Full wwPDB EM Validation Report (i)

Dec 17, 2022 – 08:09 pm GMT

PDB ID	:	6ZMR
EMDB ID	:	EMD-0668
Title	:	Porcine ATP synthase Fo domain
Authors	:	Spikes, T.E.; Montgomery, M.G.; Walker, J.E.
Deposited on	:	2020-07-03
Resolution	:	3.94 Å(reported)
Based on initial model	:	6B2Z

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:

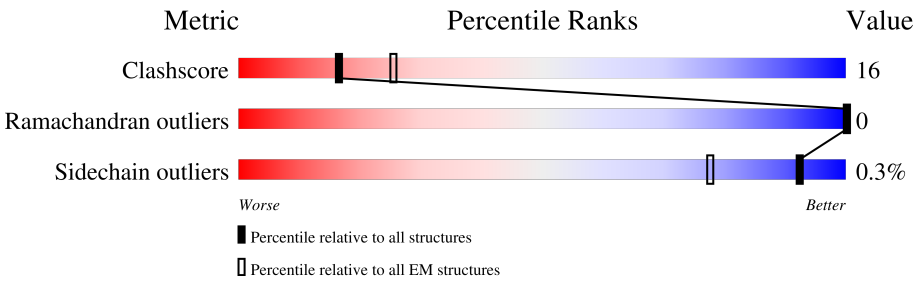
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.94 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	8	67	33% 18% 49%
2	K	75	29% 60% 39% .
2	L	75	21% 77% 21% .
2	M	75	27% 71% 29%
2	N	75	25% 68% 32%
2	O	75	35% 83% 17%
2	P	75	37% 68% 31% .
2	Q	75	21% 68% 32%

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Mol	Chain	Length	Quality of chain
2	R	75	35% 73% 27%
3	a	226	8% 98%
4	b	214	44% 56%
5	d	161	5% 20% 79%
6	e	70	60% 79% 19%
7	f	87	26% 95% 5%
8	g	102	26% 73% 27%
9	j	60	20% 80% 20%
10	k	57	40% 61% 39%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 20142 atoms, of which 10315 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 ATP synthase protein 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	8	34	574	191	291	39	50	3	0	0

- Molecule 2 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	K	74	1079	351	550	82	93	3	0	0
2	L	74	1079	351	550	82	93	3	0	0
2	M	75	1096	356	559	83	94	4	0	0
2	N	75	1096	356	559	83	94	4	0	0
2	O	75	1096	356	559	83	94	4	0	0
2	P	74	1079	351	550	82	93	3	0	0
2	Q	75	1096	356	559	83	94	4	0	0
2	R	75	1096	356	559	83	94	4	0	0

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	a	223	3594	1156	1860	275	291	12	0	0

- Molecule 4 is a protein called ATP synthase peripheral stalk-membrane subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
4	b	94	1488	486	762	110	130	0	0

- Molecule 5 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	d	34	587	197	289	46	54	1	0	0

- Molecule 6 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
6	e	57	969	301	498	88	82	0	0

- Molecule 7 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	f	83	1406	453	712	124	114	3	0	0

- Molecule 8 is a protein called ATP synthase g subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	g	74	1182	384	602	92	103	1	0	0

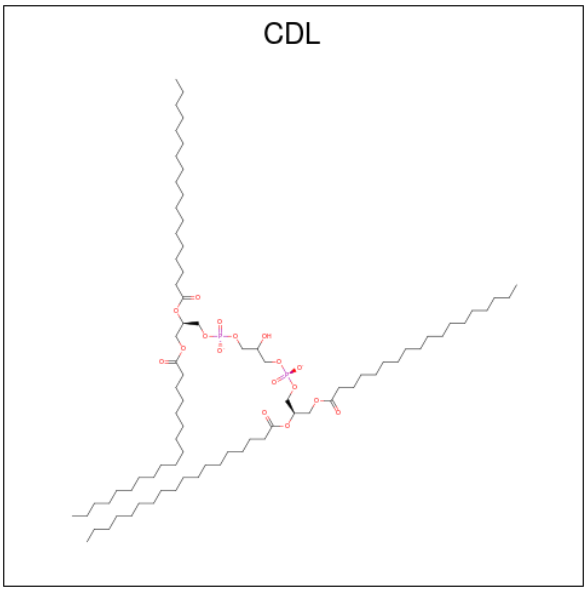
- Molecule 9 is a protein called ATP synthase j subunit (6.8PL).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	j	48	827	268	427	66	64	2	0	0

- Molecule 10 is a protein called ATP synthase membrane subunit DAPIT.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	k	35	578	187	298	46	45	2	0	0

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



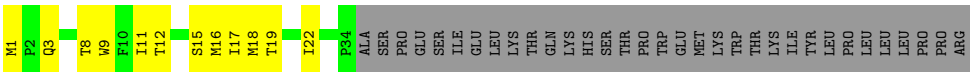
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
11	f	1	220	70	131	17	2	0

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.

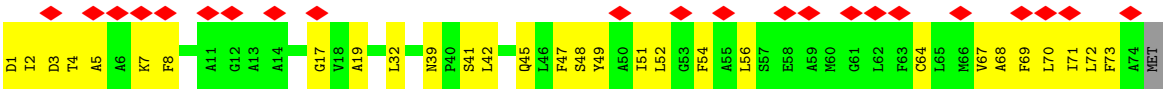
• Molecule 1: ATP synthase protein 8

Chain 8:



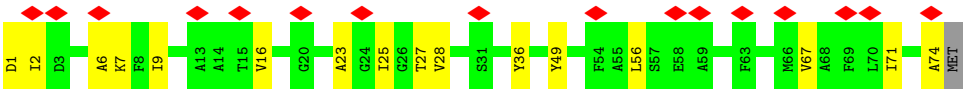
• Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain K:



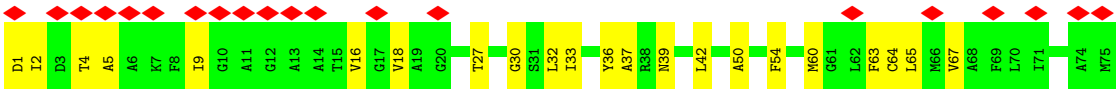
• Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain L:



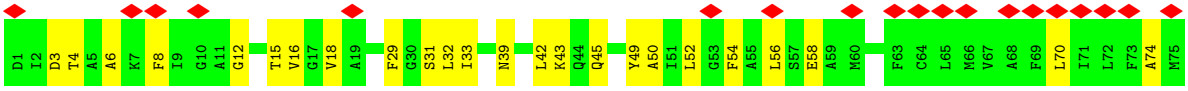
• Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain M:



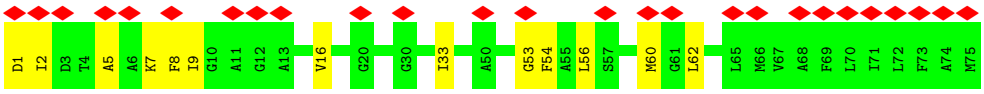
• Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain N:



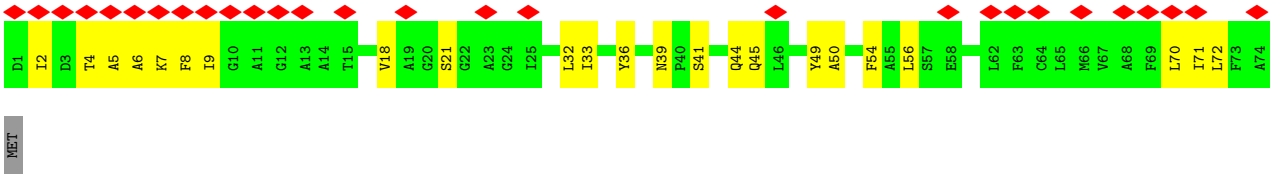
• Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain O:



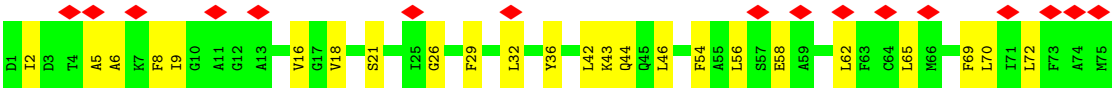
• Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain P:



