



Full wwPDB EM Validation Report ⓘ

Jun 8, 2026 – 02:35 PM EDT

PDB ID : 9ZZO / pdb_00009zzo
EMDB ID : EMD-75011
Title : MP1104-bound Kappa Opioid Receptor in complex with beta-arrestin1
Authors : Han, J.; Chen, M.; Che, T.
Deposited on : 2026-01-07
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

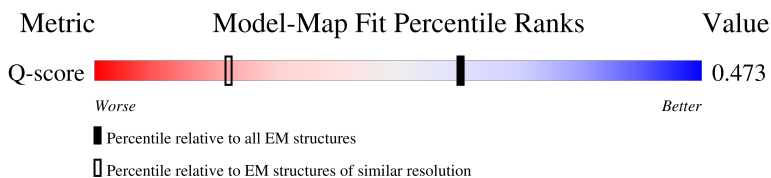
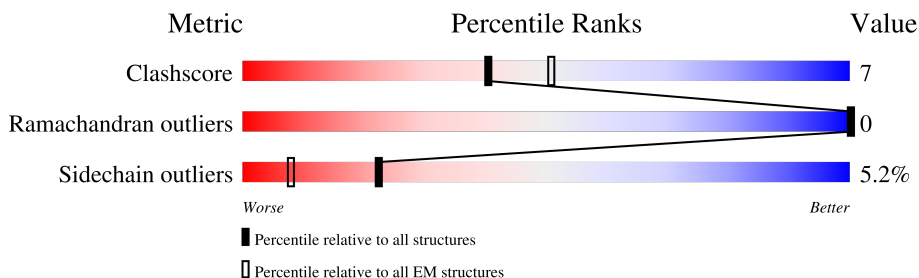
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	124	
2	C	387	
3	A	341	
4	H	241	

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Mol	Chain	Length	Quality of chain
5	L	215	 A horizontal bar chart showing the quality of chain 5. The bar is divided into three segments: a green segment representing 82%, a yellow segment representing 13%, and a small grey segment at the end. The percentages '82%' and '13%' are printed below the green and yellow segments respectively. A small black dot is visible at the end of the grey segment.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8637 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 Nanobody 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	112	Total	C	N	O	S	0	0
			820	516	146	155	3		

- Molecule 2 is a protein called Isoform 1B of Beta-arrestin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	351	Total	C	N	O	S	0	0
			2686	1727	459	498	2		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P49407
C	0	SER	-	expression tag	UNP P49407
C	1	ALA	-	expression tag	UNP P49407
C	59	ALA	CYS	conflict	UNP P49407
C	125	SER	CYS	conflict	UNP P49407
C	140	ILE	CYS	conflict	UNP P49407
C	150	VAL	CYS	conflict	UNP P49407
C	169	GLU	ARG	conflict	UNP P49407
C	242	VAL	CYS	conflict	UNP P49407
C	251	VAL	CYS	conflict	UNP P49407
C	269	SER	CYS	conflict	UNP P49407
C	378	ALA	ILE	conflict	UNP P49407
C	379	ALA	VAL	conflict	UNP P49407
C	380	ALA	PHE	conflict	UNP P49407

- Molecule 3 is a protein called Kappa-type opioid receptor, Vasopressin V2 receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	271	Total	C	N	O	P	S	0	0
			2027	1326	314	366	5	16		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	LEU	ILE	conflict	UNP P41145
A	324	CYS	SER	conflict	UNP P41145
A	393	GLY	-	expression tag	UNP P30518
A	394	GLY	-	expression tag	UNP P30518

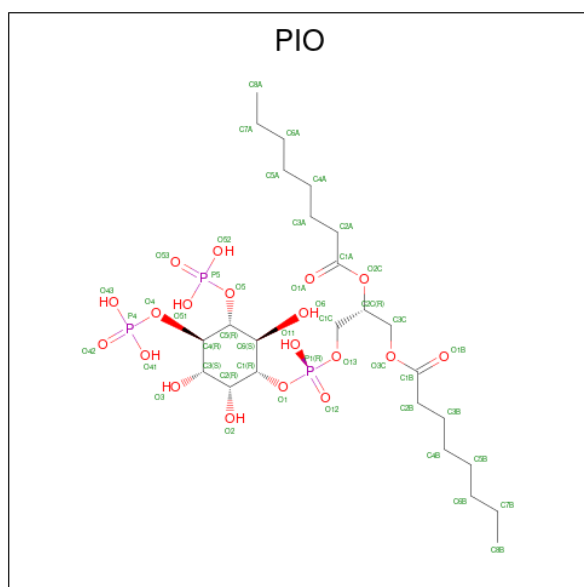
- Molecule 4 is a protein called Fab30 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	207	Total	C	N	O	S	0	0
			1514	970	252	287	5		

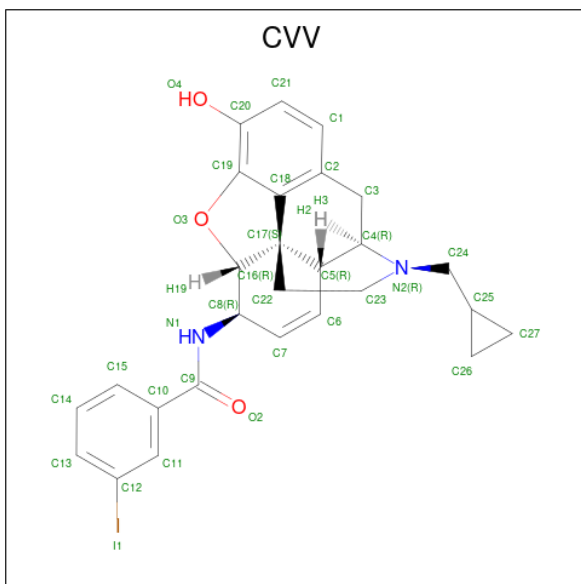
- Molecule 5 is a protein called Fab30 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	206	Total	C	N	O	S	0	0
			1510	950	257	298	5		

- Molecule 6 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃).



- Molecule 7 is N-[(5 α ,6 β)-17-(cyclopropylmethyl)-3-hydroxy-7,8-didehydro-4,5-epoxymorphinan-6-yl]-3-iodobenzamide (CCD ID: CVV) (formula: C₂₇H₂₇IN₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	I	N	O	
7	A	1	33	27	1	2	3	0

3 Residue-property plots


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.

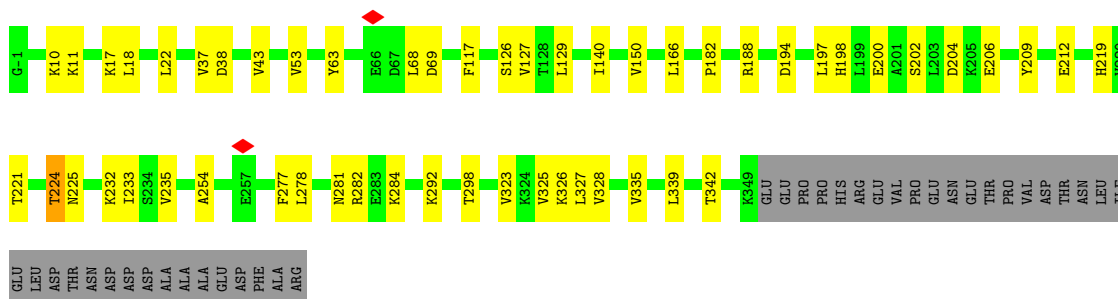
• Molecule 1: Nanobody 32

Chain E: 



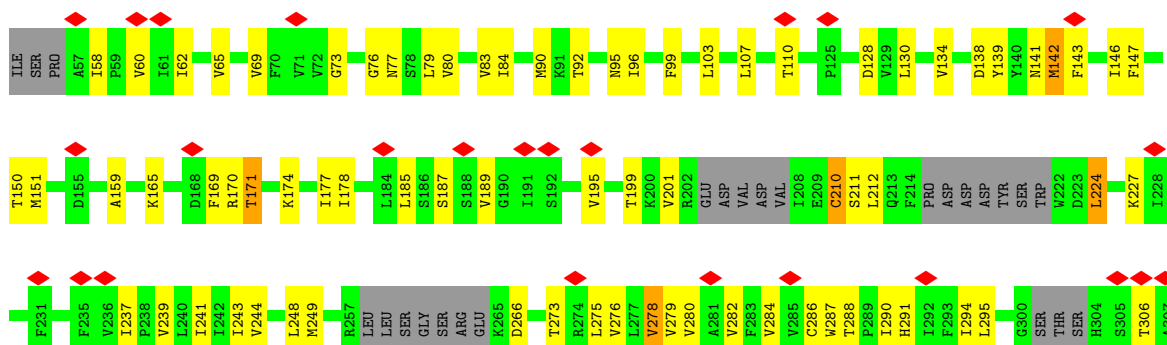
• Molecule 2: Isoform 1B of Beta-arrestin-1

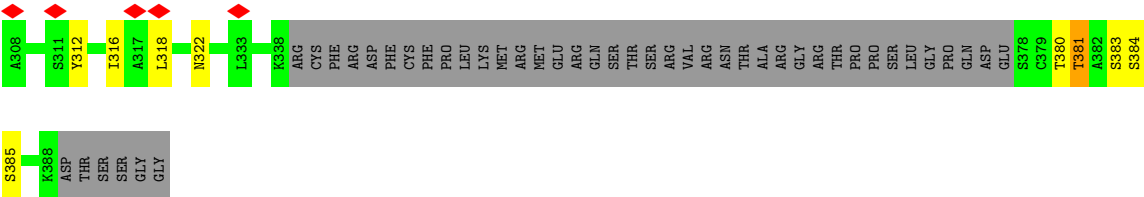
Chain C: 



