



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:51 AM UTC

PDB ID : 8JD1 / pdb_00008jd1
EMDB ID : EMD-36172
Title : Cryo-EM structure of mGlu2-mGlu3 heterodimer in Rco state
Authors : Wang, X.; Wang, M.; Xu, T.; Feng, Y.; Han, S.; Lin, S.; Zhao, Q.; Wu, B.
Deposited on : 2023-05-12
Resolution : 3.70 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

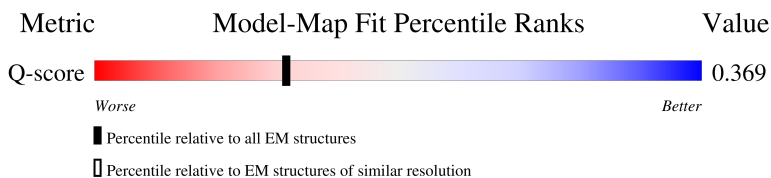
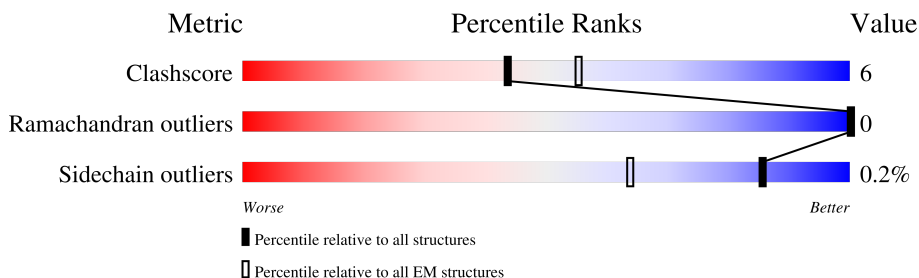
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	2	993	
2	3	993	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10766 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 2,Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	750	Total	C	N	O	S	0	0
			5121	3233	907	950	31		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	9	ASP	-	expression tag	UNP Q14416
2	10	TYR	-	expression tag	UNP Q14416
2	11	LYS	-	expression tag	UNP Q14416
2	12	ASP	-	expression tag	UNP Q14416
2	13	ASP	-	expression tag	UNP Q14416
2	14	ASP	-	expression tag	UNP Q14416
2	15	ASP	-	expression tag	UNP Q14416
2	16	GLY	-	expression tag	UNP Q14416
2	17	ALA	-	expression tag	UNP Q14416
2	18	PRO	-	expression tag	UNP Q14416
2	873	LEU	-	linker	UNP Q14416
2	874	GLU	-	linker	UNP Q14416
2	875	VAL	-	linker	UNP Q14416
2	876	LEU	-	linker	UNP Q14416
2	877	PHE	-	linker	UNP Q14416
2	878	GLN	-	linker	UNP Q14416
2	879	GLY	-	linker	UNP Q14416
2	880	PRO	-	linker	UNP Q14416
2	988	PHE	-	expression tag	UNP P62942
2	989	ALA	-	expression tag	UNP P62942
2	990	ALA	-	expression tag	UNP P62942
2	991	ALA	-	expression tag	UNP P62942
2	992	HIS	-	expression tag	UNP P62942
2	993	HIS	-	expression tag	UNP P62942
2	994	HIS	-	expression tag	UNP P62942
2	995	HIS	-	expression tag	UNP P62942
2	996	HIS	-	expression tag	UNP P62942

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Chain	Residue	Modelled	Actual	Comment	Reference
2	997	HIS	-	expression tag	UNP P62942
2	998	HIS	-	expression tag	UNP P62942
2	999	HIS	-	expression tag	UNP P62942
2	1000	HIS	-	expression tag	UNP P62942
2	1001	HIS	-	expression tag	UNP P62942

- Molecule 2 is a protein called Metabotropic glutamate receptor 3, Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	756	Total	C	N	O	S	0	0
			5429	3444	928	1022	35		

There are 41 discrepancies between the modelled and reference sequences:

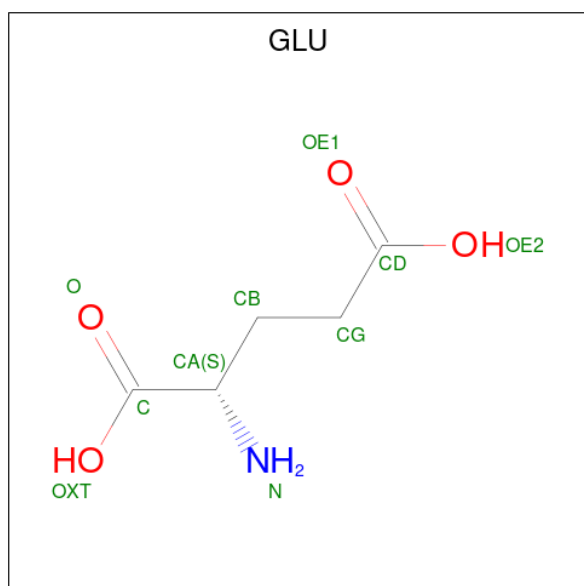
Chain	Residue	Modelled	Actual	Comment	Reference
3	-8	ASP	-	expression tag	UNP Q14832
3	-7	TYR	-	expression tag	UNP Q14832
3	-6	LYS	-	expression tag	UNP Q14832
3	-5	ASP	-	expression tag	UNP Q14832
3	-4	ASP	-	expression tag	UNP Q14832
3	-3	ASP	-	expression tag	UNP Q14832
3	-2	ASP	-	expression tag	UNP Q14832
3	-1	LYS	-	expression tag	UNP Q14832
3	0	GLY	-	expression tag	UNP Q14832
3	1	ALA	-	expression tag	UNP Q14832
3	2	PRO	-	expression tag	UNP Q14832
3	3	TRP	-	expression tag	UNP Q14832
3	4	SER	-	expression tag	UNP Q14832
3	5	HIS	-	expression tag	UNP Q14832
3	6	PRO	-	expression tag	UNP Q14832
3	7	GLN	-	expression tag	UNP Q14832
3	8	PHE	-	expression tag	UNP Q14832
3	9	GLU	-	expression tag	UNP Q14832
3	10	LYS	-	expression tag	UNP Q14832
3	11	GLY	-	expression tag	UNP Q14832
3	12	SER	-	expression tag	UNP Q14832
3	13	GLY	-	expression tag	UNP Q14832
3	14	SER	-	expression tag	UNP Q14832
3	15	TRP	-	expression tag	UNP Q14832
3	16	SER	-	expression tag	UNP Q14832
3	17	HIS	-	expression tag	UNP Q14832

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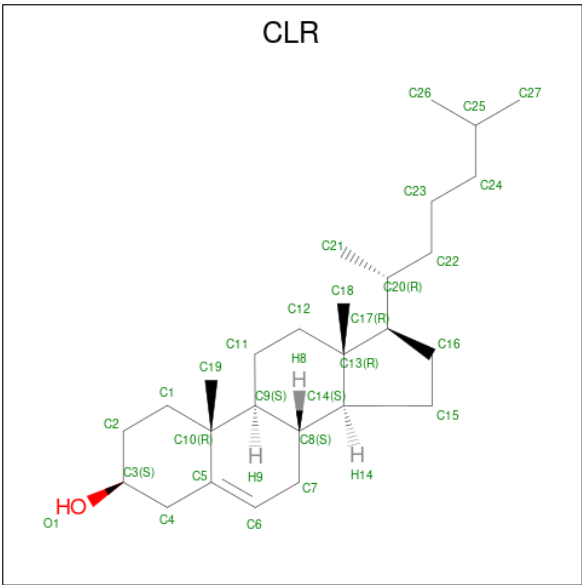
Chain	Residue	Modelled	Actual	Comment	Reference
3	18	PRO	-	expression tag	UNP Q14832
3	19	GLN	-	expression tag	UNP Q14832
3	20	PHE	-	expression tag	UNP Q14832
3	21	GLU	-	expression tag	UNP Q14832
3	22	LYS	-	expression tag	UNP Q14832
3	880	LEU	-	linker	UNP Q14832
3	881	GLU	-	linker	UNP Q14832
3	882	VAL	-	linker	UNP Q14832
3	883	LEU	-	linker	UNP Q14832
3	884	PHE	-	linker	UNP Q14832
3	885	GLN	-	linker	UNP Q14832
3	886	GLY	-	linker	UNP Q14832
3	887	PRO	-	linker	UNP Q14832
3	983	GLU	-	expression tag	UNP A0A8V8TRG9
3	984	PHE	-	expression tag	UNP A0A8V8TRG9

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	2	1	Total	C	N	O	0
			10	5	1	4	
3	3	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
4	3	1	Total	C	O	0
			28	27	1	
4	3	1	Total	C	O	0
			28	27	1	
4	3	1	Total	C	O	0
			28	27	1	
4	3	1	Total	C	O	0
			28	27	1	
4	3	1	Total	C	O	0
			28	27	1	
4	3	1	Total	C	O	0
			28	27	1	

