



Full wwPDB EM Validation Report ⓘ

Jul 2, 2026 – 09:21 PM JST

PDB ID : 9XDR / pdb_00009xdr
EMDB ID : EMD-66773
Title : Cryo-EM structure of asimadoline-BMS-986187-bound KOR-Gi1 complex
Authors : Zhao, C.; Fu, H.; Tian, X.W.; Cheng, L.; Shao, Z.H.
Deposited on : 2025-10-27
Resolution : 2.58 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:

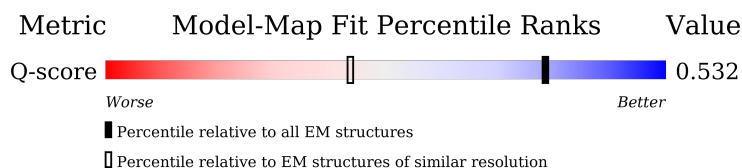
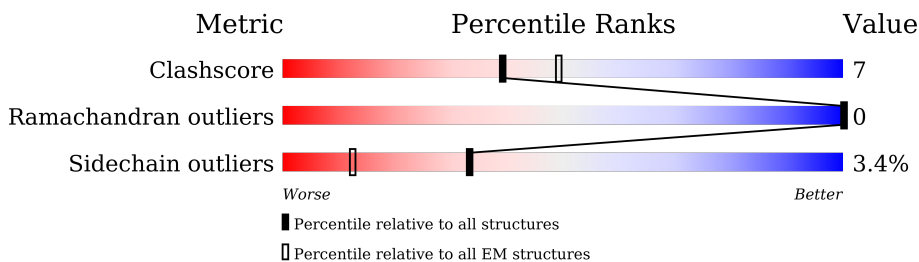
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

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 2.58 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	7675 (2.08 - 3.08)

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	A	354	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">11%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 11% 53% 10% • 36% </div> </div>
2	B	384	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">10%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 10% 70% 16% • 13% </div> </div>
3	C	71	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">46%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 46% 55% 20% • 23% </div> </div>
4	R	608	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">•</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> • 41% 6% 53% </div> </div>

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7165 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	1820	1156	302	348	14	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	conflict	UNP P63097
A	203	ALA	GLY	conflict	UNP P63097
A	245	ALA	GLU	conflict	UNP P63097
A	326	SER	ALA	conflict	UNP P63097

- 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	335	2575	1589	464	501	21	0	0

There are 45 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	341	GLY	-	expression tag	UNP P62873
B	342	GLY	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	SER	-	expression tag	UNP P62873
B	352	SER	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	GLY	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	SER	-	expression tag	UNP P62873
B	358	GLY	-	expression tag	UNP P62873
B	359	TRP	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	LYS	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	SER	-	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	C	55	427	268	75	81	3	0	0

- Molecule 4 is a protein called Soluble cytochrome b562,Kappa-type opioid receptor,Soluble cytochrome b562,Kappa-type opioid receptor,Oplophorus-luciferin 2-monooxygenase cat-

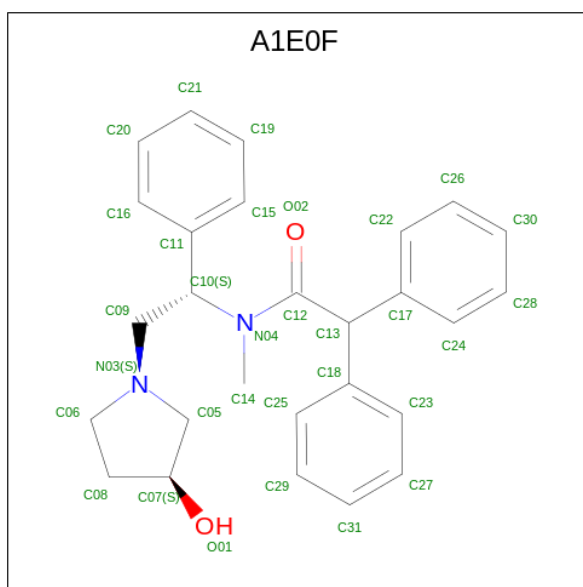
alytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	286	2277	1511	359	389	18	0	0

There are 26 discrepancies between the modelled and reference sequences:

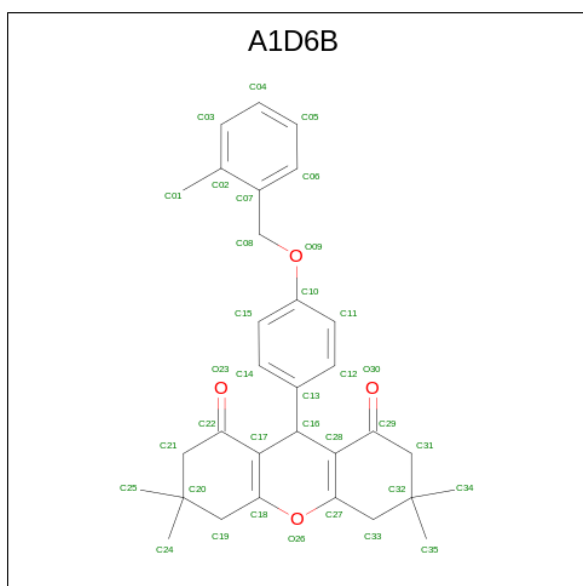
Chain	Residue	Modelled	Actual	Comment	Reference
R	-76	MET	-	initiating methionine	UNP P0ABE7
R	-75	LYS	-	expression tag	UNP P0ABE7
R	-74	THR	-	expression tag	UNP P0ABE7
R	-73	ILE	-	expression tag	UNP P0ABE7
R	-72	ILE	-	expression tag	UNP P0ABE7
R	-71	ALA	-	expression tag	UNP P0ABE7
R	-70	LEU	-	expression tag	UNP P0ABE7
R	-69	SER	-	expression tag	UNP P0ABE7
R	-68	TYR	-	expression tag	UNP P0ABE7
R	-67	ILE	-	expression tag	UNP P0ABE7
R	-66	PHE	-	expression tag	UNP P0ABE7
R	-65	CYS	-	expression tag	UNP P0ABE7
R	-64	LEU	-	expression tag	UNP P0ABE7
R	-63	VAL	-	expression tag	UNP P0ABE7
R	-62	PHE	-	expression tag	UNP P0ABE7
R	-61	ALA	-	expression tag	UNP P0ABE7
R	-60	ASP	-	expression tag	UNP P0ABE7
R	-59	TYR	-	expression tag	UNP P0ABE7
R	-58	LYS	-	expression tag	UNP P0ABE7
R	-57	ASP	-	expression tag	UNP P0ABE7
R	-56	ASP	-	expression tag	UNP P0ABE7
R	-55	ASP	-	expression tag	UNP P0ABE7
R	-54	ASP	-	expression tag	UNP P0ABE7
R	-46	TRP	MET	conflict	UNP P0ABE7
R	49	ILE	HIS	conflict	UNP P0ABE7
R	53	LEU	-	linker	UNP P0ABE7

- Molecule 5 is Asimadoline (CCD ID: A1E0F) (formula: C₂₇H₃₀N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	R	1	31	27	2	2	0

- Molecule 6 is 3,3,6,6-tetramethyl-9-[4-[(2-methylphenyl)methoxy]phenyl]-4,5,7,9-tetrahydro-2 {H}-xanthene-1,8-dione (CCD ID: A1D6B) (formula: C₃₁H₃₄O₄).

