Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 04:16 AM JST

PDB ID	:	7VV5
EMDB ID	:	EMD-32138
Title	:	Cryo-EM structure of pseudoallergen receptor MRGPRX2 complex with C48/80, state1
Authors	:	Li, Y.; Yang, F.
Deposited on	:	2021-11-04
Resolution	:	2.76 Å(reported)

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

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

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

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

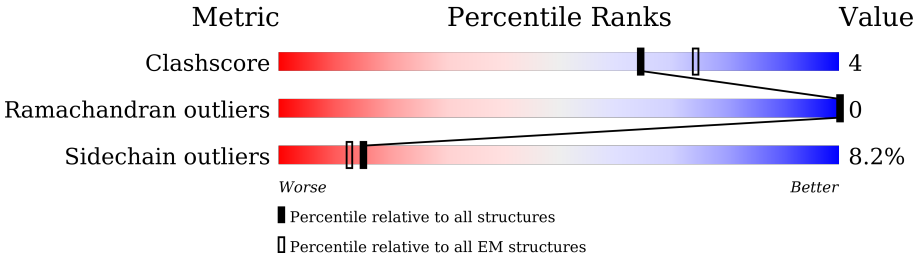
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.76 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	354	54% 9% • 36%
2	B	358	75% 18% • 5%
3	G	58	91% 5% •
4	S	285	69% 12% • 18%
5	R	330	67% 13% • 19%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8829 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	226	1813	1150	300	349	14	0	0

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	339	2598	1603	464	510	21	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	56	427	268	76	80	3	0	0

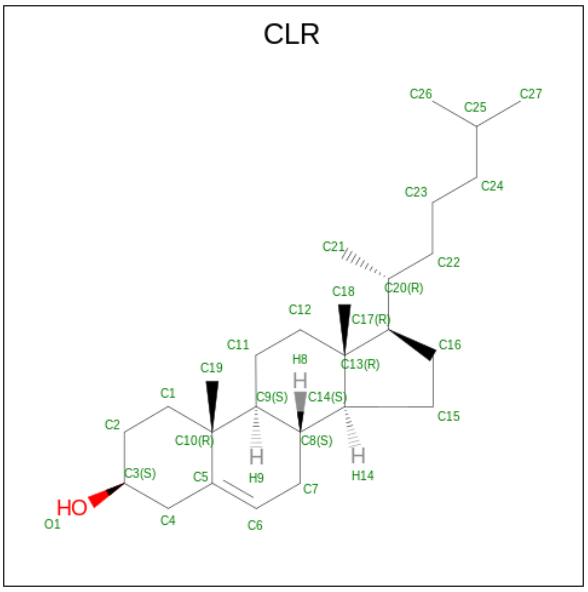
- Molecule 4 is a protein called scFv.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S	233	1786	1133	296	347	10	0	0

- Molecule 5 is a protein called Mas-related G-protein coupled receptor member X2.

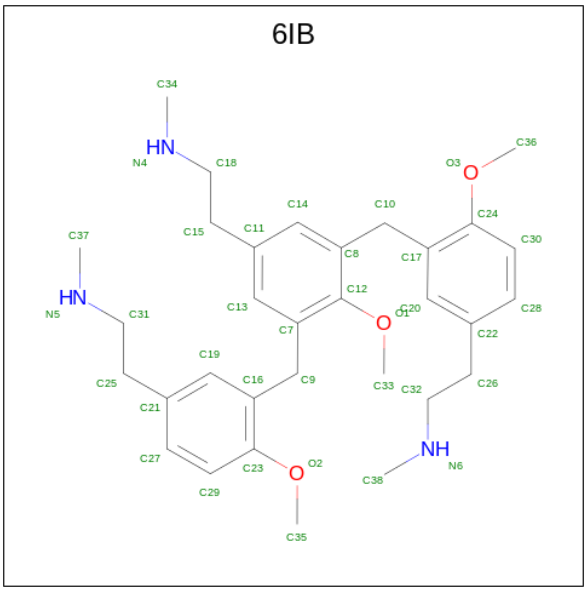
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	R	268	2139	1447	335	339	18	0	0

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	R	1	28	27	1	0

- Molecule 7 is 2-[4-methoxy-3-[[2-methoxy-3-[[2-methoxy-5-[2-(methylamino)ethyl]phenyl]methyl]-5-[2-(methylamino)ethyl]phenyl]methyl]phenyl]- {N}-methyl-ethanamine (three-letter code: 6IB) (formula: $C_{32}H_{45}N_3O_3$) (labeled as "Ligand of Interest" by depositor).



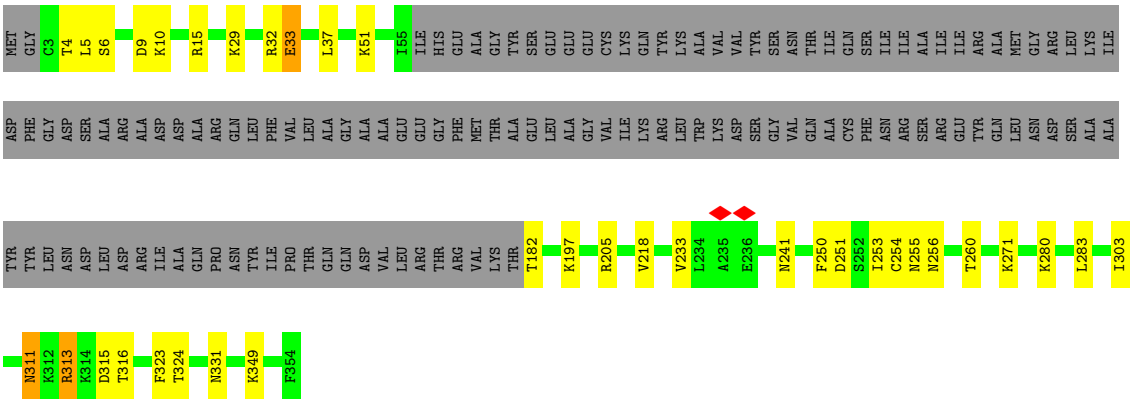
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	R	1	38	32	3	3	0

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.

