



Full wwPDB EM Validation Report ⓘ

Jun 3, 2026 – 10:12 PM JST

PDB ID : 24XY / pdb_000024xy
EMDB ID : EMD-69904
Title : P2Y13R-Gq complex bound to ADP
Authors : Oshima, H.S.; Akasaka, H.; Sano, F.K.; Nureki, O.
Deposited on : 2026-03-24
Resolution : 3.00 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 : 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) : 2.49

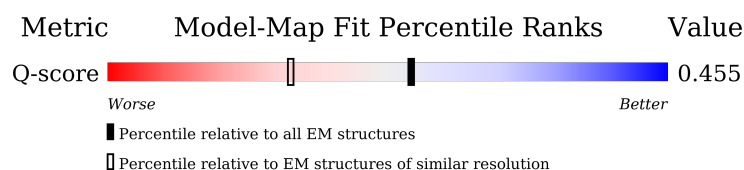
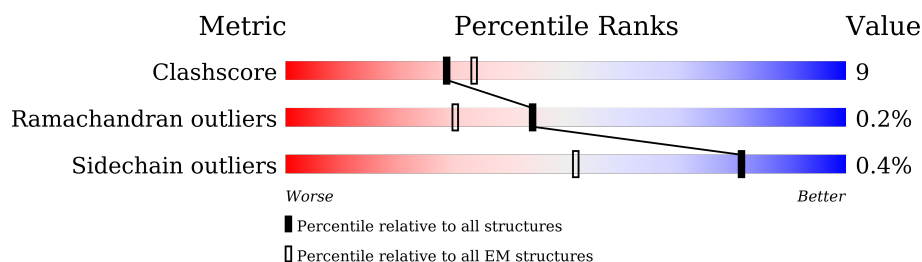
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	R	915	<div> <div>19%</div> <div>9%</div> <div>71%</div> </div>
2	A	323	<div> <div>59%</div> <div>11%</div> <div>30%</div> </div>
3	B	351	<div> <div>6%</div> <div>81%</div> <div>15%</div> </div>
4	G	68	<div> <div>18%</div> <div>75%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
5	N	137	 75% 18% 7%
6	S	260	 73% 15% 11%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9754 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 Soluble cytochrome b562,P2Y purinoceptor 13,LgBiT tag,GFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	263	Total	C	N	O	S	0	0
			2147	1458	338	338	13		

There are 83 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-108	MET	-	initiating methionine	UNP P0ABE7
R	-107	LYS	-	expression tag	UNP P0ABE7
R	-106	THR	-	expression tag	UNP P0ABE7
R	-105	ILE	-	expression tag	UNP P0ABE7
R	-104	ILE	-	expression tag	UNP P0ABE7
R	-103	ALA	-	expression tag	UNP P0ABE7
R	-102	LEU	-	expression tag	UNP P0ABE7
R	-101	SER	-	expression tag	UNP P0ABE7
R	-100	TYR	-	expression tag	UNP P0ABE7
R	-99	ILE	-	expression tag	UNP P0ABE7
R	-98	PHE	-	expression tag	UNP P0ABE7
R	-97	CYS	-	expression tag	UNP P0ABE7
R	-96	LEU	-	expression tag	UNP P0ABE7
R	-95	VAL	-	expression tag	UNP P0ABE7
R	-94	PHE	-	expression tag	UNP P0ABE7
R	-93	ALA	-	expression tag	UNP P0ABE7
R	-92	ASP	-	expression tag	UNP P0ABE7
R	-91	TYR	-	expression tag	UNP P0ABE7
R	-90	LYS	-	expression tag	UNP P0ABE7
R	-89	ASP	-	expression tag	UNP P0ABE7
R	-88	ASP	-	expression tag	UNP P0ABE7
R	-87	ASP	-	expression tag	UNP P0ABE7
R	-86	ASP	-	expression tag	UNP P0ABE7
R	-85	LYS	-	expression tag	UNP P0ABE7
R	-78	TRP	MET	engineered mutation	UNP P0ABE7
R	17	ILE	HIS	engineered mutation	UNP P0ABE7
R	21	LEU	ARG	engineered mutation	UNP P0ABE7
R	355	GLY	-	linker	UNP Q9BPV8

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Chain	Residue	Modelled	Actual	Comment	Reference
R	356	SER	-	linker	UNP Q9BPV8
R	357	GLY	-	linker	UNP Q9BPV8
R	358	GLY	-	linker	UNP Q9BPV8
R	359	GLY	-	linker	UNP Q9BPV8
R	360	GLY	-	linker	UNP Q9BPV8
R	361	SER	-	linker	UNP Q9BPV8
R	362	GLY	-	linker	UNP Q9BPV8
R	363	GLY	-	linker	UNP Q9BPV8
R	364	SER	-	linker	UNP Q9BPV8
R	365	SER	-	linker	UNP Q9BPV8
R	366	SER	-	linker	UNP Q9BPV8
R	367	GLY	-	linker	UNP Q9BPV8
R	368	GLY	-	linker	UNP Q9BPV8
R	527	GLY	-	linker	UNP Q9BPV8
R	528	GLY	-	linker	UNP Q9BPV8
R	529	SER	-	linker	UNP Q9BPV8
R	530	GLY	-	linker	UNP Q9BPV8
R	531	GLY	-	linker	UNP Q9BPV8
R	532	GLY	-	linker	UNP Q9BPV8
R	533	GLY	-	linker	UNP Q9BPV8
R	534	SER	-	linker	UNP Q9BPV8
R	535	GLY	-	linker	UNP Q9BPV8
R	536	GLY	-	linker	UNP Q9BPV8
R	537	SER	-	linker	UNP Q9BPV8
R	538	SER	-	linker	UNP Q9BPV8
R	539	SER	-	linker	UNP Q9BPV8
R	540	GLY	-	linker	UNP Q9BPV8
R	541	GLY	-	linker	UNP Q9BPV8
R	542	LEU	-	linker	UNP Q9BPV8
R	543	GLU	-	linker	UNP Q9BPV8
R	544	VAL	-	linker	UNP Q9BPV8
R	545	LEU	-	linker	UNP Q9BPV8
R	546	PHE	-	linker	UNP Q9BPV8
R	547	GLN	-	linker	UNP Q9BPV8
R	548	GLY	-	linker	UNP Q9BPV8
R	549	PRO	-	linker	UNP Q9BPV8
R	550	GLY	-	linker	UNP Q9BPV8
R	551	SER	-	linker	UNP Q9BPV8
R	552	ALA	-	linker	UNP Q9BPV8
R	553	ALA	-	linker	UNP Q9BPV8
R	554	ALA	-	linker	UNP Q9BPV8
R	555	ALA	-	linker	UNP Q9BPV8

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Chain	Residue	Modelled	Actual	Comment	Reference
R	794	SER	-	expression tag	UNP A0A5P9VSM6
R	795	GLY	-	expression tag	UNP A0A5P9VSM6
R	796	LEU	-	expression tag	UNP A0A5P9VSM6
R	797	ARG	-	expression tag	UNP A0A5P9VSM6
R	798	SER	-	expression tag	UNP A0A5P9VSM6
R	799	HIS	-	expression tag	UNP A0A5P9VSM6
R	800	HIS	-	expression tag	UNP A0A5P9VSM6
R	801	HIS	-	expression tag	UNP A0A5P9VSM6
R	802	HIS	-	expression tag	UNP A0A5P9VSM6
R	803	HIS	-	expression tag	UNP A0A5P9VSM6
R	804	HIS	-	expression tag	UNP A0A5P9VSM6
R	805	HIS	-	expression tag	UNP A0A5P9VSM6
R	806	HIS	-	expression tag	UNP A0A5P9VSM6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	226	Total	C	N	O	S	0	0
			1845	1163	328	347	7		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	SER	-	linker	UNP P59768
A	-8	GLY	-	linker	UNP P59768
A	-7	SER	-	linker	UNP P59768
A	-6	ALA	-	linker	UNP P59768
A	-5	GLY	-	linker	UNP P59768
A	-4	SER	-	linker	UNP P59768
A	-3	ALA	-	linker	UNP P59768
A	-2	GLY	-	linker	UNP P59768
A	-1	SER	-	linker	UNP P59768
A	0	ALA	-	linker	UNP P59768
A	1	MET	-	linker	UNP P59768
A	2	GLY	-	linker	UNP P59768
A	3	SER	-	linker	UNP P59768