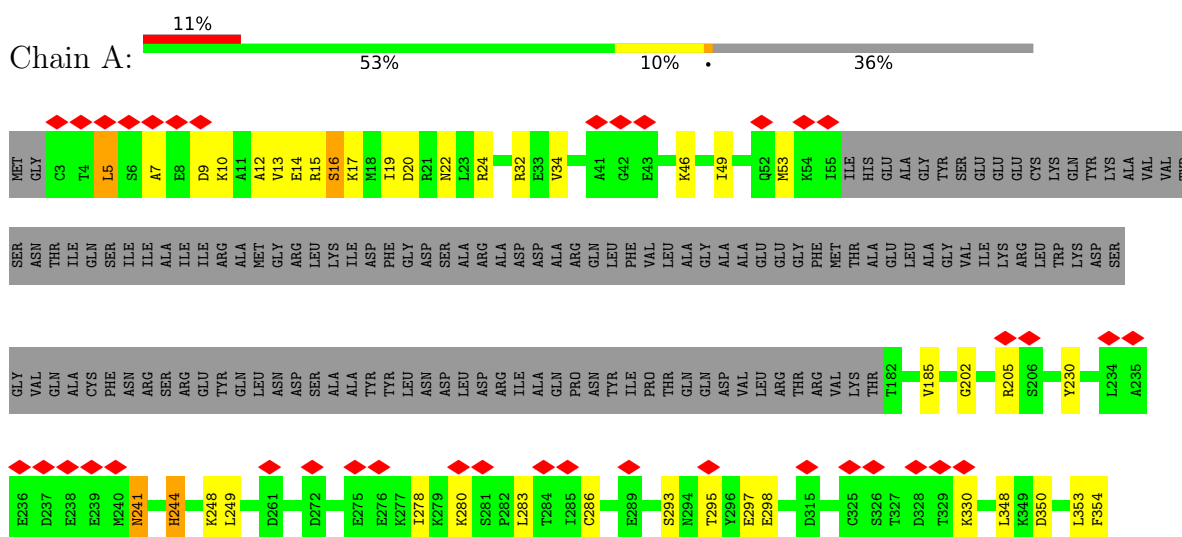


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	R	1	35	31	4	0

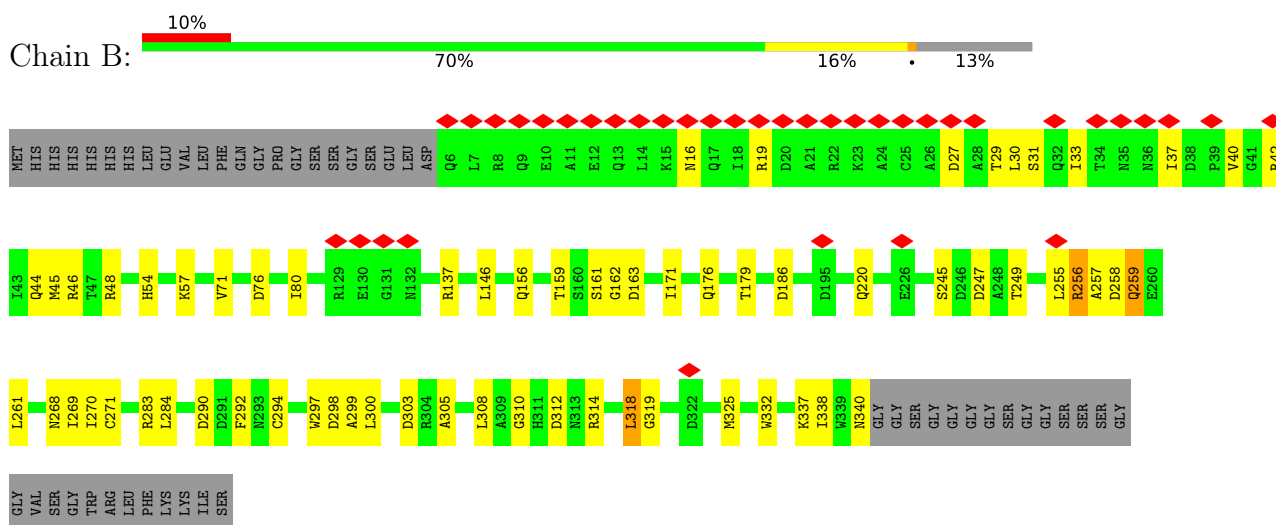
3 Residue-property plots [i](#)

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

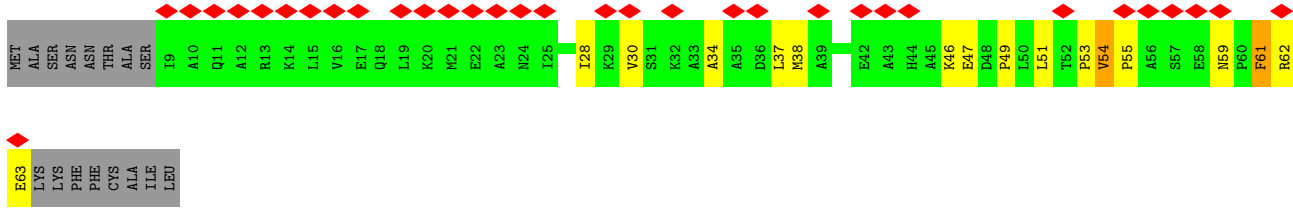


- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

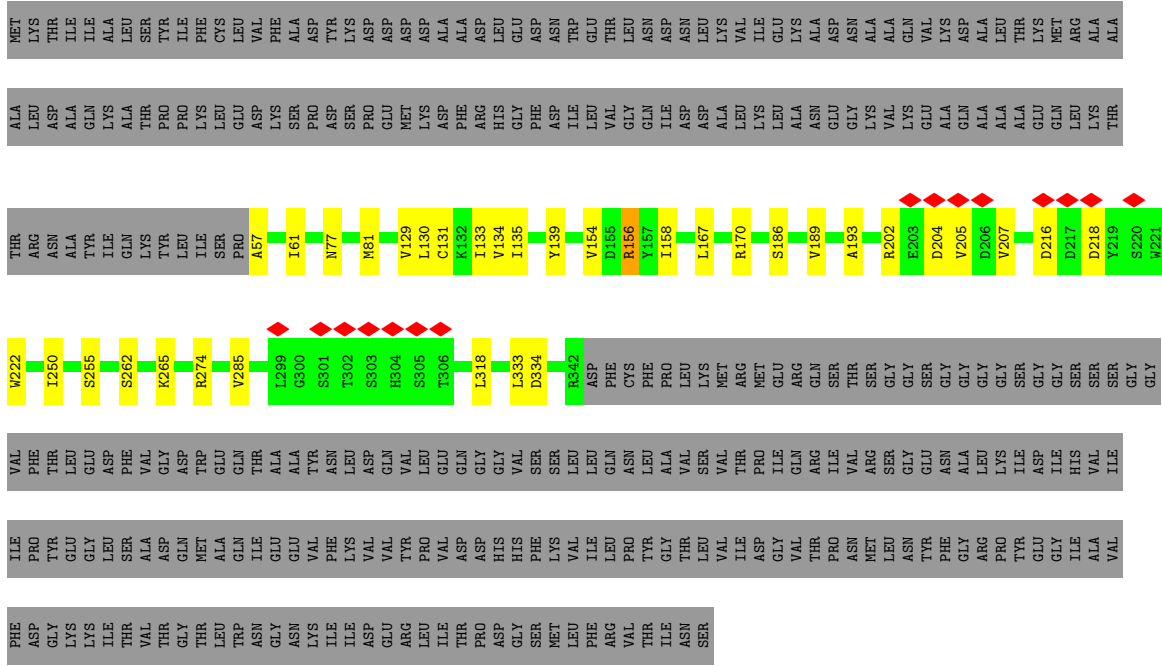
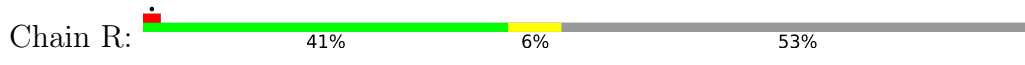


- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2





- Molecule 4: Soluble cytochrome b562,Kappa-type opioid receptor,Soluble cytochrome b562,Kappa-type opioid receptor,Oplophorus-luciferin 2-monoxygenase catalytic subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	352862	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.318	Depositor
Minimum map value	-0.377	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	228.0, 228.0, 228.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.76, 0.76, 0.76	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1D6B, A1E0F

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	0.23	0/1850	0.38	0/2482
2	B	0.39	0/2622	0.61	0/3555
3	C	0.53	0/433	0.74	0/584
4	R	0.41	0/2330	0.61	0/3176
All	All	0.37	0/7235	0.57	0/9797

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
4	R	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	256	ARG	Sidechain
4	R	156	ARG	Sidechain