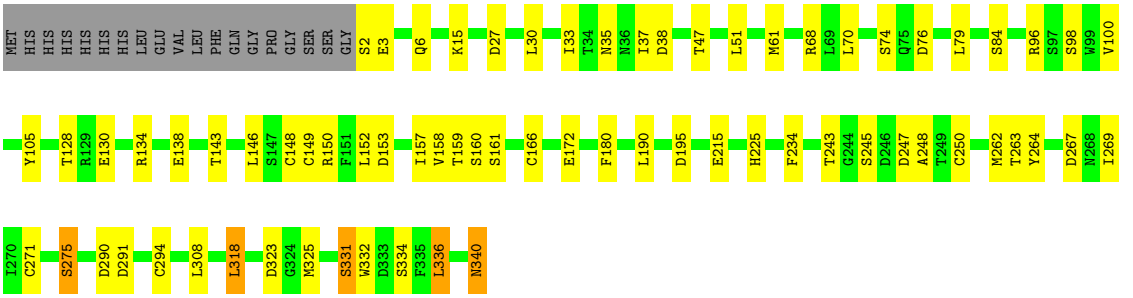
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



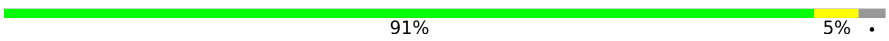
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

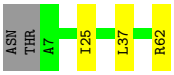
Chain B:



• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:





• Molecule 4: scFv

Chain S: 69% 12% • 18%

MET LEU LEU VAL ASN GLN SER HIS GLN GLY PHE ASN LYS GLU HIS THR SER LYS MET VAL SER ALA ILE VAL LEU TYR VAL LEU LEU ALA ALA ALA ALA HIS SER ALA PHE ALA V2 R18 A40 K43 S52 R67 F68 T69 R72 S85 T91 S105 S106

T118 V119 S120 ALA GLY GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY GLY G122 S123 A124 D125 M128 T129 T132 S133 S144 S149 S150 K151 S152 L153 T160 Y161 L162 R168 R179 S185 R190 F191 S192 T198 T201 S205 R206 L207 E210

D211 L235

• Molecule 5: Mas-related G-protein coupled receptor member X2

Chain R: 67% 13% • 19%

MET ASP PRO THR THR PRO ALA TRP GLY THR GLU SER THR THR VAL ASN GLY ASN ASP GLN ALA L22 G27 I32 I40 G44 N48 R60 V66 L79 Q82 Y89 L90 S91 S98 T107 V108 M109 S118 E126 R127 C128 R141 L153

S157 L158 L159 L160 S161 I162 L163 D174 W179 T182 F183 D184 L198 S213 L221 L226 L230 V231 C235 I241 Q242 L245 I246 L247 W248 I249 W250 S264 S268 S269 L270 Q288 W289 ARG LEU GLN GLN PRO ILE LEU LYS LEU ALA LEU GLN

ARG ALA LEU GLN ASP ILE ALA GLU VAL ASP HIS SER GLU GLY CYS PHE ARG GLN GLY THR PRO GLU MET SER ARG SER SER LEU VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	264735	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 ($e^-/Å^2$)	58	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	0.181	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	168.32, 168.32, 168.32	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	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: 6IB, CLR

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	0.47	0/1843	0.59	1/2473 (0.0%)
2	B	0.62	0/2645	0.71	5/3586 (0.1%)
3	G	0.38	0/433	0.59	0/583
4	S	0.59	0/1830	0.65	0/2481
5	R	0.45	0/2202	0.69	2/3001 (0.1%)
All	All	0.54	0/8953	0.66	8/12124 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	226	LEU	CA-CB-CG	7.42	132.37	115.30
2	B	336	LEU	CA-CB-CG	6.96	131.30	115.30
5	R	230	LEU	CA-CB-CG	6.72	130.75	115.30
2	B	318	LEU	CA-CB-CG	6.61	130.51	115.30
2	B	79	LEU	CA-CB-CG	6.43	130.09	115.30
2	B	291	ASP	CB-CG-OD1	5.60	123.34	118.30
2	B	79	LEU	CB-CG-CD2	-5.59	101.49	111.00
1	A	251	ASP	CB-CG-OD1	5.15	122.93	118.30

