



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:23 PM UTC

PDB ID : 8XQT / pdb_00008xqt
EMDB ID : EMD-38588
Title : Structure of human class T GPCR TAS2R14-Gi complex.
Authors : Hu, X.L.; Pei, Y.; Wu, L.J.; Hua, T.; Liu, Z.J.
Deposited on : 2024-01-05
Resolution : 2.94 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

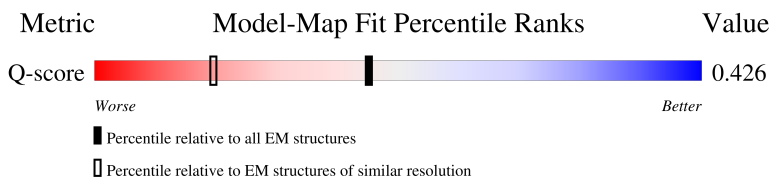
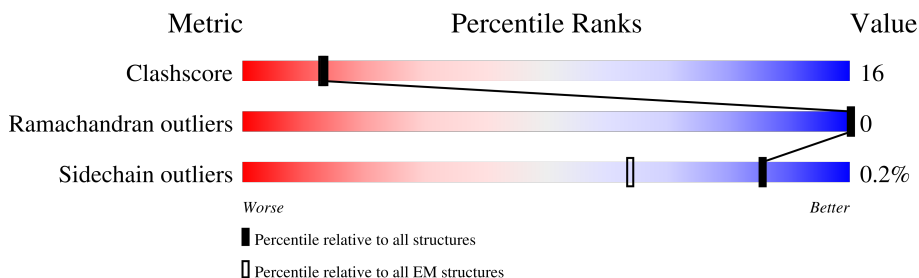
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

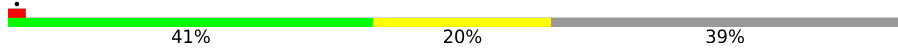
The reported resolution of this entry is 2.94 Å.

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	13068 (2.44 - 3.44)

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

Mol	Chain	Length	Quality of chain
1	A	370	
2	B	366	
3	C	71	
4	S	286	

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Mol	Chain	Length	Quality of chain
5	R	990	 A horizontal bar chart showing the quality of chain R. The bar is divided into three segments: a red segment at the beginning (18%), a green segment (10%), and a grey segment for the remainder (72%).

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8897 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
			1813	1151	300	348	14		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP P63096
A	-14	ASP	-	expression tag	UNP P63096
A	-13	TYR	-	expression tag	UNP P63096
A	-12	LYS	-	expression tag	UNP P63096
A	-11	ASP	-	expression tag	UNP P63096
A	-10	ASP	-	expression tag	UNP P63096
A	-9	ASP	-	expression tag	UNP P63096
A	-8	ASP	-	expression tag	UNP P63096
A	-7	LYS	-	expression tag	UNP P63096
A	-6	GLU	-	expression tag	UNP P63096
A	-5	ASN	-	expression tag	UNP P63096
A	-4	LEU	-	expression tag	UNP P63096
A	-3	TYR	-	expression tag	UNP P63096
A	-2	PHE	-	expression tag	UNP P63096
A	-1	GLN	-	expression tag	UNP P63096
A	0	SER	-	expression tag	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	326	SER	ALA	conflict	UNP P63096

- 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	338	Total	C	N	O	S	0	0
			2600	1604	467	508	21		

There are 26 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	56	Total	C	N	O	S	0	0
			429	269	76	81	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	232	Total	C	N	O	S	0	0
			1783	1131	295	347	10		

- Molecule 5 is a protein called Exo-alpha-sialidase,Taste receptor type 2 member 14,LgBiT.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	274	Total	C	N	O	S	0	0
			2216	1498	356	351	11		

There are 50 discrepancies between the modelled and reference sequences:

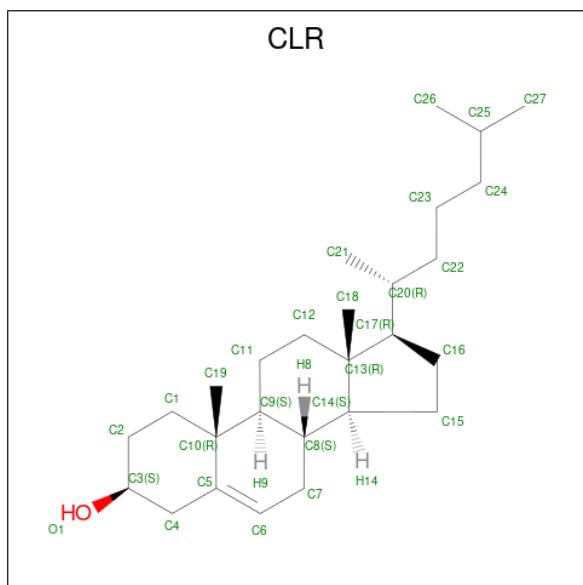
Chain	Residue	Modelled	Actual	Comment	Reference
R	-499	MET	-	initiating methionine	UNP Q59310
R	-498	LYS	-	expression tag	UNP Q59310
R	-497	THR	-	expression tag	UNP Q59310
R	-496	ILE	-	expression tag	UNP Q59310
R	-495	ILE	-	expression tag	UNP Q59310
R	-494	ALA	-	expression tag	UNP Q59310
R	-493	LEU	-	expression tag	UNP Q59310
R	-492	SER	-	expression tag	UNP Q59310
R	-491	TYR	-	expression tag	UNP Q59310
R	-490	ILE	-	expression tag	UNP Q59310
R	-489	PHE	-	expression tag	UNP Q59310
R	-488	CYS	-	expression tag	UNP Q59310
R	-487	LEU	-	expression tag	UNP Q59310
R	-486	VAL	-	expression tag	UNP Q59310
R	-485	PHE	-	expression tag	UNP Q59310
R	-484	ALA	-	expression tag	UNP Q59310
R	-483	ASP	-	expression tag	UNP Q59310
R	-482	TYR	-	expression tag	UNP Q59310
R	-481	LYS	-	expression tag	UNP Q59310
R	-480	ASP	-	expression tag	UNP Q59310
R	-479	ASP	-	expression tag	UNP Q59310
R	-478	ASP	-	expression tag	UNP Q59310
R	-477	ASP	-	expression tag	UNP Q59310
R	-476	ALA	-	expression tag	UNP Q59310
R	-475	HIS	-	expression tag	UNP Q59310
R	-474	HIS	-	expression tag	UNP Q59310
R	-473	HIS	-	expression tag	UNP Q59310
R	-472	HIS	-	expression tag	UNP Q59310
R	-471	HIS	-	expression tag	UNP Q59310
R	-470	HIS	-	expression tag	UNP Q59310
R	-469	HIS	-	expression tag	UNP Q59310
R	-468	HIS	-	expression tag	UNP Q59310
R	-467	HIS	-	expression tag	UNP Q59310
R	-466	HIS	-	expression tag	UNP Q59310
R	-465	GLU	-	expression tag	UNP Q59310
R	-464	ASN	-	expression tag	UNP Q59310
R	-463	LEU	-	expression tag	UNP Q59310

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-462	TYR	-	expression tag	UNP Q59310
R	-461	PHE	-	expression tag	UNP Q59310
R	-460	GLN	-	expression tag	UNP Q59310
R	-459	SER	-	expression tag	UNP Q59310
R	-458	GLY	-	expression tag	UNP Q59310
R	-457	ARG	-	expression tag	UNP Q59310
R	-456	ALA	-	expression tag	UNP Q59310
R	-305	SER	GLY	conflict	UNP Q59310
R	-3	GLY	-	linker	UNP Q59310
R	-2	SER	-	linker	UNP Q59310
R	-1	ALA	-	linker	UNP Q59310
R	0	GLY	-	linker	UNP Q59310
R	1	SER	-	linker	UNP Q59310

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

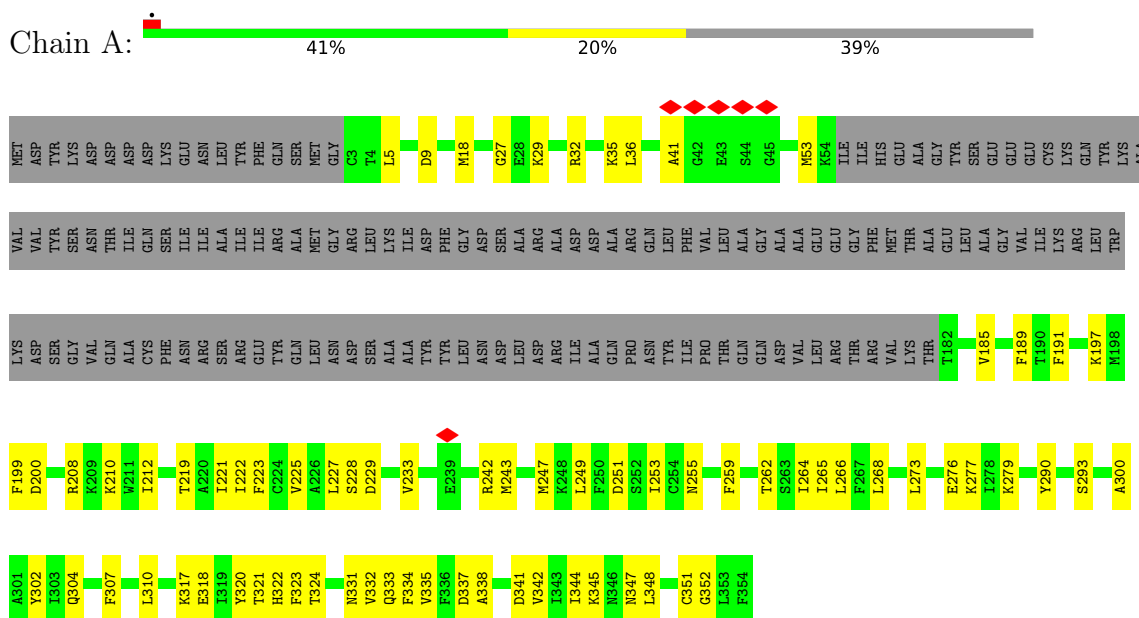


Mol	Chain	Residues	Atoms			AltConf
6	R	1	Total	C	O	0
			28	27	1	
6	R	1	Total	C	O	0
			28	27	1	