ASP	TYR	LYS	ASP	ASP	ASP	ASP	LYS	GLY	ALA	PRO	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	SER	GLY	SER	TRP	SER	SER	HIS	PRO	GLN	LEU	R30	R31	E32	E36	M48	E49	LYS	GLY	THR	GLY	THR	GLU	GLU	C57	R64	R68	L69	E70																	
	F74		I79		L85	L86	K90	L91		D97		L106		E111		R114		T118	K119	V120	ASP	GLU	ALA	HIS	GLU	TYR	MET	CYS	PRO	ASP	GLY	SER	TYR	ALA	ILE	GLN	N137	S149	Y150	S151	Q156	R162	P167	Q168	I169	A172	L178	K181	S182	R183														
	A188	R189	P192	A202	E203	L203	V213	S214	T215	V216	E219		Y222	G223	E224	Q232	R237	E245	K246	D257	R261	E262	Q265	R270	V271	V272	V273	L274	F275	M276	R282	E283	L284	I285	S294	I309	I310	Y318	I321	L325	Y336	H346																						
	R347	N348	P349	C361	S362	L363	GLN	ASN	LYS	ARG	ASN	R370	C373	Y384	E385	Q386	K389	A401	K406	M407	Q408	N414	K417	D426	L430	R465	N470	N473	W486	L490	Q508	P512	C513	M521	Q522	P523	G524	D525	N526	W529																								
	I530	C531	P536	Y537	E538	Y539	F544	T545	C546	M547	D548	C549	G550	S551	G552	W554	L565	E573	D574	A575	I583	G587	F588	M589	K608	Y626	T629	F630	S637	P638	V639	I640	R645	N664	CYS	ILE	ALA	ARG	ILE	ASP	PHE	GLY	VAL	LYS	ASN	GLY	ALA																	
	GLN	ARG	PRO	K681	S684	P685	V699	V701	S704	I708	L709	E710	A711	P712	G713	T714	Y717	R723	V726	L727	L728	S736	S740	Y743	D744	L750	V753	Y754	R759	F770	I780	L783	I792	S793	S794	D795	V798	Q799	A820																									
	I625	P630	GLN	LYS	ASN	VAL	VAL	HIS	GLU	GLY	LEU	HIS	GLU	GLU	ASN	ALA	SER	ARG	PHE	SER	VAL	GLY	THR	GLY	ASN	THR	THR	LYS	SER	GLN	SER	VAL	ALA	LEU	SER	THR	THR	THR	SER	SER	ASN	LEU	LEU	GLU	VAL	VAL	LEU	PHE	ARG	ASP	GLN	GLY	PRO											
GLU	ALA	GLN	GLU	TRP	TRP	CYS	GLU	MET	GLU	TRP	HIS	THR	GLU	GLY	LEU	THR	GLU	GLY	GLY	THR	ARG	ASN	THR	VAL	GLY	GLY	PHE	VAL	ARG	GLU	LEU	LEU	THR	VAL	VAL	CYS	ASN	GLY	ARG	GLY	PRO	GLN	THR	LEU	LEU	LYS	GLU	THR	THR	SER	PHE	ASN	GLN	ALA	ALA	TYR	GLY	ARG	GLY	ASP	GLN	LEU	GLY	PRO
GLU	ALA	GLN	GLU	TRP	TRP	CYS	GLU	MET	GLU	TRP	HIS	THR	GLU	GLY	LEU	THR	GLU	GLY	GLY	THR	ARG	ASN	THR	VAL	GLY	GLY	PHE	VAL	ARG	GLU	LEU	LEU	THR	VAL	VAL	CYS	ASN	GLY	ARG	GLY	PRO	GLN	THR	LEU	LEU	LYS	GLU	THR	THR	SER	PHE	ASN	GLN	ALA	ALA	TYR	GLY	ARG	GLY	ASP	GLN	LEU	GLY	PRO

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.237	Depositor
Minimum map value	-5.405	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.425	Depositor
Map size ($\text{\AA}$)	385.56, 385.56, 385.56	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.071, 1.071, 1.071	Depositor

5 Model quality

5.1 Standard geometry

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	2	0.10	0/5231	0.27	0/7170
2	3	0.08	0/5541	0.25	0/7569
All	All	0.09	0/10772	0.26	0/14739

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5121	0	4443	56	0
2	3	5429	0	4874	73	0
3	2	10	0	5	0	0
3	3	10	0	5	2	0
4	3	196	0	322	6	0
All	All	10766	0	9649	132	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 6.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:704:SER:HB3	2:3:708:ILE:HD12	1.72	0.70
1:2:155:LEU:HD12	1:2:160:ILE:HB	1.78	0.66
2:3:536:PRO:O	2:3:723:ARG:NH2	2.29	0.66
2:3:276:MET:HE1	2:3:284:LEU:HD22	1.80	0.63
2:3:552:GLY:HA2	2:3:726:VAL:HG21	1.81	0.63
2:3:70:GLU:OE2	2:3:348:ASN:ND2	2.31	0.62
1:2:175:LYS:NZ	1:2:181:PHE:O	2.33	0.62
2:3:85:LEU:HD21	2:3:401:ALA:HB1	1.83	0.60
2:3:48:ASN:ND2	2:3:97:ASP:OD2	2.35	0.60
1:2:471:VAL:HG22	1:2:484:LEU:HD22	1.84	0.59
4:3:1004:CLR:H273	4:3:1006:CLR:H211	1.85	0.58
2:3:192:PRO:HD3	2:3:465:ARG:HH21	1.68	0.58
2:3:111:GLU:OE2	2:3:114:ARG:NH2	2.37	0.58
2:3:408:GLN:NE2	2:3:417:LYS:O	2.37	0.57
1:2:156:ARG:NH1	1:2:177:ARG:O	2.37	0.57
2:3:270:ARG:NH2	2:3:294:SER:O	2.38	0.57
2:3:172:ALA:O	3:3:1001:GLU:N	2.37	0.57
2:3:162:ARG:NH1	2:3:183:ARG:O	2.38	0.57
2:3:538:GLU:OE2	2:3:723:ARG:NH2	2.38	0.57
1:2:245:MET:HE3	1:2:250:PHE:HE1	1.71	0.56
1:2:509:VAL:HG23	1:2:520:TRP:HZ3	1.71	0.55
2:3:203:GLU:OE1	2:3:486:TRP:NE1	2.32	0.55
2:3:257:ASP:OD2	2:3:261:ARG:NH1	2.39	0.55
2:3:384:TYR:OH	2:3:386:GLN:OE1	2.23	0.55
2:3:68:ARG:NH1	2:3:149:SER:OG	2.40	0.55
2:3:274:LEU:HD22	2:3:276:MET:HE2	1.88	0.55
2:3:626:TYR:O	2:3:629:THR:OG1	2.23	0.55
2:3:213:VAL:HG12	2:3:271:VAL:HG13	1.90	0.54
1:2:228:ALA:HB1	1:2:233:ILE:HB	1.89	0.54
2:3:792:THR:OG1	2:3:799:GLN:O	2.25	0.54
2:3:31:ARG:NH2	2:3:349:PRO:O	2.41	0.54
2:3:86:LEU:HD23	2:3:91:LEU:HD11	1.90	0.54
2:3:321:ILE:HD13	2:3:470:ASN:HD22	1.73	0.53
1:2:255:ARG:HA	1:2:258:LEU:HG	1.90	0.53
1:2:34:LEU:O	1:2:87:HIS:N	2.41	0.53
2:3:219:GLU:HA	2:3:246:LYS:HZ2	1.73	0.52
1:2:776:PHE:HA	1:2:779:ILE:HD12	1.89	0.52
1:2:724:ARG:HA	1:2:727:SER:HB3	1.90	0.52
1:2:26:LEU:HD12	1:2:343:PRO:HD3	1.91	0.52
2:3:637:SER:HB2	2:3:640:ILE:HG13	1.91	0.52
2:3:36:GLU:O	2:3:90:LYS:NZ	2.43	0.52
2:3:645:ARG:NH2	2:3:740:SER:OG	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:639:VAL:HG23	4:3:1004:CLR:H71	1.93	0.51
1:2:33:VAL:HG13	1:2:136:ILE:HG12	1.92	0.51
2:3:717:TYR:HA	2:3:728:LEU:HA	1.92	0.51
2:3:770:PHE:HB3	2:3:820:ALA:HB1	1.93	0.50
2:3:169:ILE:HG22	2:3:188:ALA:HB3	1.92	0.50
1:2:561:ILE:HB	1:2:563:TRP:HE3	1.76	0.50
2:3:232:GLN:CD	2:3:232:GLN:H	2.19	0.50
1:2:636:ARG:NH1	1:2:727:SER:OG	2.45	0.49
2:3:214:SER:HB2	2:3:272:VAL:HG12	1.95	0.49
1:2:250:PHE:HA	1:2:253:VAL:HG12	1.93	0.49
1:2:187:PRO:HD2	1:2:190:PHE:CE2	2.48	0.49
2:3:48:ASN:HB3	2:3:57:CYS:HB2	1.95	0.49
2:3:282:ARG:HA	2:3:309:ILE:HG23	1.94	0.49
1:2:197:GLU:HB3	1:2:478:LEU:HD22	1.94	0.48
1:2:140:ILE:HD13	1:2:385:VAL:HG12	1.95	0.48
2:3:79:ILE:HD12	2:3:85:LEU:HD22	1.96	0.48
2:3:711:ALA:HB3	4:3:1004:CLR:H21	1.96	0.47
2:3:551:SER:HA	2:3:723:ARG:HG2	1.97	0.47
2:3:224:GLU:OE1	2:3:246:LYS:NZ	2.48	0.47
1:2:99:LEU:HD13	1:2:154:LEU:HD22	1.96	0.47
1:2:560:TYR:N	1:2:717:VAL:O	2.45	0.47
2:3:285:ILE:HG21	2:3:310:ILE:HG22	1.97	0.47
1:2:322:TYR:OH	1:2:438:HIS:ND1	2.36	0.47
1:2:198:ILE:HD13	1:2:315:ILE:HG21	1.96	0.47
4:3:1002:CLR:H241	4:3:1003:CLR:H272	1.97	0.47
1:2:208:SER:HB3	1:2:257:LEU:HD12	1.97	0.47
2:3:325:LEU:HD13	2:3:389:LYS:HE3	1.97	0.47
2:3:704:SER:O	2:3:708:ILE:N	2.45	0.46
2:3:645:ARG:HH21	2:3:740:SER:HG	1.60	0.46
1:2:285:LEU:HD22	1:2:287:ALA:HB2	1.98	0.46
2:3:151:SER:HB2	2:3:222:TYR:HB2	1.96	0.46
2:3:523:PRO:HG2	2:3:525:ASP:OD1	2.14	0.46
1:2:473:TYR:O	1:2:479:THR:OG1	2.33	0.46
2:3:361:CYS:HB3	2:3:373:CYS:HB3	1.94	0.46
2:3:181:LYS:HA	2:3:181:LYS:HD3	1.73	0.46
2:3:684:SER:OG	2:3:685:PRO:HD3	2.16	0.46
1:2:78:LEU:HD21	1:2:389:ALA:HB1	1.98	0.46
1:2:172:LEU:HB2	1:2:183:ARG:HH21	1.80	0.46
2:3:30:ARG:NH2	2:3:32:GLU:OE1	2.39	0.45
2:3:202:ALA:HB1	2:3:237:ARG:HD2	1.97	0.45
1:2:219:THR:O	1:2:222:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:178:LEU:HB2	2:3:189:ARG:HH12	1.82	0.45
1:2:430:ALA:HB2	1:2:439:ASN:HA	1.98	0.44
2:3:246:LYS:HE3	2:3:246:LYS:HB3	1.80	0.44
2:3:554:TRP:HB2	2:3:565:LEU:HB3	1.99	0.44
2:3:521:MET:HA	2:3:544:PHE:HB2	1.99	0.44
1:2:527:PRO:C	1:2:529:GLU:H	2.26	0.44
1:2:26:LEU:HB3	1:2:88:ILE:HB	2.00	0.44
1:2:510:LYS:H	1:2:522:CYS:HA	1.82	0.44
1:2:146:ASP:OD1	1:2:146:ASP:N	2.51	0.43
1:2:564:GLY:O	1:2:566:ALA:N	2.50	0.43
1:2:72:ILE:HD11	1:2:78:LEU:HD13	1.99	0.43
2:3:167:PRO:HG2	2:3:430:LEU:HD22	2.01	0.43
2:3:318:TYR:HE1	2:3:473:ASN:HB3	1.84	0.43
2:3:203:GLU:HB3	2:3:490:LEU:HD11	2.01	0.43
2:3:539:TYR:HD1	2:3:549:CYS:HB3	1.84	0.43
1:2:561:ILE:HD12	1:2:627:PRO:HD2	2.00	0.42
2:3:529:TRP:HZ3	2:3:531:CYS:HB2	1.83	0.42
1:2:161:PRO:HB3	1:2:419:TYR:HB2	2.01	0.42
2:3:64:ARG:NH1	3:3:1001:GLU:CD	2.77	0.42
2:3:106:LEU:HG	2:3:156:GLN:HB3	2.01	0.42
1:2:211:ALA:HB3	1:2:240:LYS:HD3	2.00	0.42
1:2:143:SER:HB3	1:2:165:TYR:OH	2.19	0.42
2:3:216:VAL:HG12	2:3:245:GLU:HB2	2.01	0.42
2:3:262:GLU:O	2:3:265:GLN:HG2	2.20	0.42
1:2:61:ARG:HG2	1:2:381:VAL:HG21	2.01	0.42
2:3:545:THR:OG1	2:3:547:MET:SD	2.64	0.42
2:3:698:VAL:HA	2:3:701:VAL:HG22	2.02	0.42
1:2:485:ILE:HG22	1:2:487:TRP:H	1.83	0.42
1:2:103:LEU:HD23	1:2:103:LEU:HA	1.89	0.41
4:3:1005:CLR:H222	4:3:1005:CLR:H162	1.40	0.41
1:2:57:ARG:O	1:2:61:ARG:HD2	2.21	0.41
2:3:74:PHE:HB2	2:3:336:TYR:CD2	2.55	0.41
1:2:34:LEU:HD11	1:2:388:MET:HG2	2.02	0.41
1:2:800:LEU:O	1:2:804:VAL:N	2.43	0.41
1:2:174:ASP:OD1	1:2:174:ASP:N	2.48	0.41
1:2:746:ALA:O	1:2:749:THR:OG1	2.34	0.41
1:2:273:GLU:HG2	1:2:274:ASP:N	2.36	0.41
1:2:266:ALA:HB3	1:2:291:TRP:CD1	2.55	0.41
1:2:634:LEU:HA	1:2:637:LEU:HB2	2.03	0.41
1:2:698:LEU:HD11	4:3:1004:CLR:H152	2.01	0.41
2:3:426:ASP:OD1	2:3:426:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:467:ARG:NH2	1:2:469:GLN:OE1	2.53	0.41
2:3:285:ILE:HD13	2:3:285:ILE:HA	1.95	0.41
2:3:406:LYS:HE3	2:3:406:LYS:HB2	1.95	0.41
1:2:331:PHE:HA	1:2:334:LEU:HD13	2.04	0.40
1:2:79:LEU:HD12	1:2:84:LEU:HD11	2.04	0.40
2:3:68:ARG:HH21	2:3:389:LYS:HB2	1.86	0.40
2:3:583:ILE:O	2:3:587:GLY:N	2.42	0.40
1:2:805:VAL:O	1:2:809:LEU:N	2.54	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	2	742/993 (75%)	693 (93%)	49 (7%)	0	100	100
2	3	746/993 (75%)	694 (93%)	52 (7%)	0	100	100
All	All	1488/1986 (75%)	1387 (93%)	101 (7%)	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	2	429/813 (53%)	429 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3	510/867 (59%)	510 (100%)	0	100	100
All	All	939/1680 (56%)	939 (100%)	0	85	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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	41	HIS
1	2	339	ASN
1	2	351	GLN
1	2	365	HIS
1	2	394	ASN
2	3	315	HIS
2	3	332	GLN
2	3	360	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
4	CLR	3	1008	-	31,31,31	0.28	0	48,48,48	0.38	0
4	CLR	3	1003	-	31,31,31	0.28	0	48,48,48	0.39	0
4	CLR	3	1002	-	31,31,31	0.28	0	48,48,48	0.37	0
4	CLR	3	1006	-	31,31,31	0.28	0	48,48,48	0.38	0
3	GLU	2	1101	-	8,9,9	1.04	0	8,11,11	1.17	0
4	CLR	3	1007	-	31,31,31	0.29	0	48,48,48	0.39	0
4	CLR	3	1005	-	31,31,31	0.29	0	48,48,48	0.36	0
4	CLR	3	1004	-	31,31,31	0.29	0	48,48,48	0.39	0
3	GLU	3	1001	-	8,9,9	1.08	0	8,11,11	1.41	2 (25%)