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	A	1813	0	1788	11	0
2	B	2598	0	2493	28	0
3	G	427	0	439	0	0
4	S	1786	0	1722	12	0
5	R	2139	0	2213	19	0
6	R	28	0	46	1	0
7	R	38	0	0	5	0
All	All	8829	0	8701	73	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 4.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PHE:O	1:A:254:CYS:HB2	1.92	0.70
1:A:311:ASN:N	1:A:311:ASN:OD1	2.35	0.60
5:R:82:GLN:NE2	5:R:109:MET:SD	2.75	0.59
2:B:294:CYS:HB2	2:B:308:LEU:HB2	1.85	0.58
2:B:160:SER:HB3	2:B:190:LEU:HD13	1.85	0.57
2:B:248:ALA:HB1	2:B:269:ILE:HG22	1.87	0.57
2:B:245:SER:OG	2:B:247:ASP:OD1	2.24	0.56
4:S:40:ALA:HB3	4:S:43:LYS:HB2	1.89	0.55
7:R:402:6IB:C38	7:R:402:6IB:C35	2.85	0.54
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.90	0.54
7:R:402:6IB:C14	7:R:402:6IB:C34	2.86	0.54
7:R:402:6IB:C9	7:R:402:6IB:C33	2.86	0.54
7:R:402:6IB:C35	7:R:402:6IB:C32	2.86	0.53
4:S:91:THR:HG23	4:S:118:THR:HA	1.90	0.53
2:B:96:ARG:NH2	2:B:138:GLU:OE2	2.42	0.53
4:S:105:SER:O	4:S:179:ARG:NH2	2.39	0.53
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.91	0.52
1:A:260:THR:HG22	1:A:313:ARG:HH11	1.74	0.52
1:A:271:LYS:HD3	1:A:323:PHE:HB3	1.90	0.52
5:R:118:SER:HB2	5:R:153:LEU:HD22	1.92	0.51
2:B:225:HIS:NE2	2:B:243:THR:OG1	2.37	0.51
2:B:149:CYS:HB3	2:B:157:ILE:HD11	1.92	0.51
2:B:331:SER:OG	2:B:332:TRP:N	2.44	0.51
5:R:27:GLY:O	5:R:89:TYR:OH	2.29	0.50
2:B:166:CYS:HB2	2:B:180:PHE:HB2	1.93	0.50
4:S:149:SER:HB3	4:S:198:THR:HA	1.93	0.50
1:A:255:ASN:HD21	1:A:311:ASN:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:LEU:HD11	2:B:159:THR:HB	1.95	0.49
4:S:190:ARG:NH2	4:S:211:ASP:OD1	2.46	0.48
2:B:38:ASP:OD2	2:B:38:ASP:N	2.38	0.48
2:B:2:SER:OG	2:B:3:GLU:N	2.42	0.48
5:R:264:SER:O	5:R:268:SER:OG	2.31	0.48
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.96	0.48
5:R:241:ILE:HG22	5:R:246:ILE:HD12	1.96	0.48
5:R:288:GLN:HG2	5:R:289:TRP:HD1	1.78	0.48
1:A:29:LYS:HZ2	1:A:32:ARG:HD2	1.79	0.48
4:S:67:ARG:NH1	4:S:85:SER:O	2.47	0.47
4:S:168:ARG:NH1	4:S:210:GLU:O	2.42	0.47
5:R:107:THR:O	5:R:161:SER:OG	2.32	0.47
2:B:30:LEU:HD23	2:B:262:MET:HB2	1.96	0.47
5:R:184:ASP:OD2	7:R:402:6IB:N4	2.47	0.47
4:S:118:THR:O	4:S:118:THR:OG1	2.33	0.47
2:B:74:SER:OG	2:B:76:ASP:OD1	2.33	0.47
2:B:130:GLU:OE2	2:B:134:ARG:NH1	2.42	0.47
2:B:152:LEU:HD11	2:B:158:VAL:HG23	1.97	0.47
2:B:334:SER:OG	5:R:60:ARG:NH2	2.47	0.47
4:S:52:SER:O	4:S:72:ARG:NH1	2.48	0.47
2:B:325:MET:O	2:B:340:ASN:ND2	2.47	0.46
2:B:27:ASP:OD1	2:B:27:ASP:N	2.44	0.46
4:S:125:ASP:OD2	4:S:125:ASP:N	2.49	0.45
5:R:98:SER:O	5:R:98:SER:OG	2.32	0.45
5:R:66:VAL:HG13	6:R:401:CLR:H42	1.98	0.45
1:A:283:LEU:HD21	1:A:303:ILE:HD11	1.97	0.45
2:B:128:THR:HG22	2:B:130:GLU:H	1.81	0.45
2:B:15:LYS:HE3	2:B:15:LYS:HB2	1.79	0.45
1:A:33:GLU:OE2	1:A:197:LYS:NZ	2.46	0.45
2:B:68:ARG:O	2:B:84:SER:OG	2.30	0.44
4:S:128:MET:HE1	4:S:153:LEU:HD11	1.99	0.44
1:A:233:VAL:HA	1:A:241:ASN:HA	2.00	0.43
1:A:349:LYS:HE3	1:A:349:LYS:HB2	1.91	0.42
5:R:40:ILE:HD13	5:R:270:LEU:HG	2.01	0.42
5:R:44:GLY:O	5:R:48:ASN:ND2	2.52	0.42
5:R:242:GLN:HA	5:R:246:ILE:HB	2.01	0.42
1:A:5:LEU:HB2	1:A:10:LYS:HE3	2.02	0.41
2:B:37:ILE:HD13	2:B:37:ILE:HA	1.91	0.41
5:R:79:LEU:HD23	5:R:79:LEU:HA	1.93	0.41
5:R:231:VAL:O	5:R:235:CYS:HB2	2.21	0.41
2:B:150:ARG:HD3	2:B:150:ARG:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:18:ARG:HA	4:S:18:ARG:HD3	1.93	0.41
5:R:126:GLU:OE1	5:R:141:ARG:NH2	2.54	0.41
5:R:246:ILE:O	5:R:250:TRP:HB2	2.22	0.40
2:B:275:SER:HB2	2:B:318:LEU:HG	2.04	0.40
5:R:159:LEU:O	5:R:163:LEU:HB2	2.22	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	222/354 (63%)	216 (97%)	6 (3%)	0	100	100
2	B	337/358 (94%)	325 (96%)	12 (4%)	0	100	100
3	G	54/58 (93%)	51 (94%)	3 (6%)	0	100	100
4	S	229/285 (80%)	222 (97%)	7 (3%)	0	100	100
5	R	266/330 (81%)	252 (95%)	14 (5%)	0	100	100
All	All	1108/1385 (80%)	1066 (96%)	42 (4%)	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	A	199/305 (65%)	180 (90%)	19 (10%)	8	15
2	B	280/298 (94%)	257 (92%)	23 (8%)	11	20
3	G	44/47 (94%)	41 (93%)	3 (7%)	16	28
4	S	196/228 (86%)	179 (91%)	17 (9%)	10	18
5	R	239/292 (82%)	222 (93%)	17 (7%)	14	26
All	All	958/1170 (82%)	879 (92%)	79 (8%)	15	20

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	6	SER
1	A	9	ASP
1	A	15	ARG
1	A	33	GLU
1	A	37	LEU
1	A	51	LYS
1	A	182	THR
1	A	205	ARG
1	A	218	VAL
1	A	253	ILE
1	A	256	ASN
1	A	280	LYS
1	A	311	ASN
1	A	313	ARG
1	A	315	ASP
1	A	316	THR
1	A	324	THR
1	A	331	ASN
2	B	6	GLN
2	B	33	ILE
2	B	35	ASN
2	B	47	THR
2	B	61	MET
2	B	70	LEU
2	B	98	SER
2	B	100	VAL
2	B	105	TYR
2	B	143	THR
2	B	148	CYS
2	B	153	ASP

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Mol	Chain	Res	Type
2	B	161	SER
2	B	172	GLU
2	B	195	ASP
2	B	215	GLU
2	B	234	PHE
2	B	263	THR
2	B	267	ASP
2	B	275	SER
2	B	323	ASP
2	B	331	SER
2	B	340	ASN
3	G	25	ILE
3	G	37	LEU
3	G	62	ARG
4	S	43	LYS
4	S	69	THR
4	S	106	SER
4	S	118	THR
4	S	129	THR
4	S	132	THR
4	S	133	SER
4	S	144	SER
4	S	150	SER
4	S	152	SER
4	S	160	THR
4	S	162	LEU
4	S	185	SER
4	S	192	SER
4	S	201	THR
4	S	205	SER
4	S	207	LEU
5	R	22	LEU
5	R	32	ILE
5	R	91	SER
5	R	128	CYS
5	R	157	SER
5	R	163	LEU
5	R	174	ASP
5	R	179	TRP
5	R	182	THR
5	R	198	LEU
5	R	213	SER

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Mol	Chain	Res	Type
5	R	221	LEU
5	R	245	LEU
5	R	246	ILE
5	R	248	TRP
5	R	250	TRP
5	R	268	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	255	ASN
1	A	346	ASN
2	B	35	ASN
2	B	175	GLN
2	B	259	GLN
2	B	311	HIS
2	B	340	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
6	CLR	R	401	-	31,31,31	1.57	2 (6%)	48,48,48	1.55	6 (12%)
7	6IB	R	402	-	40,40,40	0.74	0	52,52,52	1.55	12 (23%)

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
6	CLR	R	401	-	-	9/10/68/68	0/4/4/4
7	6IB	R	402	-	-	15/26/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	401	CLR	C20-C17	7.43	1.67	1.54
6	R	401	CLR	C13-C17	2.25	1.59	1.55

