



Full wwPDB EM Validation Report ⓘ

Oct 1, 2024 – 05:47 PM JST

PDB ID : 8JXH
EMDB ID : EMD-36701
Title : rat megalin RAP complex wingA
Authors : Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on : 2023-06-30
Resolution : 3.50 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

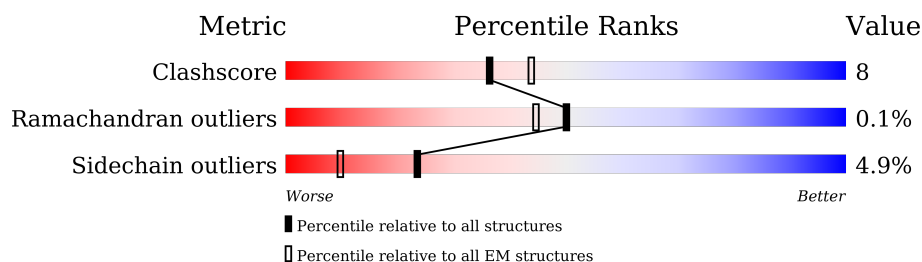
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	D	332	
2	A	4660	
2	B	4660	
3	Q	6	
4	R	5	
5	C	2	
5	F	2	
6	E	3	

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Mol	Chain	Length	Quality of chain
7	G	5	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11503 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 Alpha-2-macroglobulin receptor-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	D	105	Total	C	N	O	0	0
			895	563	163	169		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	GLY	-	expression tag	UNP Q99068
D	30	PRO	-	expression tag	UNP Q99068
D	31	LEU	-	expression tag	UNP Q99068
D	32	GLY	-	expression tag	UNP Q99068
D	33	SER	-	expression tag	UNP Q99068

- Molecule 2 is a protein called LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	151	Total	C	N	O	S	0	0
			1149	680	202	246	21		
2	B	1166	Total	C	N	O	S	0	0
			9047	5545	1608	1786	108		

- Molecule 3 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Q	6	Total	C	N	O	0	0
			30	18	6	6		

- Molecule 4 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	R	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



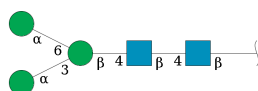
Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



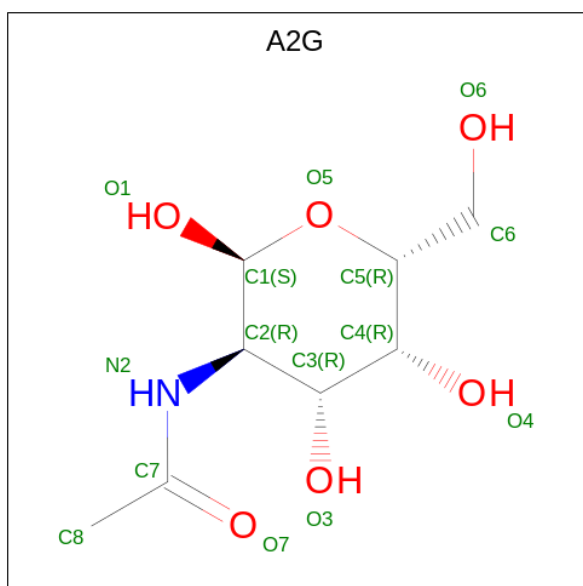
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 9 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

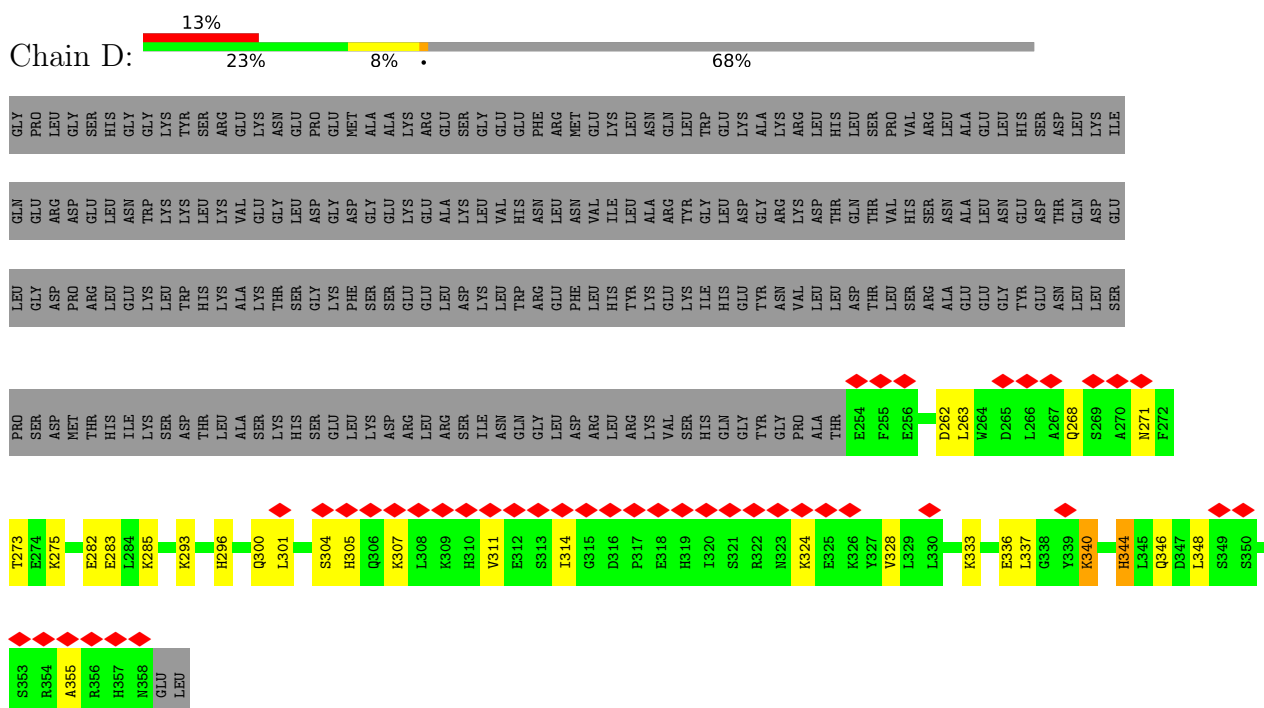
- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	A	4	Total	Ca	0
			4	4	
10	B	12	Total	Ca	0
			12	12	

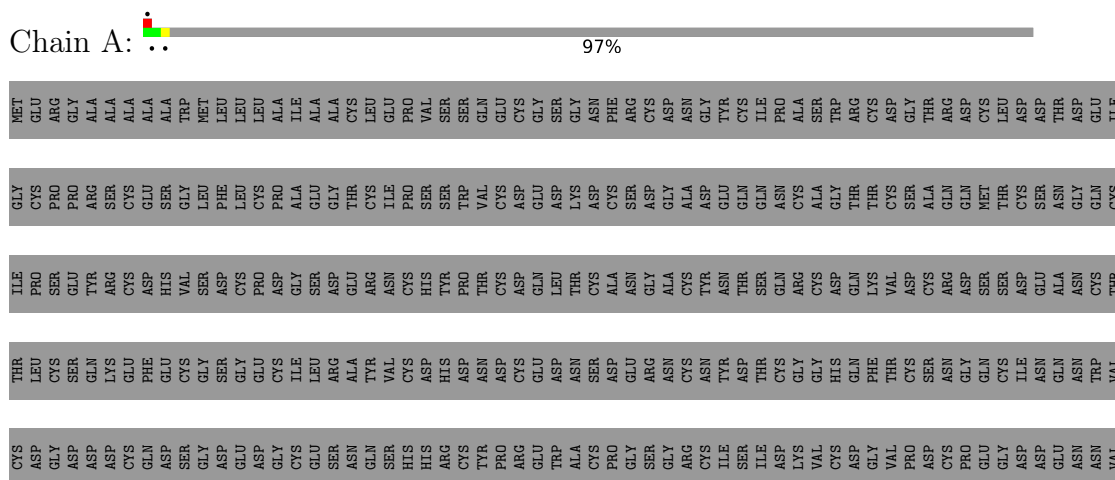
3 Residue-property plots

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: Alpha-2-macroglobulin receptor-associated protein