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	337	Total	C	N	O	S	0	0
			2591	1599	466	505	21		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	initiating methionine	UNP P54311
B	-9	HIS	-	expression tag	UNP P54311
B	-8	HIS	-	expression tag	UNP P54311
B	-7	HIS	-	expression tag	UNP P54311
B	-6	HIS	-	expression tag	UNP P54311
B	-5	HIS	-	expression tag	UNP P54311
B	-4	HIS	-	expression tag	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	51	Total	C	N	O	S	0	0
			394	248	68	75	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	68	SER	-	expression tag	UNP P63212

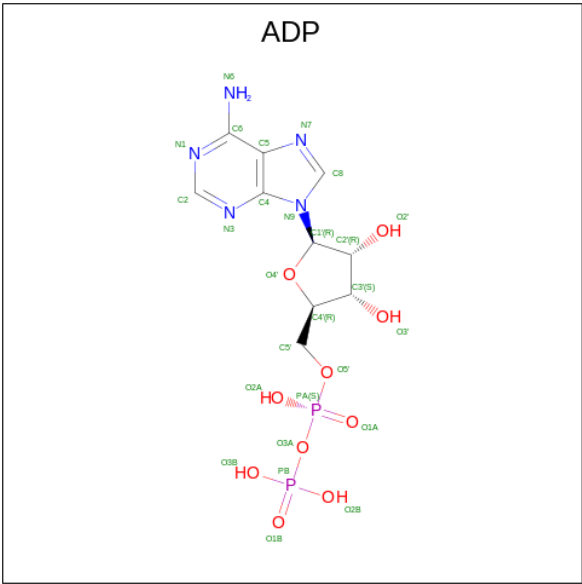
- Molecule 5 is a protein called nanobody Nb35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	128	Total	C	N	O	S	0	0
			973	605	170	192	6		

- Molecule 6 is a protein called scFv16.

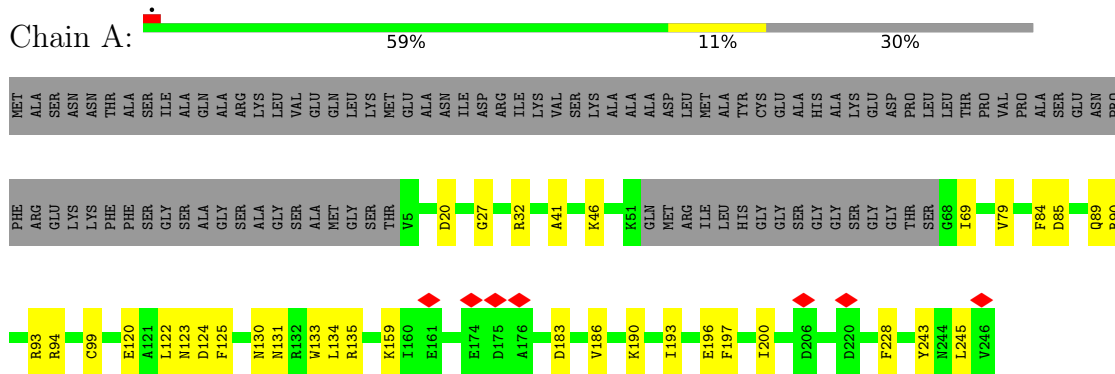
Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	231	Total	C	N	O	S	0	0
			1777	1128	294	345	10		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

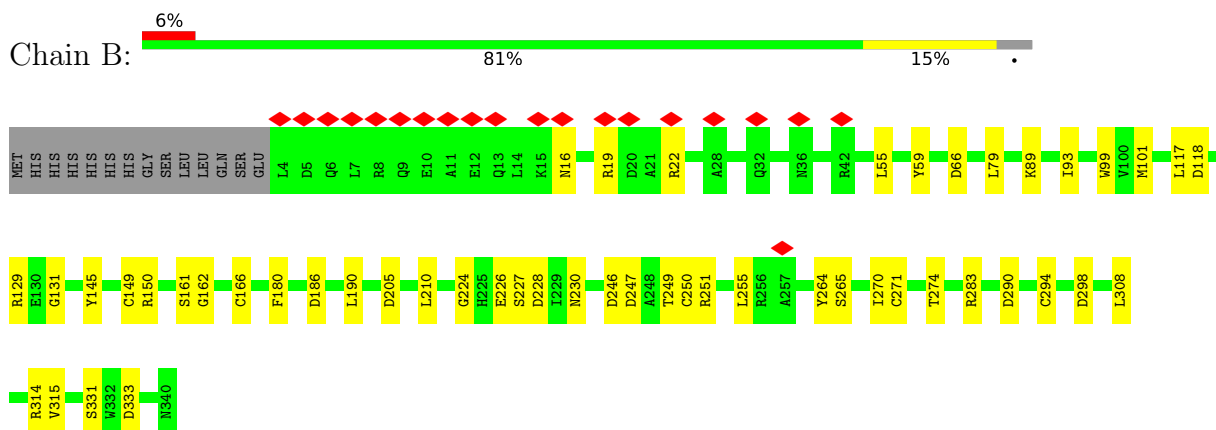


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	R	1	27	10	5	10	2	0

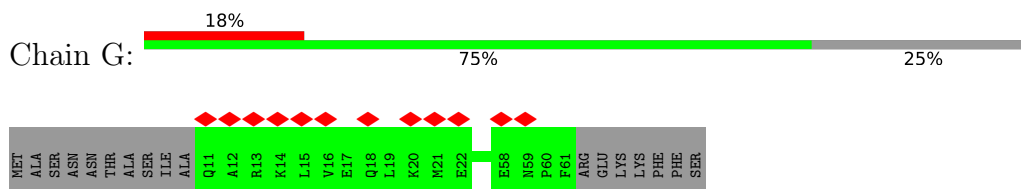
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2,miniGsqi



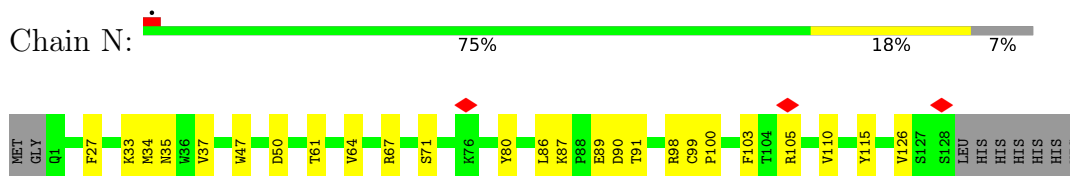
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

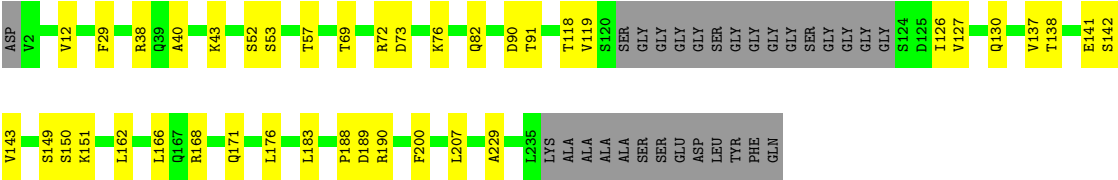


- Molecule 5: nanobody Nb35



- Molecule 6: scFv16

Chain S: 73% 15% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111828	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	51.145	Depositor
Minimum map value	-34.213	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.031	Depositor
Recommended contour level	4.05	Depositor
Map size (Å)	265.60797, 265.60797, 265.60797	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9485999, 0.9485999, 0.9485999	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: ADP

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	R	0.79	0/2210	1.24	0/3009
2	A	0.89	0/1878	1.08	0/2527
3	B	0.30	0/2638	0.65	0/3577
4	G	0.22	0/400	0.52	0/540
5	N	0.85	0/993	1.05	0/1345
6	S	0.86	0/1821	0.98	0/2469
All	All	0.72	0/9940	0.99	0/13467

There are no bond length outliers.

There are no bond angle outliers.

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	R	2147	0	2253	69	0
2	A	1845	0	1826	45	0
3	B	2591	0	2499	45	0
4	G	394	0	402	0	0
5	N	973	0	938	24	0
6	S	1777	0	1712	32	0
7	R	27	0	12	2	0
All	All	9754	0	9642	182	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 9.