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	401	CLR	C22-C20-C17	5.60	121.86	110.28
7	R	402	6IB	O2-C23-C16	3.51	120.86	115.97
6	R	401	CLR	C13-C17-C20	3.48	124.93	119.49
7	R	402	6IB	O2-C23-C29	-3.30	118.72	124.37
6	R	401	CLR	C17-C13-C14	-3.28	96.18	100.07
6	R	401	CLR	C16-C17-C20	2.77	116.44	112.15
7	R	402	6IB	C9-C16-C19	2.76	124.48	120.23
6	R	401	CLR	C4-C5-C6	-2.67	116.76	120.61
7	R	402	6IB	C35-O2-C23	-2.65	113.53	117.53
7	R	402	6IB	C10-C17-C20	2.60	124.23	120.23
7	R	402	6IB	C25-C21-C19	2.60	124.80	120.54
7	R	402	6IB	C28-C22-C20	-2.55	114.96	118.54
7	R	402	6IB	C19-C16-C23	-2.41	115.73	118.26
7	R	402	6IB	C17-C20-C22	2.29	125.36	121.76
7	R	402	6IB	C16-C19-C21	2.20	125.23	121.76
6	R	401	CLR	C2-C3-C4	-2.20	107.29	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	402	6IB	C26-C22-C20	2.15	124.08	120.54
7	R	402	6IB	C27-C21-C19	-2.06	115.66	118.54

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	401	CLR	C13-C17-C20-C22
6	R	401	CLR	C16-C17-C20-C21
6	R	401	CLR	C16-C17-C20-C22
7	R	402	6IB	C15-C18-N4-C34
7	R	402	6IB	C21-C25-C31-N5
7	R	402	6IB	C29-C23-O2-C35
6	R	401	CLR	C17-C20-C22-C23
6	R	401	CLR	C22-C23-C24-C25
7	R	402	6IB	C16-C23-O2-C35
6	R	401	CLR	C13-C17-C20-C21
6	R	401	CLR	C21-C20-C22-C23
7	R	402	6IB	C20-C22-C26-C32
7	R	402	6IB	C28-C22-C26-C32
6	R	401	CLR	C23-C24-C25-C26
7	R	402	6IB	C27-C21-C25-C31
6	R	401	CLR	C23-C24-C25-C27
7	R	402	6IB	C8-C10-C17-C24
7	R	402	6IB	C7-C12-O1-C33
7	R	402	6IB	C19-C21-C25-C31
7	R	402	6IB	C30-C24-O3-C36
7	R	402	6IB	C8-C10-C17-C20
7	R	402	6IB	C17-C24-O3-C36
7	R	402	6IB	C14-C11-C15-C18
7	R	402	6IB	C13-C11-C15-C18

There are no ring outliers.

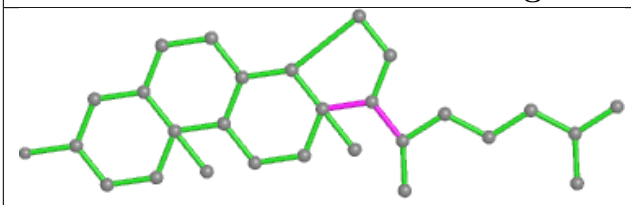
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	401	CLR	1	0
7	R	402	6IB	5	0

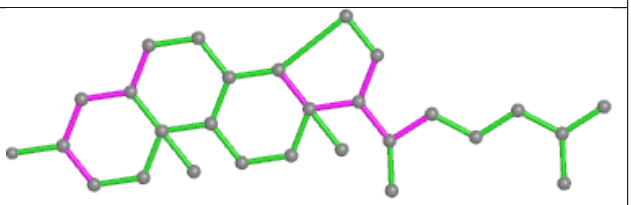
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

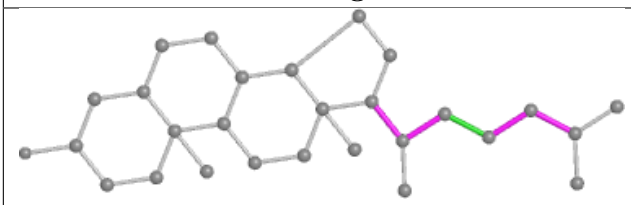
Ligand CLR R 401



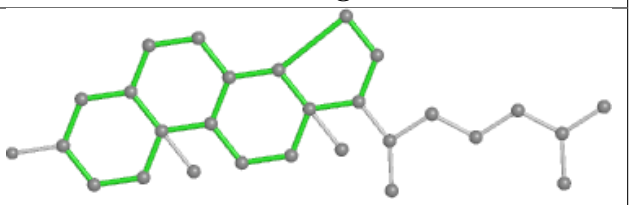
Bond lengths



Bond angles

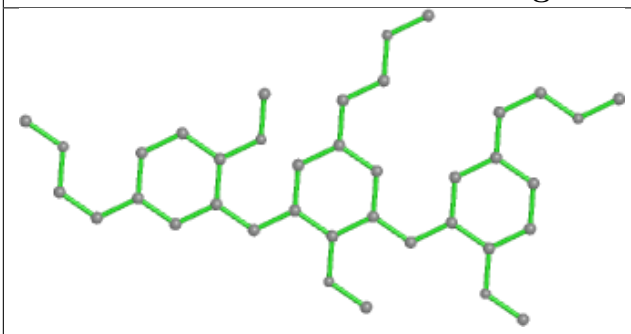


Torsions

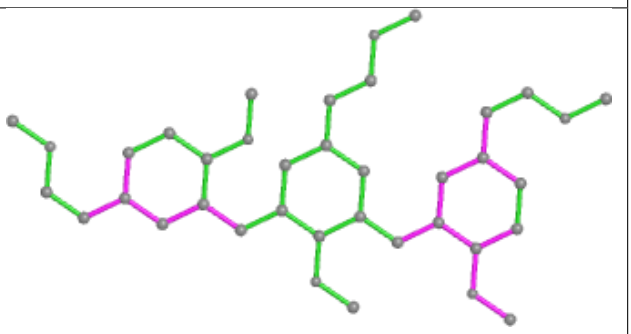


Rings

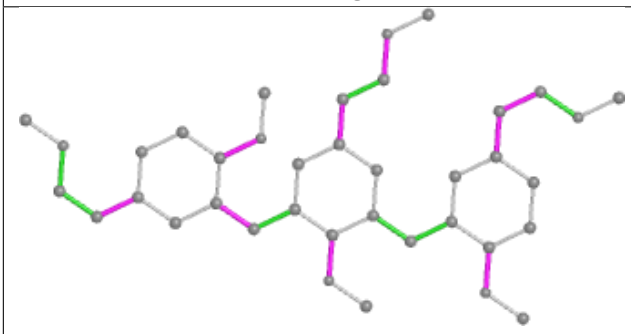
Ligand 6IB R 402



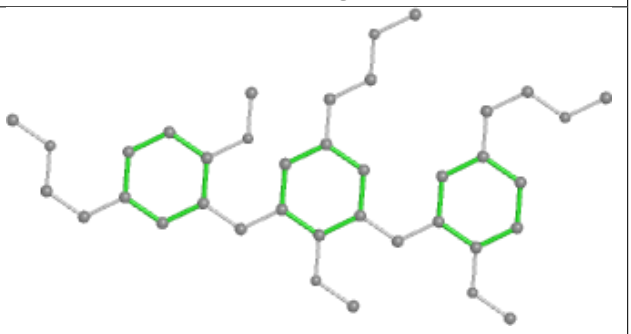
Bond lengths



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.