- Molecule 2: LDL receptor related protein 2









[illegible]

- Molecule 2: LDL receptor related protein 2

Chain B:  20% 5% 75%

P273	G274	G275	G276	G277	G278	D282	K283	G284	G285	D286	G287	D290	G291	G292	G293	G294	D295	D296	G297	N298	N299	G300	T301	S302	G303	R304	T305	G306	G307	K308	G309	V310	C311	S312	V313	L314	N315	Y318	Q319	C320	H321	Q322	F325		
THR	LEU	CYS	SER	GLN	K186	E187	F188	E189	C190	G191	S192	G193	E194	C195	I196	L197	Y200	D203	H206	E209	D210	N211	E214	R215	N216	C217	G218	Y219	D220	T221	C229	Q237	D244	E253	E257	S258	N259	Q261	H262	H263	E264	C265	Y266	T267	
ILE	PRO	SER	GLU	TVR	ARG	CYS	HIS	VAL	SER	ASP	PRO	ASP	GLY	SER	ASP	GLY	THR	GLN	LEU	THR	THR	GLN	LEU	CYS	ASN	GLY	ALA	CYS	TVR	ASN	THR	GLN	ARG	CYS	VAL	ASP	SER	GLU	ALA	ASN	CYS	TVR			
GLY	CYS	PRO	ARG	SER	CYS	GLU	SER	LEU	PHE	LEU	LEU	CYS	PRO	ALA	GLY	GLY	THR	GLY	ILE	PRO	VAL	ASP	GLY	LYS	CYS	ASP	GLY	ALA	ASP	GLU	GLN	ASN	CYS	ALA	GLY	THR	CYS	ASP	SER	GLY	ALA	THR	GLY	CYS	
MET	GLU	ARG	GLY	ALA	ALA	ALA	ALA	TRP	MET	LEU	LEU	LEU	ALA	ILE	ALA	CYS	GLY	ALA	CYS	GLN	SER	SER	GLY	ASN	PHE	ARG	CYS	ASN	GLY	CYS	ILE	PRO	ALA	SER	TRP	ARG	CYS	ASP	GLY	THR	ASP	THR	THR	GLU	TVR








PRO	PRO	ASP	CYS	ARG	GLY	CYS	MET	HIS	GLY	GLY	CYS	TYR	PHE	ASP	GLU	ASN	GLU	PRO	LEU	PRO	LYS	LYS	CYS	LYS	CYS	SER	SER	GLY	TYR	GLY	GLY	TYR	CYS	GLU	VAL	GLY	LEU	ARG	GLY	ILE	PRO	PRO	GLY	THR	THR	MET	ALA	VAL	LEU	LEU	THR	PHE	ILE	VAL	GLY	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
LEU	VAL	PRO	LEU	VAL	GLY	CYS	LEU	PHE	HIS	TYR	ASN	ARG	THR	GLY	SER	LEU	PRO	LEU	PRO	LYS	LYS	CYS	LYS	LYS	CYS	SER	SER	LEU	SER	ALA	LYS	PRO	SER	GLU	ASN	GLY	VAL	THR	PHE	ILE	ASP	VAL	ASN	ASN	VAL	MET	ASP	ILE	GLY	VAL	THR	PRO	PHE	GLY	PRO	GLU	THR	ILE	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
ILE	ASP	ARG	SER	MET	ALA	MET	ASN	GLY	GLU	HIS	ASN	PHE	VAL	MET	GLU	VAL	LYS	GLN	VAL	ILE	PHE	GLU	ILE	GLU	GLN	ASN	PRO	MET	TYR	SER	ALA	LYS	ASP	ASN	THR	SER	LYS	VAL	ALA	LEU	ALA	VAL	GLN	GLY	PRO	SER	THR	GLY	ALA	ALA	GLN	VAL	GLU	ASN	VAL	GLU	ASN	GLN	ASN	TYR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
GLY	ARG	PRO	PRO	ILE	SER	ASP	PRO	SER	LEU	PRO	ALA	VAL	LYS	ARG	ASN	LEU	THR	PRO	GLY	ALA	ASP	GLU	ILE	GLU	GLN	GLY	LYS	TRP	LYS	TRP	ASN	ILE	THR	PHE	LYS	ASN	ARG	THR	GLN	THR	THR	ASN	PHE	GLU	ASN	PRO	ILE	TYR	ALA	ALA	MET	ASP	SER	GLU	VAL	LYS	ASP	ALA	VAL	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
PRO	PRO	PRO	SER	PRO	PRO	SER	LEU	PRO	ALA	LYS	ALA	SER	LYS	ARG	ASN	LEU	THR	PRO	GLY	TYR	THR	THR	THR	GLU	ASP	THR	PHE	LYS	TRP	ASN	THR	ALA	ASN	LEU	VAL	GLU	ASP	SER	ASP	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											

- Molecule 3: unclear peptide

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: unclear peptide

Chain R:  80% 20%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100% 100%



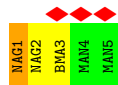
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%



- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain G:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.029	Depositor
Map size (\AA)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.411, 1.411, 1.411	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: A2G, MAN, CA, NAG, BMA

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	D	0.26	0/913	0.46	0/1220
2	A	0.31	0/1176	0.55	0/1603
2	B	0.28	0/9263	0.52	0/12565
4	R	0.19	0/7	0.43	0/8
All	All	0.28	0/11359	0.52	0/15396

