



## Full wwPDB EM Validation Report ⓘ

Apr 30, 2026 – 02:12 PM JST

PDB ID : 9XHI / pdb\_00009xhi  
EMDB ID : EMD-66875  
Title : Structure of the CCL21-CCR7-Gi-scFv16 complex  
Authors : Tsutsumi, N.; Nishikawa, K.; Fujiyoshi, Y.  
Deposited on : 2025-11-01  
Resolution : 3.20 Å (reported)  
Based on initial models : 7JHJ, .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

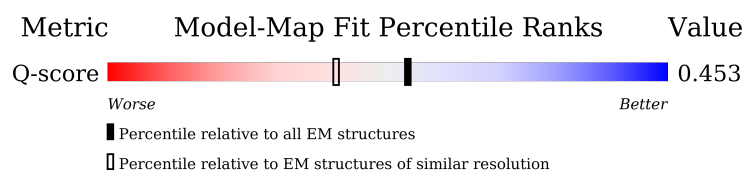
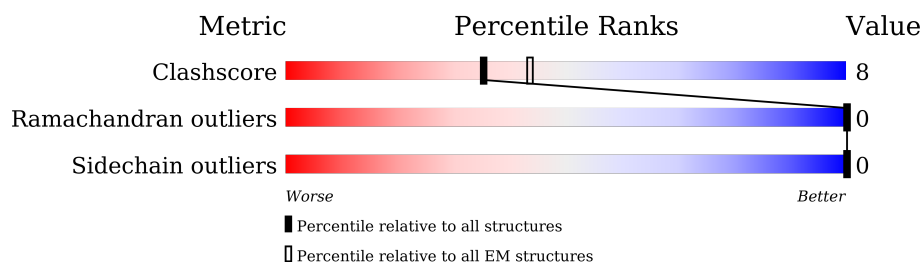
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	15020 ( 2.70 - 3.70 )

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  $\geq 3$ , 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	L	126	
2	R	551	
3	A	432	
3	C	432	

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Mol	Chain	Length	Quality of chain
4	B	371	
5	D	256	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9449 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 C-C motif chemokine 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	69	Total	C	N	O	S	0	0
			540	338	99	98	5		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	112	GLY	-	expression tag	UNP O00585
L	113	SER	-	expression tag	UNP O00585
L	114	GLY	-	expression tag	UNP O00585
L	115	SER	-	expression tag	UNP O00585
L	116	GLY	-	expression tag	UNP O00585
L	117	SER	-	expression tag	UNP O00585
L	118	ALA	-	expression tag	UNP O00585
L	119	ALA	-	expression tag	UNP O00585
L	120	ALA	-	expression tag	UNP O00585
L	121	LEU	-	expression tag	UNP O00585
L	122	GLU	-	expression tag	UNP O00585
L	123	VAL	-	expression tag	UNP O00585
L	124	LEU	-	expression tag	UNP O00585
L	125	PHE	-	expression tag	UNP O00585
L	126	GLN	-	expression tag	UNP O00585

- Molecule 2 is a protein called C-C chemokine receptor type 7,Non structural polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	304	Total	C	N	O	S	0	0
			2432	1621	389	404	18		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	16	ASP	-	expression tag	UNP P32248
R	17	TYR	-	expression tag	UNP P32248

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Chain	Residue	Modelled	Actual	Comment	Reference
R	18	LYS	-	expression tag	UNP P32248
R	19	ASP	-	expression tag	UNP P32248
R	20	ASP	-	expression tag	UNP P32248
R	21	ASP	-	expression tag	UNP P32248
R	22	ASP	-	expression tag	UNP P32248
R	23	GLY	-	expression tag	UNP P32248
R	24	SER	-	expression tag	UNP P32248
R	379	SER	-	linker	UNP P32248
R	380	ARG	-	linker	UNP P32248
R	381	GLY	-	linker	UNP P32248
R	382	SER	-	linker	UNP P32248
R	383	SER	-	linker	UNP P32248
R	384	GLY	-	linker	UNP P32248
R	385	GLY	-	linker	UNP P32248
R	386	GLY	-	linker	UNP P32248
R	387	GLY	-	linker	UNP P32248
R	388	SER	-	linker	UNP P32248
R	389	GLY	-	linker	UNP P32248
R	390	GLY	-	linker	UNP P32248
R	391	GLY	-	linker	UNP P32248
R	392	GLY	-	linker	UNP P32248
R	393	SER	-	linker	UNP P32248
R	394	SER	-	linker	UNP P32248
R	395	GLY	-	linker	UNP P32248
R	407	GLU	ARG	conflict	UNP A0A482LYE4
R	411	ALA	GLY	conflict	UNP A0A482LYE4
R	427	LEU	PHE	conflict	UNP A0A482LYE4
R	431	ALA	GLY	conflict	UNP A0A482LYE4
R	442	ARG	LEU	conflict	UNP A0A482LYE4
R	447	ALA	GLY	conflict	UNP A0A482LYE4
R	463	ALA	GLY	conflict	UNP A0A482LYE4
R	467	ALA	GLY	conflict	UNP A0A482LYE4
R	471	GLU	LYS	conflict	UNP A0A482LYE4
R	472	VAL	ILE	conflict	UNP A0A482LYE4
R	489	PRO	HIS	conflict	UNP A0A482LYE4
R	503	LEU	ILE	conflict	UNP A0A482LYE4
R	504	ASN	ASP	conflict	UNP A0A482LYE4
R	540	THR	ASN	conflict	UNP A0A482LYE4
R	545	MET	LEU	conflict	UNP A0A482LYE4
R	553	SER	-	expression tag	UNP A0A482LYE4
R	554	GLY	-	expression tag	UNP A0A482LYE4
R	555	GLY	-	expression tag	UNP A0A482LYE4

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Chain	Residue	Modelled	Actual	Comment	Reference
R	556	GLY	-	expression tag	UNP A0A482LYE4
R	557	GLY	-	expression tag	UNP A0A482LYE4
R	558	SER	-	expression tag	UNP A0A482LYE4
R	559	HIS	-	expression tag	UNP A0A482LYE4
R	560	HIS	-	expression tag	UNP A0A482LYE4
R	561	HIS	-	expression tag	UNP A0A482LYE4
R	562	HIS	-	expression tag	UNP A0A482LYE4
R	563	HIS	-	expression tag	UNP A0A482LYE4
R	564	HIS	-	expression tag	UNP A0A482LYE4
R	565	HIS	-	expression tag	UNP A0A482LYE4
R	566	HIS	-	expression tag	UNP A0A482LYE4

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2, Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	220	Total	C	N	O	S	0	0
			1743	1112	294	324	13		
3	C	52	Total	C	N	O	S	0	0
			383	241	66	73	3		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	linker	UNP P59768
A	-6	SER	-	linker	UNP P59768
A	-5	ALA	-	linker	UNP P59768
A	-4	GLY	-	linker	UNP P59768
A	-3	SER	-	linker	UNP P59768
A	-2	ALA	-	linker	UNP P59768
A	-1	GLY	-	linker	UNP P59768
A	0	SER	-	linker	UNP P59768
A	1	ALA	-	linker	UNP P59768
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
C	72	GLY	-	linker	UNP P59768
C	73	SER	-	linker	UNP P59768
C	74	ALA	-	linker	UNP P59768
C	75	GLY	-	linker	UNP P59768
C	76	SER	-	linker	UNP P59768

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Chain	Residue	Modelled	Actual	Comment	Reference
C	77	ALA	-	linker	UNP P59768
C	78	GLY	-	linker	UNP P59768
C	79	SER	-	linker	UNP P59768
C	80	ALA	-	linker	UNP P59768
C	126	ASN	SER	conflict	UNP P63097
C	282	ALA	GLY	conflict	UNP P63097
C	324	ALA	GLU	conflict	UNP P63097
C	405	SER	ALA	conflict	UNP P63097

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	337	Total	C	N	O	S	0	0
			2565	1585	462	497	21		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP P62873
B	-4	PRO	-	expression tag	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	GLY	-	expression tag	UNP P62873
B	340	GLY	-	expression tag	UNP P62873
B	341	SER	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	GLY	-	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	SER	-	expression tag	UNP P62873
B	348	GLY	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	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	VAL	-	expression tag	UNP P62873
B	356	SER	-	expression tag	UNP P62873

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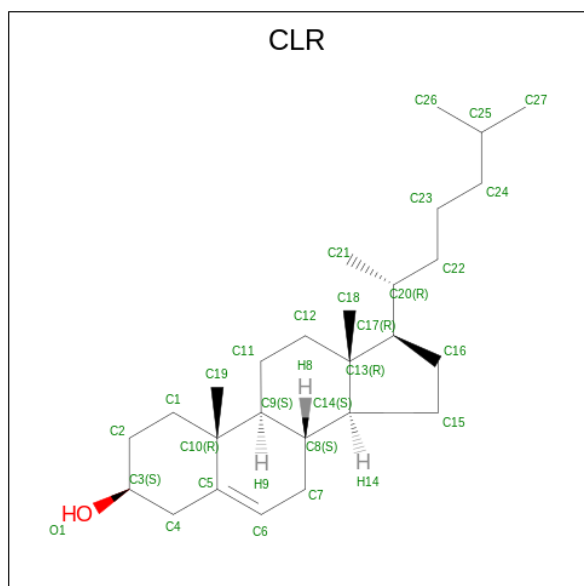
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Chain	Residue	Modelled	Actual	Comment	Reference
B	357	GLY	-	expression tag	UNP P62873
B	358	TRP	-	expression tag	UNP P62873
B	359	ARG	-	expression tag	UNP P62873
B	360	LEU	-	expression tag	UNP P62873
B	361	PHE	-	expression tag	UNP P62873
B	362	LYS	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	ILE	-	expression tag	UNP P62873
B	365	SER	-	expression tag	UNP P62873

- Molecule 5 is a protein called Antibody fragment scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	231	Total	C	N	O	S	0	0
			1758	1119	291	338	10		

