:602:FTT:C6	2.80	0.59
1:A:152:SER:O	1:A:156:LEU:HG	2.02	0.59
1:B:387:SER:HA	1:B:392:PHE:H	1.67	0.59
1:A:101:ARG:HD3	1:A:132:SER:CB	2.32	0.59
1:A:250:ILE:C	1:A:253:PRO:HD2	2.22	0.59
1:A:123:THR:HG23	1:A:124:LEU:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:O	1:A:128:ILE:HG23	2.03	0.59
1:B:307:GLN:C	1:B:309:GLN:N	2.49	0.59
2:C:3:KDO:H31	2:C:4:GMH:H72	1.84	0.59
1:A:274:SER:N	1:A:278:SER:CB	2.65	0.59
1:B:296:ARG:CG	4:B:604:FTT:C2	2.68	0.59
1:A:114:SER:O	1:A:117:ASP:N	2.35	0.59
1:A:24:LYS:O	1:A:27:LEU:HB3	2.03	0.58
1:A:343:GLU:CB	1:A:401:LEU:O	2.52	0.58
1:B:125:LEU:HA	1:B:128:ILE:HG12	1.85	0.58
1:A:273:PRO:HA	1:A:276:MET:HG2	1.86	0.58
1:A:273:PRO:O	1:A:278:SER:CB	2.52	0.58
1:A:138:SER:O	1:A:142:ALA:HB2	2.03	0.58
1:A:146:VAL:HB	1:A:304:VAL:HG21	1.85	0.58
1:B:128:ILE:HG13	1:B:129:THR:N	2.19	0.58
2:C:3:KDO:H7	2:C:3:KDO:C1	2.32	0.58
1:A:17:TRP:O	1:A:20:ILE:N	2.34	0.57
1:A:250:ILE:HG22	1:B:83:TYR:HE1	1.65	0.57
1:B:263:LEU:CB	4:B:607:FTT:C9	2.82	0.57
1:A:92:VAL:O	1:A:96:VAL:N	2.27	0.57
1:A:272:PHE:O	1:A:275:VAL:HG12	2.03	0.57
1:A:199:THR:O	1:A:203:VAL:HG12	2.03	0.57
1:B:295:MET:CE	1:B:299:LYS:CB	2.54	0.57
1:A:274:SER:HA	1:A:278:SER:N	2.20	0.57
1:B:288:PHE:CD1	4:B:606:FTT:H132	2.39	0.57
1:A:276:MET:O	1:A:276:MET:HG3	2.05	0.57
1:B:196:MET:O	1:B:200:MET:SD	2.63	0.57
1:B:284:ILE:O	1:B:287:VAL:HG22	2.04	0.57
1:B:292:ILE:CG2	6:B:605:DAO:C4	2.75	0.57
1:B:15:ARG:O	1:B:18:PRO:HD2	2.04	0.57
1:A:122:GLY:O	1:A:126:SER:CB	2.53	0.56
1:A:541:THR:O	1:A:545:ALA:N	2.25	0.56
1:A:42:THR:HA	1:A:156:LEU:CD2	2.35	0.56
1:A:254:ILE:HG13	1:A:255:ILE:N	2.19	0.56
1:A:289:SER:HA	1:A:292:ILE:HG22	1.86	0.56
1:B:247:ALA:O	1:B:250:ILE:HG12	2.05	0.56
1:B:348:THR:O	1:B:397:GLU:N	2.38	0.56
1:A:97:VAL:O	1:A:101:ARG:HG2	2.06	0.56
1:B:154:ILE:HG13	1:B:155:GLY:N	2.20	0.55
1:A:127:ARG:O	1:A:131:ASP:CB	2.55	0.55
1:A:214:HIS:O	1:A:218:LEU:CB	2.55	0.55
1:B:54:ASP:O	1:B:58:LYS:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HG3	1:A:239:LEU:N	2.22	0.55
1:A:449:GLN:O	1:A:453:ALA:HB2	2.06	0.55
1:A:140:SER:O	1:A:143:LEU:N	2.40	0.55
1:B:296:ARG:HG2	4:B:604:FTT:C3	2.37	0.55
1:A:124:LEU:HD23	1:A:124:LEU:O	2.06	0.55
1:A:63:VAL:HA	1:A:66:TRP:CE2	2.42	0.55
1:A:252:ASP:C	1:A:256:GLN:HE21	2.05	0.55
4:B:602:FTT:O2	2:C:2:PA1:N2	2.40	0.55
1:B:196:MET:C	1:B:200:MET:HE2	2.23	0.55
1:B:196:MET:CB	1:B:200:MET:HE2	2.37	0.55
1:B:359:LEU:HA	1:B:554:GLY:HA3	1.88	0.55
1:B:384:THR:O	1:B:387:SER:N	2.40	0.54
2:C:3:KDO:H5	2:C:7:KDO:C6	2.23	0.54
1:A:80:ILE:CG2	1:A:81:THR:N	2.70	0.54
1:B:274:SER:HA	1:B:278:SER:H	1.72	0.54
1:B:373:ALA:N	1:B:547:GLU:O	2.29	0.54
1:B:344:PHE:O	1:B:364:LEU:N	2.39	0.54
1:B:314:ALA:O	1:B:317:THR:OG1	2.21	0.54
1:A:144:ILE:O	1:A:148:ARG:HB2	2.08	0.53
1:A:551:VAL:HA	1:A:556:ILE:HA	1.89	0.53
1:A:273:PRO:O	1:A:278:SER:CA	2.56	0.53
1:B:561:THR:O	1:B:564:ASP:N	2.41	0.53
1:A:94:GLY:O	1:A:98:MET:CB	2.56	0.53
1:B:247:ALA:HA	1:B:250:ILE:CD1	2.39	0.53
1:B:12:THR:O	1:B:16:LEU:N	2.42	0.53
1:B:283:THR:HG23	1:B:284:ILE:N	2.23	0.53
1:A:189:PHE:O	1:A:192:ILE:HG22	2.08	0.53
1:A:422:VAL:O	1:A:504:LEU:HA	2.09	0.53
1:A:297:PRO:O	1:A:300:SER:N	2.42	0.53
1:A:51:LEU:HD13	1:B:288:PHE:HZ	1.74	0.52
1:A:86:SER:CB	1:B:249:SER:CB	2.87	0.52
1:A:256:GLN:CG	1:A:257:LEU:N	2.73	0.52
1:B:457:ALA:O	1:B:522:ALA:HB1	2.10	0.52
1:A:252:ASP:N	1:A:253:PRO:HD2	2.23	0.52
1:B:17:TRP:CE2	1:B:21:ALA:HA	2.44	0.52
1:B:261:LEU:O	1:B:265:PHE:N	2.27	0.52
3:B:601:PO4:O3	4:B:602:FTT:H22	2.09	0.52
1:B:283:THR:HG23	1:B:284:ILE:HD13	1.92	0.52
1:B:144:ILE:O	1:B:148:ARG:HB3	2.10	0.52
1:B:349:PHE:H	1:B:359:LEU:CB	2.23	0.52
1:B:518:ALA:O	1:B:522:ALA:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:SER:N	1:A:253:PRO:HD2	2.25	0.51
1:A:101:ARG:HB3	1:A:105:PHE:HE2	1.74	0.51
1:A:256:GLN:HG3	1:A:257:LEU:N	2.26	0.51
1:A:157:PHE:CB	1:A:161:PHE:CE2	2.90	0.51
3:A:608:PO4:P	2:C:1:PA1:N2	2.83	0.51
1:A:27:LEU:O	1:A:30:ALA:HB3	2.10	0.51
1:A:67:MET:O	1:A:70:VAL:HG12	2.11	0.51
1:A:540:SER:O	1:A:544:LYS:CB	2.58	0.51
1:A:238:ARG:O	1:A:241:GLY:N	2.44	0.51
1:A:128:ILE:CG1	1:A:129:THR:N	2.74	0.51
