Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:04 AM UTC

PDB ID	:	9PXV / pdb_00009pxv
EMDB ID	:	EMD-72002
Title	:	Nucleotide-free naloxone-mu opioid receptor Gi1 complex
Authors	:	Gati, C.; Han, G.W.; Khan, S.
Deposited on	:	2025-08-06
Resolution	:	3.02 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:

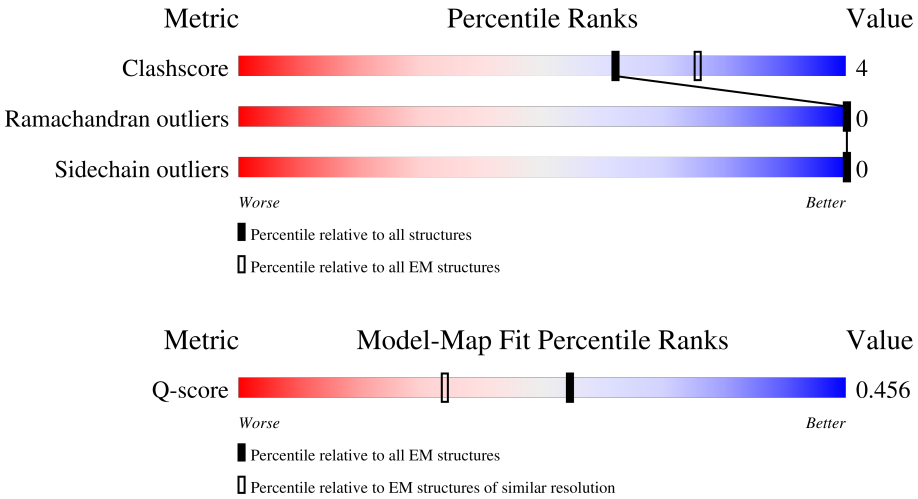
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 (i)

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

The reported resolution of this entry is 3.02 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.



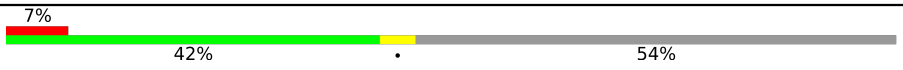
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13913 (2.52 - 3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	354	18% 57% 7% 36%
2	B	361	9% 75% 18% 7%
3	C	71	28% 69% 8% 23%
4	E	259	8% 82% 7% 10%

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Mol	Chain	Length	Quality of chain
5	R	622	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8966 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
1	A	225	Total	C	N	O	S	0	0
			1810	1151	300	346	13		

- 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
2	B	335	Total	C	N	O	S	0	0
			2572	1587	464	500	21		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP P62873
B	-19	HIS	-	expression tag	UNP P62873
B	-18	HIS	-	expression tag	UNP P62873
B	-17	HIS	-	expression tag	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	55	Total	C	N	O	S	0	0
			428	268	76	81	3		

- Molecule 4 is a protein called ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	232	Total	C	N	O	S	0	0
			1782	1131	295	346	10		

- Molecule 5 is a protein called Soluble cytochrome b562,Mu-type opioid receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	286	Total	C	N	O	S	0	0
			2294	1522	367	381	24		

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-169	MET	-	expression tag	UNP P0ABE7
R	-168	LYS	-	expression tag	UNP P0ABE7
R	-167	THR	-	expression tag	UNP P0ABE7
R	-166	ILE	-	expression tag	UNP P0ABE7
R	-165	ILE	-	expression tag	UNP P0ABE7
R	-164	ALA	-	expression tag	UNP P0ABE7
R	-163	LEU	-	expression tag	UNP P0ABE7
R	-162	SER	-	expression tag	UNP P0ABE7
R	-161	TYR	-	expression tag	UNP P0ABE7
R	-160	ILE	-	expression tag	UNP P0ABE7
R	-159	PHE	-	expression tag	UNP P0ABE7
R	-158	CYS	-	expression tag	UNP P0ABE7
R	-157	LEU	-	expression tag	UNP P0ABE7
R	-156	VAL	-	expression tag	UNP P0ABE7
R	-155	PHE	-	expression tag	UNP P0ABE7
R	-154	ALA	-	expression tag	UNP P0ABE7
R	-153	ASP	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-152	TYR	-	expression tag	UNP P0ABE7
R	-151	LYS	-	expression tag	UNP P0ABE7
R	-150	ASP	-	expression tag	UNP P0ABE7
R	-149	HIS	-	expression tag	UNP P0ABE7
R	-148	ASP	-	expression tag	UNP P0ABE7
R	-147	GLY	-	expression tag	UNP P0ABE7
R	-146	ASP	-	expression tag	UNP P0ABE7
R	-145	TYR	-	expression tag	UNP P0ABE7
R	-144	LYS	-	expression tag	UNP P0ABE7
R	-143	ASP	-	expression tag	UNP P0ABE7
R	-142	HIS	-	expression tag	UNP P0ABE7
R	-141	ASP	-	expression tag	UNP P0ABE7
R	-140	ILE	-	expression tag	UNP P0ABE7
R	-139	ASP	-	expression tag	UNP P0ABE7
R	-138	TYR	-	expression tag	UNP P0ABE7
R	-137	LYS	-	expression tag	UNP P0ABE7
R	-136	ASP	-	expression tag	UNP P0ABE7
R	-135	ASP	-	expression tag	UNP P0ABE7
R	-134	ASP	-	expression tag	UNP P0ABE7
R	-133	ASP	-	expression tag	UNP P0ABE7
R	-132	LYS	-	expression tag	UNP P0ABE7
R	-131	LEU	-	expression tag	UNP P0ABE7
R	-130	HIS	-	expression tag	UNP P0ABE7
R	-129	HIS	-	expression tag	UNP P0ABE7
R	-128	HIS	-	expression tag	UNP P0ABE7
R	-127	HIS	-	expression tag	UNP P0ABE7
R	-126	HIS	-	expression tag	UNP P0ABE7
R	-125	HIS	-	expression tag	UNP P0ABE7
R	-124	HIS	-	expression tag	UNP P0ABE7
R	-123	HIS	-	expression tag	UNP P0ABE7
R	-122	HIS	-	expression tag	UNP P0ABE7
R	-121	HIS	-	expression tag	UNP P0ABE7
R	-120	LEU	-	expression tag	UNP P0ABE7
R	-119	GLU	-	expression tag	UNP P0ABE7
R	-118	VAL	-	expression tag	UNP P0ABE7
R	-117	LEU	-	expression tag	UNP P0ABE7
R	-116	PHE	-	expression tag	UNP P0ABE7
R	-115	GLN	-	expression tag	UNP P0ABE7
R	-114	GLY	-	expression tag	UNP P0ABE7
R	-113	PRO	-	expression tag	UNP P0ABE7
R	-112	GLY	-	expression tag	UNP P0ABE7
R	-111	SER	-	expression tag	UNP P0ABE7

