



Full wwPDB EM Validation Report ⓘ

May 20, 2026 – 06:57 PM JST

PDB ID : 9WQP / pdb_00009wqp
EMDB ID : EMD-66179
Title : GRM1-Acc State Conformation 2
Authors : Lu, Y.; Wen, T.L.; Shen, Y.Q.; Yang, X.
Deposited on : 2025-09-11
Resolution : 3.20 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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

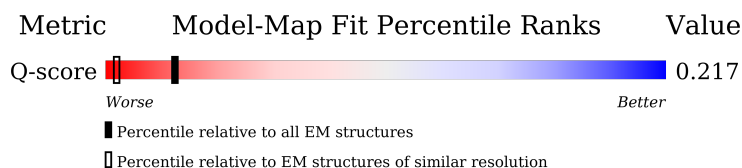
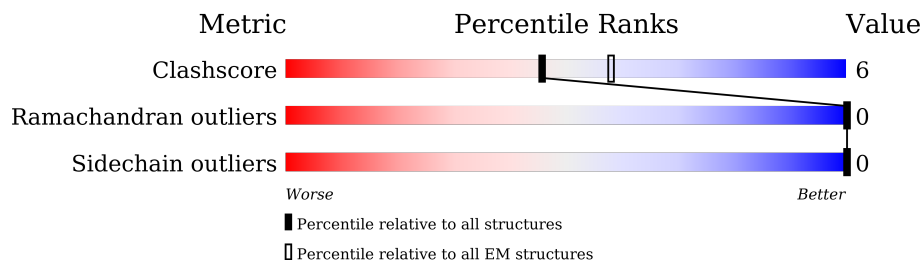
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	X	869	 11% 74% 15% 10%
1	Y	869	 11% 76% 13% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12432 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.

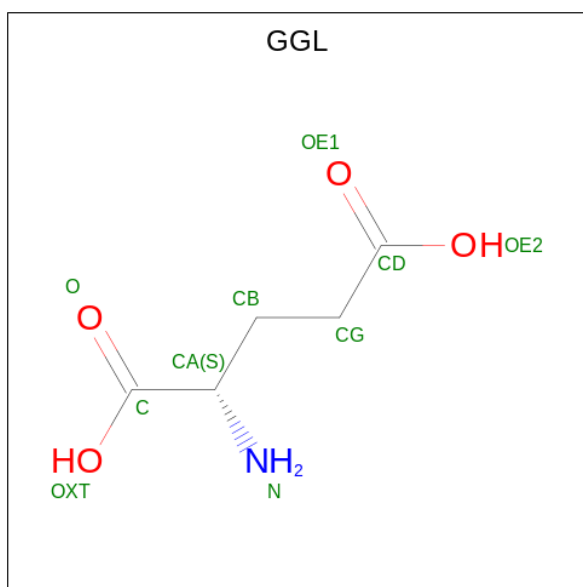
- Molecule 1 is a protein called Metabotropic glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	778	Total	C	N	O	S	0	0
			6095	3918	1017	1113	47		
1	Y	777	Total	C	N	O	S	0	0
			6121	3936	1022	1115	48		

There are 18 discrepancies between the modelled and reference sequences:

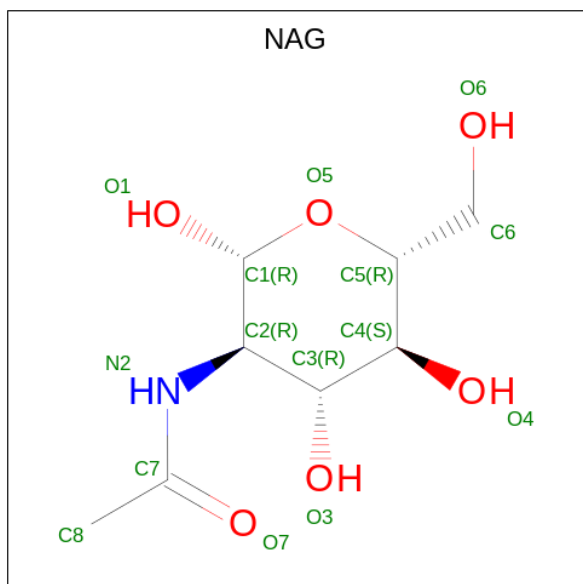
Chain	Residue	Modelled	Actual	Comment	Reference
X	22	ASP	-	expression tag	UNP Q13255
X	23	TYR	-	expression tag	UNP Q13255
X	24	LYS	-	expression tag	UNP Q13255
X	25	ASP	-	expression tag	UNP Q13255
X	26	ASP	-	expression tag	UNP Q13255
X	27	ASP	-	expression tag	UNP Q13255
X	28	ASP	-	expression tag	UNP Q13255
X	29	LYS	-	expression tag	UNP Q13255
X	30	THR	-	expression tag	UNP Q13255
Y	22	ASP	-	expression tag	UNP Q13255
Y	23	TYR	-	expression tag	UNP Q13255
Y	24	LYS	-	expression tag	UNP Q13255
Y	25	ASP	-	expression tag	UNP Q13255
Y	26	ASP	-	expression tag	UNP Q13255
Y	27	ASP	-	expression tag	UNP Q13255
Y	28	ASP	-	expression tag	UNP Q13255
Y	29	LYS	-	expression tag	UNP Q13255
Y	30	THR	-	expression tag	UNP Q13255

- Molecule 2 is GAMMA-L-GLUTAMIC ACID (CCD ID: GGL) (formula: C₅H₉NO₄).



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	X	1	Total	C	N	O	0
			14	8	1	5	

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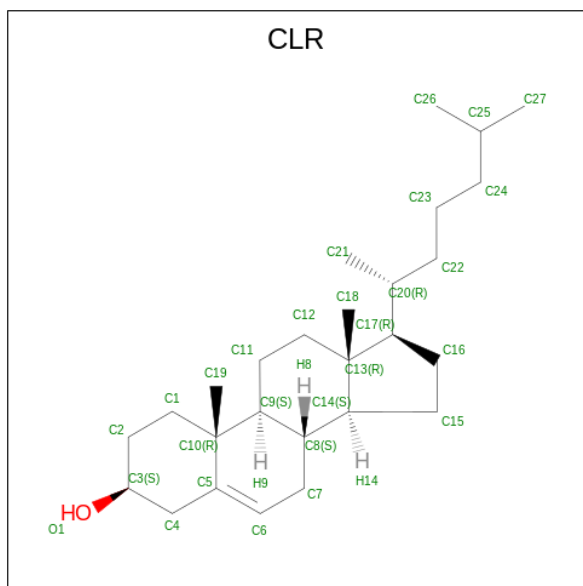
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Mol	Chain	Residues	Atoms				AltConf
3	X	1	Total	C	N	O	0
			14	8	1	5	
3	X	1	Total	C	N	O	0
			14	8	1	5	
3	X	1	Total	C	N	O	0
			14	8	1	5	
3	Y	1	Total	C	N	O	0
			14	8	1	5	
3	Y	1	Total	C	N	O	0
			14	8	1	5	
3	Y	1	Total	C	N	O	0
			14	8	1	5	
3	Y	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

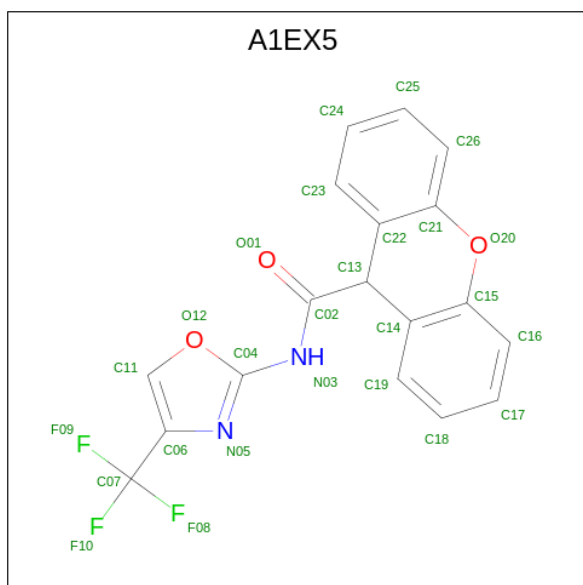
Mol	Chain	Residues	Atoms		AltConf
4	X	1	Total	Cl	0
			1	1	
4	Y	1	Total	Cl	0
			1	1	

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
5	X	1	Total	C	O	0
			28	27	1	
5	Y	1	Total	C	O	0
			28	27	1	

- Molecule 6 is N-[4-(trifluoromethyl)-1,3-oxazol-2-yl]-9H-xanthene-9-carboxamide (CCD ID: A1EX5) (formula: C₁₈H₁₁F₃N₂O₃).