All (182) 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:A:69:ILE:HD11	3:B:117:LEU:HB3	1.40	0.99
2:A:84:PHE:CE2	3:B:99:TRP:HZ2	1.99	0.79
6:S:137:VAL:HG11	6:S:207:LEU:CD1	2.13	0.79
6:S:137:VAL:HG11	6:S:207:LEU:HD13	1.67	0.76
2:A:94:ARG:NE	3:B:228:ASP:OD2	2.20	0.74
2:A:243:TYR:HB2	2:A:245:LEU:HG	1.69	0.74
1:R:267:CYS:HB3	1:R:309:ASN:HB2	1.70	0.73
2:A:99:CYS:HA	3:B:59:TYR:OH	1.89	0.73
1:R:92:MET:CE	1:R:310:ILE:HG21	2.17	0.72
3:B:230:ASN:ND2	3:B:246:ASP:OD1	2.22	0.72
1:R:40:THR:HB	1:R:43:VAL:HB	1.70	0.72
1:R:151:ASN:HD22	2:A:32:ARG:HD3	1.55	0.71
2:A:69:ILE:CD1	3:B:117:LEU:HB3	2.18	0.68
6:S:137:VAL:CG1	6:S:207:LEU:HD13	2.25	0.67
1:R:128:TYR:HD2	1:R:216:ILE:HD11	1.59	0.66
3:B:226:GLU:O	5:N:98:ARG:NH2	2.20	0.66
6:S:141:GLU:HG2	6:S:142:SER:N	2.12	0.65
2:A:20:ASP:OD1	3:B:89:LYS:NZ	2.30	0.65
2:A:122:LEU:HD11	2:A:196:GLU:HG3	1.78	0.64
6:S:141:GLU:HG2	6:S:142:SER:H	1.61	0.64
1:R:67:TRP:O	1:R:70:VAL:HG22	1.98	0.63
5:N:33:LYS:O	5:N:99:CYS:SG	2.58	0.62
1:R:92:MET:HE1	1:R:310:ILE:HG21	1.80	0.62
2:A:89:GLN:OE1	3:B:145:TYR:HD1	1.82	0.62
1:R:149:LEU:HD12	2:A:228:PHE:CE1	2.35	0.61
2:A:89:GLN:OE1	3:B:145:TYR:N	2.32	0.61
6:S:188:PRO:HB2	6:S:190:ARG:HG2	1.81	0.60
2:A:84:PHE:CZ	3:B:99:TRP:HZ2	2.20	0.59
1:R:206:HIS:HE1	7:R:901:ADP:H2'	1.68	0.59
2:A:197:PHE:O	2:A:200:ILE:HG12	2.02	0.59
6:S:162:LEU:HD22	6:S:200:PHE:CG	2.39	0.58
2:A:122:LEU:CD1	2:A:196:GLU:HG3	2.33	0.58
6:S:137:VAL:CG1	6:S:207:LEU:HD22	2.35	0.57
2:A:125:PHE:HB3	2:A:200:ILE:HD11	1.86	0.56
2:A:94:ARG:HD3	5:N:100:PRO:HG2	1.85	0.56
6:S:137:VAL:HG12	6:S:138:THR:N	2.21	0.56
1:R:267:CYS:CB	1:R:309:ASN:HB2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:69:THR:HB	6:S:82:GLN:HB3	1.87	0.55
1:R:275:ARG:O	1:R:276:VAL:C	2.49	0.55
1:R:124:TYR:HE2	1:R:275:ARG:HH11	1.55	0.55
1:R:307:ALA:O	1:R:310:ILE:HG12	2.07	0.54
6:S:168:ARG:HB2	6:S:171:GLN:HB2	1.89	0.54
6:S:73:ASP:OD2	6:S:76:LYS:HD2	2.07	0.54
1:R:216:ILE:HG13	1:R:217:PHE:N	2.21	0.53
2:A:130:ASN:HB3	5:N:105:ARG:NE	2.23	0.53
5:N:61:THR:HG22	5:N:64:VAL:HG22	1.90	0.53
1:R:92:MET:HE2	1:R:310:ILE:HG21	1.90	0.53
1:R:109:TRP:O	1:R:112:ARG:N	2.42	0.53
1:R:39:ASP:OD1	1:R:40:THR:N	2.43	0.52
1:R:280:HIS:O	1:R:281:SER:C	2.51	0.52
1:R:52:THR:HG22	1:R:100:ILE:HG21	1.92	0.51
6:S:141:GLU:CG	6:S:142:SER:H	2.23	0.51
5:N:37:VAL:HG12	5:N:47:TRP:HA	1.92	0.51
1:R:117:ARG:NH1	1:R:182:SER:O	2.43	0.51
1:R:205:TRP:O	1:R:206:HIS:C	2.53	0.50
1:R:206:HIS:O	1:R:209:VAL:HG12	2.11	0.50
1:R:289:CYS:SG	1:R:292:GLN:NE2	2.85	0.50
1:R:71:HIS:O	1:R:72:ILE:C	2.54	0.50
1:R:263:VAL:O	1:R:264:PHE:C	2.55	0.50
1:R:149:LEU:HD22	2:A:79:VAL:HG11	1.94	0.49
2:A:41:ALA:O	2:A:46:LYS:NZ	2.44	0.49
1:R:175:SER:O	1:R:176:LEU:C	2.54	0.49
5:N:67:ARG:NH2	5:N:90:ASP:OD2	2.45	0.49
1:R:232:ALA:HB2	1:R:258:PHE:HE1	1.77	0.49
6:S:137:VAL:HG11	6:S:207:LEU:CD2	2.42	0.49
1:R:51:TYR:HB2	1:R:100:ILE:HG12	1.95	0.48
3:B:227:SER:OG	5:N:100:PRO:O	2.22	0.48
1:R:146:ILE:HG22	1:R:234:LYS:HE3	1.96	0.48
3:B:16:ASN:OD1	3:B:19:ARG:NH1	2.46	0.48
6:S:52:SER:OG	6:S:53:SER:N	2.47	0.48
2:A:94:ARG:NH1	5:N:115:TYR:HE1	2.11	0.48
2:A:94:ARG:CD	5:N:100:PRO:HG2	2.43	0.48
2:A:94:ARG:HH12	5:N:115:TYR:HE1	1.59	0.48
3:B:190:LEU:C	3:B:190:LEU:HD12	2.39	0.48
3:B:250:CYS:HB2	3:B:264:TYR:HB2	1.95	0.48
6:S:137:VAL:CG1	6:S:138:THR:N	2.77	0.48
2:A:85:ASP:N	2:A:85:ASP:OD1	2.46	0.47
2:A:90:ARG:NH1	3:B:186:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:331:SER:OG	3:B:333:ASP:OD1	2.32	0.47
3:B:294:CYS:HB2	3:B:308:LEU:HB2	1.96	0.47
3:B:149:CYS:O	3:B:150:ARG:NH1	2.48	0.47
1:R:46:VAL:C	1:R:48:PRO:HD2	2.39	0.47
1:R:103:ASP:O	1:R:104:SER:C	2.56	0.47
6:S:141:GLU:CG	6:S:142:SER:N	2.76	0.47
3:B:271:CYS:HB2	3:B:290:ASP:HB2	1.95	0.47
6:S:183:LEU:HD11	6:S:189:ASP:HA	1.97	0.47
2:A:123:ASN:HD21	5:N:47:TRP:HE3	1.63	0.47
1:R:62:ASN:HB3	1:R:90:LEU:HD22	1.97	0.46
2:A:190:LYS:O	2:A:193:ILE:HG12	2.15	0.46
3:B:59:TYR:HD2	3:B:101:MET:HA	1.80	0.46
6:S:137:VAL:HG12	6:S:207:LEU:HD22	1.96	0.46
6:S:137:VAL:HG22	6:S:143:VAL:HG11	1.97	0.46
2:A:125:PHE:CD1	2:A:200:ILE:HD11	2.51	0.46
1:R:55:PHE:O	1:R:56:LEU:C	2.59	0.46
3:B:161:SER:OG	3:B:162:GLY:N	2.49	0.45
3:B:226:GLU:HG2	5:N:27:PHE:HB3	1.97	0.45
5:N:91:THR:HG22	5:N:126:VAL:H	1.80	0.45
1:R:47:PHE:N	1:R:48:PRO:CD	2.80	0.45
2:A:135:ARG:HH12	5:N:105:ARG:NH2	2.14	0.45
1:R:40:THR:O	1:R:41:ARG:C	2.59	0.45
2:A:120:GLU:HA	2:A:123:ASN:HB2	1.99	0.45
1:R:115:VAL:HA	1:R:119:SER:HB3	1.99	0.45
1:R:299:LYS:O	1:R:300:GLU:C	2.59	0.45
2:A:133:TRP:CZ3	3:B:314:ARG:HD2	2.52	0.45
3:B:19:ARG:HA	3:B:22:ARG:HG2	1.98	0.45
6:S:91:THR:HG23	6:S:118:THR:HA	1.99	0.45
1:R:55:PHE:HB2	1:R:96:LEU:HD23	1.99	0.45
3:B:166:CYS:HB2	3:B:180:PHE:HB2	1.99	0.45
1:R:212:ILE:O	1:R:216:ILE:HG23	2.16	0.45
2:A:27:GLY:HA3	3:B:55:LEU:HD12	1.99	0.45
2:A:183:ASP:HB3	2:A:186:VAL:HG23	1.99	0.44
6:S:38:ARG:NH2	6:S:90:ASP:OD1	2.50	0.44
2:A:84:PHE:CE2	3:B:99:TRP:CZ2	2.92	0.44
3:B:66:ASP:OD1	3:B:66:ASP:N	2.50	0.44
1:R:149:LEU:HB3	2:A:79:VAL:HG21	1.99	0.44
1:R:269:ALA:O	1:R:270:PRO:C	2.58	0.44
5:N:71:SER:HB3	5:N:80:TYR:HB2	2.00	0.44
2:A:84:PHE:CZ	3:B:99:TRP:CZ2	3.04	0.44
1:R:57:THR:HG22	1:R:61:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:127:VAL:HG12	6:S:150:SER:HB2	1.99	0.44
1:R:91:ILE:O	1:R:95:MET:HG2	2.18	0.44
1:R:268:PHE:O	1:R:271:PHE:N	2.47	0.44
6:S:130:GLN:HG3	6:S:229:ALA:H	1.83	0.44
2:A:131:ASN:HB3	2:A:134:LEU:HB2	2.00	0.43
5:N:35:ASN:HD22	5:N:110:VAL:HG21	1.83	0.43
1:R:109:TRP:O	1:R:110:GLN:C	2.61	0.43
1:R:109:TRP:C	1:R:111:LEU:N	2.75	0.43
2:A:130:ASN:HB3	5:N:105:ARG:CZ	2.48	0.43
1:R:65:ALA:O	1:R:68:VAL:HG22	2.18	0.43
3:B:118:ASP:OD1	3:B:118:ASP:N	2.45	0.43
2:A:243:TYR:C	2:A:245:LEU:N	2.75	0.43
3:B:145:TYR:O	3:B:162:GLY:N	2.52	0.43
2:A:159:LYS:HA	2:A:159:LYS:HD2	1.85	0.43
3:B:79:LEU:HD23	3:B:93:ILE:HD12	2.00	0.43
6:S:149:SER:OG	6:S:150:SER:N	2.51	0.43
3:B:247:ASP:HB3	3:B:249:THR:OG1	2.19	0.43
6:S:12:VAL:HB	6:S:119:VAL:HG22	2.01	0.43
1:R:107:ALA:HB1	1:R:108:PRO:CD	2.49	0.42
1:R:267:CYS:SG	1:R:309:ASN:HB2	2.59	0.42
6:S:126:ILE:HD11	6:S:151:LYS:HE3	2.00	0.42
1:R:271:PHE:O	1:R:272:HIS:C	2.58	0.42
3:B:283:ARG:NH1	3:B:298:ASP:OD1	2.53	0.42
3:B:210:LEU:HD11	3:B:255:LEU:HD22	2.00	0.42
6:S:137:VAL:HG11	6:S:207:LEU:HD22	2.01	0.42
3:B:224:GLY:O	3:B:251:ARG:NH1	2.52	0.42
1:R:276:VAL:N	1:R:277:PRO:CD	2.83	0.42
2:A:27:GLY:HA3	3:B:55:LEU:CD1	2.49	0.42
6:S:29:PHE:O	6:S:72:ARG:NH2	2.53	0.42
1:R:143:LEU:HD21	1:R:152:ILE:HD11	2.02	0.41
5:N:50:ASP:N	5:N:50:ASP:OD1	2.51	0.41
6:S:40:ALA:HB3	6:S:43:LYS:HB2	2.03	0.41
1:R:149:LEU:HD13	2:A:79:VAL:HG11	2.01	0.41
1:R:216:ILE:O	1:R:217:PHE:C	2.61	0.41
1:R:225:LEU:HA	1:R:225:LEU:HD13	1.81	0.41
1:R:206:HIS:CE1	7:R:901:ADP:H2'	2.52	0.41
2:A:130:ASN:O	5:N:105:ARG:NH2	2.54	0.41
3:B:249:THR:HG22	3:B:265:SER:HB3	2.02	0.41
3:B:290:ASP:OD1	3:B:314:ARG:NE	2.54	0.41
3:B:270:ILE:HG22	5:N:103:PHE:CE2	2.55	0.41
3:B:274:THR:OG1	3:B:315:VAL:O	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:62:ASN:HB3	1:R:90:LEU:CD2	2.50	0.41
1:R:107:ALA:HB1	1:R:108:PRO:HD2	2.03	0.41
1:R:164:SER:O	1:R:168:TRP:HD1	2.03	0.41
3:B:205:ASP:OD1	3:B:205:ASP:N	2.53	0.41
1:R:104:SER:O	1:R:105:HIS:HB2	2.20	0.41
1:R:48:PRO:O	1:R:52:THR:HG23	2.21	0.41
2:A:93:ARG:NH2	2:A:124:ASP:OD1	2.53	0.41
2:A:243:TYR:C	2:A:245:LEU:H	2.27	0.41
3:B:129:ARG:C	3:B:131:GLY:H	2.28	0.41
1:R:60:LEU:O	1:R:64:LEU:HG	2.20	0.41
5:N:87:LYS:C	5:N:89:GLU:H	2.29	0.41
1:R:46:VAL:C	1:R:48:PRO:CD	2.94	0.41
1:R:171:LEU:HD13	1:R:171:LEU:HA	1.89	0.41
6:S:166:LEU:HB2	6:S:176:LEU:HD11	2.03	0.41
1:R:92:MET:HB3	1:R:310:ILE:HD12	2.03	0.40
1:R:109:TRP:O	1:R:111:LEU:N	2.54	0.40
1:R:191:VAL:HG12	1:R:197:LEU:HD11	2.03	0.40
5:N:34:MET:HE3	5:N:34:MET:HB2	1.77	0.40
5:N:86:LEU:HD23	5:N:86:LEU:HA	1.86	0.40
1:R:177:PRO:HG2	1:R:205:TRP:CZ2	2.56	0.40
3:B:150:ARG:HA	3:B:150:ARG:HD3	1.92	0.40
6:S:52:SER:HB3	6:S:57:THR:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	R	259/915 (28%)	241 (93%)	15 (6%)	3 (1%)	10	40
2	A	222/323 (69%)	214 (96%)	8 (4%)	0	100	100
3	B	335/351 (95%)	318 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	49/68 (72%)	48 (98%)	1 (2%)	0	100	100
5	N	126/137 (92%)	123 (98%)	3 (2%)	0	100	100
6	S	227/260 (87%)	216 (95%)	11 (5%)	0	100	100
All	All	1218/2054 (59%)	1160 (95%)	55 (4%)	3 (0%)	44	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	37	PRO
1	R	277	PRO
1	R	200	PRO