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
4	CLR	3	1008	-	-	3/10/68/68	0/4/4/4
4	CLR	3	1003	-	-	3/10/68/68	0/4/4/4
4	CLR	3	1002	-	-	1/10/68/68	0/4/4/4
4	CLR	3	1006	-	-	0/10/68/68	0/4/4/4
3	GLU	2	1101	-	-	8/9/9/9	-
4	CLR	3	1007	-	-	0/10/68/68	0/4/4/4
4	CLR	3	1005	-	-	6/10/68/68	0/4/4/4
4	CLR	3	1004	-	-	6/10/68/68	0/4/4/4
3	GLU	3	1001	-	-	6/9/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	1001	GLU	OE2-CD-CG	2.14	120.76	114.00
3	3	1001	GLU	OXT-C-O	-2.07	119.37	124.08

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	2	1101	GLU	N-CA-CB-CG
3	2	1101	GLU	C-CA-CB-CG
3	3	1001	GLU	N-CA-CB-CG
3	3	1001	GLU	C-CA-CB-CG
4	3	1005	CLR	C16-C17-C20-C21
4	3	1005	CLR	C13-C17-C20-C22
4	3	1005	CLR	C13-C17-C20-C21
4	3	1005	CLR	C16-C17-C20-C22
3	3	1001	GLU	OXT-C-CA-N
4	3	1004	CLR	C17-C20-C22-C23
4	3	1005	CLR	C17-C20-C22-C23
3	2	1101	GLU	OXT-C-CA-N
4	3	1004	CLR	C21-C20-C22-C23
4	3	1005	CLR	C21-C20-C22-C23
4	3	1008	CLR	C17-C20-C22-C23
4	3	1003	CLR	C20-C22-C23-C24
4	3	1003	CLR	C22-C23-C24-C25
4	3	1008	CLR	C21-C20-C22-C23
3	2	1101	GLU	OXT-C-CA-CB
3	3	1001	GLU	OXT-C-CA-CB
3	2	1101	GLU	O-C-CA-CB
3	3	1001	GLU	O-C-CA-CB
3	2	1101	GLU	O-C-CA-N
3	3	1001	GLU	O-C-CA-N
4	3	1004	CLR	C16-C17-C20-C22
4	3	1004	CLR	C13-C17-C20-C22
4	3	1004	CLR	C16-C17-C20-C21
4	3	1004	CLR	C13-C17-C20-C21
4	3	1002	CLR	C16-C17-C20-C22
4	3	1003	CLR	C16-C17-C20-C22
4	3	1008	CLR	C16-C17-C20-C22
3	2	1101	GLU	OE2-CD-CG-CB
3	2	1101	GLU	CA-CB-CG-CD

There are no ring outliers.

6 monomers are involved in 8 short contacts:

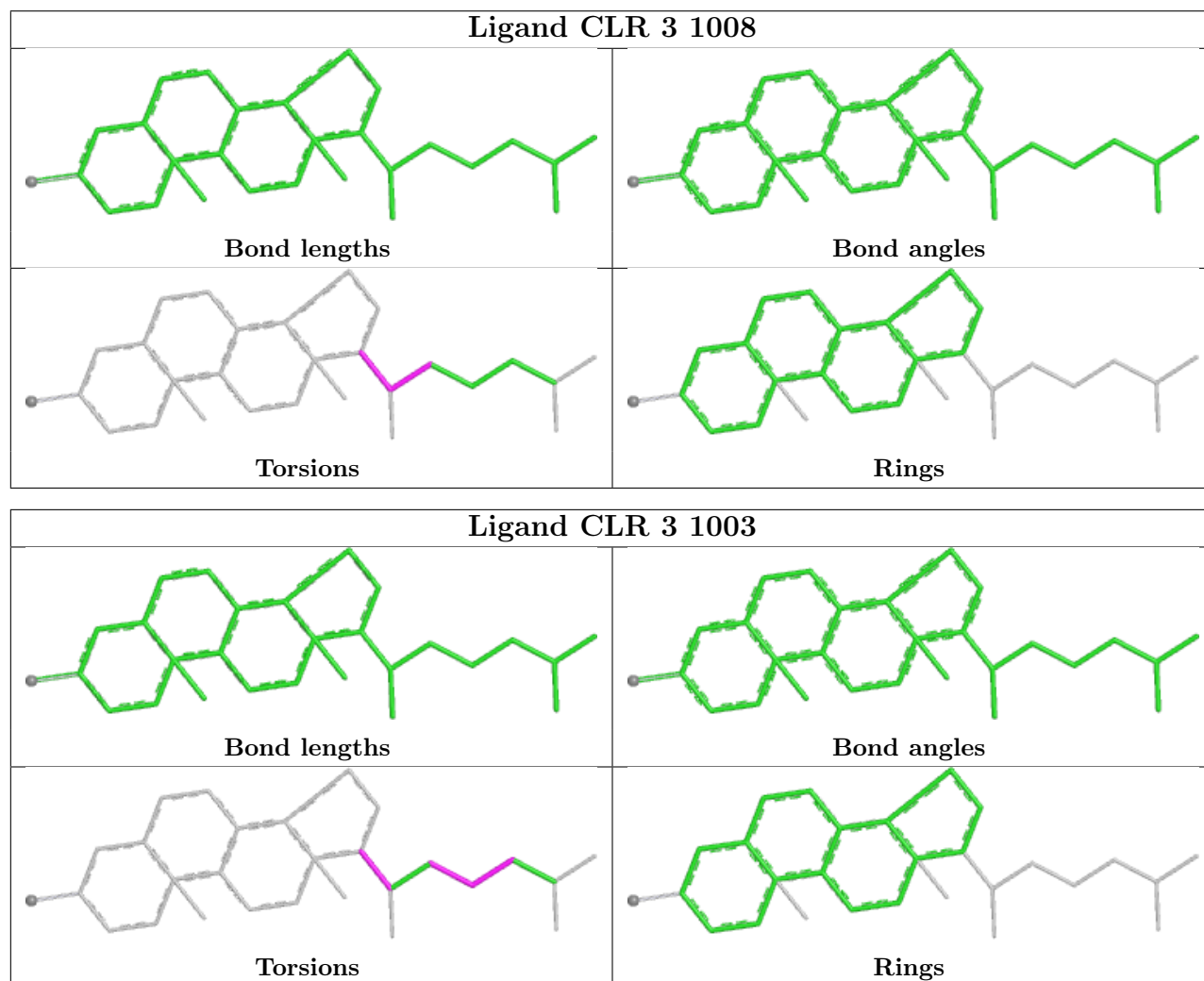
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	1003	CLR	1	0
4	3	1002	CLR	1	0
4	3	1006	CLR	1	0
4	3	1005	CLR	1	0
4	3	1004	CLR	4	0

