



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:29 AM UTC

PDB ID : 8X0F / pdb_00008x0f
EMDB ID : EMD-37977
Title : Human FL Metabotropic glutamate receptor 5, mGlu5-5M with quisqualate and PAM VU29
Authors : Vinothkumar, K.R.; Lebon, G.; Cannone, G.
Deposited on : 2023-11-04
Resolution : 3.30 Å(reported)
Based on initial model : .

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

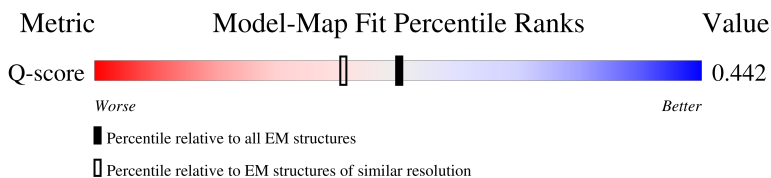
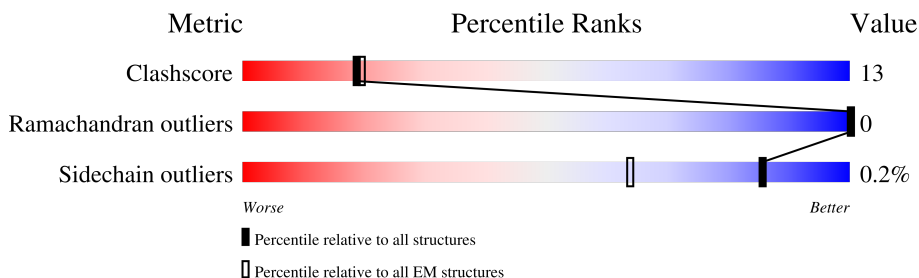
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	836	 65% 26% 9%
1	B	836	 63% 28% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12073 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.

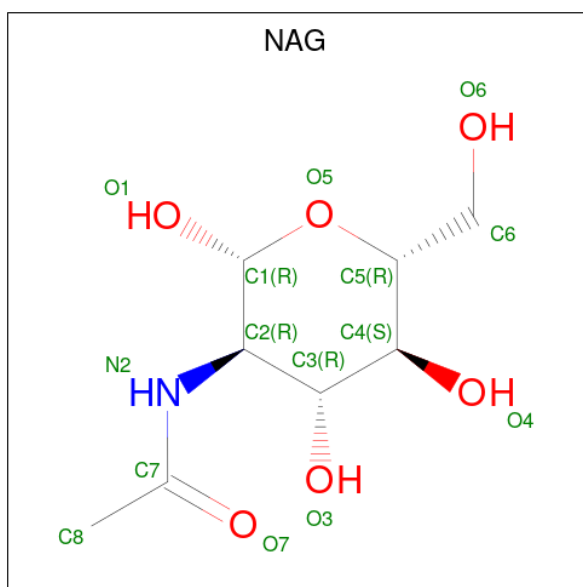
- Molecule 1 is a protein called Metabotropic glutamate receptor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	762	Total	C	N	O	S	0	0
			5995	3856	993	1089	57		
1	B	762	Total	C	N	O	S	0	0
			5995	3856	993	1089	57		

There are 14 discrepancies between the modelled and reference sequences:

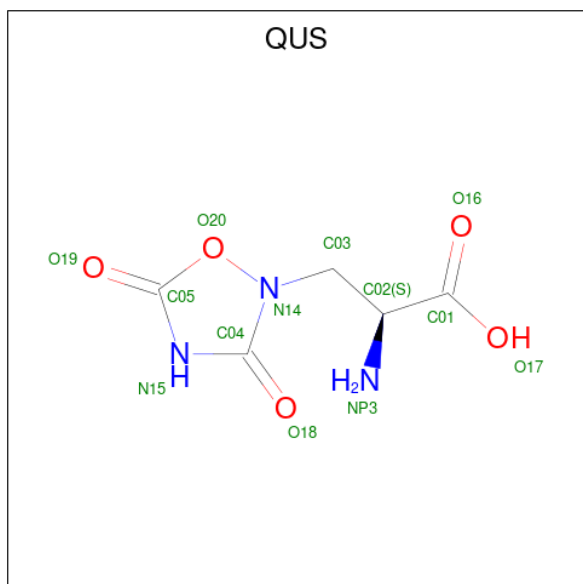
Chain	Residue	Modelled	Actual	Comment	Reference
A	350	LEU	HIS	engineered mutation	UNP P41594
A	445	ALA	ASN	engineered mutation	UNP P41594
A	742	ALA	THR	engineered mutation	UNP P41594
A	753	ALA	SER	engineered mutation	UNP P41594
A	777	ALA	THR	engineered mutation	UNP P41594
A	799	ALA	ILE	engineered mutation	UNP P41594
A	813	LEU	ALA	engineered mutation	UNP P41594
B	350	LEU	HIS	engineered mutation	UNP P41594
B	445	ALA	ASN	engineered mutation	UNP P41594
B	742	ALA	THR	engineered mutation	UNP P41594
B	753	ALA	SER	engineered mutation	UNP P41594
B	777	ALA	THR	engineered mutation	UNP P41594
B	799	ALA	ILE	engineered mutation	UNP P41594
B	813	LEU	ALA	engineered mutation	UNP P41594

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (CCD ID: QUS) (formula: $C_5H_7N_3O_5$) (labeled as "Ligand of Interest" by depositor).



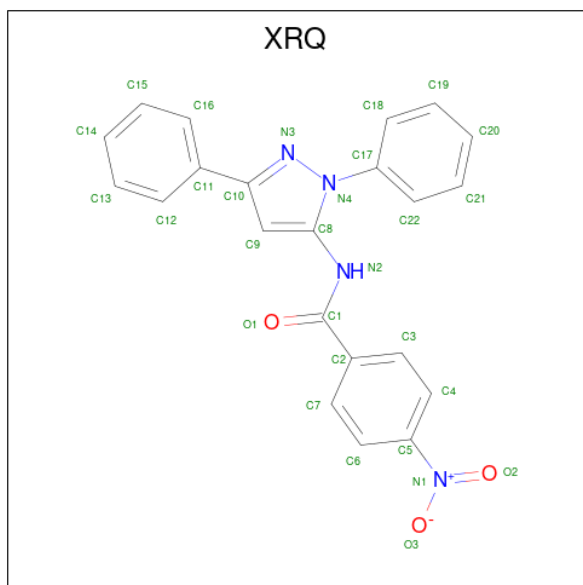
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			13	5	3	5	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	13	5	3	5	0

- Molecule 4 is N-(1,3-diphenyl-1H-pyrazol-5-yl)-4-nitrobenzamide (CCD ID: XRQ) (formula: $C_{22}H_{16}N_4O_3$) (labeled as "Ligand of Interest" by depositor).

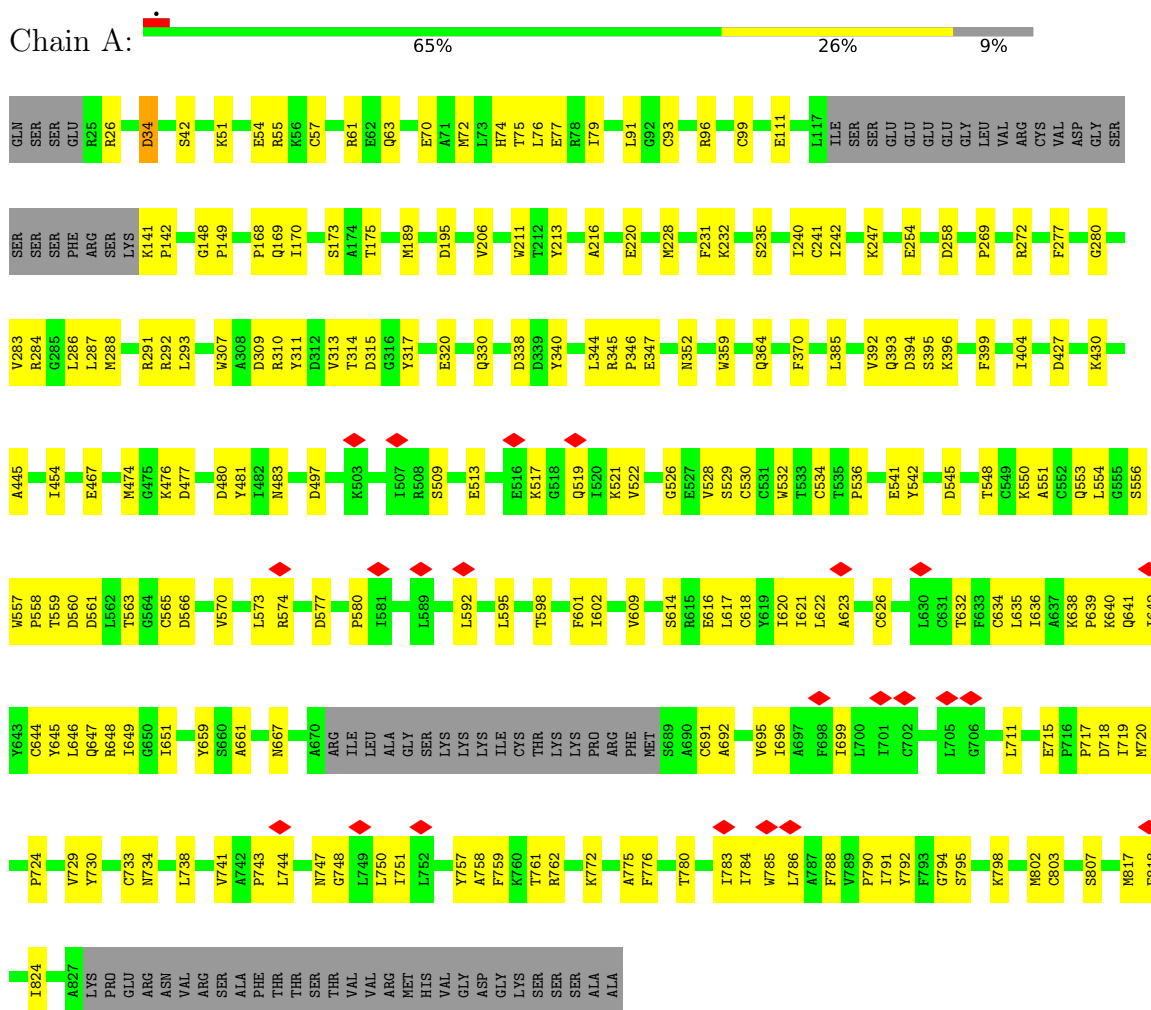


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	29	22	4	3	0

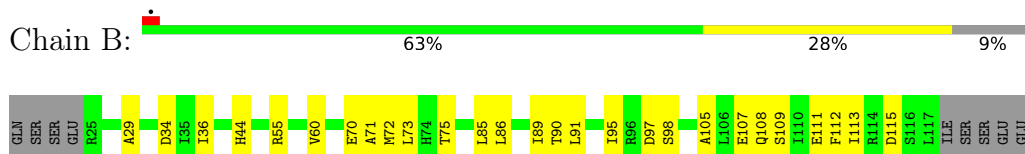
3 Residue-property plots

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: Metabotropic glutamate receptor 5