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	1820	0	1810	27	0
2	B	2575	0	2484	54	0
3	C	427	0	437	22	0
4	R	2277	0	2374	16	0
5	R	31	0	0	0	0
6	R	35	0	0	0	0
All	All	7165	0	7105	102	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 (102) 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:B:261:LEU:HD12	3:C:37:LEU:HD12	1.42	0.97
2:B:30:LEU:HD13	3:C:34:ALA:HB1	1.58	0.85
2:B:162:GLY:HA2	2:B:186:ASP:HB2	1.59	0.85
1:A:5:LEU:HD12	1:A:9:ASP:HB2	1.66	0.75
2:B:220:GLN:NE2	2:B:255:LEU:O	2.21	0.73
2:B:283:ARG:O	2:B:299:ALA:N	2.23	0.70
2:B:40:VAL:CG2	2:B:298:ASP:HB2	2.21	0.70
1:A:32:ARG:NH2	4:R:167:LEU:O	2.28	0.67
2:B:261:LEU:HD12	3:C:37:LEU:CD1	2.23	0.67
2:B:54:HIS:CE1	2:B:80:ILE:HD12	2.28	0.66
2:B:40:VAL:HG21	2:B:298:ASP:HB2	1.76	0.66
1:A:297:GLU:OE2	1:A:297:GLU:N	2.26	0.64
1:A:348:LEU:HB3	1:A:354:PHE:HB3	1.80	0.64
1:A:350:ASP:OD2	4:R:170:ARG:NH1	2.25	0.64
3:C:46:LYS:HE3	3:C:47:GLU:HG3	1.80	0.63
2:B:325:MET:HE3	3:C:49:PRO:HB2	1.80	0.62
1:A:14:GLU:OE1	1:A:17:LYS:NZ	2.34	0.61
2:B:48:ARG:HD2	3:C:63:GLU:N	2.15	0.60
2:B:310:GLY:O	2:B:337:LYS:HE3	2.01	0.59
2:B:137:ARG:NH1	2:B:171:ILE:O	2.35	0.59
2:B:37:ILE:HD13	2:B:300:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:LEU:HG	2:B:319:GLY:H	1.70	0.57
1:A:5:LEU:HG	1:A:10:LYS:H	1.70	0.56
2:B:37:ILE:CD1	2:B:300:LEU:HD13	2.35	0.56
2:B:245:SER:OG	2:B:247:ASP:OD1	2.23	0.56
2:B:261:LEU:CD1	3:C:34:ALA:HA	2.34	0.56
3:C:54:VAL:HG22	3:C:55:PRO:HD2	1.87	0.56
4:R:262:SER:HB3	4:R:265:LYS:HE2	1.87	0.56
2:B:45:MET:HG3	2:B:308:LEU:HD11	1.87	0.56
2:B:318:LEU:HG	2:B:319:GLY:N	2.23	0.53
1:A:49:ILE:O	1:A:53:MET:HG2	2.08	0.53
2:B:325:MET:HE3	2:B:325:MET:HA	1.92	0.52
4:R:129:VAL:O	4:R:133:ILE:HG13	2.09	0.52
1:A:12:ALA:O	1:A:16:SER:OG	2.26	0.52
2:B:284:LEU:HA	2:B:297:TRP:O	2.10	0.52
1:A:241:ASN:HD22	1:A:244:HIS:HD2	1.59	0.51
3:C:61:PHE:CD1	3:C:61:PHE:N	2.79	0.51
3:C:46:LYS:HE3	3:C:47:GLU:CG	2.41	0.50
1:A:9:ASP:O	1:A:13:VAL:HG23	2.11	0.50
1:A:20:ASP:O	1:A:24:ARG:HG3	2.12	0.50
2:B:261:LEU:HD11	3:C:34:ALA:CA	2.42	0.50
1:A:293:SER:OG	1:A:298:GLU:OE1	2.28	0.49
3:C:59:ASN:HB3	3:C:62:ARG:CG	2.43	0.49
2:B:259:GLN:NE2	3:C:30:VAL:HB	2.28	0.49
2:B:40:VAL:HG23	2:B:298:ASP:HB2	1.91	0.49
4:R:218:ASP:HB3	4:R:222:TRP:HD1	1.78	0.48
4:R:154:VAL:O	4:R:158:ILE:HG12	2.13	0.48
2:B:29:THR:HG22	2:B:31:SER:H	1.78	0.48
2:B:256:ARG:C	2:B:258:ASP:N	2.70	0.47
2:B:294:CYS:SG	2:B:308:LEU:HB2	2.54	0.47
1:A:19:ILE:HA	1:A:22:ASN:OD1	2.14	0.47
1:A:32:ARG:N	1:A:32:ARG:HD2	2.29	0.47
1:A:295:THR:HG23	1:A:298:GLU:H	1.79	0.47
2:B:16:ASN:OD1	2:B:19:ARG:NH1	2.47	0.47
1:A:7:ALA:HA	1:A:10:LYS:HG2	1.96	0.47
2:B:338:ILE:O	2:B:338:ILE:HG13	2.15	0.47
1:A:230:TYR:HB2	1:A:286:CYS:SG	2.55	0.46
1:A:278:ILE:HD11	1:A:283:LEU:HB2	1.97	0.46
2:B:300:LEU:HD22	3:C:38:MET:HG2	1.96	0.46
4:R:202:ARG:HG2	4:R:204:ASP:OD1	2.16	0.46
3:C:59:ASN:HB3	3:C:62:ARG:HG3	1.98	0.46
1:A:283:LEU:O	1:A:283:LEU:HG	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:LYS:HD3	2:B:332:TRP:CD2	2.52	0.45
2:B:257:ALA:HA	3:C:28:ILE:O	2.16	0.45
1:A:202:GLY:O	1:A:205:ARG:NH1	2.50	0.45
3:C:51:LEU:O	3:C:53:PRO:HD3	2.16	0.45
4:R:57:ALA:O	4:R:61:ILE:HG13	2.16	0.45
2:B:261:LEU:HA	2:B:261:LEU:HD23	1.68	0.45
2:B:137:ARG:HH11	2:B:137:ARG:HG3	1.81	0.45
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.99	0.45
2:B:162:GLY:HA2	2:B:186:ASP:CB	2.36	0.45
4:R:130:LEU:O	4:R:134:VAL:HG23	2.17	0.44
4:R:205:VAL:O	4:R:207:VAL:HG13	2.17	0.44
2:B:44:GLN:HB3	2:B:46:ARG:NH2	2.32	0.44
1:A:330:LYS:HA	1:A:330:LYS:HD2	1.81	0.43
2:B:256:ARG:C	2:B:258:ASP:H	2.26	0.43
2:B:27:ASP:OD1	3:C:30:VAL:HG12	2.19	0.43
2:B:259:GLN:HE21	3:C:30:VAL:HB	1.84	0.43
1:A:353:LEU:HD11	4:R:156:ARG:HD3	2.01	0.42
1:A:5:LEU:HD23	1:A:7:ALA:H	1.84	0.42
2:B:146:LEU:HD11	2:B:159:THR:HB	2.00	0.42
4:R:216:ASP:OD1	4:R:216:ASP:N	2.52	0.42
2:B:269:ILE:C	2:B:270:ILE:HD12	2.45	0.42
2:B:161:SER:HB3	2:B:163:ASP:OD1	2.19	0.42
1:A:15:ARG:O	1:A:19:ILE:HG13	2.20	0.42
3:C:61:PHE:H	3:C:61:PHE:HD1	1.67	0.42
2:B:30:LEU:HD22	2:B:261:LEU:HD13	2.02	0.42
2:B:30:LEU:HD12	2:B:33:ILE:HB	2.02	0.41
2:B:292:PHE:N	2:B:292:PHE:CD1	2.87	0.41
4:R:77:ASN:O	4:R:81:MET:HG3	2.20	0.41
4:R:135:ILE:HG22	4:R:193:ALA:HB1	2.01	0.41
2:B:176:GLN:OE1	2:B:179:THR:OG1	2.38	0.41
2:B:314:ARG:HE	2:B:314:ARG:HB2	1.67	0.41
2:B:76:ASP:OD1	2:B:76:ASP:N	2.54	0.41
2:B:298:ASP:HB3	2:B:303:ASP:OD1	2.21	0.41
1:A:46:LYS:O	1:A:49:ILE:HG13	2.20	0.41
4:R:318:LEU:HD23	4:R:318:LEU:HA	1.89	0.41
1:A:248:LYS:HD3	1:A:248:LYS:HA	1.80	0.41
2:B:261:LEU:HD11	3:C:34:ALA:HA	2.01	0.41
2:B:42:ARG:HA	2:B:305:ALA:O	2.21	0.40
4:R:333:LEU:HD23	4:R:333:LEU:HA	1.90	0.40
2:B:261:LEU:HD11	3:C:34:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/354 (63%)	216 (97%)	6 (3%)	0	100	100
2	B	333/384 (87%)	321 (96%)	12 (4%)	0	100	100
3	C	53/71 (75%)	47 (89%)	6 (11%)	0	100	100
4	R	284/608 (47%)	279 (98%)	5 (2%)	0	100	100
All	All	892/1417 (63%)	863 (97%)	29 (3%)	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	201/305 (66%)	193 (96%)	8 (4%)	28	52
2	B	278/313 (89%)	270 (97%)	8 (3%)	37	63
3	C	45/58 (78%)	43 (96%)	2 (4%)	25	48
4	R	260/529 (49%)	251 (96%)	9 (4%)	32	57
All	All	784/1205 (65%)	757 (97%)	27 (3%)	33	58