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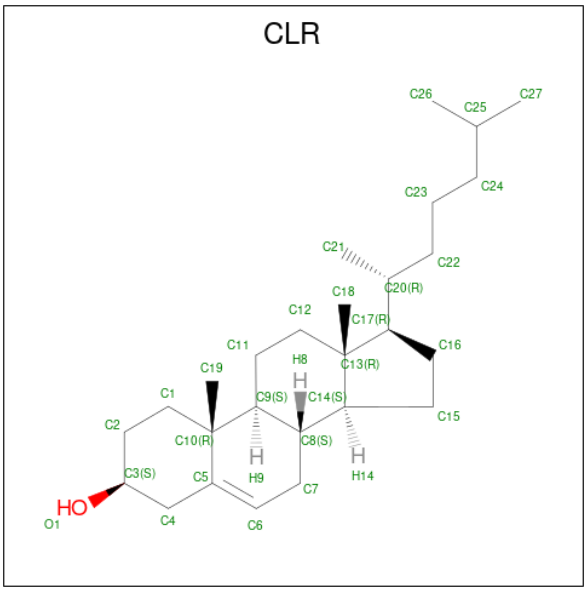
Chain	Residue	Modelled	Actual	Comment	Reference
R	-110	GLY	-	expression tag	UNP P0ABE7
R	-109	SER	-	expression tag	UNP P0ABE7
R	-102	TRP	MET	conflict	UNP P0ABE7
R	-7	ILE	-	linker	UNP P0ABE7
R	-6	GLN	-	linker	UNP P0ABE7
R	-5	LYS	-	linker	UNP P0ABE7
R	-4	TYR	-	linker	UNP P0ABE7
R	-3	LEU	-	linker	UNP P0ABE7
R	-2	GLY	-	linker	UNP P0ABE7
R	-1	THR	-	linker	UNP P0ABE7
R	0	GLY	-	linker	UNP P0ABE7
R	1	SER	-	linker	UNP P0ABE7
R	401	ALA	-	expression tag	UNP P35372
R	402	ALA	-	expression tag	UNP P35372
R	403	ALA	-	expression tag	UNP P35372
R	404	LEU	-	expression tag	UNP P35372
R	405	GLU	-	expression tag	UNP P35372
R	406	VAL	-	expression tag	UNP P35372
R	407	LEU	-	expression tag	UNP P35372
R	408	PHE	-	expression tag	UNP P35372
R	409	GLN	-	expression tag	UNP P35372
R	410	GLY	-	expression tag	UNP P35372
R	411	PRO	-	expression tag	UNP P35372
R	412	GLY	-	expression tag	UNP P35372
R	413	SER	-	expression tag	UNP P35372
R	414	TRP	-	expression tag	UNP P35372
R	415	SER	-	expression tag	UNP P35372
R	416	HIS	-	expression tag	UNP P35372
R	417	PRO	-	expression tag	UNP P35372
R	418	GLN	-	expression tag	UNP P35372
R	419	PHE	-	expression tag	UNP P35372
R	420	GLU	-	expression tag	UNP P35372
R	421	LYS	-	expression tag	UNP P35372
R	422	GLY	-	expression tag	UNP P35372
R	423	GLY	-	expression tag	UNP P35372
R	424	GLY	-	expression tag	UNP P35372
R	425	SER	-	expression tag	UNP P35372
R	426	GLY	-	expression tag	UNP P35372
R	427	GLY	-	expression tag	UNP P35372
R	428	GLY	-	expression tag	UNP P35372
R	429	SER	-	expression tag	UNP P35372
R	430	GLY	-	expression tag	UNP P35372

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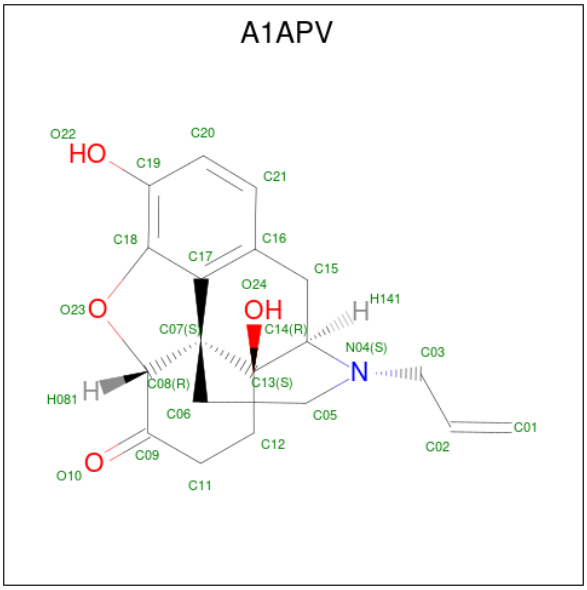
Chain	Residue	Modelled	Actual	Comment	Reference
R	431	GLY	-	expression tag	UNP P35372
R	432	SER	-	expression tag	UNP P35372
R	433	SER	-	expression tag	UNP P35372
R	434	ALA	-	expression tag	UNP P35372
R	435	TRP	-	expression tag	UNP P35372
R	436	SER	-	expression tag	UNP P35372
R	437	HIS	-	expression tag	UNP P35372
R	438	PRO	-	expression tag	UNP P35372
R	439	GLN	-	expression tag	UNP P35372
R	440	PHE	-	expression tag	UNP P35372
R	441	GLU	-	expression tag	UNP P35372
R	442	LYS	-	expression tag	UNP P35372
R	443	HIS	-	expression tag	UNP P35372
R	444	HIS	-	expression tag	UNP P35372
R	445	HIS	-	expression tag	UNP P35372
R	446	HIS	-	expression tag	UNP P35372
R	447	HIS	-	expression tag	UNP P35372
R	448	HIS	-	expression tag	UNP P35372
R	449	HIS	-	expression tag	UNP P35372
R	450	HIS	-	expression tag	UNP P35372
R	451	HIS	-	expression tag	UNP P35372
R	452	HIS	-	expression tag	UNP P35372

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 7 is Naloxone (CCD ID: A1APV) (formula: $C_{19}H_{21}NO_4$) (labeled as "Ligand of Interest" by depositor).



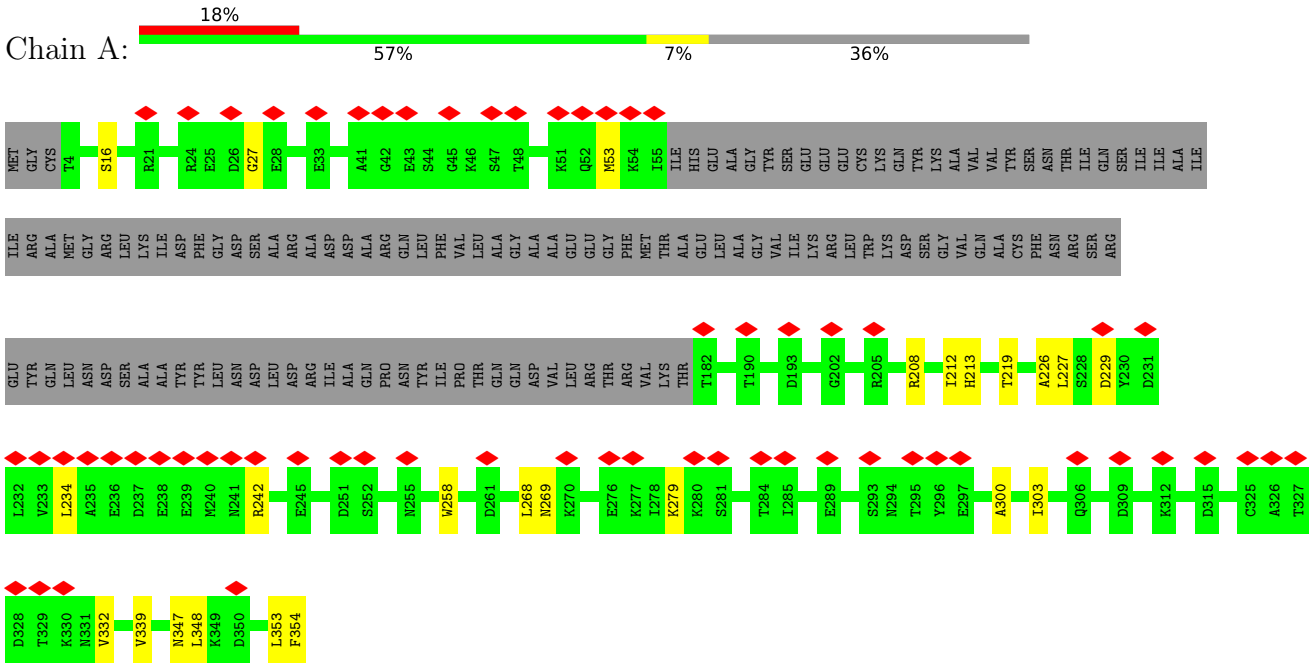
Mol	Chain	Residues	Atoms	AltConf
7	R	1	Total C N O 24 19 1 4	0

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.