• Molecule 1: Metabotropic glutamate receptor 5



VAL	VAL	ARG	VAL	ASP	GLY	SER	SER	SER	SER	PHE	ARG	SER	LYS	K141	K144	V144	G150	S151	V154	Q159	Q163	L164	F165	P168	S173	A174	T175	M189	R190	P193	S194	Q198	A199	R200	D204	R208	Y213	H218	T219	A230	P231	K232	D233	M234	S235						
G748	L749	L752	A753	K760	N763	K772	Y773	F776	A777	I783	L786	V789	F790	I791	F792	F793	Y797	K798	A799	I800	T801	M802	S807	C816	M817	F818	V819	P820	K821	V822	I825	L826	A827	LYS	PRO	GLU	ARG	ASN	VAL	ARG	SER	ALA	PHE	THR	SER	THR					
L581	A582	A583	V584	V585	F586	A587	C588	L589	G590	L591	L592	A593	T594	L595	T598	V599	V600	S614	L617	C618	I620	I621	L622	A623	G624	I625	C626	L627	G628	Y629	L630	C631	T632	I636	A637	K638	P639	K640	Q641	I642	I643	Q647	R648	Y659	S660	A661	L662	V663	A670	ARG	ILE
E491	L492	K493	M494	D495	D496	K502	K503	S504	N505	I506	I507	R508	S509	C515	E516	Q519	I520	K521	R524	V528	S529	C530	Y542	V543	F544	D545	E546	Y547	T548	C549	Q553	L554	G555	S556	W557	P558	L562	C565	D566	L567	Y572	W575	G576	D577	P578	E579	P590				
A236	I240	C241	K247	E254	D258	L261	R272	C278	M288	R292	L293	E298	S304	W307	Y311	D312	V313	T314	Y317	D333	V334	K335	L342	K343	L344	N349	L350	R351	N352	E357	Q360	H361	R362	R366	L367	F370	E373														
K374	S375	Y377	C381	L385	T389	H390	H391	D394	M397	I401	Y409	G410	N413	L418	L425	M429	K430	P431	I432	L437	L441	T444	D461	R465	Y466	E467	M470	F471	K472	E473	M474	G475	K476	D480	Y481	I482	M483	W487	D488												

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	113563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	192572	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.100	Depositor
Minimum map value	-0.434	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	346.052, 346.052, 346.052	wwPDB
Map dimensions	476, 476, 476	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	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: QUS, NAG, XHQ

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	0.28	0/6133	0.35	0/8312
1	B	0.27	0/6133	0.36	0/8312
All	All	0.27	0/12266	0.36	0/16624

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	A	5995	0	5976	154	0
1	B	5995	0	5976	157	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	13	0	6	0	0
3	B	13	0	6	0	0
4	A	29	0	0	1	0
All	All	12073	0	11990	310	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 13.