1:A:316:GLN:HA	1:A:319:PHE:HB2	1.93	0.51
1:B:67:MET:O	1:B:70:VAL:HG12	2.11	0.51
1:B:235:ASN:O	1:B:239:LEU:HG	2.11	0.51
1:A:260:SER:HB3	1:B:72:ILE:CD1	2.39	0.51
1:B:280:THR:O	1:B:284:ILE:HG12	2.11	0.51
1:A:138:SER:O	1:A:142:ALA:CB	2.59	0.51
1:A:157:PHE:CG	1:A:161:PHE:CE2	2.96	0.51
1:A:255:ILE:HG23	1:A:256:GLN:N	2.26	0.51
1:A:296:ARG:HB3	1:A:297:PRO:HD3	1.93	0.51
1:A:441:ARG:C	1:A:443:GLU:H	2.15	0.50
2:C:4:GMH:H2	2:C:7:KDO:O8	2.11	0.50
1:B:128:ILE:HG13	1:B:129:THR:H	1.75	0.50
1:A:25:ALA:HA	1:A:28:ILE:HD12	1.94	0.50
1:A:101:ARG:O	1:A:104:LEU:N	2.43	0.50
1:A:254:ILE:CG1	1:A:255:ILE:N	2.73	0.50
1:A:67:MET:HA	1:A:70:VAL:HG12	1.94	0.50
1:B:451:GLU:O	1:B:454:ALA:HB3	2.12	0.50
1:B:225:VAL:O	1:B:229:ARG:N	2.45	0.50
1:B:153:ILE:O	1:B:157:PHE:CB	2.59	0.49
1:A:49:LYS:HB3	1:A:286:VAL:CG1	2.42	0.49
1:A:100:MET:O	1:A:104:LEU:HG	2.12	0.49
1:A:33:ALA:CB	1:A:84:VAL:HG11	2.42	0.49
1:B:296:ARG:HB3	4:B:604:FTT:C5	2.42	0.49
6:B:605:DAO:C1	2:C:2:PA1:N2	2.73	0.49
1:A:40:SER:HA	1:A:74:LEU:HD21	1.94	0.49
1:A:249:SER:O	1:A:253:PRO:CG	2.60	0.49
1:B:33:ALA:O	1:B:81:THR:OG1	2.29	0.49
1:B:67:MET:HA	1:B:70:VAL:HG12	1.94	0.49
1:B:479:VAL:O	1:B:481:LEU:N	2.45	0.49
3:A:610:PO4:O4	2:C:5:GMH:H2	2.13	0.49
1:A:128:ILE:HG13	1:A:129:THR:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:MET:SD	1:B:103:ARG:NH2	2.87	0.48
1:B:519:ILE:O	1:B:523:LEU:CB	2.62	0.48
1:A:272:PHE:HA	1:A:275:VAL:HG12	1.94	0.48
1:B:251:SER:O	1:B:255:ILE:CB	2.61	0.48
1:B:296:ARG:HE	4:B:604:FTT:C1	2.25	0.48
1:B:193:SER:O	1:B:197:GLN:HB2	2.14	0.48
1:A:252:ASP:O	1:A:256:GLN:HG2	2.13	0.48
1:A:346:ASN:N	1:A:362:ILE:O	2.47	0.48
1:B:129:THR:O	1:B:133:GLU:CB	2.61	0.48
1:B:289:SER:O	1:B:293:ALA:CB	2.55	0.48
1:B:156:LEU:O	1:B:159:MET:CB	2.61	0.48
1:B:296:ARG:CG	4:B:604:FTT:C4	2.87	0.48
1:A:31:GLY:O	1:A:34:LEU:HB3	2.13	0.47
1:A:84:VAL:HG22	1:A:88:CYS:SG	2.55	0.47
1:B:261:LEU:O	1:B:264:ALA:HB3	2.13	0.47
1:B:40:SER:HA	1:B:74:LEU:HD21	1.96	0.47
1:B:236:ARG:O	1:B:239:LEU:HB2	2.14	0.47
1:B:100:MET:CE	1:B:103:ARG:HH21	2.27	0.47
1:A:123:THR:CG2	1:A:124:LEU:N	2.78	0.47
1:A:347:VAL:O	1:A:361:ASN:N	2.48	0.47
1:B:63:VAL:HA	1:B:66:TRP:HB3	1.96	0.47
1:A:74:LEU:O	1:A:75:MET:C	2.52	0.47
1:B:100:MET:CE	1:B:103:ARG:NH2	2.78	0.47
1:B:283:THR:O	1:B:287:VAL:HG13	2.15	0.47
1:B:504:LEU:O	1:B:534:VAL:HA	2.14	0.47
1:A:92:VAL:CG2	1:A:96:VAL:HG23	2.44	0.47
1:B:78:ARG:HA	1:B:81:THR:HG22	1.97	0.47
1:A:260:SER:O	1:A:264:ALA:N	2.45	0.46
1:A:292:ILE:O	1:A:295:MET:N	2.48	0.46
4:B:606:FTT:O2	2:C:1:PA1:O4	2.31	0.46
1:A:50:PRO:O	1:A:55:GLY:N	2.45	0.46
1:B:283:THR:CG2	1:B:284:ILE:N	2.79	0.46
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.97	0.46
1:B:288:PHE:CE1	4:B:606:FTT:H141	2.48	0.46
1:B:17:TRP:CZ2	1:B:21:ALA:HA	2.51	0.46
1:B:267:LEU:O	1:B:271:SER:N	2.47	0.46
1:A:69:LEU:HA	1:A:72:ILE:HG22	1.98	0.46
1:B:17:TRP:O	1:B:20:ILE:N	2.46	0.46
1:B:260:SER:O	1:B:264:ALA:N	2.37	0.46
1:B:295:MET:SD	1:B:295:MET:C	2.94	0.46
1:B:296:ARG:CG	4:B:604:FTT:C3	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLN:O	1:B:312:MET:CB	2.63	0.46
1:A:348:THR:HA	1:A:360:ARG:HA	1.97	0.46
1:A:149:GLU:CB	1:A:297:PRO:HB3	2.46	0.46
1:B:124:LEU:O	1:B:127:ARG:HB2	2.16	0.46
1:B:124:LEU:HA	1:B:127:ARG:HG2	1.98	0.46
1:B:450:ILE:O	1:B:453:ALA:HB3	2.15	0.45
1:A:333:ARG:CB	1:A:334:VAL:HA	2.47	0.45
1:B:24:LYS:O	1:B:27:LEU:N	2.49	0.45
1:A:192:ILE:HD12	1:A:192:ILE:HA	1.84	0.45
1:A:238:ARG:HD3	1:B:98:MET:HG3	1.99	0.45
1:B:144:ILE:O	1:B:148:ARG:CB	2.64	0.45
1:A:42:THR:HA	1:A:156:LEU:HD21	1.97	0.45
1:B:69:LEU:HA	1:B:72:ILE:HG22	1.98	0.45
1:A:256:GLN:CG	1:A:257:LEU:H	2.29	0.45
1:A:263:LEU:O	1:A:264:ALA:C	2.55	0.45
1:B:273:PRO:O	1:B:278:SER:N	2.49	0.45
1:B:432:THR:O	1:B:435:ASN:N	2.34	0.45
4:B:602:FTT:C1	4:B:604:FTT:C1	2.95	0.45
1:A:255:ILE:HG23	1:A:256:GLN:H	1.82	0.45
1:B:88:CYS:O	1:B:92:VAL:HG12	2.16	0.45
1:B:197:GLN:HA	1:B:200:MET:HE1	1.94	0.45
1:B:263:LEU:CD2	4:B:607:FTT:C9	2.92	0.45
1:B:550:VAL:O	1:B:556:ILE:HA	2.17	0.45
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.68	0.44