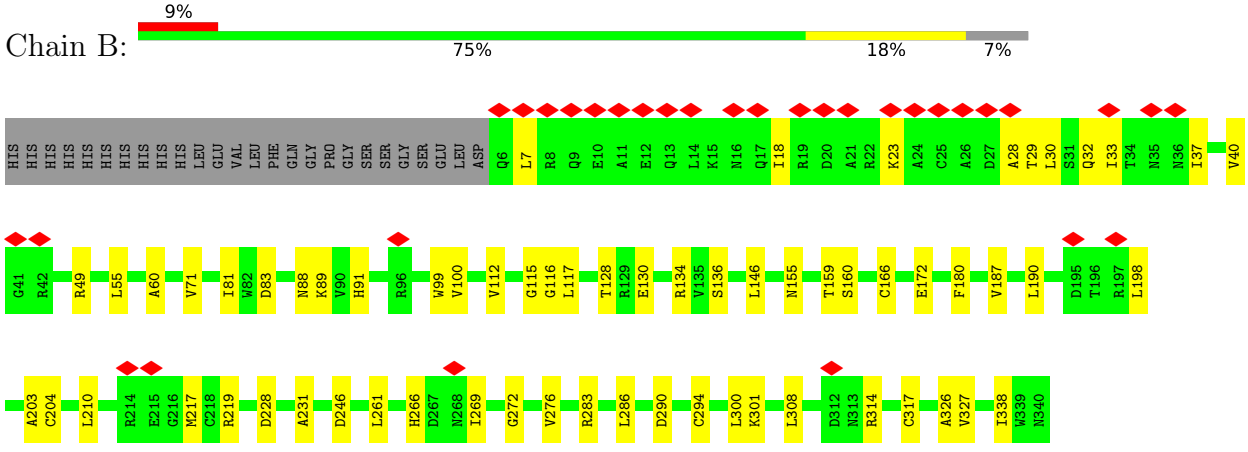
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



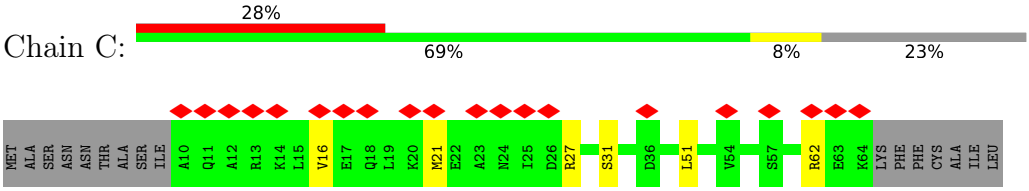
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



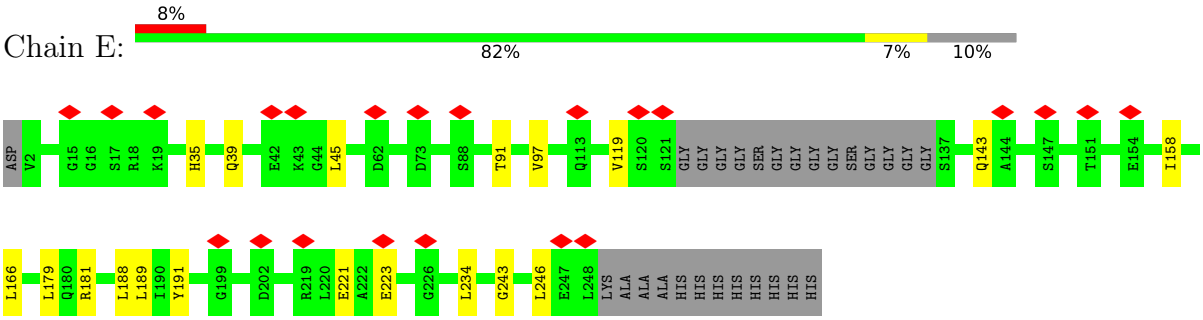
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:



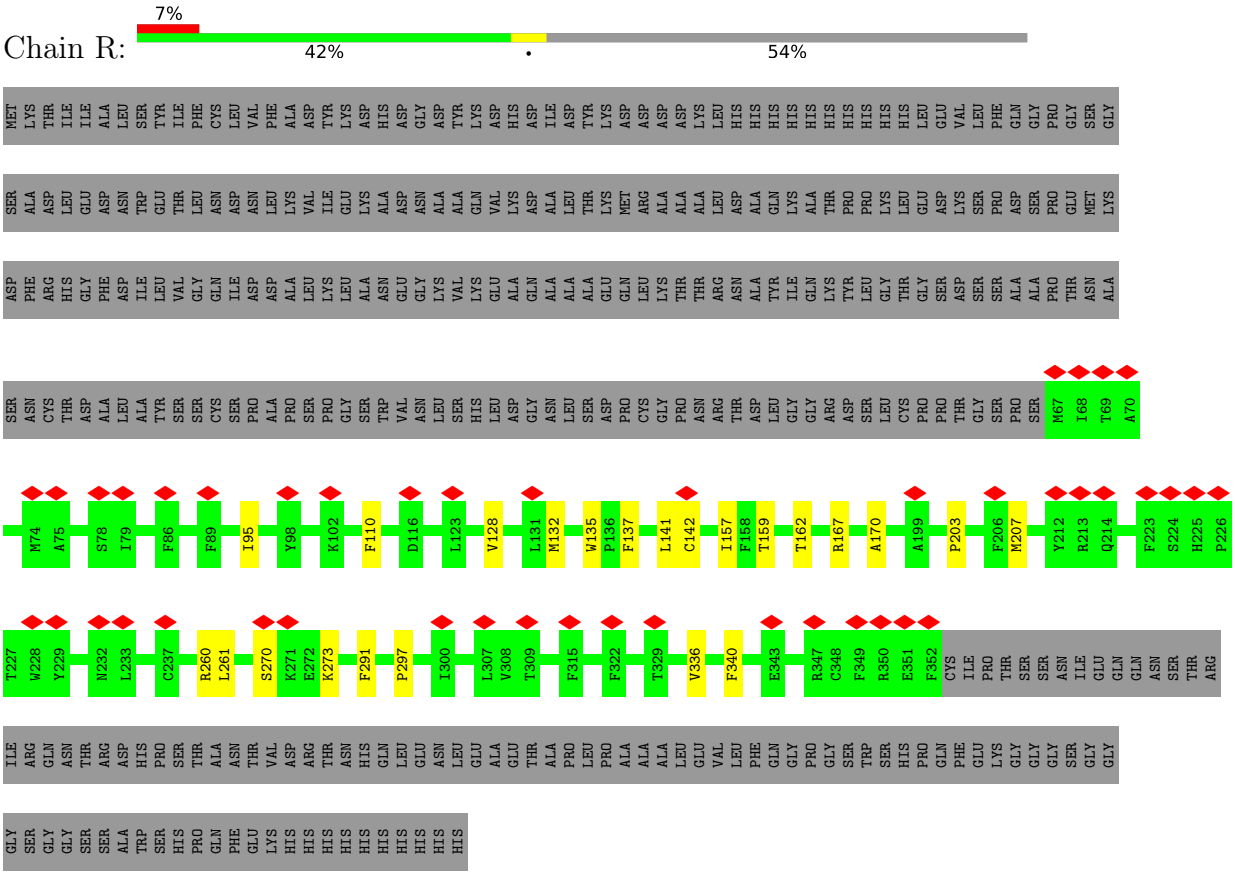
• Molecule 4: ScFv16

Chain E:



• Molecule 5: Soluble cytochrome b562,Mu-type opioid receptor

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	216557	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.608	Depositor
Minimum map value	-1.197	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	331.264, 331.264, 331.264	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.294, 1.294, 1.294	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1APV, CLR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.16	0/1840	0.34	0/2468
2	B	0.20	0/2619	0.41	0/3550
3	C	0.15	0/434	0.35	0/584
4	E	0.18	0/1826	0.38	0/2476
5	R	0.20	0/2352	0.42	0/3205
All	All	0.19	0/9071	0.39	0/12283