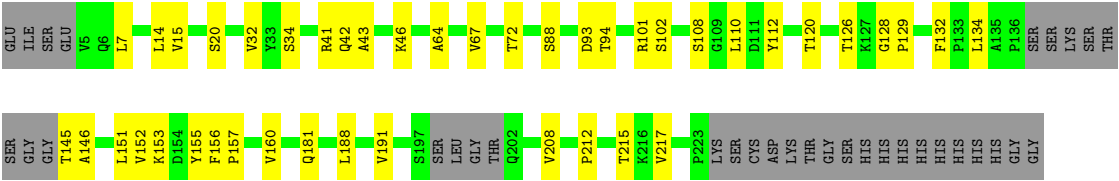
• Molecule 3: Kappa-type opioid receptor, Vasopressin V2 receptor

Chain A: 

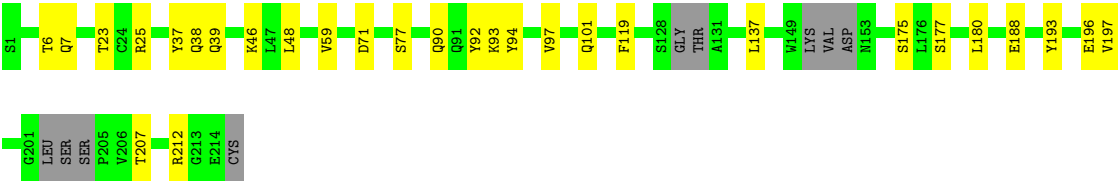
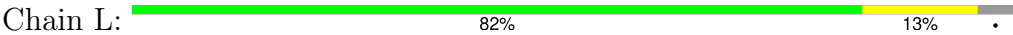




● Molecule 4: Fab30 heavy chain



● Molecule 5: Fab30 light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	163293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	36.342	Depositor
Minimum map value	-16.947	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size (\AA)	278.208, 278.208, 278.208	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.242, 1.242, 1.242	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: TPO, SEP, PIO, CVV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.11	0/836	0.32	0/1140
2	C	0.13	0/2745	0.35	0/3737
3	A	0.24	0/2010	0.62	3/2748 (0.1%)
4	H	0.12	0/1555	0.32	0/2132
5	L	0.13	0/1542	0.34	0/2101
All	All	0.16	0/8688	0.42	3/11858 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	90	MET	CA-CB-CG	5.37	124.83	114.10
3	A	142	MET	CB-CG-SD	5.21	128.32	112.70
3	A	90	MET	CB-CG-SD	5.09	127.96	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	820	0	772	15	0
2	C	2686	0	2692	32	0
3	A	2027	0	1981	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1514	0	1416	20	0
5	L	1510	0	1407	13	0
6	C	47	0	44	0	0
7	A	33	0	0	0	0
All	All	8637	0	8312	118	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 7.

All (118) 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:E:32:VAL:HG12	2:C:17:LYS:HD3	1.66	0.78
3:A:92:THR:H	3:A:95:ASN:HD21	1.34	0.72
1:E:68:THR:HB	1:E:81:GLN:HB3	1.78	0.65
3:A:165:LYS:O	3:A:169:PHE:HB2	1.98	0.64
4:H:43:ALA:HB3	4:H:46:LYS:HB2	1.81	0.63
3:A:282:VAL:O	3:A:286:CYS:HB2	1.98	0.63
2:C:232:LYS:HB3	2:C:326:LYS:HB3	1.81	0.62
2:C:37:VAL:HB	2:C:117:PHE:HB2	1.82	0.61
3:A:174:LYS:HA	3:A:177:ILE:HG12	1.86	0.58
3:A:107:LEU:HB2	3:A:141:ASN:HD22	1.69	0.56
4:H:145:THR:OG1	4:H:146:ALA:N	2.38	0.56
3:A:84:ILE:HG21	3:A:99:PHE:HB2	1.88	0.56
3:A:107:LEU:HA	3:A:110:THR:HG22	1.87	0.56
2:C:235:VAL:HB	2:C:254:ALA:HB3	1.87	0.55
3:A:107:LEU:HB2	3:A:141:ASN:ND2	2.21	0.55
2:C:235:VAL:HG22	2:C:323:VAL:HG22	1.87	0.55
2:C:53:VAL:HG22	2:C:150:VAL:HG22	1.89	0.55
4:H:129:PRO:HB3	4:H:155:TYR:HB3	1.90	0.54
3:A:65:VAL:O	3:A:69:VAL:HG12	2.08	0.54
2:C:38:ASP:N	2:C:38:ASP:OD1	2.38	0.54
2:C:233:ILE:HG13	2:C:325:VAL:HG22	1.89	0.53
2:C:188:ARG:HD3	2:C:335:VAL:HG22	1.91	0.53
1:E:2:VAL:HG11	1:E:102:LEU:HD22	1.91	0.53
1:E:19:ARG:HH11	1:E:79:TYR:HD1	1.57	0.53
4:H:101:ARG:HB3	4:H:112:TYR:HB2	1.90	0.52
5:L:92:TYR:HA	5:L:97:VAL:HG12	1.91	0.52
2:C:182:PRO:HG3	2:C:206:GLU:HG2	1.91	0.51
3:A:266:ASP:N	3:A:266:ASP:OD1	2.42	0.51
2:C:204:ASP:OD1	2:C:204:ASP:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:286:CYS:HB3	3:A:322:ASN:HB2	1.93	0.50
1:E:23:VAL:HG13	1:E:77:THR:HG22	1.92	0.50
4:H:134:LEU:HD11	4:H:151:LEU:HB2	1.92	0.50
2:C:63:TYR:HA	2:C:140:ILE:HG23	1.93	0.50
1:E:19:ARG:NE	1:E:81:GLN:OE1	2.45	0.50
3:A:146:ILE:O	3:A:150:THR:HG23	2.11	0.49
5:L:101:GLN:H	5:L:101:GLN:CD	2.19	0.49
4:H:102:SER:HB3	4:H:110:LEU:HD23	1.93	0.49
3:A:171:THR:HG23	3:A:174:LYS:HG3	1.94	0.49
3:A:103:LEU:O	3:A:107:LEU:HD12	2.13	0.49
4:H:126:THR:HG23	4:H:157:PRO:HG3	1.95	0.49
3:A:224:LEU:HA	3:A:227:LYS:HE2	1.95	0.49
3:A:286:CYS:HA	3:A:318:LEU:HD13	1.95	0.48
4:H:157:PRO:HB2	4:H:212:PRO:HG2	1.95	0.48
4:H:42:GLN:NE2	5:L:39:GLN:OE1	2.47	0.48
2:C:11:LYS:NZ	3:A:381:TPO:O3P	2.46	0.48
4:H:88:SER:O	4:H:88:SER:OG	2.30	0.48
3:A:128:ASP:OD1	3:A:128:ASP:N	2.44	0.47
2:C:323:VAL:HB	2:C:339:LEU:HB2	1.97	0.47
3:A:159:ALA:HB2	3:A:170:ARG:HD3	1.97	0.47
3:A:237:ILE:O	3:A:241:ILE:HG12	2.14	0.47
3:A:278:VAL:O	3:A:282:VAL:HG12	2.15	0.47
1:E:34:MET:HE1	1:E:97:THR:HG22	1.96	0.47
2:C:194:ASP:N	2:C:194:ASP:OD1	2.49	0.46
4:H:64:ALA:HB3	4:H:67:VAL:HG22	1.96	0.46
2:C:18:LEU:HB3	2:C:43:VAL:HG23	1.97	0.46
2:C:68:LEU:HD13	2:C:69:ASP:HB2	1.97	0.46
4:H:14:LEU:HD11	4:H:156:PHE:HE2	1.79	0.46
2:C:224:THR:OG1	2:C:225:ASN:N	2.49	0.46
3:A:290:ILE:O	3:A:294:ILE:HG12	2.15	0.46
2:C:278:LEU:HD23	2:C:282:ARG:HE	1.80	0.46
3:A:76:GLY:O	3:A:80:VAL:HG12	2.15	0.46
1:E:18:LEU:HB2	1:E:85:LEU:HD21	1.98	0.46
3:A:58:ILE:O	3:A:62:ILE:HD12	2.15	0.45
3:A:287:TRP:HE3	3:A:291:HIS:HE1	1.64	0.45
1:E:100:ARG:O	2:C:10:LYS:NZ	2.48	0.45
3:A:130:LEU:O	3:A:134:VAL:HG23	2.16	0.45
3:A:239:VAL:O	3:A:243:ILE:HG12	2.16	0.45
1:E:36:TRP:HD1	1:E:69:ILE:HD12	1.80	0.45
3:A:185:LEU:O	3:A:189:VAL:HG23	2.17	0.45
1:E:32:VAL:O	1:E:71:ARG:NH2	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:14:LEU:HD23	4:H:14:LEU:HA	1.85	0.45
2:C:198:HIS:HB3	2:C:221:THR:HB	1.99	0.45
4:H:134:LEU:HD23	5:L:119:PHE:CG	2.52	0.44
4:H:94:THR:HG23	4:H:120:THR:HA	1.99	0.44
5:L:25:ARG:NE	5:L:71:ASP:OD1	2.51	0.44
4:H:132:PHE:HB2	4:H:151:LEU:HB3	1.98	0.44
5:L:196:GLU:HA	5:L:207:THR:HG22	1.99	0.44
2:C:200:GLU:HG3	2:C:219:HIS:HD2	1.82	0.44
2:C:11:LYS:HD2	2:C:166:LEU:HD13	2.00	0.44
3:A:79:LEU:O	3:A:83:VAL:HG12	2.18	0.44
3:A:312:TYR:O	3:A:316:ILE:HG22	2.17	0.44
2:C:292:LYS:HG2	2:C:298:THR:HB	1.99	0.44
3:A:275:LEU:O	3:A:279:VAL:HG12	2.18	0.43
2:C:129:LEU:N	2:C:140:ILE:O	2.44	0.43
4:H:128:GLY:HA3	4:H:215:THR:HG21	2.00	0.43
3:A:244:VAL:O	3:A:248:LEU:HG	2.18	0.43
5:L:37:TYR:HE1	5:L:90:GLN:HG2	1.84	0.43
2:C:209:TYR:HB2	2:C:212:GLU:HG2	2.01	0.43
4:H:41:ARG:NH2	4:H:93:ASP:OD2	2.52	0.43
5:L:38:GLN:HB2	5:L:48:LEU:HD11	1.99	0.43
3:A:151:MET:HE2	3:A:178:ILE:HG12	2.01	0.43
3:A:73:GLY:O	3:A:77:ASN:ND2	2.52	0.43
4:H:7:LEU:HD11	4:H:101:ARG:HB2	2.01	0.43
5:L:48:LEU:HA	5:L:59:VAL:HG21	2.01	0.42
3:A:143:PHE:O	3:A:147:PHE:HD1	2.02	0.42
2:C:197:LEU:HD22	2:C:335:VAL:HG21	2.01	0.42
3:A:287:TRP:CE3	3:A:291:HIS:HE1	2.36	0.42
1:E:6:GLU:HA	1:E:22:CYS:HA	2.01	0.42
1:E:80:LEU:HD23	1:E:80:LEU:HA	1.94	0.42
2:C:22:LEU:HD23	2:C:22:LEU:HA	1.90	0.42
1:E:29:PHE:HB3	1:E:34:MET:HE3	2.01	0.41
2:C:197:LEU:HD21	2:C:327:LEU:HD23	2.01	0.41
2:C:281:ASN:OD1	2:C:284:LYS:NZ	2.53	0.41
3:A:62:ILE:HD12	3:A:62:ILE:H	1.85	0.41
3:A:142:MET:O	3:A:146:ILE:HG22	2.21	0.41
5:L:6:THR:HA	5:L:101:GLN:HE22	1.86	0.41
1:E:5:GLN:HB2	1:E:23:VAL:HB	2.02	0.41
2:C:198:HIS:NE2	2:C:200:GLU:OE1	2.51	0.41
3:A:241:ILE:HA	3:A:244:VAL:HG22	2.03	0.41
3:A:273:THR:HA	3:A:276:VAL:HG12	2.03	0.41
5:L:93:LYS:HG2	5:L:94:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:199:THR:HG23	3:A:210:CYS:HB3	2.03	0.40
3:A:211:SER:OG	3:A:212:LEU:N	2.54	0.40
4:H:152:VAL:HB	4:H:188:LEU:HD23	2.03	0.40
2:C:277:PHE:O	2:C:281:ASN:ND2	2.53	0.40
5:L:38:GLN:O	5:L:46:LYS:N	2.48	0.40
3:A:280:VAL:O	3:A:284:VAL:HG12	2.21	0.40
5:L:188:GLU:O	5:L:212:ARG:NH2	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	E	110/124 (89%)	105 (96%)	5 (4%)	0	100	100
2	C	349/387 (90%)	338 (97%)	11 (3%)	0	100	100
3	A	254/341 (74%)	245 (96%)	9 (4%)	0	100	100
4	H	201/241 (83%)	194 (96%)	7 (4%)	0	100	100
5	L	198/215 (92%)	188 (95%)	10 (5%)	0	100	100
All	All	1112/1308 (85%)	1070 (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	E	81/103 (79%)	77 (95%)	4 (5%)	22	47
2	C	286/340 (84%)	280 (98%)	6 (2%)	47	73
3	A	207/303 (68%)	192 (93%)	15 (7%)	13	30
4	H	155/200 (78%)	143 (92%)	12 (8%)	12	27
5	L	160/190 (84%)	151 (94%)	9 (6%)	19	40
All	All	889/1136 (78%)	843 (95%)	46 (5%)	22	44