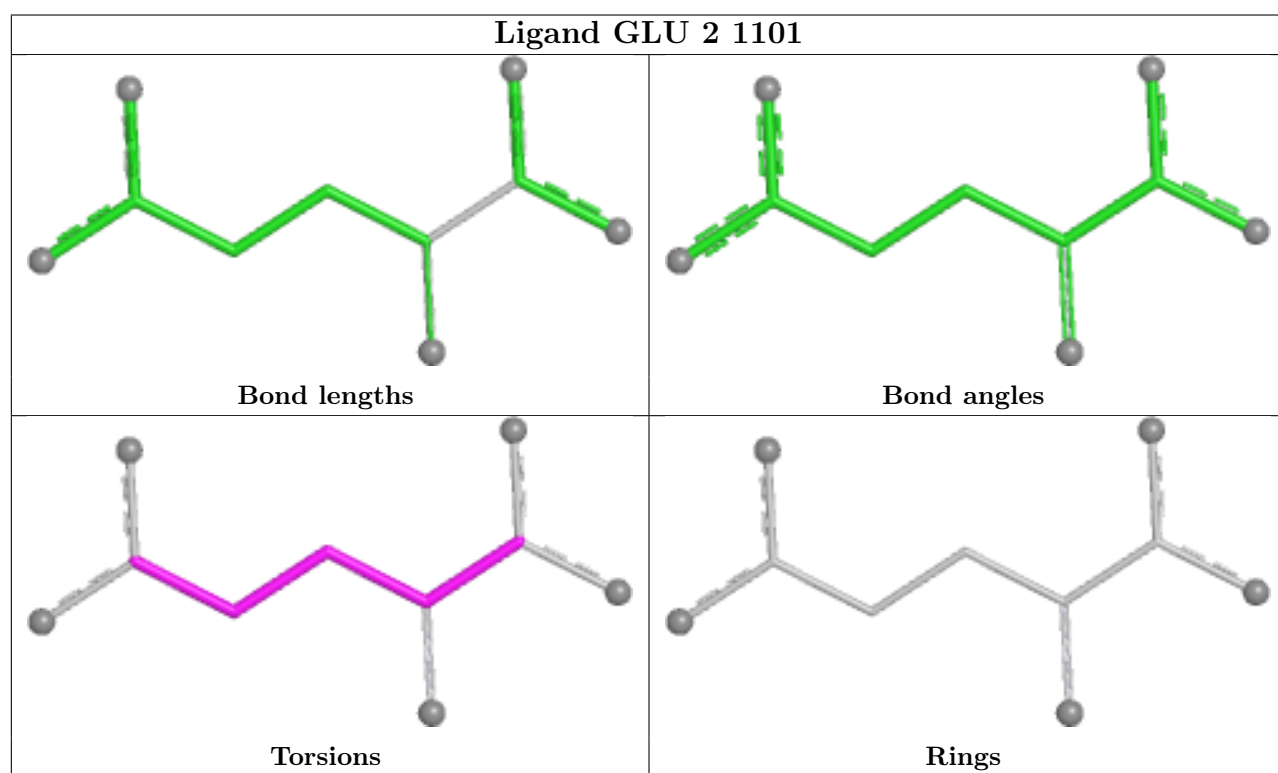
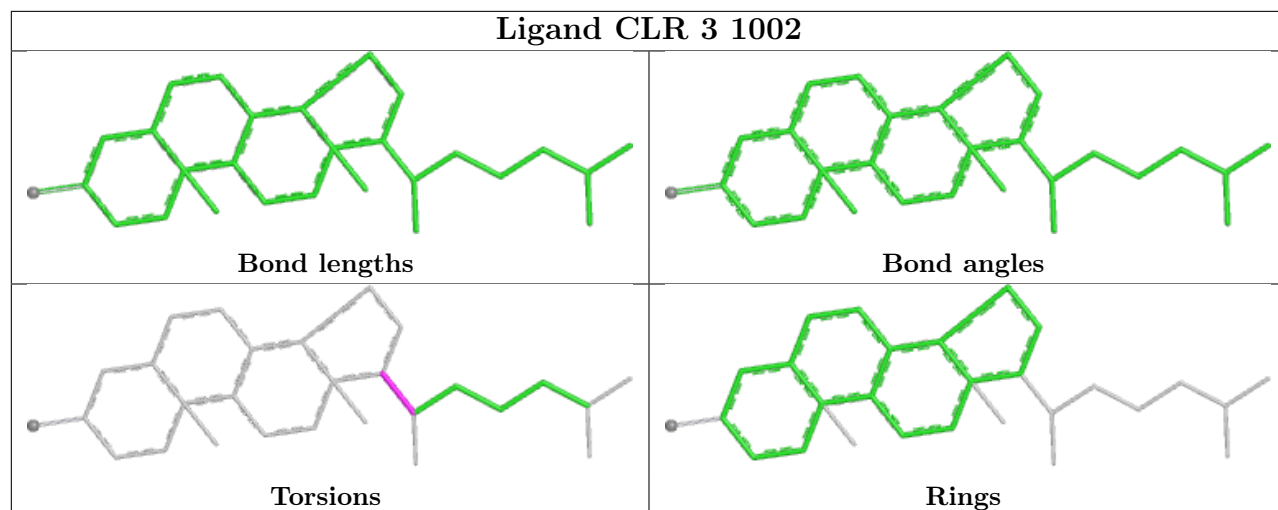
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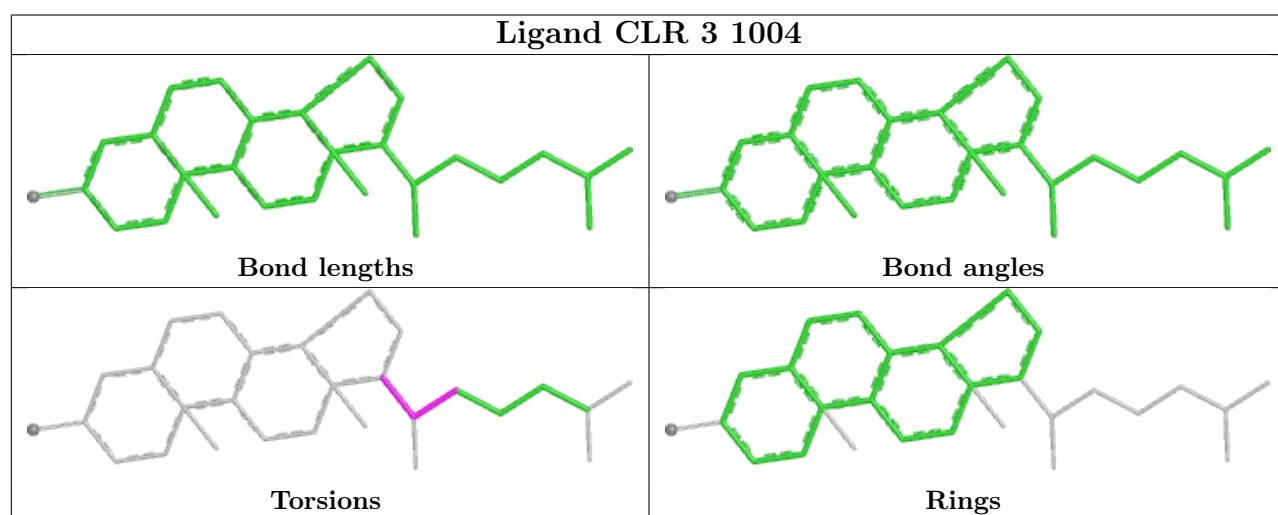
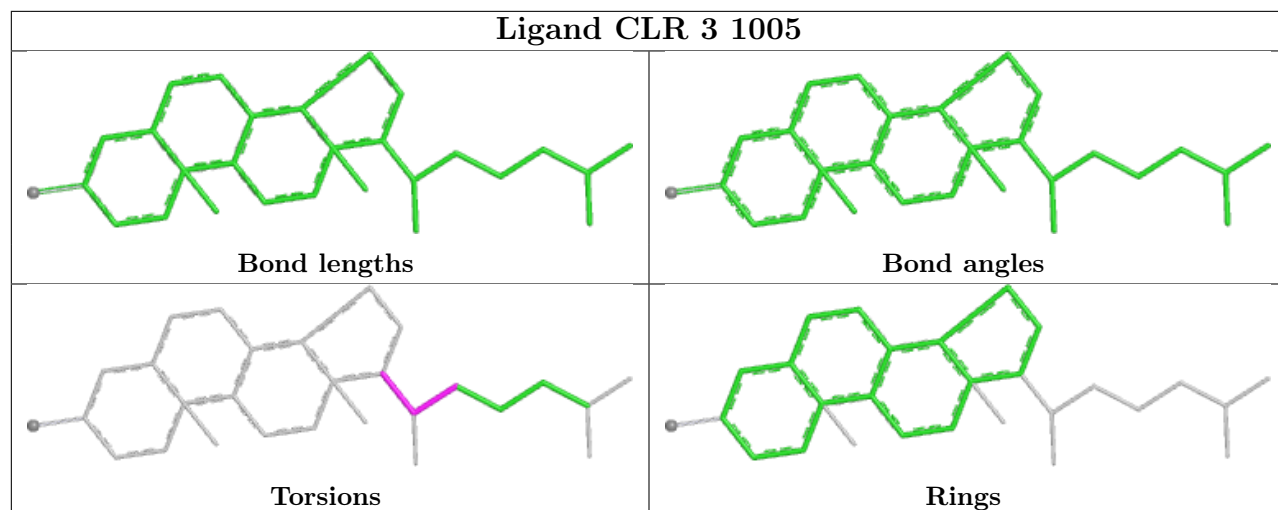
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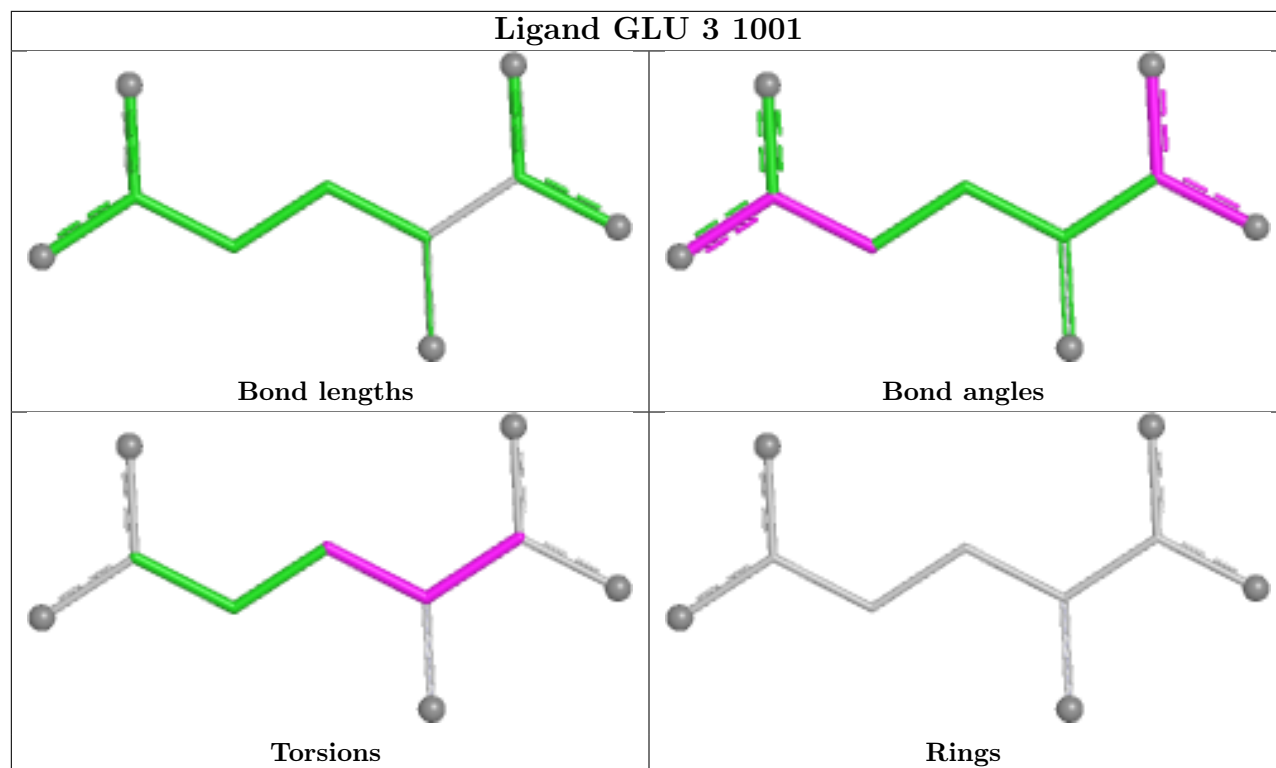
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	3	1001	GLU	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