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

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	1810	0	1799	17	0
2	B	2572	0	2480	40	0
3	C	428	0	439	7	0
4	E	1782	0	1714	10	0
5	R	2294	0	2381	14	0
6	R	56	0	92	1	0
7	R	24	0	0	0	0
All	All	8966	0	8905	76	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (76) 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:146:LEU:HD11	2:B:159:THR:HB	1.76	0.67
2:B:286:LEU:HD22	2:B:327:VAL:HG11	1.80	0.63
5:R:137:PHE:HB3	5:R:141:LEU:HD23	1.80	0.62
2:B:166:CYS:HB2	2:B:180:PHE:HB2	1.83	0.60
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.83	0.60
4:E:39:GLN:HB2	4:E:45:LEU:HD23	1.83	0.60
4:E:188:LEU:HD21	4:E:191:TYR:HB3	1.83	0.59
1:A:348:LEU:HB3	1:A:354:PHE:HB2	1.85	0.59
2:B:155:ASN:HD21	2:B:172:GLU:HG2	1.68	0.59
5:R:157:ILE:HD12	5:R:291:PHE:HE1	1.67	0.59
2:B:115:GLY:HA3	2:B:146:LEU:HD23	1.85	0.58
1:A:226:ALA:HA	1:A:269:ASN:HB2	1.85	0.57
4:E:143:GLN:HG3	4:E:243:GLY:H	1.71	0.56
2:B:30:LEU:HD12	2:B:261:LEU:HD22	1.87	0.55
2:B:290:ASP:HA	2:B:314:ARG:HG3	1.88	0.55
2:B:100:VAL:HA	2:B:116:GLY:HA3	1.87	0.55
2:B:294:CYS:HB2	2:B:308:LEU:HB2	1.88	0.54
2:B:283:ARG:HD3	3:C:51:LEU:HD11	1.90	0.54
2:B:37:ILE:HG22	2:B:301:LYS:HD3	1.90	0.53
1:A:347:ASN:HB3	5:R:170:ALA:HB1	1.90	0.53
5:R:203:PRO:O	5:R:207:MET:HB2	2.09	0.53
2:B:30:LEU:HD21	2:B:300:LEU:HD13	1.91	0.51
4:E:179:LEU:HB2	4:E:189:LEU:HD11	1.93	0.51
1:A:234:LEU:HD13	1:A:242:ARG:HG2	1.93	0.51
2:B:83:ASP:HB3	2:B:88:ASN:HB2	1.92	0.50
5:R:95:ILE:HD13	5:R:110:PHE:HB2	1.92	0.50
2:B:134:ARG:HH12	2:B:136:SER:HB3	1.76	0.49
1:A:229:ASP:HB2	1:A:242:ARG:HB2	1.93	0.49
2:B:198:LEU:HD22	2:B:210:LEU:HD21	1.95	0.48
1:A:16:SER:HB2	2:B:89:LYS:H	1.77	0.48
2:B:49:ARG:HH22	3:C:62:ARG:H	1.62	0.48
2:B:29:THR:HG23	2:B:32:GLN:H	1.78	0.48
2:B:204:CYS:HA	2:B:228:ASP:HB2	1.95	0.48
2:B:187:VAL:HA	2:B:203:ALA:HA	1.96	0.48
1:A:27:GLY:HA3	2:B:55:LEU:HD13	1.96	0.47
4:E:158:ILE:HD11	4:E:246:LEU:HD11	1.97	0.47
2:B:210:LEU:HD22	2:B:219:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:35:HIS:HB2	4:E:97:VAL:HB	1.96	0.47
2:B:231:ALA:HB1	2:B:276:VAL:HG22	1.97	0.46
2:B:23:LYS:HD3	2:B:23:LYS:HA	1.76	0.46
5:R:159:THR:HA	5:R:162:THR:HG22	1.97	0.46
1:A:348:LEU:HD11	5:R:261:LEU:HD21	1.98	0.46
4:E:179:LEU:HD22	4:E:181:ARG:HE	1.81	0.46
2:B:71:VAL:HG21	2:B:112:VAL:HG21	1.97	0.46
2:B:217:MET:HB2	3:C:21:MET:HE1	1.98	0.46
2:B:246:ASP:HA	2:B:272:GLY:HA3	1.99	0.45
2:B:18:ILE:HG23	3:C:27:ARG:HH22	1.82	0.45
2:B:81:ILE:HD13	2:B:91:HIS:HB2	1.97	0.45
1:A:229:ASP:HB2	1:A:242:ARG:HD3	1.98	0.45
2:B:40:VAL:HG13	2:B:283:ARG:HE	1.82	0.45
1:A:300:ALA:HA	1:A:303:ILE:HG22	1.99	0.44
2:B:7:LEU:HG	3:C:16:VAL:HG21	2.00	0.44
2:B:28:ALA:HB3	3:C:31:SER:HB2	1.99	0.44
2:B:217:MET:HE2	3:C:21:MET:HE1	1.99	0.44
5:R:336:VAL:HG23	5:R:340:PHE:HD2	1.83	0.44
1:A:219:THR:HG21	1:A:339:VAL:HG13	2.00	0.43
2:B:99:TRP:HB3	2:B:117:LEU:HD13	2.00	0.43
1:A:227:LEU:HD21	1:A:268:LEU:HD13	2.00	0.43
1:A:353:LEU:HD21	5:R:167:ARG:HD3	2.00	0.43
1:A:213:HIS:HB3	1:A:258:TRP:CE2	2.54	0.43
4:E:91:THR:HB	4:E:119:VAL:H	1.83	0.43
5:R:260:ARG:HD3	5:R:260:ARG:HA	1.87	0.43
5:R:297:PRO:HB3	6:R:502:CLR:H222	2.00	0.42
1:A:53:MET:HG2	1:A:332:VAL:HG12	2.01	0.42
4:E:221:GLU:HG3	4:E:223:GLU:H	1.83	0.42
5:R:270:SER:HB3	5:R:273:LYS:HG3	2.02	0.42
5:R:135:TRP:NE1	5:R:142:CYS:HB3	2.35	0.42
2:B:60:ALA:HA	2:B:317:CYS:HB3	2.01	0.42
2:B:266:HIS:HB3	2:B:269:ILE:HG22	2.02	0.42
1:A:208:ARG:O	1:A:212:ILE:HB	2.21	0.41
4:E:166:LEU:HA	4:E:234:LEU:HD22	2.03	0.41
2:B:326:ALA:HB1	2:B:338:ILE:HG23	2.02	0.41
1:A:279:LYS:HA	1:A:279:LYS:HD2	1.94	0.41
2:B:128:THR:HG22	2:B:130:GLU:H	1.86	0.41
5:R:128:VAL:O	5:R:132:MET:HG3	2.21	0.41
2:B:30:LEU:HA	2:B:33:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/354 (62%)	214 (97%)	7 (3%)	0	100	100
2	B	333/361 (92%)	314 (94%)	19 (6%)	0	100	100
3	C	53/71 (75%)	53 (100%)	0	0	100	100
4	E	228/259 (88%)	219 (96%)	9 (4%)	0	100	100
5	R	284/622 (46%)	275 (97%)	9 (3%)	0	100	100
All	All	1119/1667 (67%)	1075 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/305 (65%)	199 (100%)	0	100	100
2	B	277/301 (92%)	277 (100%)	0	100	100
3	C	45/58 (78%)	45 (100%)	0	100	100
4	E	196/209 (94%)	196 (100%)	0	100	100
5	R	258/539 (48%)	258 (100%)	0	100	100
All	All	975/1412 (69%)	975 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	306	GLN
2	B	16	ASN
2	B	44	GLN
2	B	293	ASN
4	E	82	GLN
5	R	126	GLN
5	R	129	ASN
5	R	185	ASN
5	R	330	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)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	CLR	R	502	-	31,31,31	0.38	0	48,48,48	0.79	0
7	A1APV	R	503	-	28,28,28	1.07	2 (7%)	45,46,46	1.14	3 (6%)
6	CLR	R	501	-	31,31,31	0.41	0	48,48,48	0.73	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	R	502	-	-	3/10/68/68	0/4/4/4
7	A1APV	R	503	-	-	0/3/58/58	0/6/5/5
6	CLR	R	501	-	-	3/10/68/68	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	503	A1APV	C16-C17	-2.37	1.35	1.39
7	R	503	A1APV	C07-C08	-2.12	1.52	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	503	A1APV	O23-C08-C09	3.03	111.02	108.51
7	R	503	A1APV	C06-C07-C08	-2.20	109.61	111.97
6	R	501	CLR	C21-C20-C17	2.14	116.09	112.88
7	R	503	A1APV	C15-C16-C21	2.01	126.96	121.58

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	502	CLR	C17-C20-C22-C23
6	R	501	CLR	C23-C24-C25-C27
6	R	501	CLR	C23-C24-C25-C26
6	R	501	CLR	C22-C23-C24-C25
6	R	502	CLR	C22-C23-C24-C25
6	R	502	CLR	C21-C20-C22-C23

There are no ring outliers.