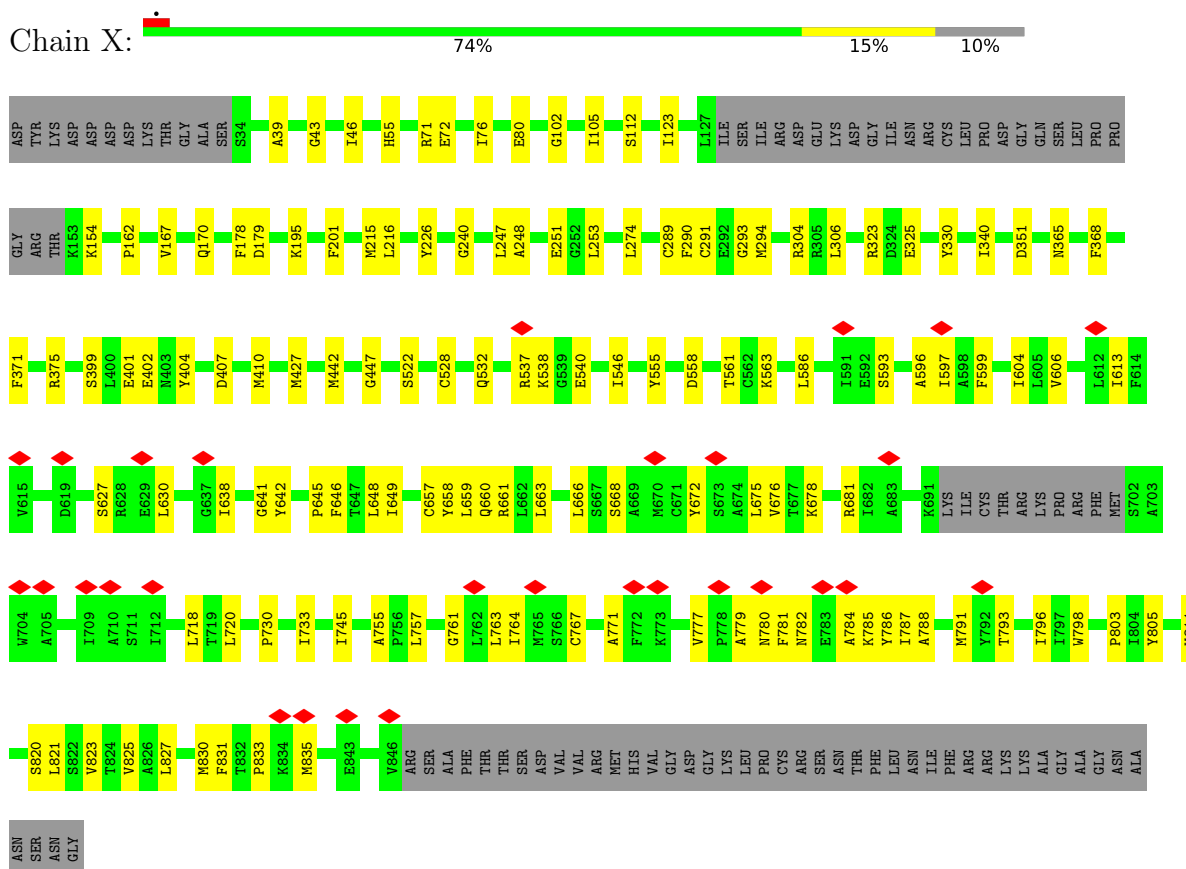


Mol	Chain	Residues	Atoms					AltConf
6	X	1	Total	C	F	N	O	0
			26	18	3	2	3	

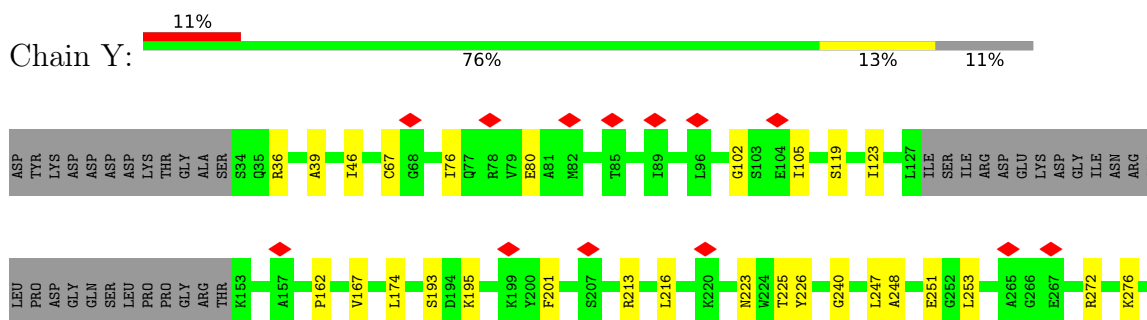
3 Residue-property plots [i](#)

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

• Molecule 1: Metabotropic glutamate receptor 1



• Molecule 1: Metabotropic glutamate receptor 1



ALA	GLY	ALA	GLY	ASN	ALA	ASN	ASN	SER	ASN	GLY																																																																			
Y805	K811	C816	F817	A818	V819	V823	A826	M830	K834	M835	Y836	A840	K841	P842	E843	R844	N845	V846	ARG	SER	ALA	PHE	THR	THR	SER	ASP	VAL	VAL	ARG	MET	HIS	VAL	GLY	ASP	GLY	LYS	LEU	PRO	CYS	ARG	SER	ASN	THR	PHE	LEU	ASN	ILE	PHE	ARG	ARG	LYS	LYS																									
L886	ALA	GLY	SER	LYS	LYS	LYS	ILE	CYS	THR	ARG	LYS	P698	R699	A705	Q706	V707	I712	Q717	P732	K740	V754	L757	G758	G761	L762	M765	S766	C767	T768	Y769	Y770	A771	F772	K773	N776	N780	K785	M791	L796	I797	W798	V802	P803	I804																																	
C601	L602	L605	V606	T607	L608	F609	V610	T611	L612	I613	F614	Y617	R618	D619	T620	P621	V622	V623	K624	S625	S626	S627	R628	E629	L630	C631	Y632	I633	I634	L635	G641	P645	T653	S656	R661	S668	A669	M670	C671	Y672	S673	A674	L675	V676	T677	K678	T679	A683	R684	I685																											
K283	C289	F290	C291	E292	G293	R304	D318	A321	D322	Y330	G336	D351	D352	Y353	F354	L355	K356	L357	N362	N365	F371	C378	R379	L385	E386	K391	R392	T395	G396	N397	L400	E401	D407	S408	K409	M410	G411	N415	A416	A419	G423	A430	G434	G437	K449	D452	S458	E466	V467	W468	E471	K472	G473	D474	Q485	R491	E502	G503	K511	I512	S522	V523	C524	C528	Q532	Y555	D558	T561	C562	K563	P571	G577	I581	E592	A598	F599	S600

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	6000	Depositor
Maximum defocus (nm)	19000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (\AA)	357.12, 357.12, 357.12	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.93, 0.93, 0.93	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, NAG, A1EX5, GGL, CL

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	X	0.22	0/6231	0.30	0/8458
1	Y	0.19	0/6260	0.27	0/8496
All	All	0.20	0/12491	0.29	0/16954