All (310) 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:609:VAL:HG11	1:A:824:ILE:HG21	1.68	0.75
1:B:410:GLY:HA2	1:B:444:THR:HG21	1.70	0.74
1:B:70:GLU:OE2	1:B:352:ASN:ND2	2.21	0.73
1:B:648:ARG:HH22	1:B:717:PRO:HA	1.55	0.72
1:A:644:CYS:HB2	1:A:648:ARG:HH12	1.55	0.71
1:B:467:GLU:OE2	1:B:483:ASN:ND2	2.24	0.70
1:A:556:SER:HB3	1:A:565:CYS:HB3	1.72	0.70
1:A:747:ASN:O	1:A:751:ILE:HD12	1.92	0.70
1:A:517:LYS:NZ	1:A:534:CYS:SG	2.61	0.69
1:A:785:TRP:HE3	1:A:786:LEU:HD22	1.58	0.68
1:B:200:ARG:NH2	1:B:204:ASP:OD1	2.28	0.67
1:A:70:GLU:OE2	1:A:352:ASN:ND2	2.28	0.67
1:A:338:ASP:OD1	1:A:393:GLN:NE2	2.28	0.67
1:A:560:ASP:OD1	1:A:561:ASP:N	2.27	0.67
1:B:743:PRO:O	1:B:747:ASN:ND2	2.27	0.67
1:B:802:MET:HE2	1:B:802:MET:HA	1.76	0.67
1:A:640:LYS:HA	1:A:719:ILE:HD11	1.76	0.67
1:A:614:SER:HB2	1:A:617:LEU:HB2	1.76	0.66
1:B:55:ARG:NH1	1:B:107:GLU:OE1	2.28	0.66
1:A:313:VAL:HG23	1:A:314:THR:HG23	1.78	0.66
1:B:313:VAL:HG23	1:B:314:THR:HG23	1.78	0.66
1:A:291:ARG:NE	1:A:320:GLU:OE2	2.27	0.65
1:B:366:ARG:NH2	1:B:377:TYR:O	2.29	0.65
1:B:175:THR:HG22	1:B:195:ASP:HB3	1.79	0.65
1:B:620:ILE:HD11	1:B:661:ALA:HB2	1.78	0.64
1:B:528:VAL:HG13	1:B:530:CYS:H	1.62	0.64
1:B:817:MET:HG2	1:B:818:PHE:HD1	1.62	0.64
1:A:307:TRP:NE1	1:A:481:TYR:OH	2.31	0.63
1:B:614:SER:HB3	1:B:617:LEU:HB2	1.80	0.63
1:A:646:LEU:HA	1:A:649:ILE:HG12	1.80	0.63
1:B:736:THR:HG23	1:B:739:GLY:H	1.64	0.63
1:B:544:PHE:H	1:B:549:CYS:HA	1.63	0.62
1:A:467:GLU:OE1	1:A:483:ASN:ND2	2.32	0.62
1:B:258:ASP:OD1	1:B:292:ARG:NH2	2.31	0.62
1:A:553:GLN:OE1	1:A:553:GLN:N	2.23	0.62
1:B:720:MET:SD	1:B:720:MET:N	2.72	0.62
1:B:366:ARG:HE	1:B:375:SER:HA	1.65	0.62
1:A:557:TRP:O	1:A:566:ASP:N	2.24	0.62
1:A:213:TYR:N	1:A:509:SER:O	2.27	0.61
1:B:502:LYS:HD2	1:B:504:SER:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ARG:NH2	1:B:389:THR:O	2.33	0.60
1:B:594:THR:O	1:B:598:THR:HG23	2.00	0.60
1:B:716:PRO:O	1:B:734:ASN:ND2	2.34	0.60
1:A:718:ASP:O	1:A:734:ASN:N	2.35	0.60
1:A:743:PRO:O	1:A:747:ASN:ND2	2.34	0.60
1:B:394:ASP:N	1:B:394:ASP:OD1	2.32	0.60
1:B:254:GLU:OE1	1:B:292:ARG:NH1	2.34	0.59
1:B:643:TYR:O	1:B:647:GLN:HG2	2.02	0.59
1:B:557:TRP:N	1:B:566:ASP:O	2.34	0.59
1:A:632:THR:HG21	1:A:807:SER:HB2	1.84	0.59
1:A:638:LYS:HD3	1:A:639:PRO:HD2	1.85	0.59
1:A:641:GLN:NE2	1:A:717:PRO:O	2.34	0.59
1:A:26:ARG:NH2	1:A:55:ARG:O	2.35	0.59
1:B:198:GLN:OE1	1:B:304:SER:OG	2.21	0.59
1:B:333:ASP:OD1	1:B:333:ASP:N	2.35	0.59
1:A:542:TYR:HB3	1:A:558:PRO:HB3	1.85	0.59
1:B:425:LEU:HB3	1:B:430:LYS:HE2	1.84	0.58
1:B:763:ASN:O	1:B:772:LYS:NZ	2.35	0.58
1:A:96:ARG:NH1	1:A:111:GLU:OE1	2.36	0.58
1:A:497:ASP:OD1	1:A:497:ASP:N	2.33	0.58
1:B:474:MET:N	1:B:474:MET:SD	2.76	0.57
1:B:515:CYS:HB2	1:B:520:ILE:HD12	1.86	0.57
1:A:347:GLU:HA	1:A:370:PHE:HZ	1.69	0.57
1:A:529:SER:O	1:A:529:SER:OG	2.19	0.57
1:B:219:THR:HG23	1:B:278:CYS:HA	1.87	0.57
1:A:623:ALA:HA	1:A:626:CYS:SG	2.44	0.57
1:B:115:ASP:OD2	1:B:141:LYS:N	2.38	0.57
1:A:258:ASP:OD1	1:A:292:ARG:NH2	2.27	0.56
1:B:491:GLU:OE2	1:B:493:LYS:NZ	2.34	0.56
1:A:776:PHE:O	1:A:780:THR:HG23	2.05	0.56
1:B:86:LEU:HD13	1:B:89:ILE:HD11	1.86	0.56
1:B:208:ARG:NH2	1:B:494:MET:O	2.38	0.56
1:B:174:ALA:O	1:B:190:ARG:NH1	2.31	0.56
1:B:623:ALA:O	1:B:627:LEU:HD22	2.05	0.56
1:B:488:ASP:OD1	1:B:488:ASP:N	2.36	0.56
1:B:553:GLN:N	1:B:553:GLN:OE1	2.39	0.56
1:B:586:PHE:CE1	1:B:807:SER:HB2	2.41	0.56
1:A:394:ASP:OD1	1:A:394:ASP:N	2.38	0.55
1:B:230:ALA:O	1:B:234:MET:HG2	2.06	0.55
1:A:635:LEU:HB3	1:A:803:CYS:SG	2.46	0.55
1:A:307:TRP:CD1	1:A:313:VAL:HG21	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLY:HA2	1:B:524:ARG:HH12	1.71	0.55
1:B:34:ASP:OD2	1:B:90:THR:N	2.30	0.55
1:A:542:TYR:OH	1:A:550:LYS:NZ	2.36	0.55
1:A:621:ILE:HG23	1:A:661:ALA:HB3	1.89	0.55
1:A:284:ARG:HH12	1:A:315:ASP:H	1.54	0.55
1:A:667:ASN:HA	1:A:757:TYR:OH	2.07	0.55
1:B:641:GLN:HG2	1:B:717:PRO:HG2	1.89	0.55
1:B:628:GLY:O	1:B:632:THR:HG23	2.07	0.54
1:A:175:THR:HG22	1:A:195:ASP:HB3	1.89	0.54
1:A:519:GLN:HE21	1:A:536:PRO:HB3	1.71	0.54
1:A:601:PHE:HE2	1:A:618:CYS:HB3	1.71	0.54
1:B:558:PRO:HA	1:B:565:CYS:HA	1.89	0.54
1:B:542:TYR:HB3	1:B:558:PRO:HB3	1.89	0.54
1:A:561:ASP:OD2	1:A:563:THR:OG1	2.20	0.54
1:B:418:LEU:HD22	1:B:429:MET:HG3	1.90	0.54
1:A:254:GLU:OE1	1:A:292:ARG:NH1	2.41	0.53
1:B:704:GLN:O	1:B:707:ILE:HG13	2.07	0.53
1:B:381:CYS:HB2	1:B:385:LEU:HD12	1.91	0.53
1:B:272:ARG:NE	1:B:298:GLU:OE2	2.37	0.53
1:B:465:ARG:HG2	1:B:488:ASP:HB3	1.89	0.53
1:B:691:CYS:O	1:B:693:GLN:NE2	2.42	0.53
1:B:367:LEU:HD12	1:B:370:PHE:CE2	2.44	0.53
1:A:741:VAL:HA	1:A:744:LEU:HB2	1.91	0.53
1:A:63:GLN:NE2	1:A:392:VAL:O	2.29	0.52
1:A:715:GLU:HG3	1:A:734:ASN:HD22	1.74	0.52
1:A:76:LEU:HD12	1:A:93:CYS:HB3	1.92	0.52
1:A:791:ILE:O	1:A:795:SER:OG	2.25	0.52
1:A:311:TYR:OH	1:A:480:ASP:OD1	2.26	0.52
1:A:598:THR:HG22	1:A:622:LEU:HD13	1.91	0.52
1:A:792:TYR:O	1:A:798:LYS:NZ	2.42	0.52
1:B:553:GLN:O	1:B:556:SER:OG	2.28	0.52
1:A:220:GLU:HG3	1:A:247:LYS:HE2	1.93	0.51
1:B:360:GLN:NE2	1:B:373:GLU:O	2.35	0.51
1:A:719:ILE:HA	1:A:733:CYS:HA	1.93	0.51
1:A:232:LYS:HG2	1:A:242:ILE:HD13	1.92	0.51
1:B:556:SER:HB2	1:B:565:CYS:SG	2.51	0.51
1:A:288:MET:HA	1:A:317:TYR:CE2	2.46	0.51
1:B:272:ARG:HD2	1:B:507:ILE:HB	1.92	0.51
1:A:573:LEU:HB3	1:A:636:ILE:HG13	1.92	0.50
1:B:495:ASP:N	1:B:495:ASP:OD1	2.42	0.50
1:B:344:LEU:HD22	1:B:349:ASN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LYS:HE3	1:A:54:GLU:HB2	1.93	0.50
1:A:758:ALA:O	1:A:761:THR:OG1	2.23	0.50
1:B:98:SER:HB2	1:B:105:ALA:HB2	1.94	0.50
1:B:519:GLN:HG2	1:B:562:LEU:HD11	1.93	0.50
1:B:572:TYR:HB3	1:B:731:LEU:HD21	1.93	0.50
1:A:474:MET:HE2	1:A:474:MET:HA	1.94	0.50
1:A:647:GLN:O	1:A:651:ILE:HG22	2.11	0.50
1:B:168:PRO:HG2	1:B:437:LEU:HD23	1.94	0.50
1:A:592:LEU:HD23	1:A:595:LEU:HD21	1.94	0.49
1:B:707:ILE:O	1:B:711:LEU:HD22	2.11	0.49
1:B:773:TYR:HA	1:B:776:PHE:CD1	2.47	0.49
1:B:789:VAL:HG13	1:B:793:PHE:HD2	1.77	0.49
1:A:574:ARG:HG3	1:A:577:ASP:HB2	1.95	0.49
1:B:817:MET:HG2	1:B:818:PHE:CD1	2.47	0.49
1:B:622:LEU:O	1:B:625:ILE:HG22	2.12	0.49
1:A:616:GLU:O	1:A:620:ILE:HG12	2.13	0.49
1:B:29:ALA:HB3	1:B:95:ILE:HB	1.93	0.49
1:B:553:GLN:NE2	1:B:555:GLY:O	2.45	0.49
1:B:502:LYS:NZ	1:B:504:SER:O	2.32	0.48
1:B:724:PRO:HG2	1:B:728:GLU:HG3	1.95	0.48
1:A:577:ASP:HB3	1:A:580:PRO:HD2	1.95	0.48
1:A:72:MET:HE2	1:A:93:CYS:HB2	1.94	0.48
1:A:427:ASP:HA	1:A:430:LYS:HD2	1.94	0.48
1:A:759:PHE:O	1:A:762:ARG:NE	2.45	0.48
1:A:34:ASP:OD1	1:A:34:ASP:N	2.34	0.48
1:A:645:TYR:CD2	1:A:717:PRO:HG2	2.47	0.48
1:A:785:TRP:HD1	4:A:903:XRQ:C18	2.27	0.48
1:A:541:GLU:HA	1:A:551:ALA:HA	1.96	0.48
1:A:570:VAL:HG23	1:A:729:VAL:HG13	1.96	0.48
1:A:79:ILE:HG21	1:A:91:LEU:HD12	1.96	0.48
1:B:659:TYR:O	1:B:663:VAL:HG23	2.14	0.47
1:B:487:TRP:HA	1:B:491:GLU:O	2.14	0.47
1:B:85:LEU:HD11	1:B:409:TYR:CZ	2.49	0.47
1:A:346:PRO:HG3	1:A:359:TRP:CD1	2.49	0.47
1:B:97:ASP:O	1:B:108:GLN:HG3	2.14	0.47
1:B:413:ASN:ND2	1:B:444:THR:HG22	2.30	0.47
1:A:659:TYR:OH	1:A:751:ILE:HA	2.15	0.47
1:B:235:SER:OG	1:B:236:ALA:N	2.47	0.47
1:B:797:TYR:O	1:B:799:ALA:N	2.45	0.47
1:A:148:GLY:N	1:A:170:ILE:O	2.41	0.47
1:B:60:VAL:HG21	1:B:357:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLY:O	1:B:173:SER:OG	2.33	0.47
1:A:521:LYS:HZ1	1:A:548:THR:C	2.23	0.47
1:B:618:CYS:HA	1:B:621:ILE:HG22	1.95	0.47
1:A:645:TYR:O	1:A:649:ILE:HG23	2.15	0.46
1:B:159:GLN:OE1	1:B:163:GLN:HB3	2.15	0.46
1:B:107:GLU:O	1:B:111:GLU:HG2	2.15	0.46
1:B:506:ILE:HD12	1:B:506:ILE:HA	1.78	0.46
1:B:557:TRP:CD2	1:B:558:PRO:HD2	2.50	0.46
1:B:529:SER:O	1:B:529:SER:OG	2.25	0.46
1:A:173:SER:HB2	1:A:396:LYS:HD3	1.98	0.46
1:A:696:ILE:HA	1:A:699:ILE:HG12	1.96	0.46
1:A:691:CYS:SG	1:A:692:ALA:N	2.87	0.46
1:B:335:LYS:HB2	1:B:335:LYS:HE2	1.74	0.46
1:B:821:LYS:O	1:B:825:ILE:HG12	2.16	0.46
1:B:175:THR:HG23	1:B:193:PRO:O	2.16	0.45
1:B:213:TYR:O	1:B:509:SER:HB2	2.15	0.45
1:A:240:ILE:HG22	1:A:241:CYS:H	1.81	0.45
1:A:717:PRO:HA	1:A:734:ASN:CG	2.42	0.45
1:A:720:MET:HE1	1:A:734:ASN:HA	1.98	0.45
1:B:73:LEU:HB3	1:B:351:ARG:HH11	1.80	0.45
1:A:598:THR:O	1:A:602:ILE:HG12	2.17	0.45
1:B:91:LEU:HD12	1:B:91:LEU:HA	1.72	0.45
1:B:496:ASP:OD1	1:B:496:ASP:N	2.49	0.45
1:B:580:PRO:HB3	1:B:636:ILE:CD1	2.46	0.45
1:A:635:LEU:HA	1:A:647:GLN:OE1	2.17	0.45
1:B:72:MET:HA	1:B:75:THR:HG22	1.98	0.45
1:A:293:LEU:HD12	1:A:293:LEU:O	2.17	0.45
1:A:667:ASN:OD1	1:A:757:TYR:OH	2.26	0.45
1:A:748:GLY:HA2	1:A:751:ILE:HD12	1.97	0.45
1:A:522:VAL:HG13	1:A:532:TRP:CB	2.47	0.45
1:A:75:THR:HG21	1:A:404:ILE:HD13	1.98	0.45
1:B:545:ASP:OD1	1:B:547:TYR:N	2.47	0.45
1:A:330:GLN:HB2	1:A:467:GLU:HG3	1.98	0.45
1:A:206:VAL:HG13	1:A:211:TRP:HB2	1.97	0.45
1:A:559:THR:OG1	1:A:561:ASP:OD1	2.26	0.45
1:A:738:LEU:HA	1:A:741:VAL:HG22	1.97	0.44
1:A:744:LEU:HD23	1:A:744:LEU:HA	1.82	0.44
1:B:556:SER:HA	1:B:567:LEU:HA	1.99	0.44
1:A:780:THR:O	1:A:783:ILE:HG22	2.17	0.44
1:B:670:ALA:HB2	1:B:760:LYS:HE2	1.99	0.44
1:B:586:PHE:CD1	1:B:586:PHE:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PHE:O	1:A:235:SER:HB3	2.18	0.44
1:B:579:GLU:HB3	1:B:580:PRO:HD3	2.00	0.44
1:B:713:ILE:HD13	1:B:713:ILE:HA	1.85	0.44
1:B:311:TYR:OH	1:B:480:ASP:OD1	2.32	0.44
1:B:288:MET:HA	1:B:317:TYR:CE2	2.52	0.44
1:A:141:LYS:HA	1:A:142:PRO:HD3	1.91	0.44
1:A:634:CYS:SG	1:A:646:LEU:HD11	2.57	0.44
1:A:772:LYS:HB3	1:A:772:LYS:HE2	1.73	0.44
1:B:113:ILE:HG21	1:B:165:PHE:CE1	2.53	0.44
1:B:472:LYS:HB3	1:B:472:LYS:HE2	1.87	0.44
1:A:74:HIS:HB2	1:A:340:TYR:CE2	2.53	0.43
1:A:228:MET:CE	1:A:277:PHE:HB2	2.48	0.43
1:A:641:GLN:NE2	1:A:717:PRO:HB2	2.33	0.43
1:A:785:TRP:CE3	1:A:786:LEU:HD22	2.46	0.43
1:B:44:HIS:NE2	1:B:357:GLU:OE2	2.44	0.43
1:B:71:ALA:HB1	1:B:401:ILE:HD11	2.00	0.43
1:A:711:LEU:O	1:A:715:GLU:N	2.52	0.43
1:A:640:LYS:HG3	1:A:642:ILE:HG22	2.00	0.43
1:B:738:LEU:HA	1:B:741:VAL:HG12	1.99	0.43
1:A:74:HIS:ND1	1:A:77:GLU:OE1	2.45	0.43
1:B:692:ALA:O	1:B:696:ILE:HG23	2.18	0.43
1:A:554:LEU:HD12	1:A:554:LEU:O	2.18	0.43
1:B:639:PRO:O	1:B:719:ILE:HG12	2.19	0.43
1:A:396:LYS:HG2	1:A:399:PHE:HD2	1.83	0.43
1:A:790:PRO:O	1:A:794:GLY:N	2.50	0.43
1:B:218:HIS:CE1	1:B:247:LYS:HG2	2.54	0.43
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.79	0.43
1:A:692:ALA:HA	1:A:695:VAL:HG22	2.01	0.43
1:B:577:ASP:HB3	1:B:580:PRO:HD2	2.01	0.43
1:A:659:TYR:CD1	1:A:750:LEU:HB3	2.54	0.43
1:A:283:VAL:O	1:A:287:LEU:HG	2.19	0.42
1:B:777:ALA:HB2	1:B:816:CYS:HB2	2.00	0.42
1:A:269:PRO:O	1:A:272:ARG:NH2	2.46	0.42
1:B:200:ARG:HD2	1:B:200:ARG:HA	1.74	0.42
1:A:757:TYR:O	1:A:761:THR:HG23	2.19	0.42
1:B:394:ASP:OD1	1:B:397:MET:HE3	2.19	0.42
1:B:397:MET:O	1:B:401:ILE:HG12	2.18	0.42
1:B:575:TRP:HZ3	1:B:584:VAL:HG11	1.84	0.42
1:A:563:THR:OG1	1:A:563:THR:O	2.36	0.42
1:A:783:ILE:HD12	1:A:783:ILE:HA	1.87	0.42
1:B:521:LYS:HD2	1:B:549:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLY:HA3	1:A:310:ARG:NH2	2.35	0.42
1:A:288:MET:HG2	1:A:317:TYR:CZ	2.53	0.42
1:A:545:ASP:HB3	1:A:548:THR:HG23	2.01	0.42
1:A:553:GLN:HG2	1:A:554:LEU:H	1.85	0.42
1:B:307:TRP:CD1	1:B:313:VAL:HG21	2.54	0.42
1:B:572:TYR:CE2	1:B:638:LYS:HG2	2.54	0.42
1:B:272:ARG:CZ	1:B:507:ILE:HD12	2.49	0.42
1:B:621:ILE:HD12	1:B:661:ALA:HB3	2.02	0.42
1:B:791:ILE:HG22	1:B:801:THR:HB	2.02	0.42
1:A:57:CYS:HB3	1:A:99:CYS:HB3	1.83	0.42
1:A:284:ARG:NH1	1:A:313:VAL:O	2.53	0.42
1:A:476:LYS:HG3	1:A:477:ASP:OD2	2.20	0.42
1:A:617:LEU:O	1:A:621:ILE:HG12	2.20	0.42
1:A:720:MET:SD	1:A:720:MET:N	2.93	0.42
1:B:109:SER:O	1:B:113:ILE:HG12	2.19	0.42
1:B:470:ASN:N	1:B:482:ILE:O	2.53	0.42
1:B:590:GLY:HA3	1:B:629:TYR:CZ	2.54	0.42
1:A:513:GLU:CD	1:A:513:GLU:H	2.27	0.42
1:A:761:THR:C	1:A:762:ARG:HG2	2.45	0.42
1:B:476:LYS:HD2	1:B:476:LYS:HA	1.90	0.42
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.79	0.41
1:B:85:LEU:HD21	1:B:409:TYR:CE1	2.55	0.41
1:B:461:ASP:OD1	1:B:461:ASP:N	2.53	0.41
1:B:586:PHE:O	1:B:589:LEU:HG	2.20	0.41
1:A:780:THR:O	1:A:784:ILE:HG22	2.20	0.41
1:B:189:MET:HE3	1:B:441:LEU:HB3	2.02	0.41
1:B:503:LYS:HD3	1:B:503:LYS:HA	1.73	0.41
1:A:309:ASP:OD1	1:A:395:SER:OG	2.29	0.41
1:A:528:VAL:O	1:A:530:CYS:N	2.52	0.41
1:B:151:SER:HB3	1:B:154:VAL:HB	2.02	0.41
1:B:247:LYS:HE3	1:B:247:LYS:HB2	1.69	0.41
1:B:261:LEU:HB3	1:B:293:LEU:HD21	2.02	0.41
1:B:508:ARG:H	1:B:508:ARG:HG3	1.56	0.41
1:B:640:LYS:H	1:B:643:TYR:HB2	1.85	0.41
1:B:817:MET:C	1:B:820:PRO:HD2	2.46	0.41
1:A:445:ALA:HA	1:A:454:ILE:O	2.21	0.41
1:A:622:LEU:HG	1:A:818:PHE:CZ	2.56	0.41
1:A:724:PRO:HG2	1:A:730:TYR:CE2	2.55	0.41
1:B:109:SER:O	1:B:112:PHE:HB2	2.21	0.41
1:B:240:ILE:HG22	1:B:241:CYS:H	1.85	0.41
1:A:345:ARG:HE	1:A:345:ARG:HB3	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLN:H	1:A:364:GLN:HG2	1.59	0.41
1:A:574:ARG:O	1:A:580:PRO:HG2	2.21	0.41
1:A:635:LEU:HD21	1:A:802:MET:HB3	2.01	0.41
1:A:788:PHE:HB2	1:A:791:ILE:HD12	2.02	0.41
1:B:720:MET:HE1	1:B:734:ASN:HB3	2.02	0.41
1:A:42:SER:O	1:A:61:ARG:HD3	2.21	0.41
1:A:149:PRO:HD2	1:A:169:GLN:NE2	2.35	0.41
1:A:216:ALA:HB1	1:A:228:MET:SD	2.61	0.41
1:A:758:ALA:HB1	1:A:775:ALA:HA	2.03	0.41
1:B:86:LEU:HB3	1:B:89:ILE:HG12	2.02	0.41
1:B:600:VAL:HG11	1:B:822:VAL:HG13	2.02	0.41
1:B:821:LYS:HA	1:B:821:LYS:HD2	1.97	0.41
1:A:195:ASP:OD2	1:A:195:ASP:C	2.64	0.41
1:B:543:VAL:HA	1:B:549:CYS:HB3	2.03	0.41
1:B:742:ALA:HB3	1:B:743:PRO:HD3	2.02	0.41
1:B:545:ASP:OD1	1:B:548:THR:N	2.54	0.40
1:B:232:LYS:HE2	1:B:232:LYS:HB2	1.89	0.40
1:B:342:LEU:HD21	1:B:391:HIS:CD2	2.56	0.40
1:A:621:ILE:HD12	1:A:817:MET:HG3	2.04	0.40
1:B:36:ILE:O	1:B:144:VAL:HG12	2.21	0.40
1:A:51:LYS:HD2	1:A:51:LYS:HA	1.93	0.40
1:A:168:PRO:HB3	1:A:189:MET:HE1	2.04	0.40
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.85	0.40
1:B:642:ILE:H	1:B:642:ILE:HG12	1.71	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	756/836 (90%)	691 (91%)	65 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	756/836 (90%)	692 (92%)	64 (8%)	0	100	100
All	All	1512/1672 (90%)	1383 (92%)	129 (8%)	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	A	658/723 (91%)	656 (100%)	2 (0%)	86	86
1	B	658/723 (91%)	657 (100%)	1 (0%)	87	88
All	All	1316/1446 (91%)	1313 (100%)	3 (0%)	85	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	385	LEU
1	B	432	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	412	HIS
1	A	737	ASN
1	B	53	HIS
1	B	157	GLN