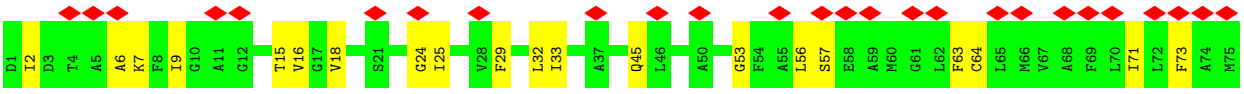
• Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain Q:



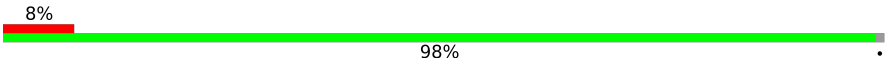
• Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

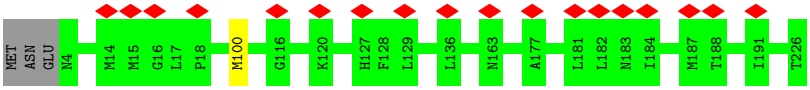
Chain R:



• Molecule 3: ATP synthase subunit a

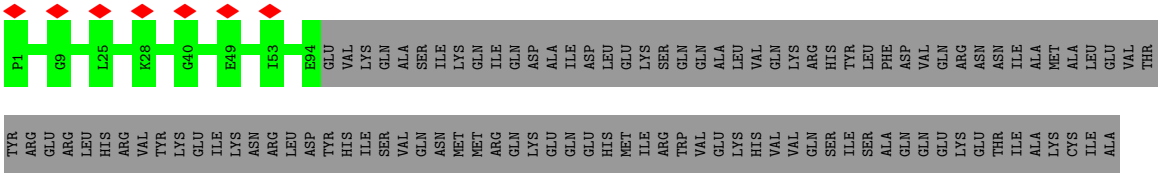
Chain a:

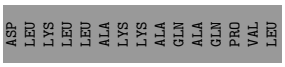




• Molecule 4: ATP synthase peripheral stalk-membrane subunit b

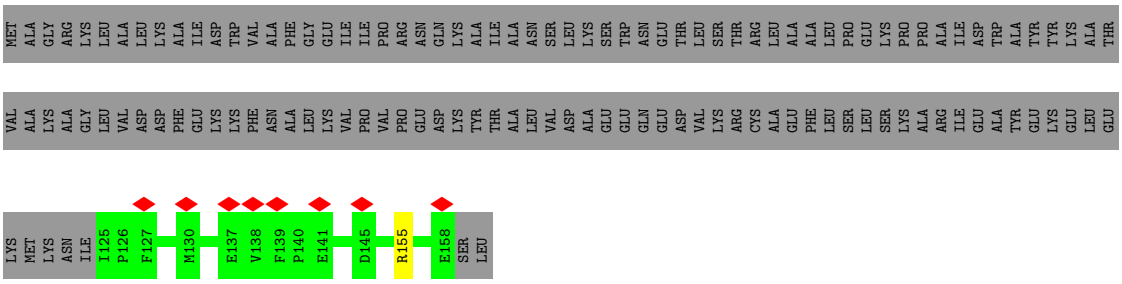
Chain b:





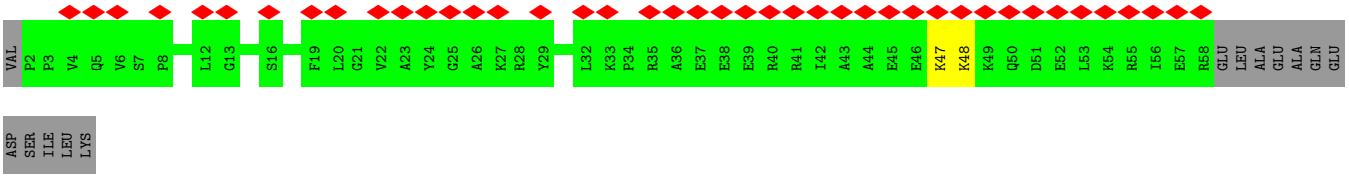
• Molecule 5: ATP synthase subunit d, mitochondrial

Chain d:



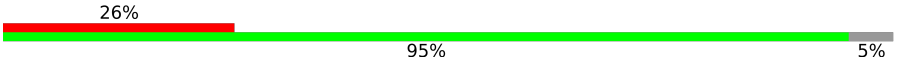
• Molecule 6: ATP synthase subunit e, mitochondrial

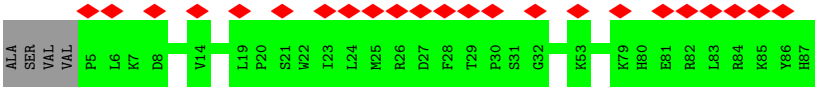
Chain e:



• Molecule 7: ATP synthase subunit f, mitochondrial

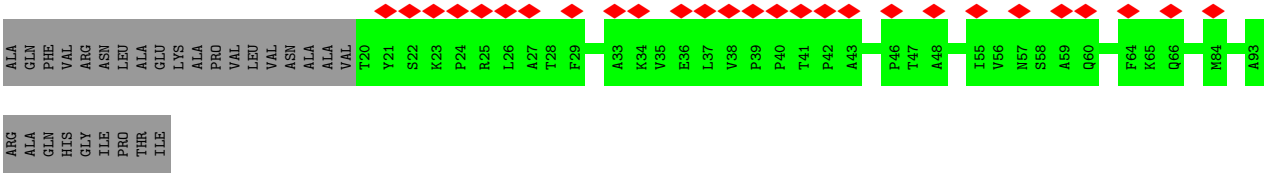
Chain f:





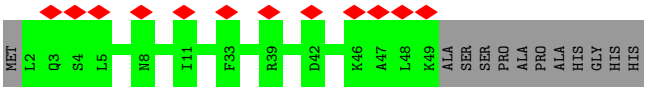
• Molecule 8: ATP synthase g subunit

Chain g:



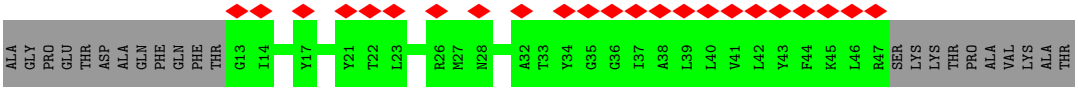
• Molecule 9: ATP synthase j subunit (6.8PL)

Chain j:



• Molecule 10: ATP synthase membrane subunit DAPIT

Chain k:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	167954	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 ($e^-/Å^2$)	50	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	0.186	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0286	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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: M3L, CDL