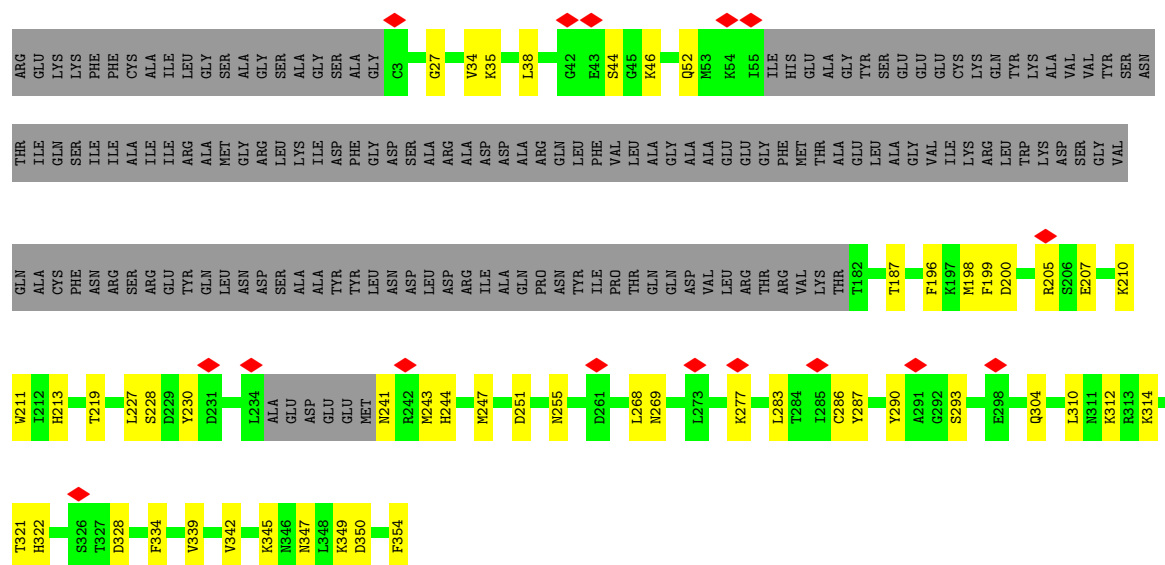
- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



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

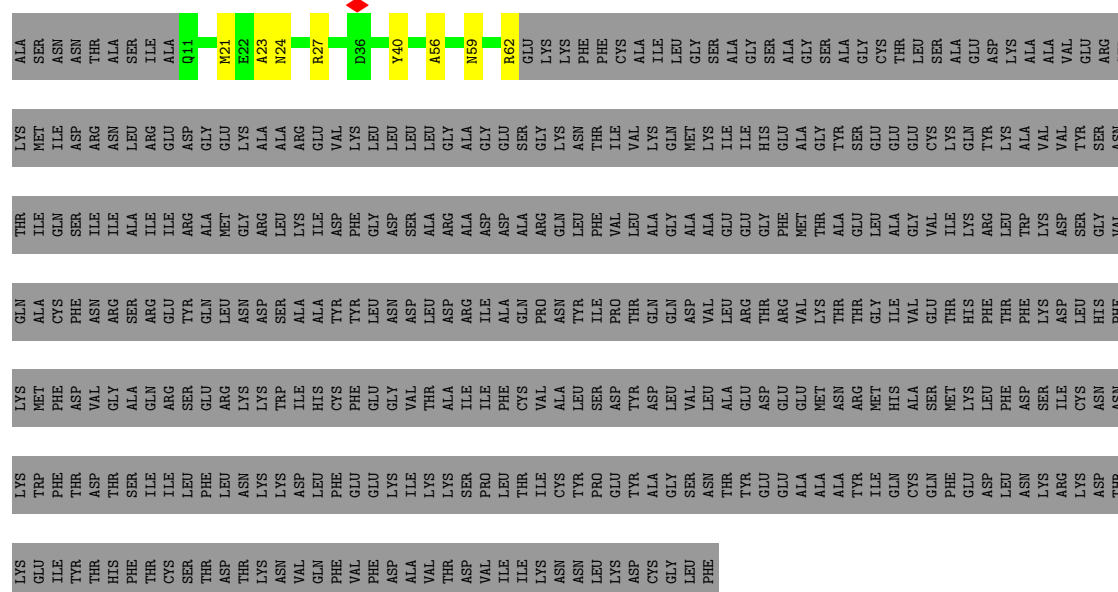






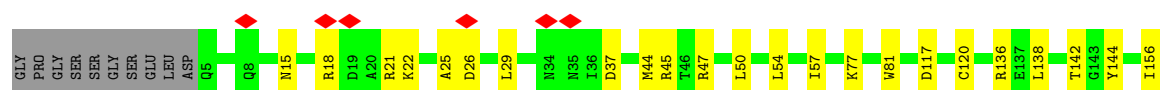
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2, Guanine nucleotide-binding protein G(i) subunit alpha-1

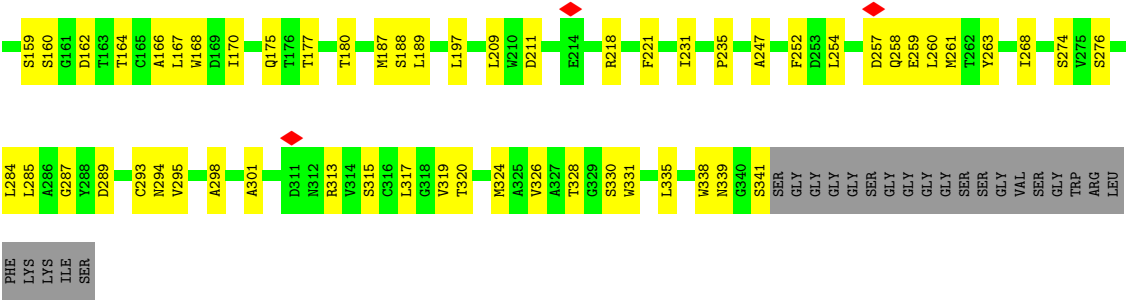
Chain C:  10% 88%



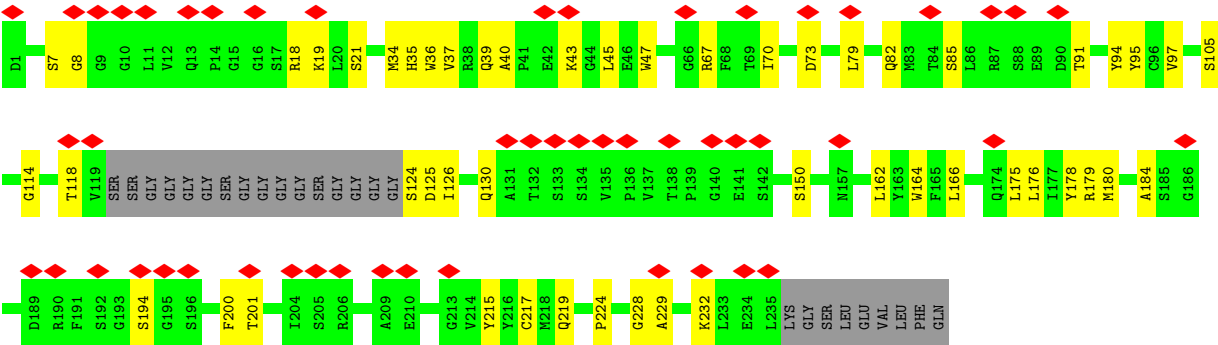
- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:  70% 21% 9%





● Molecule 5: Antibody fragment scFv16



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	195011	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CryoSPARC patch CTF estimation and global/local CTF refinements	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	63291	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.564	Depositor
Minimum map value	-0.445	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	252.8, 252.8, 252.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.9875, 0.9875, 0.9875	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: 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	L	0.17	0/550	0.46	0/741
2	R	0.18	0/2487	0.38	0/3378
3	A	0.13	0/1772	0.31	0/2380
3	C	0.11	0/389	0.25	0/529
4	B	0.12	0/2612	0.33	0/3543
5	D	0.12	0/1802	0.35	0/2446
All	All	0.14	0/9612	0.35	0/13017

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	L	540	0	542	8	0
2	R	2432	0	2543	25	0
3	A	1743	0	1726	37	0
3	C	383	0	372	6	0
4	B	2565	0	2467	52	0
5	D	1758	0	1689	31	0
6	R	28	0	46	1	0
All	All	9449	0	9385	149	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 8.