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	D	895	0	885	15	0
2	A	1149	0	967	21	0
2	B	9047	0	8299	129	0
3	Q	30	0	8	0	0
4	R	28	0	12	1	0
5	C	28	0	25	0	0
5	F	28	0	25	4	0
6	E	39	0	34	0	0
7	G	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	28	0	26	1	0
8	B	28	0	26	0	0
9	A	14	0	12	0	0
9	B	112	0	96	7	0
10	A	4	0	0	0	0
10	B	12	0	0	0	0
All	All	11503	0	10467	165	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (165) 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:B:1149:THR:OG1	9:B:4707:A2G:C1	1.73	1.36
2:B:1109:THR:OG1	9:B:4706:A2G:C1	1.78	1.32
2:B:1109:THR:CB	9:B:4706:A2G:C1	2.49	0.90
2:A:2786:GLU:HG2	2:A:2788:THR:H	1.36	0.87
2:A:2805:ASN:HD22	2:A:2812:THR:HG23	1.51	0.74
2:B:353:ILE:HG12	2:B:356:ILE:HB	1.70	0.74
2:A:2827:PHE:HB3	2:A:2836:CYS:HB2	1.69	0.73
2:B:715:LYS:HB2	2:B:955:SER:HB2	1.77	0.67
1:D:282:GLU:HA	1:D:285:LYS:HZ3	1.60	0.67
2:B:1149:THR:CB	9:B:4707:A2G:C1	2.71	0.67
2:B:1105:ALA:HB3	9:B:4710:A2G:H3	1.75	0.67
2:B:190:CYS:SG	2:B:191:GLY:N	2.70	0.65
2:B:1109:THR:HB	9:B:4706:A2G:C1	2.27	0.65
2:B:343:ARG:HD3	2:B:344:THR:HG23	1.79	0.64
1:D:283:GLU:HG2	1:D:348:LEU:HD21	1.81	0.62
2:B:451:ASP:OD2	2:B:453:ASN:ND2	2.32	0.62
2:B:1045:ASP:HA	2:B:1070:ALA:HB2	1.81	0.62
2:A:2760:ARG:NH2	2:A:2774:ALA:O	2.32	0.62
2:B:766:LYS:HD3	2:B:777:ILE:HD11	1.81	0.61
2:B:811:ARG:NH1	2:B:814:ASP:OD1	2.33	0.61
2:B:807:VAL:HG13	2:B:821:ILE:HB	1.83	0.61
2:B:825:ASN:O	2:B:826:ASN:ND2	2.34	0.60
2:B:616:THR:HG22	2:B:623:VAL:HG22	1.83	0.60
2:B:534:GLN:N	2:B:534:GLN:OE1	2.33	0.59
2:B:574:ASP:OD1	2:B:577:TYR:N	2.28	0.59
2:B:713:SER:HB3	2:B:745:ILE:HD13	1.85	0.59
2:B:863:ILE:HG22	2:B:864:VAL:HG23	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:ASP:OD1	1:D:263:LEU:N	2.36	0.58
2:B:503:LEU:HD13	2:B:543:ASP:HA	1.86	0.58
2:A:2737:CYS:HA	2:A:2740:HIS:HB3	1.84	0.58
2:B:381:GLY:O	2:B:382:GLN:HG3	2.03	0.58
2:B:486:LYS:HG2	2:B:736:THR:HG21	1.85	0.57
2:B:431:HIS:HD2	2:B:434:LYS:H	1.50	0.57
2:B:886:VAL:HG12	2:B:893:ILE:HG12	1.86	0.56
1:D:283:GLU:OE1	1:D:344:HIS:NE2	2.34	0.56
2:B:738:SER:HB3	2:B:739:PRO:HD3	1.87	0.56
2:B:1088:ARG:HH11	2:B:1088:ARG:HB3	1.71	0.56
2:B:616:THR:HB	2:B:644:PRO:HB2	1.88	0.55
2:A:2810:ASN:HB2	8:A:4702:NAG:O5	2.07	0.55
2:B:272:CYS:HB2	2:B:295:ASP:HB3	1.88	0.55
2:B:738:SER:HB3	2:B:739:PRO:CD	2.37	0.55
2:B:349:ASP:OD1	2:B:364:ARG:NH1	2.40	0.54
2:B:299:ASN:OD1	2:B:301:THR:OG1	2.25	0.54
2:B:725:LEU:HD11	2:B:949:ILE:HD12	1.91	0.53
2:B:1064:ASN:HB2	5:F:1:NAG:H2	1.89	0.53
2:B:543:ASP:OD1	2:B:545:SER:OG	2.26	0.53
2:B:318:TYR:CG	2:B:332:PRO:HD3	2.44	0.53
2:B:963:ASP:HB3	2:B:966:LEU:HD23	1.90	0.53
2:B:526:SER:HB2	2:B:558:PRO:HB2	1.91	0.53
2:B:1003:MET:HG2	2:B:1012:CYS:HB3	1.90	0.52
1:D:324:LYS:O	1:D:328:VAL:HG22	2.10	0.52
2:B:735:VAL:HG11	2:B:756:TYR:CZ	2.45	0.52
5:F:1:NAG:O4	5:F:2:NAG:N2	2.41	0.51
2:B:928:THR:HG21	2:B:957:MET:O	2.10	0.51
2:B:214:GLU:OE1	2:B:219:TYR:OH	2.29	0.51
2:B:1040:SER:O	2:B:1042:PHE:N	2.44	0.50
2:B:1157:CYS:HB3	2:B:1160:HIS:HB3	1.93	0.50
2:A:2779:ARG:NH1	2:A:2794:CYS:SG	2.69	0.50
2:B:426:MET:HB3	2:B:442:PRO:HD3	1.93	0.50
2:B:257:GLU:OE2	2:B:260:GLN:HB3	2.11	0.50
2:B:1188:CYS:HB2	2:B:1194:LYS:HE2	1.93	0.50
2:B:872:ASN:OD1	4:R:2:ASN:ND2	2.40	0.49
2:A:2747:PHE:HB3	2:A:2755:VAL:HG13	1.95	0.49
1:D:304:SER:HA	1:D:307:LYS:HB2	1.95	0.48
2:B:431:HIS:CD2	2:B:434:LYS:H	2.32	0.48
2:B:475:TRP:CZ2	2:B:656:PRO:HD2	2.48	0.48
1:D:311:VAL:HA	1:D:314:ILE:HD12	1.96	0.48
2:B:433:GLN:HE22	7:G:1:NAG:H5	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ASN:OD1	2:B:211:ASN:ND2	2.27	0.48
2:B:779:ALA:HB1	2:B:1036:LYS:HG2	1.94	0.48
2:B:793:ILE:HG21	2:B:971:ASN:OD1	2.14	0.47
2:B:1024:GLN:O	2:B:1025:CYS:HB3	2.15	0.47
2:B:1140:ASP:OD1	2:B:1140:ASP:N	2.41	0.47
2:B:341:ASP:HB2	2:B:343:ARG:HG3	1.97	0.47
2:B:538:GLU:HA	2:B:550:LEU:H	1.80	0.47
2:B:852:ARG:NH1	2:B:898:LEU:O	2.44	0.47
2:B:1124:PRO:HD2	2:B:1127:TRP:CE3	2.50	0.47
2:B:331:CYS:HB2	2:B:332:PRO:HD2	1.97	0.47
2:B:846:ARG:HB3	2:B:847:PRO:HD3	1.97	0.47
2:B:474:ASP:HB3	2:B:479:LYS:HB2	1.97	0.47
2:B:407:ASP:N	2:B:407:ASP:OD1	2.36	0.47
2:B:1236:PHE:N	2:B:1245:ILE:O	2.39	0.47
2:B:266:TYR:HB3	2:B:267:PRO:HD2	1.96	0.46
2:A:2830:CYS:HB2	2:A:2835:ILE:HD11	1.97	0.46
2:B:1134:ASP:N	2:B:1134:ASP:OD1	2.49	0.46
2:A:2785:THR:HA	2:A:2796:PRO:HA	1.97	0.46
2:B:1275:THR:HA	2:B:1287:LYS:HE3	1.97	0.46
2:B:396:ILE:HG22	2:B:405:VAL:HG22	1.97	0.46
2:B:609:PHE:HB2	2:B:649:VAL:HG11	1.97	0.46
2:B:1091:ASP:OD1	2:B:1091:ASP:N	2.48	0.45
2:B:562:THR:HG23	2:B:608:LEU:HD23	1.98	0.45
2:B:263:HIS:HB3	2:B:265:CYS:SG	2.57	0.45
2:B:781:ARG:NH2	2:B:1023:GLN:O	2.50	0.45
1:D:293:LYS:NZ	2:B:203:ASP:OD2	2.45	0.45
2:B:426:MET:HB3	2:B:442:PRO:CD	2.47	0.45
2:B:1226:ARG:HG3	2:B:1232:HIS:CE1	2.52	0.45
1:D:273:THR:HG22	1:D:275:LYS:H	1.82	0.45
2:A:2787:PHE:CZ	2:A:2814:ASP:HA	2.51	0.45
2:B:237:GLN:HE21	2:B:539:ARG:HH21	1.65	0.45
2:B:266:TYR:CE2	2:B:353:ILE:HA	2.52	0.45
2:B:844:TRP:HB2	2:B:870:TRP:HA	1.99	0.45
2:B:866:THR:OG1	2:B:1257:CYS:O	2.35	0.45
2:B:1081:PRO:HD2	2:B:1084:TRP:CE3	2.52	0.45
2:B:573:VAL:HB	2:B:603:PRO:HB2	2.00	0.44
2:B:367:ARG:NE	2:B:367:ARG:HA	2.32	0.44
2:B:990:VAL:HG21	2:B:996:VAL:HG13	1.98	0.44
1:D:296:HIS:O	1:D:300:GLN:HG3	2.17	0.44
2:A:2772:ASP:OD1	2:A:2772:ASP:N	2.50	0.44
2:B:699:ASP:OD2	2:B:702:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1064:ASN:HB2	5:F:1:NAG:C2	2.47	0.44
2:B:1207:ARG:NH1	2:B:1219:ASP:O	2.37	0.44
2:B:781:ARG:HB2	2:B:817:ARG:NH2	2.33	0.44
2:B:681:ASN:ND2	2:B:686:TYR:O	2.49	0.44
2:B:1088:ARG:HB3	2:B:1088:ARG:NH1	2.31	0.44
2:B:308:MET:HG3	2:B:322:GLN:HB3	2.00	0.43
2:A:2827:PHE:CE2	2:A:2838:PRO:HG3	2.53	0.43
2:A:2829:LYS:HA	2:A:2835:ILE:O	2.18	0.43
2:B:451:ASP:HB3	2:B:454:GLY:O	2.19	0.43
2:A:2828:THR:O	2:A:2836:CYS:HA	2.18	0.43
2:B:244:ASP:N	2:B:253:GLU:OE1	2.51	0.43
1:D:333:LYS:NZ	2:B:206:ASN:O	2.46	0.43
2:B:270:TRP:CH2	2:B:272:CYS:HA	2.54	0.42
2:B:1172:ASP:OD1	2:B:1172:ASP:N	2.51	0.42
2:B:1194:LYS:H	2:B:1194:LYS:HG2	1.63	0.42
2:B:421:ASN:ND2	2:B:444:GLN:OE1	2.52	0.42
5:F:1:NAG:H82	5:F:2:NAG:H61	2.01	0.42
2:B:1234:ASP:O	2:B:1247:ASN:HB2	2.20	0.42
2:A:2767:CYS:HB2	2:A:2772:ASP:OD1	2.19	0.42
2:B:818:ARG:NH2	2:B:1000:PRO:O	2.52	0.42
2:B:931:ARG:NH2	2:B:1213:ASP:OD1	2.53	0.42
2:B:510:HIS:HB3	2:B:528:TRP:NE1	2.35	0.42
2:B:1281:ASN:HD21	2:B:1283:ASN:HD21	1.67	0.42
2:B:367:ARG:HH11	2:B:367:ARG:HG2	1.85	0.42
2:B:780:ASN:CG	2:B:781:ARG:HG3	2.41	0.42
2:A:2827:PHE:HE2	2:A:2838:PRO:HG3	1.85	0.41
2:B:405:VAL:HG23	2:B:416:LEU:HB2	2.01	0.41
2:B:1040:SER:C	2:B:1042:PHE:N	2.73	0.41
2:B:318:TYR:CD2	2:B:319:GLN:HB2	2.55	0.41
1:D:268:GLN:HE21	1:D:268:GLN:HB3	1.59	0.41
2:A:2779:ARG:CZ	2:A:2779:ARG:HB3	2.50	0.41
2:A:2837:VAL:HG21	2:A:2849:CYS:HA	2.01	0.41
2:B:424:MET:O	2:B:441:ASP:HA	2.20	0.41
2:B:826:ASN:HB3	2:B:844:TRP:NE1	2.35	0.41
2:B:738:SER:CB	2:B:739:PRO:CD	2.98	0.41
2:B:1109:THR:HB	9:B:4706:A2G:C5	2.51	0.41
1:D:336:GLU:HG3	1:D:340:LYS:NZ	2.36	0.41
2:B:739:PRO:HG2	2:B:761:LYS:NZ	2.36	0.41
2:B:1046:GLY:HA3	2:B:1081:PRO:HD3	2.01	0.41
2:B:846:ARG:O	2:B:846:ARG:NE	2.54	0.41
2:B:357:CYS:HB3	2:B:370:CYS:HB3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:PHE:CZ	2:B:638:HIS:HB2	2.56	0.41
2:B:1281:ASN:HD21	2:B:1283:ASN:ND2	2.18	0.41
2:A:2779:ARG:NH1	2:A:2779:ARG:HB3	2.36	0.41
2:B:442:PRO:HA	2:B:468:PRO:HD2	2.02	0.41
2:B:476:ILE:HG22	2:B:660:ASN:HB3	2.02	0.41
2:B:197:LEU:HD12	2:B:200:TYR:CE2	2.56	0.41
2:B:473:VAL:HG12	2:B:480:LEU:HD13	2.02	0.41
2:B:890:PHE:HB2	2:B:892:LYS:HE2	2.03	0.41
2:B:372:CYS:HB3	2:B:376:TYR:HB3	2.02	0.40
2:B:790:PHE:CE2	2:B:792:TRP:HA	2.56	0.40
2:A:2825:PRO:C	2:A:2827:PHE:H	2.24	0.40
2:B:444:GLN:O	2:B:445:GLU:HB2	2.21	0.40
1:D:301:LEU:O	1:D:305:HIS:HB2	2.21	0.40
2:B:1227:PRO:HB2	2:B:1230:MET:HB2	2.03	0.40
1:D:271:ASN:ND2	1:D:355:ALA:O	2.32	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	D	103/332 (31%)	101 (98%)	2 (2%)	0	100	100
2	A	149/4660 (3%)	135 (91%)	14 (9%)	0	100	100
2	B	1162/4660 (25%)	1084 (93%)	77 (7%)	1 (0%)	48	79
4	R	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1415/9657 (15%)	1321 (93%)	93 (7%)	1 (0%)	50	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1041	PHE