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	8	0.44	0/291	0.66	0/396
2	K	0.34	0/526	0.47	0/711
2	L	0.35	0/526	0.48	0/711
2	M	0.37	0/534	0.49	0/721
2	N	0.41	0/534	0.52	0/721
2	O	0.39	0/534	0.53	0/721
2	P	0.37	0/526	0.51	0/711
2	Q	0.42	0/534	0.50	0/721
2	R	0.39	0/534	0.47	0/721
3	a	0.37	0/1774	0.53	1/2424 (0.0%)
4	b	0.36	0/744	0.47	0/1011
5	d	0.32	0/309	0.49	0/420
6	e	0.29	0/479	0.49	0/639
7	f	0.39	0/712	0.47	0/955
8	g	0.31	0/595	0.45	0/812
9	j	0.37	0/410	0.45	0/552
10	k	0.31	0/285	0.44	0/382
All	All	0.37	0/9847	0.50	1/13329 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	100	MET	CA-CB-CG	5.72	123.03	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8	283	291	291	10	0
2	K	529	550	550	35	0
2	L	529	550	550	15	0
2	M	537	559	559	25	0
2	N	537	559	559	30	0
2	O	537	559	559	20	0
2	P	529	550	550	25	0
2	Q	537	559	559	34	0
2	R	537	559	559	32	0
3	a	1734	1860	1860	0	0
4	b	726	762	762	0	0
5	d	298	289	289	0	0
6	e	471	498	498	0	0
7	f	694	712	712	0	0
8	g	580	602	601	0	0
9	j	400	427	427	0	0
10	k	280	298	298	0	0
11	f	89	131	125	0	0
All	All	9827	10315	10308	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:36:TYR:OH	2:R:45:GLN:OE1	1.91	0.88
2:K:72:LEU:HD22	2:K:73:PHE:CE2	2.19	0.78
2:K:7:LYS:NZ	2:K:72:LEU:O	2.13	0.77
2:M:36:TYR:CE2	2:N:42:LEU:HD13	2.21	0.76
2:O:54:PHE:CZ	2:P:56:LEU:HD12	2.21	0.76
2:Q:43:M3L:HM22	2:R:45:GLN:NE2	2.01	0.76
2:Q:18:VAL:O	2:Q:21:SER:OG	2.04	0.73
2:Q:18:VAL:HG21	2:R:64:CYS:SG	2.28	0.73
2:Q:9:ILE:HD13	2:R:9:ILE:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:37:ALA:O	2:N:39:ASN:ND2	2.21	0.73
2:L:1:ASP:OD1	2:L:2:ILE:N	2.23	0.72
2:O:5:ALA:HB1	2:P:6:ALA:CB	2.21	0.71
2:N:3:ASP:OD1	2:N:4:THR:N	2.24	0.70
2:M:32:LEU:HD12	2:M:50:ALA:CB	2.22	0.69
2:K:1:ASP:O	2:K:4:THR:OG1	2.11	0.69
2:K:52:LEU:HD22	2:R:29:PHE:CE1	2.28	0.67
2:P:18:VAL:O	2:P:21:SER:N	2.27	0.67
2:Q:65:LEU:HD22	2:R:63:PHE:CE2	2.30	0.67
2:L:27:THR:HA	2:M:27:THR:HG21	1.78	0.66
2:P:54:PHE:CE1	2:Q:56:LEU:HD23	2.32	0.64
2:K:54:PHE:CZ	2:L:56:LEU:HD12	2.33	0.63
2:Q:43:M3L:HM22	2:R:45:GLN:HE21	1.63	0.63
2:K:67:VAL:O	2:K:71:ILE:HD12	1.99	0.63
2:L:36:TYR:OH	2:M:42:LEU:HD22	1.99	0.62
2:M:16:VAL:HG13	2:N:16:VAL:HG13	1.80	0.62
1:8:18:MET:O	1:8:22:ILE:N	2.32	0.62
2:P:2:ILE:HG13	2:Q:2:ILE:HD13	1.83	0.61
2:M:54:PHE:HZ	2:N:56:LEU:HD12	1.66	0.60
2:Q:5:ALA:HB1	2:R:6:ALA:HB2	1.83	0.60
2:K:56:LEU:HD23	2:R:25:ILE:CG2	2.31	0.60
2:P:32:LEU:HD22	2:P:50:ALA:CB	2.32	0.60
2:K:49:TYR:CE1	2:R:32:LEU:HD21	2.37	0.59
2:N:52:LEU:HD23	2:N:56:LEU:HD23	1.85	0.59
2:M:32:LEU:HD12	2:M:50:ALA:HB2	1.84	0.58
2:M:36:TYR:OH	2:N:42:LEU:HD22	2.03	0.58
2:Q:44:GLN:N	2:Q:44:GLN:OE1	2.32	0.58
2:M:1:ASP:OD1	2:M:2:ILE:N	2.36	0.58
2:M:30:GLY:O	2:N:31:SER:OG	2.23	0.57
2:R:16:VAL:HG12	2:R:16:VAL:O	2.05	0.57
2:M:5:ALA:HB1	2:N:6:ALA:HB2	1.86	0.57
2:Q:42:LEU:HD12	2:Q:42:LEU:O	2.04	0.57
2:P:44:GLN:OE1	2:P:45:GLN:N	2.37	0.56
1:8:15:SER:O	1:8:16:MET:C	2.44	0.56
2:M:16:VAL:HG13	2:N:16:VAL:CG1	2.36	0.56
2:O:2:ILE:HD12	2:P:2:ILE:HG21	1.89	0.55
2:P:36:TYR:HE2	2:Q:42:LEU:HD13	1.73	0.54
2:K:5:ALA:HB1	2:L:6:ALA:HB2	1.90	0.54
2:Q:65:LEU:HD22	2:R:63:PHE:HE2	1.69	0.54
2:O:56:LEU:HD23	2:O:56:LEU:O	2.07	0.53
2:K:72:LEU:O	2:K:72:LEU:HD23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:29:PHE:CD2	2:O:53:GLY:HA2	2.44	0.53
2:R:15:THR:HG22	2:R:15:THR:O	2.09	0.53
2:N:42:LEU:O	2:N:43:M3L:C	2.57	0.52
2:Q:9:ILE:CD1	2:R:9:ILE:HG22	2.37	0.52
2:K:56:LEU:HD23	2:R:25:ILE:HG23	1.90	0.52
2:O:2:ILE:CD1	2:P:2:ILE:HG21	2.41	0.51
2:O:5:ALA:HB1	2:P:6:ALA:HB2	1.90	0.51
2:M:30:GLY:HA2	2:M:33:ILE:HD12	1.93	0.51
2:P:7:LYS:HG2	2:P:72:LEU:HD12	1.92	0.51
2:P:33:ILE:HG21	2:Q:32:LEU:HA	1.93	0.51
2:M:54:PHE:CZ	2:N:56:LEU:HD12	2.45	0.50
2:O:54:PHE:HZ	2:P:56:LEU:HD12	1.74	0.50
2:N:32:LEU:CD1	2:N:50:ALA:HB2	2.40	0.50
2:P:54:PHE:CZ	2:Q:56:LEU:HD23	2.46	0.50
2:R:71:ILE:HG13	2:R:71:ILE:O	2.12	0.50
2:K:7:LYS:HZ1	2:K:8:PHE:HE1	1.59	0.50
2:Q:8:PHE:CE1	2:R:7:LYS:HD2	2.47	0.49
2:K:47:PHE:HD1	2:L:49:TYR:HH	1.59	0.49
2:K:69:PHE:O	2:K:72:LEU:N	2.45	0.49
2:N:32:LEU:HD12	2:N:50:ALA:HB2	1.94	0.49
2:O:33:ILE:HD11	2:P:49:TYR:HB3	1.94	0.49
2:O:1:ASP:OD2	2:O:2:ILE:N	2.44	0.49
2:K:54:PHE:HZ	2:L:56:LEU:HD12	1.75	0.49
2:K:64:CYS:SG	2:R:18:VAL:HG11	2.52	0.49
1:8:1:MET:SD	2:Q:70:LEU:HD11	2.53	0.48
2:N:54:PHE:CZ	2:O:56:LEU:HD11	2.48	0.48
2:R:7:LYS:HE2	2:R:73:PHE:HA	1.95	0.48
1:8:8:THR:O	1:8:9:TRP:C	2.51	0.48
2:K:67:VAL:HG11	2:R:15:THR:HG21	1.95	0.48
2:L:16:VAL:HG12	2:L:16:VAL:O	2.13	0.48
2:Q:9:ILE:HD13	2:R:9:ILE:CG2	2.40	0.48
1:8:18:MET:HA	1:8:22:ILE:HG12	1.95	0.48
2:N:3:ASP:OD1	2:N:4:THR:HG23	2.14	0.48
2:L:23:ALA:O	2:L:27:THR:HG23	2.14	0.47
2:K:41:SER:C	2:K:42:LEU:HD22	2.35	0.47
2:Q:70:LEU:HD23	2:Q:70:LEU:C	2.35	0.47
2:K:42:LEU:HD12	2:K:45:GLN:NE2	2.30	0.46
2:L:67:VAL:O	2:L:71:ILE:HG12	2.15	0.46
2:O:8:PHE:HD1	2:P:71:ILE:HD12	1.79	0.46
2:L:7:LYS:HD3	2:L:71:ILE:O	2.16	0.46
2:P:70:LEU:C	2:P:70:LEU:HD23	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:42:LEU:HD12	2:Q:46:LEU:HG	1.96	0.46
2:N:29:PHE:O	2:N:33:ILE:HD12	2.15	0.46
2:M:64:CYS:O	2:M:67:VAL:HG12	2.16	0.46
2:Q:54:PHE:HE1	2:R:56:LEU:HD22	1.81	0.46
2:N:45:GLN:O	2:N:49:TYR:CD1	2.68	0.46
2:P:5:ALA:HB1	2:Q:6:ALA:HB2	1.98	0.46
2:K:1:ASP:OD1	2:K:3:ASP:N	2.48	0.45
2:O:16:VAL:O	2:O:16:VAL:HG12	2.16	0.45
2:K:52:LEU:HD22	2:R:29:PHE:CZ	2.51	0.45
2:K:1:ASP:O	2:L:2:ILE:HD12	2.17	0.45
2:L:25:ILE:O	2:L:28:VAL:HG12	2.17	0.44
2:O:62:LEU:HD23	2:O:62:LEU:O	2.18	0.44
2:N:18:VAL:HG22	2:O:60:MET:CE	2.47	0.44
2:P:2:ILE:HD12	2:P:2:ILE:H	1.82	0.44
2:M:5:ALA:CB	2:N:6:ALA:HB2	2.47	0.44
2:N:58:GLU:HA	2:N:58:GLU:OE2	2.17	0.44
2:K:1:ASP:OD1	2:K:2:ILE:N	2.50	0.44
2:R:25:ILE:HD11	2:R:57:SER:OG	2.18	0.44
2:Q:58:GLU:O	2:Q:62:LEU:HG	2.18	0.43
1:8:16:MET:O	1:8:17:ILE:C	2.56	0.43
2:P:9:ILE:CD1	2:Q:9:ILE:CG2	2.96	0.43
2:N:70:LEU:O	2:N:74:ALA:N	2.51	0.43
2:K:52:LEU:HD22	2:R:29:PHE:HE1	1.79	0.43
2:M:36:TYR:HE2	2:N:42:LEU:HD13	1.79	0.43
2:N:29:PHE:HD2	2:O:53:GLY:HA2	1.82	0.43
2:L:9:ILE:HD11	2:M:9:ILE:HG21	2.00	0.43
2:K:17:GLY:O	2:K:19:ALA:N	2.51	0.42
2:M:1:ASP:O	2:M:4:THR:OG1	2.30	0.42
2:M:5:ALA:HA	2:N:6:ALA:CB	2.49	0.42
2:K:41:SER:O	2:K:42:LEU:HD22	2.19	0.42
2:K:67:VAL:O	2:K:68:ALA:C	2.57	0.42
1:8:3:GLN:OE1	1:8:3:GLN:N	2.49	0.42
2:K:67:VAL:O	2:K:70:LEU:HG	2.19	0.42
2:N:54:PHE:HZ	2:O:56:LEU:HD11	1.83	0.42
1:8:18:MET:O	1:8:19:THR:C	2.58	0.42
1:8:18:MET:O	1:8:22:ILE:HB	2.19	0.42
2:K:39:ASN:O	2:K:41:SER:N	2.53	0.42
2:M:32:LEU:C	2:M:32:LEU:HD23	2.40	0.42
2:N:8:PHE:HE1	2:O:7:LYS:HD3	1.84	0.42
2:Q:29:PHE:CD1	2:R:53:GLY:HA2	2.55	0.42
2:K:42:LEU:O	2:K:45:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:60:MET:HA	2:M:63:PHE:HB3	2.01	0.41
2:P:9:ILE:CD1	2:Q:9:ILE:HG21	2.50	0.41
2:Q:26:GLY:HA3	2:R:24:GLY:HA2	2.02	0.41
1:8:11:ILE:HG23	1:8:12:THR:N	2.34	0.41
2:K:48:SER:HA	2:K:51:ILE:HG12	2.01	0.41
2:Q:69:PHE:O	2:Q:72:LEU:N	2.54	0.41
2:L:7:LYS:NZ	2:L:74:ALA:O	2.31	0.41
2:P:4:THR:O	2:P:8:PHE:HD2	2.03	0.41
2:K:2:ILE:HD13	2:R:2:ILE:HG22	2.01	0.41
2:Q:16:VAL:O	2:Q:16:VAL:HG22	2.20	0.41
2:K:32:LEU:HA	2:R:33:ILE:HG21	2.02	0.41
2:N:12:GLY:O	2:N:15:THR:HG22	2.21	0.41
2:K:39:ASN:OD1	2:K:42:LEU:HD23	2.20	0.41
2:M:39:ASN:OD1	2:M:39:ASN:O	2.39	0.41
2:P:39:ASN:O	2:P:41:SER:N	2.54	0.41
2:Q:5:ALA:HB1	2:R:6:ALA:CB	2.51	0.41
2:Q:29:PHE:HD1	2:R:53:GLY:CA	2.33	0.40
2:N:18:VAL:HG22	2:O:60:MET:HE3	2.04	0.40
2:K:56:LEU:HD23	2:R:25:ILE:HG21	2.00	0.40
2:Q:42:LEU:HD11	2:Q:46:LEU:HD21	2.03	0.40
2:M:18:VAL:HG11	2:M:65:LEU:HD21	2.04	0.40
2:O:9:ILE:HD11	2:P:6:ALA:HA	2.03	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	8	32/67 (48%)	21 (66%)	11 (34%)	0	100	100
2	K	71/75 (95%)	64 (90%)	7 (10%)	0	100	100
2	L	71/75 (95%)	68 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
2	N	72/75 (96%)	67 (93%)	5 (7%)	0	100	100
2	O	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
2	P	71/75 (95%)	66 (93%)	5 (7%)	0	100	100
2	Q	72/75 (96%)	67 (93%)	5 (7%)	0	100	100
2	R	72/75 (96%)	63 (88%)	9 (12%)	0	100	100
3	a	221/226 (98%)	195 (88%)	26 (12%)	0	100	100
4	b	92/214 (43%)	80 (87%)	12 (13%)	0	100	100
5	d	32/161 (20%)	28 (88%)	4 (12%)	0	100	100
6	e	55/70 (79%)	53 (96%)	2 (4%)	0	100	100
7	f	81/87 (93%)	73 (90%)	8 (10%)	0	100	100
8	g	72/102 (71%)	68 (94%)	4 (6%)	0	100	100
9	j	46/60 (77%)	40 (87%)	6 (13%)	0	100	100
10	k	33/57 (58%)	31 (94%)	2 (6%)	0	100	100
All	All	1237/1644 (75%)	1119 (90%)	118 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	8	34/66 (52%)	34 (100%)	0	100	100
2	K	49/50 (98%)	49 (100%)	0	100	100
2	L	49/50 (98%)	49 (100%)	0	100	100
2	M	50/50 (100%)	50 (100%)	0	100	100
2	N	50/50 (100%)	50 (100%)	0	100	100
2	O	50/50 (100%)	50 (100%)	0	100	100
2	P	49/50 (98%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	50/50 (100%)	50 (100%)	0	100	100
2	R	50/50 (100%)	50 (100%)	0	100	100
3	a	196/199 (98%)	196 (100%)	0	100	100
4	b	78/187 (42%)	78 (100%)	0	100	100
5	d	34/139 (24%)	33 (97%)	1 (3%)	42	64
6	e	48/59 (81%)	46 (96%)	2 (4%)	30	56
7	f	72/75 (96%)	72 (100%)	0	100	100
8	g	63/84 (75%)	63 (100%)	0	100	100
9	j	43/51 (84%)	43 (100%)	0	100	100
10	k	29/46 (63%)	29 (100%)	0	100	100
All	All	994/1306 (76%)	991 (100%)	3 (0%)	92	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	d	155	ARG
6	e	47	LYS
6	e	48	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	8	30	ASN
2	K	45	GLN
5	d	129	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	$\#\|Z\| > 2$
2	M3L	M	43	2	10,11,12	0.58	0	9,14,16	0.55	0
2	M3L	P	43	2	10,11,12	0.51	0	9,14,16	0.55	0
2	M3L	K	43	2	10,11,12	0.49	0	9,14,16	0.53	0
2	M3L	L	43	2	10,11,12	0.55	0	9,14,16	0.52	0
2	M3L	Q	43	2	10,11,12	0.49	0	9,14,16	0.74	0
2	M3L	O	43	2	10,11,12	0.53	0	9,14,16	0.67	0
2	M3L	N	43	2	10,11,12	0.47	0	9,14,16	0.40	0
2	M3L	R	43	2	10,11,12	0.57	0	9,14,16	0.60	0