5.3.2 Protein sidechains ⓘ

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	R	242/792 (31%)	238 (98%)	4 (2%)	53	78
2	A	200/272 (74%)	200 (100%)	0	100	100
3	B	280/293 (96%)	280 (100%)	0	100	100
4	G	42/56 (75%)	42 (100%)	0	100	100
5	N	106/114 (93%)	106 (100%)	0	100	100
6	S	196/209 (94%)	196 (100%)	0	100	100
All	All	1066/1736 (61%)	1062 (100%)	4 (0%)	81	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	225	LEU
1	R	275	ARG
1	R	301	THR
1	R	310	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	105	HIS
1	R	151	ASN
1	R	206	HIS
1	R	210	ASN
1	R	211	ASN
1	R	284	ASN
2	A	214	HIS
3	B	175	GLN
3	B	225	HIS
3	B	340	ASN
4	G	18	GLN
5	N	5	GLN
5	N	77	ASN
6	S	77	ASN
6	S	182	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	R	901	-	27,29,29	0.48	0	42,45,45	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	R	901	-	-	6/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	901	ADP	C5'-O5'-PA-O2A
7	R	901	ADP	PA-O3A-PB-O1B
7	R	901	ADP	PB-O3A-PA-O1A
7	R	901	ADP	C5'-O5'-PA-O3A
7	R	901	ADP	C5'-O5'-PA-O1A
7	R	901	ADP	PB-O3A-PA-O2A