5.3.3 RNA ⓘ

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](#)

5 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$
3	QUS	B	902	-	9,13,13	1.26	1 (11%)	10,18,18	1.99	4 (40%)
3	QUS	A	902	-	9,13,13	1.27	1 (11%)	10,18,18	2.06	4 (40%)
2	NAG	A	901	1	14,14,15	0.19	0	17,19,21	0.56	0
2	NAG	B	901	1	14,14,15	0.60	1 (7%)	17,19,21	0.42	0
4	XRQ	A	903	-	32,32,32	0.81	1 (3%)	41,44,44	0.95	2 (4%)

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
3	QUS	B	902	-	-	0/6/8/8	0/1/1/1
3	QUS	A	902	-	-	2/6/8/8	0/1/1/1
2	NAG	A	901	1	-	4/6/23/26	0/1/1/1
2	NAG	B	901	1	-	2/6/23/26	0/1/1/1
4	XRQ	A	903	-	-	4/18/20/20	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	XRQ	C9-C8	3.85	1.41	1.37
3	B	902	QUS	C04-N14	-2.72	1.34	1.39
3	A	902	QUS	C04-N14	-2.68	1.34	1.39
2	B	901	NAG	O5-C1	-2.15	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	QUS	O20-N14-C03	4.58	122.94	113.83
3	B	902	QUS	O20-N14-C03	4.32	122.41	113.83
4	A	903	XRQ	C10-N3-N4	3.75	106.98	104.81
3	A	902	QUS	O20-C05-N15	2.82	108.69	106.14
3	B	902	QUS	O20-C05-N15	2.78	108.64	106.14
3	A	902	QUS	N15-C04-N14	2.52	108.51	106.10
3	B	902	QUS	N15-C04-N14	2.40	108.40	106.10
4	A	903	XRQ	N2-C8-N4	2.13	123.71	120.11
3	B	902	QUS	C04-N15-C05	-2.07	109.11	112.62
3	A	902	QUS	C04-N15-C05	-2.05	109.14	112.62

There are no chirality outliers.

All (12) torsion outliers are listed below:

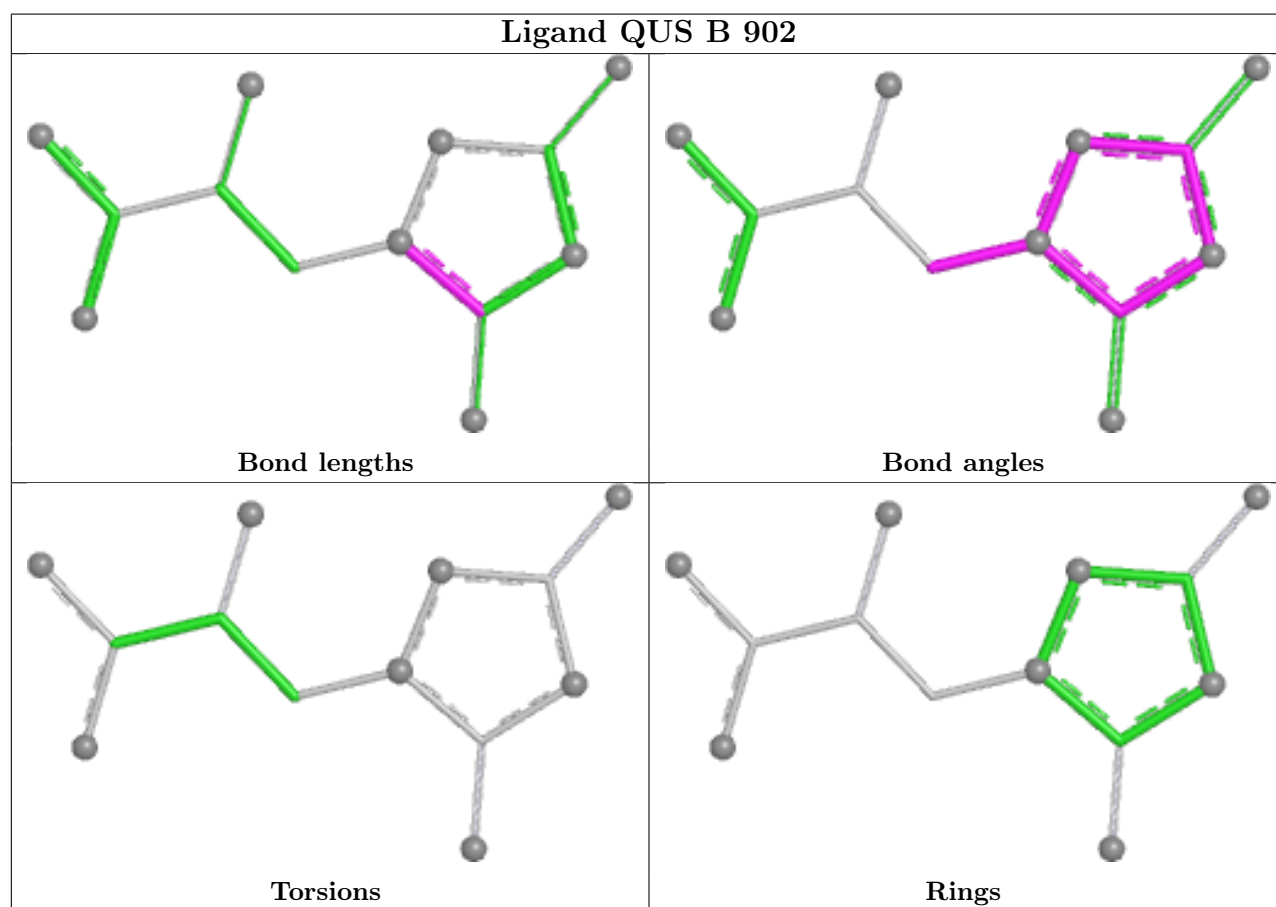
Mol	Chain	Res	Type	Atoms
4	A	903	XRQ	C2-C1-N2-C8
4	A	903	XRQ	O1-C1-N2-C8
4	A	903	XRQ	C9-C8-N2-C1
4	A	903	XRQ	N4-C8-N2-C1
2	B	901	NAG	O5-C5-C6-O6
2	B	901	NAG	C4-C5-C6-O6
2	A	901	NAG	O5-C5-C6-O6
2	A	901	NAG	C4-C5-C6-O6
2	A	901	NAG	C1-C2-N2-C7
2	A	901	NAG	C3-C2-N2-C7
3	A	902	QUS	C01-C02-C03-N14
3	A	902	QUS	O16-C01-C02-NP3