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	X	6095	0	6077	84	0
1	Y	6121	0	6124	68	0
2	X	10	0	7	0	0
2	Y	10	0	7	0	0
3	X	56	0	52	0	0
3	Y	56	0	52	2	0
4	X	1	0	0	1	0
4	Y	1	0	0	0	0
5	X	28	0	46	4	0
5	Y	28	0	46	2	0
6	X	26	0	0	3	0
All	All	12432	0	12411	154	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 (154) 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:Y:223:ASN:HD21	3:Y:2003:NAG:C1	1.41	1.33
1:Y:630:LEU:HD13	1:Y:678:LYS:HB2	1.64	0.79
1:X:323:ARG:NH1	1:X:325:GLU:OE2	2.26	0.69
1:Y:757:LEU:HD21	1:Y:802:VAL:HG22	1.75	0.68
1:X:528:CYS:HB3	1:X:532:GLN:HB2	1.75	0.68
1:X:661:ARG:HH11	1:X:730:PRO:HB3	1.60	0.67
1:Y:216:LEU:HD22	1:Y:247:LEU:HB3	1.77	0.66
1:Y:407:ASP:HB3	1:Y:410:MET:HE2	1.78	0.66
1:Y:679:THR:HB	1:Y:770:TYR:CG	2.31	0.65
1:Y:39:ALA:HB3	1:Y:105:ILE:HB	1.79	0.65
1:X:240:GLY:HA3	1:X:290:PHE:CE2	2.33	0.64
1:Y:641:GLY:HA3	1:Y:823:VAL:HG11	1.78	0.64
1:X:666:LEU:HD21	1:X:718:LEU:HD13	1.80	0.64
1:Y:240:GLY:HA3	1:Y:290:PHE:CE2	2.33	0.64
1:Y:767:CYS:HB3	1:Y:791:MET:HG3	1.78	0.64
1:X:216:LEU:HD22	1:X:247:LEU:HB3	1.80	0.63
1:X:675:LEU:HD13	1:X:791:MET:HE3	1.81	0.61
1:X:558:ASP:OD1	1:X:561:THR:OG1	2.17	0.61
1:Y:629:GLU:HG2	1:Y:707:VAL:HG21	1.83	0.60
1:X:407:ASP:HB3	1:X:410:MET:HE2	1.84	0.60
1:X:803:PRO:HG3	5:Y:2007:CLR:H121	1.82	0.60
1:Y:675:LEU:HD13	1:Y:791:MET:HE1	1.84	0.59
1:X:676:VAL:HG21	1:X:763:LEU:HD22	1.86	0.58
1:X:720:LEU:HD21	1:X:755:ALA:HB1	1.86	0.58
1:X:638:ILE:HD13	1:X:827:LEU:HB2	1.86	0.57
1:X:399:SER:OG	1:X:401:GLU:OE1	2.22	0.56
1:Y:119:SER:HB2	1:Y:174:LEU:HD23	1.87	0.56
1:Y:558:ASP:OD1	1:Y:561:THR:OG1	2.22	0.56
1:X:657:CYS:HB2	1:X:730:PRO:HB2	1.89	0.55
1:Y:685:ILE:HG22	1:Y:686:LEU:HG	1.89	0.55
1:X:798:TRP:HB2	6:X:2008:A1EX5:N05	2.22	0.55
1:X:782:ASN:ND2	1:X:785:LYS:HB2	2.23	0.54
1:X:72:GLU:OE2	1:X:375:ARG:NH1	2.41	0.54
1:X:195:LYS:NZ	1:X:201:PHE:O	2.41	0.54
1:Y:633:ILE:HG23	1:Y:670:MET:HE2	1.89	0.54
1:Y:379:ARG:HG3	1:Y:386:GLU:HG3	1.91	0.53
1:X:304:ARG:HE	1:X:330:TYR:HD1	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:618:ARG:HA	1:Y:623:VAL:HG11	1.90	0.53
1:Y:80:GLU:OE2	1:Y:365:ASN:ND2	2.29	0.53
1:Y:611:THR:HG23	1:Y:635:LEU:HD13	1.90	0.53
1:Y:617:TYR:O	1:Y:623:VAL:HG21	2.09	0.53
1:X:375:ARG:NH2	1:X:402:GLU:O	2.42	0.53
1:X:767:CYS:HB3	1:X:791:MET:HG3	1.92	0.52
1:Y:622:VAL:O	1:Y:626:SER:OG	2.21	0.52
1:X:351:ASP:OD1	1:X:404:TYR:OH	2.23	0.52
1:X:80:GLU:OE2	1:X:365:ASN:ND2	2.37	0.52
1:X:427:MET:HG2	1:X:442:MET:HE3	1.92	0.51
1:X:675:LEU:HD11	1:X:830:MET:HE1	1.91	0.51
1:X:827:LEU:HD12	1:X:831:PHE:HD2	1.75	0.51
1:X:294:MET:HG2	4:X:2006:CL:CL	2.47	0.51
1:X:777:VAL:HG21	1:X:784:ALA:HB3	1.92	0.51
1:X:274:LEU:HD23	1:X:306:LEU:HD12	1.92	0.51
1:X:39:ALA:HB3	1:X:105:ILE:HB	1.93	0.50
1:X:658:TYR:CD1	1:X:730:PRO:HG2	2.47	0.50
1:X:668:SER:HB3	6:X:2008:A1EX5:C16	2.42	0.50
1:X:226:TYR:O	1:X:522:SER:OG	2.18	0.50
1:X:248:ALA:HB1	1:X:253:LEU:HB2	1.93	0.50
1:X:781:PHE:CE2	1:X:786:TYR:HE2	2.30	0.50
1:Y:272:ARG:HD3	1:Y:276:LYS:HZ2	1.75	0.50
1:X:216:LEU:HD21	1:X:251:GLU:HG3	1.93	0.49
1:X:761:GLY:HA2	6:X:2008:A1EX5:F10	2.02	0.49
1:X:771:ALA:HB1	1:X:788:ALA:HB2	1.93	0.49
1:Y:379:ARG:NH2	1:Y:391:LYS:O	2.42	0.49
1:Y:805:TYR:CE1	1:Y:811:LYS:HB3	2.47	0.49
1:Y:613:ILE:HG13	1:Y:835:MET:HE1	1.95	0.49
1:X:678:LYS:O	1:X:681:ARG:HG2	2.13	0.48
1:Y:669:ALA:HB2	1:Y:717:GLN:HG2	1.95	0.48
1:X:648:LEU:HD23	1:X:660:GLN:OE1	2.13	0.48
1:Y:226:TYR:O	1:Y:522:SER:OG	2.18	0.48
1:X:796:ILE:HD13	1:Y:796:ILE:HD13	1.96	0.48
1:X:365:ASN:HB3	1:X:368:PHE:HB2	1.96	0.47
1:Y:225:THR:HA	1:Y:253:LEU:HD22	1.96	0.47
1:X:597:ILE:HD12	1:X:646:PHE:CE1	2.49	0.47
1:Y:36:ARG:NH1	1:Y:67:CYS:SG	2.87	0.47
1:X:55:HIS:CE1	1:X:71:ARG:HG2	2.50	0.47
1:Y:798:TRP:O	1:Y:802:VAL:HG23	2.14	0.47
1:X:215:MET:HG2	1:X:340:ILE:HD12	1.97	0.47
1:Y:248:ALA:HB1	1:Y:253:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:46:ILE:HD13	1:Y:102:GLY:HA3	1.97	0.46
1:Y:555:TYR:CE1	1:Y:563:LYS:HB3	2.50	0.46
1:Y:631:CYS:SG	1:Y:834:LYS:NZ	2.88	0.46
1:Y:679:THR:HB	1:Y:770:TYR:CD2	2.49	0.46
1:X:555:TYR:CE1	1:X:563:LYS:HB3	2.51	0.46
1:Y:76:ILE:HG13	1:Y:371:PHE:HB2	1.98	0.46
1:Y:289:CYS:HB3	1:Y:291:CYS:SG	2.55	0.46
1:X:793:THR:HG21	1:X:825:VAL:HG11	1.97	0.46
1:X:786:TYR:CE2	1:X:833:PRO:HG2	2.51	0.46
1:X:76:ILE:HG13	1:X:371:PHE:HB2	1.98	0.45
1:X:596:ALA:HB3	1:X:649:ILE:HD11	1.97	0.45
1:X:606:VAL:HG12	1:X:827:LEU:HD21	1.98	0.45
1:X:43:GLY:O	1:X:154:LYS:NZ	2.37	0.45
1:Y:528:CYS:HB3	1:Y:532:GLN:HB2	1.97	0.45
1:Y:162:PRO:HG3	1:Y:167:VAL:HG12	1.98	0.45
1:Y:378:CYS:HB3	1:Y:392:ARG:HH11	1.82	0.45
1:Y:216:LEU:HD21	1:Y:251:GLU:HG3	1.98	0.45
1:X:784:ALA:HA	1:X:787:ILE:HB	1.98	0.45
1:Y:645:PRO:HB3	1:Y:816:CYS:HB3	1.98	0.44
1:Y:195:LYS:NZ	1:Y:201:PHE:O	2.51	0.44
1:X:289:CYS:HB3	1:X:291:CYS:SG	2.57	0.44
1:X:733:ILE:HG13	1:X:745:ILE:HG13	1.99	0.44
1:Y:213:ARG:NH2	1:Y:216:LEU:HD23	2.31	0.44
1:Y:619:ASP:O	1:Y:624:LYS:HD2	2.18	0.44
1:Y:826:ALA:O	1:Y:830:MET:HB2	2.17	0.44
1:Y:836:TYR:O	1:Y:840:ALA:HB3	2.17	0.44
1:Y:653:THR:H	1:Y:656:SER:HG	1.66	0.44
1:Y:653:THR:HA	1:Y:732:PRO:HG3	2.00	0.44
1:Y:458:SER:HB2	1:Y:468:TRP:HB3	2.01	0.43
1:X:123:ILE:HD13	1:X:178:PHE:CD1	2.53	0.43
1:Y:304:ARG:HE	1:Y:330:TYR:HD1	1.67	0.43
1:Y:119:SER:O	1:Y:123:ILE:HG13	2.18	0.43
1:X:757:LEU:HB3	1:X:798:TRP:CZ3	2.54	0.43
5:X:2007:CLR:H162	5:X:2007:CLR:H222	1.52	0.43
5:X:2007:CLR:H193	5:X:2007:CLR:H111	1.80	0.43
1:Y:819:VAL:O	1:Y:823:VAL:HG22	2.18	0.43
1:X:659:LEU:HD23	1:X:659:LEU:HA	1.81	0.42
1:X:162:PRO:HG3	1:X:167:VAL:HG12	2.01	0.42
1:X:763:LEU:HD23	1:X:763:LEU:HA	1.80	0.42
5:Y:2007:CLR:H183	5:Y:2007:CLR:H20	1.70	0.42
1:X:112:SER:HB3	1:X:170:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:581:ILE:HD13	1:Y:740:LYS:O	2.19	0.42
1:Y:571:PRO:HA	1:Y:577:GLY:O	2.20	0.42
1:X:613:ILE:HD13	1:X:613:ILE:HA	1.89	0.42
1:X:672:TYR:CZ	1:X:764:ILE:HD11	2.54	0.42
1:X:796:ILE:HD13	1:Y:796:ILE:HG21	2.00	0.42
1:Y:620:THR:HB	1:Y:845:ASN:OD1	2.18	0.42
1:X:46:ILE:HD13	1:X:102:GLY:HA3	2.02	0.42
1:X:627:SER:O	1:X:630:LEU:N	2.53	0.42
1:X:179:ASP:O	1:X:447:GLY:HA3	2.20	0.42
1:X:657:CYS:O	1:X:660:GLN:HG2	2.20	0.41
1:X:796:ILE:CD1	1:Y:796:ILE:HD13	2.49	0.41
1:Y:780:ASN:OD1	1:Y:780:ASN:N	2.53	0.41
1:X:642:TYR:O	1:X:645:PRO:HD2	2.21	0.41
1:Y:592:GLU:H	1:Y:592:GLU:CD	2.28	0.41
1:X:663:LEU:HD23	1:X:663:LEU:HA	1.79	0.41
1:X:821:LEU:HD23	1:X:821:LEU:HA	1.92	0.41
1:Y:193:SER:HB3	1:Y:472:LYS:HD3	2.01	0.41
1:X:641:GLY:HA3	1:X:823:VAL:HG11	2.02	0.41
1:Y:485:GLN:NE2	1:Y:511:LYS:O	2.50	0.41
1:X:604:ILE:HG13	1:X:642:TYR:HB3	2.02	0.41
5:X:2007:CLR:H183	5:X:2007:CLR:H20	1.90	0.41
1:X:586:LEU:HD12	1:X:586:LEU:HA	1.89	0.41
1:X:805:TYR:CE1	1:X:811:LYS:HB3	2.56	0.41
1:X:835:MET:H	1:X:835:MET:HG2	1.64	0.41
5:X:2007:CLR:H232	5:X:2007:CLR:H262	1.80	0.41
1:X:293:GLY:HA3	1:X:323:ARG:HH21	1.86	0.41
1:X:599:PHE:CD2	1:X:820:SER:HB3	2.56	0.41
1:Y:672:TYR:O	1:Y:676:VAL:HG23	2.21	0.41
1:X:538:LYS:C	1:X:540:GLU:H	2.28	0.40
1:X:779:ALA:O	1:X:780:ASN:HB2	2.21	0.40
1:Y:283:LYS:NZ	1:Y:524:CYS:O	2.43	0.40
1:Y:395:THR:HB	3:Y:2004:NAG:H83	2.03	0.40
1:X:537:ARG:HD2	1:X:546:ILE:HG13	2.03	0.40
1:X:593:SER:O	1:X:597:ILE:HG12	2.22	0.40
1:Y:605:LEU:HD23	1:Y:605:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	772/869 (89%)	742 (96%)	30 (4%)	0	100	100
1	Y	771/869 (89%)	748 (97%)	23 (3%)	0	100	100
All	All	1543/1738 (89%)	1490 (97%)	53 (3%)	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	X	668/753 (89%)	668 (100%)	0	100	100
1	Y	676/753 (90%)	676 (100%)	0	100	100
All	All	1344/1506 (89%)	1344 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	84	HIS
1	X	182	GLN
1	Y	84	HIS
1	Y	223	ASN
1	Y	231	HIS
1	Y	435	HIS