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	90	THR
1	E	100	ARG
1	E	101	SER
1	E	108	THR
2	C	126	SER
2	C	127	VAL
2	C	202	SER
2	C	224	THR
2	C	328	VAL
2	C	342	THR
3	A	60	VAL
3	A	96	ILE
3	A	138	ASP
3	A	139	TYR
3	A	171	THR
3	A	187	SER
3	A	195	VAL
3	A	201	VAL
3	A	210	CYS
3	A	224	LEU
3	A	249	MET
3	A	278	VAL
3	A	288	THR
3	A	295	LEU
3	A	306	THR
4	H	15	VAL
4	H	20	SER
4	H	32	VAL
4	H	34	SER
4	H	72	THR
4	H	108	SER

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Mol	Chain	Res	Type
4	H	153	LYS
4	H	160	VAL
4	H	181	GLN
4	H	191	VAL
4	H	208	VAL
4	H	217	VAL
5	L	7	GLN
5	L	23	THR
5	L	77	SER
5	L	137	LEU
5	L	175	SER
5	L	177	SER
5	L	180	LEU
5	L	193	TYR
5	L	197	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	5	GLN
2	C	111	HIS
2	C	130	GLN
2	C	210	HIS
2	C	245	ASN
2	C	248	GLN
3	A	95	ASN
3	A	162	HIS
4	H	38	HIS
5	L	7	GLN
5	L	101	GLN
5	L	161	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](#)

5 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$
3	SEP	A	383	3	8,9,10	1.61	1 (12%)	7,12,14	1.29	1 (14%)
3	TPO	A	380	3	8,10,11	1.11	0	10,14,16	2.09	1 (10%)
3	SEP	A	384	3	8,9,10	1.60	1 (12%)	7,12,14	1.34	1 (14%)
3	SEP	A	385	3	8,9,10	1.61	1 (12%)	7,12,14	1.26	1 (14%)
3	TPO	A	381	3	8,10,11	1.10	0	10,14,16	2.12	1 (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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	A	383	3	-	0/6/8/10	-
3	TPO	A	380	3	-	2/9/11/13	-
3	SEP	A	384	3	-	1/6/8/10	-
3	SEP	A	385	3	-	0/6/8/10	-
3	TPO	A	381	3	-	0/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	385	SEP	P-O1P	3.53	1.61	1.50
3	A	383	SEP	P-O1P	3.51	1.61	1.50
3	A	384	SEP	P-O1P	3.49	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	381	TPO	P-OG1-CB	-6.12	106.70	123.33
3	A	380	TPO	P-OG1-CB	-5.96	107.14	123.33
3	A	384	SEP	OG-CB-CA	2.92	110.98	108.14
3	A	383	SEP	OG-CB-CA	2.78	110.85	108.14
3	A	385	SEP	OG-CB-CA	2.68	110.75	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	380	TPO	N-CA-CB-OG1
3	A	384	SEP	N-CA-CB-OG
3	A	380	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	381	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	PIO	C	401	-	47,47,47	2.68	9 (19%)	62,65,65	1.56	15 (24%)
7	CVV	A	401	-	38,39,39	2.08	12 (31%)	58,61,61	2.05	19 (32%)

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	PIO	C	401	-	-	24/44/68/68	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CVV	A	401	-	-	7/12/63/63	0/8/7/7

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	PIO	P4-O4	11.77	1.80	1.59
6	C	401	PIO	P5-O5	9.72	1.76	1.59
7	A	401	CVV	C9-N1	4.91	1.45	1.34
7	A	401	CVV	C8-N1	3.84	1.51	1.46
6	C	401	PIO	C6-C5	3.79	1.62	1.52
7	A	401	CVV	C1-C21	3.66	1.44	1.38
6	C	401	PIO	P1-O13	3.62	1.73	1.59
7	A	401	CVV	C10-C9	3.61	1.58	1.50
6	C	401	PIO	O4-C4	-3.61	1.31	1.44
7	A	401	CVV	C17-C5	-3.45	1.49	1.54
6	C	401	PIO	C5-C4	3.11	1.58	1.52
6	C	401	PIO	C2-C1	3.06	1.60	1.52
6	C	401	PIO	O5-C5	-2.97	1.33	1.44
7	A	401	CVV	C3-C4	2.96	1.60	1.54
7	A	401	CVV	C21-C20	2.67	1.44	1.39
6	C	401	PIO	C3-C4	2.58	1.59	1.52
7	A	401	CVV	C24-N2	-2.54	1.42	1.47
7	A	401	CVV	C5-C6	-2.44	1.45	1.50
7	A	401	CVV	C23-N2	2.28	1.51	1.47
7	A	401	CVV	C19-C18	2.25	1.41	1.38
7	A	401	CVV	C11-C10	2.03	1.42	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	401	CVV	C3-C4-N2	-4.63	107.68	115.77
7	A	401	CVV	C10-C9-N1	4.53	125.43	117.04
6	C	401	PIO	O2C-C1A-C2A	4.34	120.88	111.48
7	A	401	CVV	O3-C19-C20	4.31	133.68	126.14
7	A	401	CVV	O3-C16-C17	-4.19	99.06	105.84
7	A	401	CVV	C17-C5-C4	3.47	109.25	106.68
6	C	401	PIO	O2C-C1A-O1A	-3.40	115.76	123.70
6	C	401	PIO	C2-C3-C4	3.35	117.27	109.68
7	A	401	CVV	C22-C17-C16	-3.27	108.80	111.68
6	C	401	PIO	P4-O4-C4	3.17	131.91	123.43
7	A	401	CVV	C20-C19-C18	-3.14	117.15	120.97
7	A	401	CVV	O3-C19-C18	-3.13	109.18	112.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	401	CVV	C17-C5-C6	3.07	114.07	109.96
7	A	401	CVV	O2-C9-N1	-3.01	116.75	122.47
6	C	401	PIO	O1-C1-C2	2.89	114.85	108.73
6	C	401	PIO	O52-P5-O51	2.87	118.57	107.80
6	C	401	PIO	O5-C5-C6	-2.83	102.74	108.73
7	A	401	CVV	C22-C17-C18	2.83	116.23	111.90
7	A	401	CVV	C4-C5-C6	-2.80	110.38	114.13
7	A	401	CVV	C17-C16-C8	2.76	116.25	112.65
7	A	401	CVV	C24-N2-C4	-2.75	108.43	113.44
6	C	401	PIO	O13-P1-O12	-2.64	98.47	108.94
6	C	401	PIO	O11-P1-O12	2.60	124.52	112.44
7	A	401	CVV	C19-C18-C2	2.57	126.36	123.04
7	A	401	CVV	C8-N1-C9	2.39	126.69	121.97
7	A	401	CVV	C25-C24-N2	-2.34	109.31	113.42
6	C	401	PIO	P5-O5-C5	2.24	129.42	123.43
6	C	401	PIO	O5-P5-O53	-2.22	101.41	109.33
7	A	401	CVV	O4-C20-C19	2.22	125.01	119.58
7	A	401	CVV	C23-N2-C24	-2.18	107.78	111.82
6	C	401	PIO	O3-C3-C2	-2.12	105.38	110.38
6	C	401	PIO	O11-P1-O13	-2.08	98.13	107.57
6	C	401	PIO	C6-C1-C2	2.01	113.65	110.86
6	C	401	PIO	O41-P4-O42	2.01	118.66	110.83