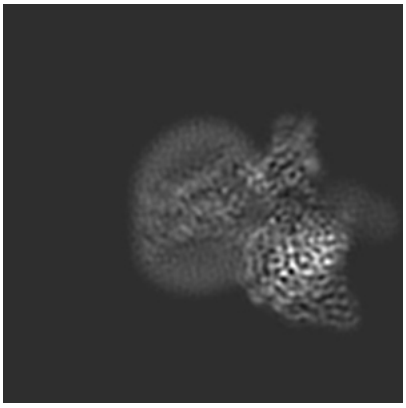
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32138. These allow visual inspection of the internal detail of the map and identification of artifacts.

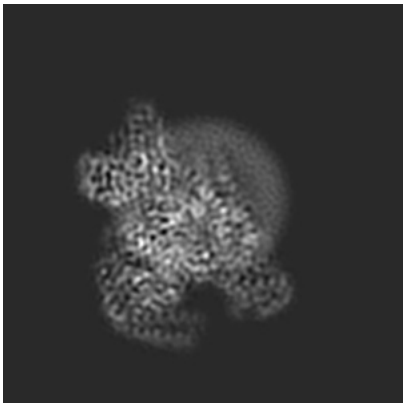
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

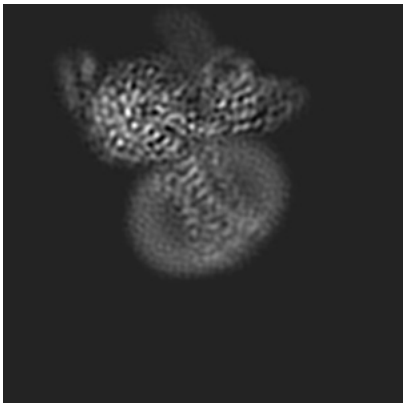
6.1.1 Primary map



X



Y

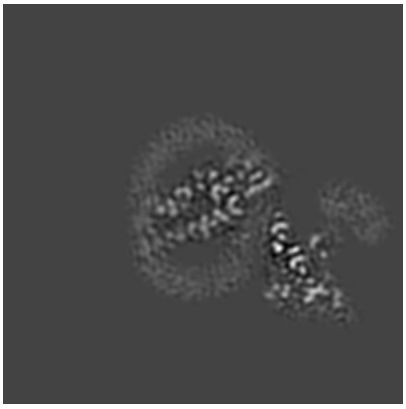


Z

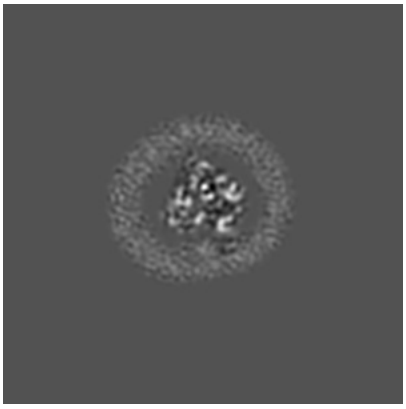
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

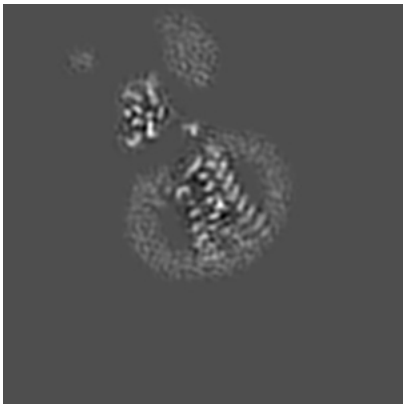
6.2.1 Primary map



X Index: 80



Y Index: 80

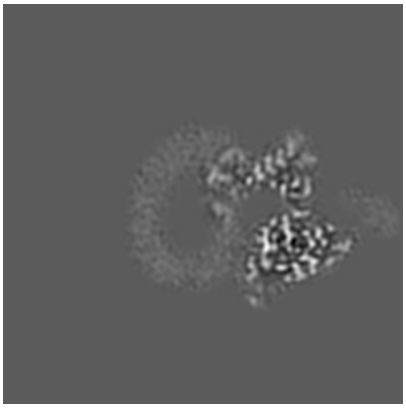


Z Index: 80

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

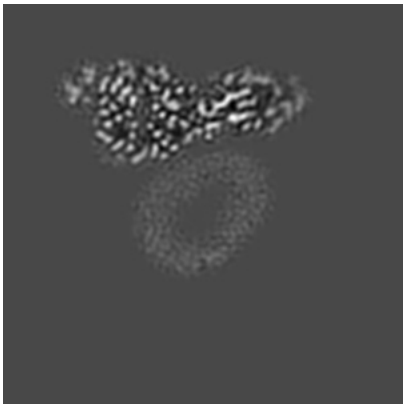
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 65

Y Index: 111

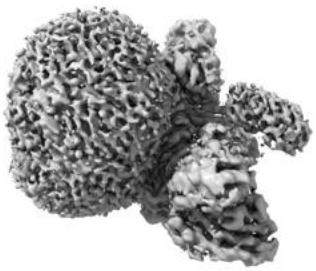


Z Index: 57

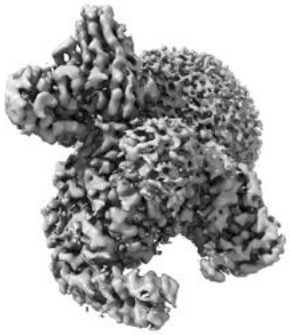
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

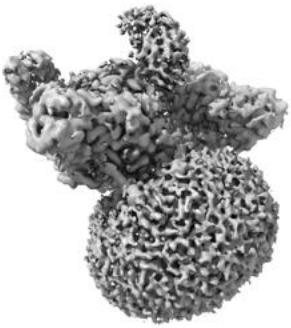
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