All (149) 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)
5:D:94:TYR:O	5:D:114:GLY:HA2	1.92	0.70
5:D:37:VAL:HG12	5:D:47:TRP:HA	1.77	0.66
2:R:92:MET:HG3	2:R:175:SER:HB3	1.82	0.62
3:C:59:ASN:O	3:C:62:ARG:NH1	2.35	0.60
5:D:19:LYS:HB3	5:D:82:GLN:HG3	1.82	0.60
4:B:29:LEU:HD23	4:B:261:MET:HB2	1.84	0.59
4:B:328:THR:OG1	4:B:338:TRP:NE1	2.35	0.57
5:D:8:GLY:O	5:D:18:ARG:NH2	2.36	0.57
4:B:162:ASP:OD1	4:B:164:THR:OG1	2.23	0.57
2:R:103:ALA:O	2:R:139:SER:OG	2.23	0.56
3:A:38:LEU:HB2	3:A:198:MET:HE3	1.87	0.56
5:D:94:TYR:O	5:D:114:GLY:CA	2.52	0.56
4:B:57:ILE:O	4:B:315:SER:OG	2.20	0.56
4:B:319:VAL:HG22	4:B:326:VAL:HG22	1.87	0.56
4:B:164:THR:HG22	4:B:180:THR:HG22	1.88	0.56
4:B:209:LEU:HD22	4:B:254:LEU:HD12	1.89	0.55
2:R:72:GLY:O	2:R:76:ASN:ND2	2.38	0.55
2:R:253:ALA:O	2:R:258:ARG:NH1	2.40	0.55
3:A:52:GLN:NE2	3:A:328:ASP:O	2.40	0.55
2:R:247:ILE:HG12	2:R:262:ILE:HD13	1.90	0.54
4:B:247:ALA:HB1	4:B:268:ILE:HG22	1.90	0.54
3:A:304:GLN:HG3	3:A:321:THR:HG21	1.89	0.54
4:B:50:LEU:HB2	4:B:335:LEU:HB2	1.89	0.54
5:D:162:LEU:HB3	5:D:180:MET:HB2	1.90	0.53
3:A:247:MET:SD	3:A:287:TYR:OH	2.65	0.53
4:B:276:SER:HB2	4:B:317:LEU:HD22	1.89	0.53
4:B:339:ASN:ND2	3:C:59:ASN:OD1	2.42	0.53
5:D:34:MET:HG3	5:D:79:LEU:HD22	1.89	0.52
5:D:37:VAL:HG23	5:D:95:TYR:HB2	1.91	0.52
2:R:68:ILE:HG21	2:R:316:CYS:HB3	1.91	0.52
5:D:180:MET:HE2	5:D:200:PHE:HB2	1.91	0.52
3:A:241:ASN:ND2	3:A:286:CYS:SG	2.83	0.52
5:D:166:LEU:HB2	5:D:176:LEU:HD11	1.91	0.52
3:A:34:VAL:HG13	3:A:219:THR:HG21	1.92	0.52
4:B:285:LEU:HG	4:B:295:VAL:HG22	1.91	0.52
3:A:339:VAL:HA	3:A:342:VAL:HG12	1.92	0.51
5:D:67:ARG:NH1	5:D:85:SER:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:91:THR:HG23	5:D:118:THR:HA	1.93	0.51
3:A:283:LEU:HG	3:A:287:TYR:HB2	1.92	0.51
4:B:160:SER:OG	4:B:162:ASP:OD1	2.28	0.51
2:R:157:ALA:O	3:A:347:ASN:ND2	2.40	0.51
5:D:178:TYR:HD2	5:D:179:ARG:HD3	1.76	0.51
1:L:47:SER:HB2	2:R:41:TYR:HE2	1.76	0.51
5:D:105:SER:O	5:D:179:ARG:NH1	2.43	0.51
5:D:130:GLN:HE22	5:D:228:GLY:HA3	1.76	0.51
5:D:130:GLN:NE2	5:D:217:CYS:SG	2.84	0.50
4:B:293:CYS:SG	4:B:294:ASN:N	2.84	0.50
5:D:40:ALA:HB3	5:D:43:LYS:HB3	1.94	0.50
4:B:221:PHE:HE1	4:B:257:ASP:HA	1.77	0.49
3:A:46:LYS:NZ	3:A:200:ASP:OD1	2.44	0.49
4:B:330:SER:OG	4:B:331:TRP:N	2.46	0.49
5:D:219:GLN:NE2	5:D:224:PRO:O	2.45	0.49
3:A:44:SER:O	3:A:269:ASN:ND2	2.38	0.49
5:D:35:HIS:HB2	5:D:97:VAL:HB	1.94	0.48
3:A:241:ASN:HD22	3:A:244:HIS:HD2	1.61	0.48
2:R:144:MET:HG3	2:R:231:GLY:HA2	1.93	0.48
3:A:247:MET:HE3	3:A:310:LEU:HD21	1.94	0.48
4:B:320:THR:OG1	4:B:324:MET:N	2.47	0.48
5:D:175:LEU:HD22	5:D:184:ALA:HB2	1.96	0.48
4:B:166:ALA:HB1	4:B:175:GLN:HE22	1.78	0.48
2:R:202:SER:HB3	2:R:209:ARG:HH21	1.79	0.48
5:D:73:ASP:N	5:D:73:ASP:OD1	2.46	0.48
6:R:601:CLR:H162	6:R:601:CLR:H221	1.57	0.47
3:C:23:ALA:HA	3:C:27:ARG:HH22	1.79	0.47
1:L:15:ARG:HH12	2:R:43:LEU:HB3	1.80	0.47
4:B:47:ARG:NH2	4:B:341:SER:OG	2.48	0.47
2:R:56:PHE:O	2:R:60:PHE:HB2	2.15	0.47
3:A:35:LYS:HB3	3:A:199:PHE:HE2	1.79	0.47
4:B:21:ARG:O	4:B:258:GLN:NE2	2.47	0.47
4:B:274:SER:O	4:B:287:GLY:N	2.48	0.46
3:A:27:GLY:HA3	4:B:54:LEU:HD12	1.98	0.46
4:B:284:LEU:HB2	4:B:298:ALA:HB2	1.97	0.46
5:D:39:GLN:HB3	5:D:45:LEU:HD13	1.96	0.46
3:A:210:LYS:O	3:A:213:HIS:NE2	2.48	0.46
3:A:228:SER:HB3	3:A:277:LYS:HD2	1.97	0.46
3:A:230:TYR:HB3	3:A:243:MET:HE2	1.97	0.45
4:B:120:CYS:HB3	4:B:138:LEU:HB2	1.98	0.45
4:B:289:ASP:HA	4:B:313:ARG:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:12:TYR:CG	1:L:54:ASP:HB2	2.51	0.45
1:L:39:ILE:HG13	1:L:53:ALA:HB3	1.98	0.45
2:R:332:LYS:NZ	3:A:350:ASP:OD1	2.42	0.45
4:B:197:LEU:HD13	4:B:209:LEU:HD21	1.98	0.45
5:D:7:SER:N	5:D:21:SER:O	2.47	0.45
3:A:228:SER:O	3:A:277:LYS:NZ	2.46	0.45
4:B:167:LEU:HB3	4:B:177:THR:HB	1.99	0.45
4:B:263:TYR:HD1	4:B:301:ALA:HA	1.82	0.45
2:R:260:LYS:HD3	3:A:354:PHE:CD1	2.51	0.44
4:B:235:PRO:HB2	3:C:40:TYR:HE2	1.81	0.44
4:B:159:SER:HB3	4:B:189:LEU:HD23	2.00	0.44
4:B:252:PHE:HE1	4:B:259:GLU:HG2	1.81	0.44
1:L:32:LEU:HD22	2:R:212:LEU:HD12	2.00	0.44
5:D:39:GLN:HB3	5:D:45:LEU:HA	1.99	0.44
2:R:308:TYR:O	2:R:312:TYR:HB2	2.18	0.44
4:B:144:TYR:OH	4:B:187:MET:SD	2.64	0.44
5:D:164:TRP:HZ3	5:D:215:TYR:HB3	1.82	0.44
3:A:251:ASP:O	3:A:255:ASN:ND2	2.51	0.44
2:R:202:SER:OG	2:R:203:SER:N	2.48	0.44
2:R:56:PHE:O	2:R:60:PHE:CB	2.65	0.43
2:R:96:TYR:HB3	2:R:150:ILE:HG12	2.00	0.43
4:B:22:LYS:HA	4:B:22:LYS:HD2	1.81	0.43
3:A:205:ARG:HH12	4:B:142:THR:HB	1.84	0.43
4:B:156:ILE:HG22	4:B:168:TRP:HB2	2.01	0.43
1:L:31:SER:N	1:L:34:CYS:O	2.36	0.43
3:A:187:THR:HB	3:A:198:MET:HB3	2.00	0.43
3:A:196:PHE:HE2	3:A:339:VAL:HG21	1.83	0.43
4:B:211:ASP:OD2	4:B:218:ARG:NH2	2.51	0.43
4:B:37:ASP:OD1	4:B:37:ASP:N	2.51	0.43
1:L:40:LEU:HB3	1:L:50:GLU:HB3	2.01	0.42
4:B:50:LEU:HD23	4:B:81:TRP:CD2	2.54	0.42
4:B:117:ASP:OD1	4:B:117:ASP:N	2.52	0.42
3:A:196:PHE:CE2	3:A:339:VAL:HG21	2.54	0.42
4:B:15:ASN:OD1	4:B:18:ARG:NH2	2.52	0.42
3:C:56:ALA:O	3:C:62:ARG:NH1	2.52	0.42
5:D:194:SER:OG	5:D:201:THR:OG1	2.38	0.42
3:A:210:LYS:HD2	4:B:187:MET:SD	2.60	0.42
4:B:136:ARG:NE	4:B:170:ILE:O	2.52	0.42
2:R:116:TYR:HE2	2:R:123:VAL:HG22	1.83	0.42
5:D:232:LYS:HB2	5:D:232:LYS:HE2	1.86	0.42
3:A:349:LYS:HE3	3:A:349:LYS:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:314:LYS:HA	3:A:314:LYS:HD2	1.86	0.41
4:B:324:MET:HE2	4:B:324:MET:HB2	1.86	0.41
3:A:227:LEU:HD11	3:A:268:LEU:HB3	2.01	0.41
3:C:21:MET:HA	3:C:24:ASN:HD21	1.85	0.41
1:L:25:TYR:OH	1:L:68:ASP:OD1	2.31	0.41
4:B:77:LYS:HD3	4:B:77:LYS:HA	1.78	0.41
4:B:44:MET:HE1	4:B:285:LEU:HD21	2.02	0.41
2:R:84:ILE:HG13	2:R:85:TYR:CD1	2.55	0.41
3:A:342:VAL:HG23	3:A:345:LYS:HE2	2.02	0.41
4:B:25:ALA:HB2	4:B:258:GLN:HE22	1.86	0.41
5:D:36:TRP:HD1	5:D:70:ILE:HD12	1.86	0.41
2:R:65:TYR:HD2	2:R:115:ALA:HB2	1.85	0.41
5:D:130:GLN:OE1	5:D:229:ALA:N	2.53	0.41
2:R:144:MET:HE3	2:R:318:ARG:HE	1.85	0.41
3:A:35:LYS:HB3	3:A:199:PHE:CE2	2.55	0.41
3:A:312:LYS:HB2	3:A:312:LYS:HE2	1.89	0.41
4:B:29:LEU:HB2	4:B:260:LEU:HD12	2.02	0.41
4:B:188:SER:HB3	4:B:231:ILE:HG22	2.02	0.41
5:D:124:SER:OG	5:D:125:ASP:N	2.54	0.41
5:D:126:ILE:HG23	5:D:150:SER:HB3	2.02	0.41
2:R:331:VAL:HG12	2:R:334:ARG:HH21	1.85	0.41
2:R:77:GLY:HA2	2:R:80:VAL:HG22	2.03	0.40
3:A:207:GLU:O	3:A:211:TRP:NE1	2.54	0.40
4:B:26:ASP:OD1	4:B:26:ASP:N	2.45	0.40
4:B:175:GLN:NE2	4:B:177:THR:O	2.53	0.40
3:A:290:TYR:OH	3:A:293:SER:O	2.39	0.40
4:B:47:ARG:HD3	4:B:47:ARG:HA	1.82	0.40
3:A:322:HIS:HB2	3:A:334:PHE:CE2	2.57	0.40
3:A:328:ASP:OD1	3:A:328:ASP:N	2.53	0.40
4:B:45:ARG:HG3	4:B:47:ARG:HE	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	L	67/126 (53%)	59 (88%)	8 (12%)	0	100	100
2	R	302/551 (55%)	290 (96%)	12 (4%)	0	100	100
3	A	214/432 (50%)	206 (96%)	8 (4%)	0	100	100
3	C	50/432 (12%)	50 (100%)	0	0	100	100
4	B	335/371 (90%)	325 (97%)	10 (3%)	0	100	100
5	D	227/256 (89%)	220 (97%)	7 (3%)	0	100	100
All	All	1195/2168 (55%)	1150 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	L	59/103 (57%)	59 (100%)	0	100	100
2	R	270/480 (56%)	270 (100%)	0	100	100
3	A	188/364 (52%)	188 (100%)	0	100	100
3	C	38/364 (10%)	38 (100%)	0	100	100
4	B	274/300 (91%)	274 (100%)	0	100	100
5	D	191/208 (92%)	191 (100%)	0	100	100
All	All	1020/1819 (56%)	1020 (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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
2	R	99	ASN