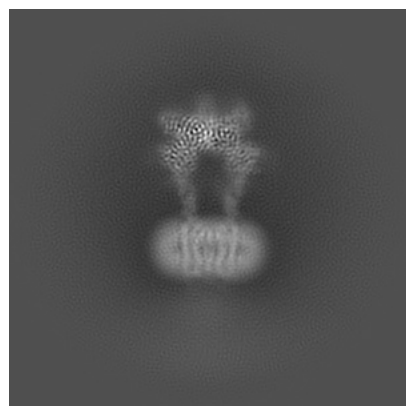
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36172. These allow visual inspection of the internal detail of the map and identification of artifacts.

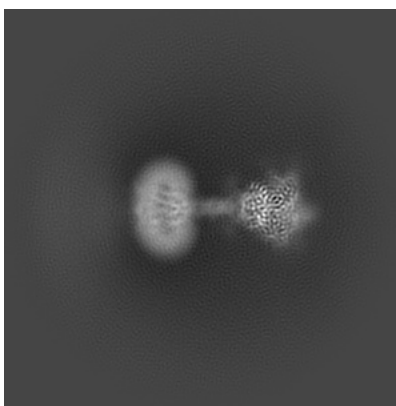
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

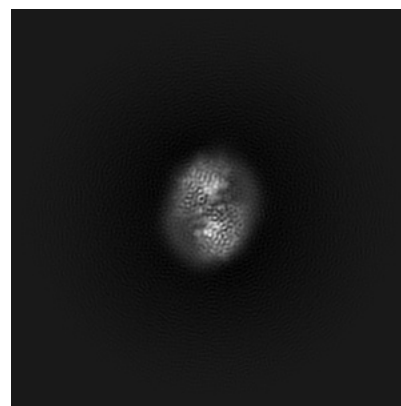
6.1.1 Primary map



X

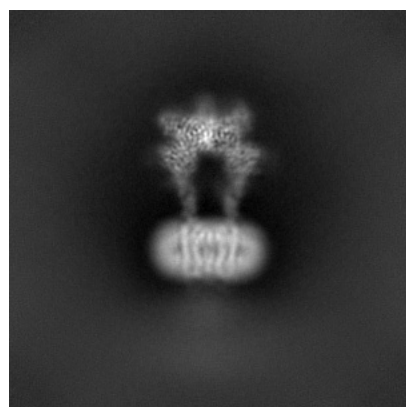


Y

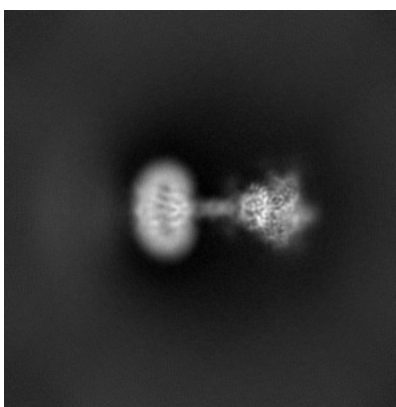


Z

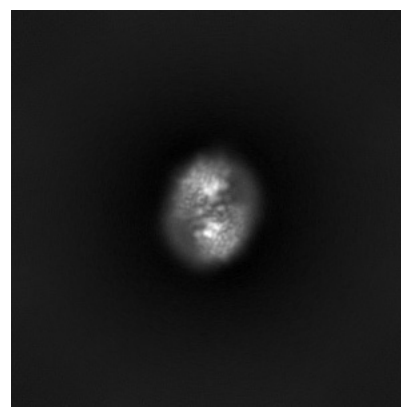
6.1.2 Raw map



X



Y

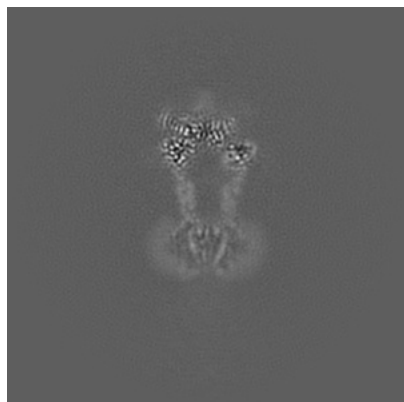


Z

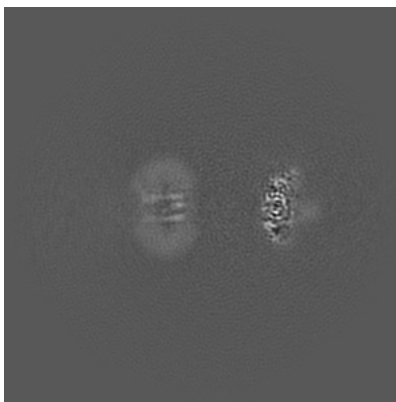
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

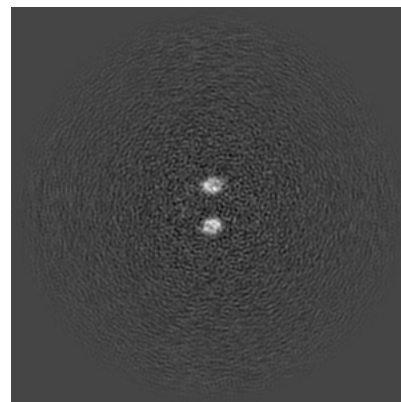
6.2.1 Primary map



X Index: 180

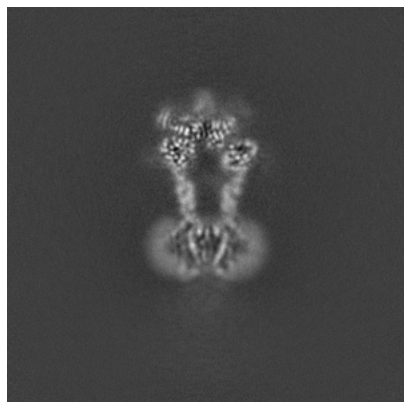


Y Index: 180

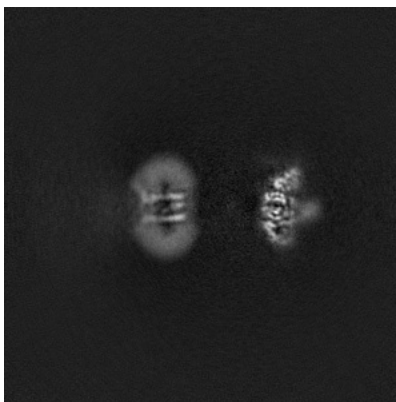


Z Index: 180

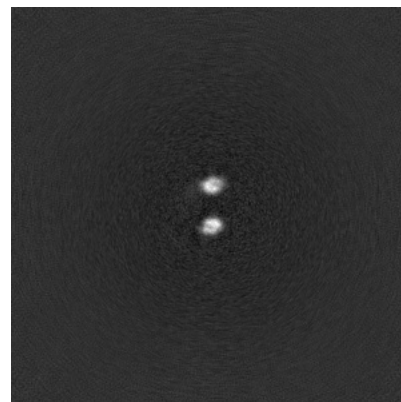
6.2.2 Raw map



X Index: 180



Y Index: 180

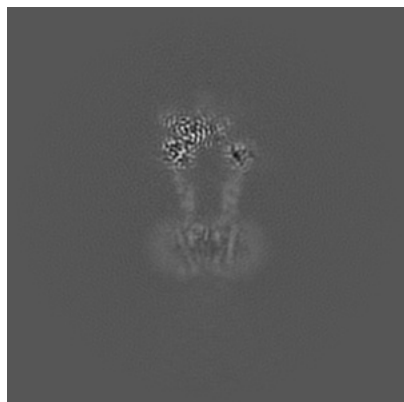


Z Index: 180

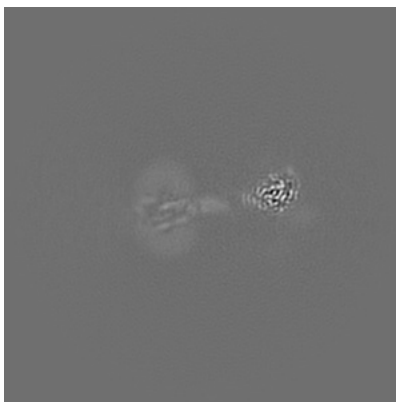
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