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	16	SER

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Mol	Chain	Res	Type
1	A	34	VAL
1	A	185	VAL
1	A	241	ASN
1	A	244	HIS
1	A	249	LEU
1	A	280	LYS
2	B	71	VAL
2	B	156	GLN
2	B	249	THR
2	B	259	GLN
2	B	268	ASN
2	B	312	ASP
2	B	318	LEU
2	B	340	ASN
3	C	54	VAL
3	C	61	PHE
4	R	131	CYS
4	R	139	TYR
4	R	186	SER
4	R	189	VAL
4	R	250	ILE
4	R	255	SER
4	R	274	ARG
4	R	285	VAL
4	R	334	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	244	HIS
1	A	255	ASN
1	A	304	GLN
1	A	333	GLN
1	A	346	ASN
1	A	347	ASN
2	B	88	ASN
2	B	110	ASN
2	B	230	ASN
2	B	259	GLN
2	B	268	ASN
3	C	59	ASN

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Mol	Chain	Res	Type
4	R	77	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 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
5	A1E0F	R	601	-	33,34,34	6.71	25 (75%)	40,46,46	1.09	3 (7%)
6	A1D6B	R	602	-	39,39,39	1.47	8 (20%)	60,60,60	2.30	8 (13%)

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
5	A1E0F	R	601	-	-	1/28/37/37	0/4/4/4
6	A1D6B	R	602	-	-	3/9/57/57	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	601	A1E0F	C05-N03	-15.84	1.26	1.47
5	R	601	A1E0F	C09-N03	-13.66	1.22	1.47
5	R	601	A1E0F	C08-C07	-9.84	1.21	1.50
5	R	601	A1E0F	C23-C18	8.50	1.52	1.39
5	R	601	A1E0F	C24-C17	8.48	1.52	1.39
5	R	601	A1E0F	C16-C11	8.46	1.52	1.39
5	R	601	A1E0F	C22-C17	8.39	1.52	1.39
5	R	601	A1E0F	C25-C18	8.27	1.52	1.39
5	R	601	A1E0F	C15-C11	8.26	1.52	1.39
5	R	601	A1E0F	C05-C07	8.01	1.64	1.52
5	R	601	A1E0F	C28-C24	6.44	1.52	1.38
5	R	601	A1E0F	C27-C23	6.42	1.52	1.38
5	R	601	A1E0F	C19-C15	6.42	1.52	1.38
5	R	601	A1E0F	C20-C16	6.36	1.52	1.38
5	R	601	A1E0F	C26-C22	6.35	1.52	1.38
5	R	601	A1E0F	C29-C25	6.28	1.52	1.38
5	R	601	A1E0F	C19-C21	5.64	1.53	1.38
5	R	601	A1E0F	C30-C28	5.61	1.52	1.38
5	R	601	A1E0F	C30-C26	5.56	1.52	1.38
5	R	601	A1E0F	C31-C27	5.48	1.52	1.38
5	R	601	A1E0F	C31-C29	5.37	1.52	1.38
5	R	601	A1E0F	C21-C20	5.33	1.52	1.38
5	R	601	A1E0F	C12-N04	4.20	1.45	1.35
6	R	602	A1D6B	C33-C27	3.61	1.53	1.49
6	R	602	A1D6B	C22-C17	3.52	1.52	1.45
6	R	602	A1D6B	C29-C28	3.36	1.52	1.45
6	R	602	A1D6B	C19-C18	3.25	1.52	1.49
6	R	602	A1D6B	C17-C18	-2.82	1.30	1.34
5	R	601	A1E0F	O01-C07	2.57	1.51	1.43
6	R	602	A1D6B	O26-C27	2.39	1.40	1.38
5	R	601	A1E0F	O02-C12	-2.10	1.18	1.22
6	R	602	A1D6B	O23-C22	-2.09	1.18	1.23
6	R	602	A1D6B	O30-C29	-2.07	1.18	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	602	A1D6B	O26-C18-C17	9.06	128.71	122.69
6	R	602	A1D6B	O26-C18-C19	-6.98	104.02	111.22
6	R	602	A1D6B	C27-O26-C18	-6.56	112.53	118.01
6	R	602	A1D6B	O26-C27-C33	5.77	117.16	111.22
6	R	602	A1D6B	C33-C27-C28	-4.84	118.89	125.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	602	A1D6B	C33-C32-C31	4.02	114.77	108.12
5	R	601	A1E0F	C06-N03-C09	-3.44	108.35	113.10
6	R	602	A1D6B	C19-C20-C21	3.10	113.25	108.12
6	R	602	A1D6B	C16-C17-C18	-3.06	120.49	122.56
5	R	601	A1E0F	C14-N04-C10	2.29	121.78	117.73
5	R	601	A1E0F	C06-C08-C07	2.12	106.91	104.17

There are no chirality outliers.

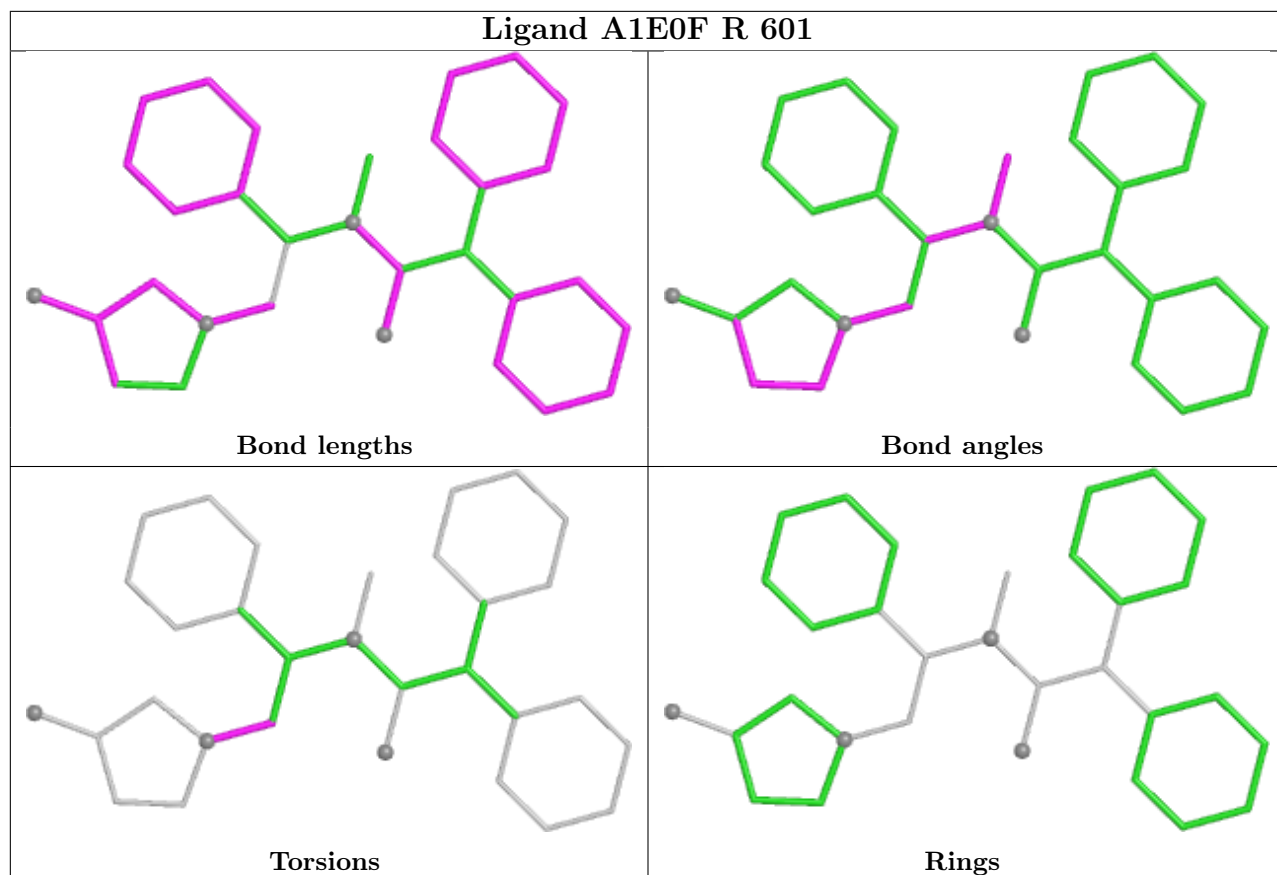
All (4) torsion outliers are listed below:

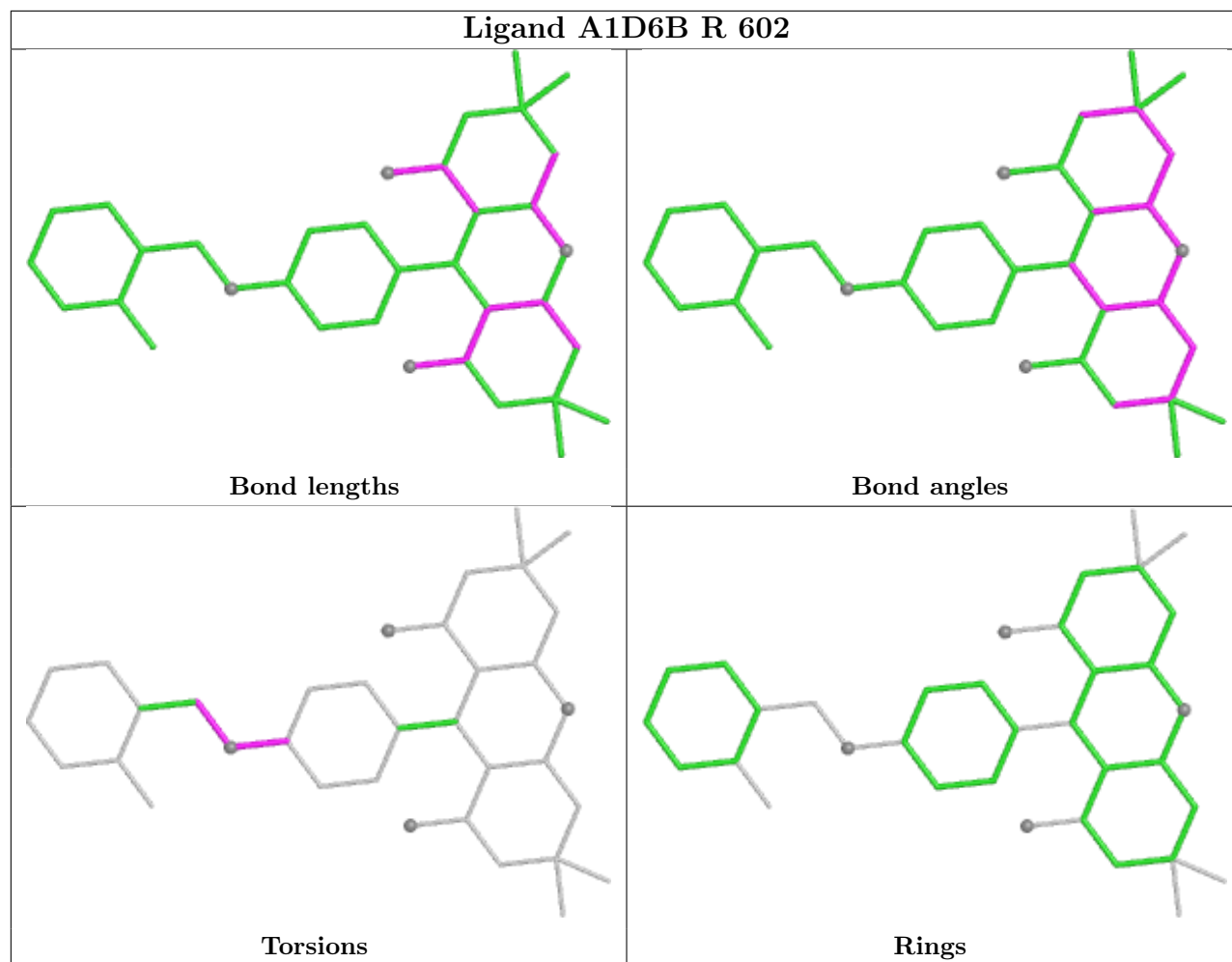
Mol	Chain	Res	Type	Atoms
5	R	601	A1E0F	C10-C09-N03-C05
6	R	602	A1D6B	C11-C10-O09-C08
6	R	602	A1D6B	C15-C10-O09-C08
6	R	602	A1D6B	C07-C08-O09-C10

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.

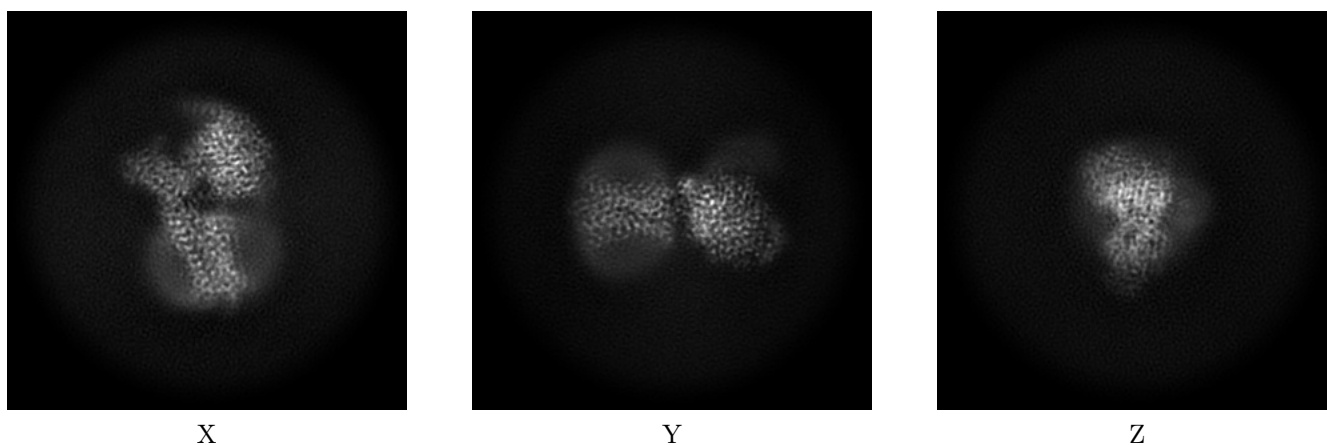
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66773. 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](#)