1:A:63:VAL:O	1:A:66:TRP:NE1	2.50	0.44
1:B:296:ARG:HB2	4:B:604:FTT:C3	2.41	0.44
1:A:435:ASN:HA	1:A:438:ALA:CB	2.48	0.44
1:B:386:ALA:O	1:B:390:THR:N	2.50	0.44
1:A:56:PHE:O	1:A:59:THR:N	2.49	0.44
1:B:233:VAL:O	1:B:236:ARG:HB2	2.17	0.44
1:A:491:ILE:O	1:A:494:ALA:HB3	2.18	0.44
1:A:139:SER:O	1:A:142:ALA:HB3	2.17	0.44
1:A:280:THR:O	1:A:284:ILE:HG12	2.18	0.44
1:B:27:LEU:HG	1:B:92:VAL:HG11	1.98	0.44
1:B:130:TYR:O	1:B:134:GLN:HB2	2.17	0.44
1:B:512:ASP:O	1:B:516:GLU:N	2.51	0.44
1:A:47:LEU:O	1:A:50:PRO:HD2	2.17	0.44
1:A:175:ALA:HB1	1:A:298:LEU:CD1	2.48	0.44
1:A:40:SER:CA	1:A:74:LEU:HD21	2.48	0.43
1:A:513:THR:HA	1:A:516:GLU:CB	2.48	0.43
1:B:344:PHE:N	1:B:364:LEU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLY:HA2	1:A:153:ILE:HG12	2.00	0.43
1:B:256:GLN:O	1:B:257:LEU:C	2.54	0.43
1:A:489:ILE:O	1:A:492:ALA:N	2.51	0.43
1:B:256:GLN:CD	4:B:607:FTT:H42	2.08	0.43
1:B:114:SER:C	1:B:117:ASP:H	2.21	0.43
1:A:61:ARG:NH2	1:B:275:VAL:CB	2.82	0.43
1:B:295:MET:HE1	1:B:299:LYS:H	1.84	0.43
1:B:250:ILE:O	1:B:254:ILE:HG12	2.17	0.43
1:B:247:ALA:HA	1:B:250:ILE:HD13	2.00	0.43
1:A:33:ALA:HB2	1:A:84:VAL:HG11	2.00	0.43
1:A:192:ILE:HG12	1:A:247:ALA:HB3	2.00	0.43
1:B:157:PHE:O	1:B:160:MET:N	2.52	0.42
1:A:123:THR:CG2	1:A:124:LEU:H	2.31	0.42
1:A:237:MET:HB3	1:B:98:MET:HE1	2.00	0.42
1:A:238:ARG:H	1:B:98:MET:HE3	1.85	0.42
1:A:257:LEU:CD1	1:B:75:MET:C	2.73	0.42
1:A:574:GLN:O	1:A:577:LYS:N	2.50	0.42
1:A:80:ILE:CG2	1:A:81:THR:H	2.32	0.42
1:A:92:VAL:O	1:A:96:VAL:HG23	2.19	0.42
1:B:232:LYS:O	1:B:236:ARG:N	2.33	0.42
1:B:236:ARG:HA	1:B:239:LEU:HD12	2.01	0.42
1:B:360:ARG:N	1:B:554:GLY:O	2.23	0.42
1:A:214:HIS:O	1:A:214:HIS:ND1	2.53	0.42
1:B:63:VAL:O	1:B:66:TRP:HB3	2.20	0.42
1:A:242:MET:SD	1:B:91:TRP:HA	2.60	0.42
1:A:116:PHE:HD2	1:B:214:HIS:ND1	2.16	0.42
1:B:140:SER:O	1:B:144:ILE:HG23	2.20	0.42
1:B:247:ALA:C	1:B:250:ILE:HG12	2.39	0.42
2:C:3:KDO:H4	2:C:7:KDO:H32	1.75	0.42
1:A:435:ASN:HA	1:A:438:ALA:HB3	2.01	0.42
1:A:259:ALA:O	1:A:262:ALA:CB	2.67	0.42
1:A:38:ALA:HB1	1:A:152:SER:HA	2.01	0.42
1:B:61:ARG:HA	1:B:64:LEU:CB	2.50	0.42
1:A:263:LEU:HD12	1:A:263:LEU:N	2.35	0.41
1:A:342:VAL:O	1:A:365:LYS:HA	2.20	0.41
1:B:233:VAL:HA	1:B:236:ARG:HB2	2.00	0.41
1:B:333:ARG:HA	1:B:334:VAL:C	2.40	0.41
1:B:452:GLU:O	1:B:455:ARG:N	2.53	0.41
1:A:61:ARG:HH21	1:B:275:VAL:CB	2.32	0.41
1:B:171:LEU:O	1:B:174:LEU:N	2.44	0.41
1:A:319:PHE:O	1:A:323:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:601:PO4:P	2:C:2:PA1:O3	2.79	0.41
1:A:53:ASP:OD2	1:A:282:GLY:N	2.54	0.41
4:B:602:FTT:C1	2:C:2:PA1:N2	2.83	0.41
1:B:54:ASP:O	1:B:56:PHE:N	2.53	0.41
1:B:313:ALA:O	1:B:317:THR:HG23	2.19	0.41
1:A:51:LEU:CD1	1:B:288:PHE:HZ	2.32	0.41
1:B:307:GLN:HG2	1:B:308:PHE:N	2.36	0.41
1:A:84:VAL:O	1:A:88:CYS:SG	2.79	0.41
2:C:3:KDO:O4	2:C:4:GMH:O6	2.38	0.41
1:A:25:ALA:O	1:A:28:ILE:HB	2.21	0.41
1:A:440:ALA:O	1:A:441:ARG:CB	2.68	0.41
1:A:146:VAL:HG13	1:A:147:VAL:N	2.36	0.40
1:A:158:ILE:O	1:A:162:TYR:N	2.47	0.40
1:A:174:LEU:O	1:A:177:ILE:N	2.51	0.40
1:A:475:GLY:O	1:A:478:GLY:N	2.52	0.40
1:A:257:LEU:HD11	1:B:75:MET:CA	2.49	0.40
1:B:98:MET:O	1:B:102:ARG:HG2	2.20	0.40
1:B:489:ILE:O	1:B:492:ALA:N	2.53	0.40
1:B:513:THR:O	1:B:516:GLU:N	2.55	0.40
1:B:517:ARG:O	1:B:521:ALA:HB3	2.22	0.40
1:A:101:ARG:O	1:A:104:LEU:HB2	2.21	0.40
1:A:299:LYS:O	1:A:303:ASN:ND2	2.55	0.40
1:B:232:LYS:O	1:B:236:ARG:HG3	2.22	0.40
2:C:3:KDO:O5	2:C:3:KDO:O7	2.06	0.40
1:B:415:LEU:O	1:B:418:GLN:N	2.53	0.40
2:C:3:KDO:O4	2:C:4:GMH:C1	2.69	0.40
2:C:6:GMH:H4	2:C:7:KDO:O1B	2.21	0.40
1:A:432:THR:O	1:A:435:ASN:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/605 (94%)	488 (86%)	74 (13%)	4 (1%)	22	62
1	B	568/605 (94%)	489 (86%)	75 (13%)	4 (1%)	22	62
All	All	1134/1210 (94%)	977 (86%)	149 (13%)	8 (1%)	26	62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	308	PHE
1	B	440	ALA
1	B	534	VAL
1	A	443	GLU
1	A	227	THR
1	A	431	ASP
1	A	519	ILE
1	B	413	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/517 (21%)	107 (98%)	2 (2%)	59	76
1	B	99/517 (19%)	95 (96%)	4 (4%)	31	57
All	All	208/1034 (20%)	202 (97%)	6 (3%)	45	64