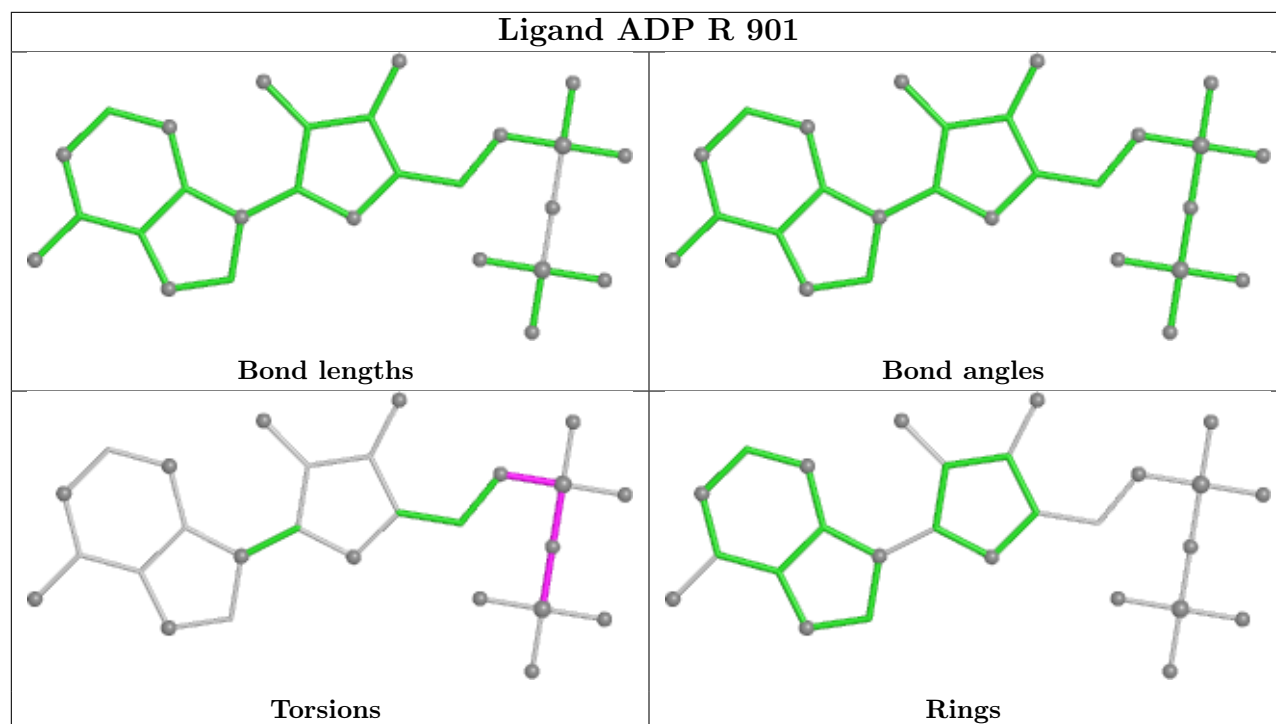
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	901	ADP	2	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 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.

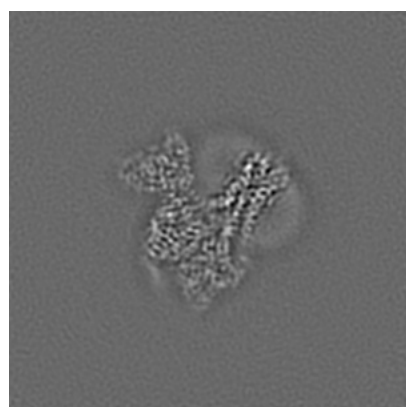
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69904. These allow visual inspection of the internal detail of the map and identification of artifacts.

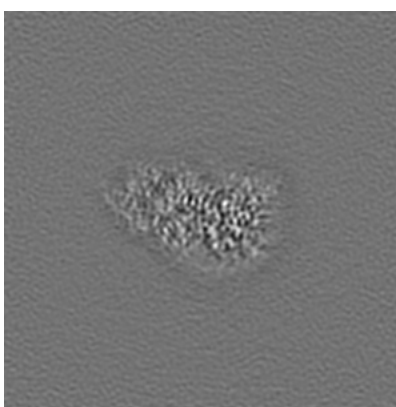
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

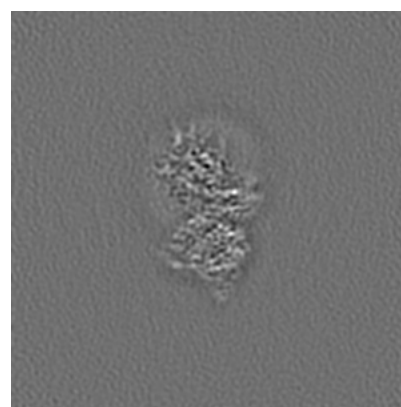
6.1.1 Primary map



X



Y

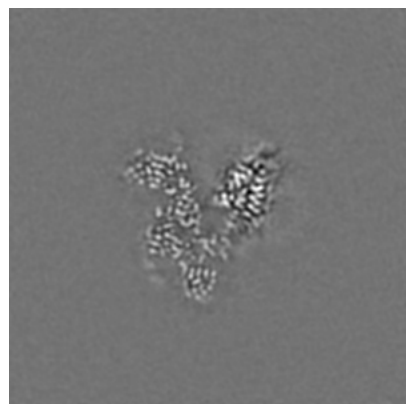


Z

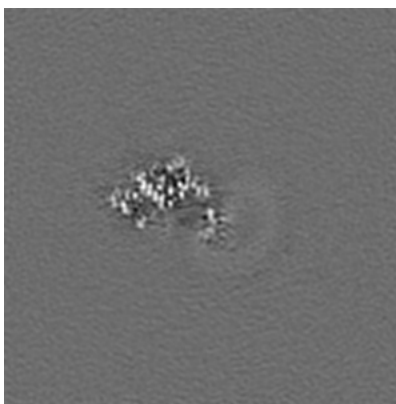
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

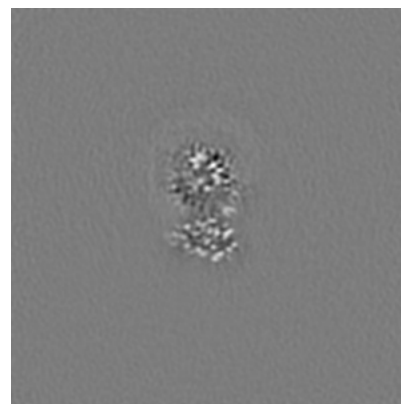
6.2.1 Primary map



X Index: 140



Y Index: 140

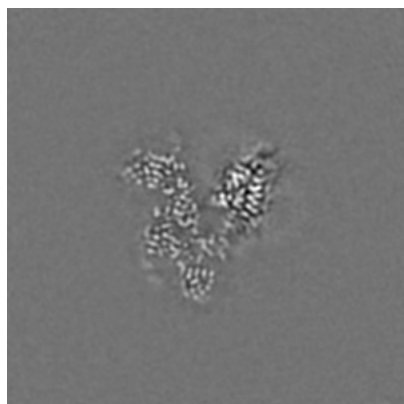


Z Index: 140

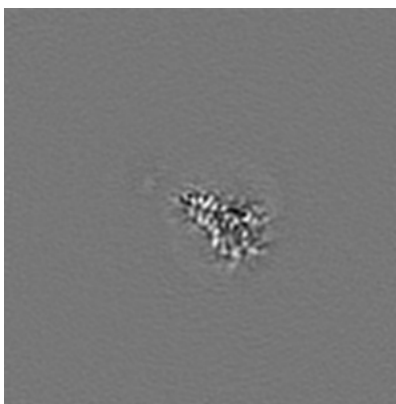
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