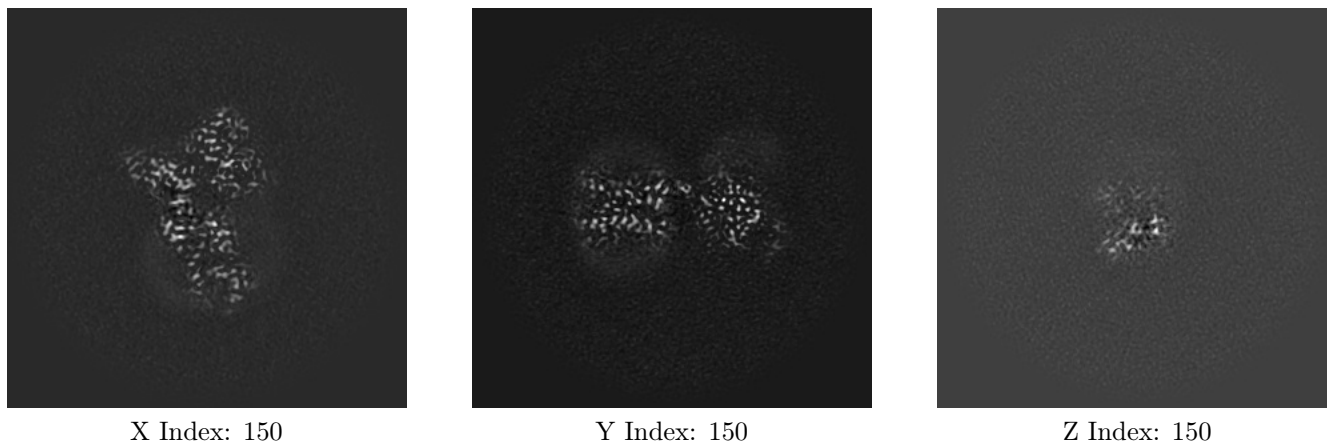
6.1.1 Primary map



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

6.2 Central slices [i](#)

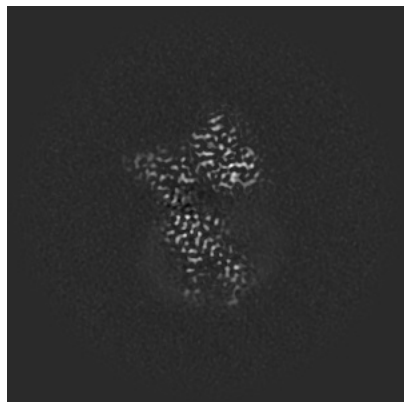
6.2.1 Primary map



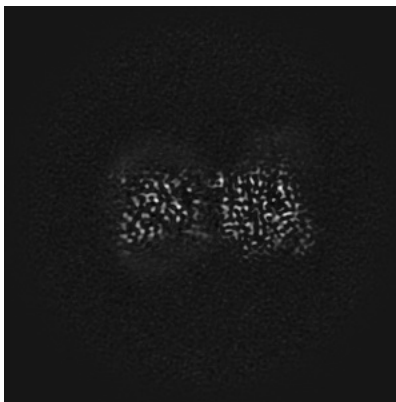
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

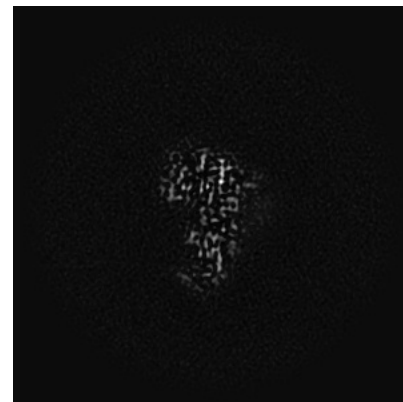
6.3.1 Primary map



X Index: 156



Y Index: 159

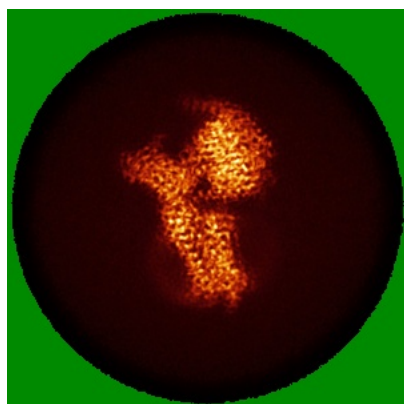


Z Index: 180

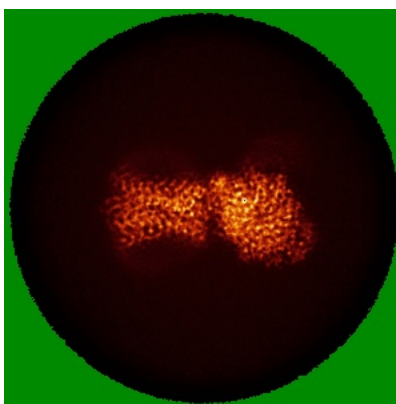
The images above show the largest variance slices of the map in three orthogonal directions.

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

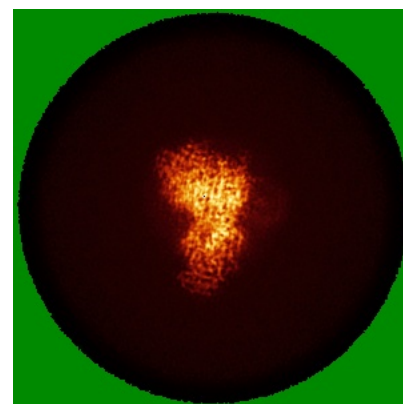
6.4.1 Primary map



X



Y

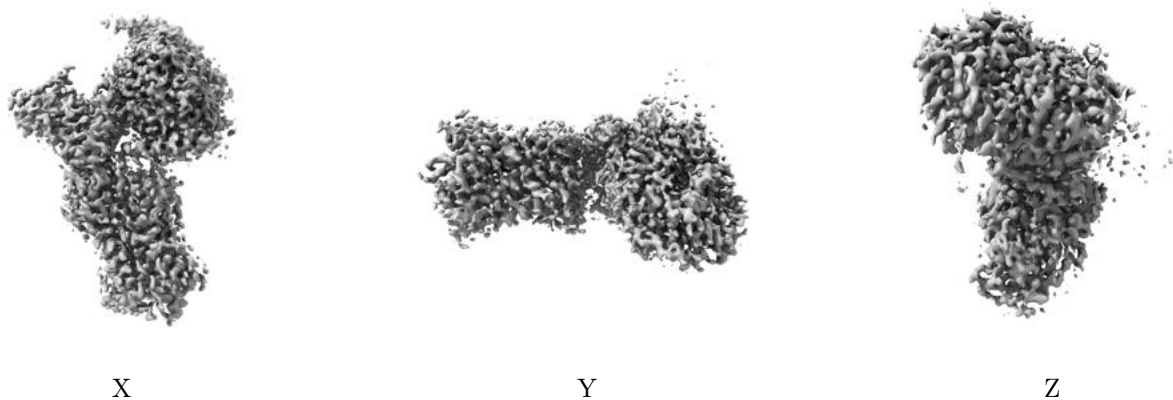


Z

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

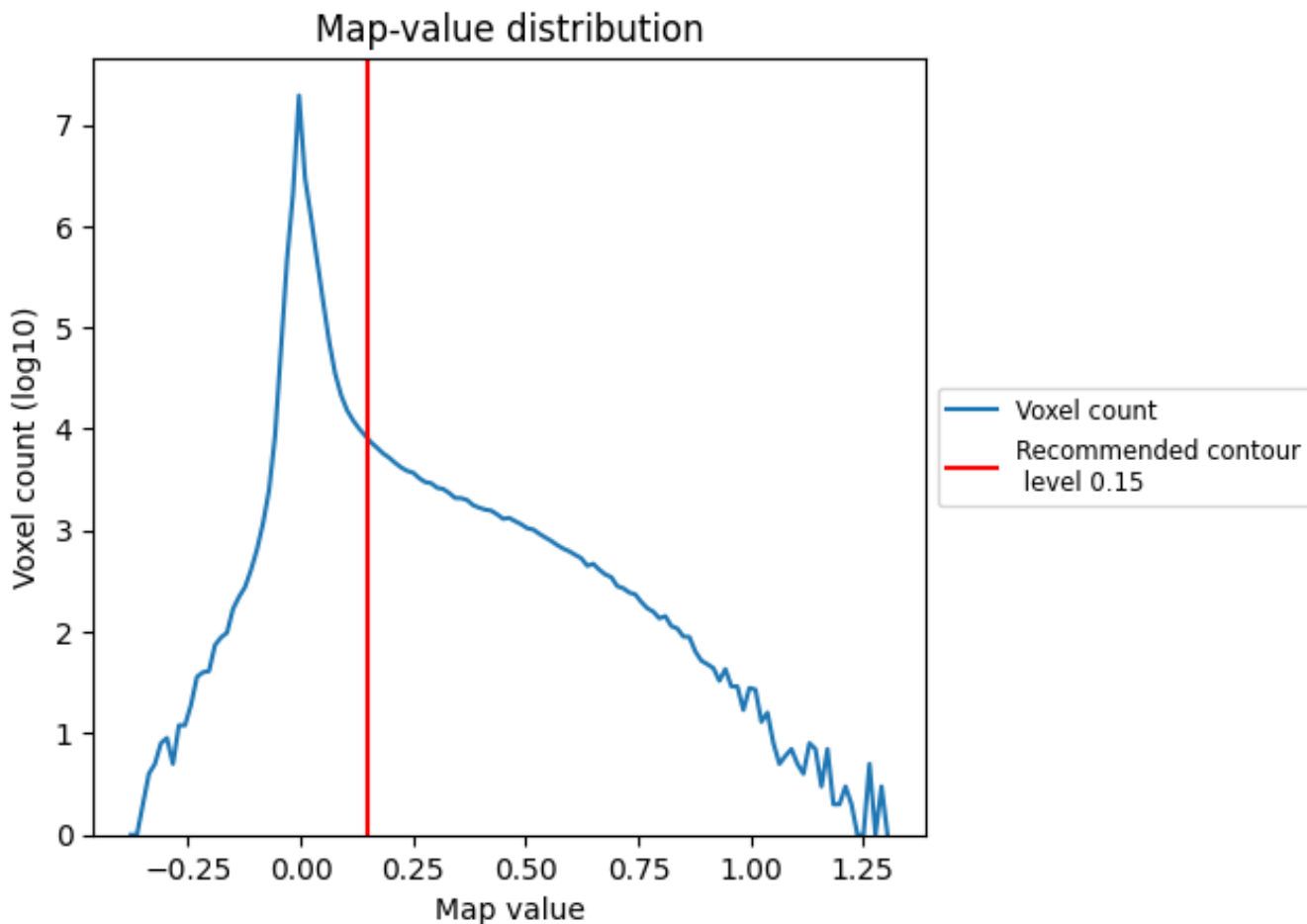
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