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	TRP
1	A	265	PHE
1	B	87	TYR
1	B	148	ARG
1	B	295	MET
1	B	307	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	256	GLN
1	B	305	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)

7 monosaccharides 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	$\#\|Z\| > 2$
2	PA1	C	1	4,2,3	12,12,12	1.14	1 (8%)	16,17,17	1.47	2 (12%)
2	PA1	C	2	4,2,3	11,11,12	2.16	2 (18%)	12,15,17	3.67	3 (25%)
2	KDO	C	3	2	14,14,16	1.56	3 (21%)	19,20,24	1.74	4 (21%)
2	GMH	C	4	2,3	13,13,14	0.89	0	17,18,20	1.31	2 (11%)
2	GMH	C	5	2,3	13,13,14	1.23	1 (7%)	17,18,20	1.33	2 (11%)
2	GMH	C	6	2	13,13,14	0.74	0	17,18,20	1.05	2 (11%)
2	KDO	C	7	2	15,15,16	1.20	2 (13%)	19,21,24	1.26	2 (10%)

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
2	PA1	C	1	4,2,3	-	0/2/22/22	0/1/1/1
2	PA1	C	2	4,2,3	1/1/4/5	0/2/19/22	0/1/1/1
2	KDO	C	3	2	-	4/8/24/30	0/1/1/1
2	GMH	C	4	2,3	-	0/6/23/26	0/1/1/1
2	GMH	C	5	2,3	-	2/6/23/26	1/1/1/1
2	GMH	C	6	2	-	3/6/23/26	0/1/1/1
2	KDO	C	7	2	-	5/10/26/30	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	PA1	O5-C5	5.10	1.53	1.43
2	C	2	PA1	O5-C1	4.39	1.50	1.43
2	C	5	GMH	O5-C5	3.64	1.47	1.43
2	C	3	KDO	O5-C5	2.93	1.49	1.43
2	C	3	KDO	O6-C6	2.91	1.48	1.44
2	C	1	PA1	C1-C2	-2.69	1.49	1.52
2	C	7	KDO	C4-C5	2.54	1.56	1.52
2	C	3	KDO	O6-C2	2.33	1.46	1.43
2	C	7	KDO	O6-C2	2.02	1.46	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	PA1	O5-C5-C6	-10.31	91.04	107.20
2	C	2	PA1	C4-C3-C2	-4.95	103.01	111.37
2	C	2	PA1	C1-O5-C5	4.72	118.58	112.19
2	C	3	KDO	O6-C6-C5	3.83	113.25	107.87
2	C	4	GMH	C1-C2-C3	3.64	114.14	109.67
2	C	1	PA1	C1-C2-C3	-3.43	106.09	110.60
2	C	5	GMH	C6-C5-C4	-3.19	108.74	114.03
2	C	1	PA1	O5-C1-C2	-3.08	105.91	109.51
2	C	3	KDO	O5-C5-C4	3.07	115.87	109.99
2	C	3	KDO	O1A-C1-C2	-2.85	115.84	122.57
2	C	7	KDO	C3-C4-C5	2.61	114.47	110.69
2	C	3	KDO	C6-O6-C2	2.61	116.91	111.34
2	C	4	GMH	C6-C5-C4	-2.52	109.85	114.03
2	C	7	KDO	O1A-C1-C2	-2.36	116.99	122.57
2	C	5	GMH	C2-C3-C4	-2.35	106.82	110.89
2	C	6	GMH	C1-O5-C5	2.24	115.14	111.48
2	C	6	GMH	C6-C5-C4	-2.08	110.59	114.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	PA1	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	KDO	C5-C6-C7-O7
2	C	3	KDO	C5-C6-C7-C8
2	C	7	KDO	C5-C6-C7-O7
2	C	7	KDO	C5-C6-C7-C8
2	C	7	KDO	O6-C6-C7-O7
2	C	7	KDO	O6-C6-C7-C8
2	C	3	KDO	O6-C6-C7-C8
2	C	6	GMH	O6-C6-C7-O7
2	C	5	GMH	O5-C5-C6-O6
2	C	5	GMH	C5-C6-C7-O7
2	C	6	GMH	C5-C6-C7-O7
2	C	3	KDO	O1B-C1-C2-O6
2	C	6	GMH	C4-C5-C6-O6
2	C	7	KDO	O1A-C1-C2-O6

All (1) ring outliers are listed below:

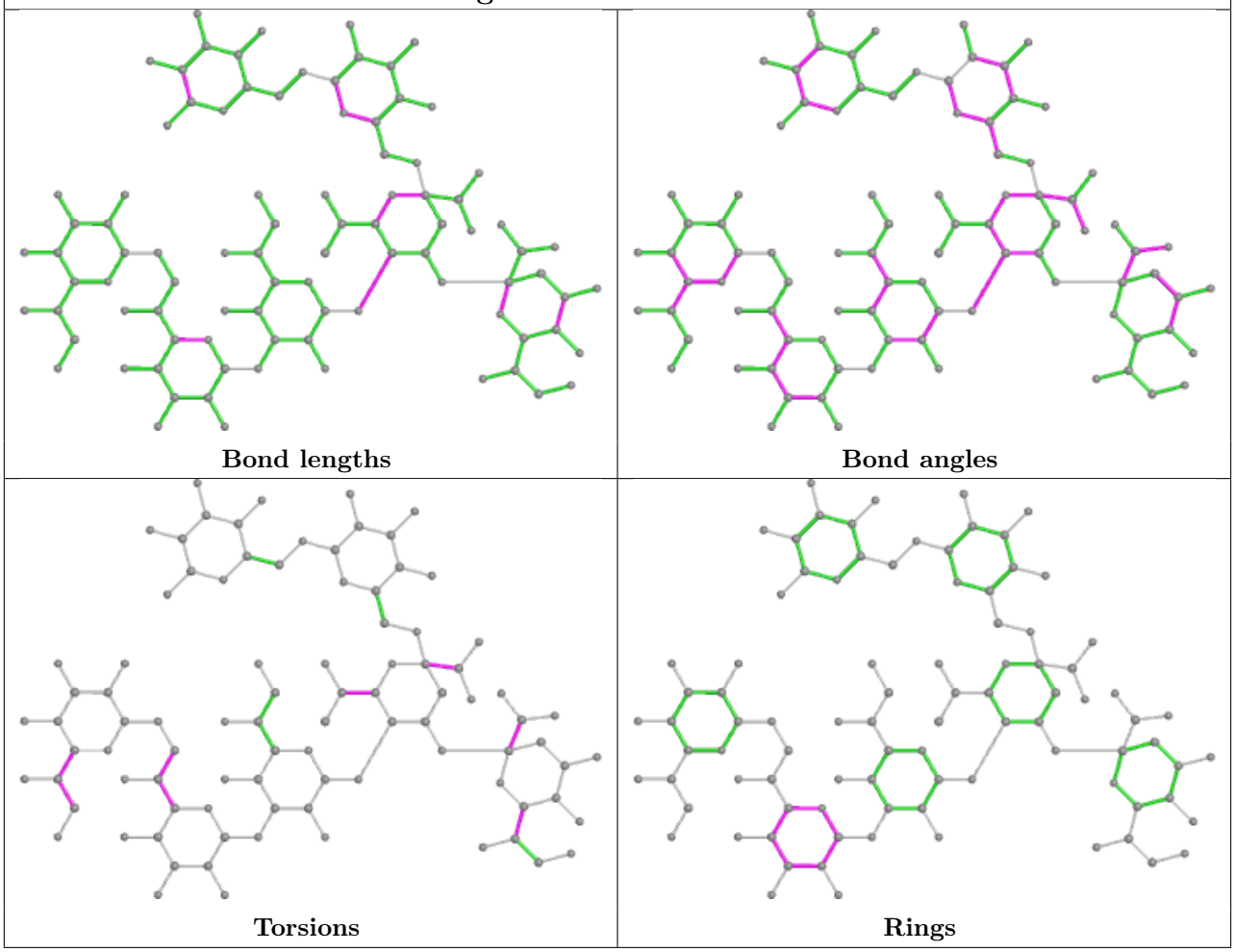
Mol	Chain	Res	Type	Atoms
2	C	5	GMH	C1-C2-C3-C4-C5-O5