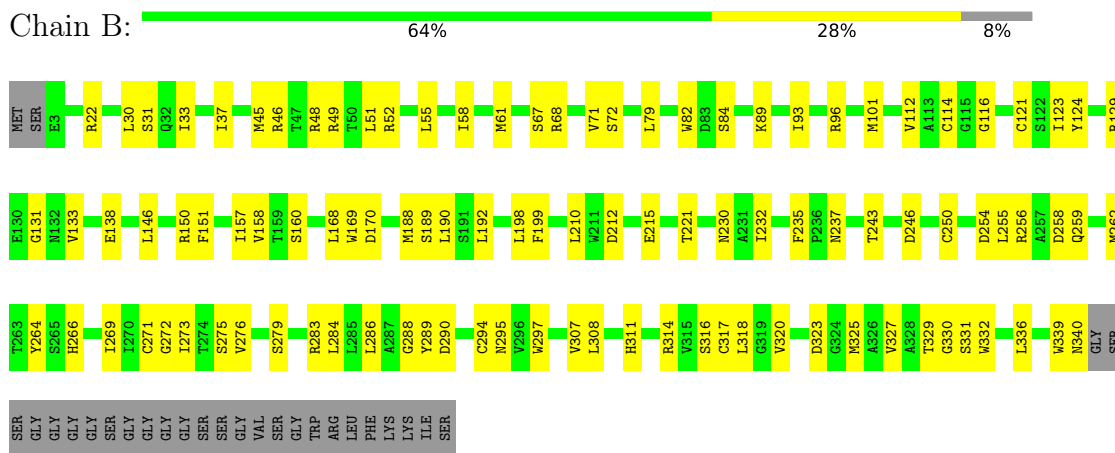
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



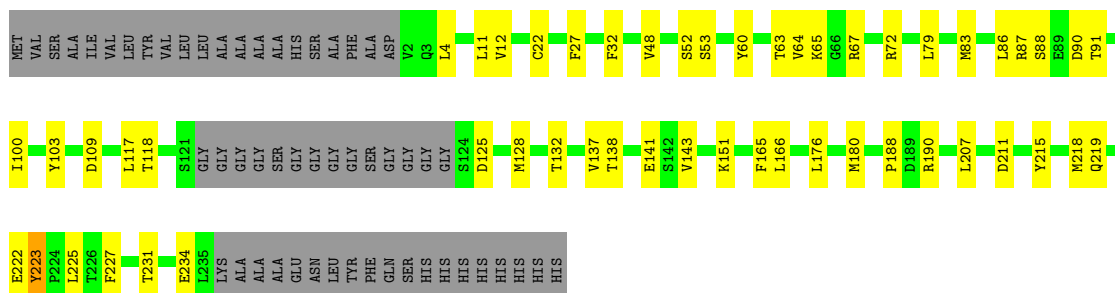
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



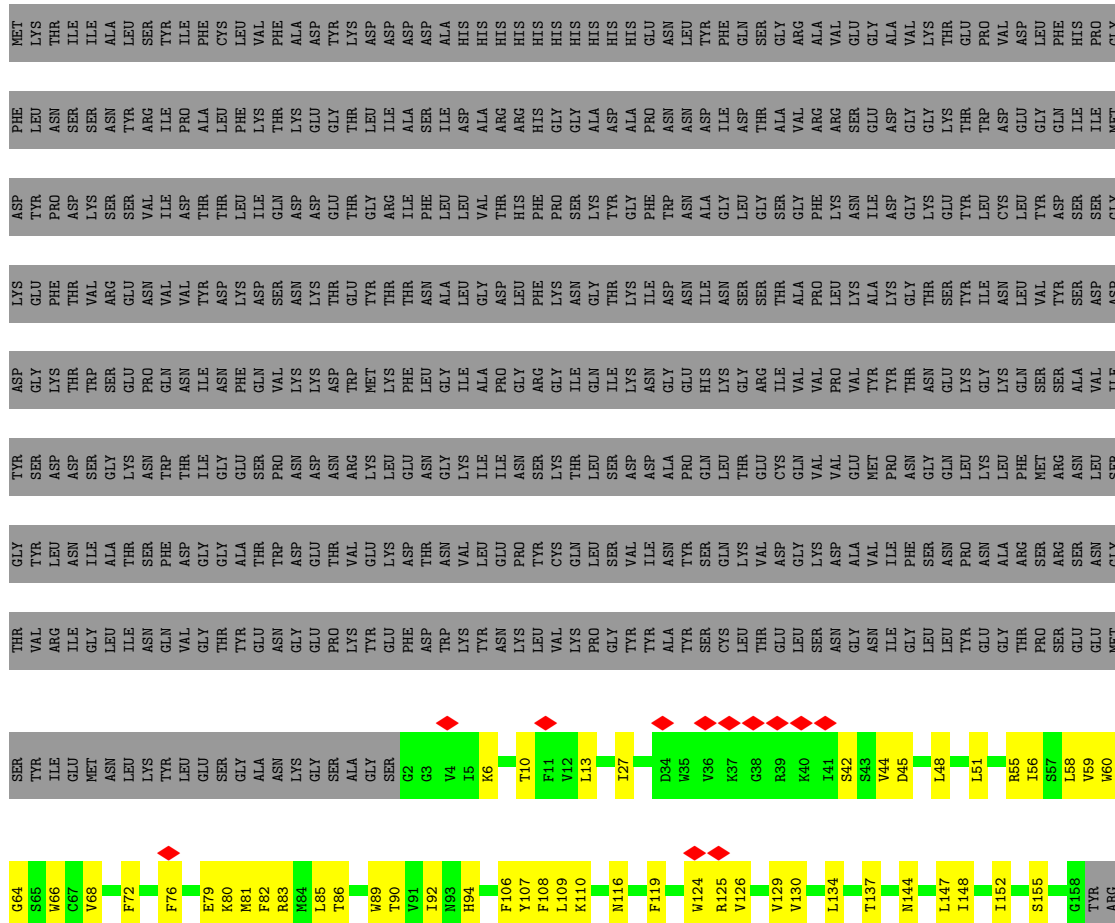
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



Chain S:



Chain R: 18% 10% 72%



ASN	LYS	THR	CYS	SER	SER	ASP	SER	SER	ASN	F172	T173	R174	F175	S176		I179	V180	L181		T184	V185	F186		L195		F198		L201	I202	F203	S204	M205	W206	K207		M212	Q213	H214	T215	V216	LYS	ILE	SER	GLY	ASP	ALA	SER	THR	LYS	ALA	ALA	HIS	R228		K231		F236	F237	L238	L239			
Y240		F243	S244	L245	S246	F247	F248	I249	S250	V251	W252	T253	S254	E255	R256	L257	E258	E259		I263	L264	S265	Q266	V267	M268	G269	M270		C275	H276	S277	C278	V279	L280	I281	L282	G283	N284	K285	K286	L287	R288		L296	W297	L298	R299	TYR	MET	PHE	LYS	ASP	GLY	PRO	GLY	PRO	SER	GLY	HIS	LYS			
GLU	PHE	ARG	GLU	SER	SER	GLY	SER	GLY	SER	GLY	SER	GLY	SER	SER	GLY	SER	GLY	SER	SER	VAL	PHE	THR	LEU	GLU	ASP	PHE	VAL	GLY	ASP	TRP	ALA	GLU	GLN	THR	ALA	ALA	LYS	TYR	ASN	LEU	VAL	ASP	GLN	VAL	LEU	LEU	GLU	GLN	GLY	GLY	VAL	SER	SER	LEU	LEU	LEU	GLN	ASN	LEU	ALA	VAL	VAL	
THR	PRO	ILE	GLN	ARG	ILE	VAL	ARG	SER	GLY	ASN	ALA	LEU	LYS	PRO	ILE	ASP	ILE	HIS	VAL	ILE	ILE	PRO	GLY	GLY	GLY	LEU	SER	VAL	ASP	GLN	MET	ALA	GLN	ILE	ASN	GLY	GLU	VAL	PHE	LYS	VAL	VAL	TYR	PRO	VAL	ASP	GLY	HIS	HIS	PHE	LYS	VAL	VAL	LEU	ILE	LEU	PRO	VAL	TYR	GLY	THR	LEU	VAL
ILE	ASP	GLY	VAL	THR	PRO	ASN	MET	LEU	ASN	TYR	PHE	GLY	ARG	PRO	TYR	GLU	ILE	ALA	VAL	PHE	ASP	GLY	LYS	LYS	ILE	THR	VAL	THR	GLY	THR	LEU	TRP	ASN	GLY	ASN	LYS	ILE	ILE	ILE	ASP	GLY	ARG	LEU	ILE	THR	PRO	ASP	GLY	SER	MET	LEU	PHE	ARG	VAL	THR	ILE	ASN	SER					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	419690	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.813	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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	A	0.15	0/1843	0.32	0/2473
2	B	0.13	0/2647	0.31	0/3589
3	C	0.08	0/435	0.20	0/587
4	S	0.13	0/1827	0.31	0/2477
5	R	0.16	0/2271	0.38	1/3077 (0.0%)
All	All	0.14	0/9023	0.33	1/12203 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	212	MET	CB-CG-SD	-5.09	97.44	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1813	0	1799	76	0
2	B	2600	0	2505	85	0
3	C	429	0	441	10	0
4	S	1783	0	1717	37	0
5	R	2216	0	2351	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	56	0	92	15	0
All	All	8897	0	8905	286	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 16.