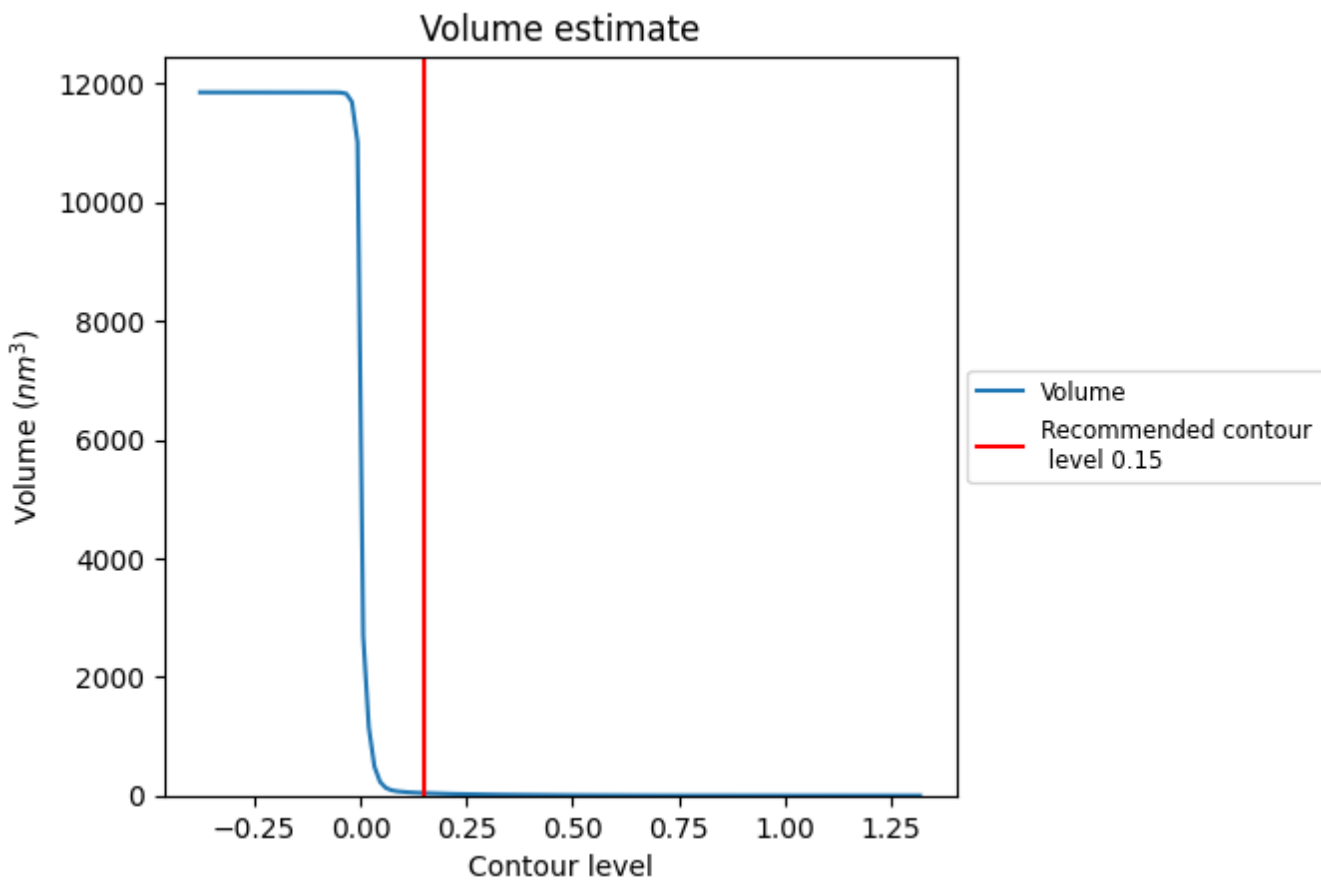
This section contains the results of statistical analysis of the map.

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.

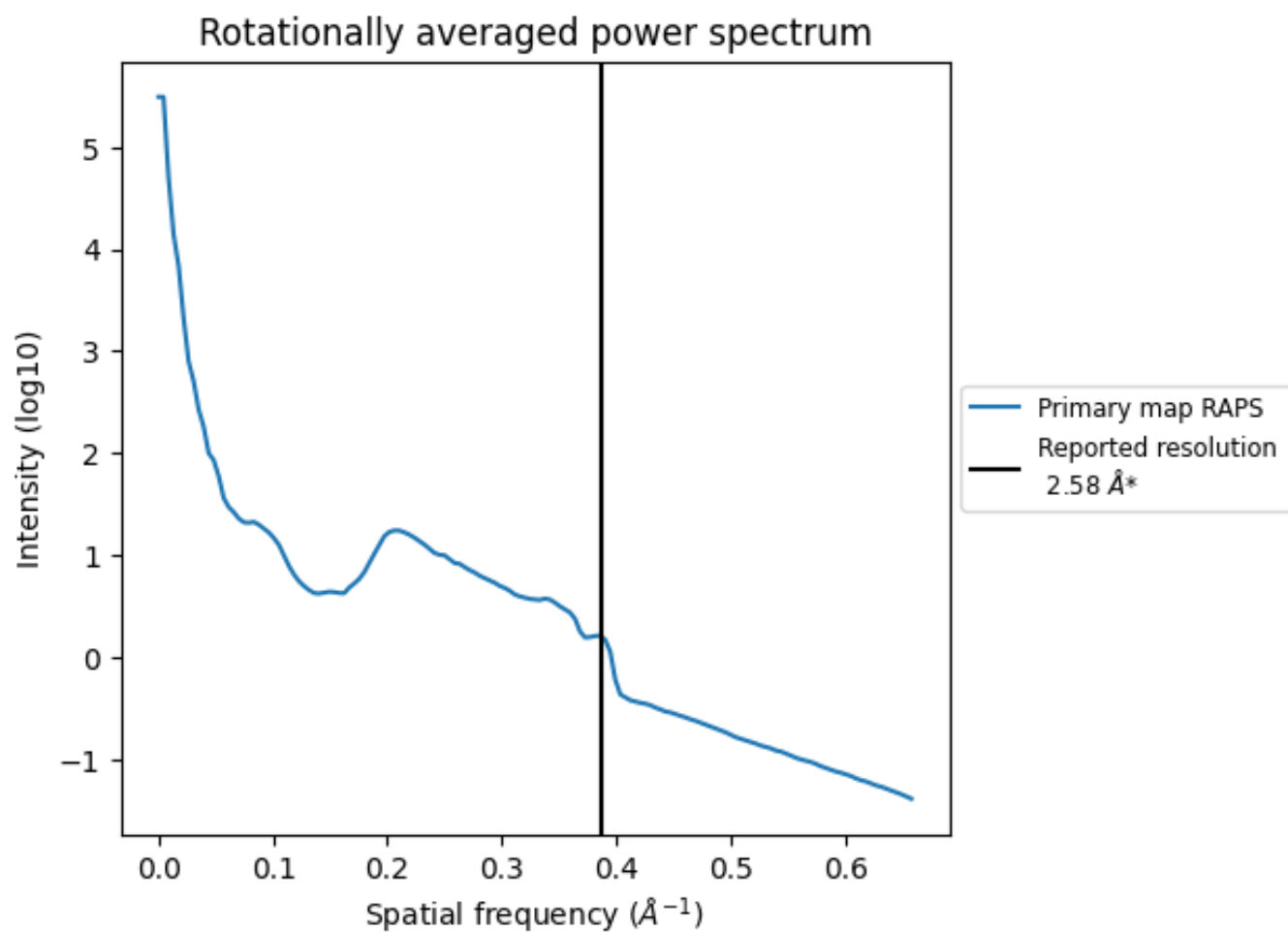
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 41 nm^3 ; this corresponds to an approximate mass of 37 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 0.388 Å⁻¹