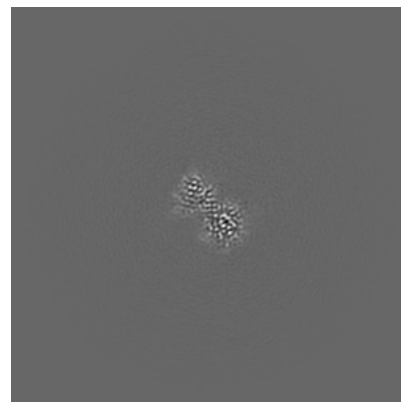
6.3.1 Primary map



X Index: 183

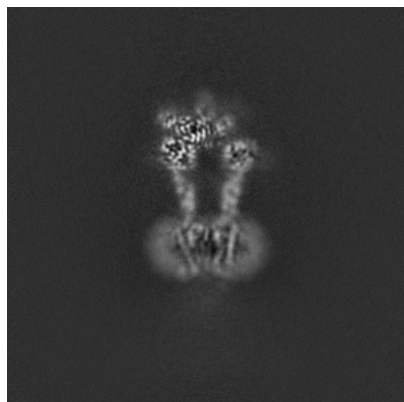


Y Index: 166

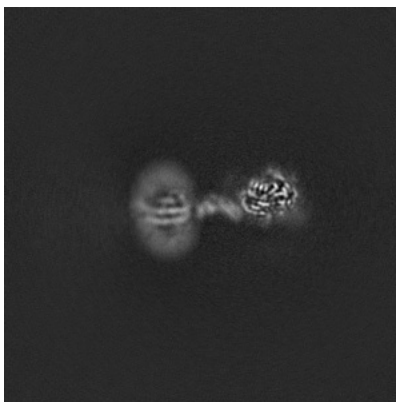


Z Index: 246

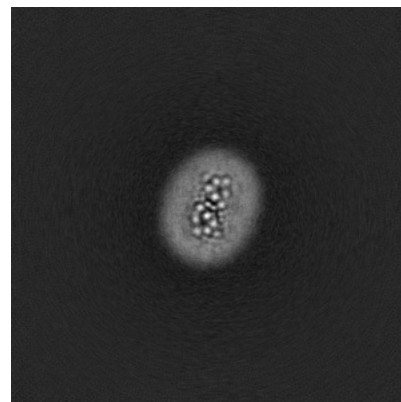
6.3.2 Raw map



X Index: 183



Y Index: 158

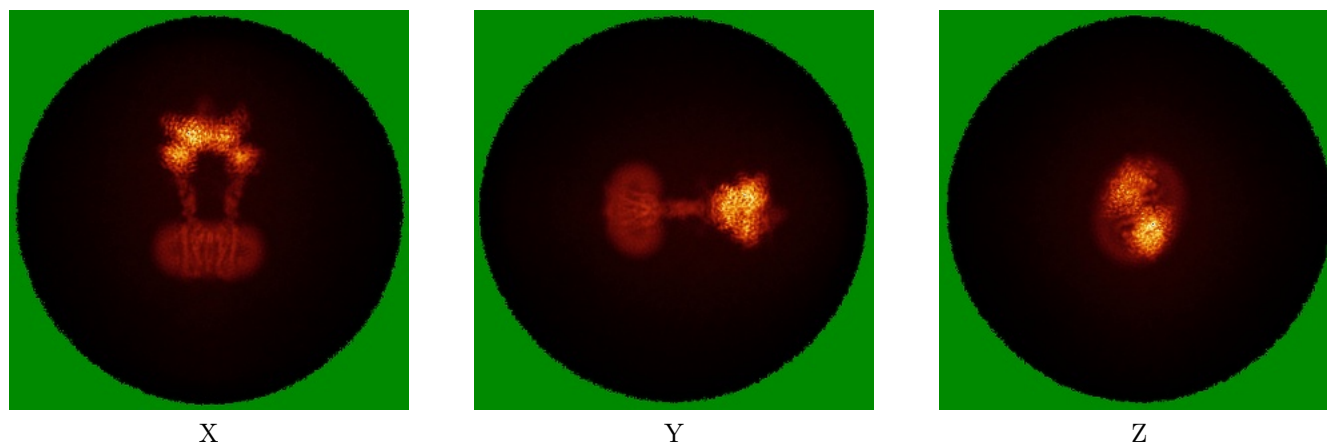


Z Index: 154

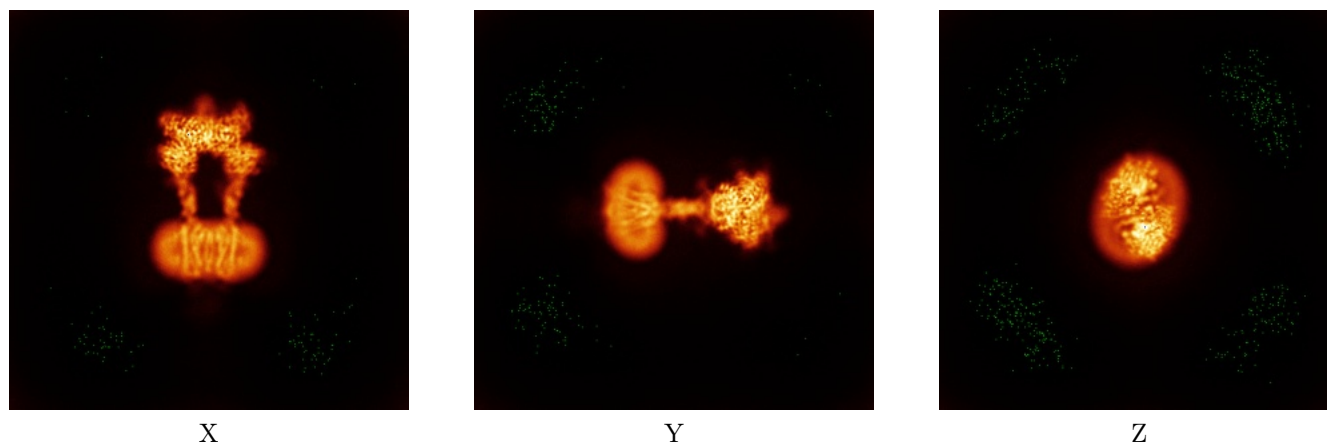
The images above show the largest variance slices of the map in three orthogonal directions.

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.

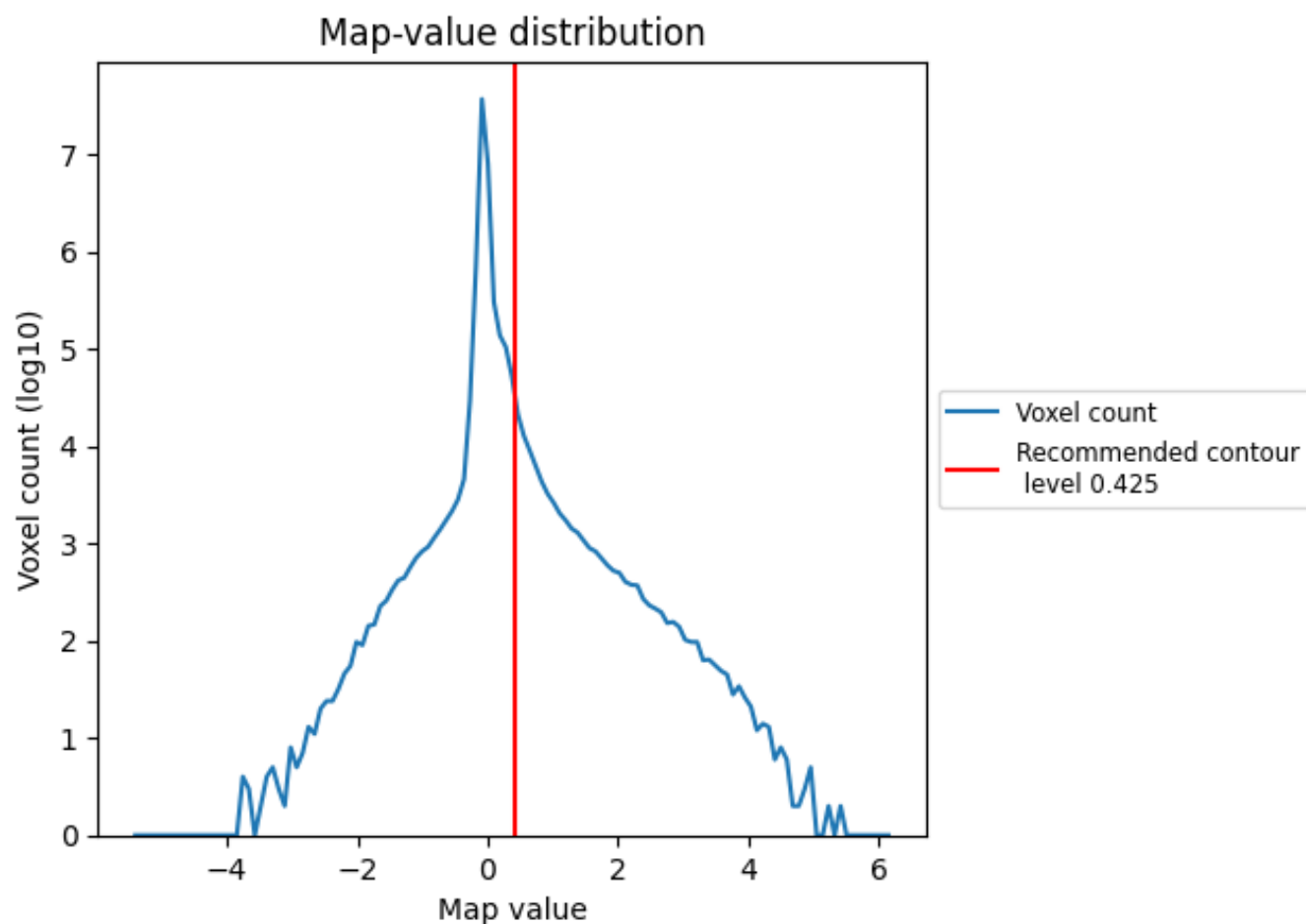
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