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Mol	Chain	Res	Type
1	Y	496	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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	A1EX5	X	2008	-	28,29,29	2.01	7 (25%)	36,43,43	1.53	8 (22%)
3	NAG	X	2005	1	14,14,15	0.20	0	17,19,21	0.48	0
3	NAG	X	2004	1	14,14,15	0.20	0	17,19,21	0.41	0
2	GGL	X	2001	-	8,9,9	1.02	0	10,11,11	1.18	0
3	NAG	Y	2002	1	14,14,15	0.22	0	17,19,21	0.49	0
3	NAG	Y	2005	1	14,14,15	0.20	0	17,19,21	0.52	0
2	GGL	Y	2001	-	8,9,9	1.02	0	10,11,11	1.21	0
3	NAG	X	2003	1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	Y	2004	1	14,14,15	0.25	0	17,19,21	0.52	0
5	CLR	X	2007	-	31,31,31	1.14	3 (9%)	48,48,48	1.70	11 (22%)
5	CLR	Y	2007	-	31,31,31	1.16	3 (9%)	48,48,48	1.69	10 (20%)
3	NAG	X	2002	1	14,14,15	0.25	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	Y	2003	1	14,14,15	0.25	0	17,19,21	0.46	0

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	A1EX5	X	2008	-	-	9/14/26/26	0/4/4/4
3	NAG	X	2005	1	-	2/6/23/26	0/1/1/1
3	NAG	X	2004	1	-	0/6/23/26	0/1/1/1
2	GGL	X	2001	-	-	2/9/9/9	-
3	NAG	Y	2002	1	-	3/6/23/26	0/1/1/1
3	NAG	Y	2005	1	-	1/6/23/26	0/1/1/1
2	GGL	Y	2001	-	-	4/9/9/9	-
3	NAG	X	2003	1	-	2/6/23/26	0/1/1/1
3	NAG	Y	2004	1	-	3/6/23/26	0/1/1/1
5	CLR	X	2007	-	-	5/10/68/68	0/4/4/4
5	CLR	Y	2007	-	-	7/10/68/68	0/4/4/4
3	NAG	X	2002	1	-	3/6/23/26	0/1/1/1
3	NAG	Y	2003	1	-	2/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	2008	A1EX5	C04-N03	5.06	1.44	1.36
6	X	2008	A1EX5	C02-N03	4.75	1.45	1.36
6	X	2008	A1EX5	O20-C15	3.44	1.44	1.38
6	X	2008	A1EX5	O20-C21	3.36	1.43	1.38
5	Y	2007	CLR	C13-C17	-3.27	1.48	1.55
6	X	2008	A1EX5	O12-C11	-3.18	1.31	1.37
5	X	2007	CLR	C13-C17	-3.11	1.49	1.55
5	Y	2007	CLR	C16-C15	3.00	1.62	1.54
5	X	2007	CLR	C16-C15	2.90	1.61	1.54
6	X	2008	A1EX5	O01-C02	-2.43	1.18	1.23
5	X	2007	CLR	C7-C6	2.31	1.55	1.50
5	Y	2007	CLR	C7-C6	2.30	1.55	1.50
6	X	2008	A1EX5	C07-C06	2.12	1.52	1.48

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	2007	CLR	C13-C17-C20	-4.97	111.70	119.49
6	X	2008	A1EX5	O12-C04-N05	-4.94	107.79	115.44
5	Y	2007	CLR	C13-C14-C8	-3.71	108.89	114.38
5	X	2007	CLR	C16-C15-C14	-3.43	98.33	105.13
5	X	2007	CLR	C13-C17-C20	-3.40	114.17	119.49
5	Y	2007	CLR	C3-C4-C5	-3.39	106.27	112.03
5	X	2007	CLR	C4-C5-C10	3.29	120.78	116.42
5	Y	2007	CLR	C17-C13-C14	3.05	103.69	100.07
5	X	2007	CLR	C3-C4-C5	-3.01	106.92	112.03
5	X	2007	CLR	C13-C14-C8	-2.96	110.00	114.38
5	Y	2007	CLR	C11-C9-C10	-2.91	109.25	113.08
5	Y	2007	CLR	C14-C8-C9	-2.88	105.24	109.09
5	Y	2007	CLR	C21-C20-C17	-2.85	108.55	112.92
6	X	2008	A1EX5	C13-C02-N03	2.84	117.66	114.52
5	X	2007	CLR	C15-C14-C8	-2.76	114.53	119.08
5	X	2007	CLR	C10-C9-C8	-2.70	108.68	112.73
5	X	2007	CLR	C16-C17-C20	-2.67	108.02	112.15
6	X	2008	A1EX5	C23-C22-C13	-2.66	119.02	125.52
5	X	2007	CLR	C11-C9-C10	-2.60	109.66	113.08
5	Y	2007	CLR	C11-C12-C13	-2.57	108.38	112.78
5	X	2007	CLR	C4-C5-C6	-2.55	116.93	120.61
5	Y	2007	CLR	C16-C15-C14	-2.50	100.18	105.13
6	X	2008	A1EX5	C22-C13-C14	2.37	111.14	106.39
6	X	2008	A1EX5	C19-C14-C13	-2.36	119.76	125.52
5	X	2007	CLR	C17-C13-C14	2.35	102.85	100.07
6	X	2008	A1EX5	O12-C04-N03	2.25	126.65	118.38
5	Y	2007	CLR	C15-C14-C8	-2.23	115.41	119.08
6	X	2008	A1EX5	C23-C22-C21	2.16	120.18	117.75
6	X	2008	A1EX5	C11-O12-C04	2.11	109.25	104.98