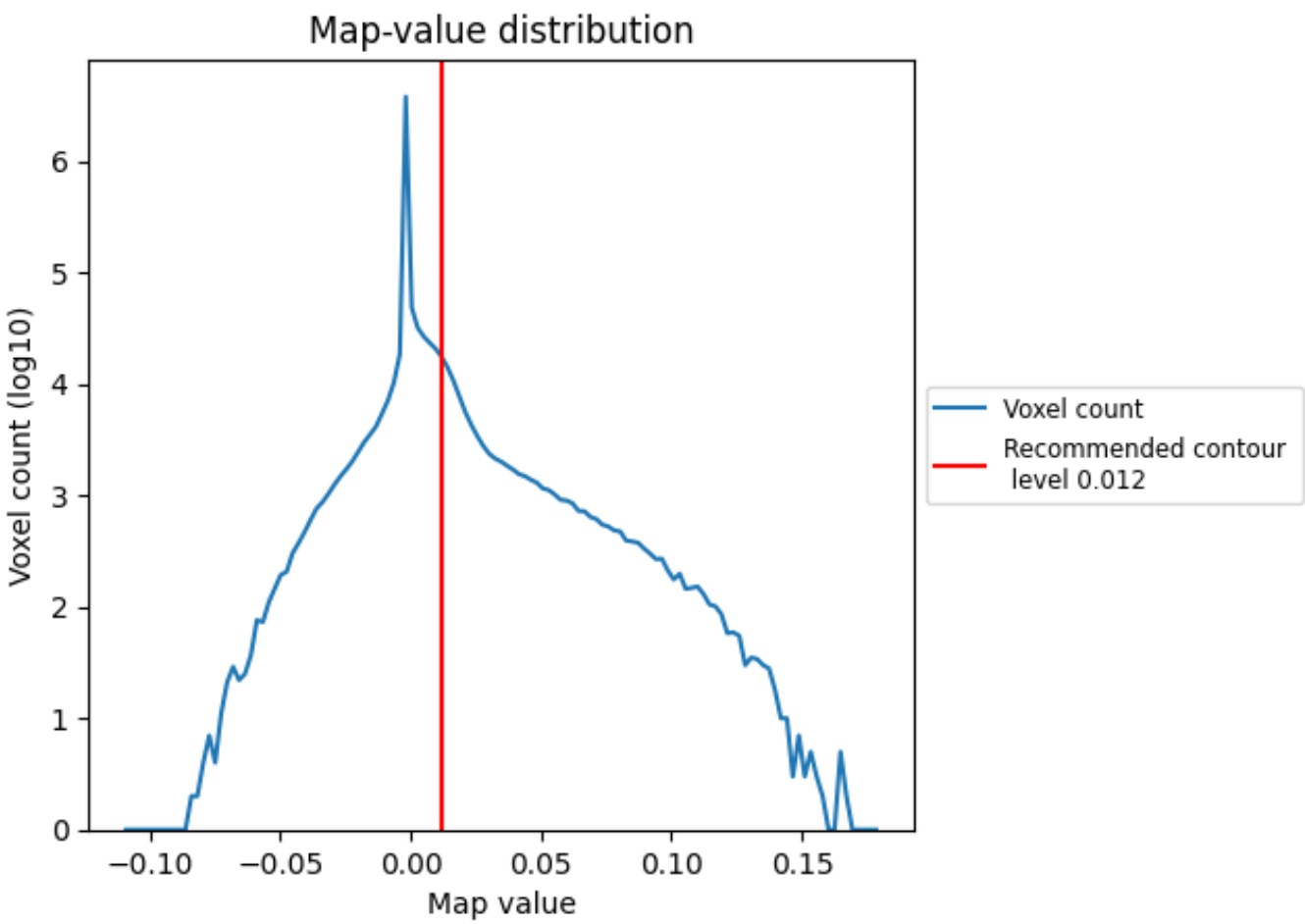
6.5 Mask visualisation (i)

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

7 Map analysis (i)

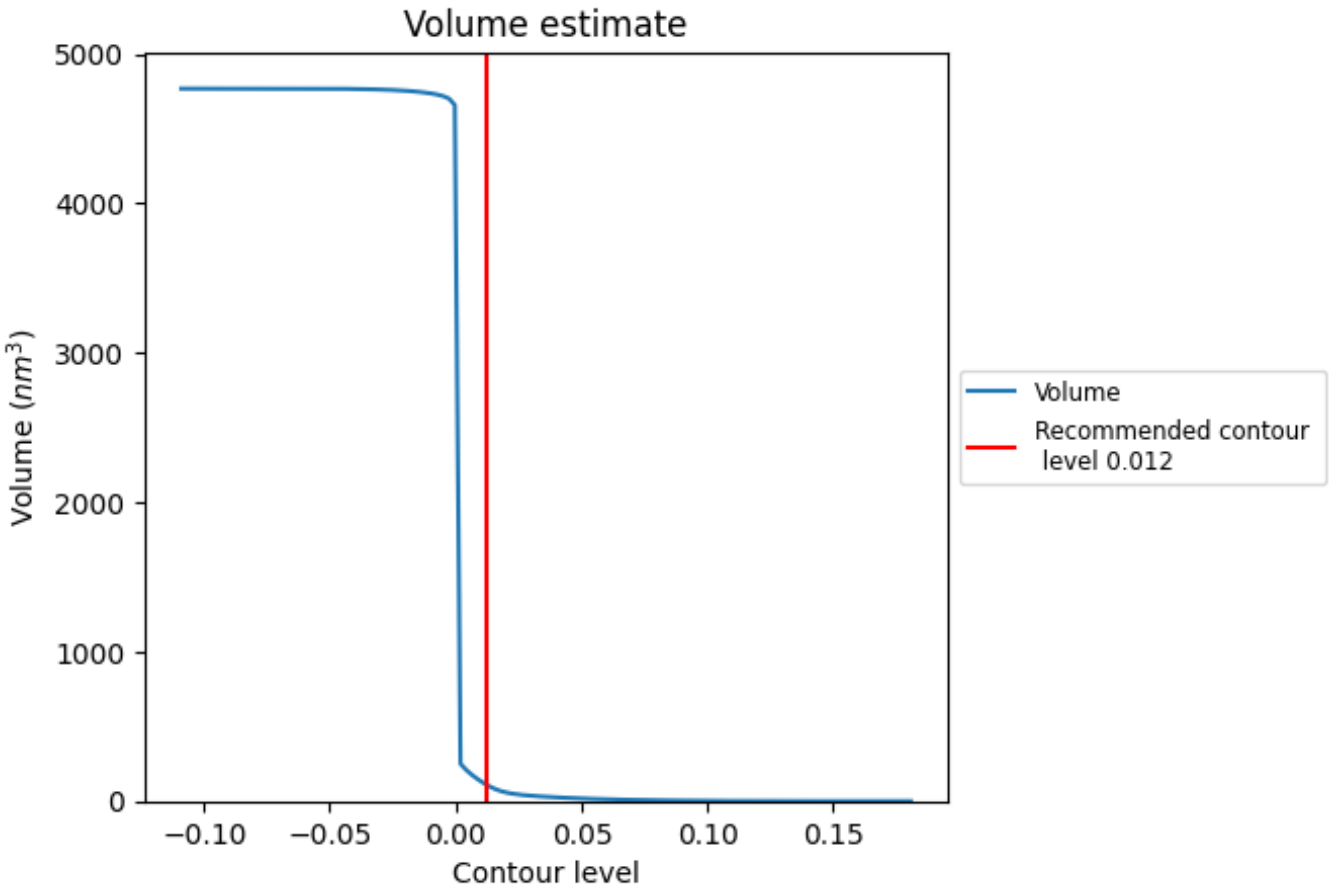
This section contains the results of statistical analysis of the map.