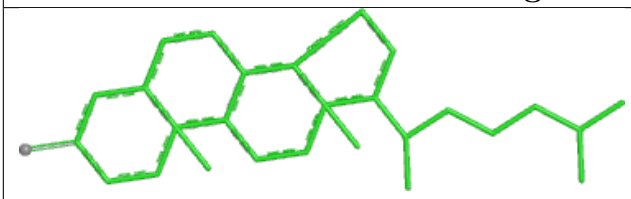
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	502	CLR	1	0

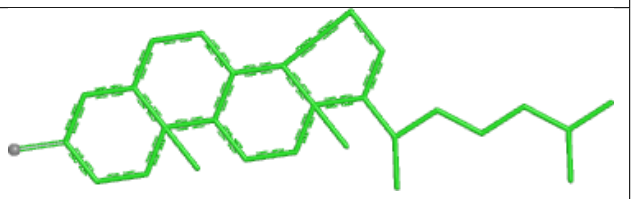
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

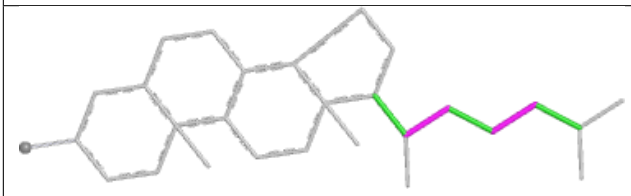
Ligand CLR R 502



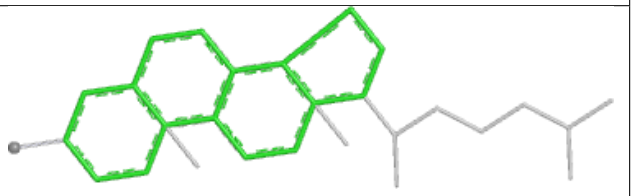
Bond lengths



Bond angles

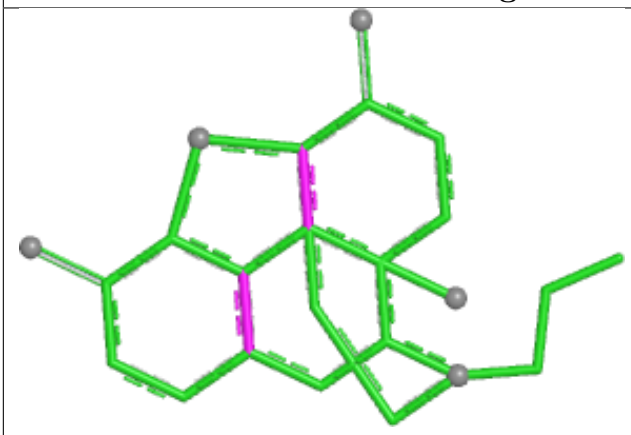


Torsions

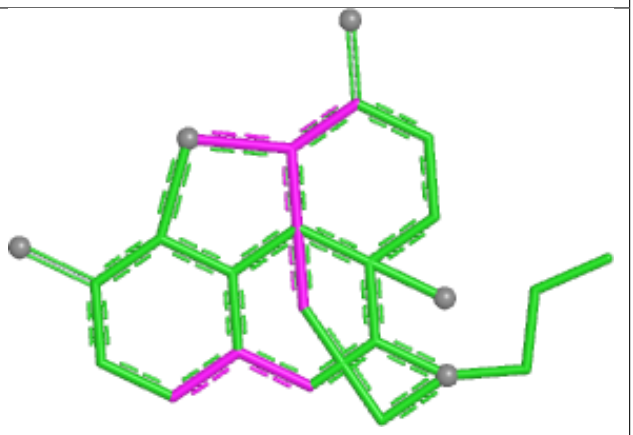


Rings

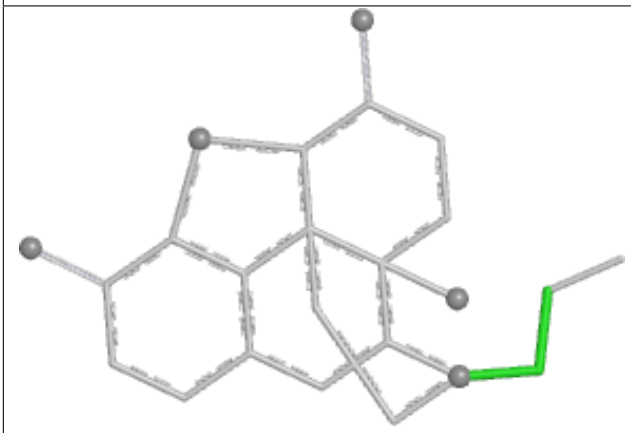
Ligand A1APV R 503



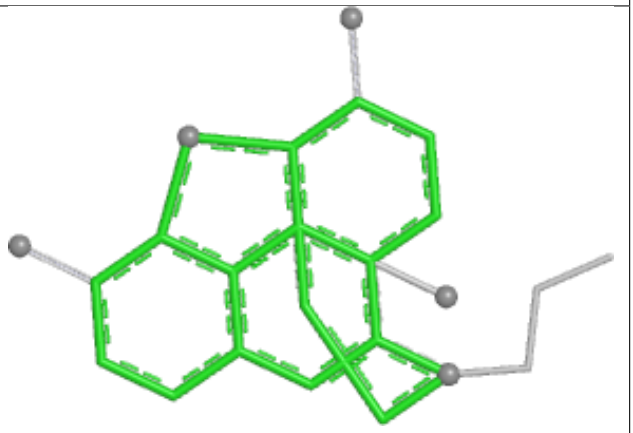
Bond lengths



Bond angles

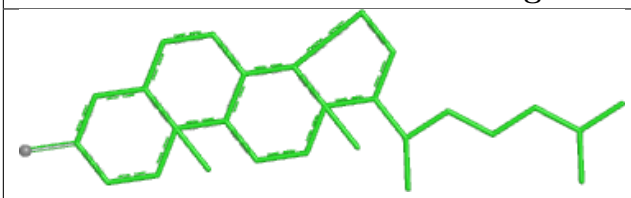


Torsions

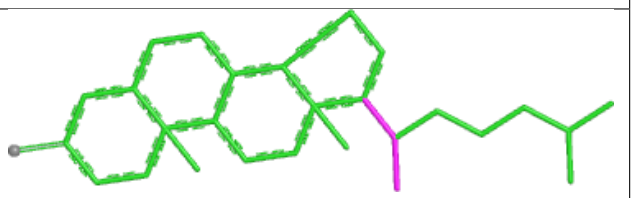


Rings

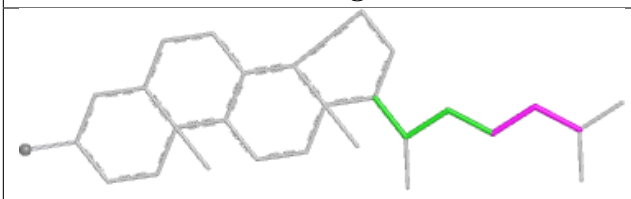
Ligand CLR R 501



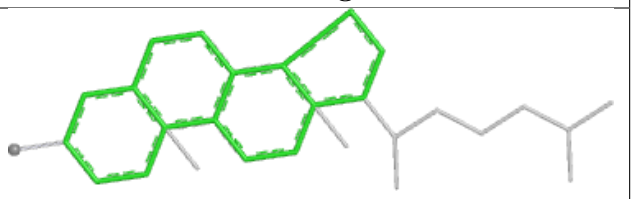
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

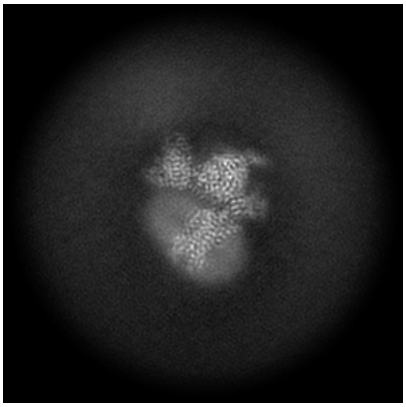
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-72002. These allow visual inspection of the internal detail of the map and identification of artifacts.