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	401	PIO	C1-O1-P1-O13
6	C	401	PIO	C1C-O13-P1-O1
6	C	401	PIO	C1C-O13-P1-O11
6	C	401	PIO	C2A-C1A-O2C-C2C
6	C	401	PIO	O1A-C1A-O2C-C2C
6	C	401	PIO	C2B-C1B-O3C-C3C
6	C	401	PIO	O1B-C1B-O3C-C3C
7	A	401	CVV	C15-C10-C9-O2
7	A	401	CVV	C15-C10-C9-N1
7	A	401	CVV	C11-C10-C9-O2
7	A	401	CVV	C11-C10-C9-N1
6	C	401	PIO	C1A-C2A-C3A-C4A
6	C	401	PIO	C2B-C3B-C4B-C5B
6	C	401	PIO	C4A-C5A-C6A-C7A
6	C	401	PIO	C1C-C2C-C3C-O3C

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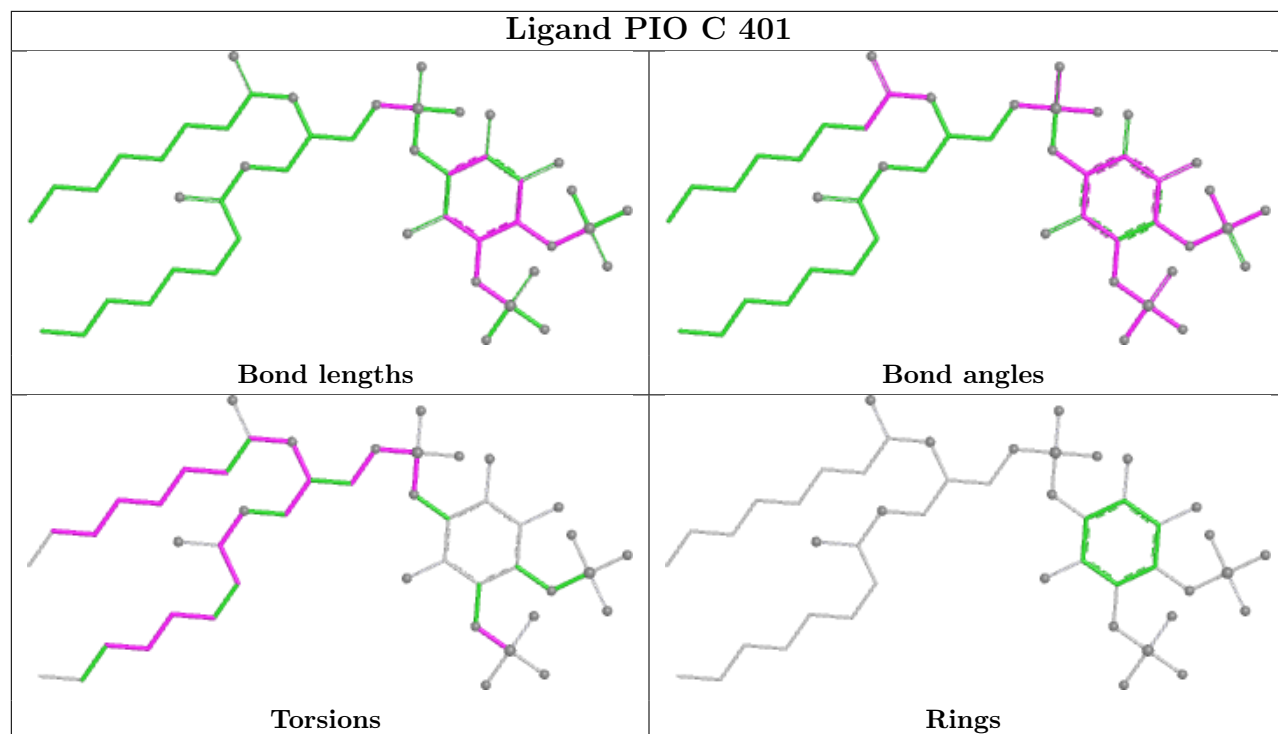
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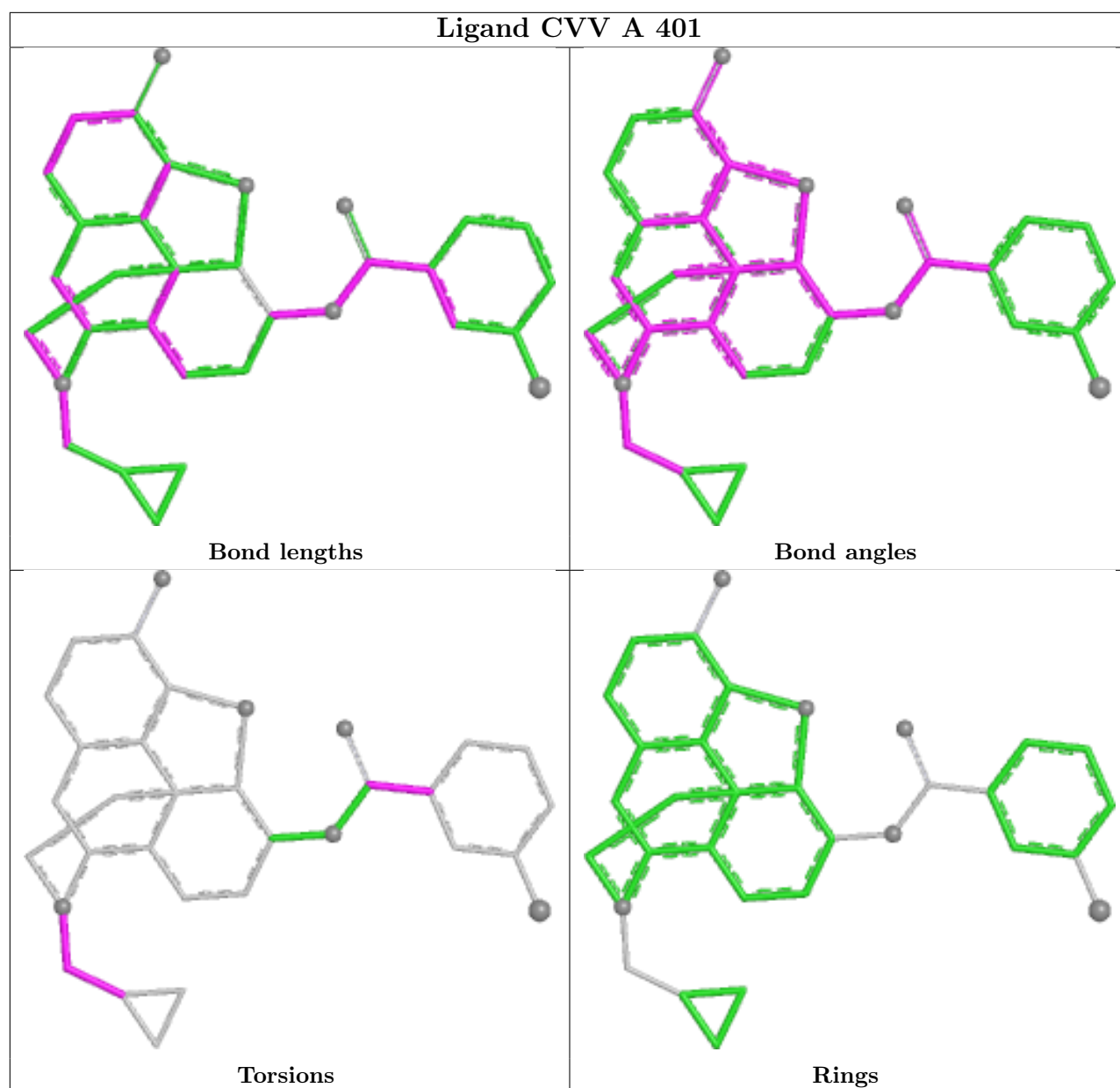
Mol	Chain	Res	Type	Atoms
6	C	401	PIO	C3B-C4B-C5B-C6B
6	C	401	PIO	C3C-C2C-O2C-C1A
6	C	401	PIO	C3A-C4A-C5A-C6A
6	C	401	PIO	C2C-C1C-O13-P1
6	C	401	PIO	C5A-C6A-C7A-C8A
6	C	401	PIO	C4B-C5B-C6B-C7B
6	C	401	PIO	C2A-C3A-C4A-C5A
7	A	401	CVV	C25-C24-N2-C23
6	C	401	PIO	C1C-O13-P1-O12
6	C	401	PIO	O2C-C2C-C3C-O3C
7	A	401	CVV	N2-C24-C25-C26
6	C	401	PIO	C1-O1-P1-O12
6	C	401	PIO	O3C-C1B-C2B-C3B
7	A	401	CVV	C25-C24-N2-C4
6	C	401	PIO	C5-O5-P5-O53
6	C	401	PIO	O1B-C1B-C2B-C3B

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 than 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.





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.