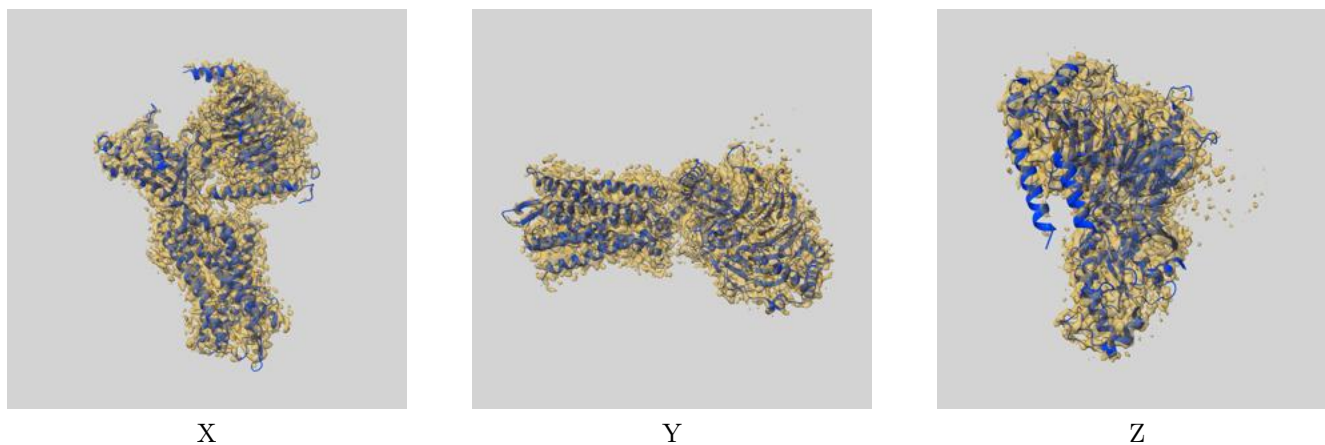
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

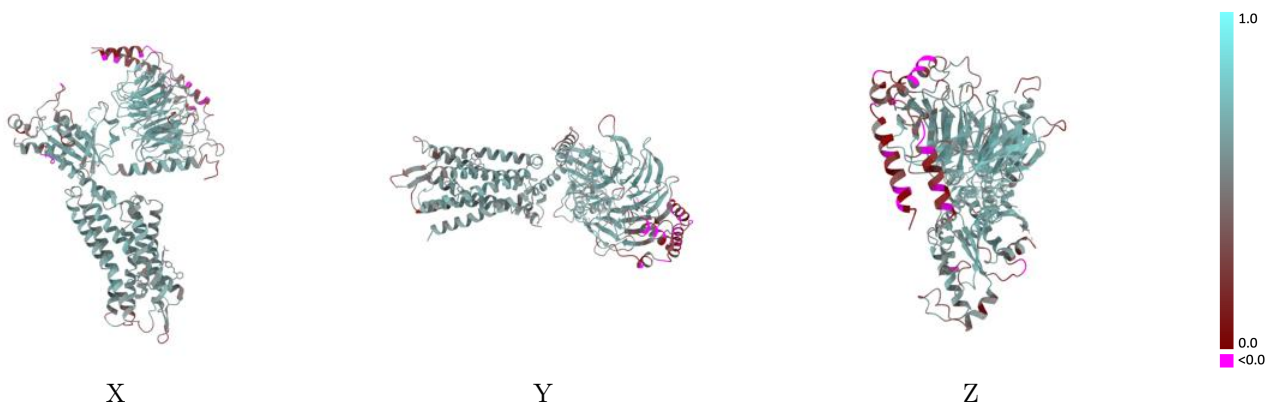
This section contains information regarding the fit between EMDB map EMD-66773 and PDB model 9XDR. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.15 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](#)



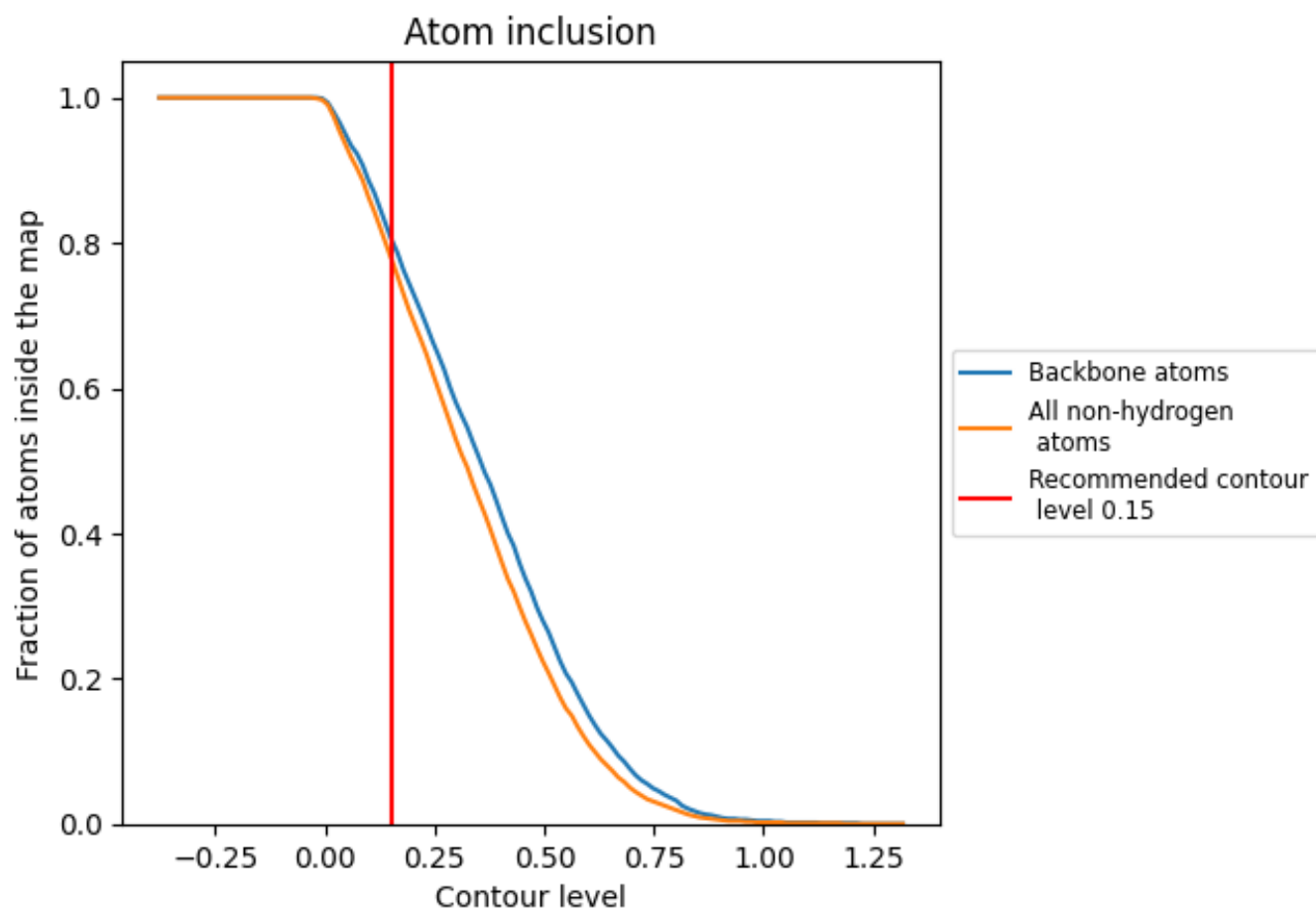
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).











9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.5320
A	 0.7420	 0.5340
B	 0.8240	 0.5490
C	 0.3860	 0.2440
R	 0.8340	 0.5640