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	M3L	M	43	2	-	1/9/10/12	-
2	M3L	P	43	2	-	1/9/10/12	-
2	M3L	K	43	2	-	1/9/10/12	-
2	M3L	L	43	2	-	0/9/10/12	-
2	M3L	Q	43	2	-	1/9/10/12	-
2	M3L	O	43	2	-	7/9/10/12	-
2	M3L	N	43	2	-	4/9/10/12	-
2	M3L	R	43	2	-	3/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	43	M3L	C-CA-CB-CG
2	R	43	M3L	C-CA-CB-CG
2	O	43	M3L	CG-CD-CE-NZ
2	O	43	M3L	CD-CE-NZ-CM2
2	O	43	M3L	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
2	O	43	M3L	CD-CE-NZ-CM1
2	O	43	M3L	CD-CE-NZ-CM3
2	O	43	M3L	CE-CD-CG-CB
2	M	43	M3L	CG-CD-CE-NZ
2	N	43	M3L	CA-CB-CG-CD
2	N	43	M3L	CD-CE-NZ-CM1
2	K	43	M3L	CA-CB-CG-CD
2	P	43	M3L	CG-CD-CE-NZ
2	R	43	M3L	CE-CD-CG-CB
2	N	43	M3L	CD-CE-NZ-CM2
2	Q	43	M3L	CA-CB-CG-CD
2	N	43	M3L	CD-CE-NZ-CM3
2	R	43	M3L	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	43	M3L	2	0
2	N	43	M3L	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CDL	f	101	-	88,88,99	0.97	6 (6%)	94,100,111	1.07	5 (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
11	CDL	f	101	-	-	43/99/99/110	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	f	101	CDL	OA6-CA4	-2.69	1.39	1.46
11	f	101	CDL	OB8-CB7	2.56	1.40	1.33
11	f	101	CDL	OB6-CB4	-2.56	1.40	1.46
11	f	101	CDL	OB6-CB5	2.44	1.41	1.34
11	f	101	CDL	OA8-CA7	2.42	1.40	1.33
11	f	101	CDL	OA8-CA6	-2.14	1.40	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	f	101	CDL	OA6-CA5-C11	4.79	121.83	111.50
11	f	101	CDL	OB6-CB5-C51	3.71	119.49	111.50
11	f	101	CDL	OA8-CA7-C31	2.34	119.26	111.91
11	f	101	CDL	OB8-CB7-C71	2.20	118.81	111.91
11	f	101	CDL	CA4-OA6-CA5	-2.07	112.69	117.79