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Mol	Chain	Res	Type
2	R	286	GLN
2	R	335	ASN
3	A	195	HIS
3	A	241	ASN
3	A	306	GLN
4	B	31	GLN
4	B	155	GLN
4	B	175	GLN
4	B	294	ASN
3	C	18	GLN
3	C	24	ASN
3	C	44	HIS

### 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	$\# Z  > 2$
6	CLR	R	601	-	31,31,31	0.72	1 (3%)	48,48,48	1.29	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	R	601	-	-	7/10/68/68	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	601	CLR	C4-C3	2.06	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	601	CLR	C13-C17-C20	-3.89	113.39	119.49
6	R	601	CLR	C4-C5-C6	-3.33	115.81	120.61
6	R	601	CLR	C10-C9-C8	-3.00	108.24	112.73
6	R	601	CLR	C13-C14-C8	-2.63	110.49	114.38
6	R	601	CLR	C11-C9-C10	-2.04	110.39	113.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	601	CLR	C13-C17-C20-C22
6	R	601	CLR	C17-C20-C22-C23
6	R	601	CLR	C13-C17-C20-C21
6	R	601	CLR	C21-C20-C22-C23
6	R	601	CLR	C16-C17-C20-C22
6	R	601	CLR	C16-C17-C20-C21
6	R	601	CLR	C20-C22-C23-C24

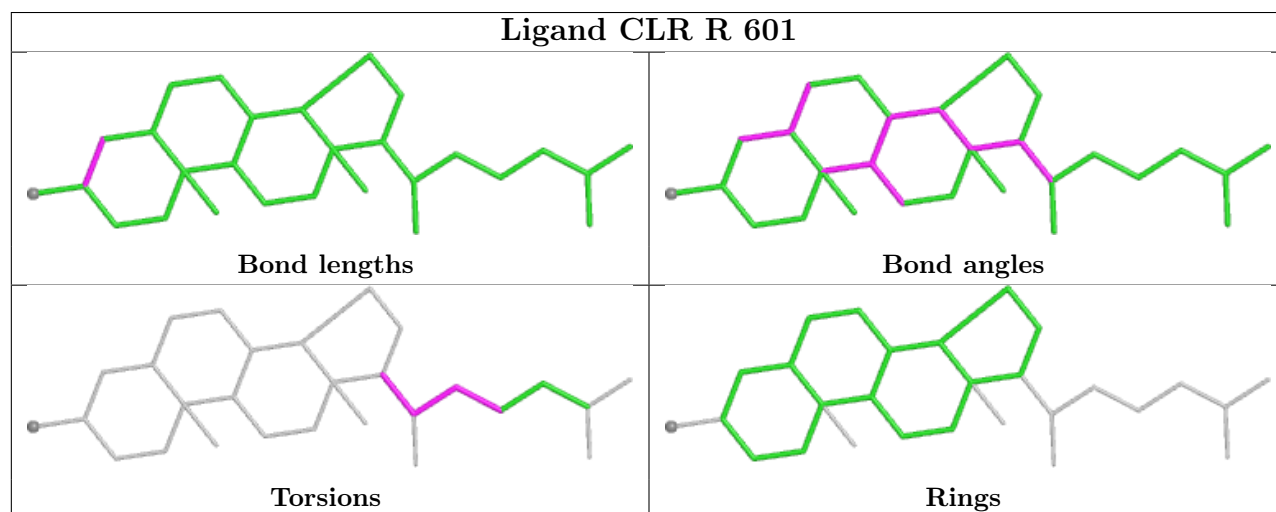
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	601	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 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.

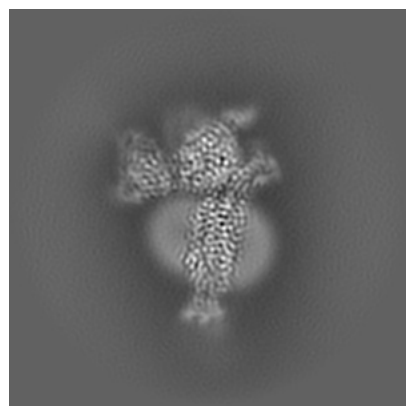
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66875. These allow visual inspection of the internal detail of the map and identification of artifacts.

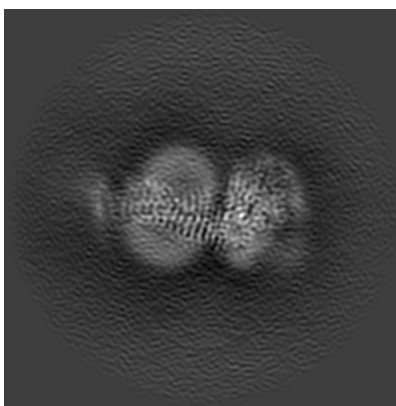
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

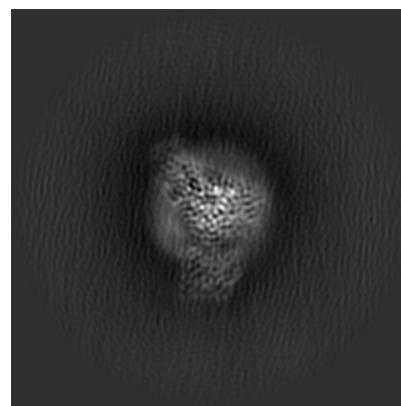
#### 6.1.1 Primary map



X

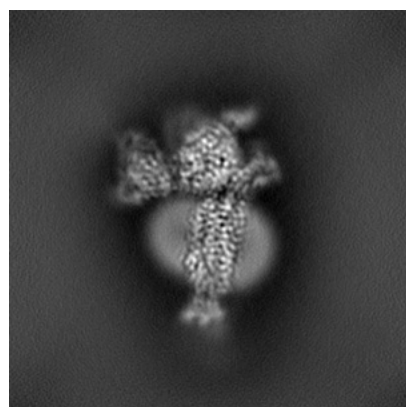


Y

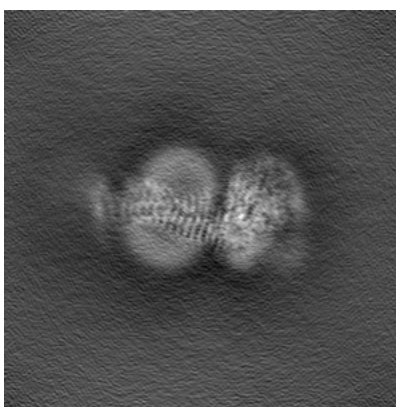


Z

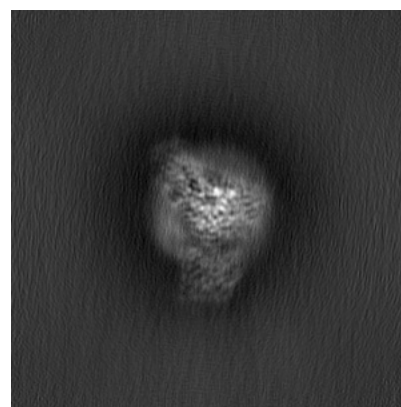
#### 6.1.2 Raw map



X



Y

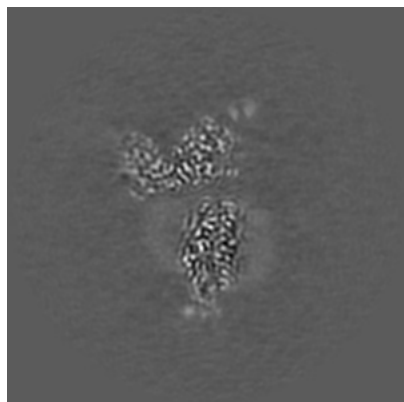


Z

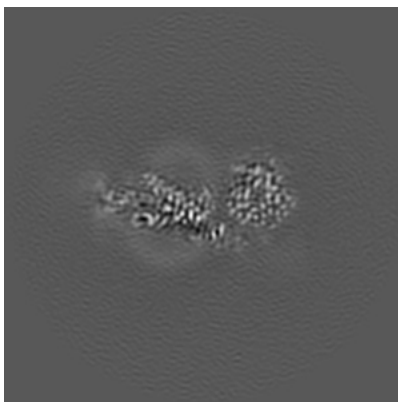
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