7 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	PA1	7	0
2	C	7	KDO	13	0
2	C	5	GMH	2	0
2	C	3	KDO	17	0
2	C	4	GMH	10	0
2	C	6	GMH	3	0
2	C	1	PA1	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
3	PO4	B	601	2	0,3,4	-	-	0,3,6	-	-
4	FTT	B	607	2	10,10,16	0.73	0	10,10,17	0.91	0
3	PO4	A	610	2	0,3,4	-	-	0,3,6	-	-
5	MYR	B	603	4	5,5,15	0.45	0	4,4,15	0.95	0
4	FTT	B	602	2,5	7,7,16	0.65	0	6,7,17	1.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FTT	B	604	6,2	6,6,16	0.65	0	6,6,17	0.95	0
3	PO4	A	608	2	0,3,4	-	-	0,3,6	-	-
6	DAO	B	605	4	7,7,13	0.46	0	6,6,13	0.75	0
3	PO4	A	609	2	0,3,4	-	-	0,3,6	-	-
4	FTT	B	606	2	15,15,16	0.40	0	15,15,17	1.13	1 (6%)

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
4	FTT	B	607	2	-	3/9/9/15	-
5	MYR	B	603	4	-	2/2/3/13	-
4	FTT	B	602	2,5	-	5/6/6/15	-
4	FTT	B	604	6,2	-	1/5/5/15	-
6	DAO	B	605	4	-	4/4/5/11	-
4	FTT	B	606	2	-	6/14/14/15	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	606	FTT	C3-C2-C1	-2.04	109.16	112.75

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	602	FTT	C1-C2-C3-C4
4	B	602	FTT	C1-C2-C3-O3
4	B	602	FTT	C2-C3-C4-C5
4	B	607	FTT	C1-C2-C3-C4
4	B	607	FTT	C1-C2-C3-O3
5	B	603	MYR	C1-C2-C3-C4
6	B	605	DAO	C1-C2-C3-C4
4	B	602	FTT	O3-C3-C4-C5
4	B	602	FTT	C3-C4-C5-C6
4	B	606	FTT	C10-C11-C12-C13
4	B	607	FTT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
6	B	605	DAO	C3-C4-C5-C6
6	B	605	DAO	C4-C5-C6-C7
6	B	605	DAO	C2-C3-C4-C5
5	B	603	MYR	C2-C3-C4-C5
4	B	606	FTT	C11-C10-C9-C8
4	B	606	FTT	C4-C5-C6-C7
4	B	604	FTT	O2-C1-C2-C3
4	B	606	FTT	C7-C8-C9-C10
4	B	606	FTT	C3-C4-C5-C6
4	B	606	FTT	C9-C10-C11-C12

There are no ring outliers.

9 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	PO4	2	0
4	B	607	FTT	11	0
3	A	610	PO4	1	0
4	B	602	FTT	5	0
4	B	604	FTT	19	0
3	A	608	PO4	3	0
6	B	605	DAO	12	0
3	A	609	PO4	1	0
4	B	606	FTT	12	0

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.

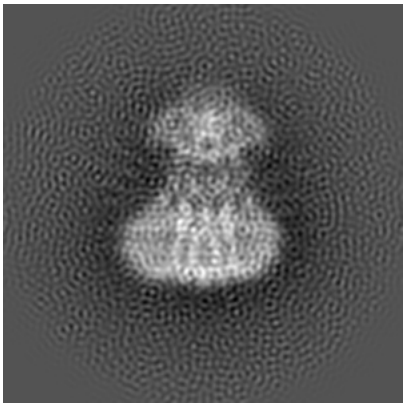
6 Map visualisation (i)

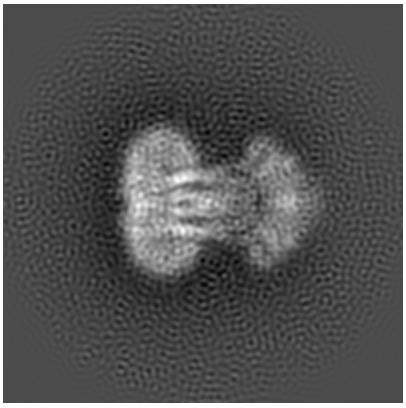
This section contains visualisations of the EMDB entry EMD-8469. These allow visual inspection of the internal detail of the map and identification of artifacts.

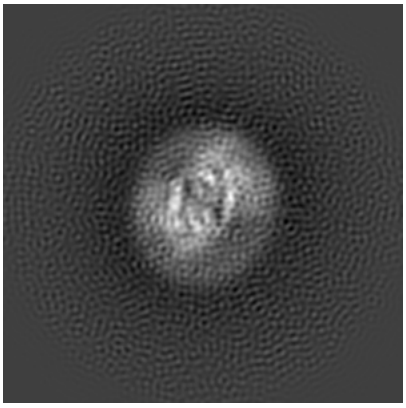
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

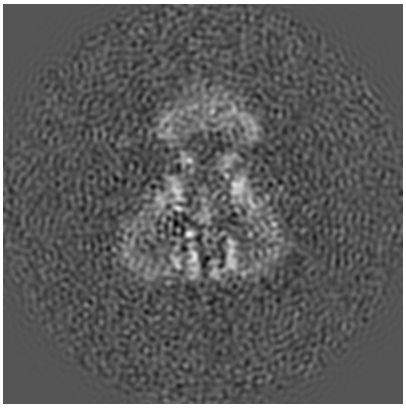

Y

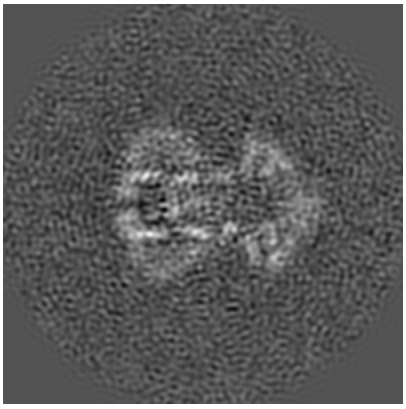

Z

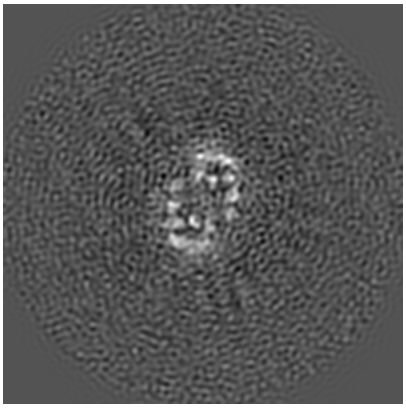
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 96

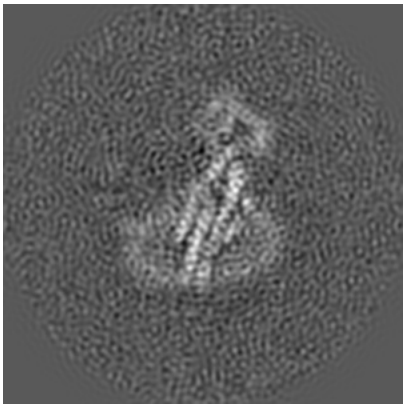

Y Index: 96


Z Index: 96

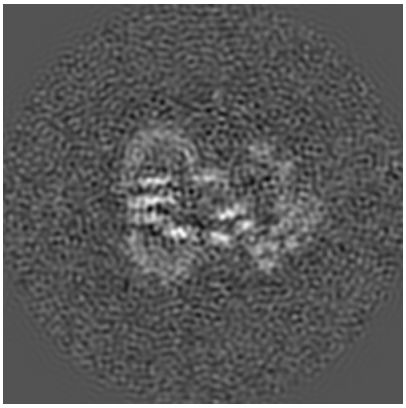
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