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	D	99/299 (33%)	95 (96%)	4 (4%)	27	56
2	A	135/4089 (3%)	125 (93%)	10 (7%)	11	36
2	B	1025/4089 (25%)	977 (95%)	48 (5%)	22	51
4	R	1/1 (100%)	1 (100%)	0	100	100
All	All	1260/8478 (15%)	1198 (95%)	62 (5%)	23	50

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	337	LEU
1	D	340	LYS
1	D	344	HIS
1	D	346	GLN
2	A	2741	THR
2	A	2753	ARG
2	A	2779	ARG
2	A	2781	CYS
2	A	2812	THR
2	A	2813	SER
2	A	2823	CYS
2	A	2836	CYS
2	A	2837	VAL
2	A	2854	ASP
2	B	187	GLU
2	B	217	CYS
2	B	221	THR
2	B	229	CYS
2	B	257	GLU
2	B	272	CYS
2	B	278	CYS

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Mol	Chain	Res	Type
2	B	343	ARG
2	B	350	ASP
2	B	353	ILE
2	B	368	HIS
2	B	407	ASP
2	B	421	ASN
2	B	466	ASP
2	B	489	ARG
2	B	516	LEU
2	B	563	LEU
2	B	595	ARG
2	B	617	ASP
2	B	643	ARG
2	B	690	CYS
2	B	715	LYS
2	B	741	PHE
2	B	746	ASP
2	B	835	THR
2	B	839	MET
2	B	846	ARG
2	B	849	LYS
2	B	861	MET
2	B	891	ASP
2	B	895	HIS
2	B	899	ASP
2	B	928	THR
2	B	946	MET
2	B	966	LEU
2	B	995	ARG
2	B	1003	MET
2	B	1010	MET
2	B	1088	ARG
2	B	1091	ASP
2	B	1126	ASP
2	B	1134	ASP
2	B	1172	ASP
2	B	1201	CYS
2	B	1300	MET
2	B	1312	HIS
2	B	3169	CYS
2	B	3187	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	D	268	GLN
1	D	294	HIS
2	A	2740	HIS
2	A	2808	HIS
2	B	315	ASN
2	B	363	ASN
2	B	412	ASN
2	B	421	ASN
2	B	431	HIS
2	B	433	GLN
2	B	444	GLN
2	B	507	ASN
2	B	826	ASN
2	B	1192	GLN
2	B	1283	ASN

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 ⓘ

12 monosaccharides 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	$\# Z > 2$
5	NAG	C	1	5,2	14,14,15	0.35	0	17,19,21	1.17	2 (11%)
5	NAG	C	2	5	14,14,15	0.33	0	17,19,21	0.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	E	1	6,2	14,14,15	0.28	0	17,19,21	0.80	0
6	NAG	E	2	6	14,14,15	0.46	0	17,19,21	1.26	4 (23%)
6	BMA	E	3	6	11,11,12	0.29	0	15,15,17	1.09	2 (13%)
5	NAG	F	1	5,2	14,14,15	0.79	1 (7%)	17,19,21	1.93	3 (17%)
5	NAG	F	2	5	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
7	NAG	G	1	7,2	14,14,15	0.49	0	17,19,21	1.63	2 (11%)
7	NAG	G	2	7	14,14,15	0.49	0	17,19,21	1.30	3 (17%)
7	BMA	G	3	7	11,11,12	0.45	0	15,15,17	1.08	1 (6%)
7	MAN	G	4	7	11,11,12	0.34	0	15,15,17	0.92	0
7	MAN	G	5	7	11,11,12	0.22	0	15,15,17	0.60	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
5	NAG	C	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
6	NAG	E	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
6	BMA	E	3	6	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	F	2	5	-	5/6/23/26	0/1/1/1
7	NAG	G	1	7,2	-	1/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	BMA	G	3	7	-	2/2/19/22	0/1/1/1
7	MAN	G	4	7	-	0/2/19/22	0/1/1/1
7	MAN	G	5	7	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	NAG	C1-C2	2.52	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1	NAG	C1-O5-C5	5.96	120.27	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1	NAG	C4-C3-C2	-3.92	105.27	111.02
7	G	2	NAG	C1-O5-C5	2.97	116.21	112.19
7	G	3	BMA	C1-C2-C3	2.92	113.25	109.67
5	F	1	NAG	C3-C4-C5	-2.90	105.07	110.24
6	E	2	NAG	C1-O5-C5	2.72	115.87	112.19
7	G	1	NAG	C2-N2-C7	-2.53	119.29	122.90
7	G	2	NAG	O5-C1-C2	-2.42	107.47	111.29
6	E	3	BMA	C1-C2-C3	2.41	112.63	109.67
5	C	2	NAG	C1-O5-C5	2.41	115.46	112.19
6	E	3	BMA	C1-O5-C5	2.39	115.43	112.19
6	E	2	NAG	C2-N2-C7	-2.35	119.56	122.90
7	G	2	NAG	C2-N2-C7	-2.29	119.64	122.90
6	E	2	NAG	O5-C1-C2	-2.28	107.68	111.29
5	C	1	NAG	C1-O5-C5	2.24	115.22	112.19
5	F	2	NAG	O5-C5-C6	2.23	110.70	107.20
5	C	1	NAG	C4-C3-C2	-2.21	107.78	111.02
5	F	1	NAG	O5-C1-C2	2.07	114.55	111.29
6	E	2	NAG	C1-C2-N2	2.02	113.94	110.49