All (286) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:MET:HE2	1:A:189:PHE:CZ	1.68	1.26
1:A:227:LEU:HD21	1:A:268:LEU:HD22	1.45	0.98
1:A:53:MET:HE2	1:A:189:PHE:HZ	0.83	0.98
1:A:53:MET:CE	1:A:189:PHE:HZ	1.77	0.97
1:A:53:MET:HE1	1:A:335:VAL:HG11	1.47	0.96
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.48	0.95
1:A:53:MET:CE	1:A:189:PHE:CZ	2.52	0.92
1:A:227:LEU:HD11	1:A:268:LEU:HB3	1.56	0.88
4:S:166:LEU:HD13	4:S:215:TYR:CZ	2.10	0.87
5:R:55:ARG:HH12	5:R:276:HIS:HB3	1.38	0.87
2:B:330:GLY:HA2	2:B:336:LEU:HD23	1.59	0.85
2:B:330:GLY:CA	2:B:336:LEU:HD23	2.06	0.84
1:A:53:MET:HG3	1:A:332:VAL:HG22	1.60	0.84
5:R:236:PHE:HB2	5:R:279:VAL:HG21	1.63	0.81
5:R:64:GLY:O	5:R:68:VAL:HG23	1.81	0.80
1:A:227:LEU:CD2	1:A:268:LEU:HD22	2.12	0.79
2:B:198:LEU:HD23	2:B:210:LEU:HD21	1.65	0.76
2:B:330:GLY:HA3	2:B:336:LEU:CD2	2.16	0.76
2:B:290:ASP:HA	2:B:314:ARG:HG3	1.71	0.71
5:R:180:VAL:HG22	6:R:501:CLR:H121	1.74	0.70
5:R:10:THR:HG23	5:R:66:TRP:HH2	1.57	0.69
4:S:67:ARG:NH2	4:S:90:ASP:OD2	2.25	0.68
2:B:330:GLY:HA3	2:B:336:LEU:HD23	1.76	0.67
2:B:325:MET:O	2:B:340:ASN:ND2	2.28	0.66
2:B:289:TYR:OH	2:B:297:TRP:NE1	2.22	0.66
1:A:227:LEU:CD1	1:A:268:LEU:HB3	2.26	0.65
1:A:53:MET:HE1	1:A:335:VAL:CG1	2.24	0.65
2:B:198:LEU:HD23	2:B:210:LEU:CD2	2.27	0.65
1:A:227:LEU:HD21	1:A:268:LEU:HB3	1.79	0.64
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.78	0.64
2:B:101:MET:HG3	2:B:116:GLY:HA2	1.79	0.64
2:B:30:LEU:HD23	2:B:262:MET:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:151:LYS:NZ	4:S:222:GLU:OE2	2.31	0.63
4:S:219:GLN:HE21	4:S:225:LEU:HA	1.63	0.63
1:A:227:LEU:HD21	1:A:268:LEU:CD2	2.23	0.63
5:R:48:LEU:HD13	5:R:287:LEU:HD11	1.79	0.63
5:R:109:LEU:HD12	5:R:126:VAL:HG13	1.81	0.63
5:R:62:ILE:HD11	5:R:266:GLN:HA	1.80	0.62
3:C:17:GLU:HA	3:C:20:LYS:HE3	1.80	0.62
2:B:198:LEU:CD2	2:B:210:LEU:HD21	2.29	0.62
4:S:166:LEU:HD13	4:S:215:TYR:CE1	2.34	0.62
2:B:72:SER:HB2	2:B:336:LEU:HD11	1.80	0.61
1:A:338:ALA:O	1:A:342:VAL:HG23	2.01	0.61
4:S:166:LEU:HD13	4:S:215:TYR:CE2	2.35	0.61
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.83	0.60
5:R:48:LEU:HD22	5:R:280:LEU:HD21	1.82	0.60
5:R:237:PHE:CE2	6:R:502:CLR:H9	2.36	0.60
2:B:330:GLY:CA	2:B:336:LEU:CD2	2.72	0.60
2:B:71:VAL:HG21	2:B:112:VAL:HG21	1.82	0.60
1:A:210:LYS:HD3	2:B:188:MET:SD	2.42	0.60
5:R:175:PHE:O	5:R:179:ILE:HG13	2.02	0.60
4:S:166:LEU:CD1	4:S:215:TYR:CE1	2.85	0.60
5:R:245:LEU:HD12	5:R:249:ILE:HG13	1.83	0.60
1:A:251:ASP:O	1:A:255:ASN:ND2	2.35	0.59
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.84	0.59
5:R:62:ILE:HG12	5:R:266:GLN:HG3	1.85	0.59
1:A:208:ARG:O	1:A:212:ILE:HB	2.02	0.59
2:B:96:ARG:NH1	2:B:138:GLU:OE2	2.36	0.59
2:B:311:HIS:NE2	2:B:329:THR:O	2.36	0.59
4:S:48:VAL:HG13	4:S:64:VAL:HG11	1.84	0.59
1:A:341:ASP:OD1	1:A:345:LYS:HG3	2.03	0.58
5:R:237:PHE:HE2	6:R:502:CLR:H9	1.68	0.58
5:R:268:MET:HE3	5:R:268:MET:HA	1.86	0.58
1:A:290:TYR:OH	1:A:293:SER:O	2.22	0.57
5:R:250:SER:OG	5:R:254:SER:O	2.21	0.57
2:B:58:ILE:O	2:B:316:SER:OG	2.17	0.57
2:B:232:ILE:HD12	2:B:243:THR:HG22	1.86	0.57
5:R:250:SER:HB3	5:R:256:ARG:NH2	2.20	0.57
1:A:324:THR:HG23	1:A:331:ASN:HD21	1.69	0.57
5:R:155:SER:HA	5:R:174:ARG:HH12	1.70	0.56
5:R:42:SER:N	5:R:45:ASP:OD2	2.34	0.56
2:B:323:ASP:OD1	2:B:323:ASP:N	2.32	0.56
1:A:219:THR:O	1:A:342:VAL:HG11	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:247:PHE:HD2	5:R:268:MET:HG2	1.71	0.56
2:B:22:ARG:NH2	2:B:221:THR:O	2.39	0.56
5:R:79:GLU:HA	5:R:82:PHE:CE2	2.41	0.56
4:S:12:VAL:HG11	4:S:86:LEU:HD12	1.87	0.56
2:B:286:LEU:HB3	2:B:318:LEU:HD21	1.88	0.56
5:R:275:CYS:O	5:R:279:VAL:HG23	2.07	0.55
5:R:44:VAL:O	5:R:48:LEU:HG	2.07	0.55
4:S:166:LEU:CD1	4:S:215:TYR:CZ	2.88	0.54
2:B:93:ILE:HG12	2:B:133:VAL:HG11	1.90	0.54
5:R:58:LEU:HD12	5:R:92:ILE:HG23	1.90	0.54
3:C:26:ASP:OD1	3:C:26:ASP:N	2.41	0.54
5:R:94:HIS:CD2	5:R:137:THR:HG23	2.42	0.54
1:A:247:MET:HB3	1:A:310:LEU:HD11	1.89	0.53
1:A:227:LEU:CG	1:A:268:LEU:HB3	2.38	0.53
2:B:129:ARG:HG2	2:B:129:ARG:HH11	1.72	0.53
1:A:227:LEU:HD11	1:A:268:LEU:CB	2.35	0.53
2:B:160:SER:CB	2:B:190:LEU:HD23	2.30	0.53
2:B:254:ASP:OD2	3:C:33:ALA:HB1	2.09	0.53
4:S:60:TYR:HB2	4:S:65:LYS:HD2	1.91	0.53
5:R:251:VAL:HG13	5:R:252:TRP:CD1	2.44	0.53
1:A:36:LEU:HD13	1:A:222:ILE:HD11	1.90	0.53
1:A:266:LEU:N	1:A:320:TYR:O	2.41	0.53
5:R:89:TRP:CZ2	6:R:501:CLR:H152	2.43	0.53
2:B:22:ARG:O	2:B:259:GLN:NE2	2.42	0.53
2:B:295:ASN:OD1	2:B:307:VAL:HG12	2.09	0.52
5:R:277:SER:O	5:R:281:ILE:HG13	2.08	0.52
1:A:347:ASN:ND2	5:R:110:LYS:O	2.43	0.52
2:B:79:LEU:HD11	2:B:114:CYS:HB3	1.91	0.52
4:S:143:VAL:HG22	4:S:207:LEU:HD11	1.89	0.52
1:A:276:GLU:HA	1:A:279:LYS:HD3	1.90	0.52
1:A:53:MET:CE	1:A:189:PHE:CE2	2.92	0.52
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.91	0.52
5:R:56:ILE:HG13	5:R:60:TRP:HD1	1.75	0.52
1:A:249:LEU:O	1:A:253:ILE:HG22	2.10	0.52
4:S:63:THR:O	4:S:67:ARG:NH1	2.43	0.51
2:B:31:SER:OG	2:B:262:MET:SD	2.67	0.51
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.91	0.51
4:S:109:ASP:OD1	4:S:109:ASP:N	2.36	0.51
5:R:203:PHE:CZ	5:R:207:LYS:HD2	2.45	0.51
5:R:212:MET:HA	5:R:215:THR:HB	1.93	0.51
5:R:86:THR:O	5:R:90:THR:OG1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:76:PHE:HA	5:R:81:MET:SD	2.50	0.51
2:B:275:SER:O	2:B:288:GLY:N	2.37	0.51
2:B:33:ILE:HD12	3:C:34:ALA:HB3	1.92	0.51
5:R:125:ARG:O	5:R:129:VAL:HG23	2.10	0.50
5:R:179:ILE:HD12	5:R:180:VAL:N	2.25	0.50
1:A:5:LEU:HD22	1:A:9:ASP:HB3	1.93	0.50
2:B:198:LEU:HD23	2:B:210:LEU:CG	2.42	0.50
2:B:67:SER:O	2:B:67:SER:OG	2.26	0.50
1:A:228:SER:O	1:A:277:LYS:NZ	2.41	0.50
2:B:258:ASP:OD2	3:C:27:ARG:NH1	2.38	0.50
5:R:44:VAL:HG23	5:R:106:PHE:CE2	2.47	0.50
5:R:80:LYS:HA	5:R:80:LYS:HE2	1.94	0.50
4:S:32:PHE:CD2	4:S:100:ILE:HB	2.46	0.50
5:R:176:SER:HA	5:R:179:ILE:HD11	1.93	0.50
5:R:6:LYS:NZ	5:R:259:GLU:O	2.45	0.49
5:R:27:ILE:HD11	5:R:281:ILE:HG12	1.93	0.49
1:A:185:VAL:HG22	1:A:200:ASP:HB3	1.93	0.49
2:B:129:ARG:HG2	2:B:129:ARG:NH1	2.27	0.49
5:R:236:PHE:HE1	5:R:275:CYS:HB2	1.77	0.49
1:A:351:CYS:HA	5:R:44:VAL:HG21	1.95	0.49
2:B:158:VAL:HG12	2:B:190:LEU:HD22	1.93	0.49
5:R:263:ILE:HG23	5:R:264:LEU:HD12	1.94	0.49
1:A:27:GLY:HA3	2:B:55:LEU:HD13	1.93	0.49
1:A:225:VAL:HG21	1:A:307:PHE:CE1	2.47	0.49
2:B:72:SER:CB	2:B:336:LEU:HD11	2.42	0.49
5:R:198:PHE:O	5:R:202:ILE:HG12	2.13	0.48
5:R:237:PHE:HZ	6:R:502:CLR:H14	1.77	0.48
1:A:191:PHE:CD1	1:A:332:VAL:CG1	2.96	0.48
2:B:61:MET:HB3	2:B:317:CYS:SG	2.54	0.48
1:A:341:ASP:OD1	1:A:341:ASP:O	2.32	0.48
5:R:268:MET:HB3	6:R:501:CLR:H221	1.94	0.48
2:B:273:ILE:HG13	2:B:289:TYR:CE2	2.49	0.48
4:S:22:CYS:HB3	4:S:79:LEU:HB3	1.94	0.48
1:A:221:ILE:HD13	1:A:253:ILE:HD11	1.96	0.48
1:A:228:SER:CB	1:A:273:LEU:HD12	2.44	0.47
2:B:112:VAL:HG12	2:B:124:TYR:HB2	1.95	0.47
2:B:131:GLY:HA3	4:S:32:PHE:CZ	2.48	0.47
5:R:243:PHE:HB3	5:R:268:MET:HE1	1.95	0.47
1:A:191:PHE:CD1	1:A:332:VAL:HG11	2.49	0.47