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	f	101	CDL	O1-C1-CA2-OA2
11	f	101	CDL	OA6-CA4-CA6-OA8
11	f	101	CDL	OA9-CA7-OA8-CA6
11	f	101	CDL	C31-CA7-OA8-CA6
11	f	101	CDL	CB2-C1-CA2-OA2
11	f	101	CDL	OB6-CB4-CB6-OB8
11	f	101	CDL	CA5-C11-C12-C13
11	f	101	CDL	CB5-C51-C52-C53
11	f	101	CDL	CA7-C31-C32-C33
11	f	101	CDL	CA2-OA2-PA1-OA5
11	f	101	CDL	C33-C34-C35-C36
11	f	101	CDL	C39-C40-C41-C42

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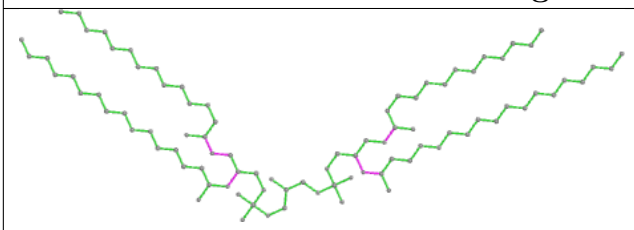
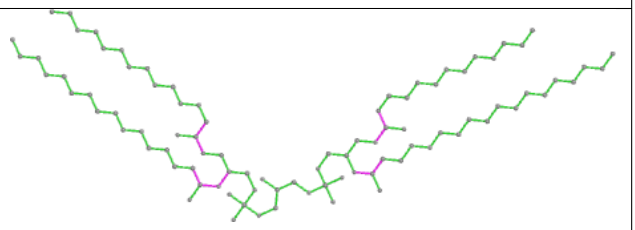
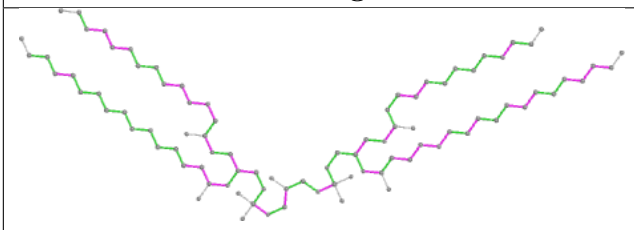
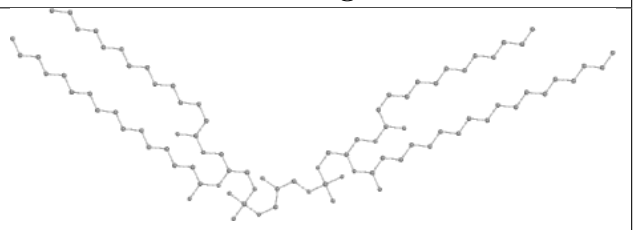
Mol	Chain	Res	Type	Atoms
11	f	101	CDL	C78-C79-C80-C81
11	f	101	CDL	C31-C32-C33-C34
11	f	101	CDL	C58-C59-C60-C61
11	f	101	CDL	C11-CA5-OA6-CA4
11	f	101	CDL	OA7-CA5-OA6-CA4
11	f	101	CDL	C51-CB5-OB6-CB4
11	f	101	CDL	OB7-CB5-OB6-CB4
11	f	101	CDL	C62-C63-C64-C65
11	f	101	CDL	C38-C39-C40-C41
11	f	101	CDL	C55-C56-C57-C58
11	f	101	CDL	CA3-CA4-CA6-OA8
11	f	101	CDL	C20-C21-C22-C23
11	f	101	CDL	C71-CB7-OB8-CB6
11	f	101	CDL	CB3-CB4-CB6-OB8
11	f	101	CDL	C32-C33-C34-C35
11	f	101	CDL	OA5-CA3-CA4-OA6
11	f	101	CDL	C51-C52-C53-C54
11	f	101	CDL	C53-C54-C55-C56
11	f	101	CDL	OB9-CB7-OB8-CB6
11	f	101	CDL	C72-C73-C74-C75
11	f	101	CDL	C63-C64-C65-C66
11	f	101	CDL	CA2-OA2-PA1-OA3
11	f	101	CDL	CB2-OB2-PB2-OB3
11	f	101	CDL	OA5-CA3-CA4-CA6
11	f	101	CDL	C64-C65-C66-C67
11	f	101	CDL	C12-C11-CA5-OA6
11	f	101	CDL	C71-C72-C73-C74
11	f	101	CDL	CB2-OB2-PB2-OB5
11	f	101	CDL	C52-C53-C54-C55
11	f	101	CDL	C59-C60-C61-C62
11	f	101	CDL	C37-C38-C39-C40

There are no ring outliers.

No monomer is involved in short contacts.

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 CDL f 101	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

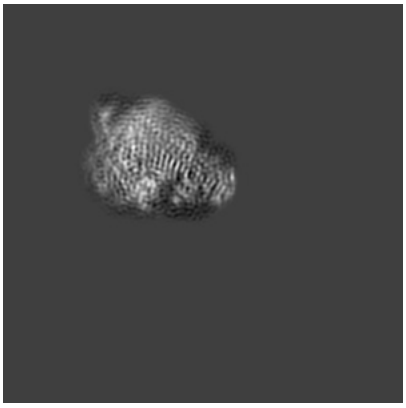
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0668. These allow visual inspection of the internal detail of the map and identification of artifacts.