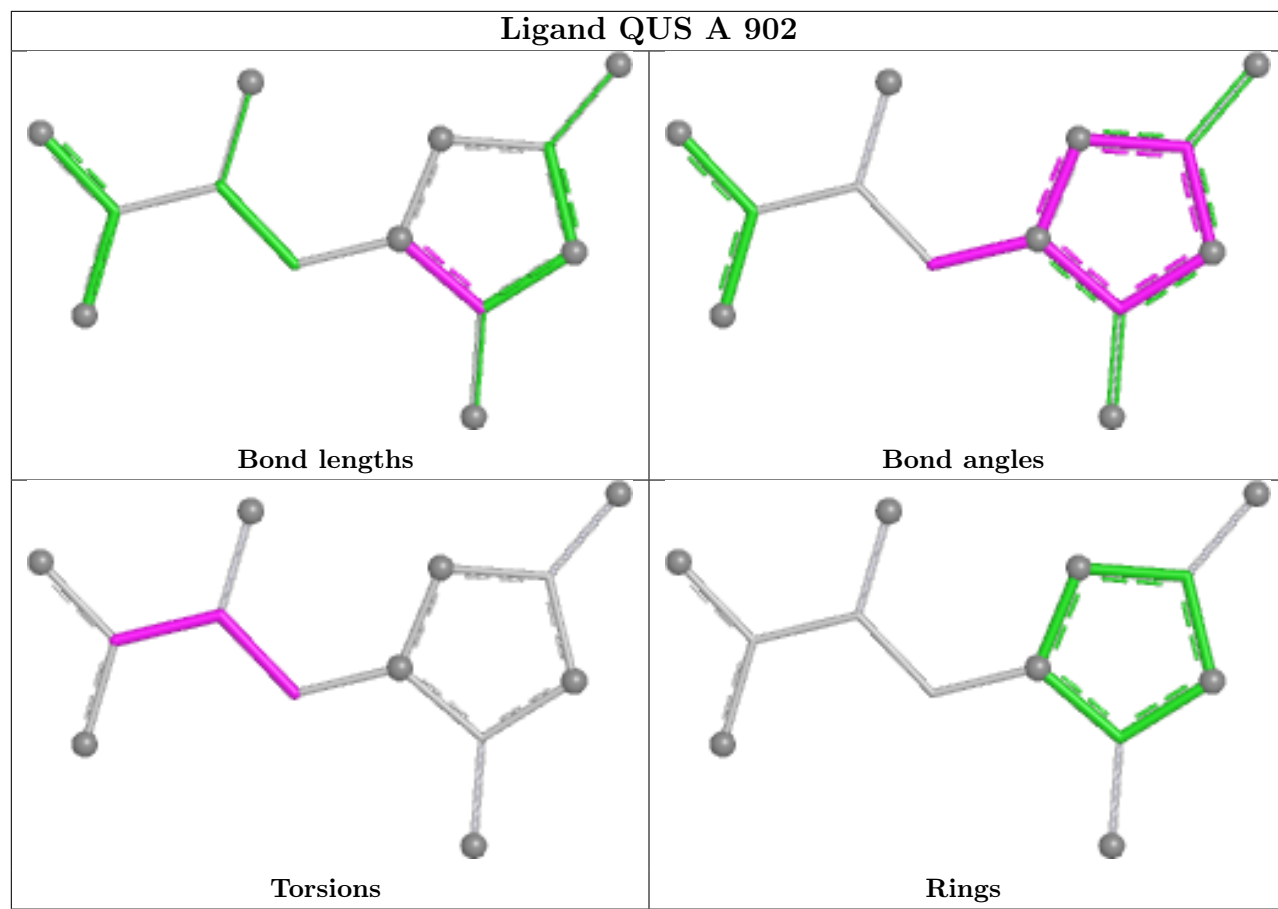
There are no ring outliers.

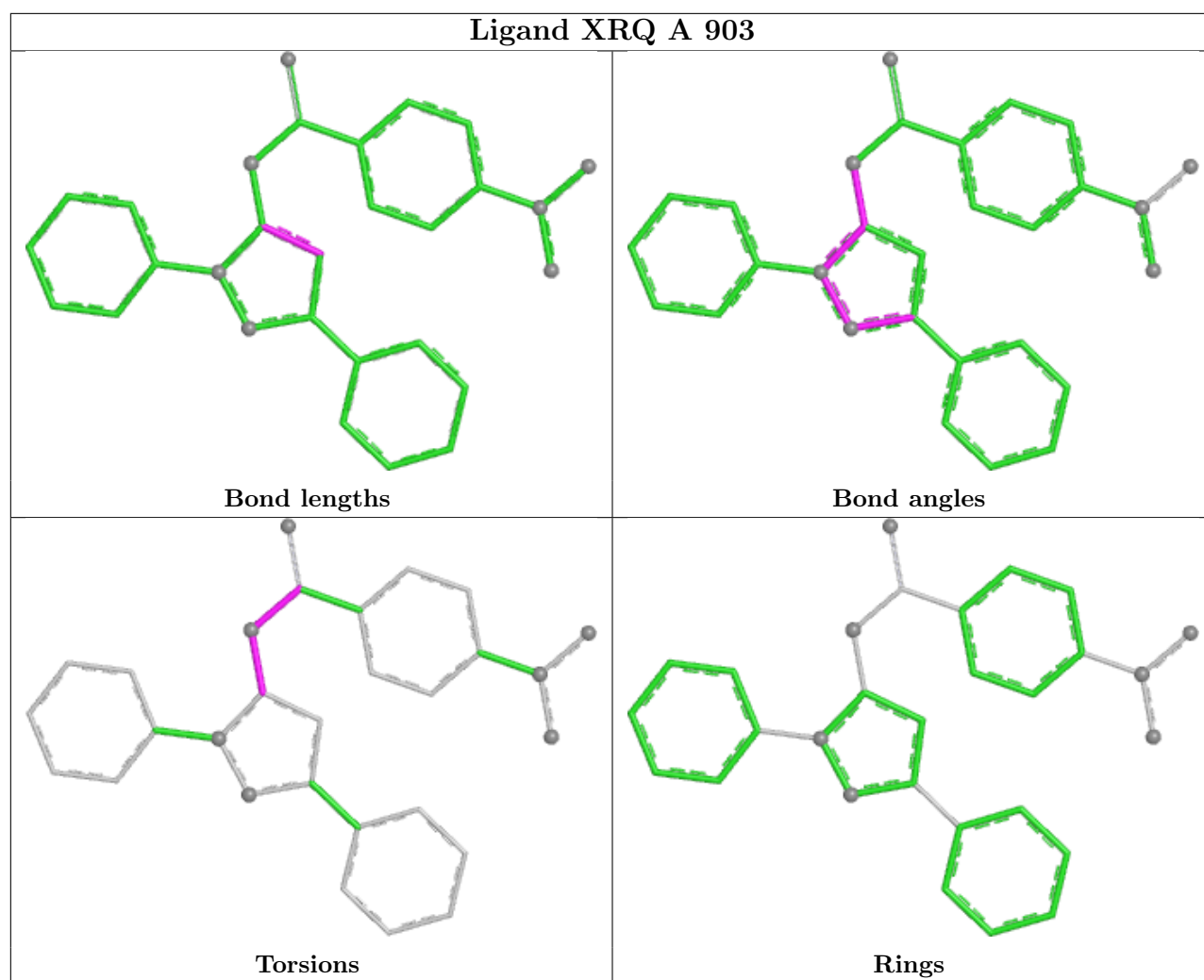
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	XRQ	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.

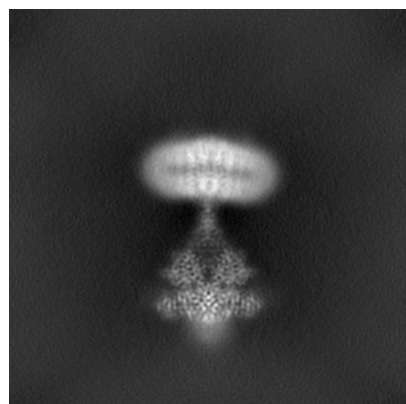
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37977. These allow visual inspection of the internal detail of the map and identification of artifacts.

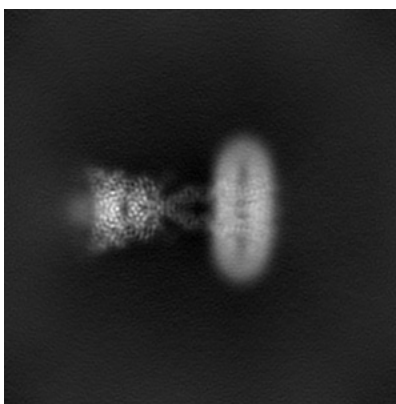
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

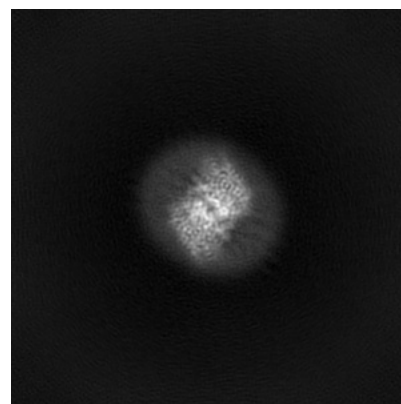
6.1.1 Primary map



X

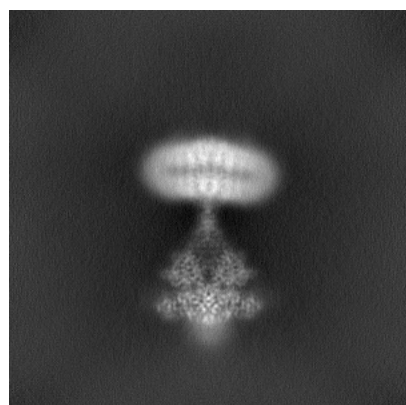


Y

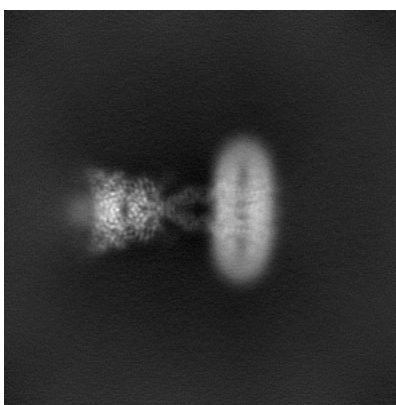


Z

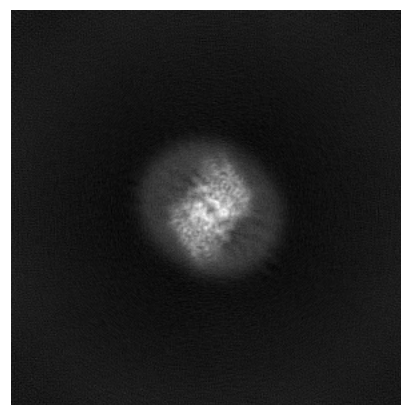
6.1.2 Raw map



X



Y

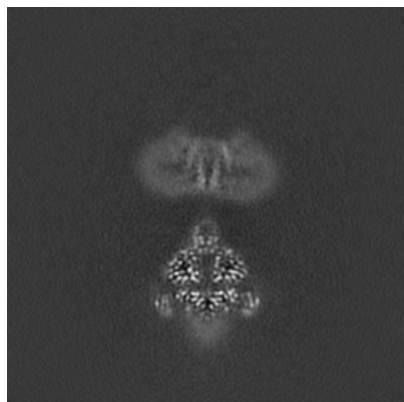


Z

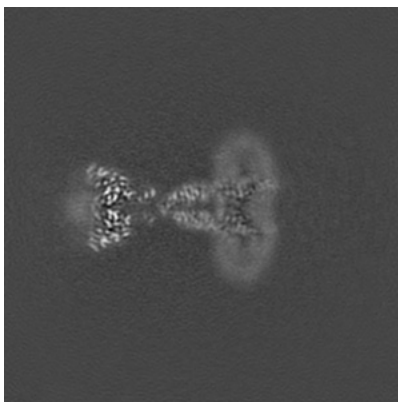
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