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Y	2001	GGL	C-CA-CB-CG
6	X	2008	A1EX5	N05-C04-N03-C02
6	X	2008	A1EX5	O12-C04-N03-C02
6	X	2008	A1EX5	N05-C06-C07-F08
6	X	2008	A1EX5	N05-C06-C07-F10
5	Y	2007	CLR	C13-C17-C20-C21
3	Y	2002	NAG	O5-C5-C6-O6
5	Y	2007	CLR	C16-C17-C20-C21
5	Y	2007	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
3	X	2003	NAG	O5-C5-C6-O6
3	Y	2003	NAG	O5-C5-C6-O6
3	X	2002	NAG	O5-C5-C6-O6
3	Y	2002	NAG	C4-C5-C6-O6
5	Y	2007	CLR	C21-C20-C22-C23
3	Y	2004	NAG	O5-C5-C6-O6
5	Y	2007	CLR	C16-C17-C20-C22
3	Y	2004	NAG	C4-C5-C6-O6
3	X	2002	NAG	C4-C5-C6-O6
3	X	2003	NAG	C4-C5-C6-O6
3	Y	2003	NAG	C4-C5-C6-O6
5	X	2007	CLR	C22-C23-C24-C25
5	X	2007	CLR	C13-C17-C20-C21
6	X	2008	A1EX5	C11-C06-C07-F08
6	X	2008	A1EX5	C11-C06-C07-F09
6	X	2008	A1EX5	C11-C06-C07-F10
5	Y	2007	CLR	C20-C22-C23-C24
5	X	2007	CLR	C16-C17-C20-C21
6	X	2008	A1EX5	N05-C06-C07-F09
5	X	2007	CLR	C13-C17-C20-C22
2	X	2001	GGL	CA-CB-CG-CD
2	Y	2001	GGL	CA-CB-CG-CD
3	Y	2004	NAG	C3-C2-N2-C7
5	Y	2007	CLR	C17-C20-C22-C23
2	Y	2001	GGL	OE2-CD-CG-CB
2	Y	2001	GGL	OE1-CD-CG-CB
2	X	2001	GGL	C-CA-CB-CG
3	X	2002	NAG	C3-C2-N2-C7
3	X	2005	NAG	C3-C2-N2-C7
3	Y	2002	NAG	C3-C2-N2-C7
3	Y	2005	NAG	C3-C2-N2-C7
6	X	2008	A1EX5	N03-C02-C13-C22
5	X	2007	CLR	C16-C17-C20-C22
3	X	2005	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 11 short contacts:

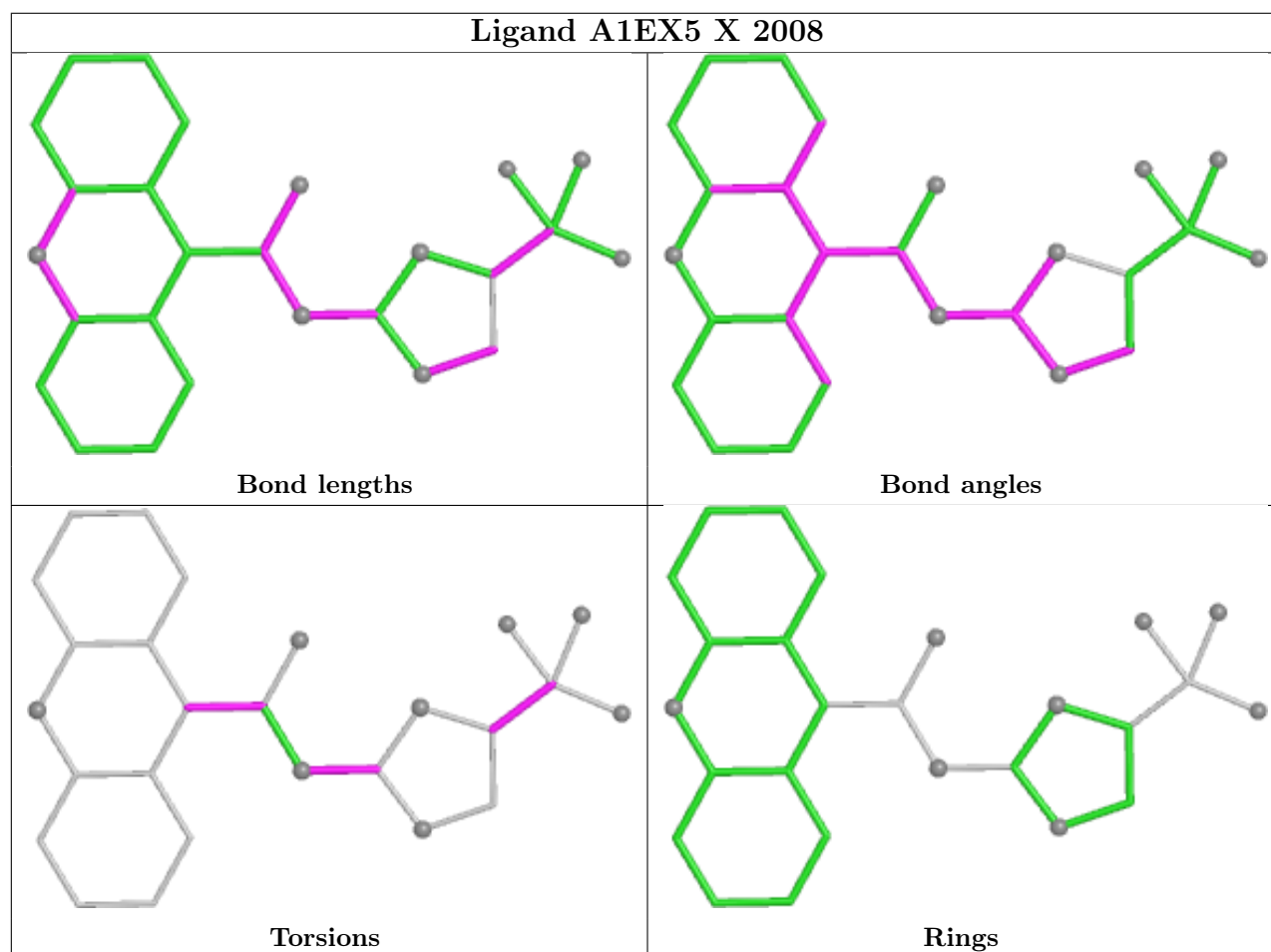
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	2008	A1EX5	3	0
3	Y	2004	NAG	1	0
5	X	2007	CLR	4	0

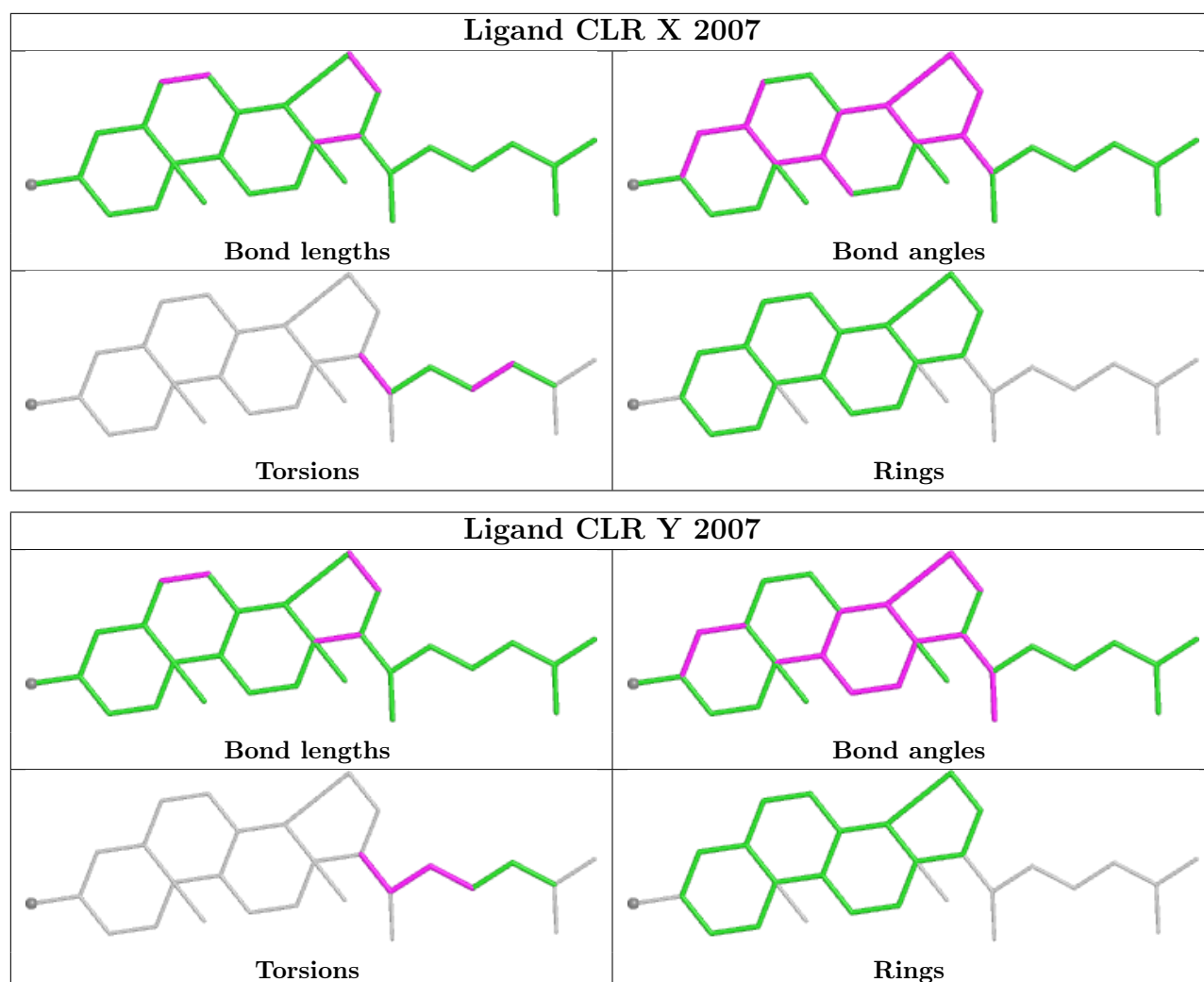
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	2007	CLR	2	0
3	Y	2003	NAG	1	0

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.