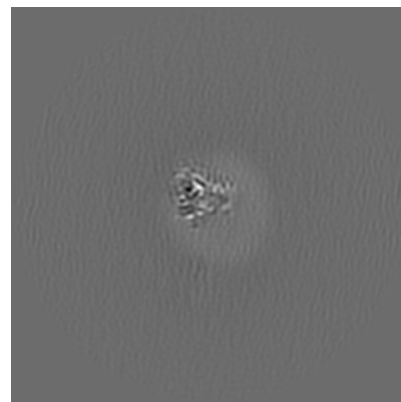
### 6.2.1 Primary map



X Index: 128

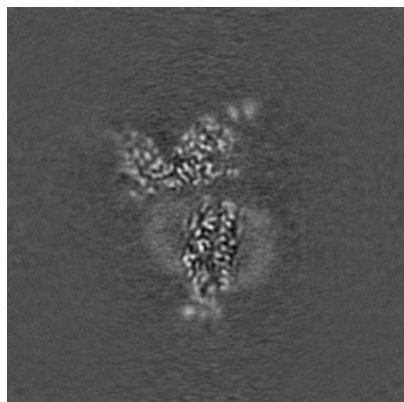


Y Index: 128

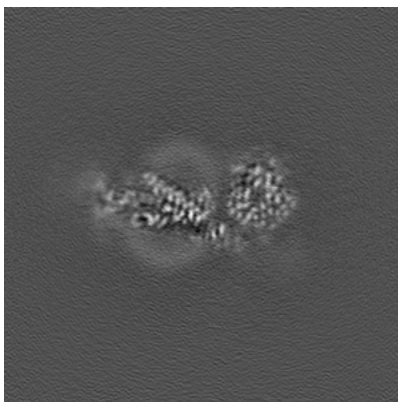


Z Index: 128

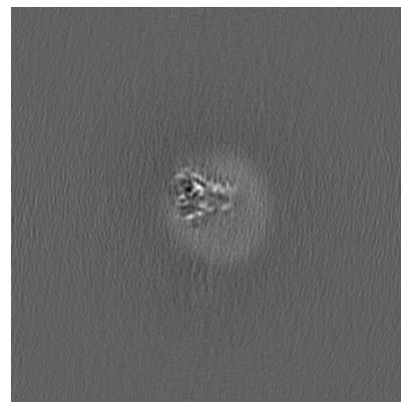
### 6.2.2 Raw map



X Index: 128



Y Index: 128



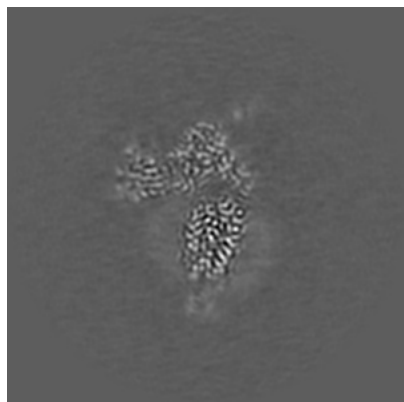
Z Index: 128

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

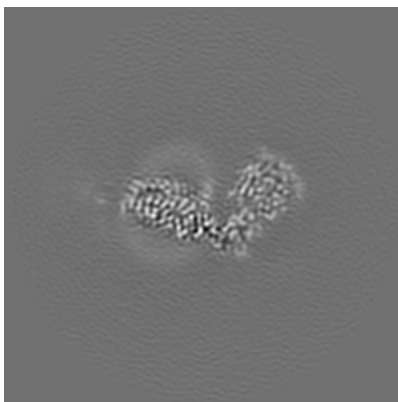


## 6.3 Largest variance slices [i](#)

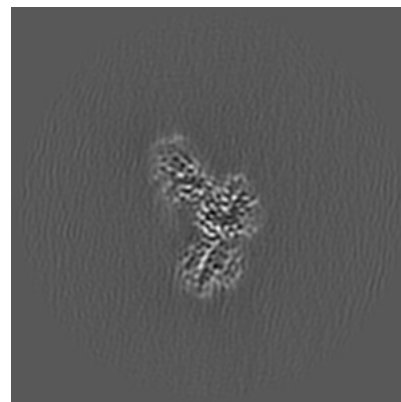
### 6.3.1 Primary map



X Index: 122

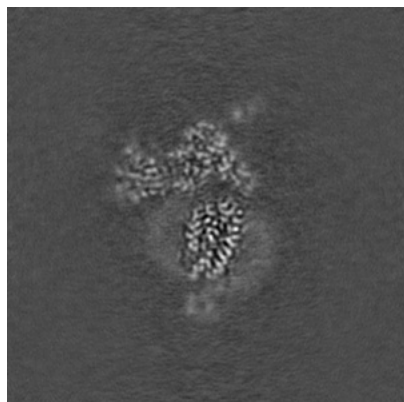


Y Index: 138

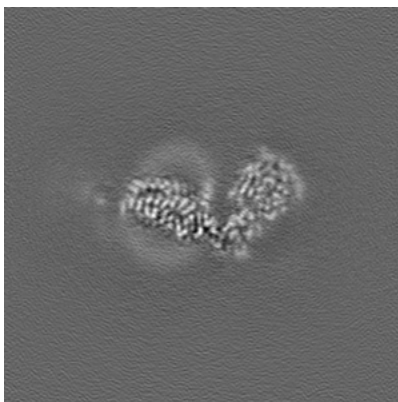


Z Index: 151

### 6.3.2 Raw map



X Index: 122



Y Index: 138



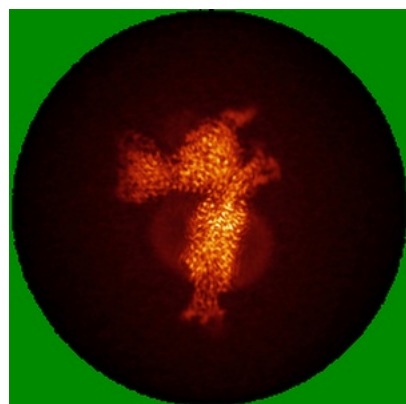
Z Index: 150

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

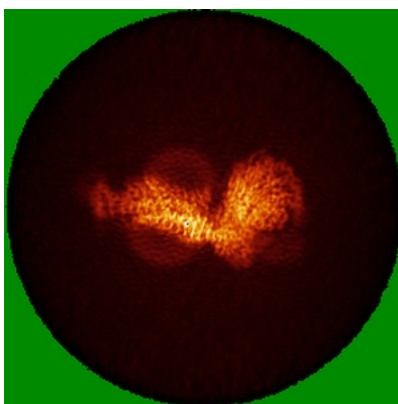


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

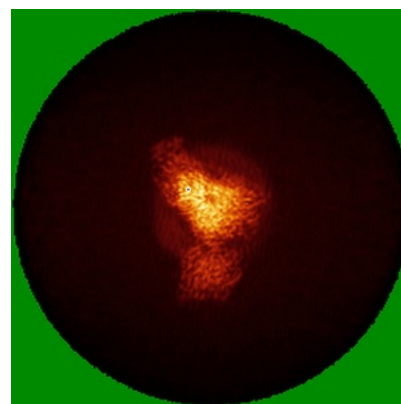
### 6.4.1 Primary map



X

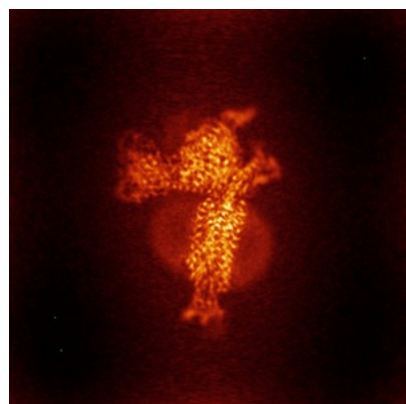


Y

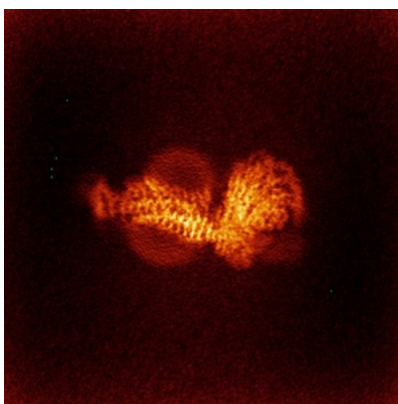


Z

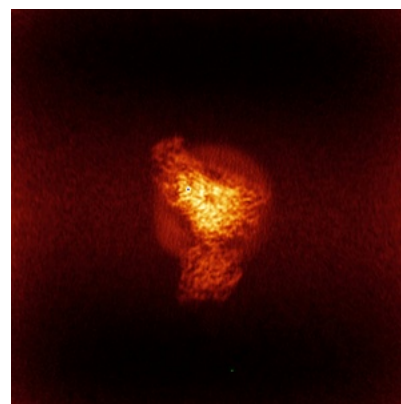
### 6.4.2 Raw map



X



Y



Z

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

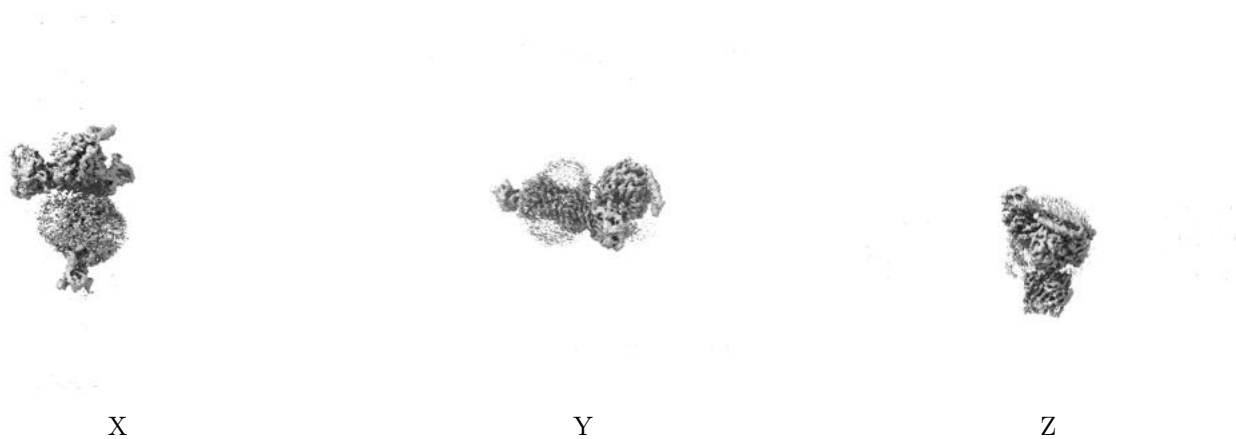
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