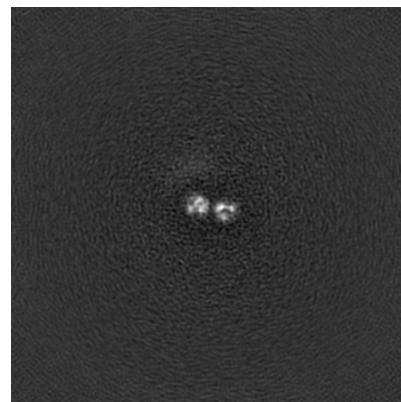
6.2.1 Primary map



X Index: 238

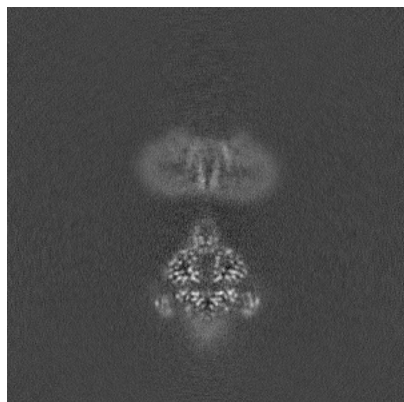


Y Index: 238

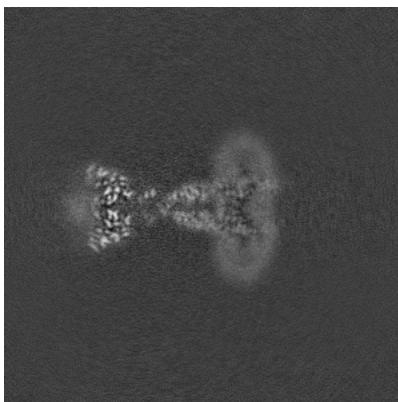


Z Index: 238

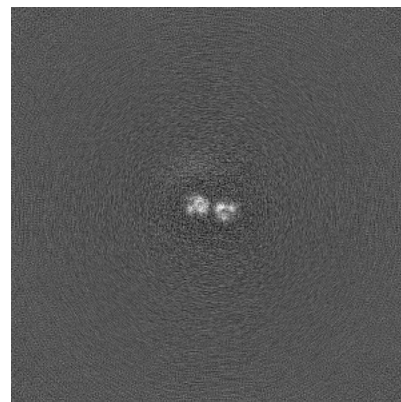
6.2.2 Raw map



X Index: 238



Y Index: 238

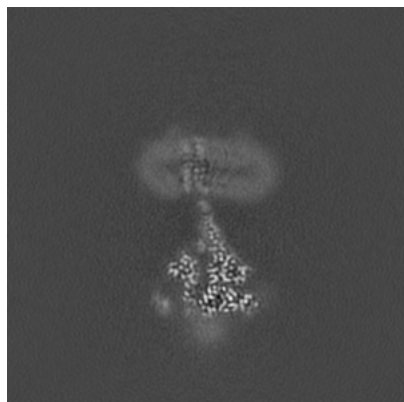


Z Index: 238

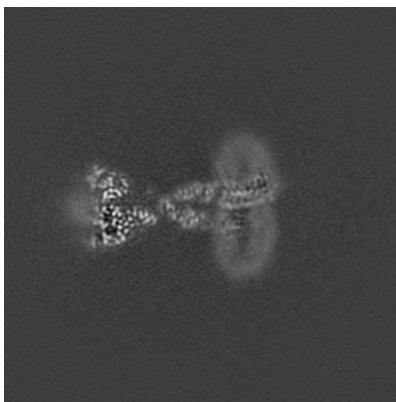
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

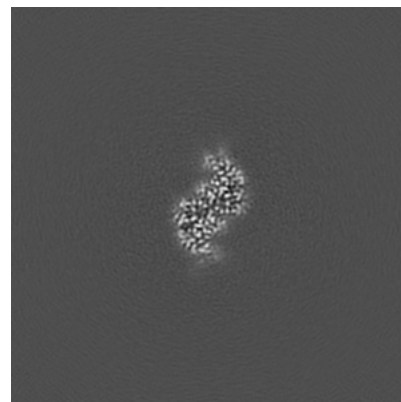
6.3.1 Primary map



X Index: 245

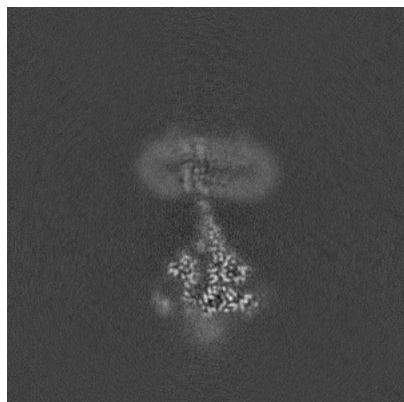


Y Index: 232

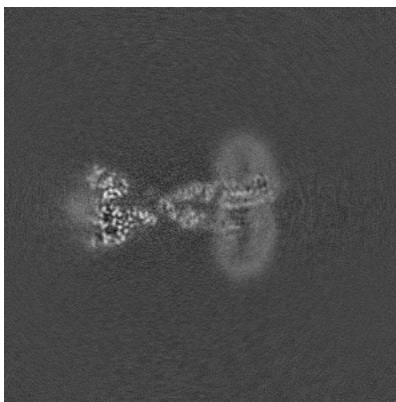


Z Index: 128

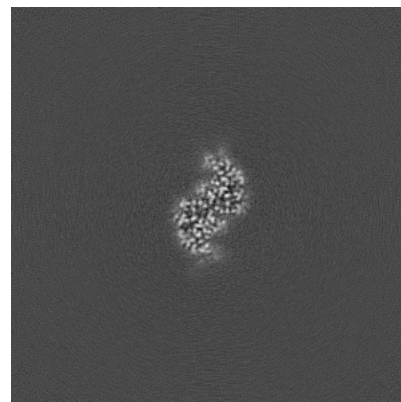
6.3.2 Raw map



X Index: 245



Y Index: 232



Z Index: 128

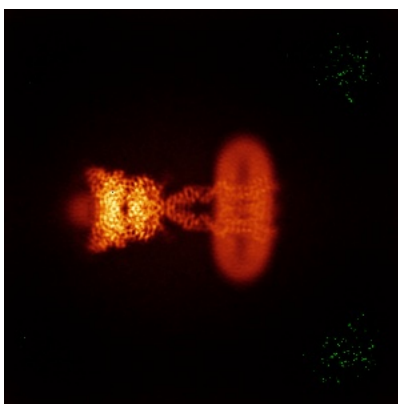
The images above show the largest variance slices of the map in three orthogonal directions.

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

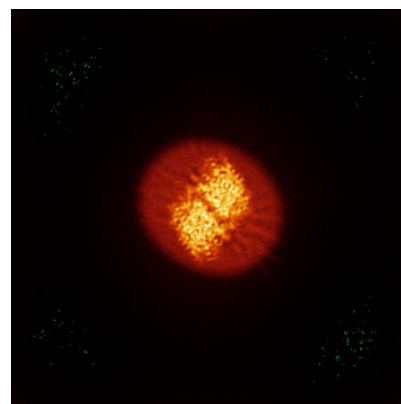
6.4.1 Primary map



X

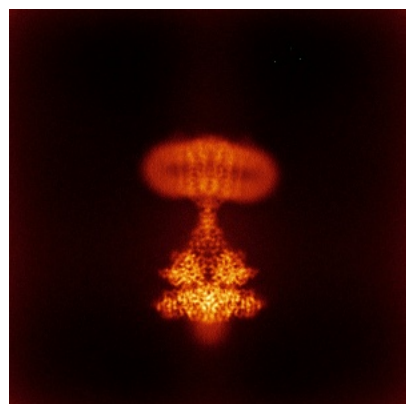


Y

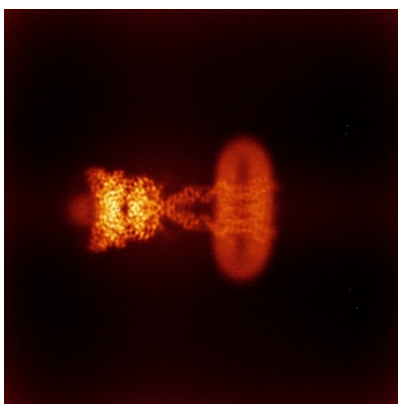


Z

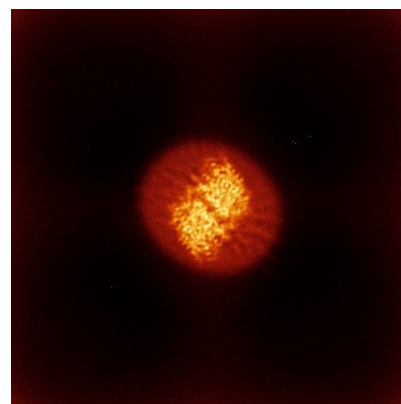
6.4.2 Raw map



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.

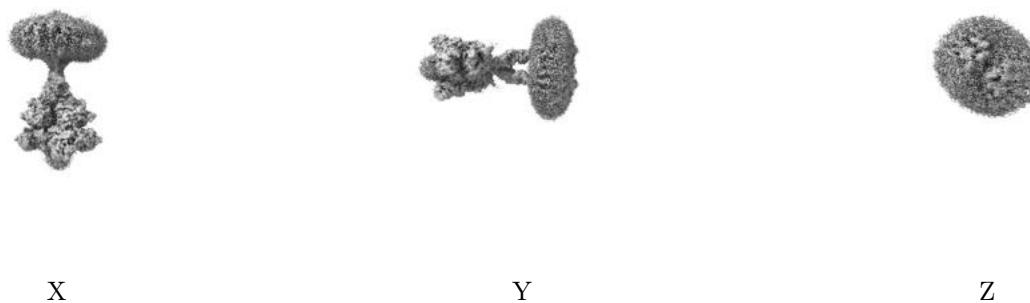
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