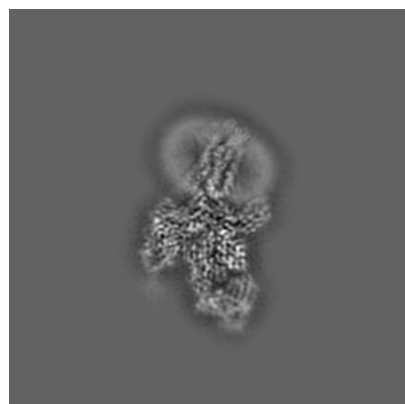
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75011. These allow visual inspection of the internal detail of the map and identification of artifacts.

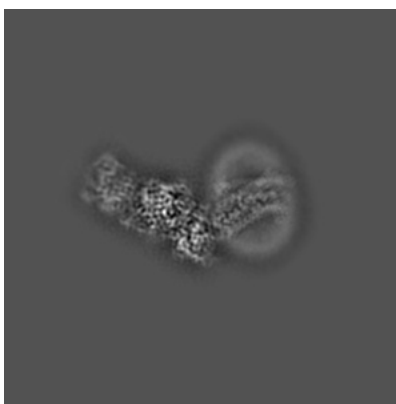
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

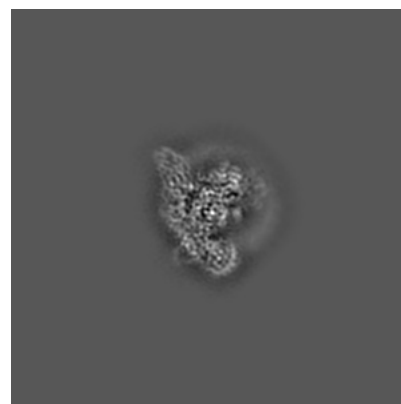
6.1.1 Primary map



X

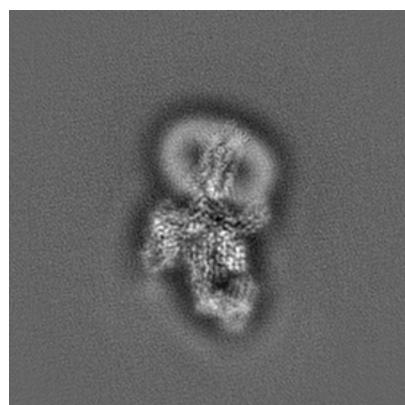


Y

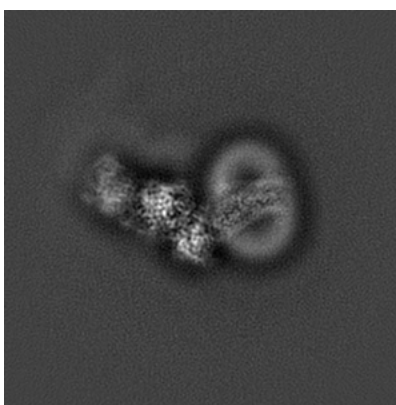


Z

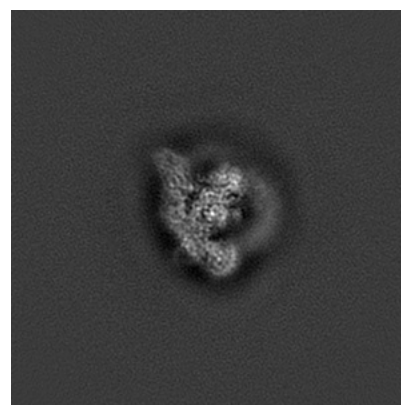
6.1.2 Raw map



X



Y

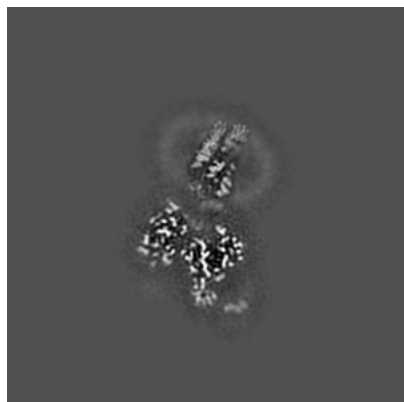


Z

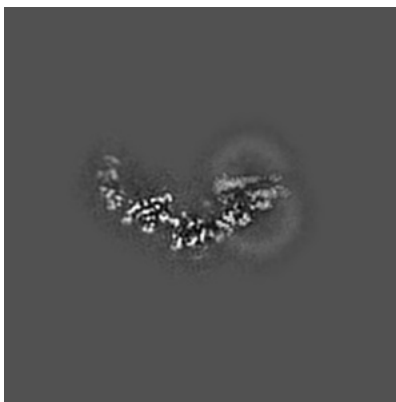
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

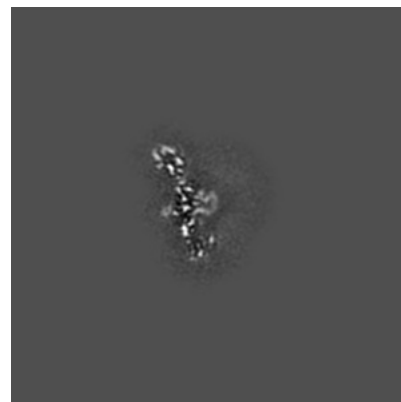
6.2.1 Primary map



X Index: 112

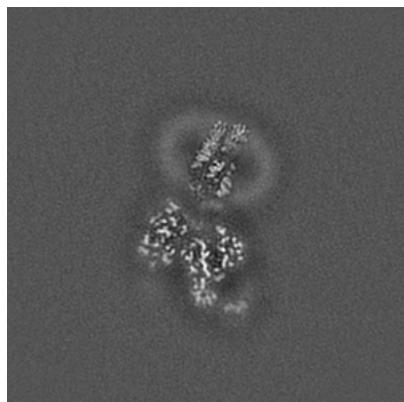


Y Index: 112

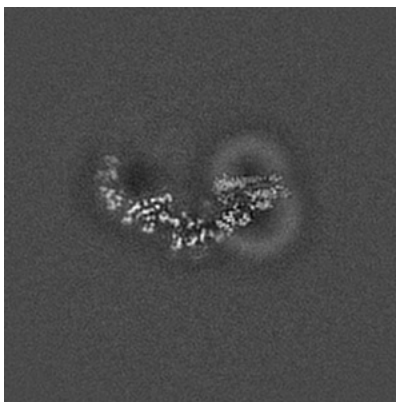


Z Index: 112

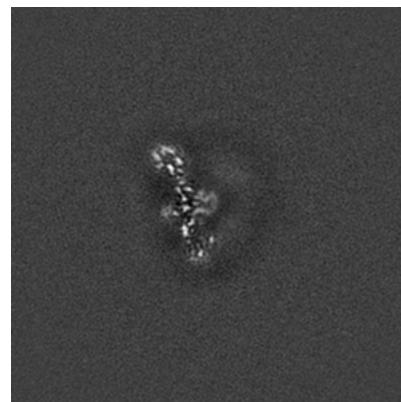
6.2.2 Raw map



X Index: 112



Y Index: 112

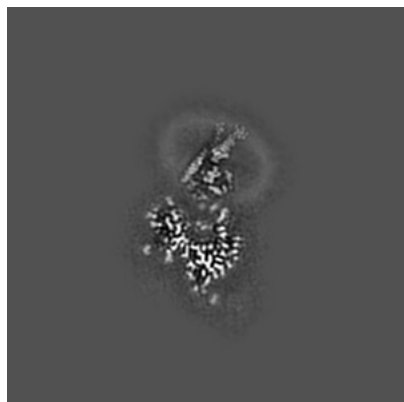


Z Index: 112

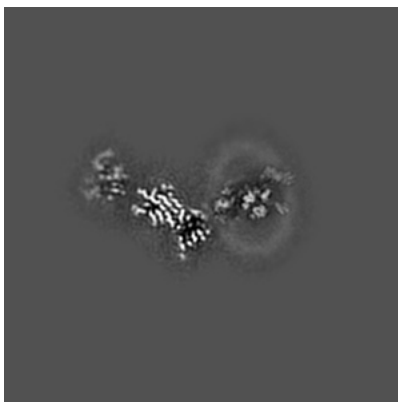
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