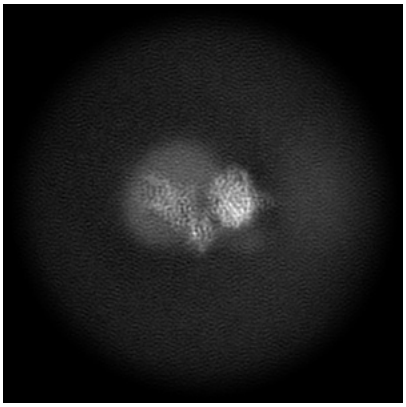
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

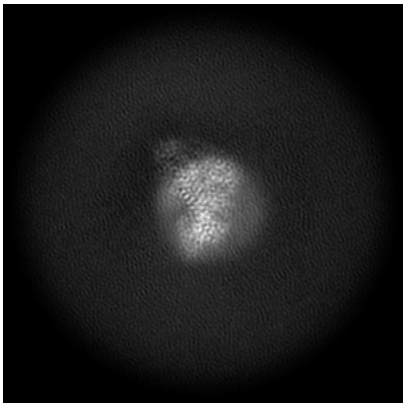
6.1.1 Primary map



X



Y

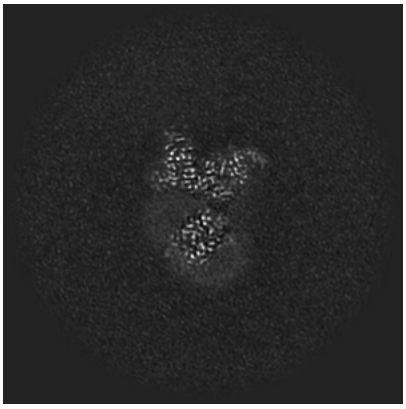


Z

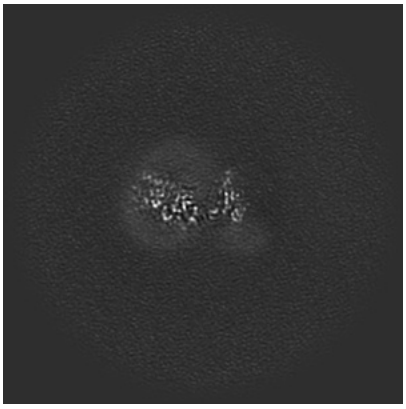
The images above show the map projected in three orthogonal directions.

6.2 Central slices

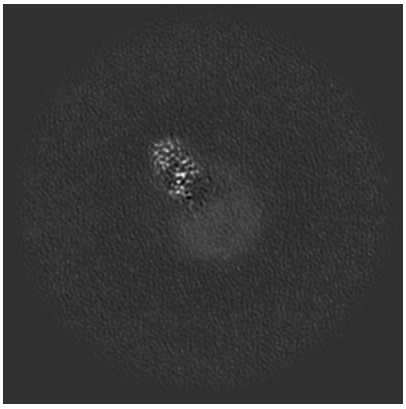
6.2.1 Primary map



X Index: 128



Y Index: 128

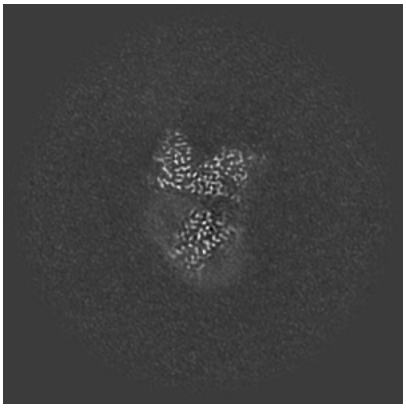


Z Index: 128

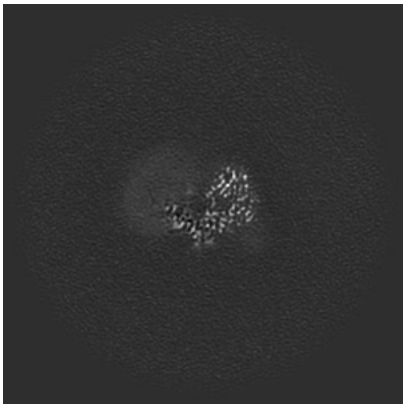
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

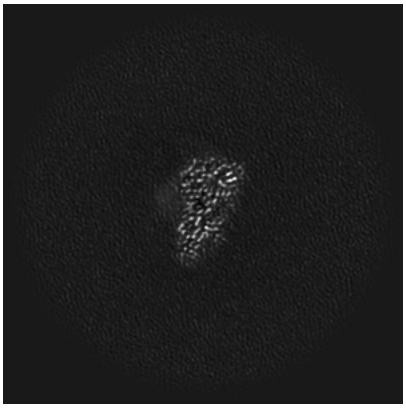
6.3.1 Primary map



X Index: 126



Y Index: 143

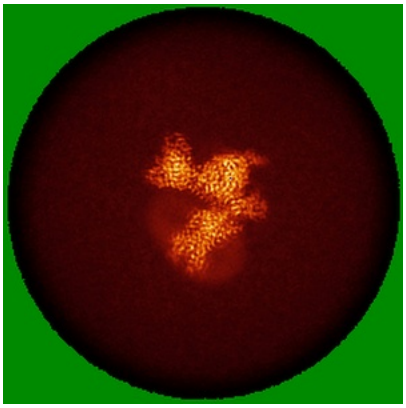


Z Index: 147

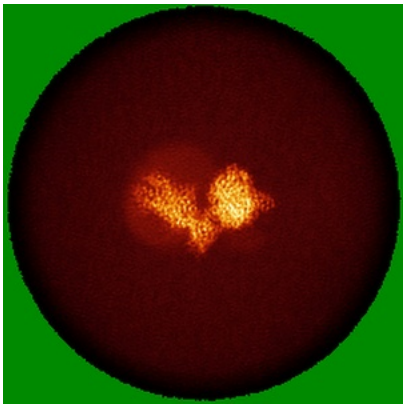
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

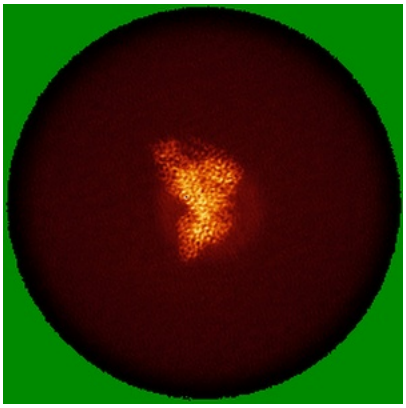
6.4.1 Primary map



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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

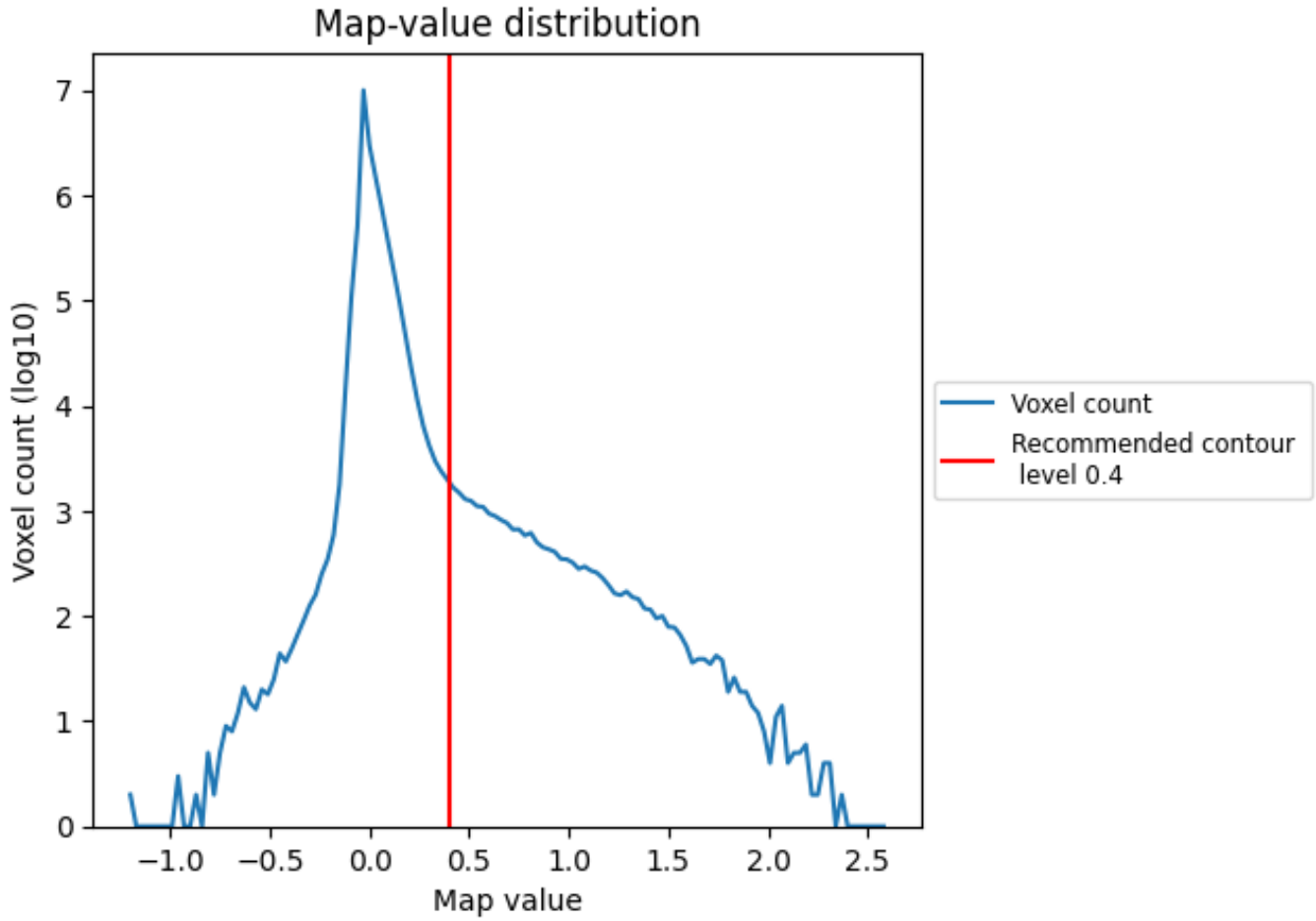
6.6 Mask visualisation (i)