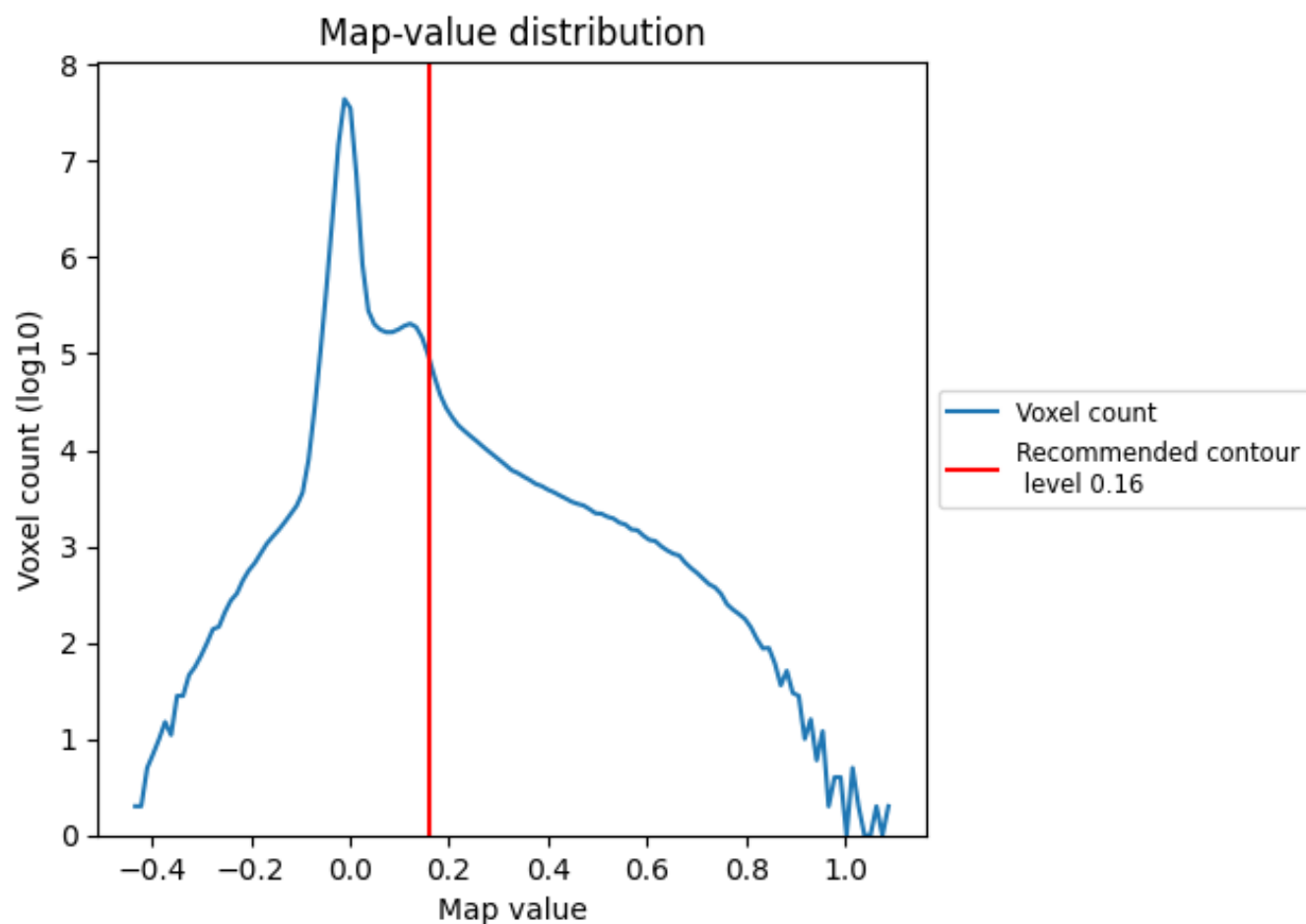
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

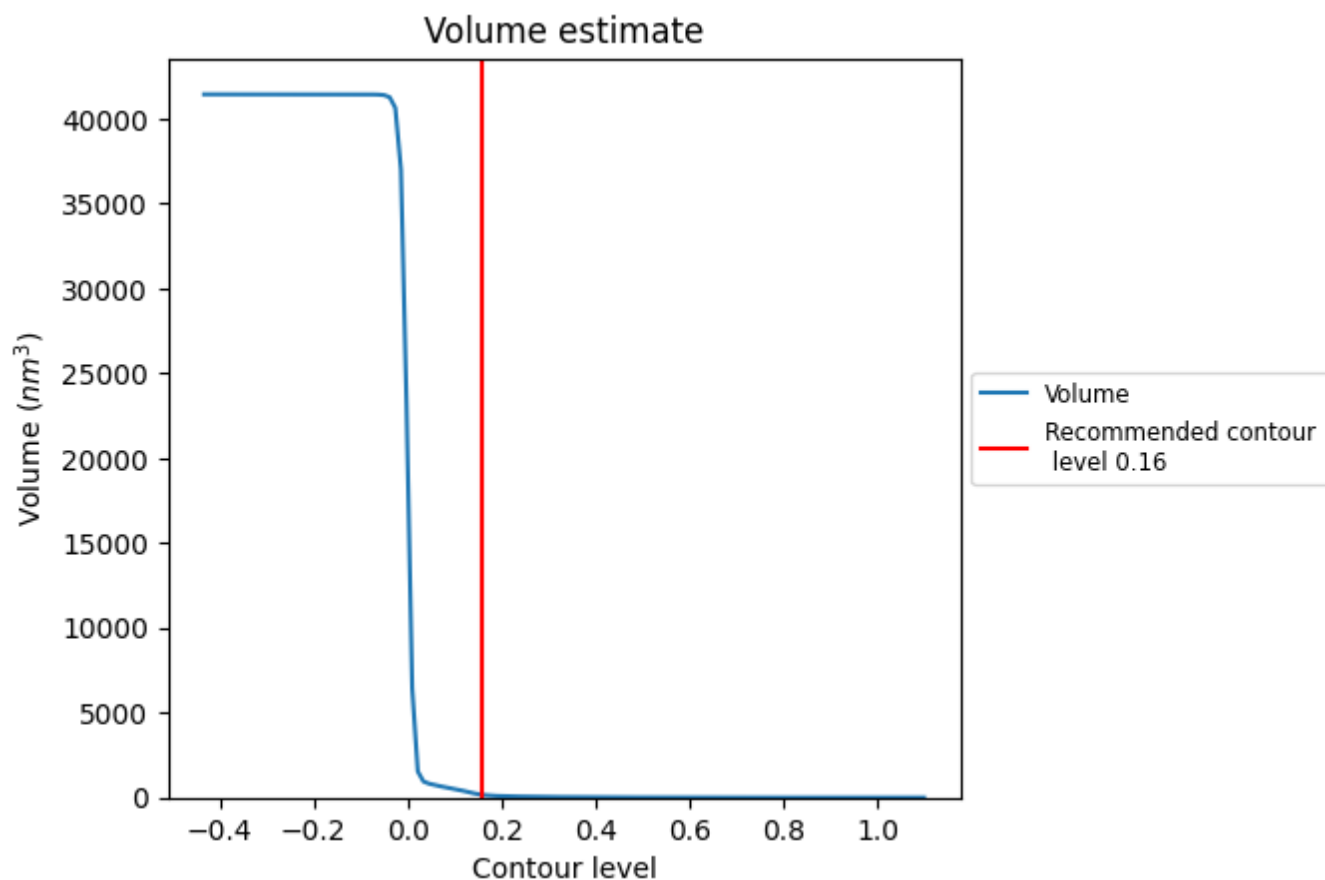
This section contains the results of statistical analysis of the map.

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.

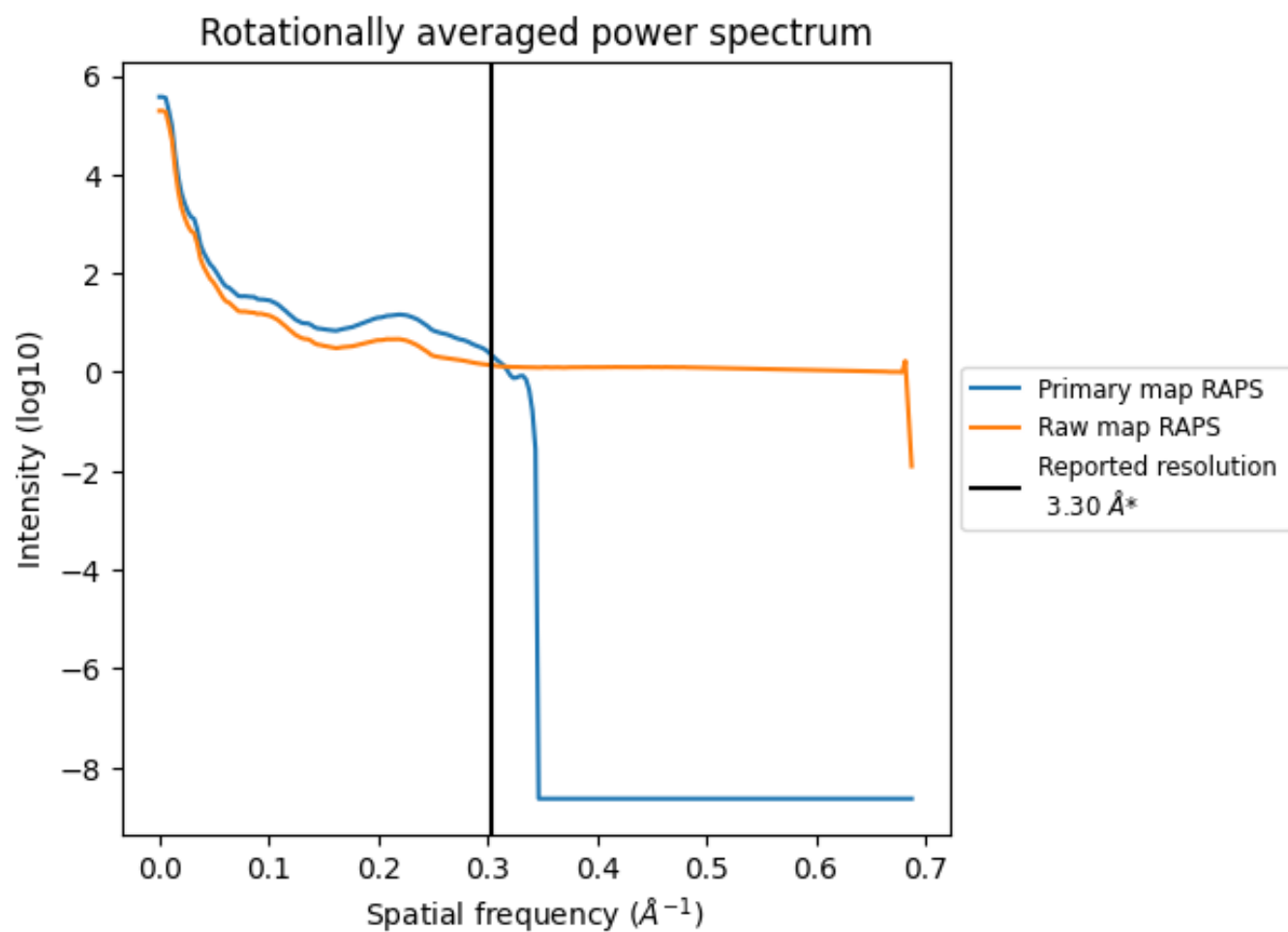
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160 nm^3 ; this corresponds to an approximate mass of 145 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 ⓘ