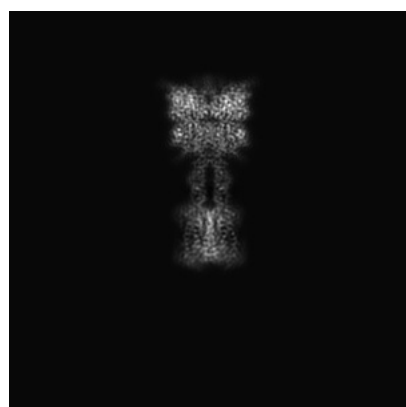
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66179. These allow visual inspection of the internal detail of the map and identification of artifacts.

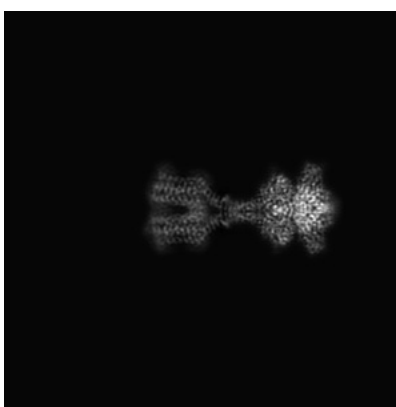
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

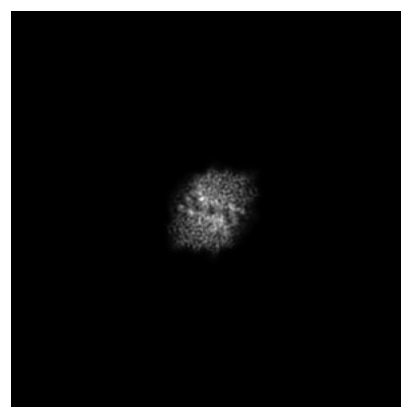
6.1.1 Primary map



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: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices [i](#)

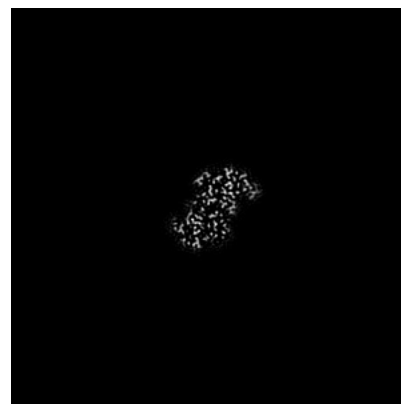
6.3.1 Primary map



X Index: 197



Y Index: 203

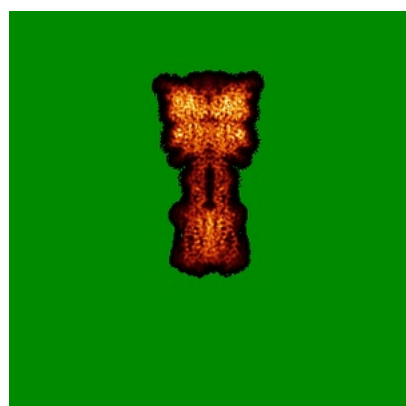


Z Index: 290

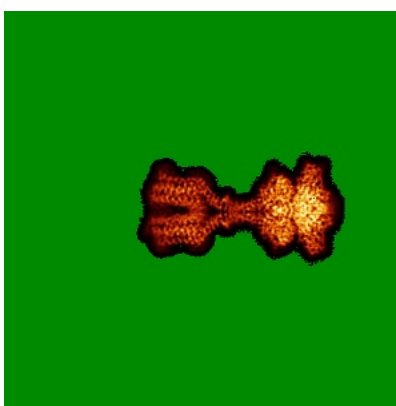
The images above show the largest variance slices of the map in three orthogonal directions.

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

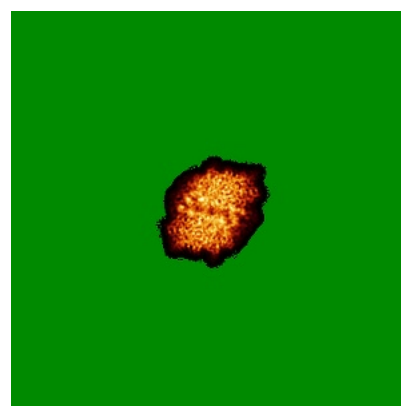
6.4.1 Primary map



X



Y

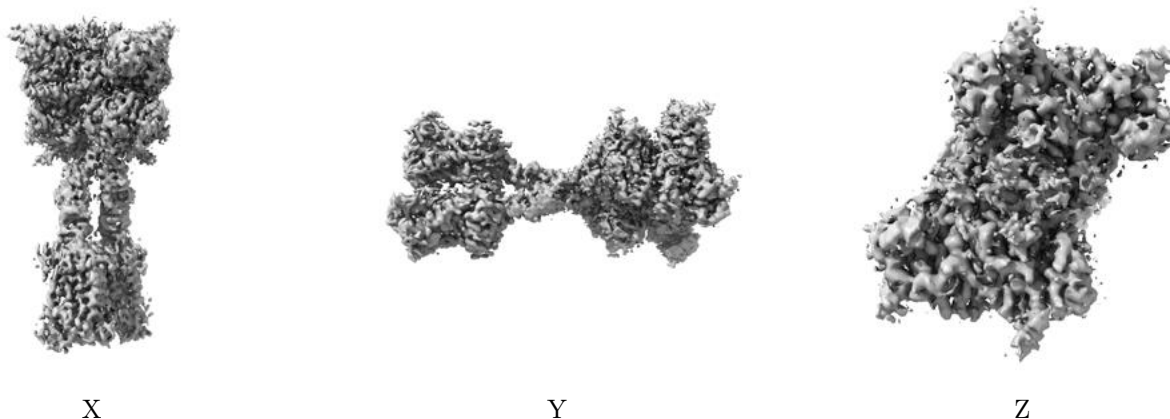


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

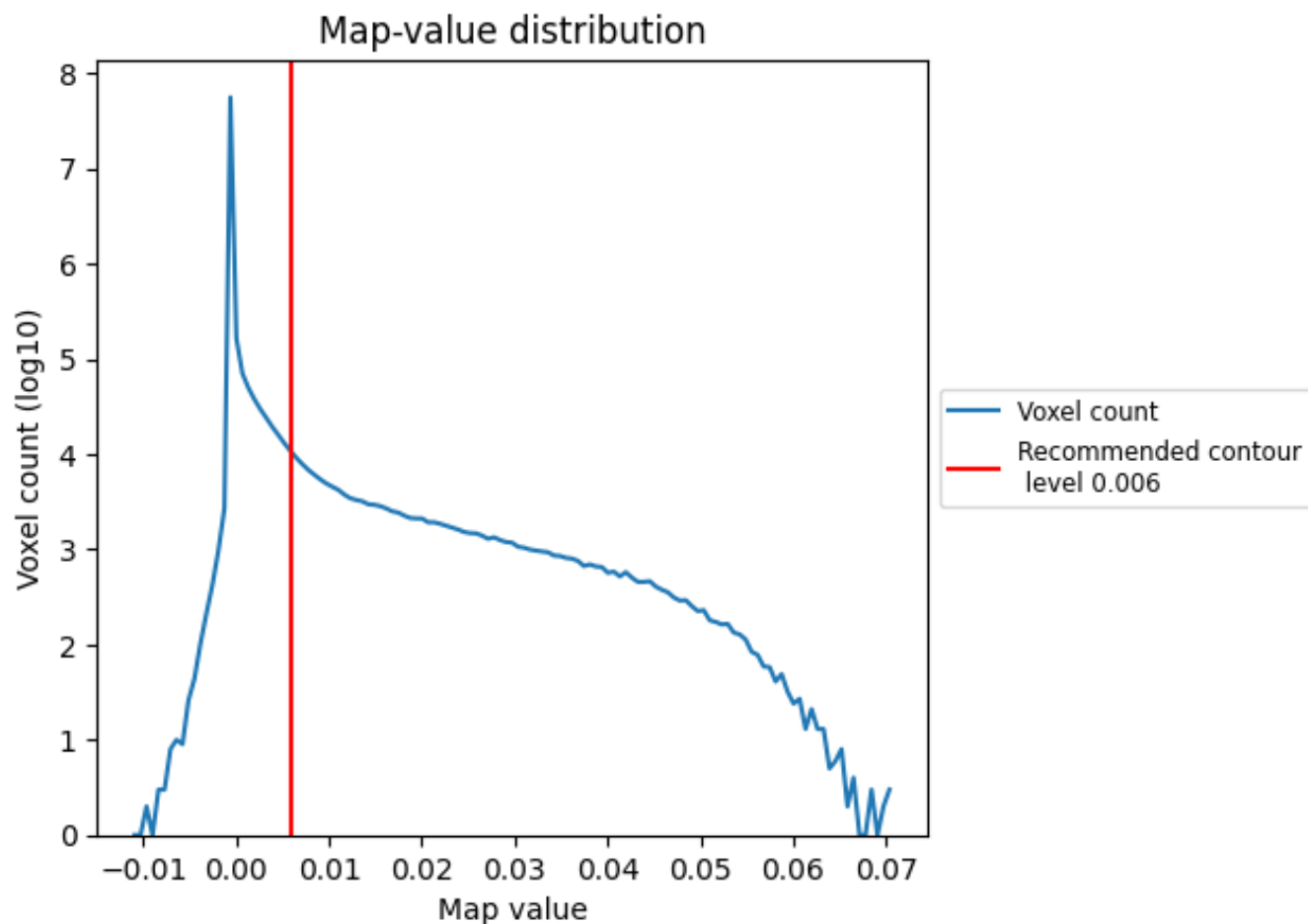
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