There are no chirality outliers.

All (14) torsion outliers are listed below:

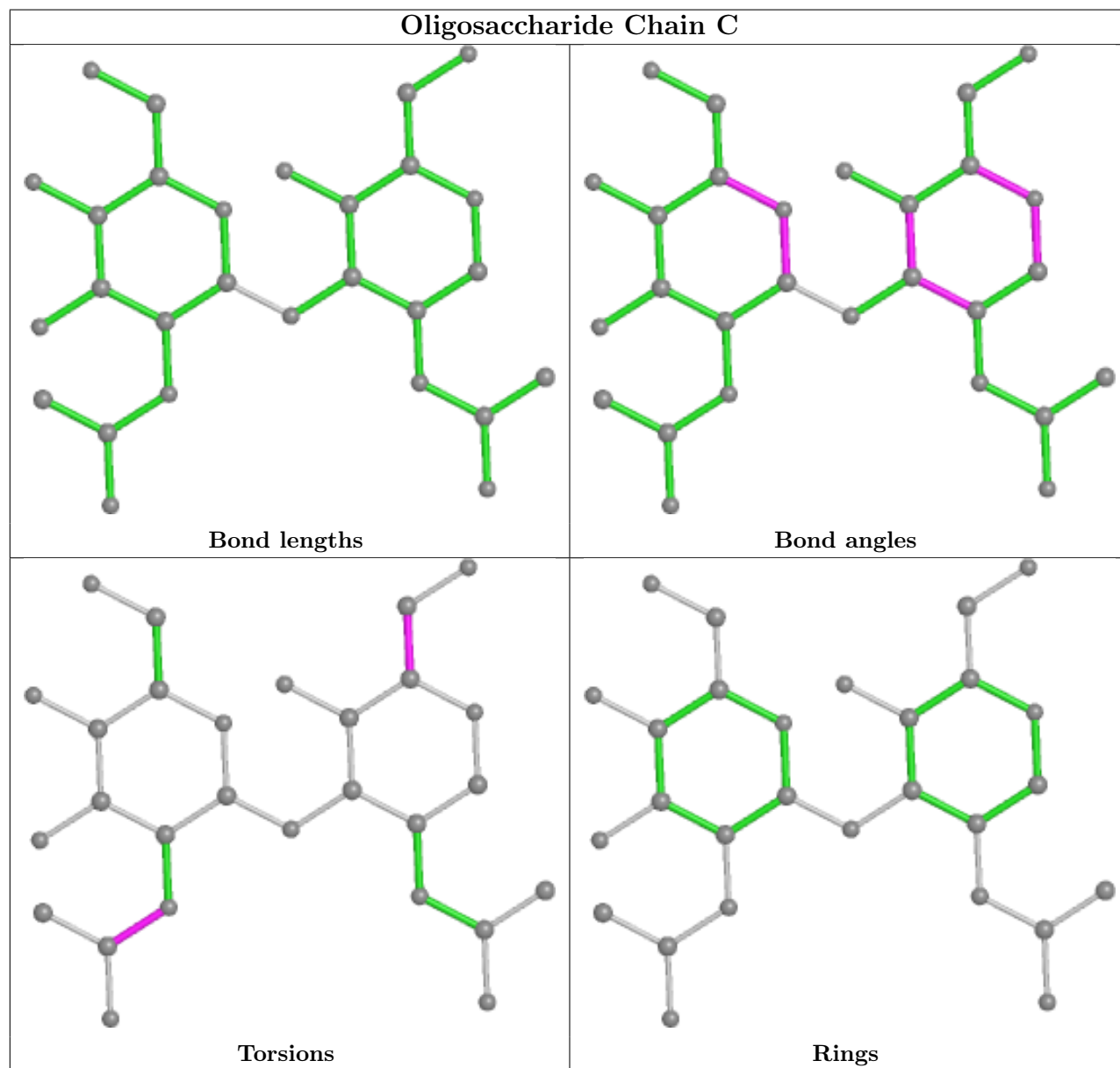
Mol	Chain	Res	Type	Atoms
5	F	2	NAG	C3-C2-N2-C7
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
5	C	2	NAG	C8-C7-N2-C2
5	C	2	NAG	O7-C7-N2-C2
7	G	3	BMA	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	F	1	NAG	C3-C2-N2-C7
7	G	1	NAG	C8-C7-N2-C2
5	C	1	NAG	C4-C5-C6-O6
7	G	3	BMA	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6

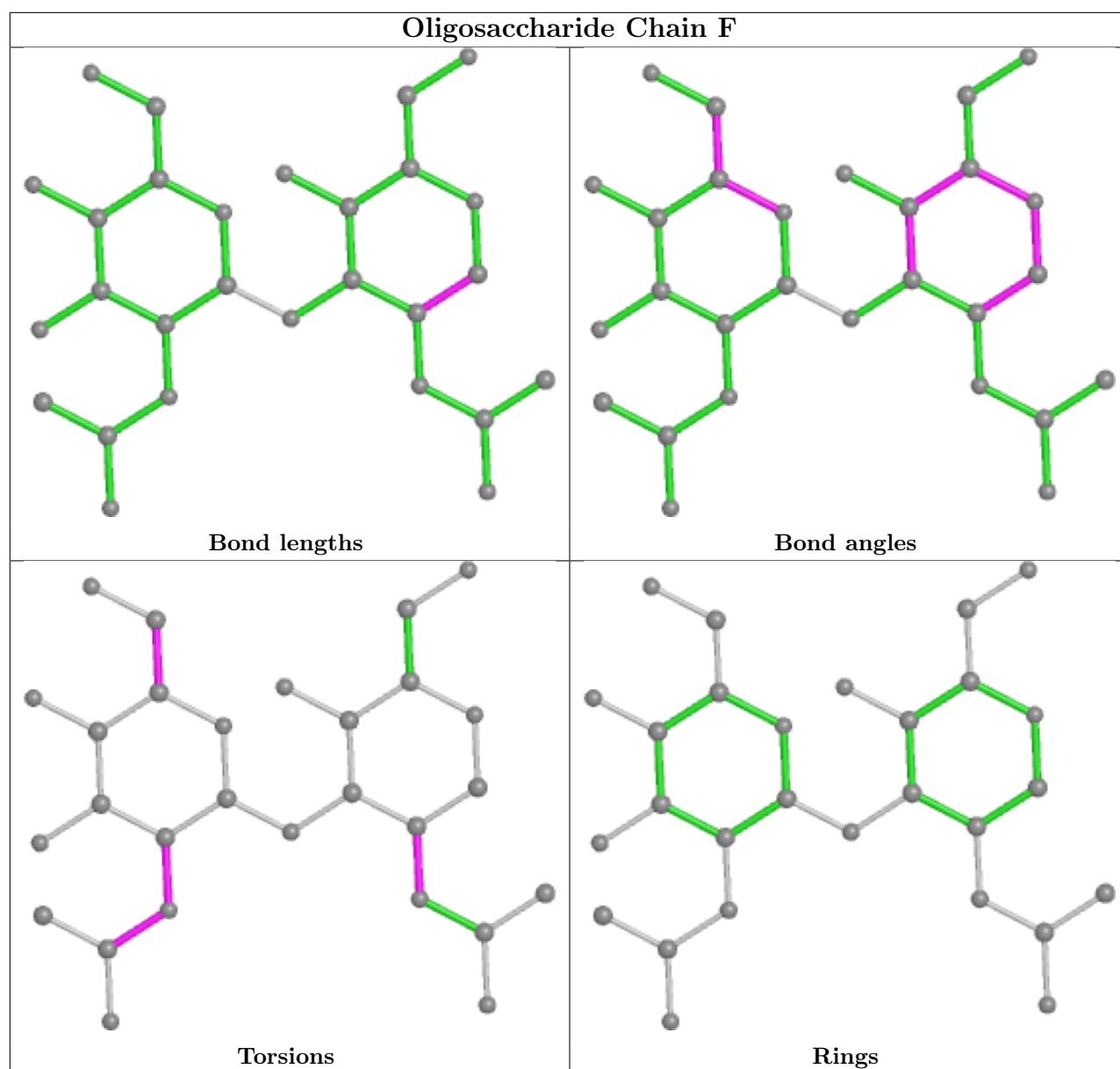
There are no ring outliers.