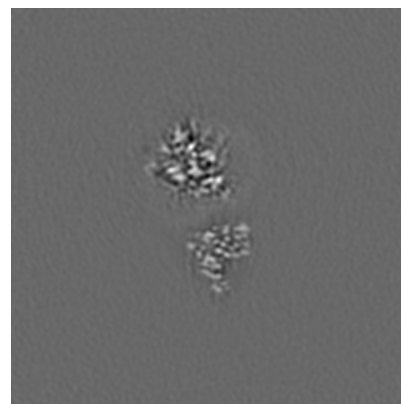
6.3.1 Primary map



X Index: 140



Y Index: 170

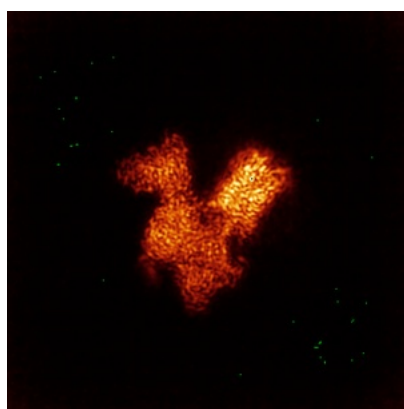


Z Index: 159

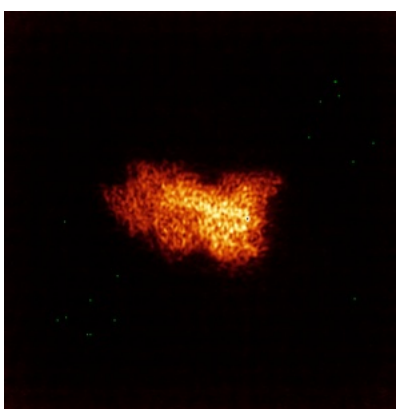
The images above show the largest variance slices of the map in three orthogonal directions.

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

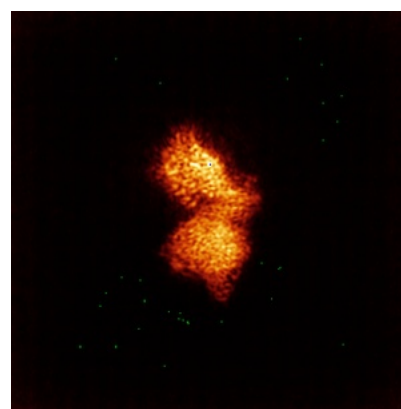
6.4.1 Primary map



X



Y

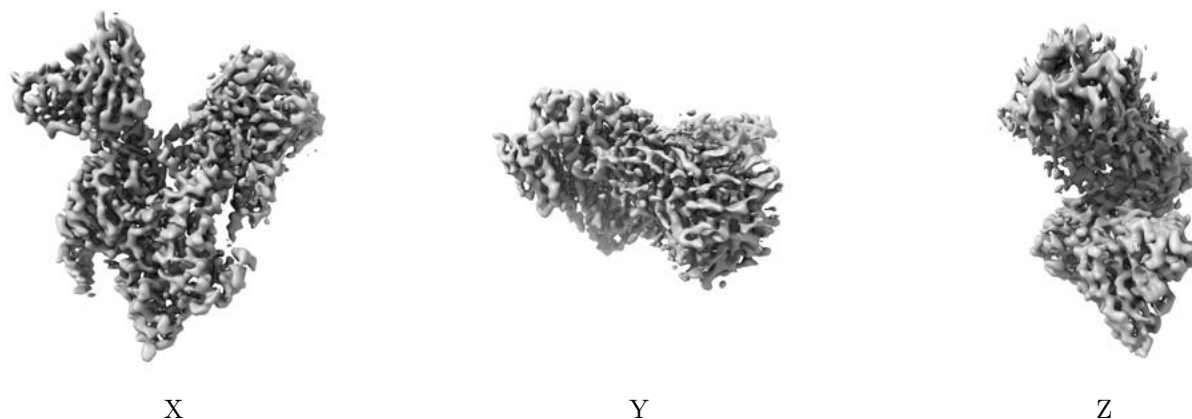


Z

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

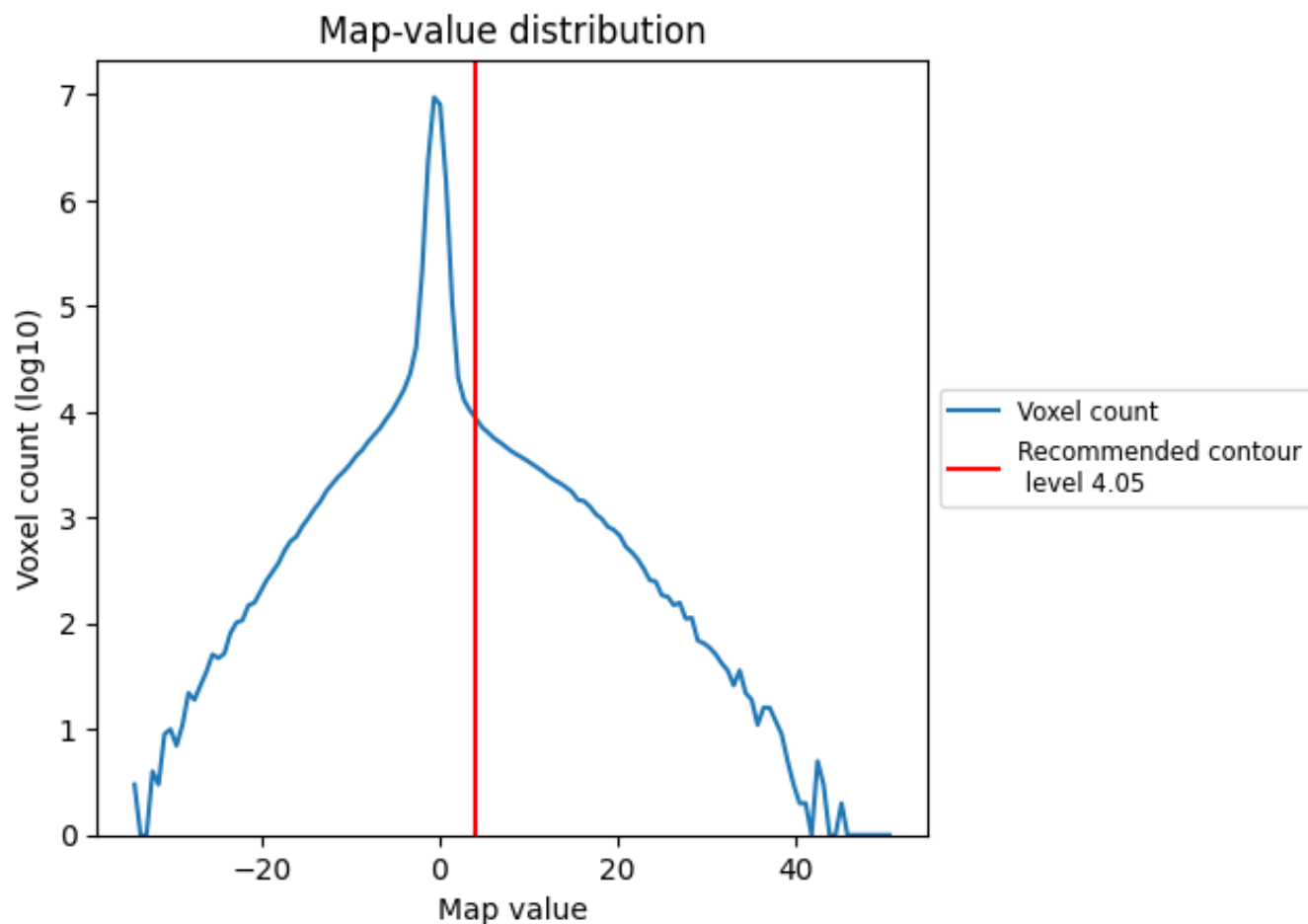
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