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.

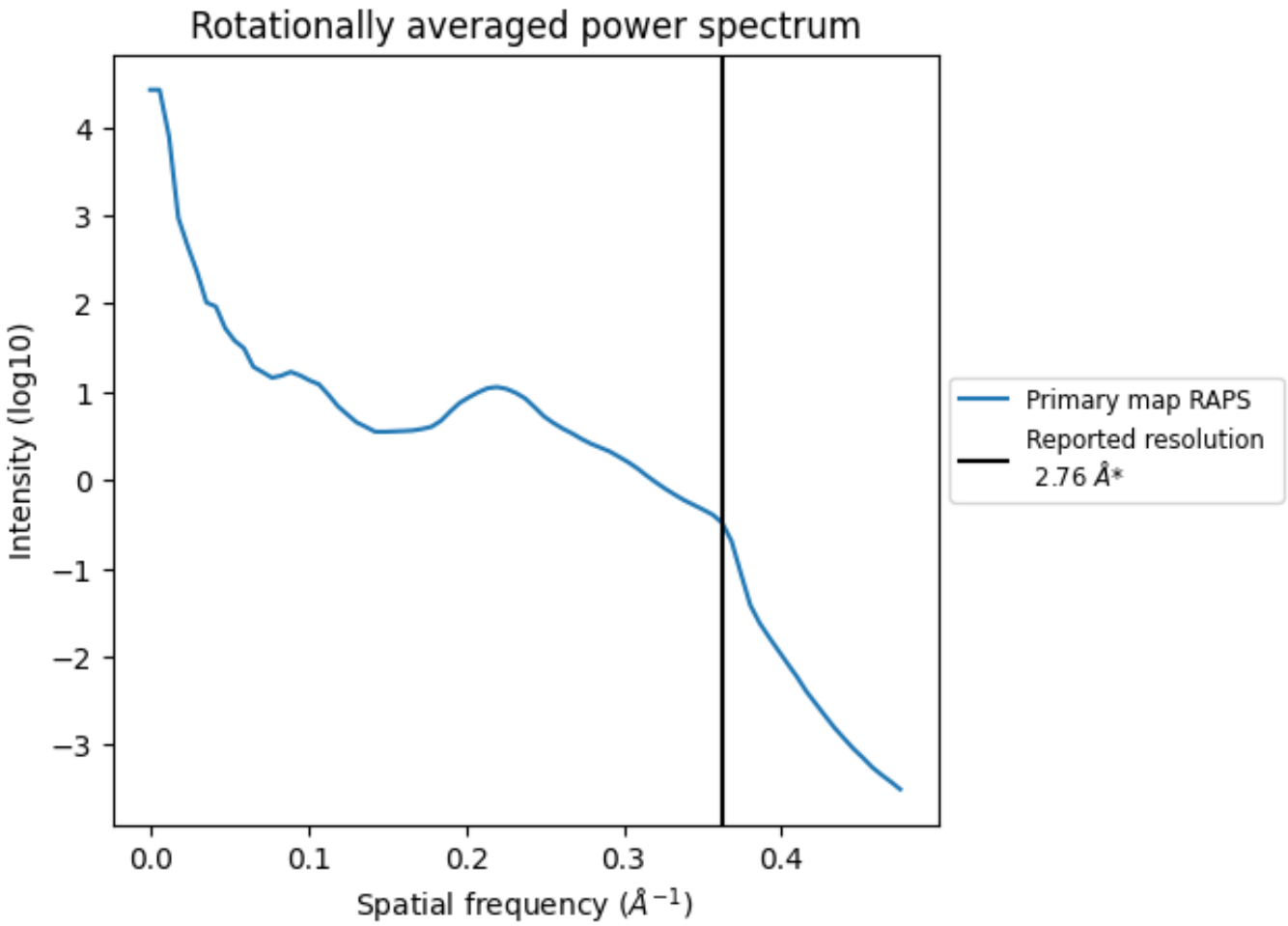
7.2 Volume estimate (i)



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 102 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 0.362 Å^{-1}

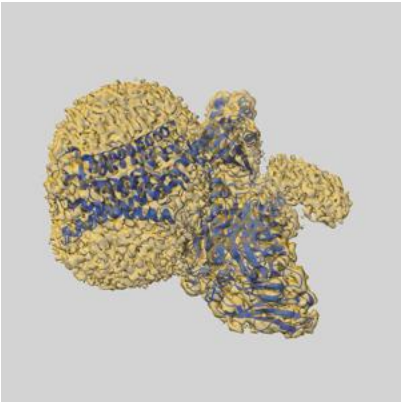
8 Fourier-Shell correlation (i)

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

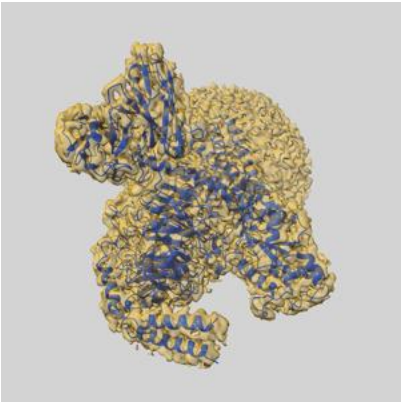
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32138 and PDB model 7VV5. Per-residue inclusion information can be found in section 3 on page 6.

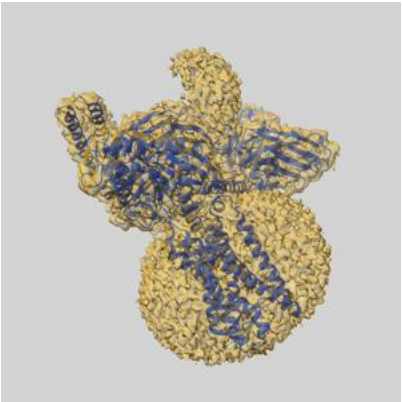
9.1 Map-model overlay (i)