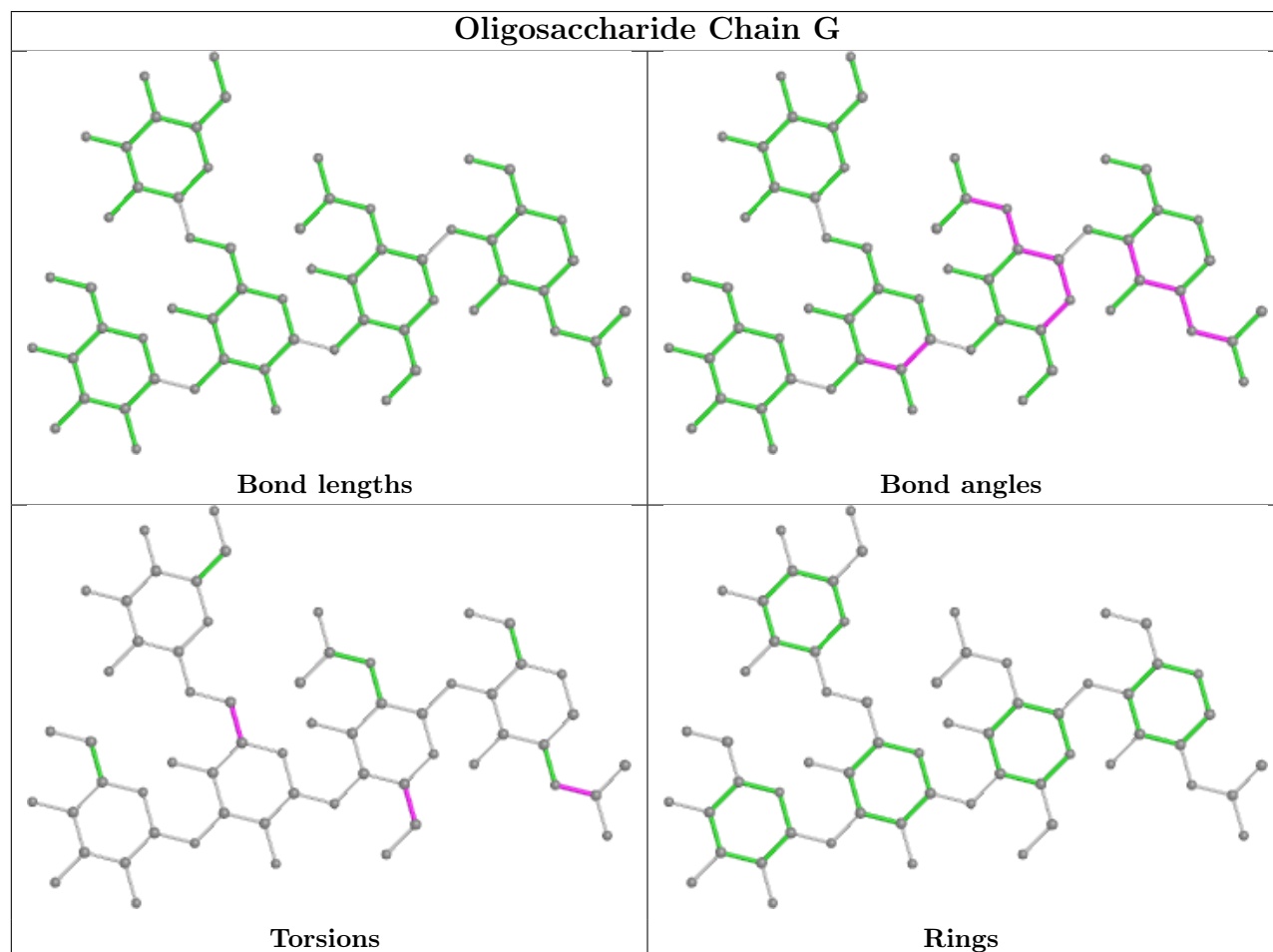
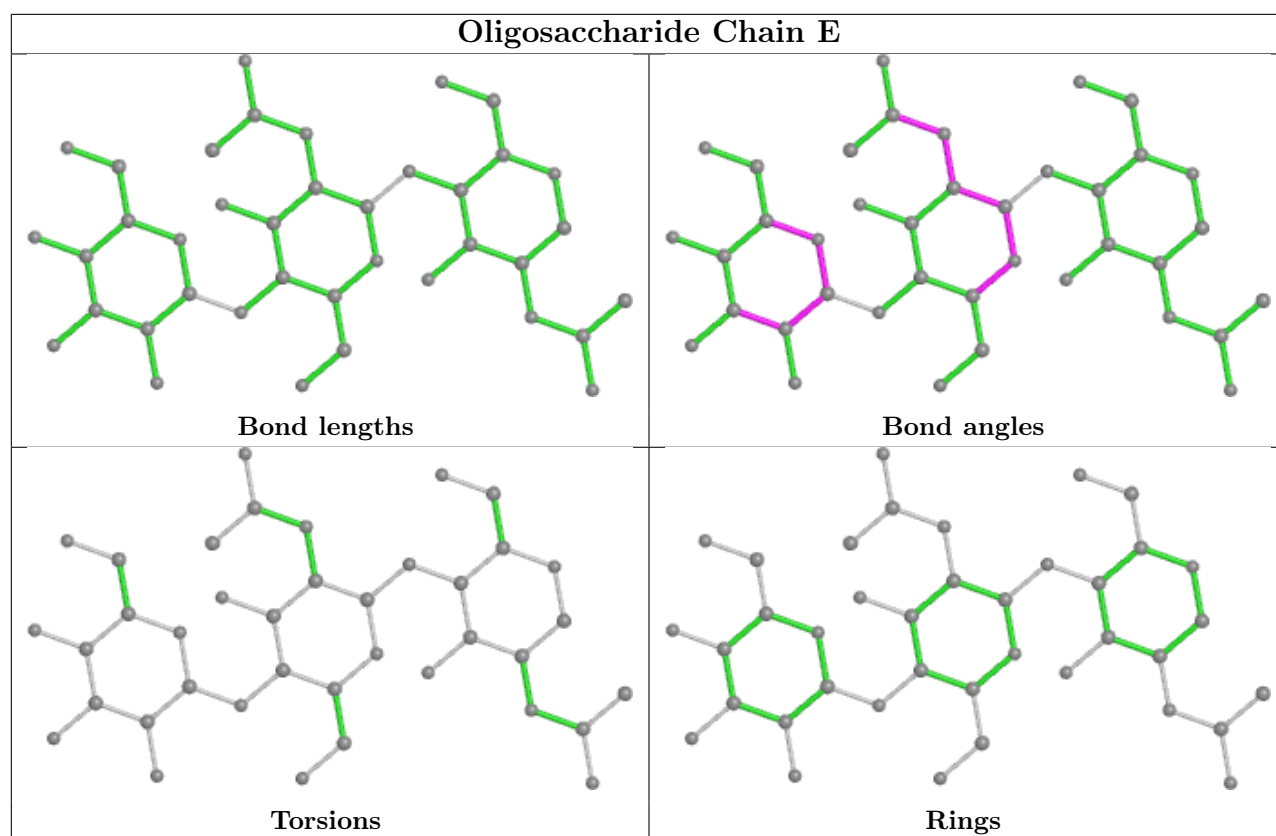
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2	NAG	2	0
7	G	1	NAG	1	0
5	F	1	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry