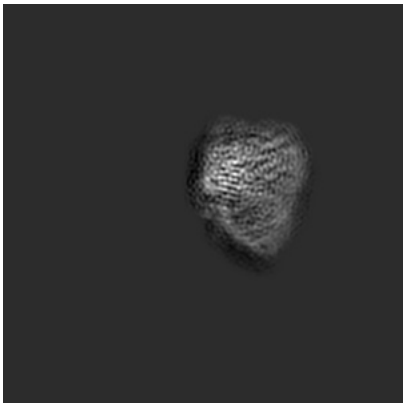
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

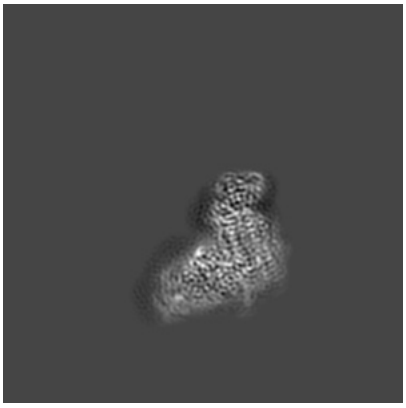
6.1.1 Primary map



X



Y

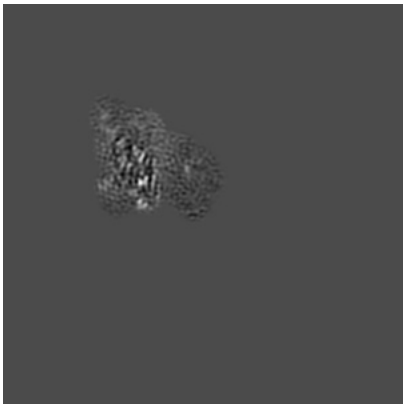


Z

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

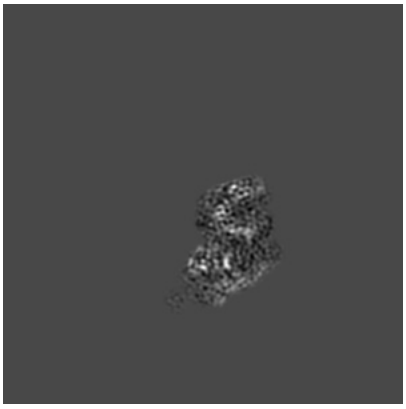
6.2 Central slices (i)

6.2.1 Primary map



X Index: 120

Y Index: 120

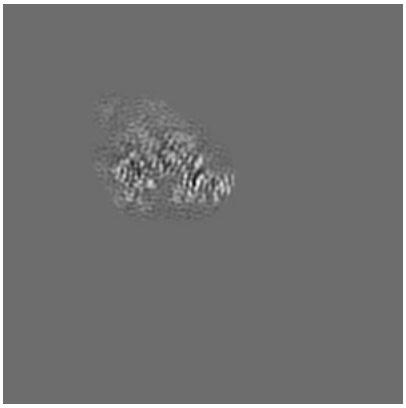


Z Index: 120

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

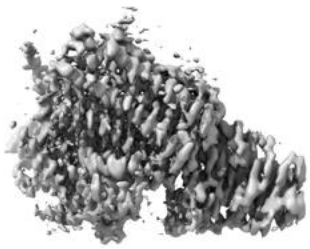
Y Index: 78

Z Index: 134

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 0.0286. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

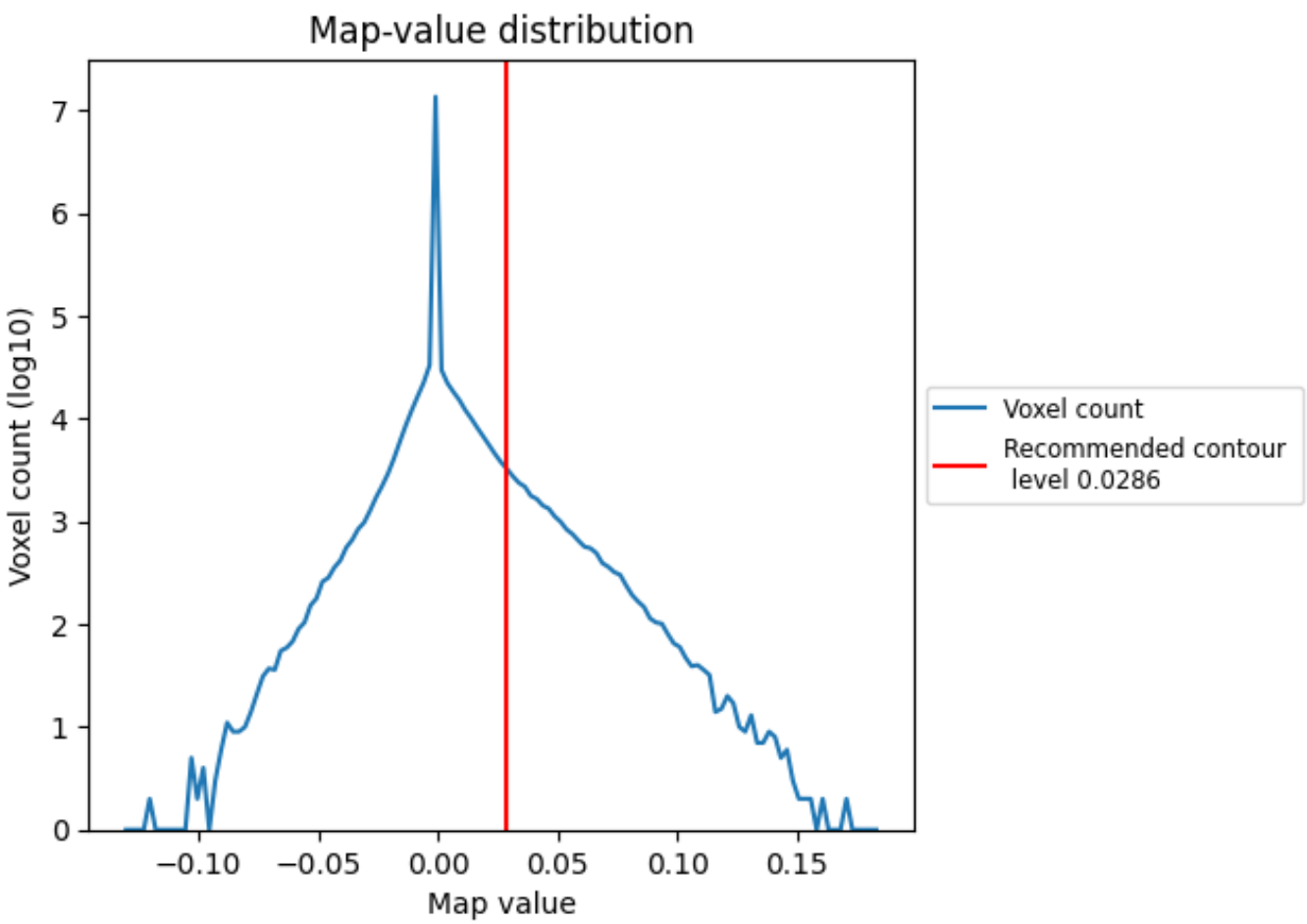
6.5 Mask visualisation (i)