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

7 Map analysis

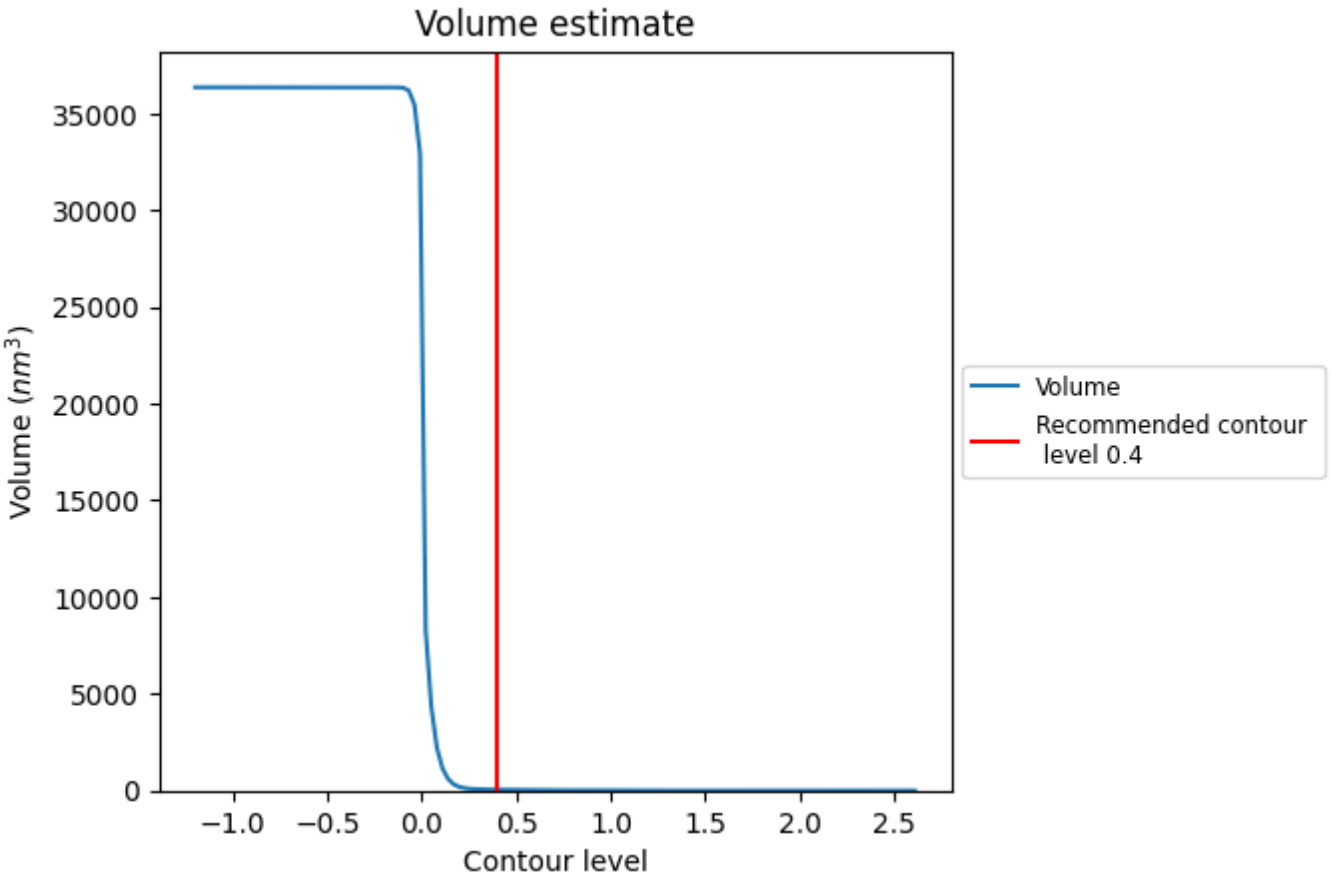
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

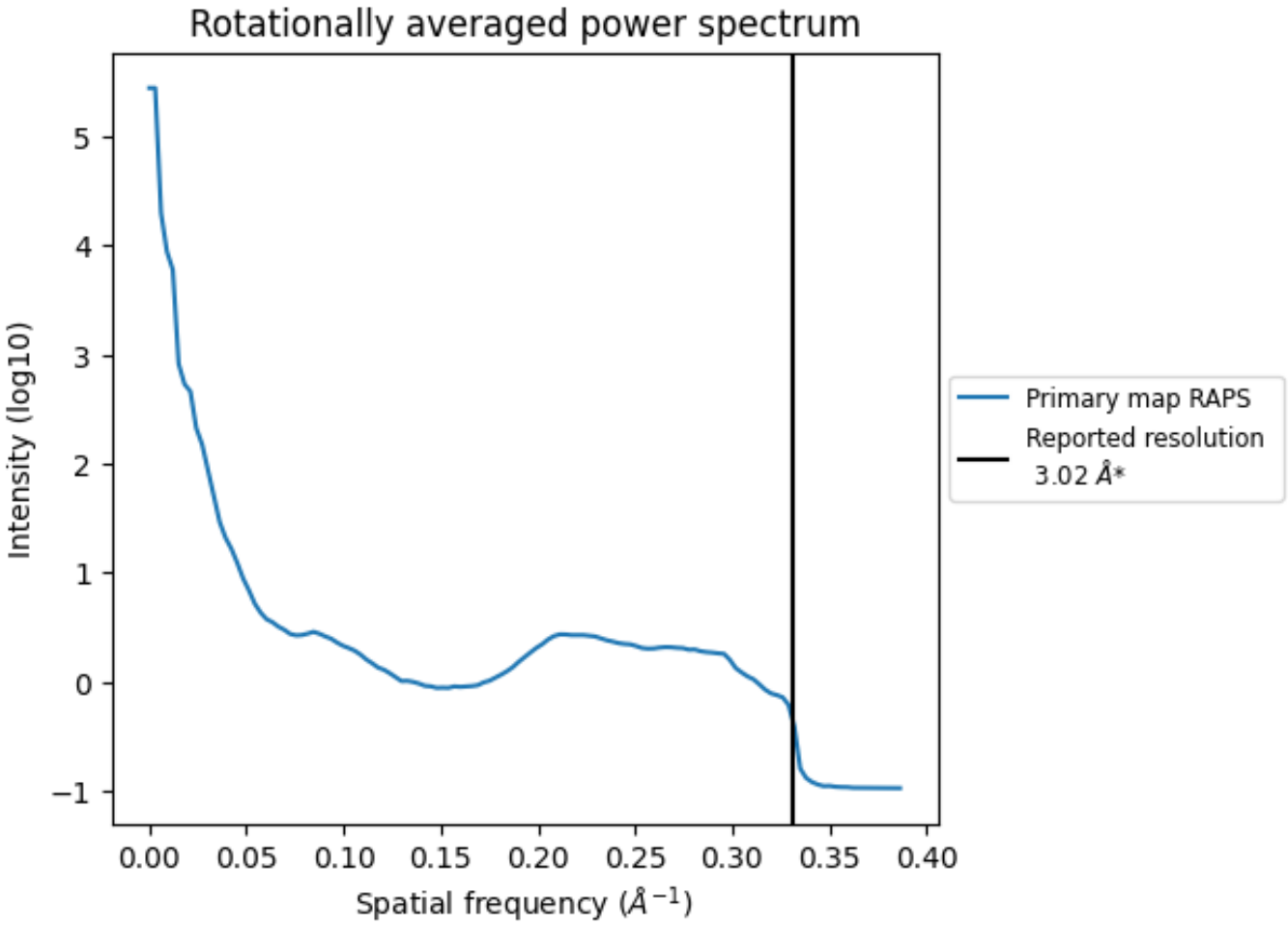
7.2 Volume estimate (i)