Of 29 ligands modelled in this entry, 16 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
9	A2G	B	4705	2	14,14,15	0.40	0	17,19,21	0.53	0
9	A2G	B	4710	2	14,14,15	0.40	0	17,19,21	0.79	1 (5%)
9	A2G	B	4704	2	14,14,15	0.44	0	17,19,21	0.87	1 (5%)
9	A2G	B	4707	-	14,14,15	0.40	0	17,19,21	1.68	3 (17%)
9	A2G	B	4706	-	14,14,15	0.39	0	17,19,21	2.02	3 (17%)
9	A2G	B	4708	2	14,14,15	0.40	0	17,19,21	1.11	1 (5%)
8	NAG	A	4702	2	14,14,15	0.40	0	17,19,21	1.05	2 (11%)
9	A2G	A	4703	2	14,14,15	0.42	0	17,19,21	0.69	1 (5%)
8	NAG	B	4702	2	14,14,15	0.38	0	17,19,21	1.18	2 (11%)
9	A2G	B	4703	2	14,14,15	0.41	0	17,19,21	0.73	0
9	A2G	B	4709	2	14,14,15	0.40	0	17,19,21	0.42	0
8	NAG	B	4701	2	14,14,15	0.30	0	17,19,21	0.64	0
8	NAG	A	4701	2	14,14,15	0.37	0	17,19,21	1.28	3 (17%)

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
9	A2G	B	4705	2	-	0/6/23/26	0/1/1/1
9	A2G	B	4710	2	-	1/6/23/26	0/1/1/1
9	A2G	B	4704	2	-	0/6/23/26	0/1/1/1
9	A2G	B	4707	-	-	1/6/23/26	0/1/1/1
9	A2G	B	4706	-	-	0/6/23/26	0/1/1/1
9	A2G	B	4708	2	-	2/6/23/26	0/1/1/1
8	NAG	A	4702	2	-	0/6/23/26	0/1/1/1
9	A2G	A	4703	2	-	2/6/23/26	0/1/1/1
8	NAG	B	4702	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A2G	B	4703	2	-	3/6/23/26	0/1/1/1
9	A2G	B	4709	2	-	1/6/23/26	0/1/1/1
8	NAG	B	4701	2	-	3/6/23/26	0/1/1/1
8	NAG	A	4701	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	4706	A2G	O5-C1-C2	7.42	123.01	111.29
9	B	4707	A2G	O5-C1-C2	6.06	120.86	111.29
9	B	4708	A2G	O5-C1-C2	3.98	117.58	111.29
9	B	4704	A2G	O5-C1-C2	-3.24	106.18	111.29
8	B	4702	NAG	C1-O5-C5	-3.16	107.91	112.19
8	B	4702	NAG	O5-C5-C6	3.07	112.02	107.20
9	B	4706	A2G	C1-O5-C5	2.99	116.24	112.19
8	A	4702	NAG	O5-C1-C2	-2.65	107.10	111.29
9	B	4707	A2G	C1-C2-N2	2.31	114.43	110.49
8	A	4702	NAG	O5-C5-C6	2.28	110.79	107.20
8	A	4701	NAG	C2-N2-C7	2.21	126.05	122.90
8	A	4701	NAG	O5-C1-C2	-2.18	107.84	111.29
9	B	4707	A2G	C1-O5-C5	2.16	115.11	112.19
9	B	4710	A2G	O5-C1-C2	2.08	114.57	111.29
9	A	4703	A2G	O5-C1-C2	-2.06	108.04	111.29
9	B	4706	A2G	C1-C2-N2	2.02	113.94	110.49
8	A	4701	NAG	C1-C2-N2	2.02	113.93	110.49

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	4702	NAG	C8-C7-N2-C2
8	B	4702	NAG	O7-C7-N2-C2
8	B	4701	NAG	C8-C7-N2-C2
9	B	4703	A2G	C1-C2-N2-C7
8	B	4701	NAG	O7-C7-N2-C2
8	B	4702	NAG	C1-C2-N2-C7
8	B	4701	NAG	C1-C2-N2-C7
9	B	4708	A2G	C1-C2-N2-C7
8	B	4702	NAG	O5-C5-C6-O6
9	B	4710	A2G	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	B	4709	A2G	O5-C5-C6-O6
9	B	4707	A2G	O5-C5-C6-O6
9	B	4703	A2G	O5-C5-C6-O6
8	A	4701	NAG	C3-C2-N2-C7
9	A	4703	A2G	C3-C2-N2-C7
9	B	4703	A2G	C3-C2-N2-C7
9	B	4708	A2G	C3-C2-N2-C7
9	A	4703	A2G	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	4710	A2G	1	0
9	B	4707	A2G	2	0
9	B	4706	A2G	4	0
8	A	4702	NAG	1	0

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.

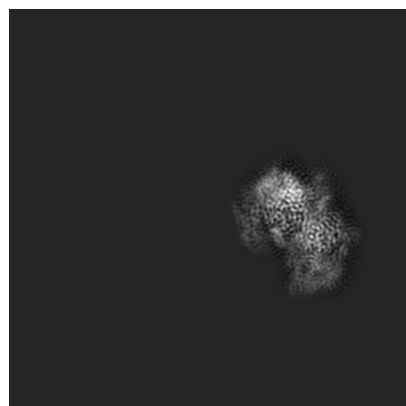
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36701. These allow visual inspection of the internal detail of the map and identification of artifacts.

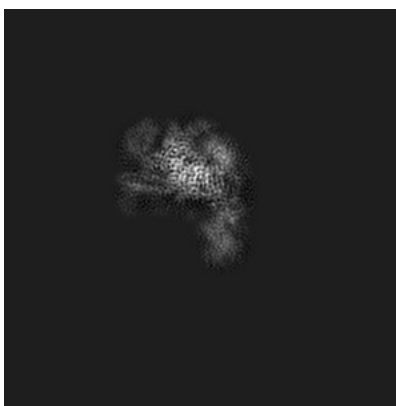
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