1:A:300:ALA:HB1	1:A:323:PHE:CE2	2.49	0.47
5:R:179:ILE:HD12	5:R:180:VAL:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:PHE:CG	1:A:332:VAL:HG12	2.49	0.47
1:A:259:PHE:HB3	1:A:262:THR:HB	1.94	0.47
3:C:16:VAL:O	3:C:20:LYS:HG3	2.15	0.47
5:R:248:PHE:O	5:R:251:VAL:HG12	2.15	0.47
1:A:227:LEU:CD2	1:A:268:LEU:HB3	2.43	0.47
5:R:282:LEU:O	5:R:288:ARG:NH1	2.47	0.47
5:R:276:HIS:CE1	6:R:502:CLR:H221	2.50	0.47
6:R:502:CLR:H211	6:R:502:CLR:H263	1.96	0.47
1:A:304:GLN:HG3	1:A:321:THR:HG21	1.96	0.47
2:B:68:ARG:HD3	4:S:103:TYR:CZ	2.50	0.47
2:B:188:MET:HE3	2:B:188:MET:HB3	1.58	0.47
5:R:85:LEU:HG	6:R:501:CLR:H41	1.97	0.47
2:B:294:CYS:HB3	2:B:308:LEU:HB2	1.96	0.46
2:B:212:ASP:HB3	2:B:215:GLU:HB2	1.98	0.46
5:R:13:LEU:HD13	5:R:266:GLN:OE1	2.14	0.46
1:A:341:ASP:OD2	1:A:345:LYS:HE2	2.15	0.46
1:A:29:LYS:HB2	1:A:29:LYS:NZ	2.31	0.46
2:B:52:ARG:HG2	2:B:52:ARG:HH11	1.80	0.46
4:S:125:ASP:OD1	4:S:125:ASP:N	2.48	0.46
5:R:48:LEU:HD11	5:R:284:ASN:ND2	2.30	0.46
5:R:237:PHE:HA	5:R:240:TYR:HB3	1.98	0.46
2:B:37:ILE:HD11	2:B:283:ARG:NH1	2.30	0.46
5:R:6:LYS:HD2	5:R:6:LYS:HA	1.77	0.46
5:R:86:THR:HG23	6:R:501:CLR:H192	1.97	0.46
2:B:158:VAL:HG23	2:B:168:LEU:HD13	1.98	0.46
2:B:331:SER:OG	2:B:332:TRP:N	2.49	0.46
5:R:59:VAL:HG22	5:R:270:MET:HE1	1.96	0.46
3:C:23:ALA:HA	3:C:27:ARG:HH22	1.81	0.46
2:B:157:ILE:HG22	2:B:169:TRP:HB2	1.98	0.46
4:S:218:MET:HE2	4:S:227:PHE:CZ	2.51	0.45
1:A:223:PHE:CZ	1:A:249:LEU:HD23	2.51	0.45
2:B:289:TYR:CE1	2:B:295:ASN:HB2	2.51	0.45
1:A:233:VAL:O	1:A:242:ARG:NH2	2.49	0.45
4:S:11:LEU:HD22	4:S:118:THR:HB	1.99	0.45
1:A:18:MET:SD	4:S:53:SER:O	2.74	0.45
2:B:71:VAL:HG22	2:B:79:LEU:HD22	1.99	0.45
2:B:246:ASP:HA	2:B:272:GLY:HA3	1.98	0.45
5:R:108:PHE:HA	5:R:201:LEU:HD12	1.99	0.45
5:R:10:THR:HG23	5:R:66:TRP:CH2	2.44	0.45
5:R:184:THR:HG21	5:R:248:PHE:CZ	2.52	0.45
6:R:502:CLR:H262	6:R:502:CLR:H232	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:SER:OG	2:B:230:ASN:O	2.33	0.45
2:B:250:CYS:SG	2:B:273:ILE:HG12	2.57	0.45
2:B:256:ARG:HB3	3:C:28:ILE:HG12	1.98	0.44
2:B:273:ILE:HG21	2:B:276:VAL:HG23	1.99	0.44
2:B:329:THR:OG1	2:B:339:TRP:NE1	2.46	0.44
5:R:247:PHE:HA	5:R:256:ARG:NH2	2.31	0.44
1:A:32:ARG:HE	5:R:124:TRP:HE1	1.66	0.44
5:R:80:LYS:HE2	5:R:83:ARG:HE	1.81	0.44
1:A:221:ILE:HD11	1:A:259:PHE:CD2	2.52	0.44
2:B:45:MET:HG3	2:B:339:TRP:HB3	1.99	0.44
1:A:35:LYS:HB3	1:A:199:PHE:HE2	1.82	0.44
1:A:225:VAL:HG21	1:A:307:PHE:CZ	2.52	0.44
2:B:235:PHE:HD1	2:B:237:ASN:H	1.64	0.44
5:R:83:ARG:HG3	5:R:152:ILE:HG21	1.99	0.44
4:S:166:LEU:HB2	4:S:176:LEU:HD11	1.99	0.44
5:R:13:LEU:HD21	5:R:267:VAL:HA	1.99	0.44
1:A:273:LEU:HA	1:A:276:GLU:HB3	1.99	0.44
2:B:79:LEU:HB2	2:B:93:ILE:HB	1.99	0.44
5:R:155:SER:HA	5:R:174:ARG:HH22	1.82	0.44
1:A:318:GLU:CD	1:A:345:LYS:HE3	2.43	0.44
4:S:165:PHE:CE1	4:S:218:MET:HE3	2.53	0.44
5:R:198:PHE:CE1	5:R:202:ILE:HG13	2.53	0.44
1:A:341:ASP:OD1	1:A:345:LYS:HE2	2.17	0.44
4:S:190:ARG:NH2	4:S:211:ASP:OD2	2.51	0.43
1:A:227:LEU:HD21	1:A:268:LEU:CB	2.48	0.43
1:A:264:ILE:HG13	1:A:317:LYS:NZ	2.34	0.43
2:B:289:TYR:HE1	2:B:295:ASN:HB2	1.82	0.43
5:R:236:PHE:CE1	5:R:275:CYS:HB2	2.52	0.43
5:R:247:PHE:CG	5:R:264:LEU:HB3	2.53	0.43
2:B:273:ILE:HD12	2:B:273:ILE:N	2.33	0.43
1:A:290:TYR:HD1	1:A:302:TYR:HD2	1.67	0.43
2:B:82:TRP:CH2	2:B:89:LYS:HE3	2.53	0.43
4:S:52:SER:O	4:S:72:ARG:NH1	2.52	0.43
4:S:132:THR:HB	4:S:231:THR:HG23	2.01	0.43
4:S:138:THR:HG22	4:S:141:GLU:HB2	2.00	0.43
1:A:266:LEU:HD23	1:A:321:THR:HG22	2.00	0.43
2:B:279:SER:HB2	2:B:284:LEU:HB2	2.01	0.43
5:R:51:LEU:HD11	5:R:55:ARG:HE	1.84	0.43
1:A:53:MET:O	1:A:53:MET:HG2	2.17	0.43
5:R:267:VAL:HG12	5:R:268:MET:SD	2.59	0.43
5:R:107:TYR:CE2	6:R:502:CLR:H261	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:134:LEU:HA	5:R:137:THR:HB	2.01	0.43
5:R:144:ASN:O	5:R:148:ILE:HG13	2.19	0.43
1:A:322:HIS:HB2	1:A:334:PHE:CE2	2.54	0.42
1:A:320:TYR:HB3	1:A:334:PHE:HZ	1.83	0.42
5:R:181:LEU:HA	5:R:252:TRP:CZ2	2.54	0.42
5:R:195:LEU:HD23	6:R:502:CLR:C6	2.49	0.42
2:B:266:HIS:HB3	2:B:269:ILE:HG12	2.01	0.42
5:R:13:LEU:HD23	5:R:13:LEU:HA	1.87	0.42
2:B:150:ARG:HG3	2:B:190:LEU:HD12	2.01	0.42
4:S:4:LEU:HD21	4:S:27:PHE:HZ	1.83	0.42
5:R:58:LEU:O	5:R:62:ILE:HG22	2.20	0.42
5:R:110:LYS:HB3	5:R:110:LYS:HE3	1.82	0.42
2:B:49:ARG:HE	2:B:49:ARG:HB2	1.68	0.42
4:S:137:VAL:HG21	4:S:207:LEU:HD22	2.02	0.42
5:R:147:LEU:HD12	5:R:186:PHE:CZ	2.54	0.42
1:A:221:ILE:O	1:A:265:ILE:N	2.42	0.42
4:S:137:VAL:HG22	4:S:234:GLU:O	2.20	0.41
2:B:46:ARG:HB2	2:B:48:ARG:NH1	2.36	0.41
2:B:121:CYS:HB2	2:B:146:LEU:HD21	2.02	0.41
2:B:192:LEU:HD23	2:B:199:PHE:HB3	2.02	0.41
1:A:259:PHE:N	1:A:259:PHE:CD1	2.84	0.41
4:S:180:MET:HE2	4:S:180:MET:HB3	1.84	0.41
1:A:344:ILE:HD13	5:R:205:MET:HE1	2.02	0.41
2:B:61:MET:HB3	2:B:61:MET:HE3	1.89	0.41
4:S:88:SER:O	4:S:91:THR:HG22	2.21	0.41
5:R:237:PHE:CZ	6:R:502:CLR:H14	2.55	0.41
1:A:333:GLN:O	1:A:337:ASP:OD1	2.38	0.41
4:S:188:PRO:HB2	4:S:190:ARG:HD3	2.02	0.41
4:S:223:TYR:O	4:S:225:LEU:N	2.52	0.41
1:A:243:MET:O	1:A:247:MET:HG3	2.20	0.41
5:R:180:VAL:HG11	5:R:251:VAL:HG11	2.02	0.41
2:B:123:ILE:HG23	2:B:151:PHE:HZ	1.86	0.41
1:A:41:ALA:HB2	1:A:249:LEU:HD22	2.02	0.41
1:A:191:PHE:CD1	1:A:332:VAL:HG12	2.56	0.41
2:B:49:ARG:HH21	3:C:61:PHE:HA	1.86	0.41
2:B:84:SER:HB3	3:C:61:PHE:HE1	1.85	0.41
5:R:179:ILE:HD13	6:R:501:CLR:H112	2.02	0.41
2:B:170:ASP:C	2:B:170:ASP:OD1	2.64	0.41
4:S:128:MET:CE	4:S:219:GLN:HB3	2.51	0.41
5:R:130:VAL:O	5:R:134:LEU:HG	2.21	0.41
5:R:147:LEU:HA	5:R:147:LEU:HD23	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:72:PHE:HD1	5:R:72:PHE:HA	1.76	0.40
1:A:197:LYS:HZ2	1:A:197:LYS:HG2	1.74	0.40
1:A:227:LEU:HD21	1:A:268:LEU:CG	2.50	0.40
1:A:229:ASP:OD2	1:A:242:ARG:HD2	2.22	0.40
5:R:116:ASN:HB3	5:R:119:PHE:CG	2.56	0.40
5:R:59:VAL:HG13	5:R:270:MET:HE1	2.02	0.40
1:A:348:LEU:O	1:A:352:GLY:N	2.55	0.40
4:S:83:MET:HE1	4:S:117:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/370 (60%)	214 (97%)	7 (3%)	0	100	100
2	B	336/366 (92%)	321 (96%)	15 (4%)	0	100	100
3	C	54/71 (76%)	54 (100%)	0	0	100	100
4	S	228/286 (80%)	218 (96%)	10 (4%)	0	100	100
5	R	268/990 (27%)	266 (99%)	2 (1%)	0	100	100
All	All	1107/2083 (53%)	1073 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/322 (62%)	201 (100%)	0	100	100
2	B	281/298 (94%)	281 (100%)	0	100	100
3	C	45/58 (78%)	45 (100%)	0	100	100
4	S	197/229 (86%)	195 (99%)	2 (1%)	68	81
5	R	249/864 (29%)	249 (100%)	0	100	100
All	All	973/1771 (55%)	971 (100%)	2 (0%)	85	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	S	87	ARG
4	S	223	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	HIS
2	B	156	GLN
4	S	82	GLN
5	R	94	HIS
5	R	151	HIS
5	R	208	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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	CLR	R	501	-	31,31,31	0.26	0	48,48,48	0.47	0
6	CLR	R	502	-	31,31,31	0.36	0	48,48,48	1.04	3 (6%)