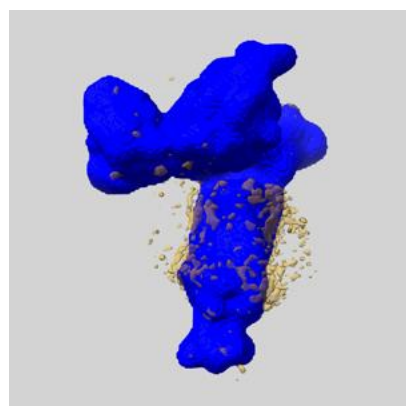
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

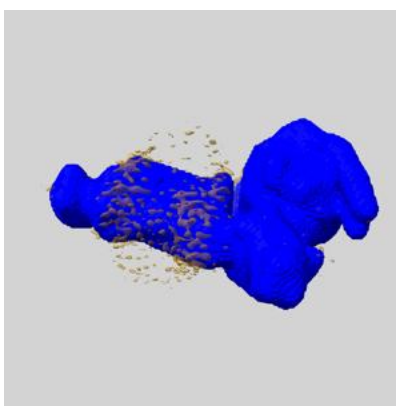
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

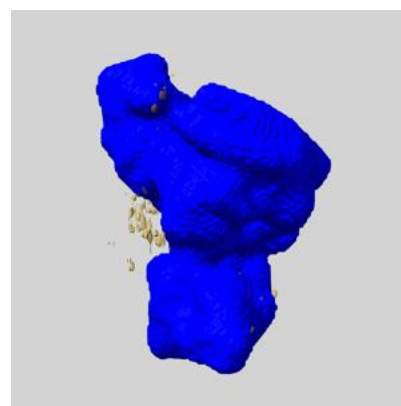
### 6.6.1 emd\_66875\_msk\_2.map [i](#)



X

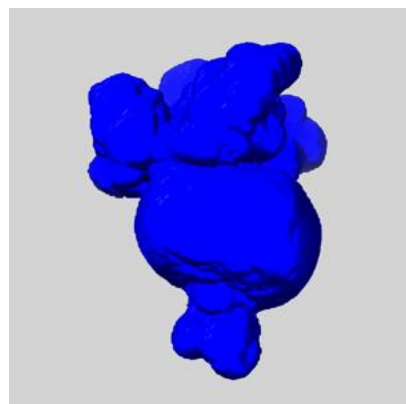


Y

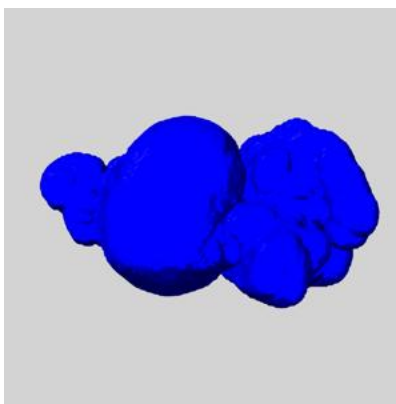


Z

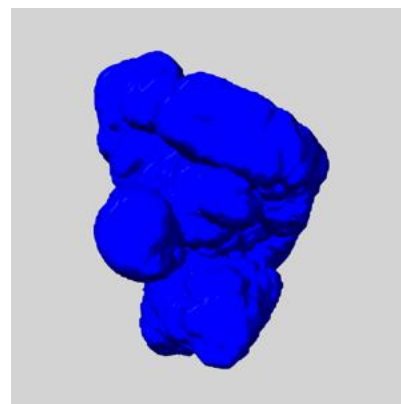
### 6.6.2 emd\_66875\_msk\_1.map [i](#)