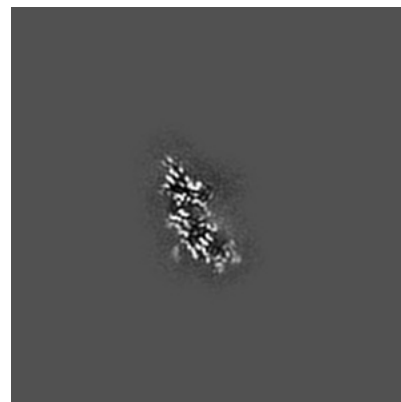
6.3.1 Primary map



X Index: 109

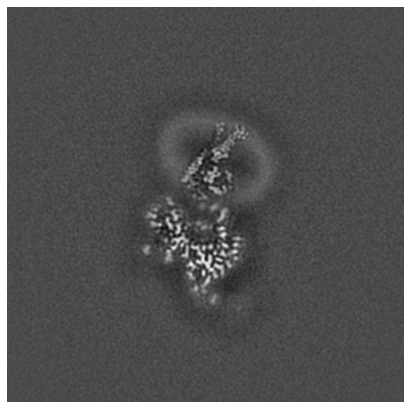


Y Index: 120

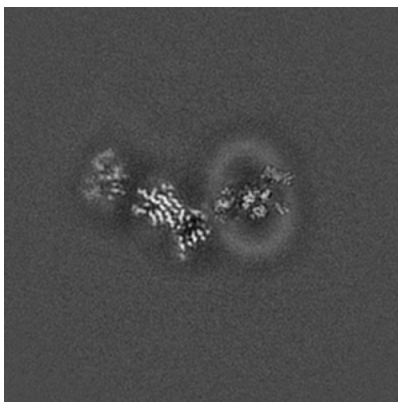


Z Index: 101

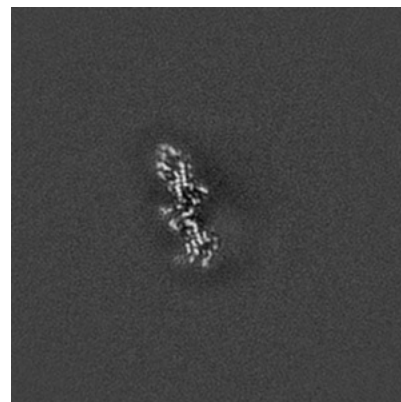
6.3.2 Raw map



X Index: 109



Y Index: 120

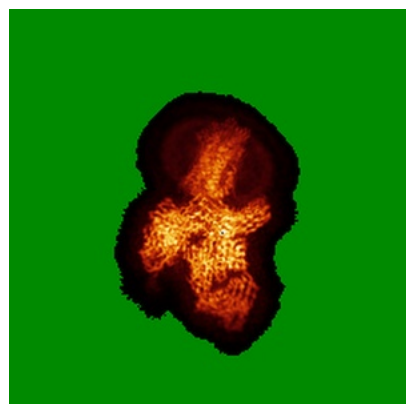


Z Index: 107

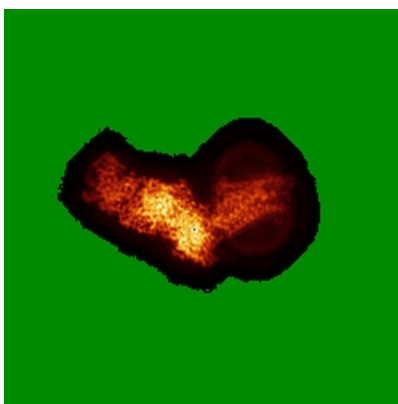
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

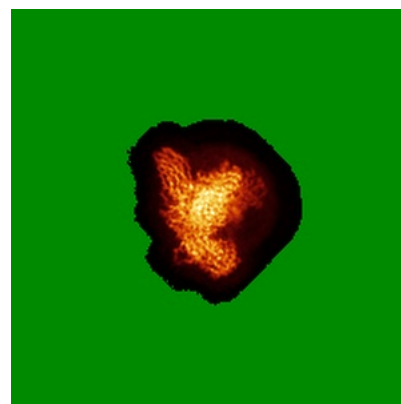
6.4.1 Primary map



X

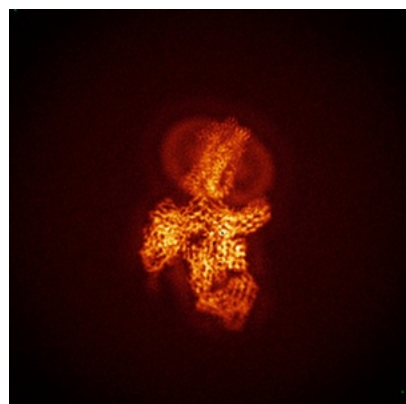


Y

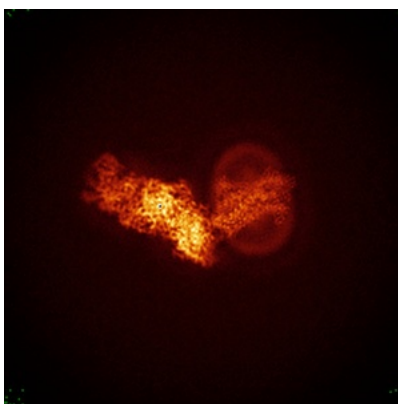


Z

6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

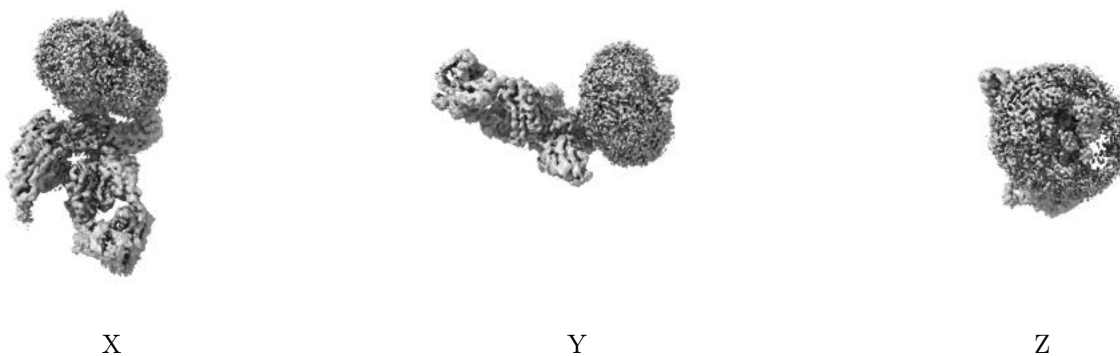
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

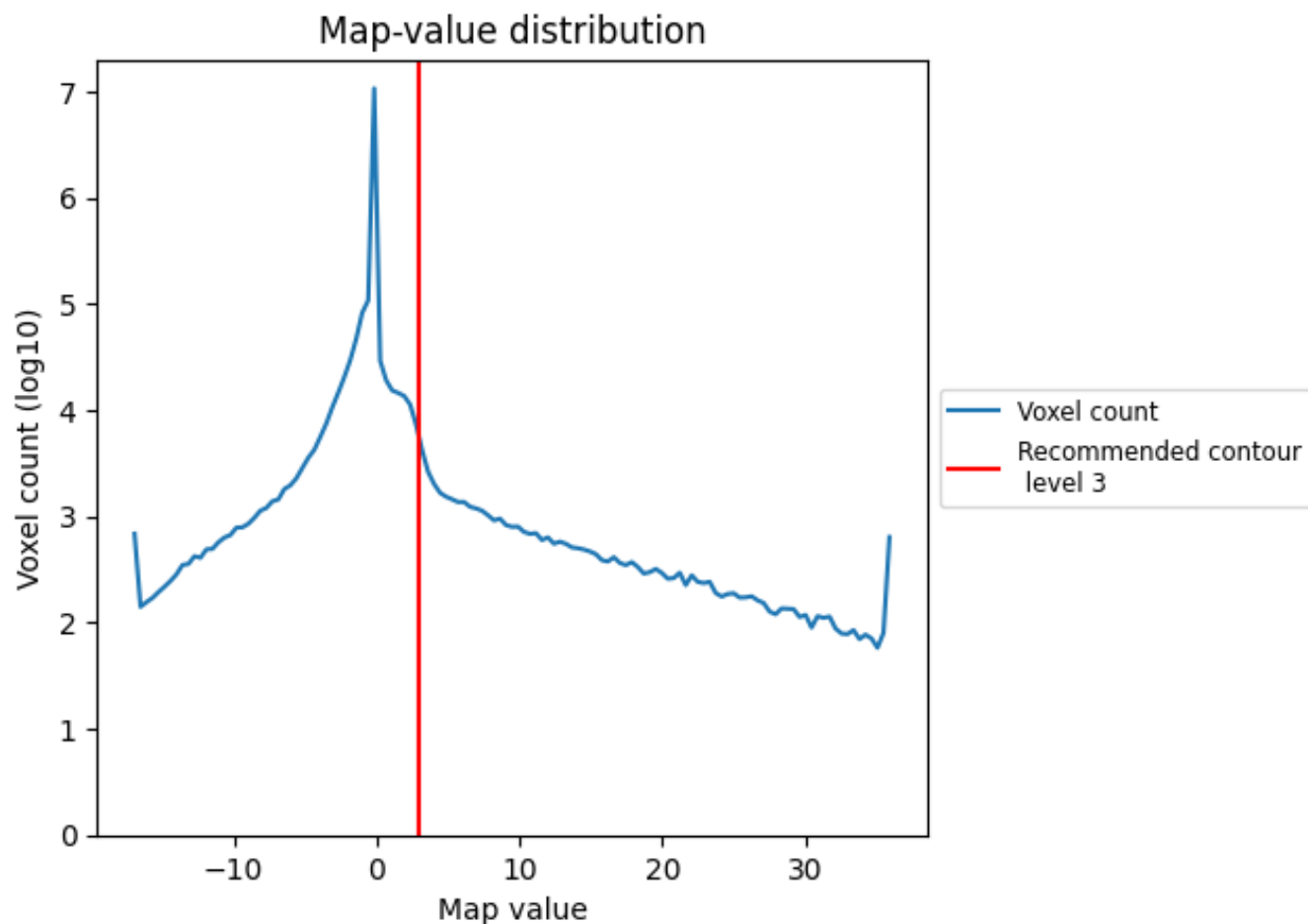
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