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

7 Map analysis (i)

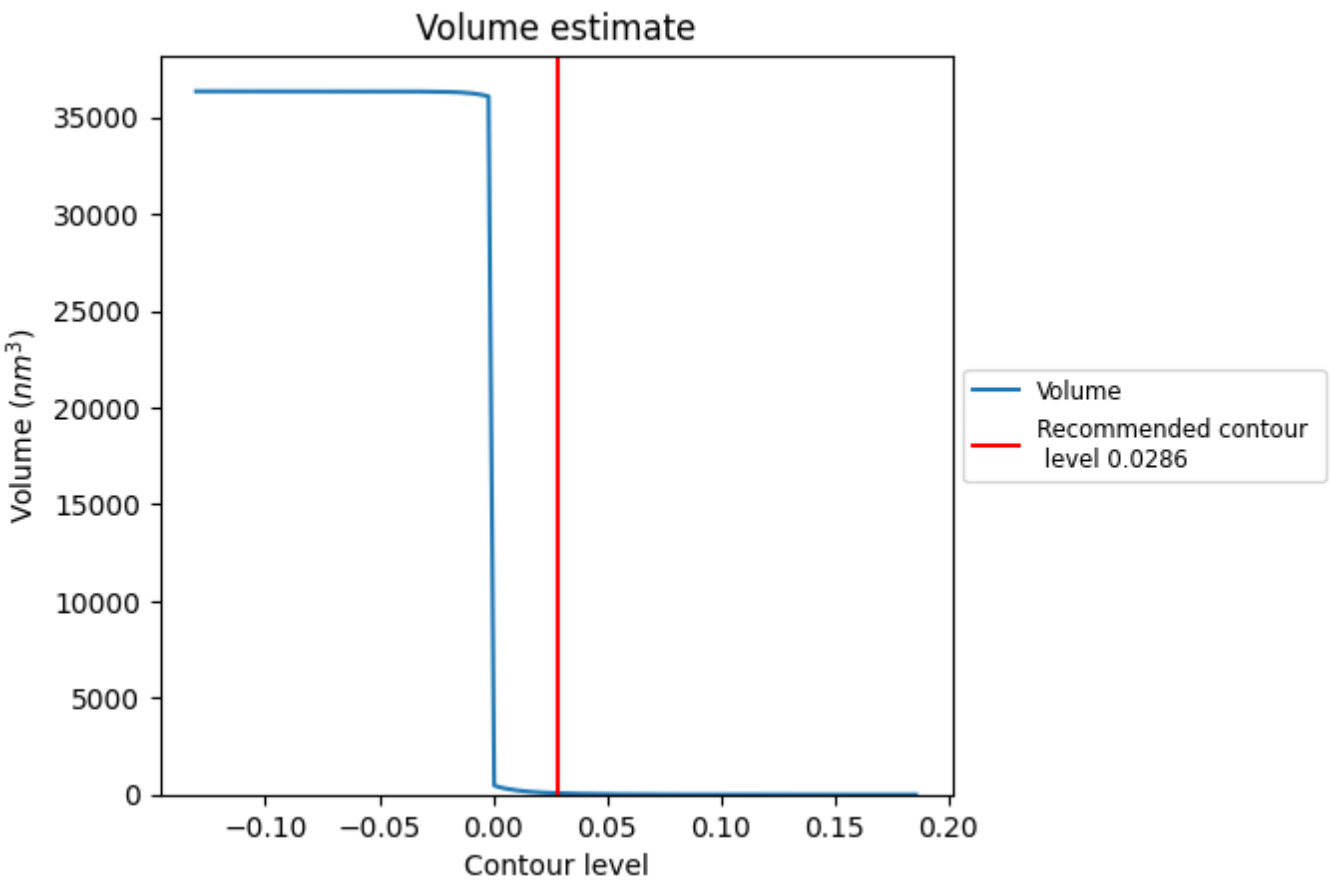
This section contains the results of statistical analysis of the map.

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.

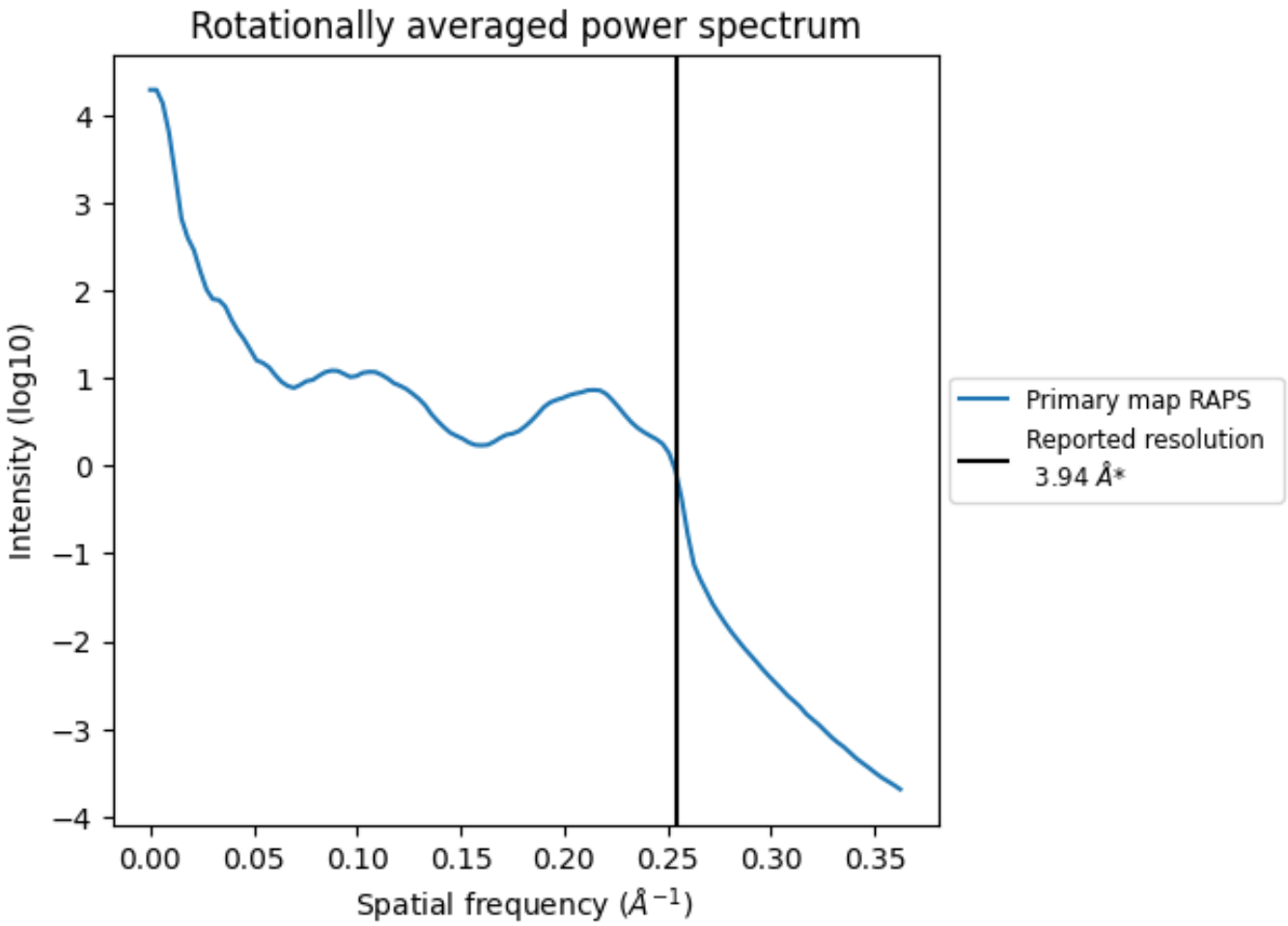
7.2 Volume estimate (i)



The volume at the recommended contour level is 69 nm^3; this corresponds to an approximate mass of 62 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 0.254 Å^{-1}

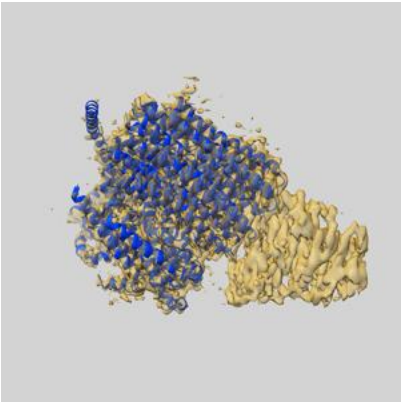
8 Fourier-Shell correlation (i)

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

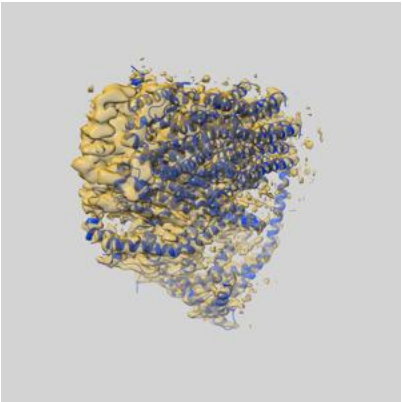
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0668 and PDB model 6ZMR. Per-residue inclusion information can be found in section 3 on page 7.