X



Y

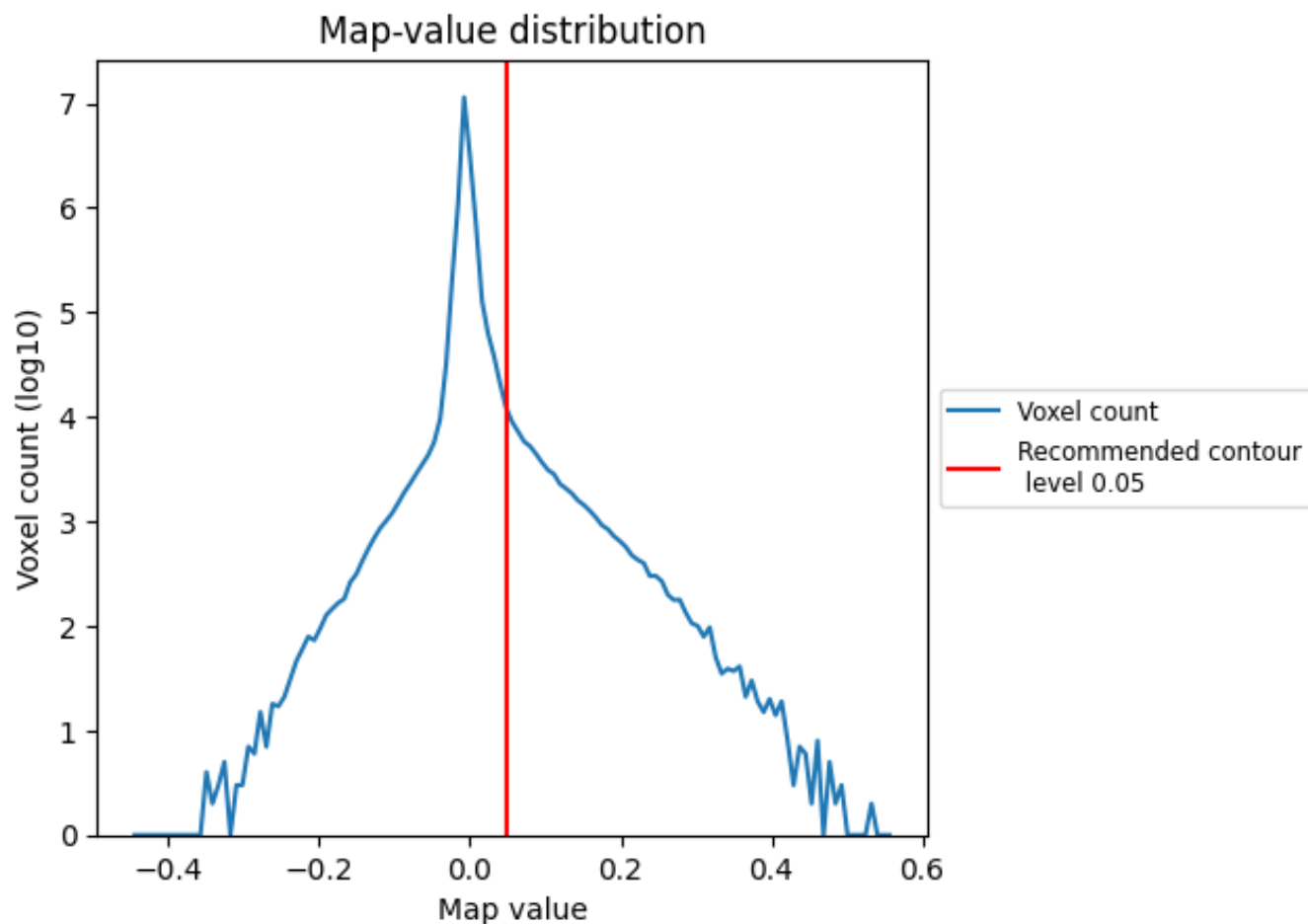


Z

## 7 Map analysis [i](#)

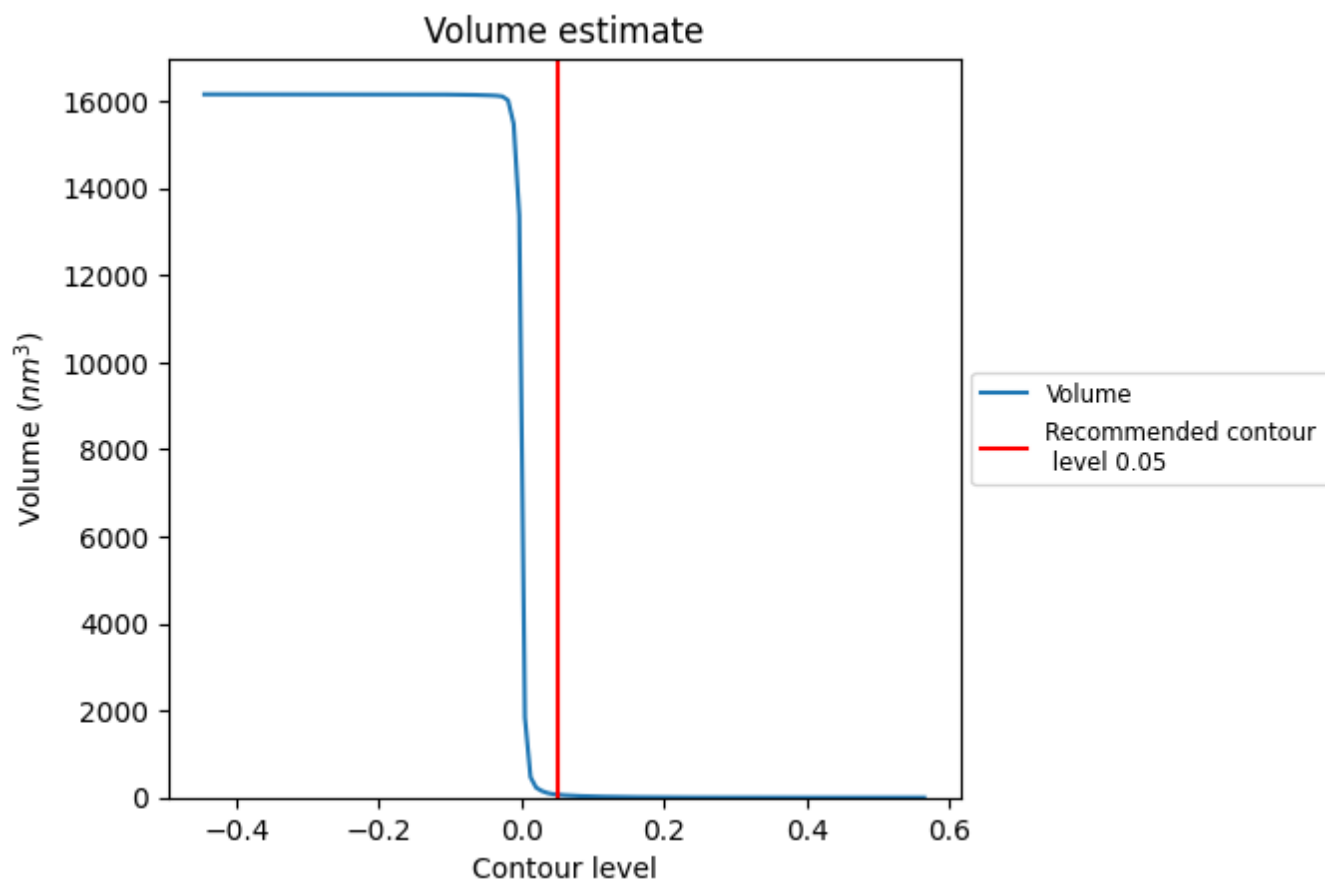
This section contains the results of statistical analysis of the map.

### 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.

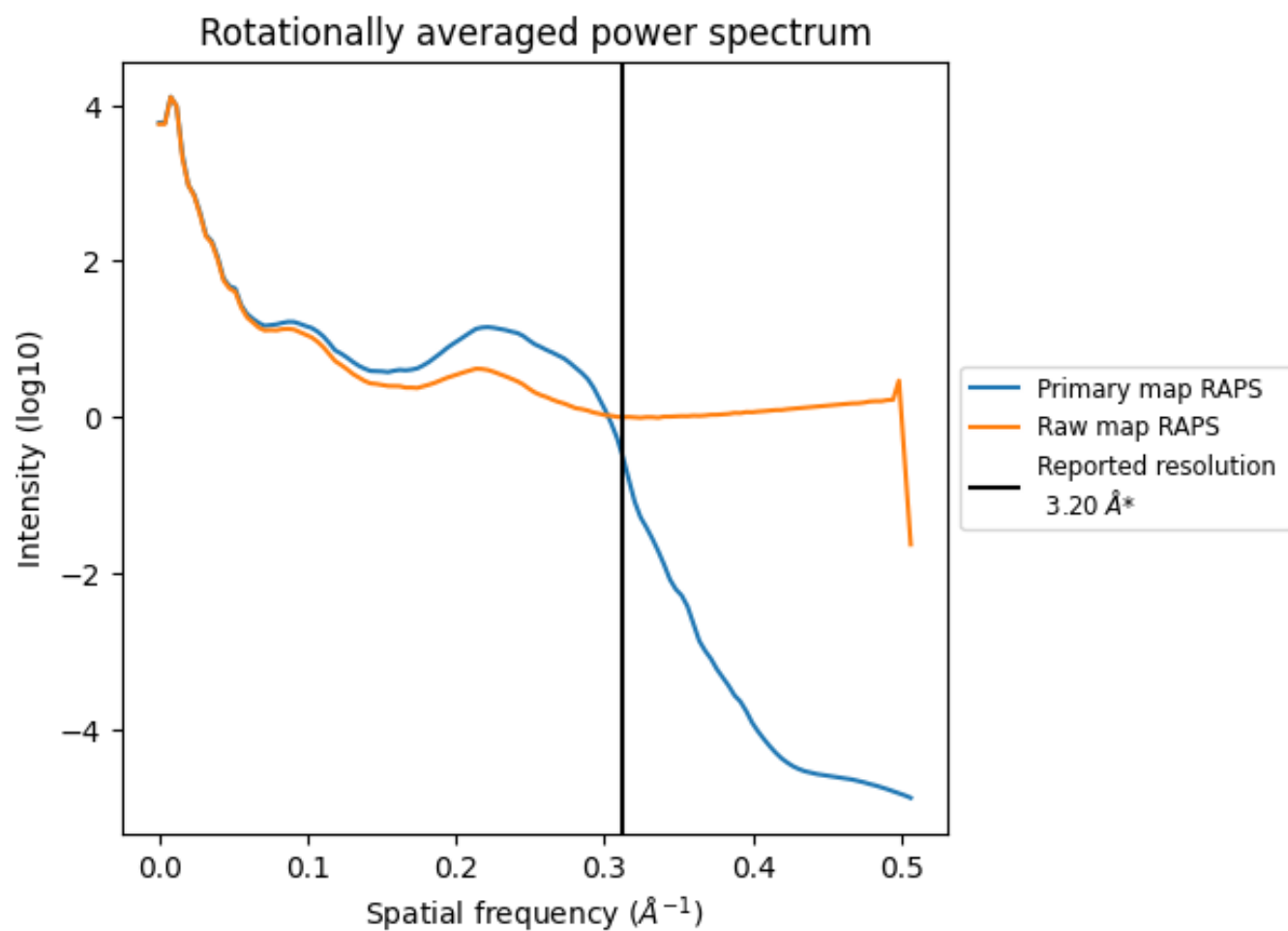
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm<sup>3</sup>; this corresponds to an approximate mass of 60 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 ⓘ

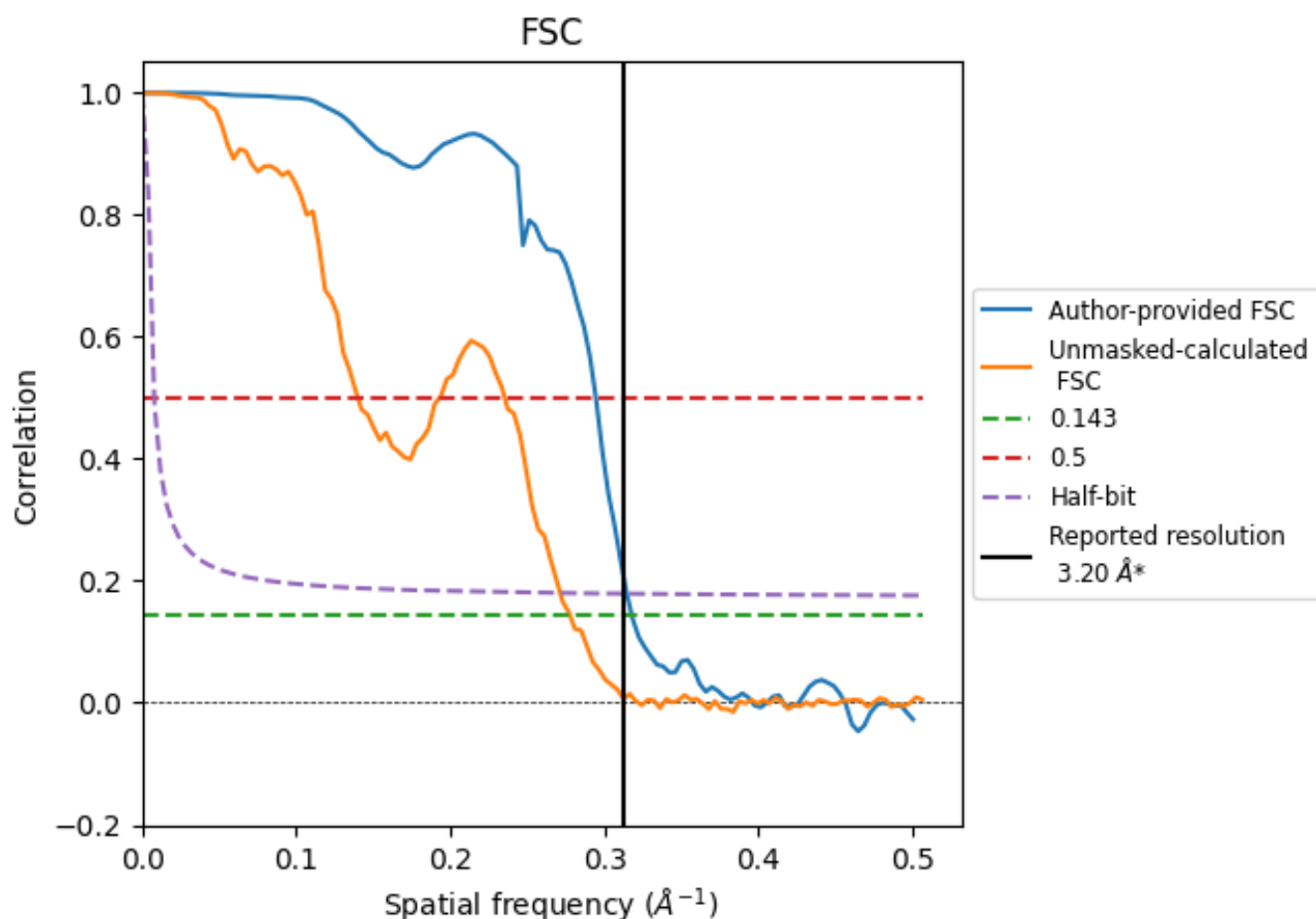


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.40	3.18
Unmasked-calculated*	3.60	7.14	3.69