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	501	-	-	5/10/68/68	0/4/4/4
6	CLR	R	502	-	-	9/10/68/68	0/4/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	R	502	CLR	C7-C8-C9	2.43	112.53	109.72
6	R	502	CLR	C14-C8-C9	-2.31	106.06	109.09
6	R	502	CLR	C10-C9-C8	2.31	116.09	112.71

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	502	CLR	C16-C17-C20-C21
6	R	501	CLR	C13-C17-C20-C21
6	R	502	CLR	C13-C17-C20-C21
6	R	501	CLR	C16-C17-C20-C21
6	R	501	CLR	C13-C17-C20-C22

Continued on next page...

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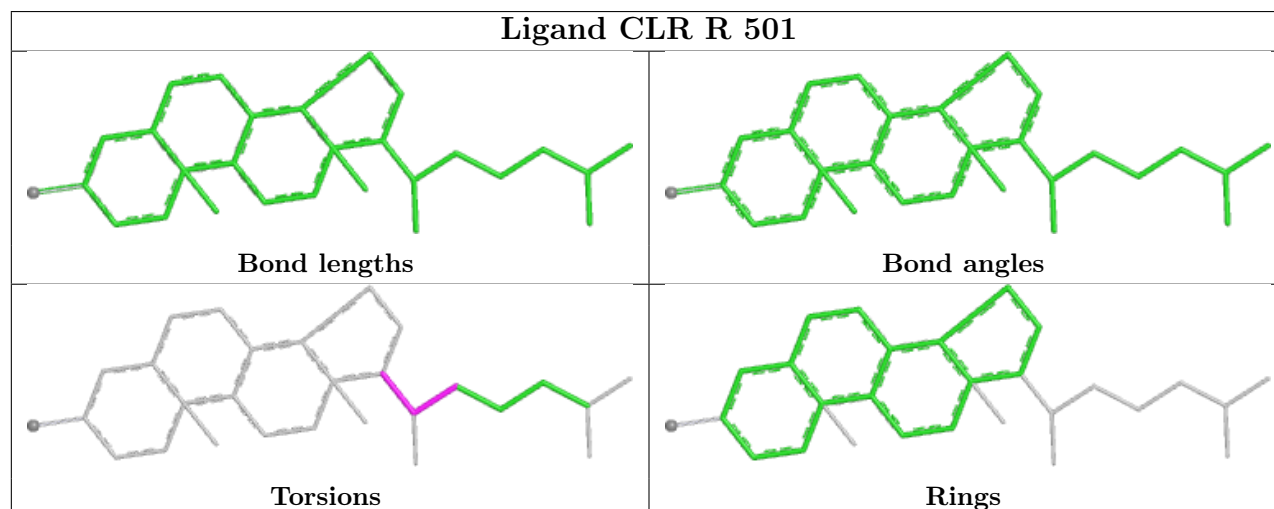
Mol	Chain	Res	Type	Atoms
6	R	502	CLR	C13-C17-C20-C22
6	R	501	CLR	C16-C17-C20-C22
6	R	502	CLR	C16-C17-C20-C22
6	R	502	CLR	C22-C23-C24-C25
6	R	502	CLR	C20-C22-C23-C24
6	R	502	CLR	C23-C24-C25-C26
6	R	501	CLR	C21-C20-C22-C23
6	R	502	CLR	C17-C20-C22-C23
6	R	502	CLR	C21-C20-C22-C23

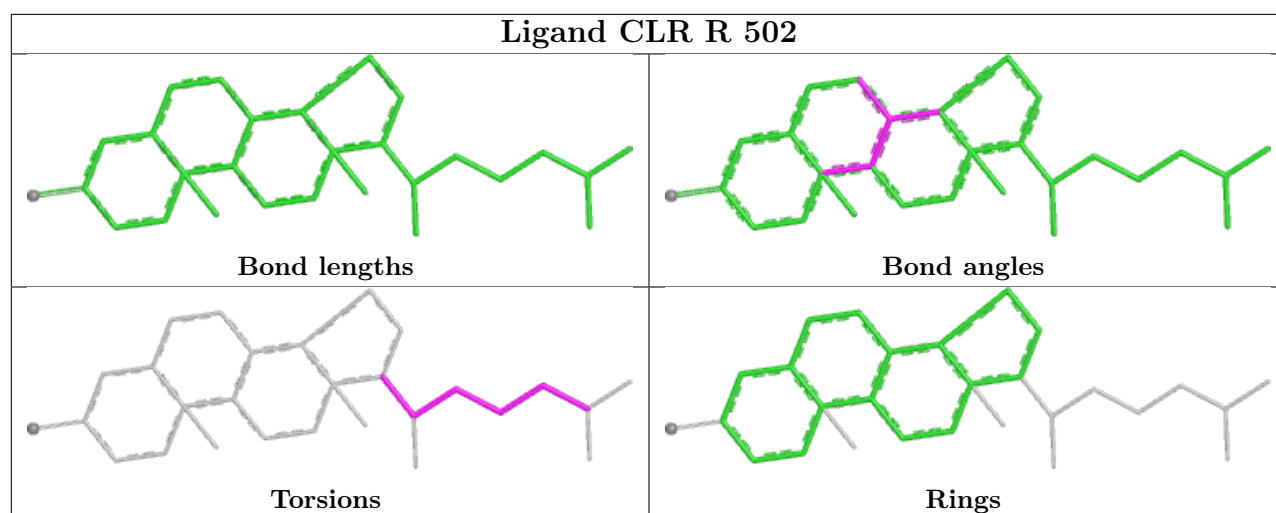
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	501	CLR	6	0
6	R	502	CLR	9	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-38588. These allow visual inspection of the internal detail of the map and identification of artifacts.