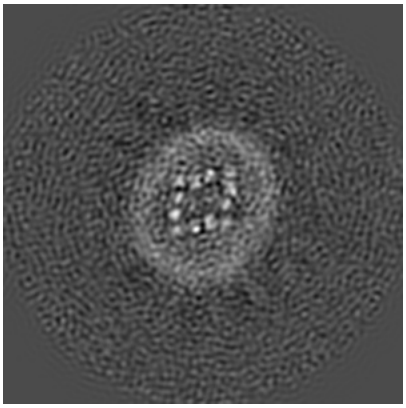
6.3.1 Primary map



X Index: 107



Y Index: 91



Z Index: 85

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 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

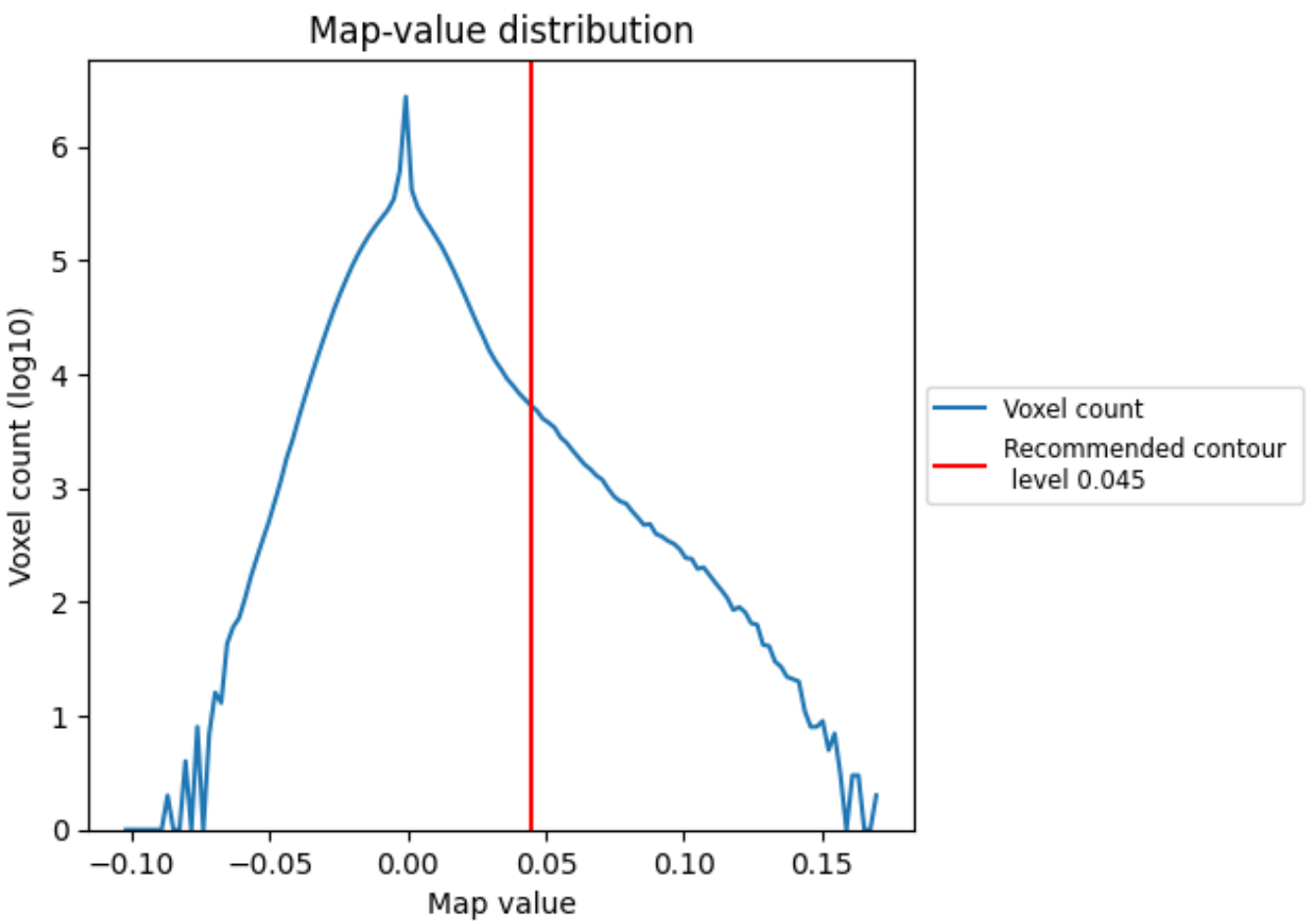
6.5 Mask visualisation (i)

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

7 Map analysis (i)

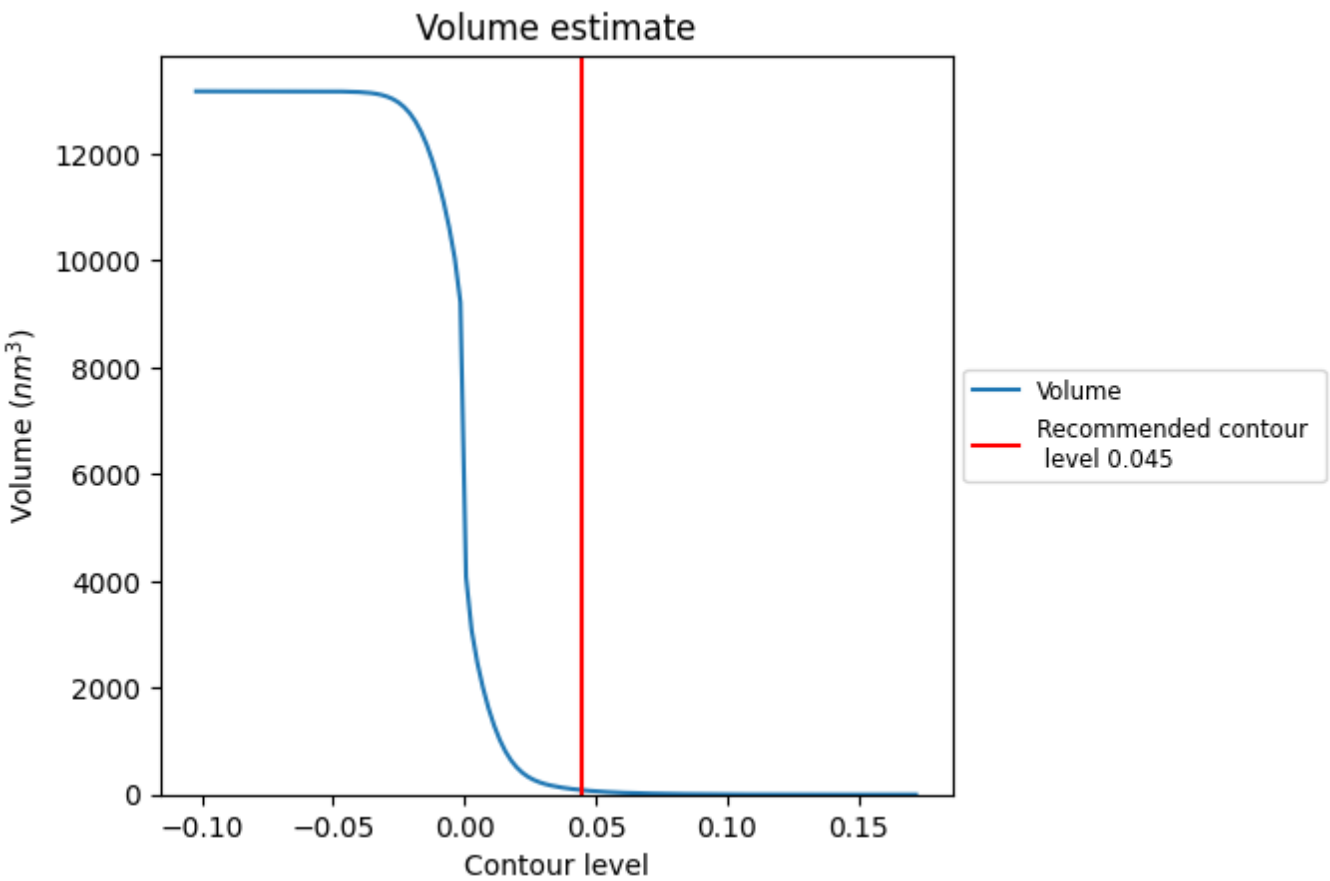
This section contains the results of statistical analysis of the map.