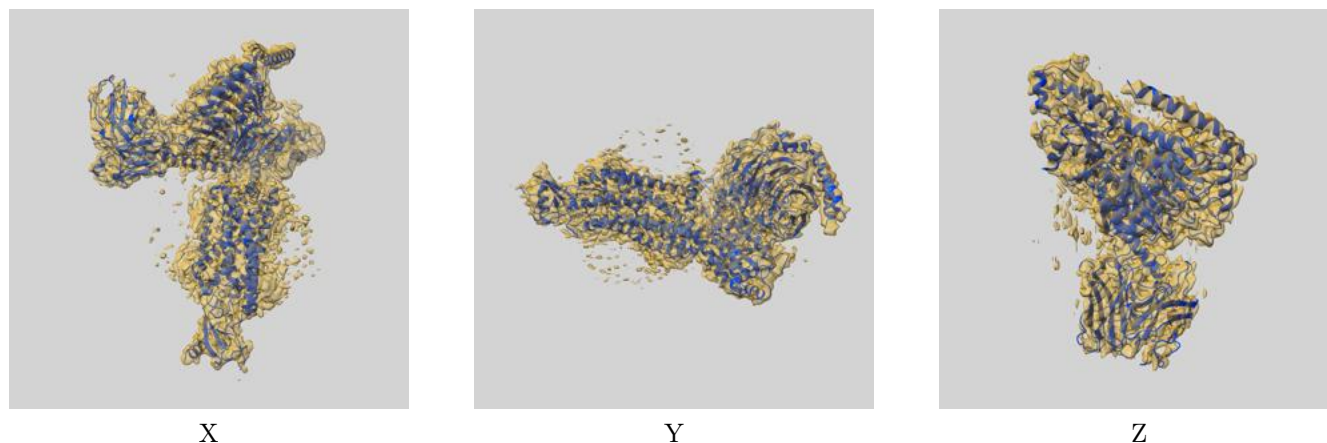
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 3.2 by more than 10 %



## 9 Map-model fit [i](#)

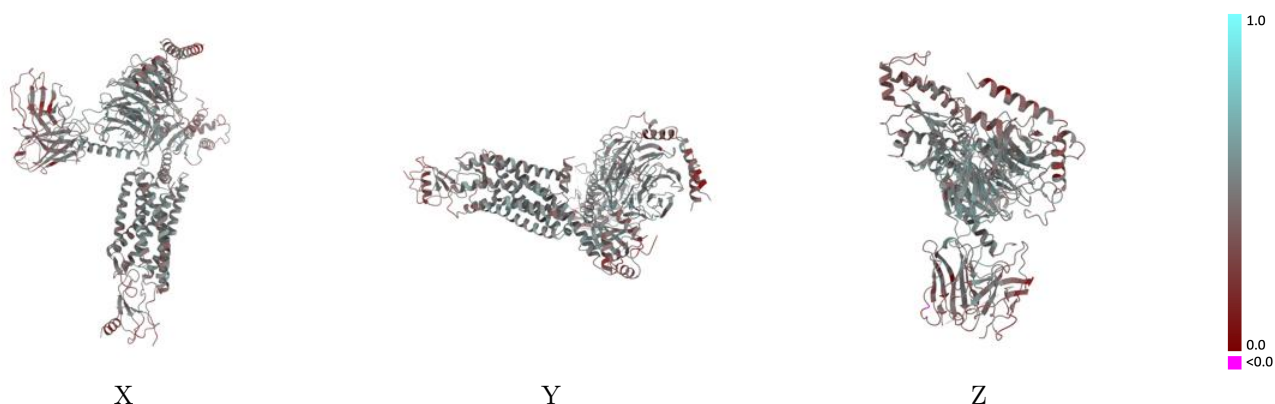
This section contains information regarding the fit between EMDB map EMD-66875 and PDB model 9XHI. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

### 9.1 Map-model overlay [i](#)



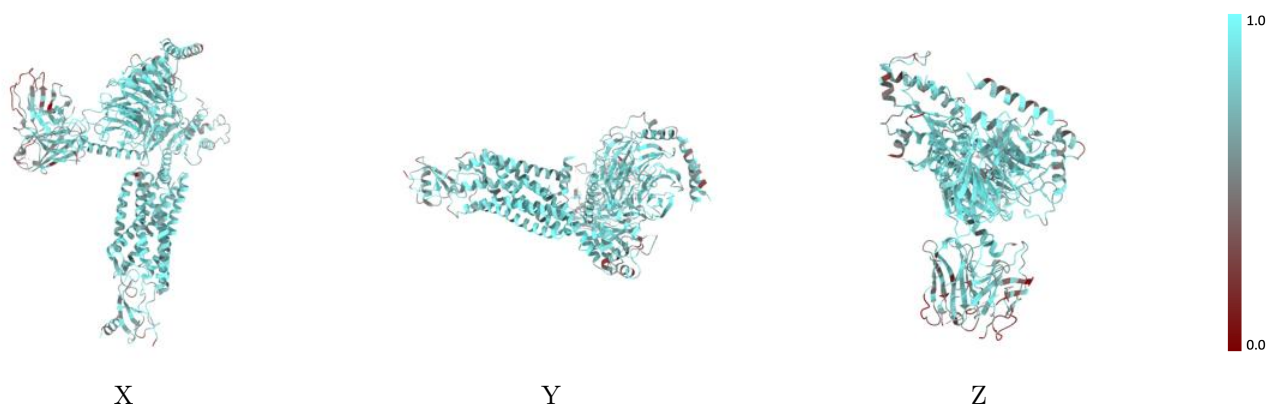
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



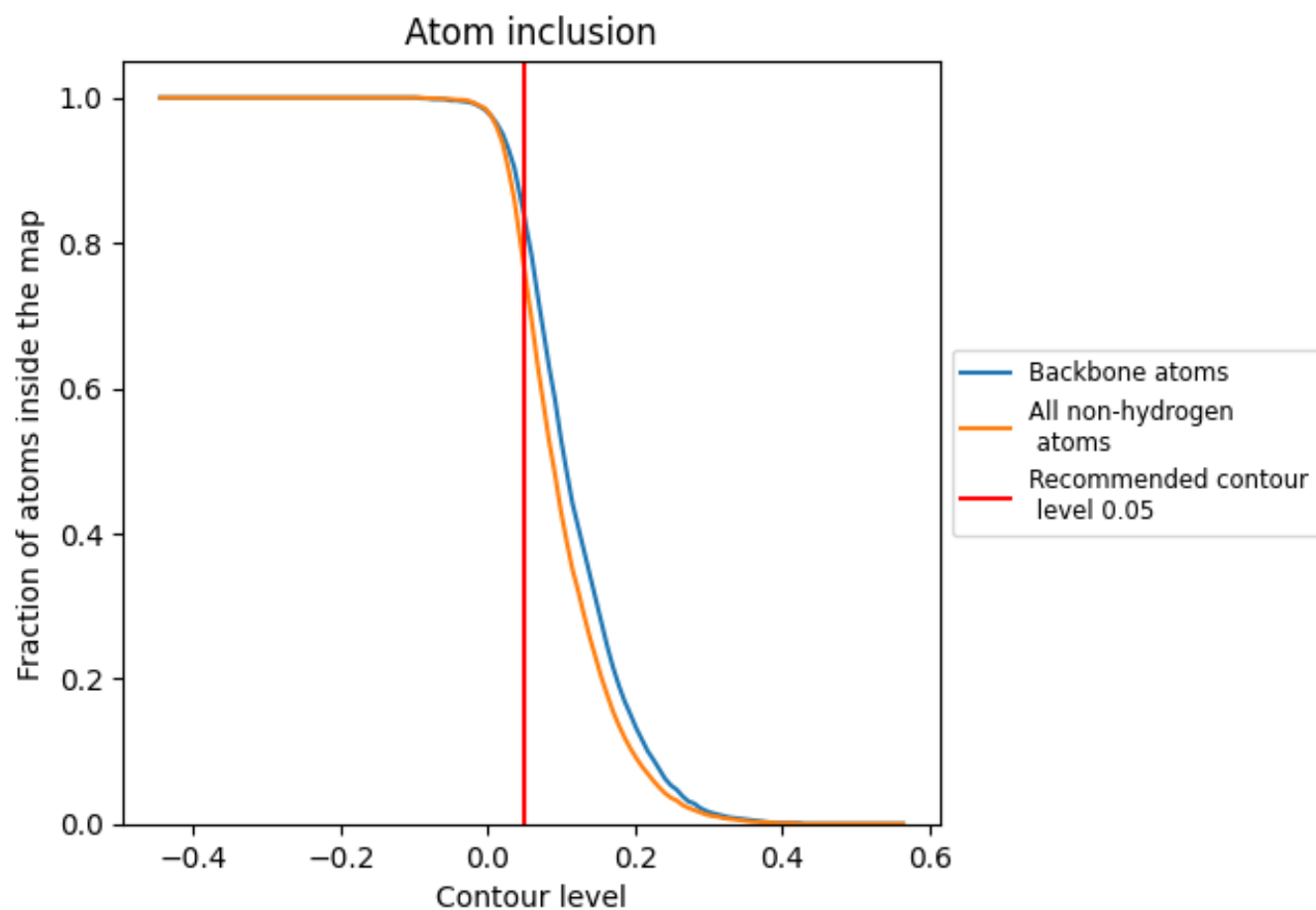
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7610	<div></div> 0.4530
A	<div></div> 0.7400	<div></div> 0.4460
B	<div></div> 0.8220	<div></div> 0.4920
C	<div></div> 0.7350	<div></div> 0.4040
D	<div></div> 0.6420	<div></div> 0.4030
L	<div></div> 0.7000	<div></div> 0.3880
R	<div></div> 0.8160	<div></div> 0.4770