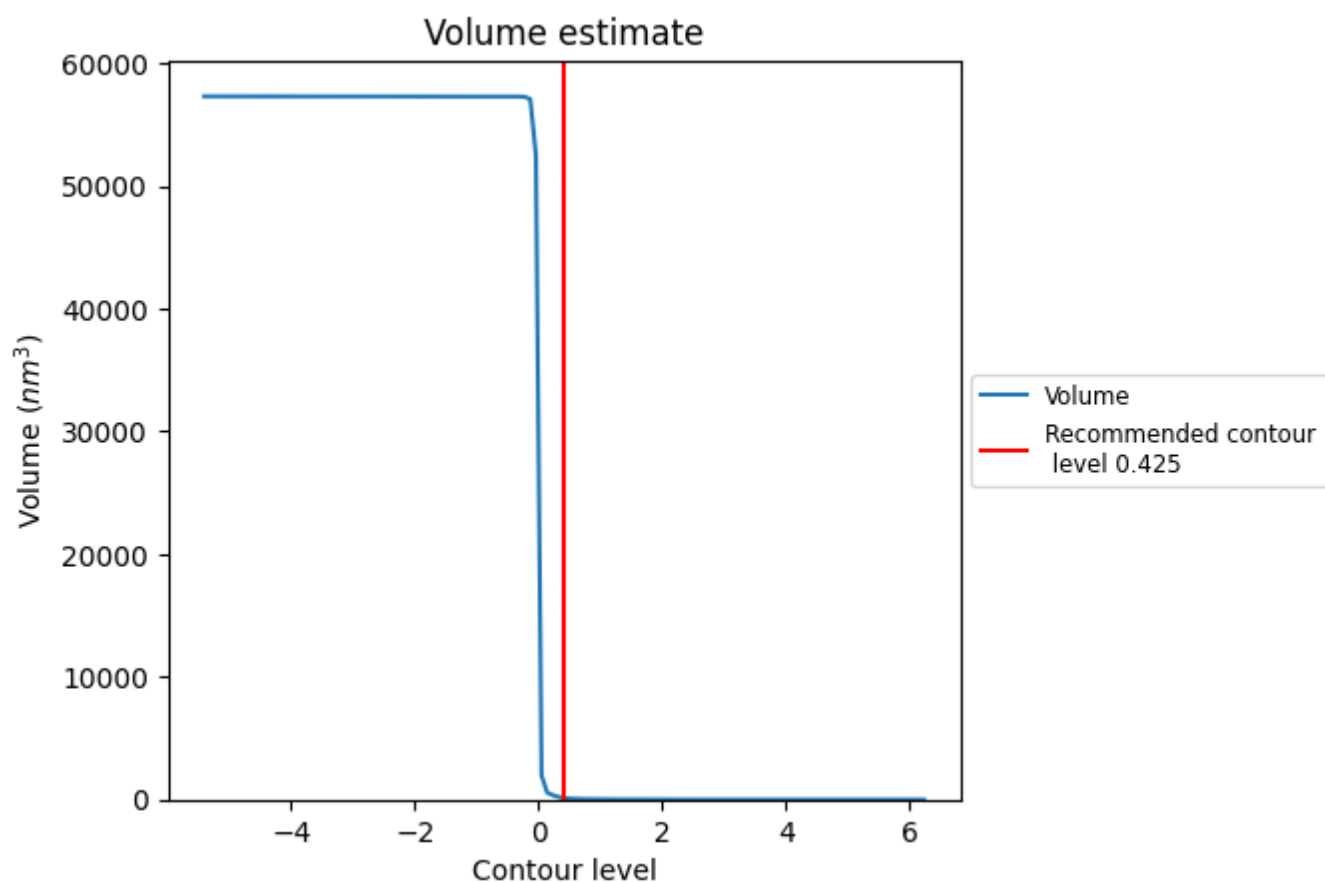
This section contains the results of statistical analysis of the map.

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.

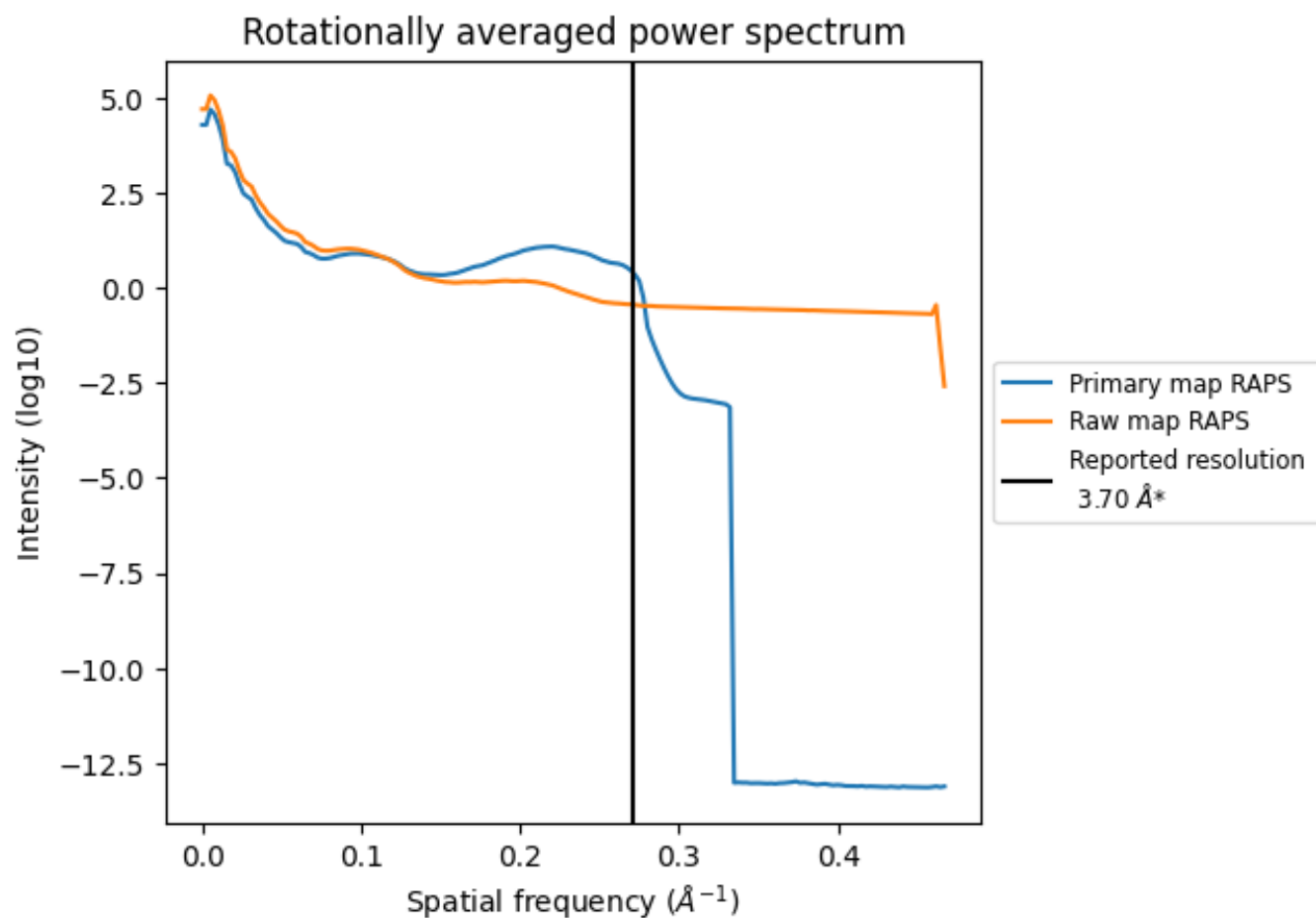
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 ⓘ

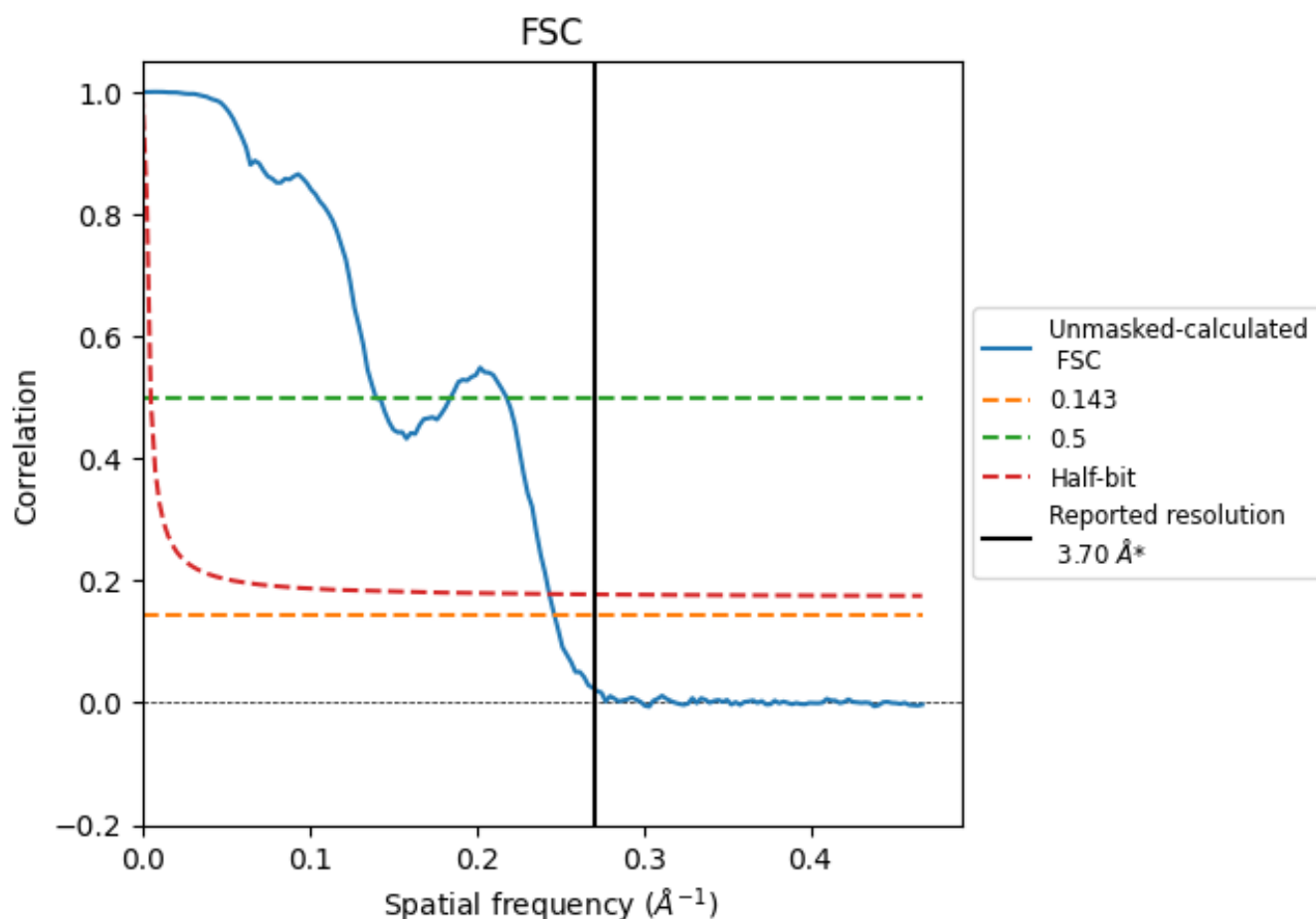


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 $0.270 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