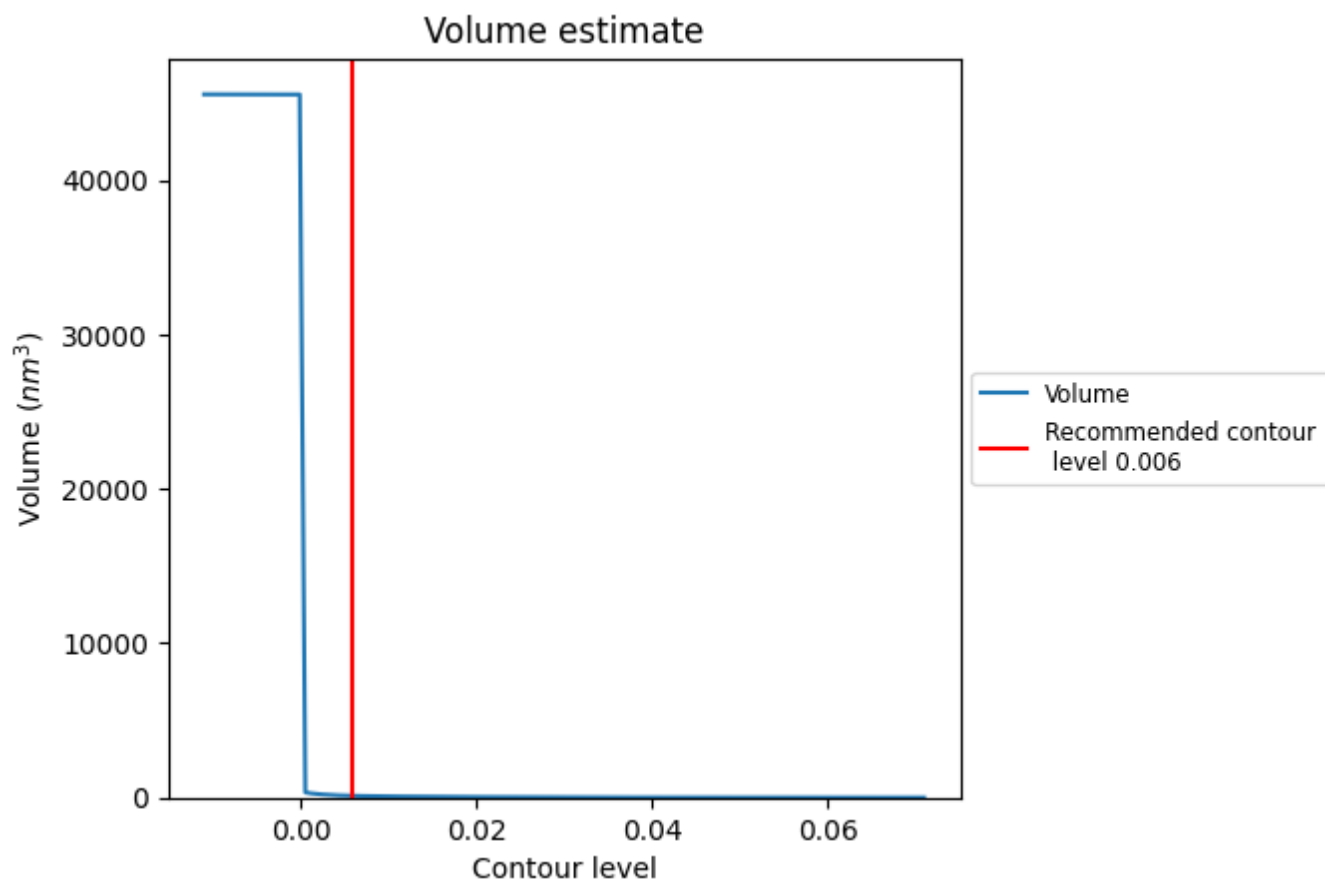
This section contains the results of statistical analysis of the map.

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.

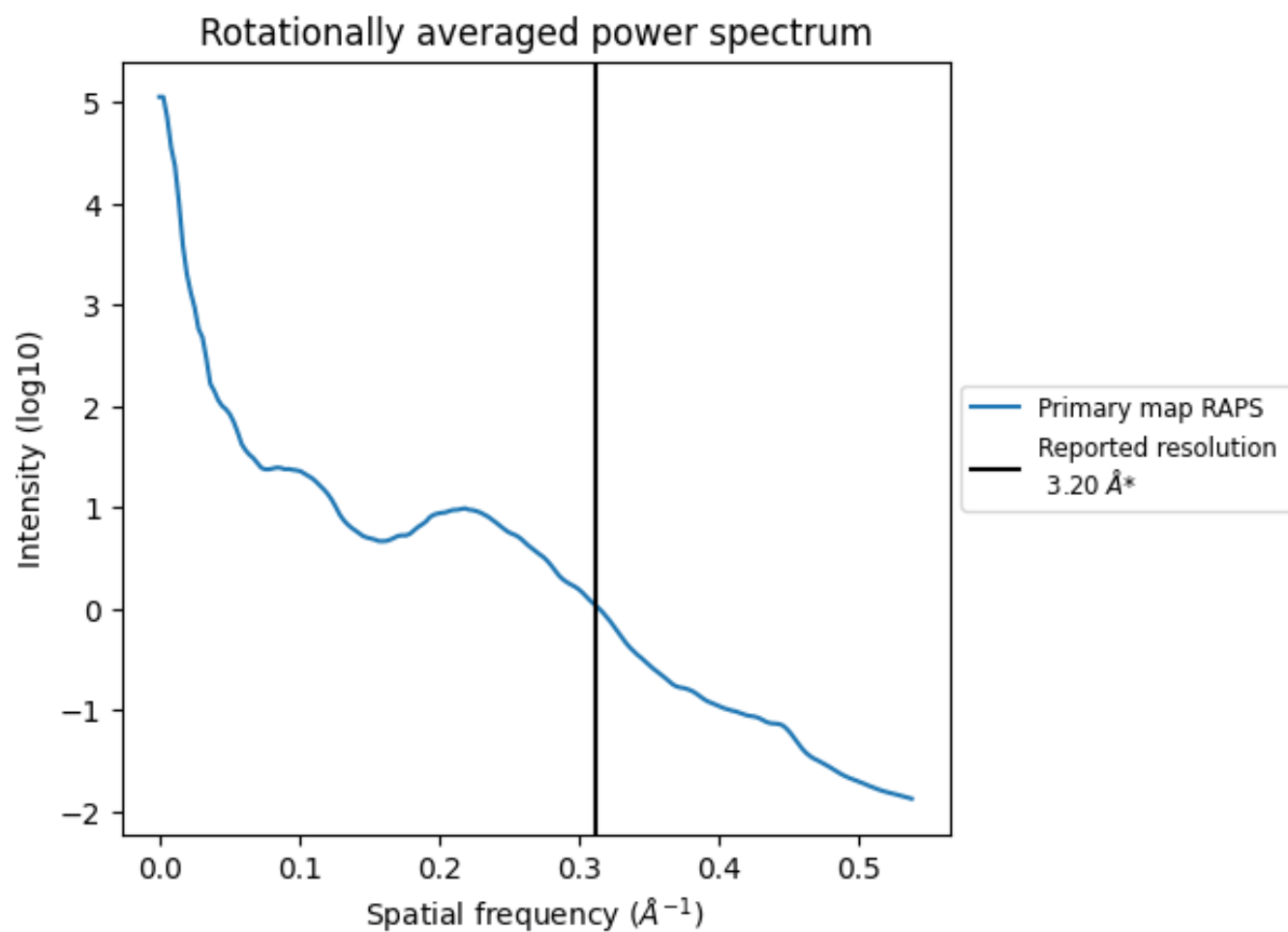
7.2 Volume estimate [i](#)



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 0.312 Å⁻¹

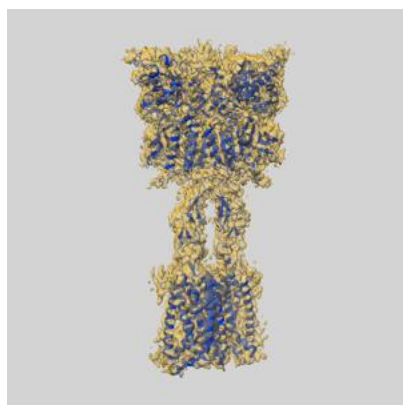
8 Fourier-Shell correlation

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

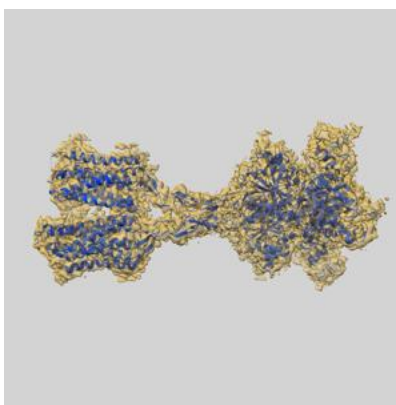
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66179 and PDB model 9WQP. Per-residue inclusion information can be found in section [3](#) on page [7](#).