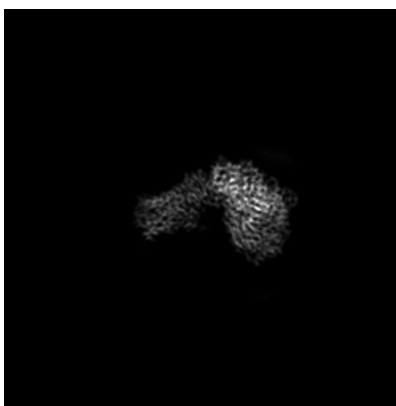
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

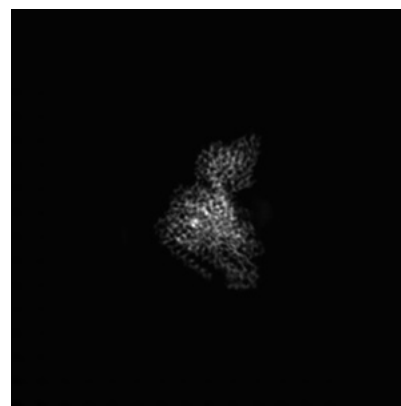
6.1.1 Primary map



X

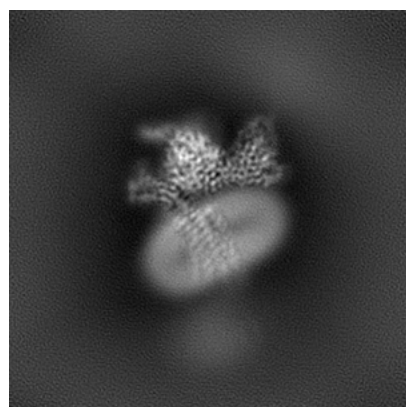


Y

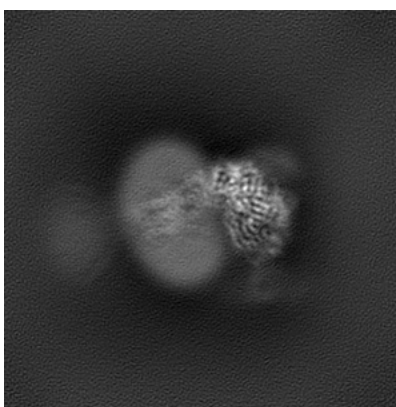


Z

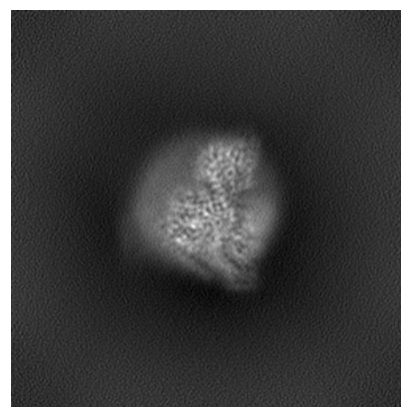
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

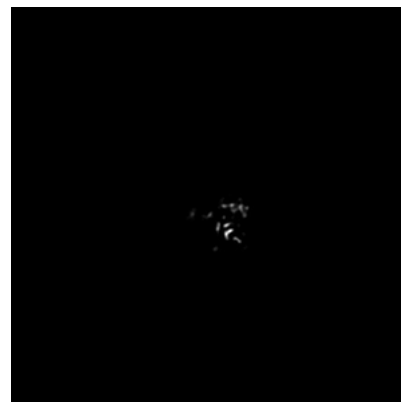
6.2.1 Primary map



X Index: 128

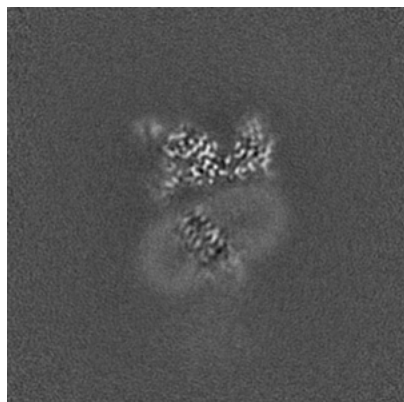


Y Index: 128

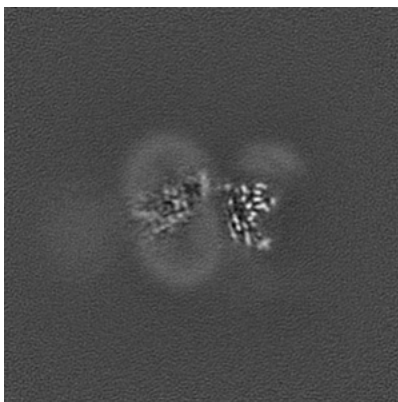


Z Index: 128

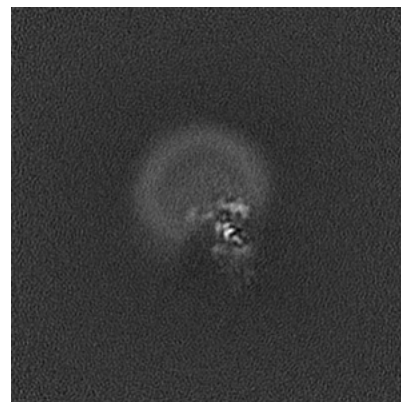
6.2.2 Raw map



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: 131

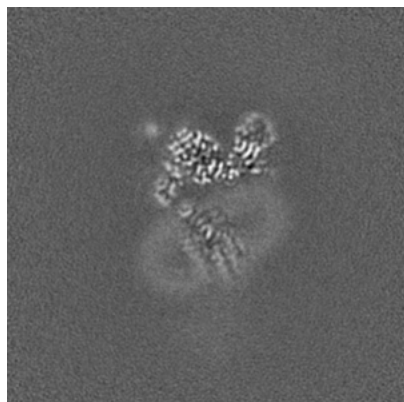


Y Index: 117

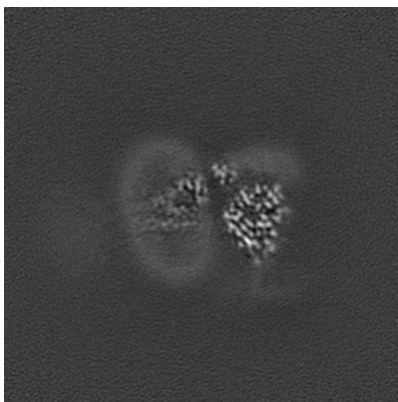


Z Index: 153

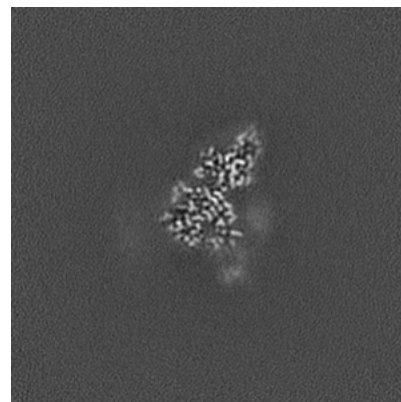
6.3.2 Raw map



X Index: 131



Y Index: 117

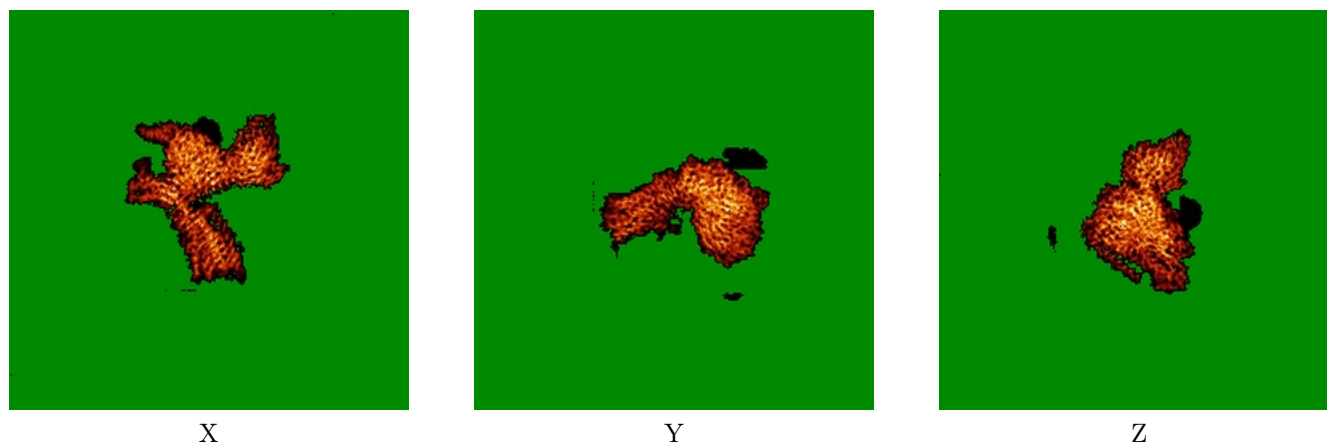


Z Index: 154

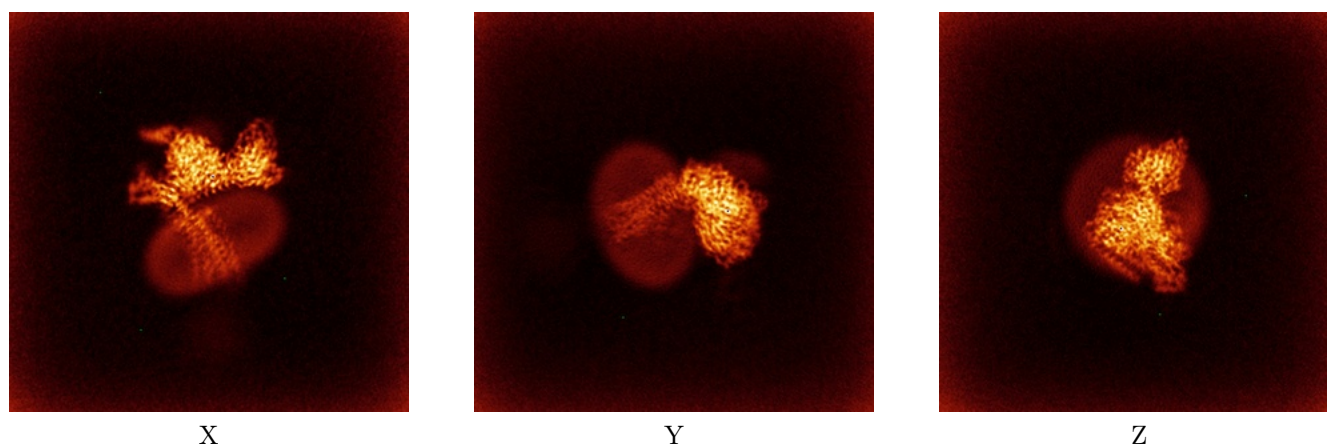
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