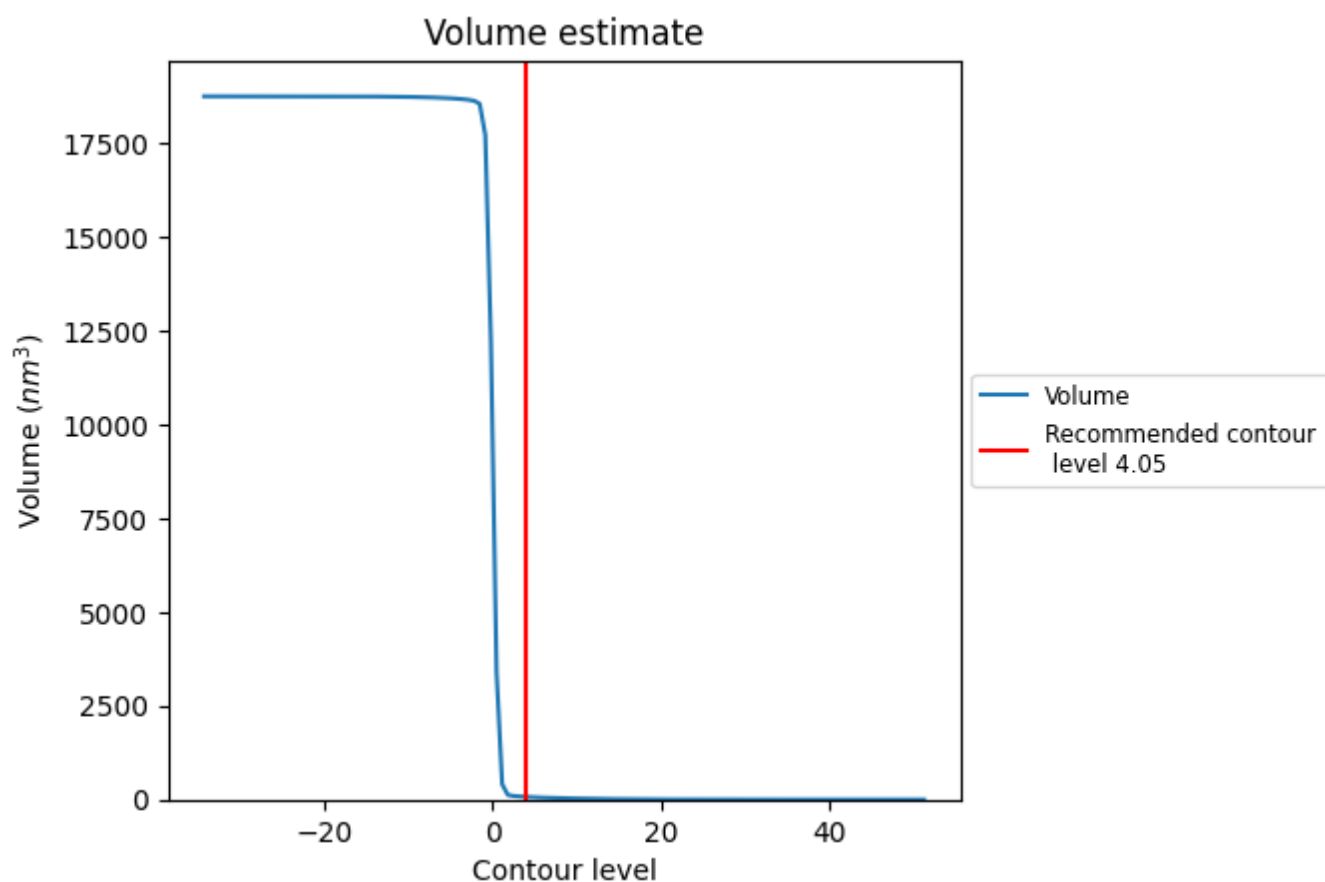
This section contains the results of statistical analysis of the map.

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.

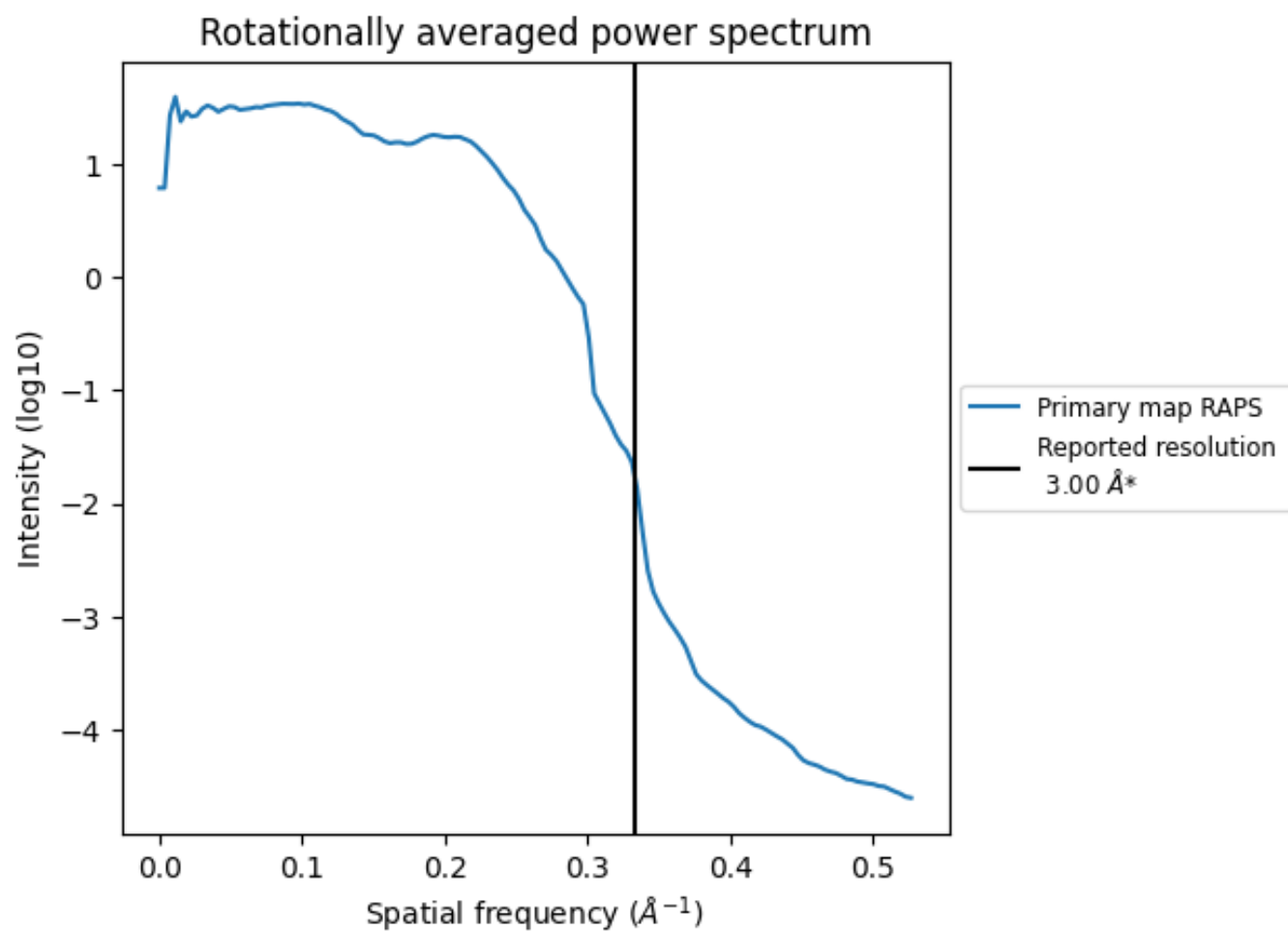
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm^3 ; this corresponds to an approximate mass of 63 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 0.333 Å⁻¹

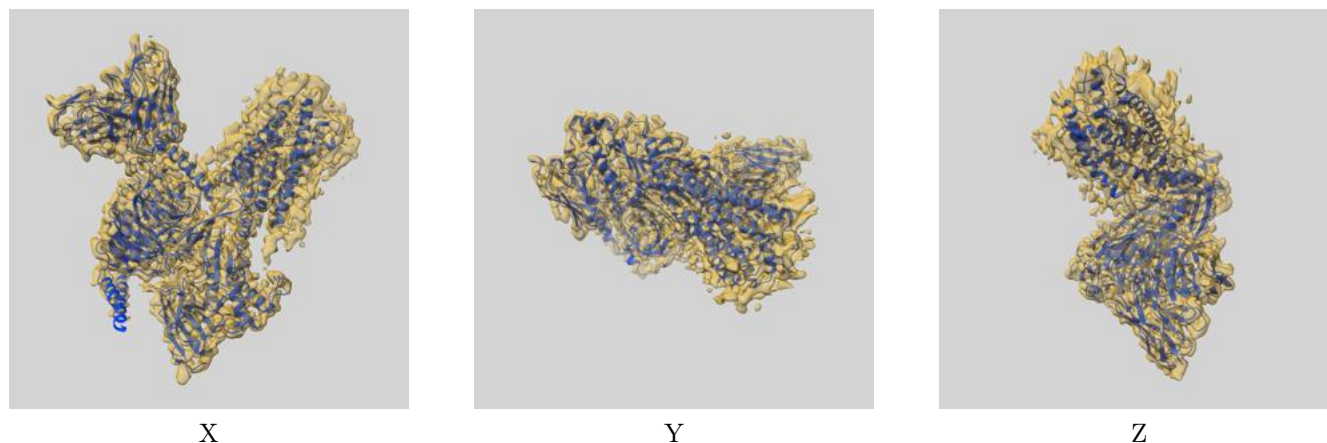
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