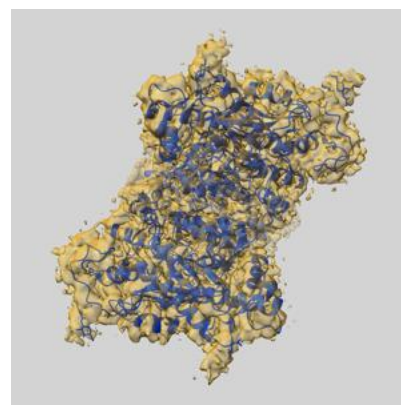
9.1 Map-model overlay [i](#)



X



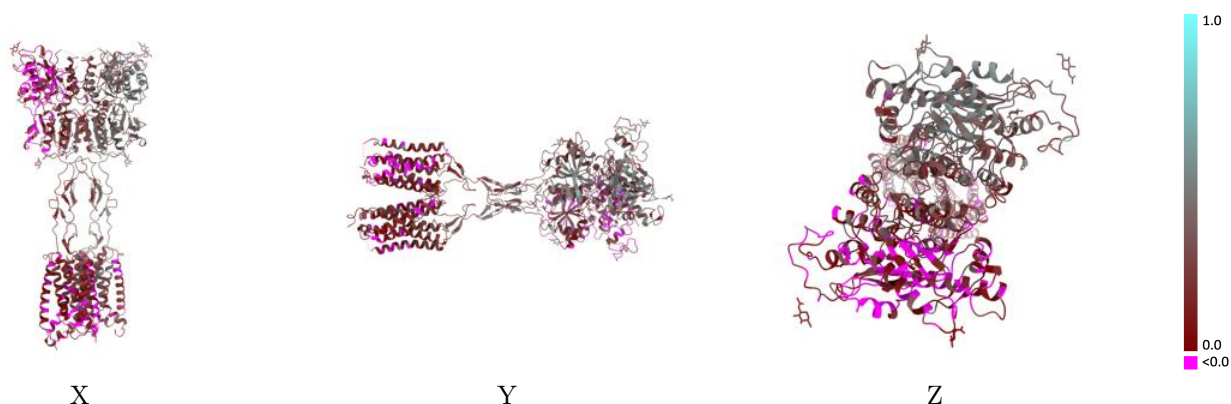
Y



Z

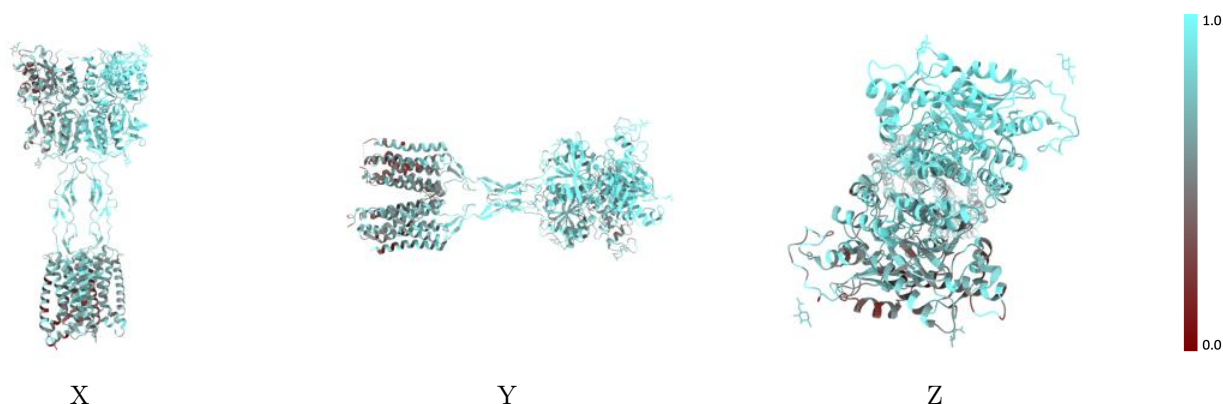
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



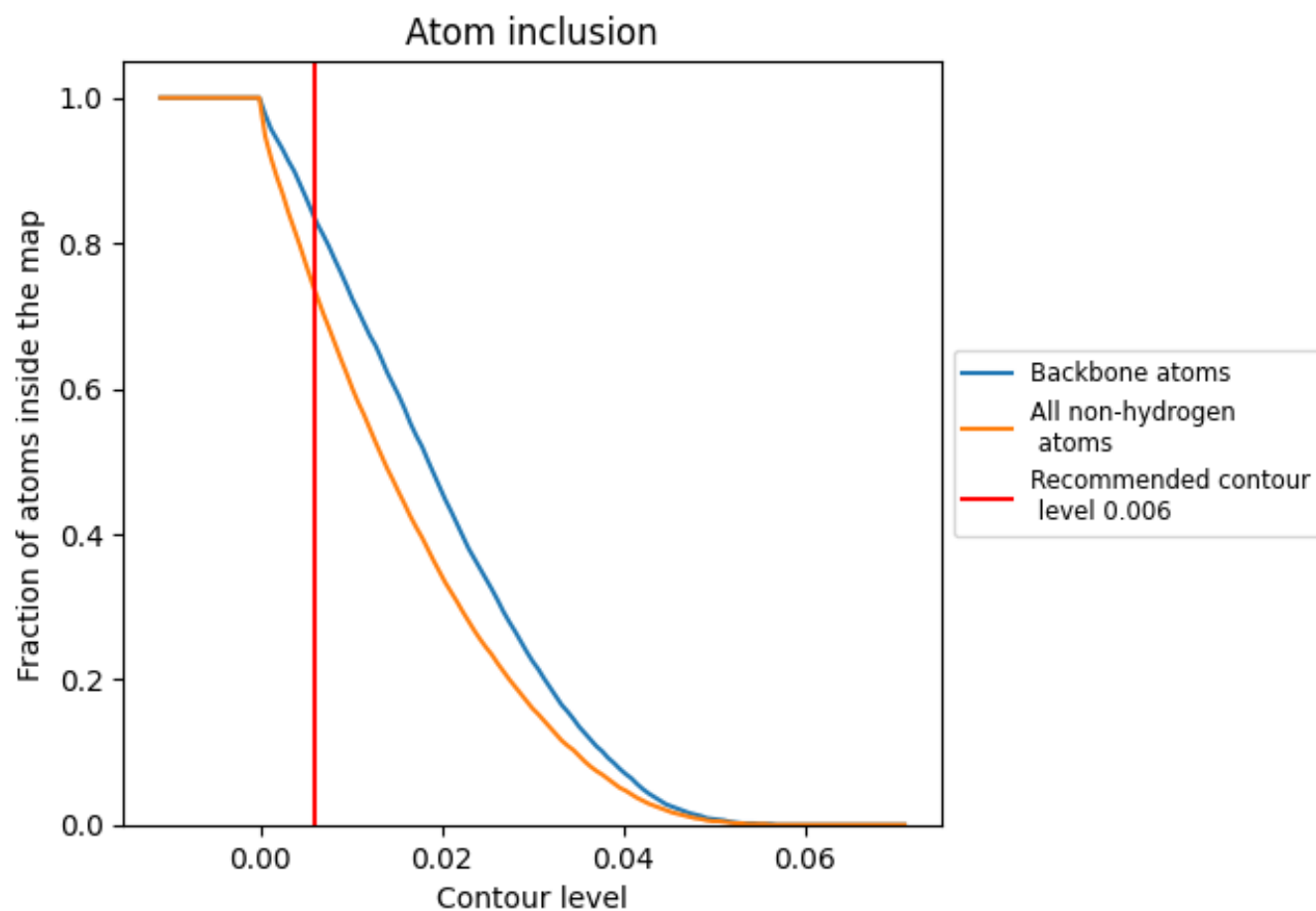
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7360	<div></div> 0.2170
X	<div></div> 0.8100	<div></div> 0.3220
Y	<div></div> 0.6630	<div></div> 0.1120