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.

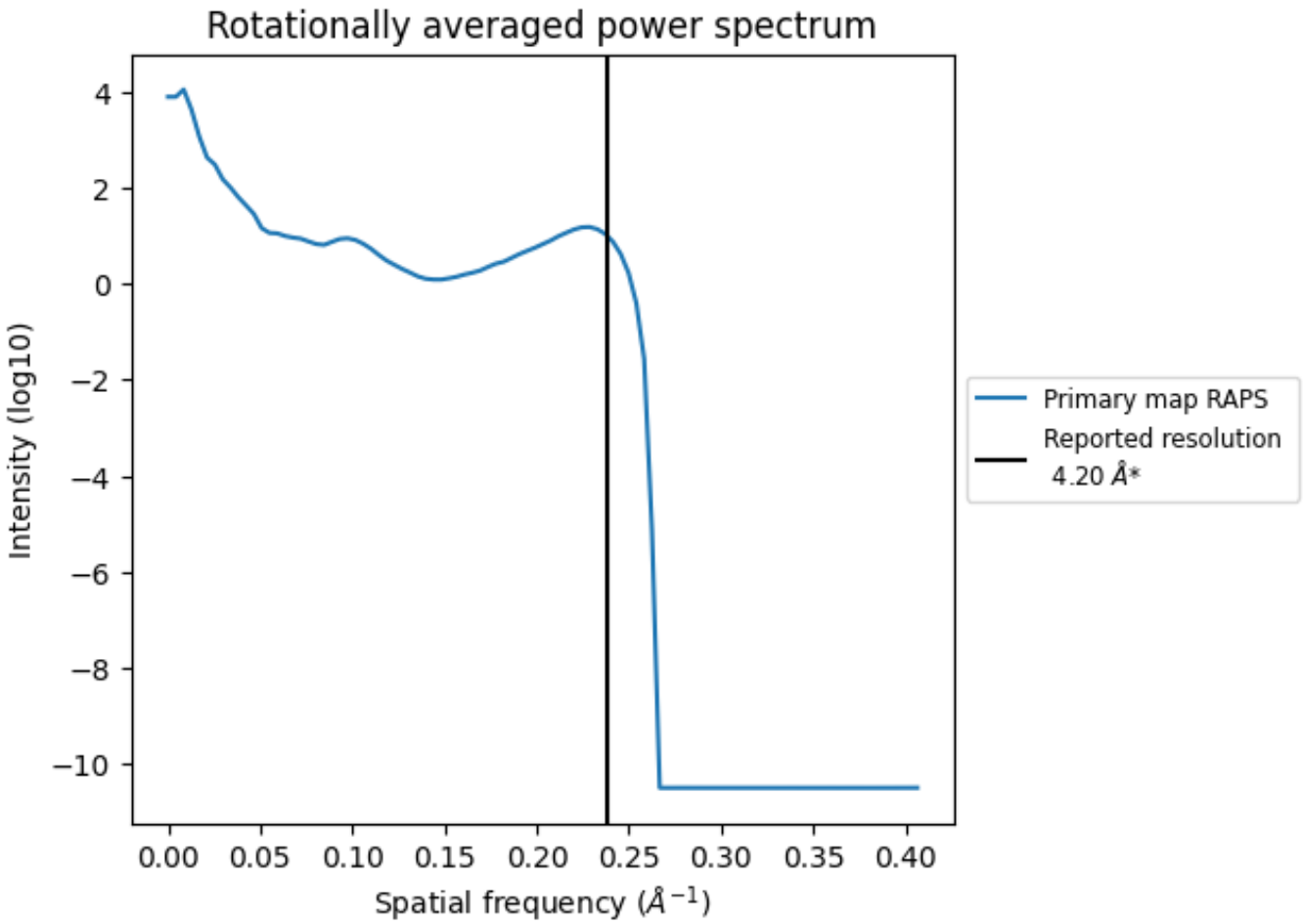
7.2 Volume estimate (i)



The volume at the recommended contour level is 83 nm^3; this corresponds to an approximate mass of 75 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)

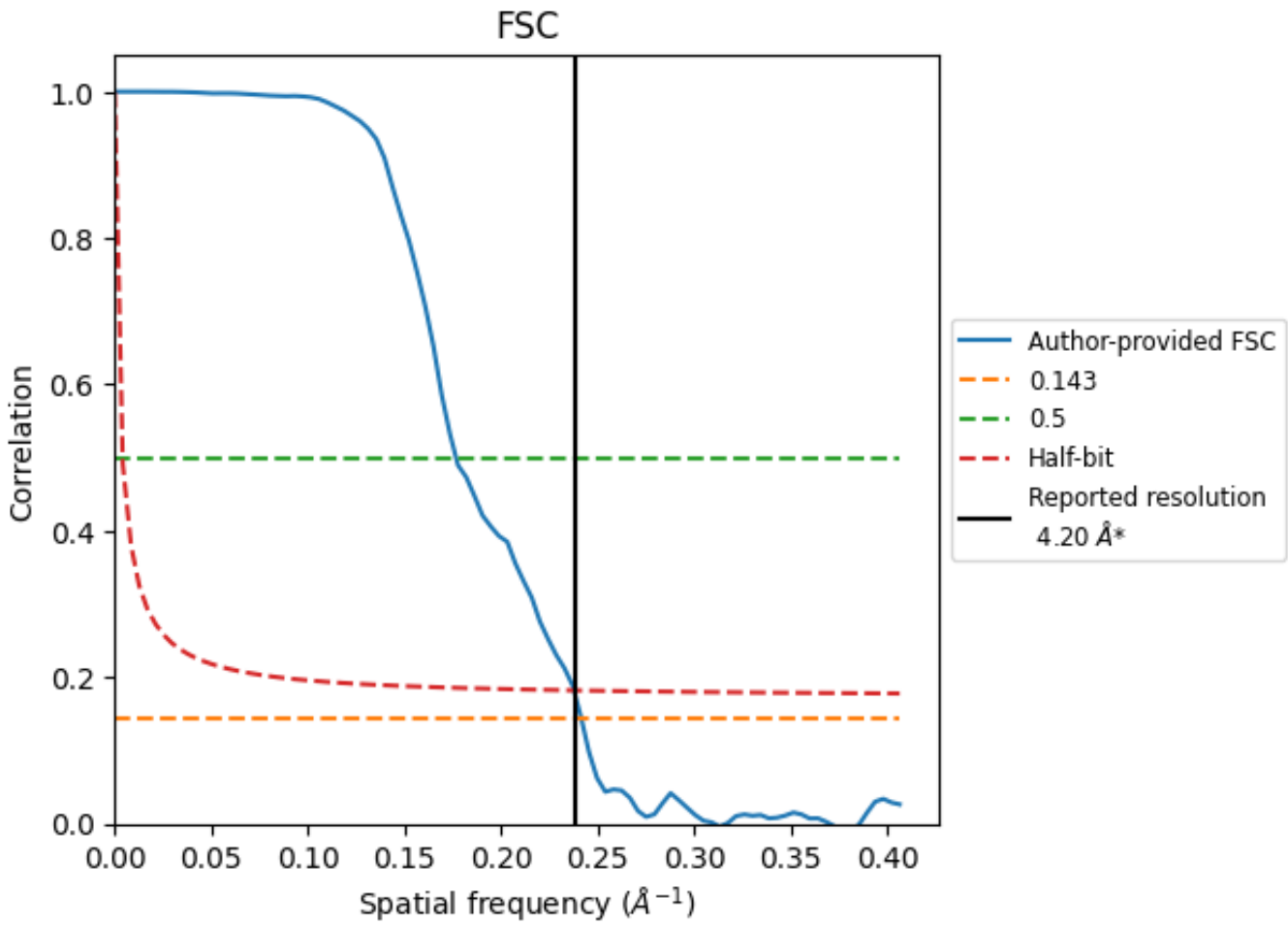


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

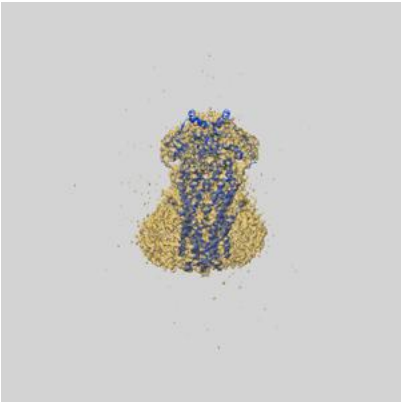
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.14	5.66	4.21
Unmasked-calculated*	-	-	-