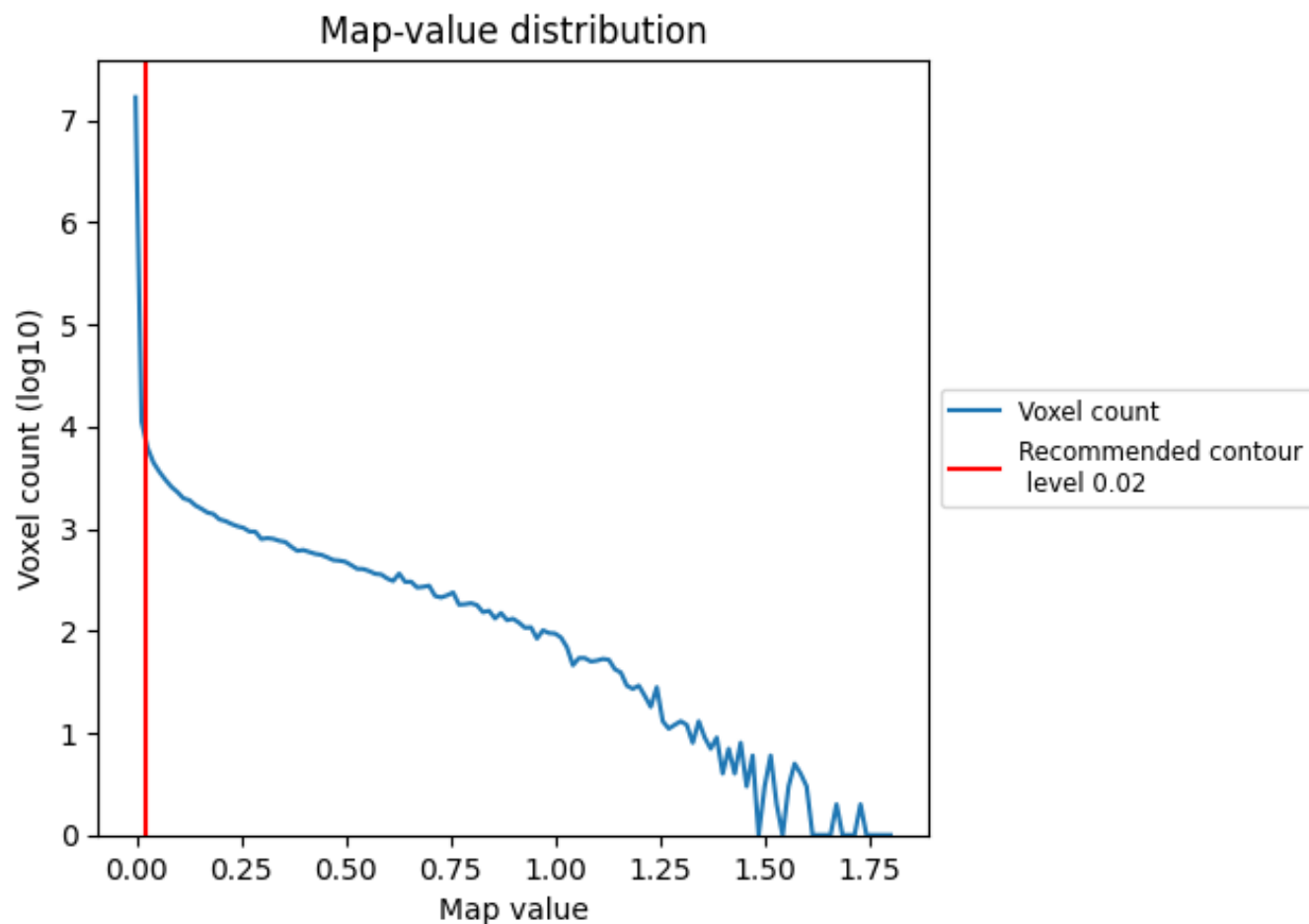
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

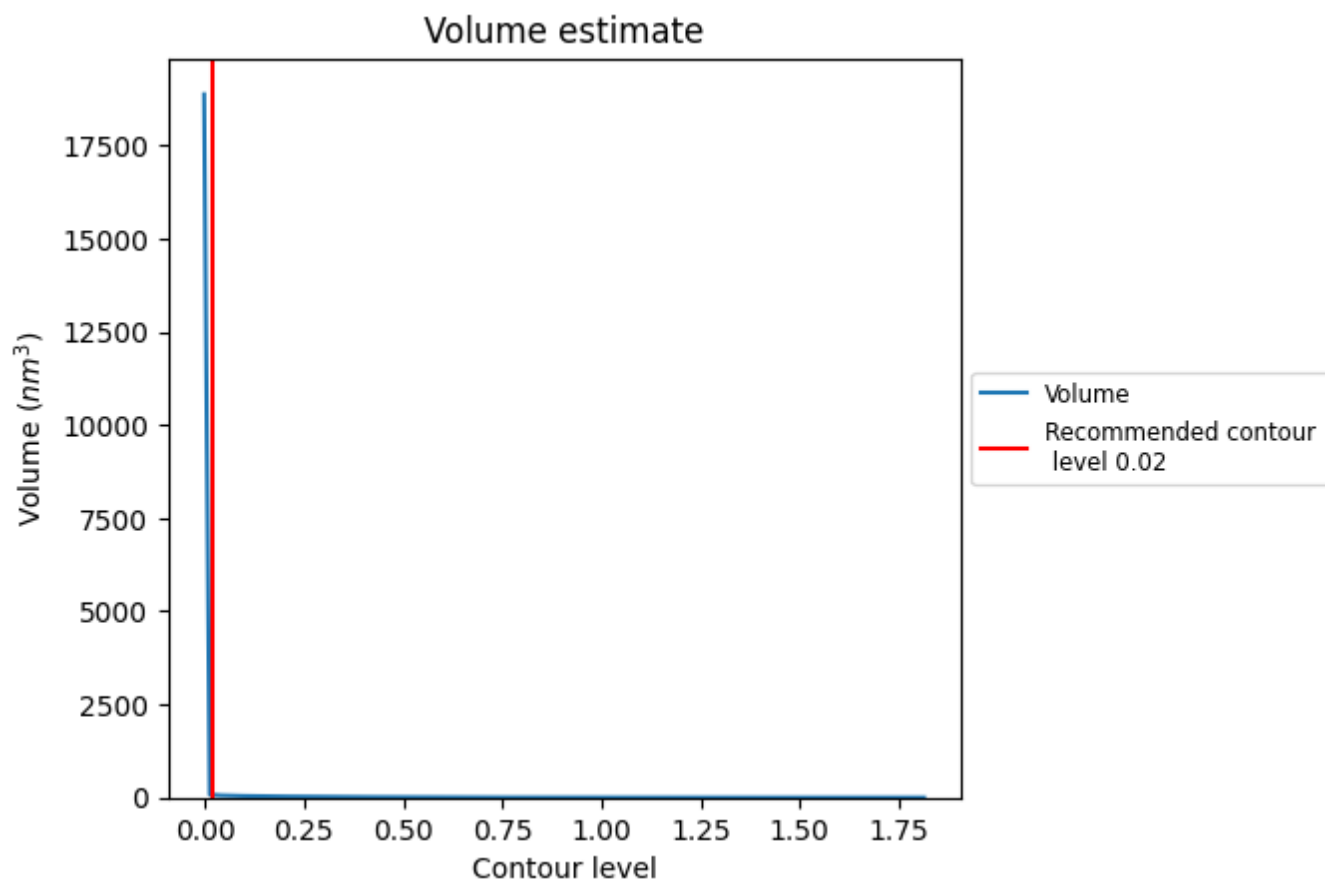
This section contains the results of statistical analysis of the map.

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.

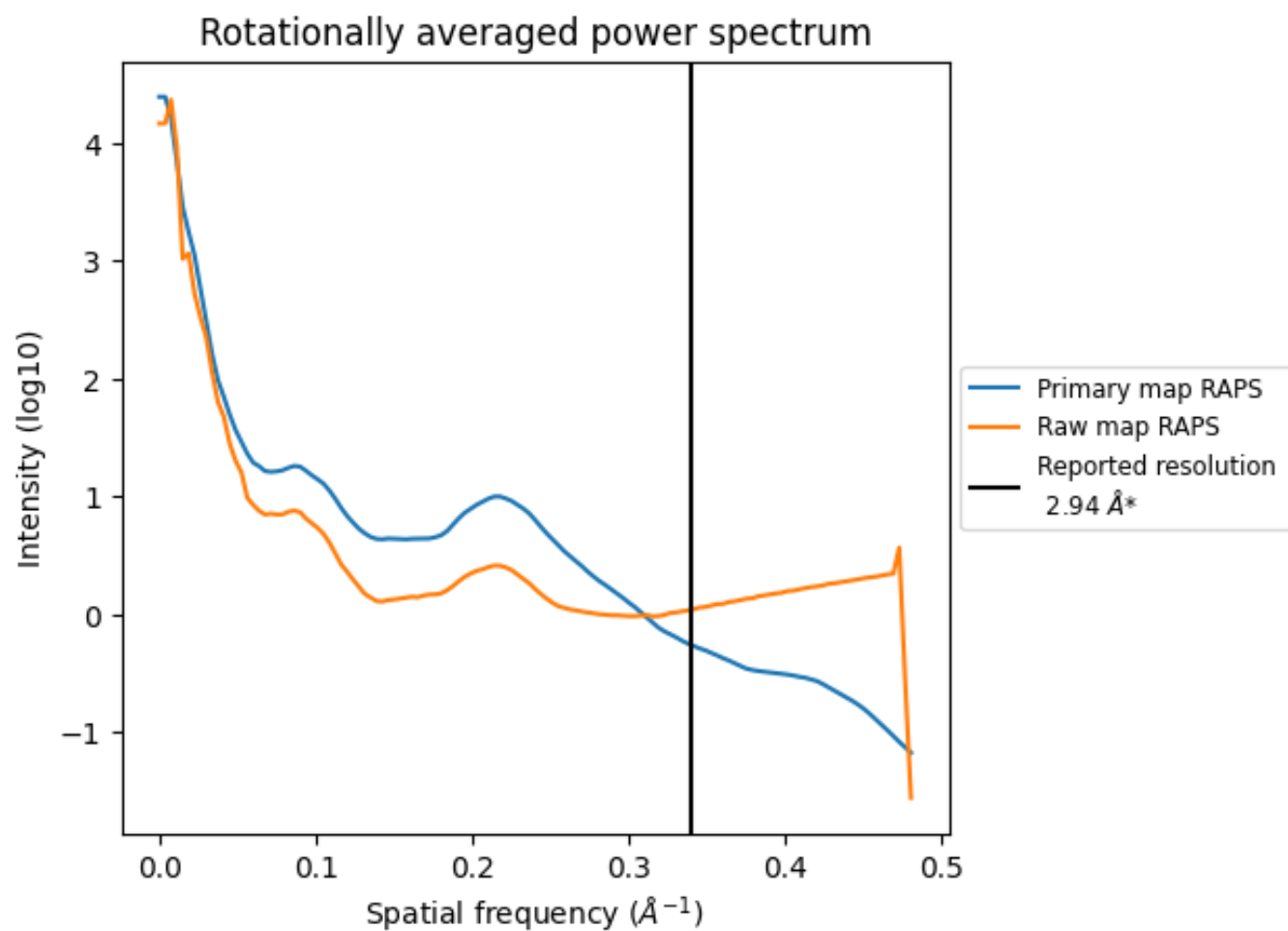
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm^3 ; this corresponds to an approximate mass of 64 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 ⓘ