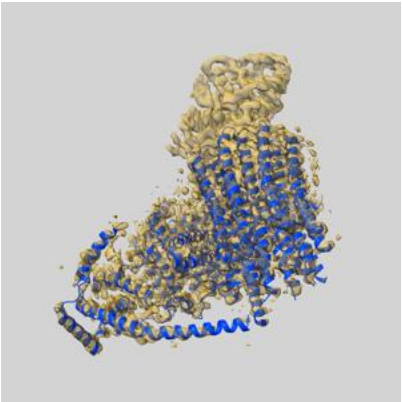
9.1 Map-model overlay (i)



X



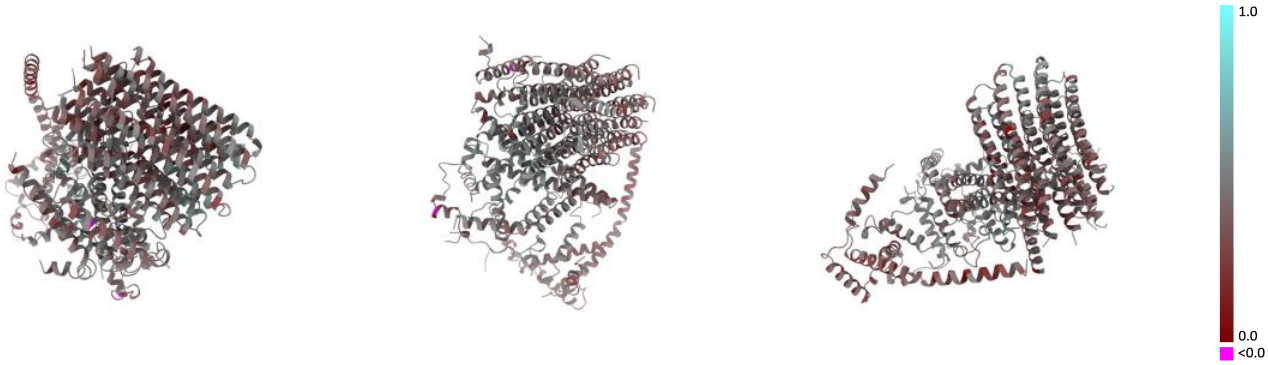
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0286 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.

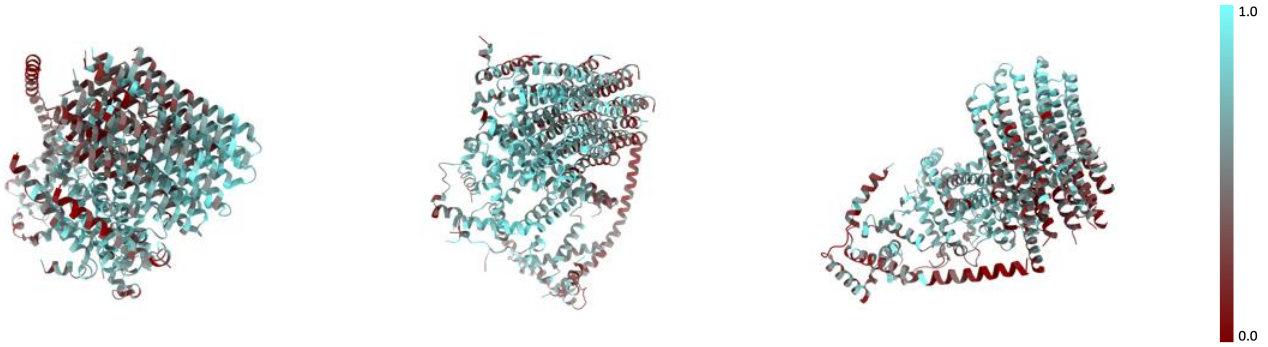
9.2 Q-score mapped to coordinate model (i)



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.

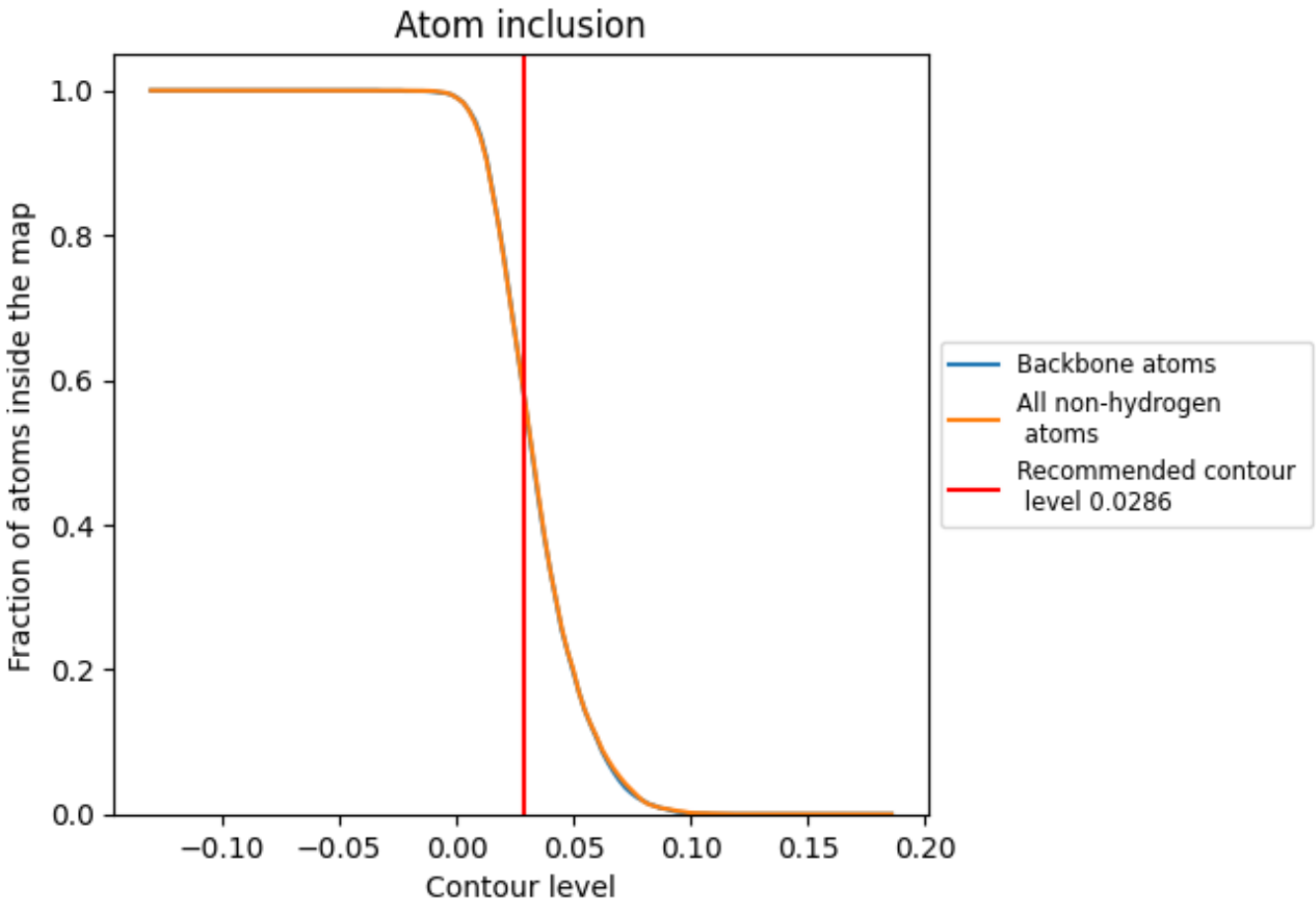
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0286).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 58% 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 (0.0286) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5847	0.4150
8	0.7357	0.4700
K	0.5448	0.3880
L	0.6171	0.4130
M	0.5779	0.4060
N	0.5553	0.4100
O	0.5253	0.4220
P	0.5276	0.4180
Q	0.6585	0.4330
R	0.5460	0.3910
a	0.7157	0.4540
b	0.6838	0.4370
d	0.5802	0.3940
e	0.2517	0.3300
f	0.5707	0.4380
g	0.4712	0.3410
j	0.5564	0.4050
k	0.3125	0.4000