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

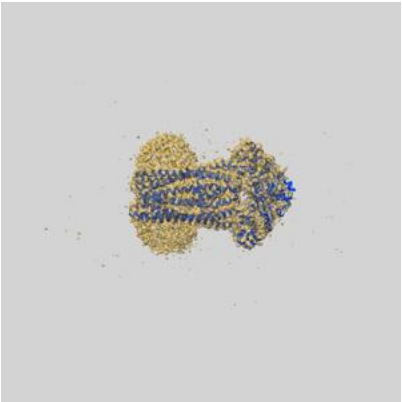
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8469 and PDB model 5TV4. Per-residue inclusion information can be found in section 3 on page 9.

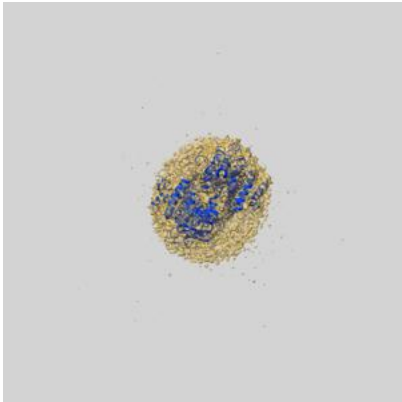
9.1 Map-model overlay (i)



X



Y



Z

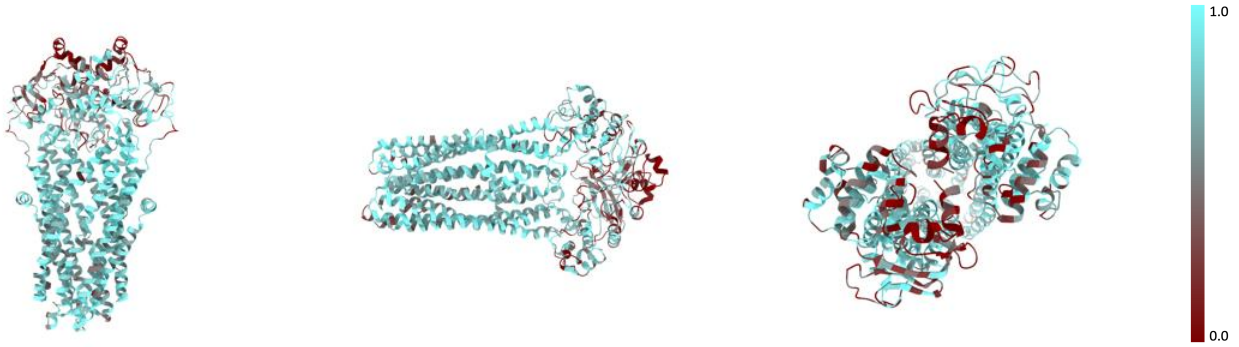
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

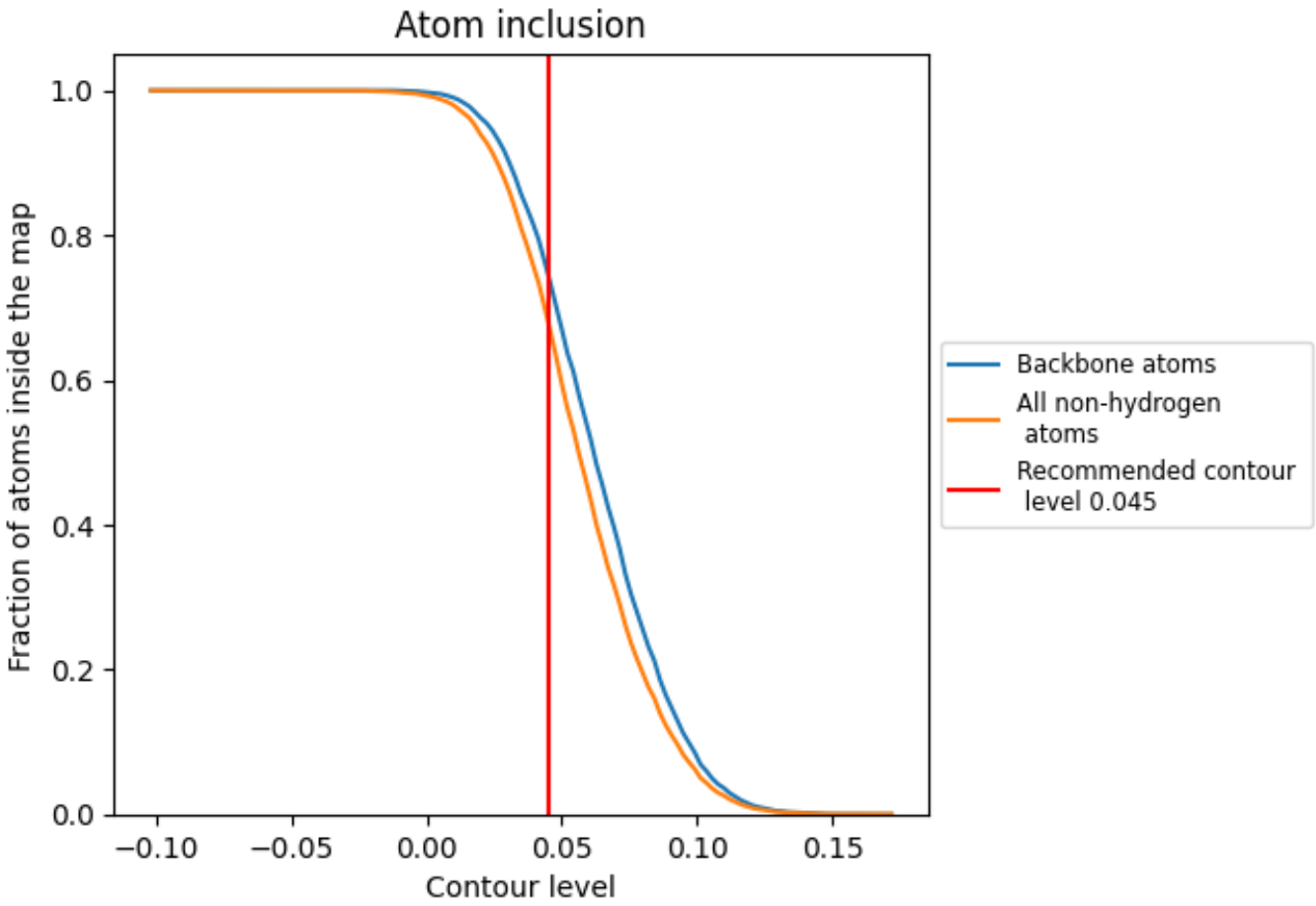
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 68% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6782	0.3080
A	0.6700	0.3010
B	0.6880	0.3130
C	0.6154	0.4260