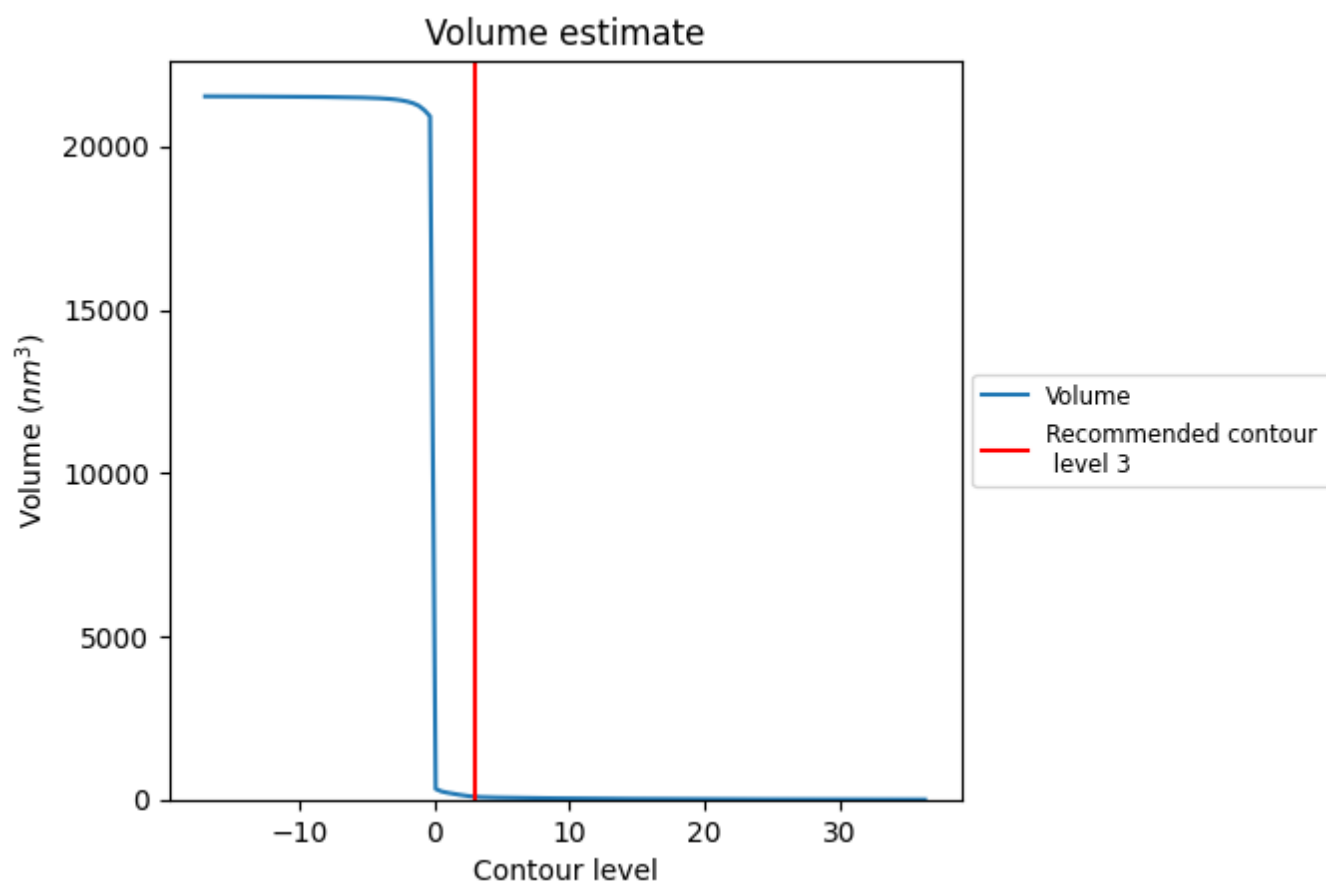
This section contains the results of statistical analysis of the map.

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.

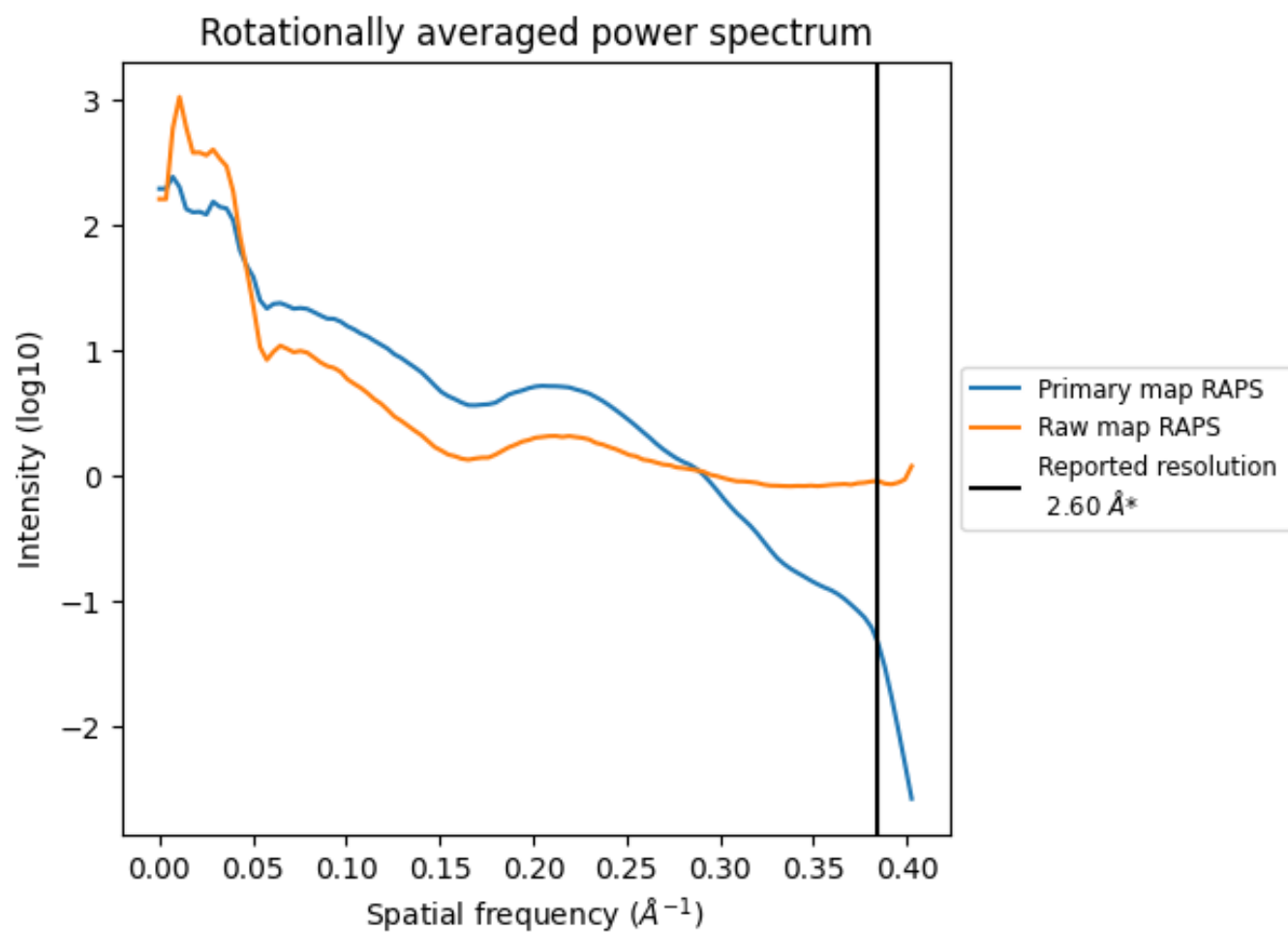
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm^3 ; this corresponds to an approximate mass of 79 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 ⓘ

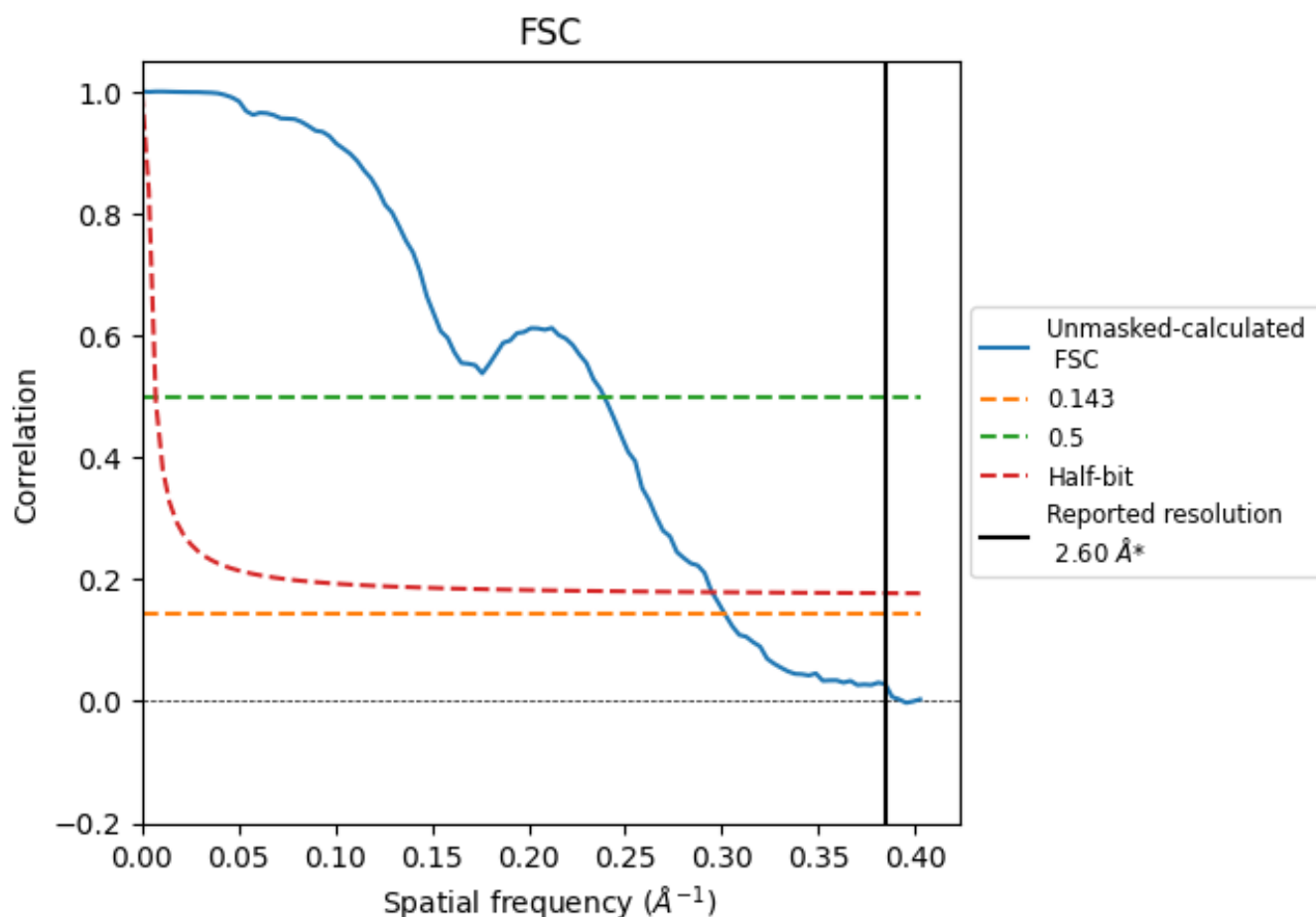


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

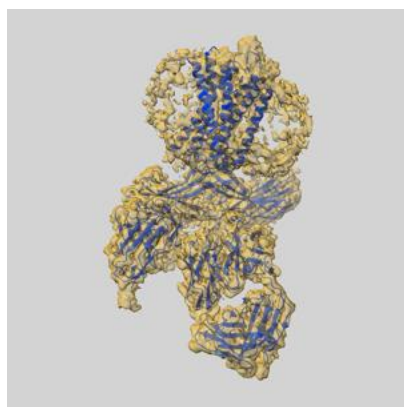
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.32	4.18	3.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.32 differs from the reported value 2.6 by more than 10 %