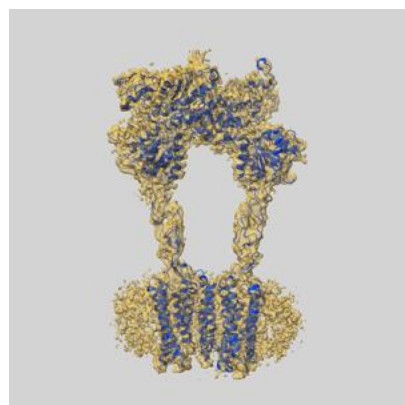
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	7.15	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

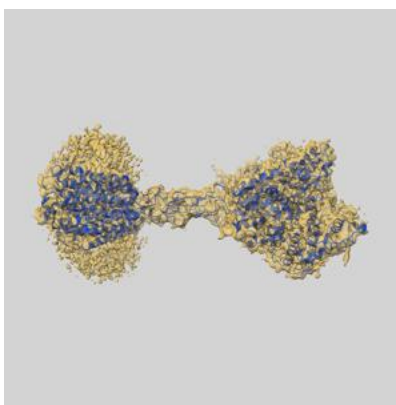
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36172 and PDB model 8JD1. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

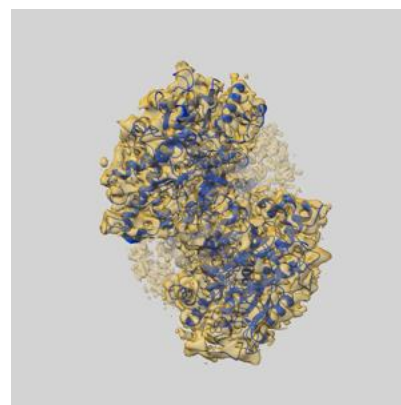
9.1 Map-model overlay [i](#)



X



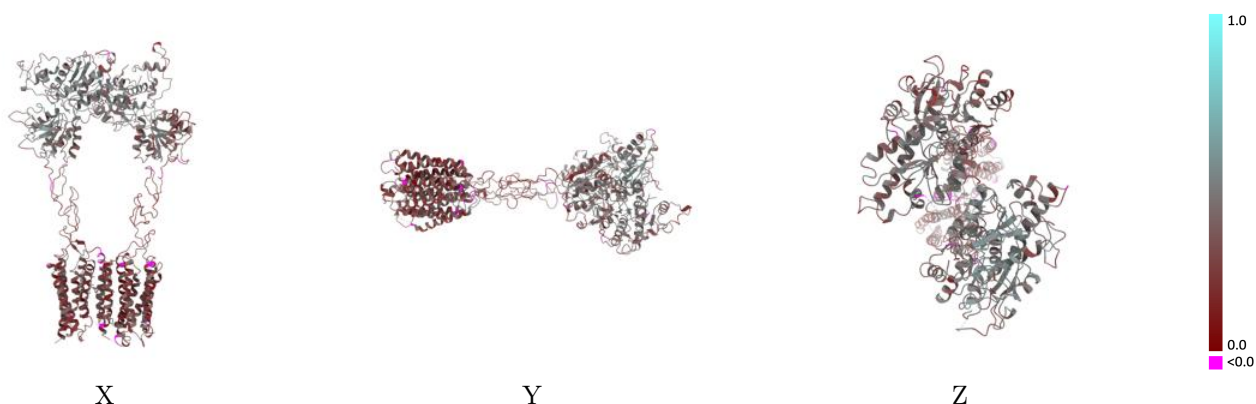
Y



Z

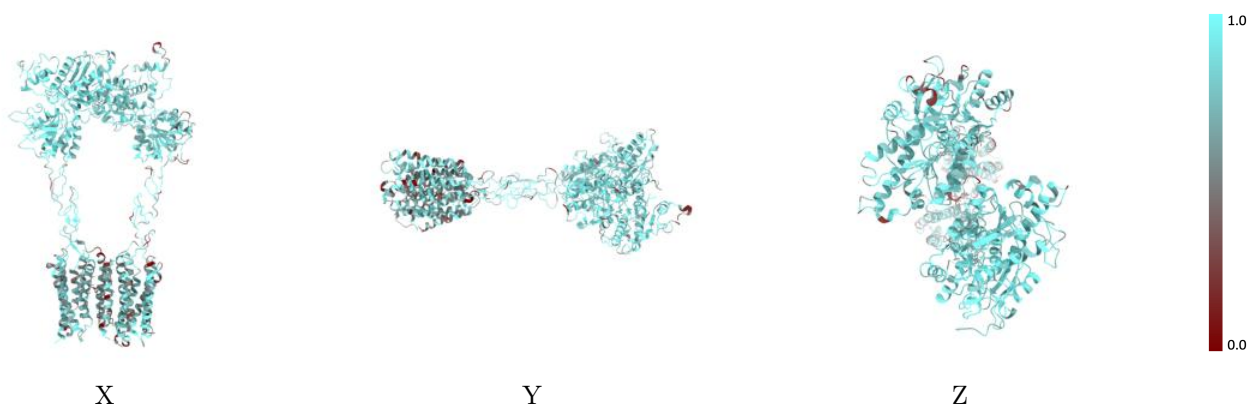
The images above show the 3D surface view of the map at the recommended contour level 0.425 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



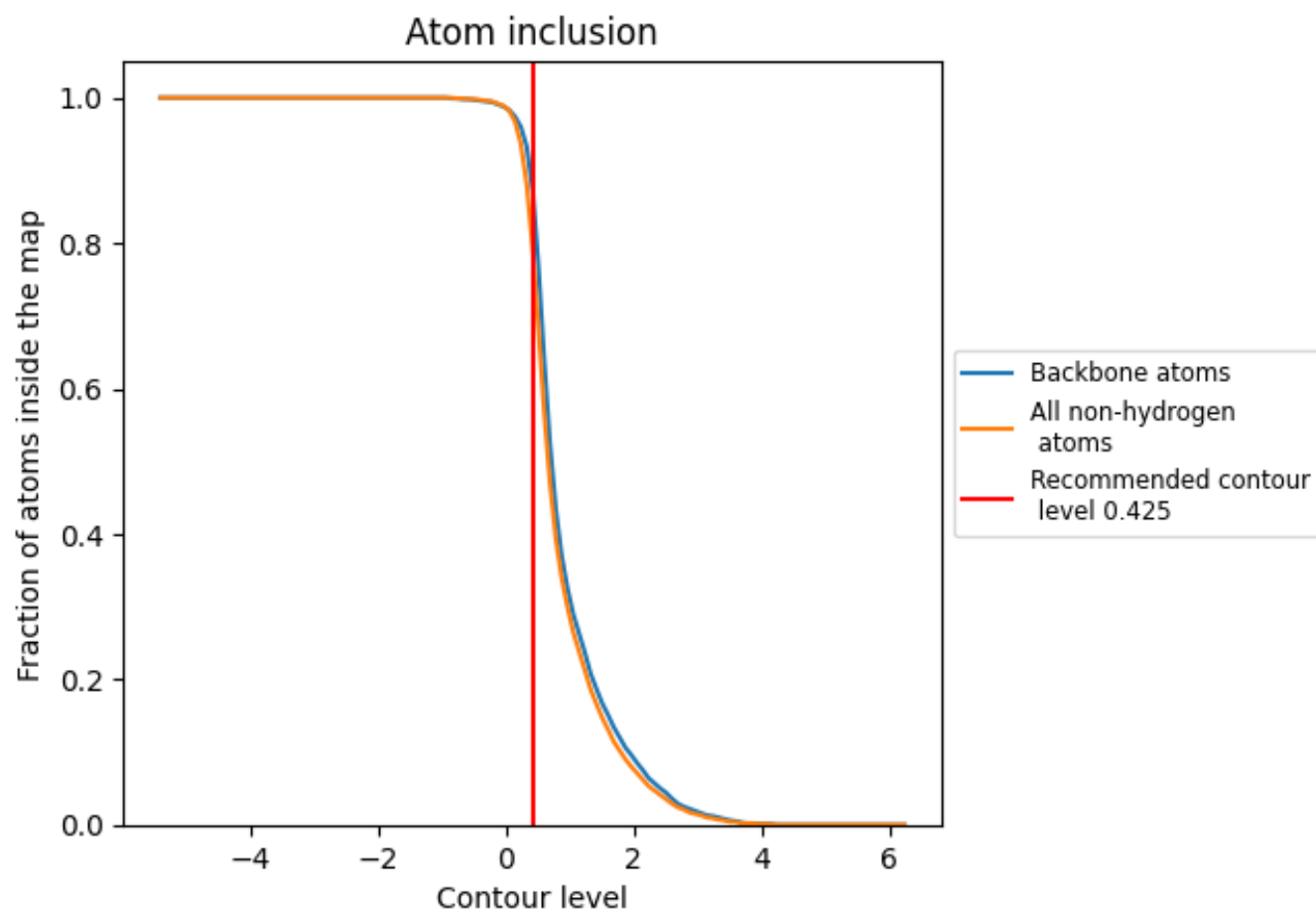
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.425).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.425) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7840	0.3690
2	0.7780	0.3510
3	0.7900	0.3850