The volume at the recommended contour level is 47 nm^3; this corresponds to an approximate mass of 42 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 0.331 Å^{-1}

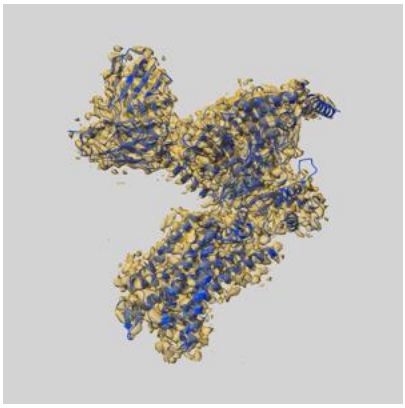
8 Fourier-Shell correlation (i)

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

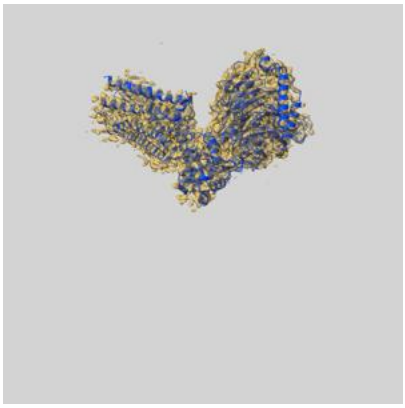
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-72002 and PDB model 9PXV. Per-residue inclusion information can be found in section 3 on page 10.

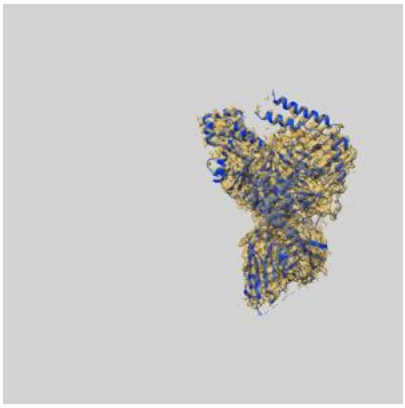
9.1 Map-model overlay



X



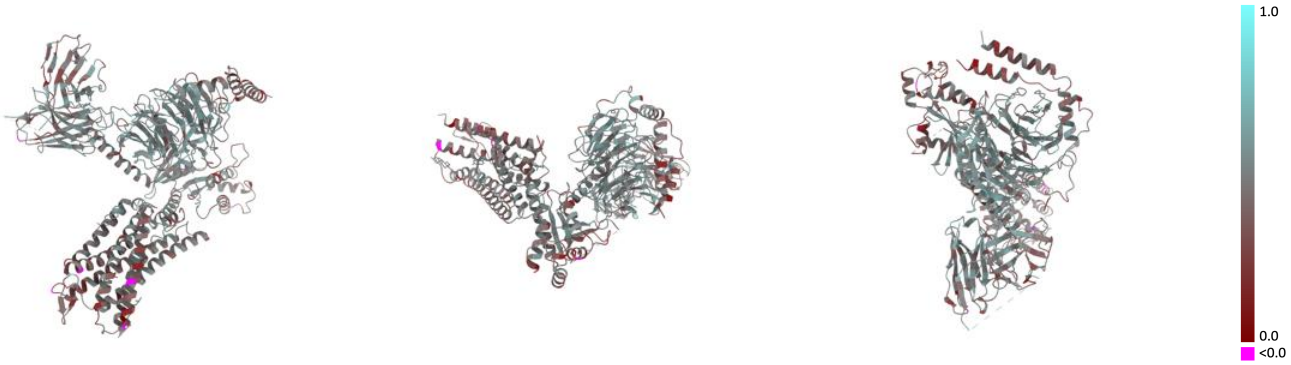
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



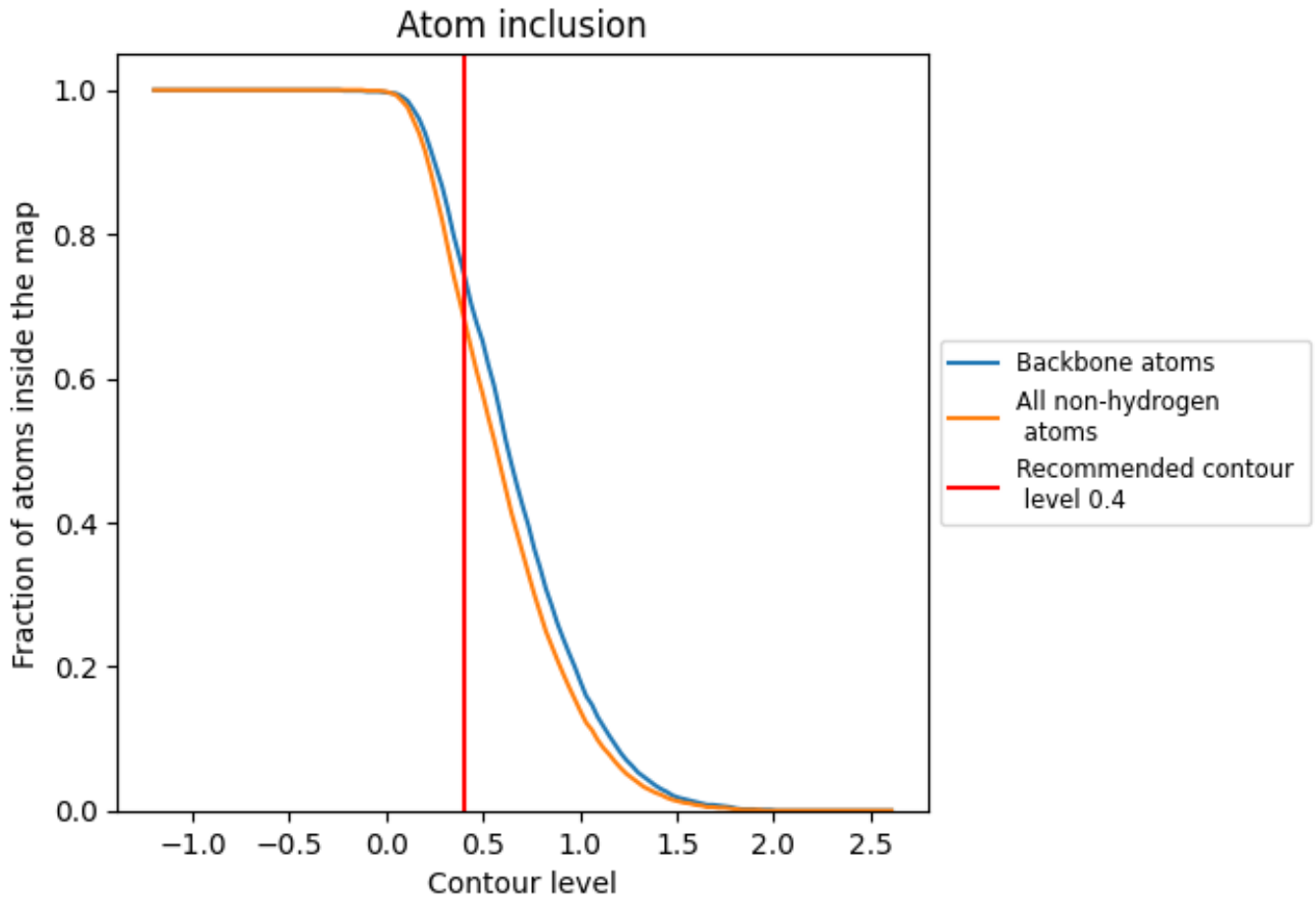
X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.4560
A	0.6010	0.4350
B	0.7630	0.5040
C	0.5270	0.4050
E	0.7390	0.4800
R	0.6560	0.4110