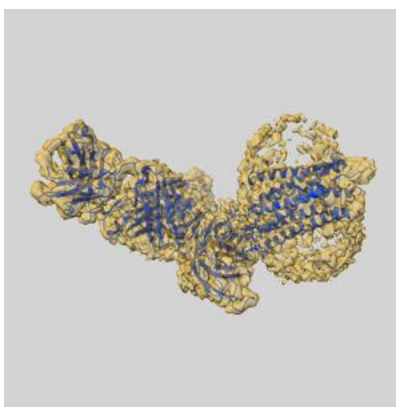
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75011 and PDB model 9ZZO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

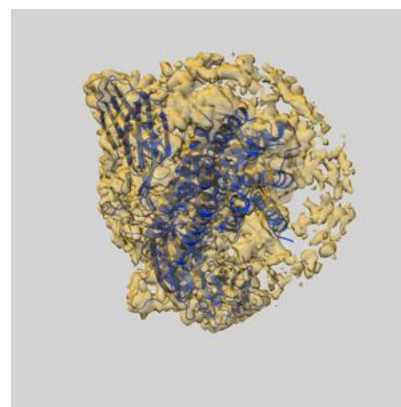
9.1 Map-model overlay [i](#)



X



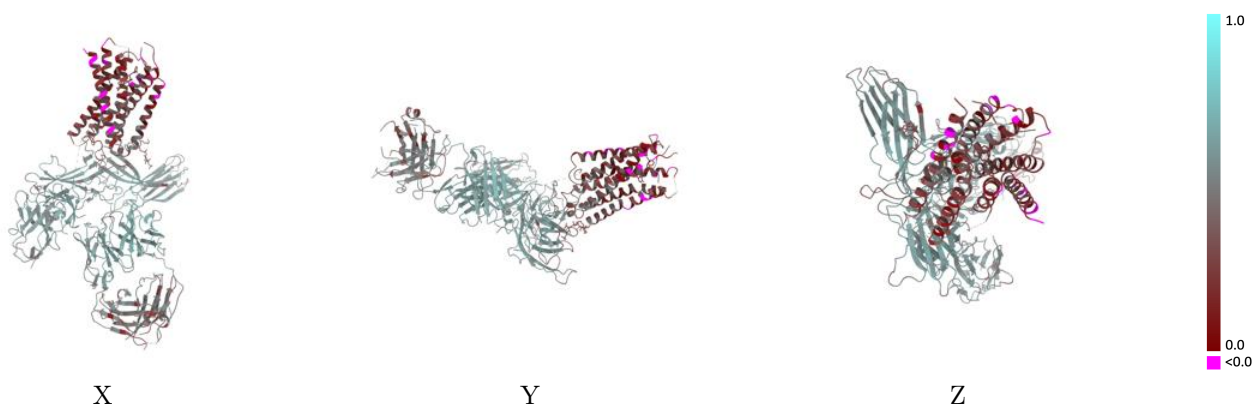
Y



Z

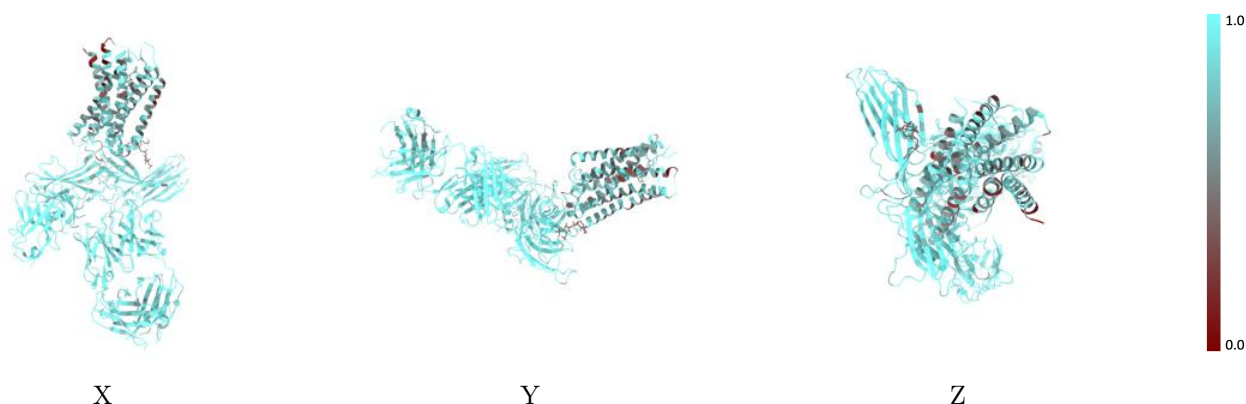
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



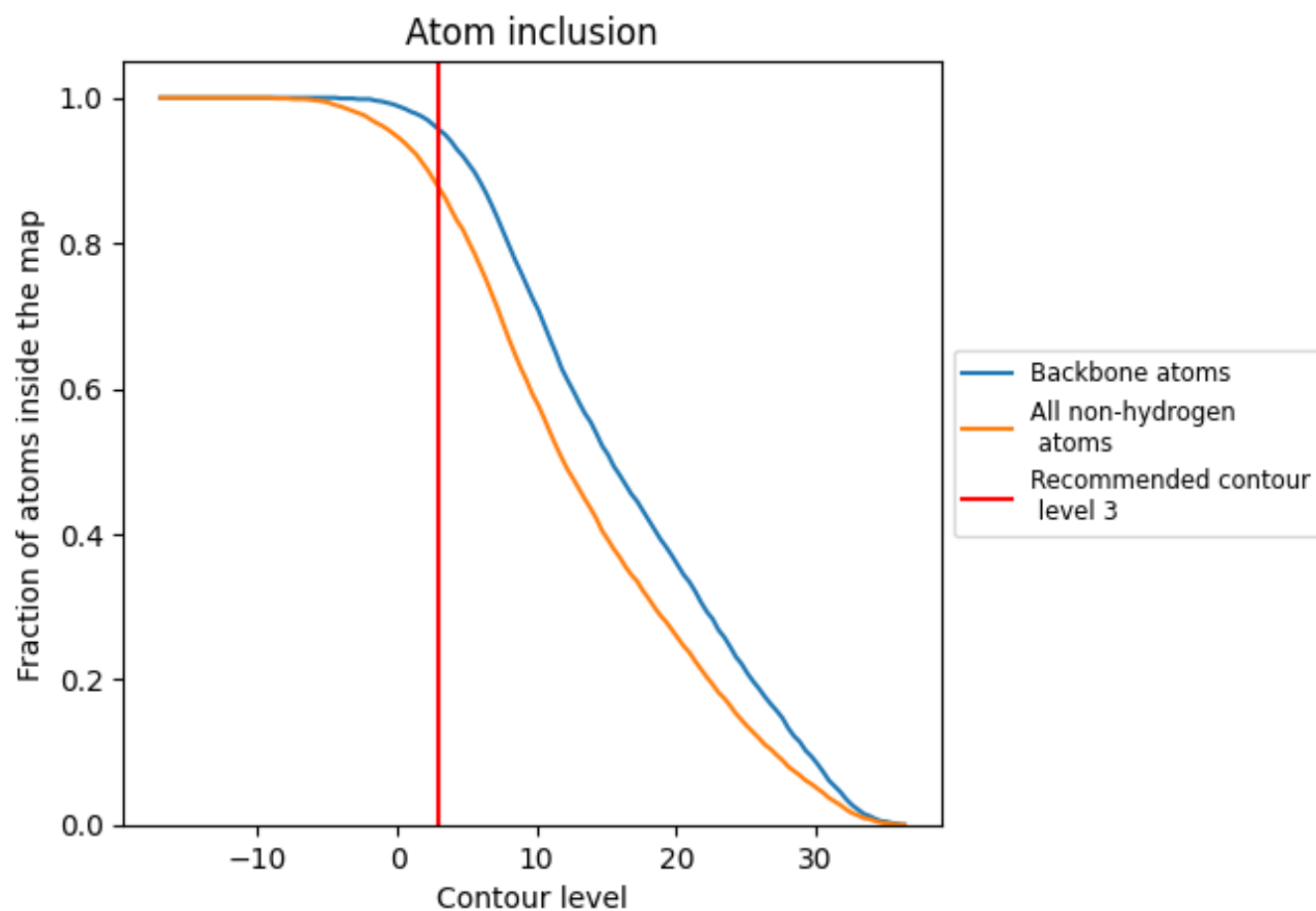
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8760	<div></div> 0.4730
A	<div></div> 0.7230	<div></div> 0.2830
C	<div></div> 0.9110	<div></div> 0.5360
E	<div></div> 0.9460	<div></div> 0.5420
H	<div></div> 0.9470	<div></div> 0.5370
L	<div></div> 0.9140	<div></div> 0.5130