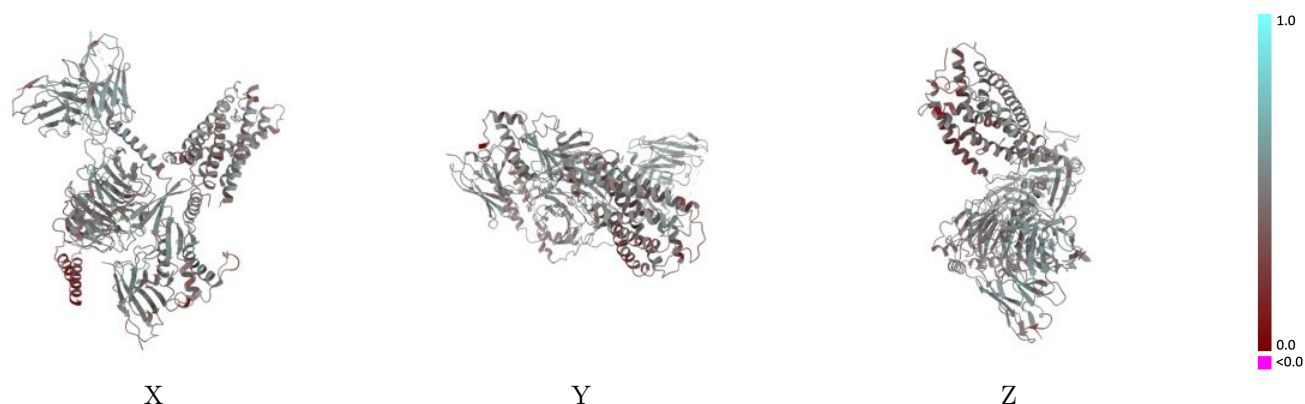
This section contains information regarding the fit between EMDB map EMD-69904 and PDB model 24XY. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



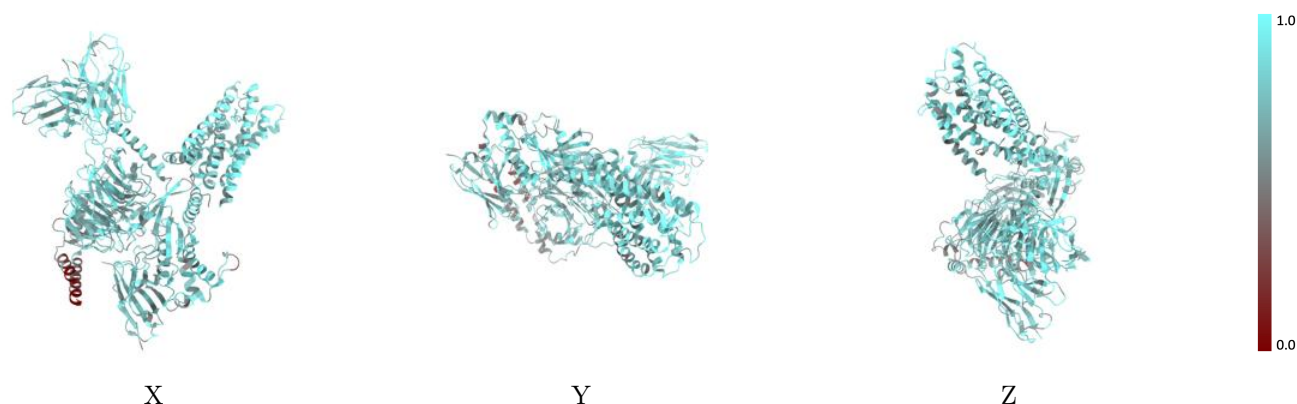
The images above show the 3D surface view of the map at the recommended contour level 4.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



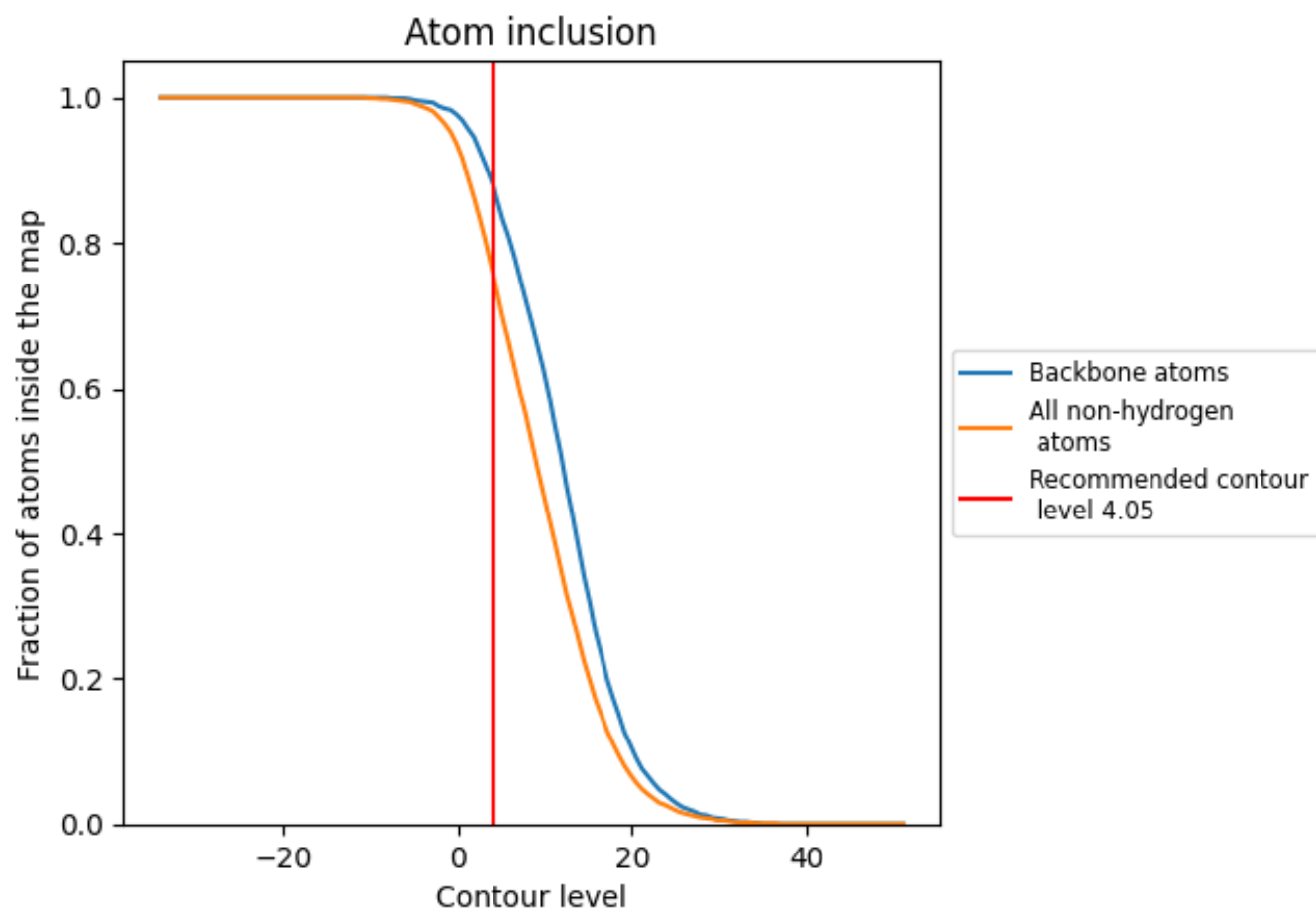
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 76% 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 (4.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7560	<div><div></div></div> 0.4550
A	<div><div></div></div> 0.7570	<div><div></div></div> 0.4680
B	<div><div></div></div> 0.7240	<div><div></div></div> 0.4430
G	<div><div></div></div> 0.5320	<div><div></div></div> 0.3700
N	<div><div></div></div> 0.7560	<div><div></div></div> 0.4820
R	<div><div></div></div> 0.7950	<div><div></div></div> 0.4210
S	<div><div></div></div> 0.8060	<div><div></div></div> 0.5050

1.0

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