X



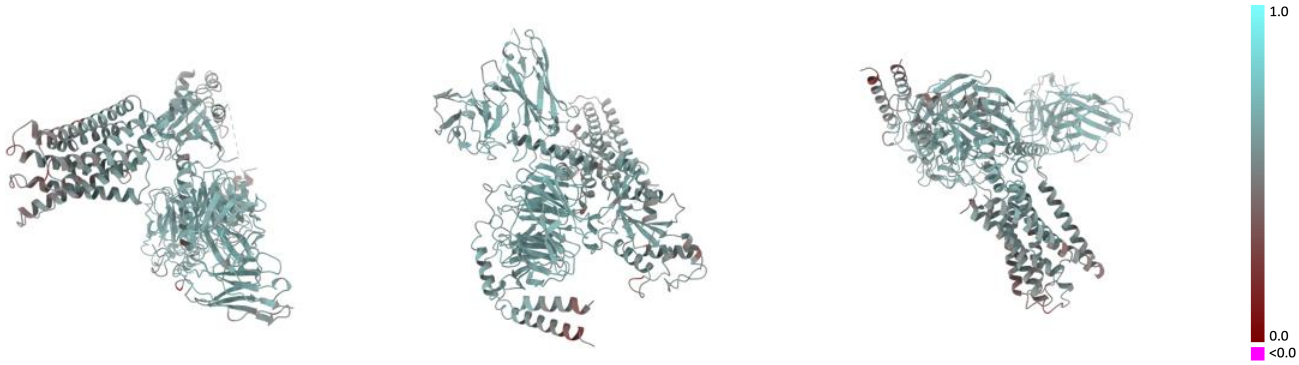
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

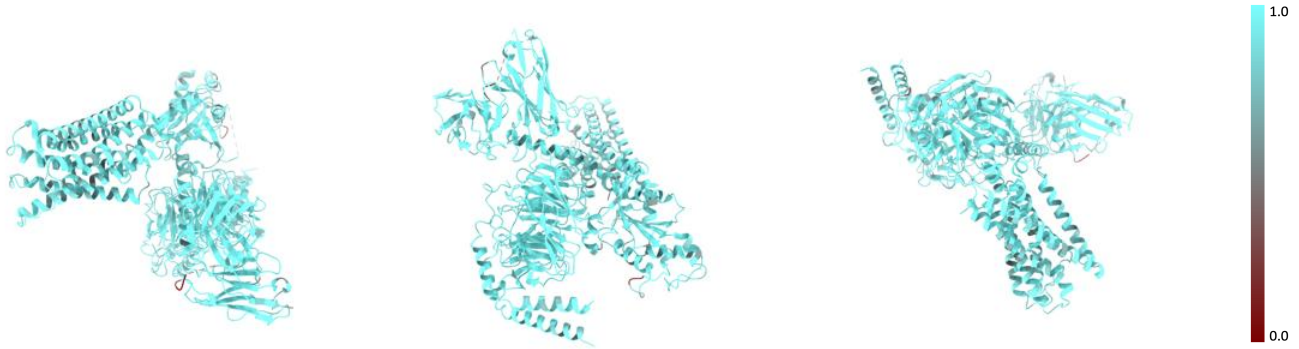
9.2 Q-score mapped to coordinate model (i)



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.

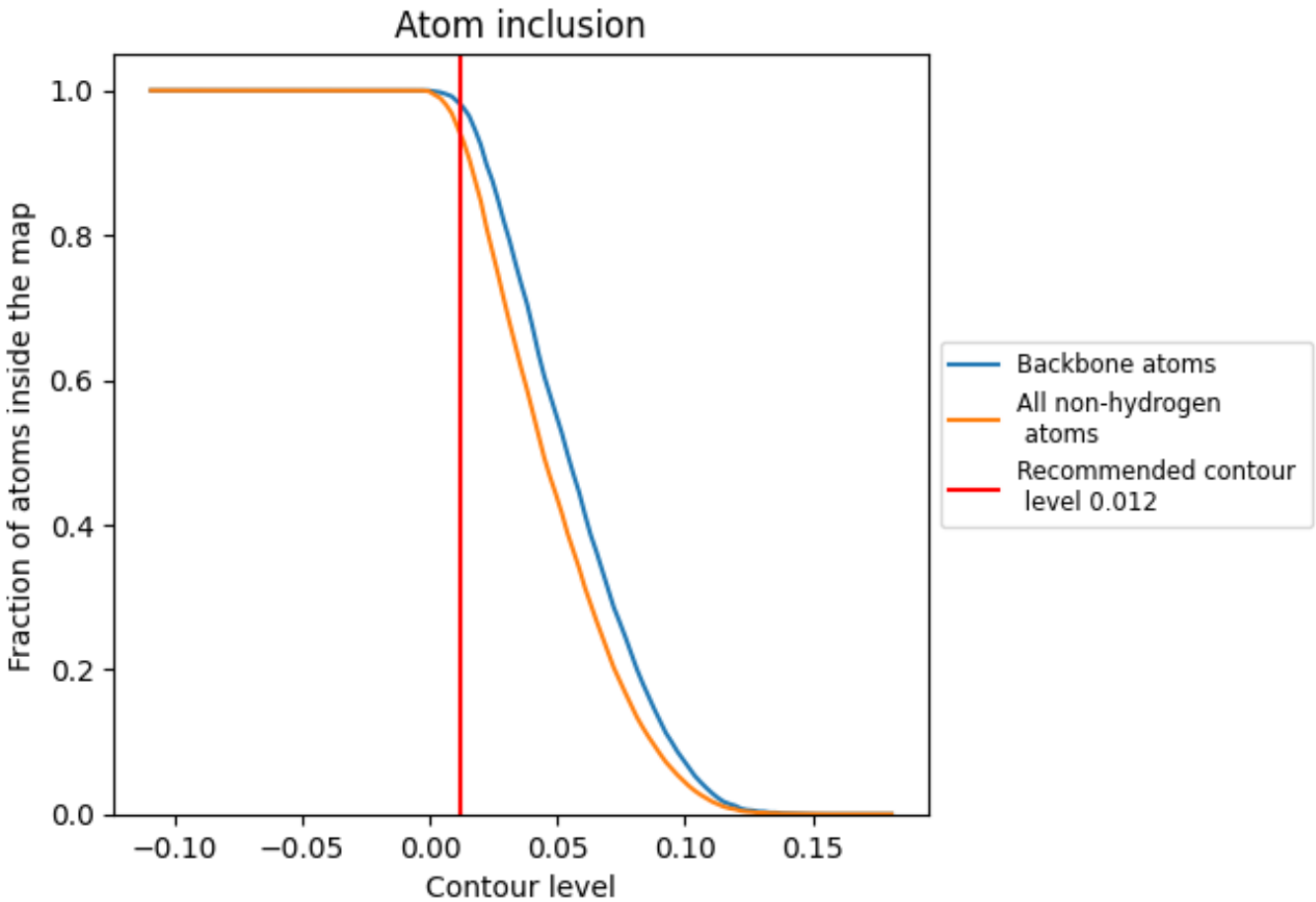
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9403	0.5750
A	0.9122	0.5640
B	0.9720	0.6130
G	0.9357	0.5600
R	0.9122	0.5200
S	0.9588	0.6000