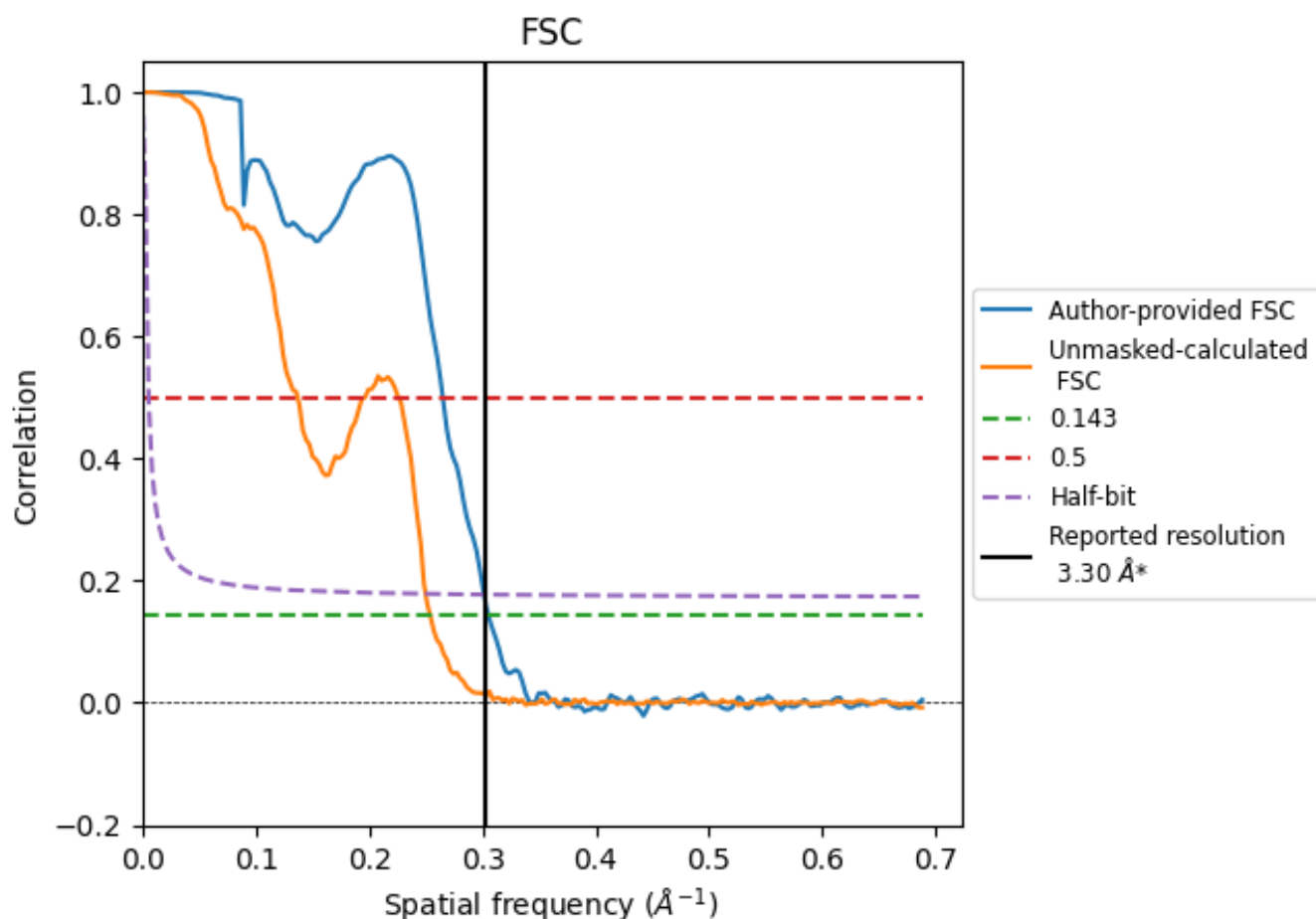


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

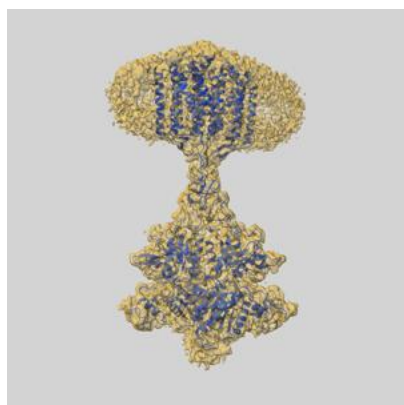
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.77	3.32
Unmasked-calculated*	3.94	7.30	4.00

*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 3.94 differs from the reported value 3.3 by more than 10 %

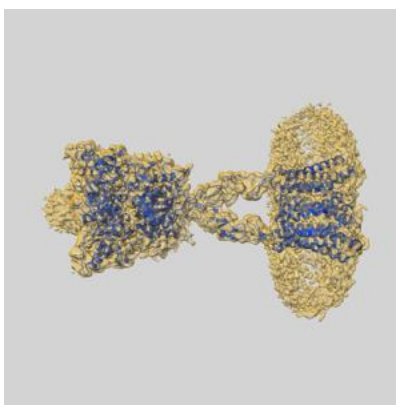
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37977 and PDB model 8X0F. Per-residue inclusion information can be found in section [3](#) on page [6](#).

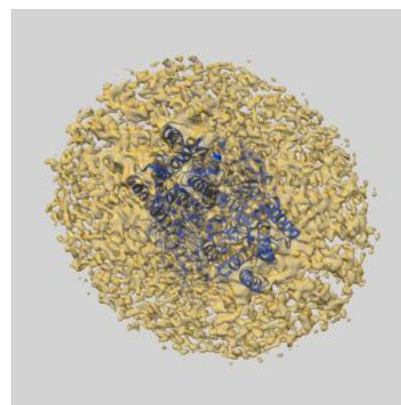
9.1 Map-model overlay [i](#)



X



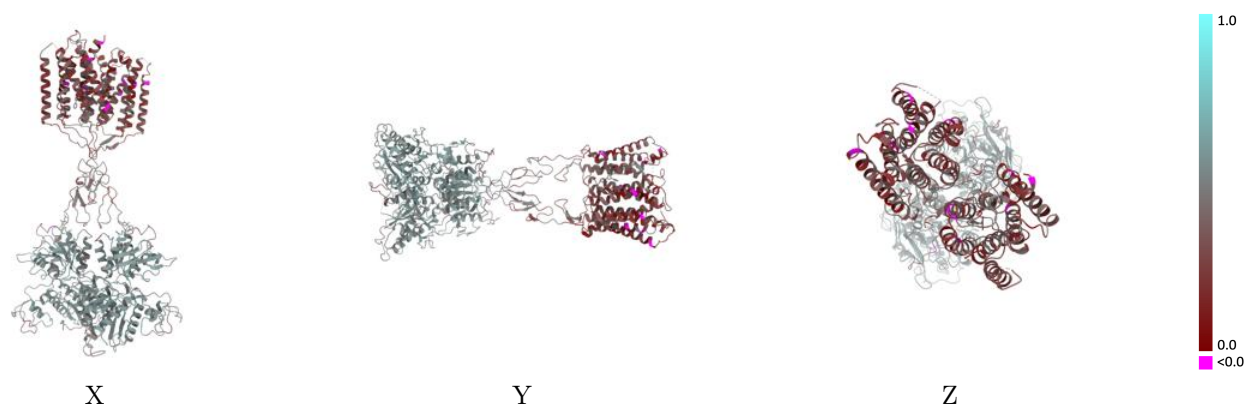
Y



Z

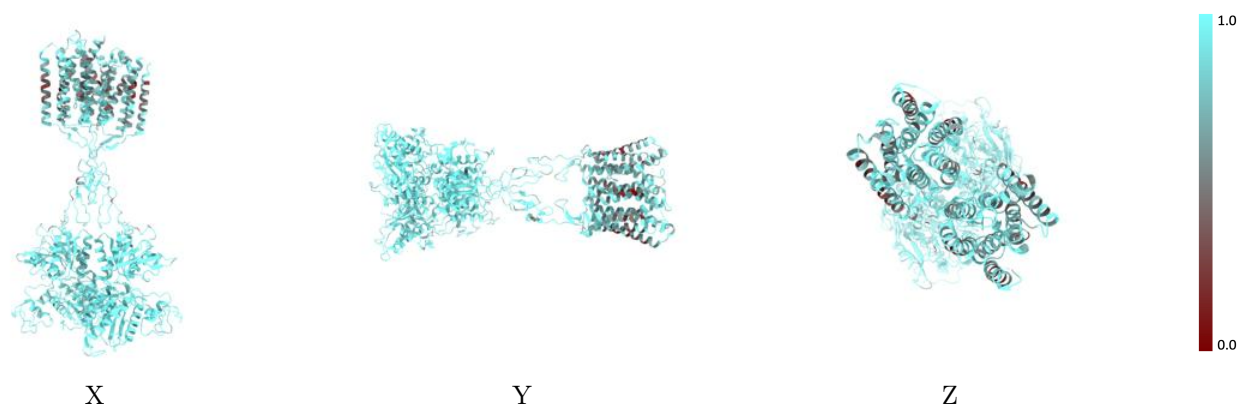
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



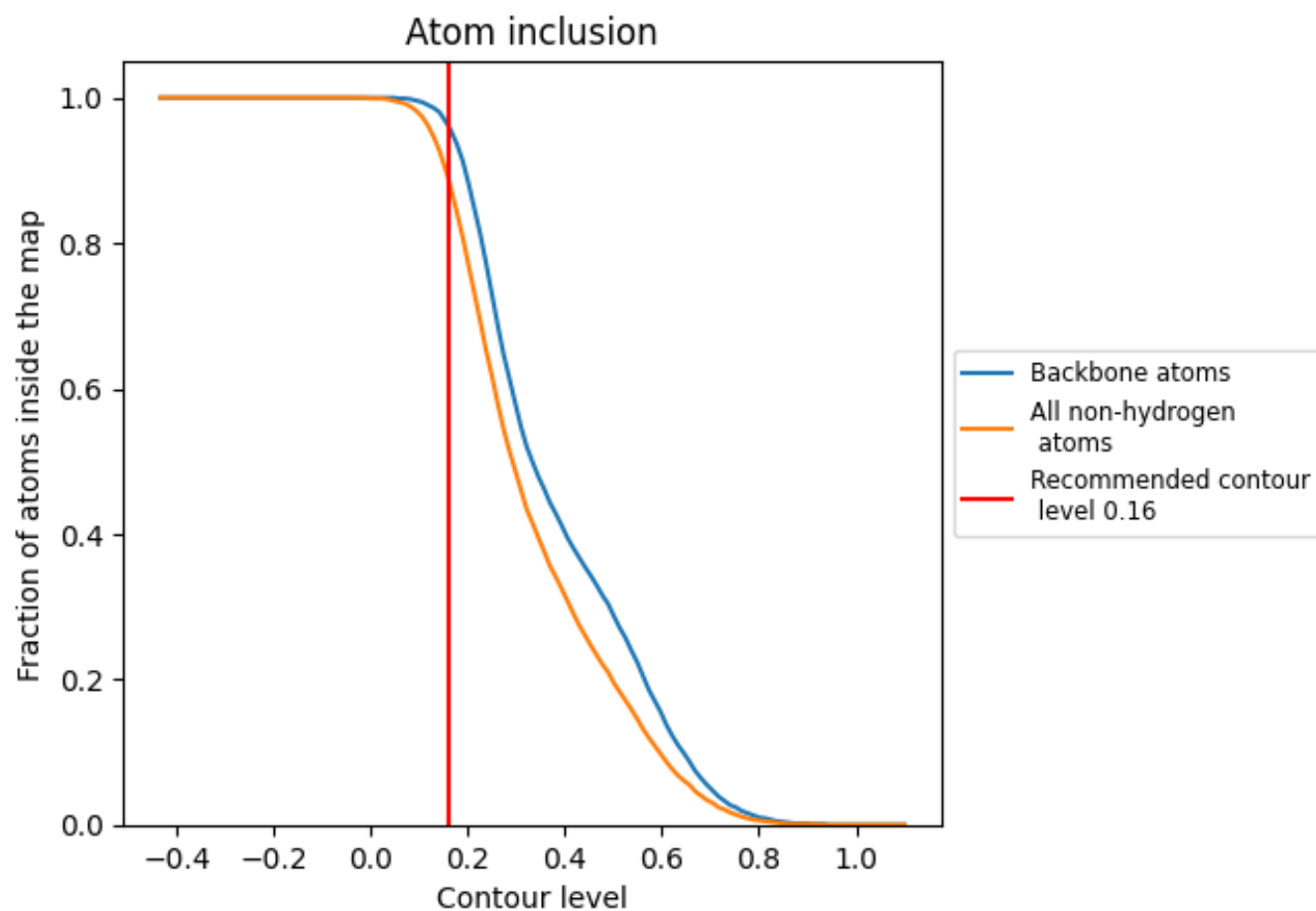
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8880	0.4420
A	0.8880	0.4450
B	0.8870	0.4390