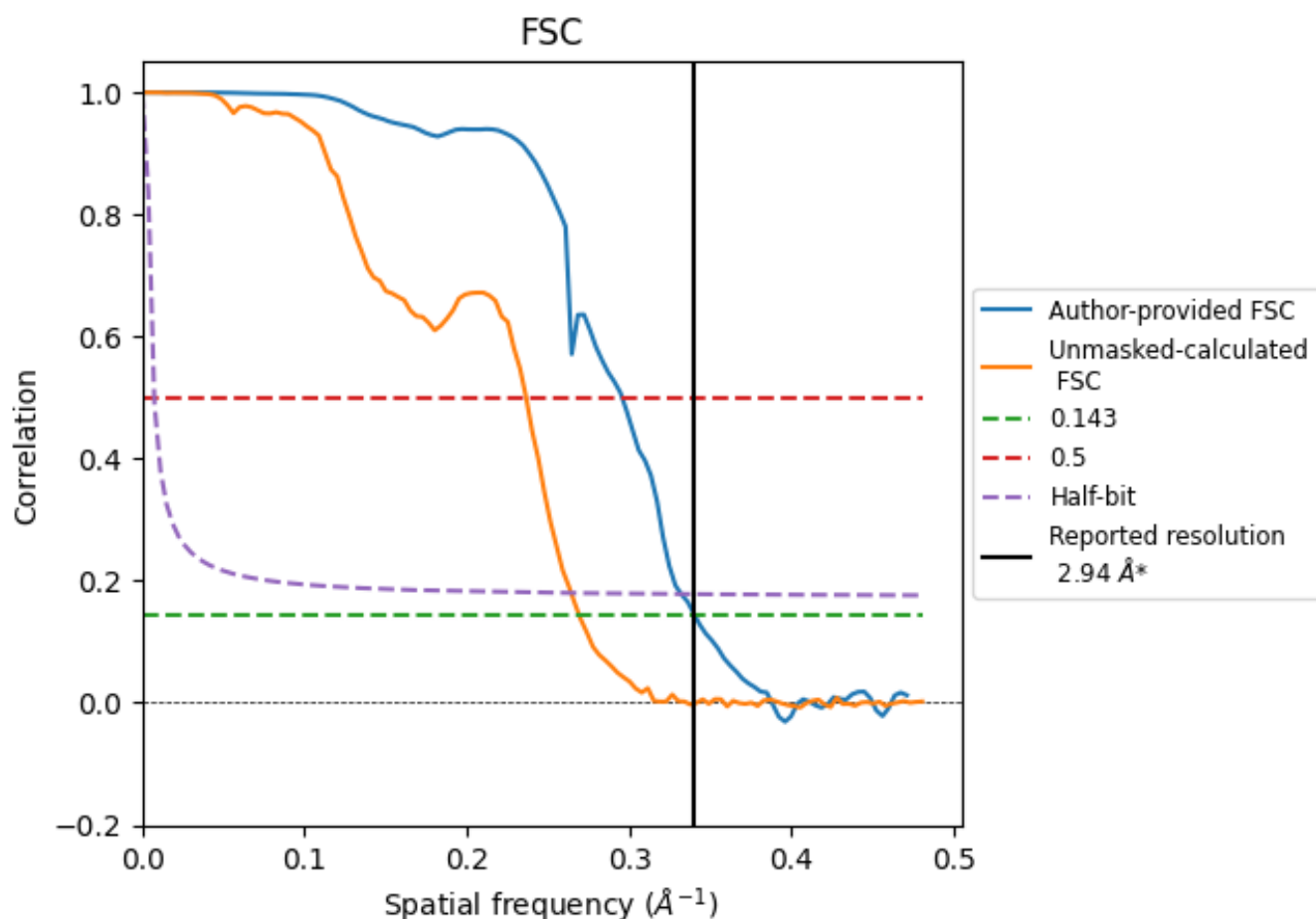


*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

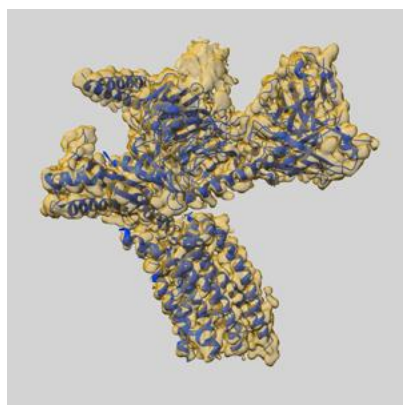
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.94	3.38	3.01
Unmasked-calculated*	3.71	4.22	3.78

*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 3.71 differs from the reported value 2.94 by more than 10 %

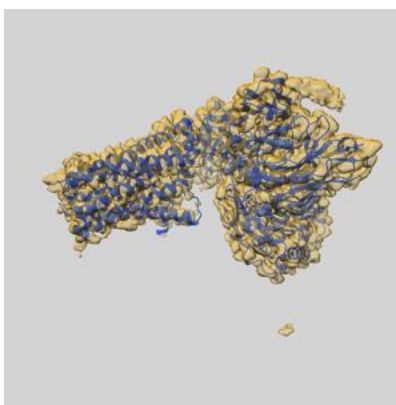
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38588 and PDB model 8XQT. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

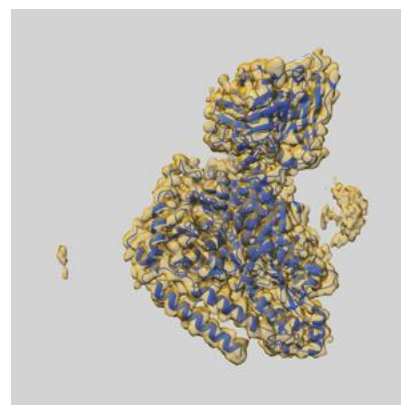
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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](#)

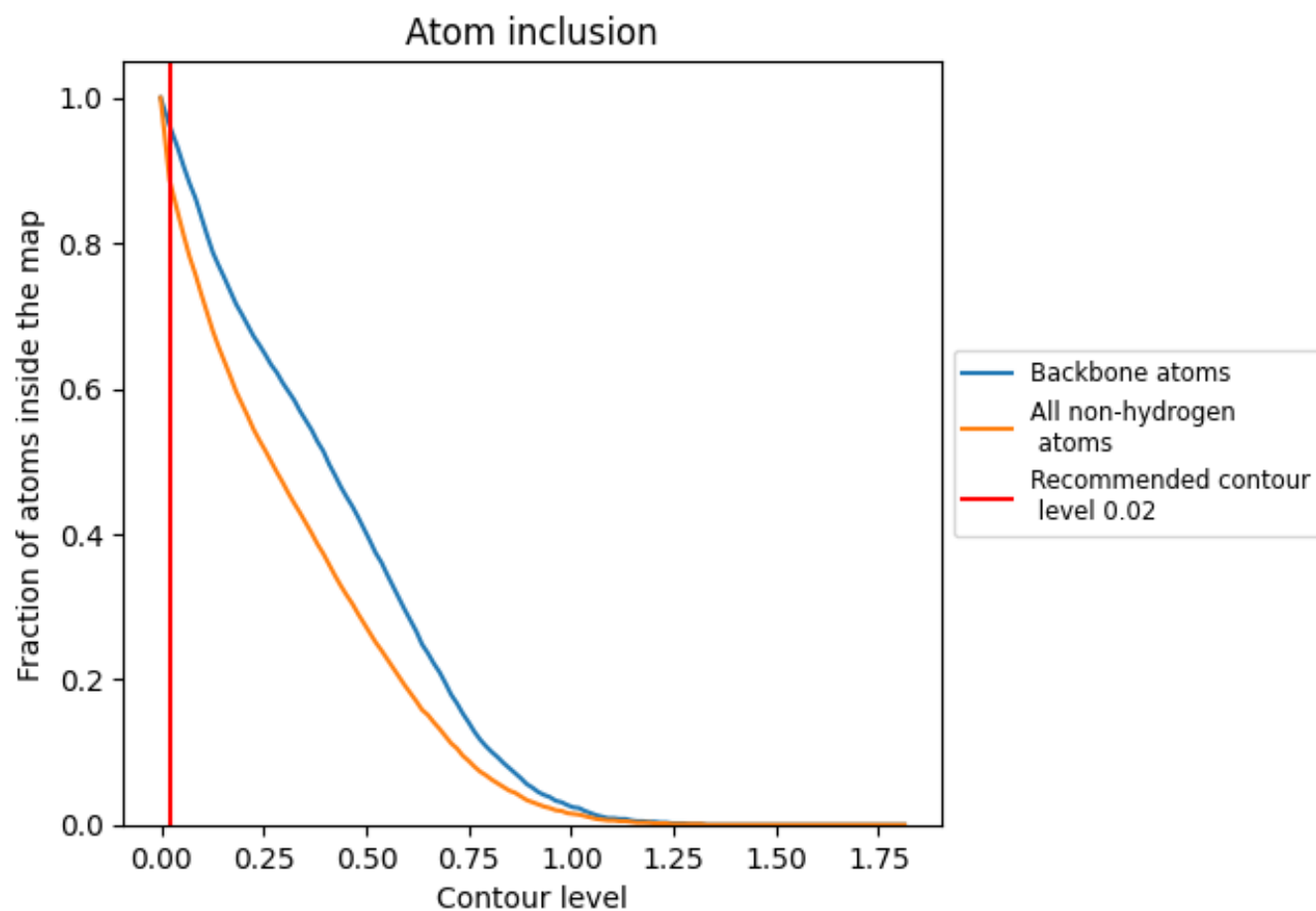


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8870	0.4260
A	0.8780	0.4290
B	0.9540	0.5190
C	0.8770	0.4390
R	0.7710	0.2470
S	0.9510	0.5120