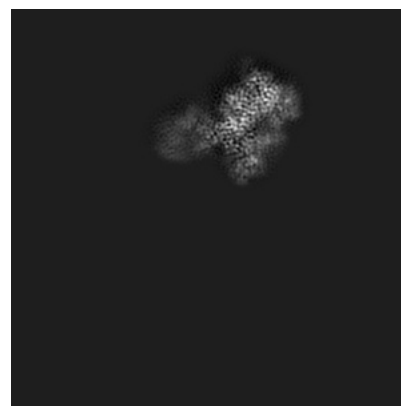
6.1.1 Primary map



X

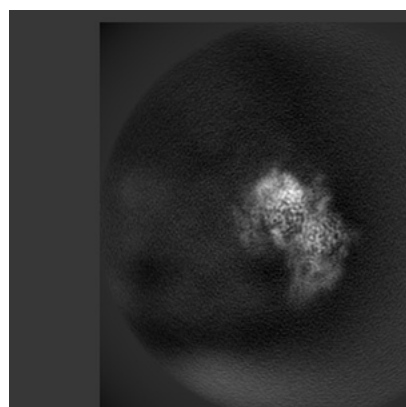


Y

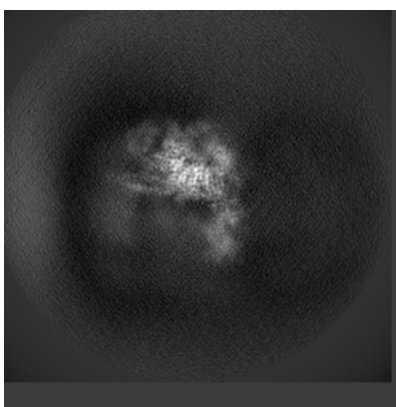


Z

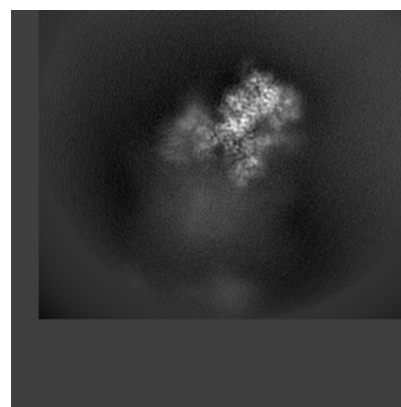
6.1.2 Raw map



X



Y

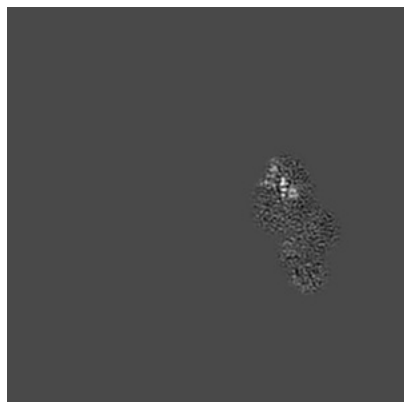


Z

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

6.2 Central slices [i](#)

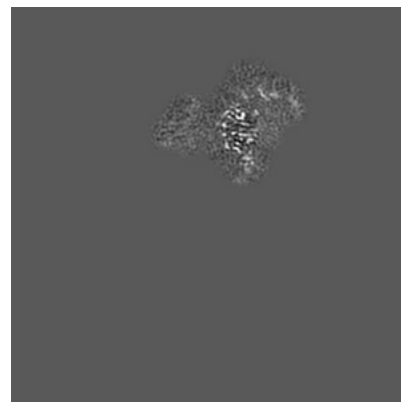
6.2.1 Primary map



X Index: 130

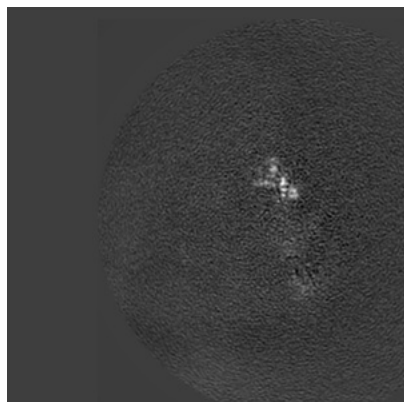


Y Index: 130

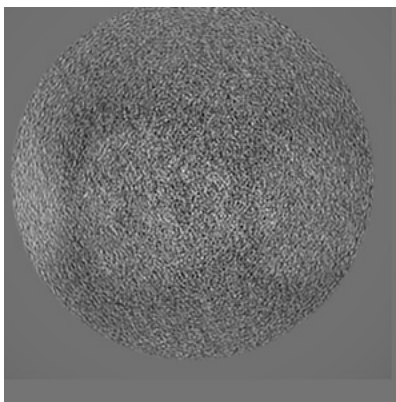


Z Index: 130

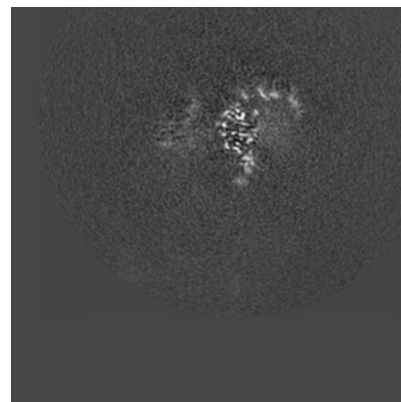
6.2.2 Raw map



X Index: 130



Y Index: 130

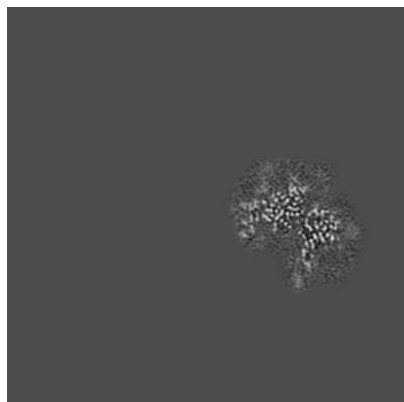


Z Index: 130

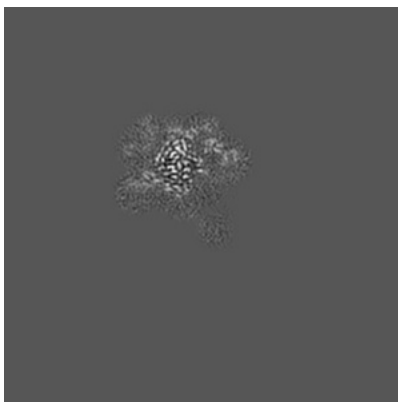
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

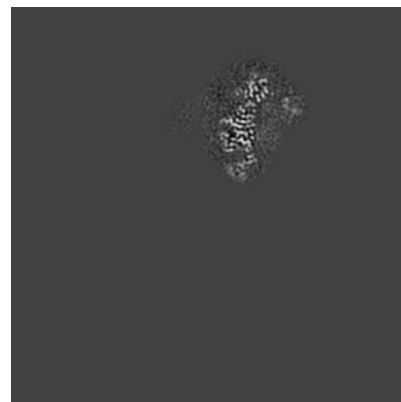
6.3.1 Primary map



X Index: 153

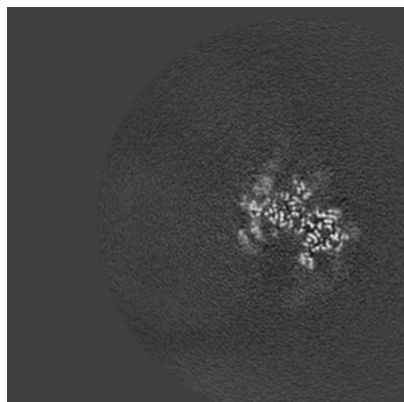


Y Index: 200

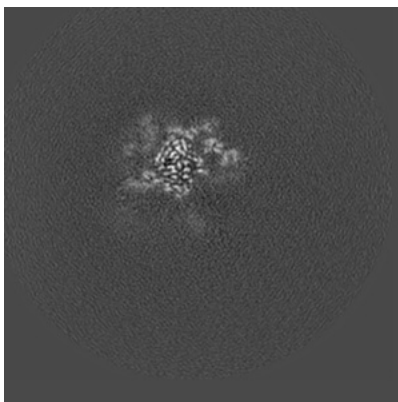


Z Index: 124

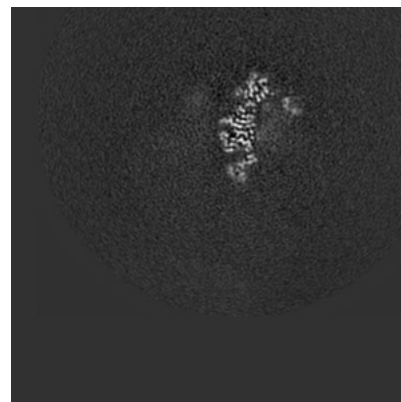
6.3.2 Raw map



X Index: 156



Y Index: 200

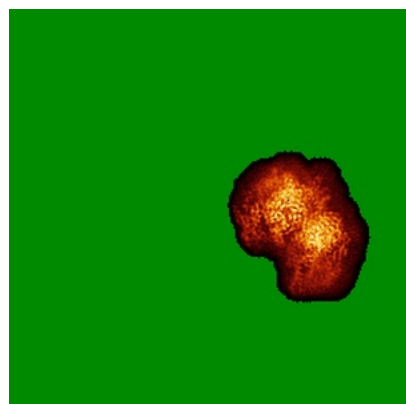


Z Index: 124

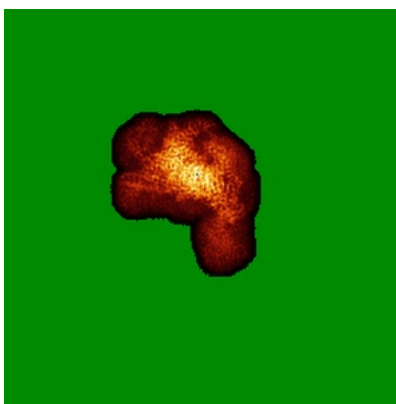
The images above show the largest variance slices of the map in three orthogonal directions.

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

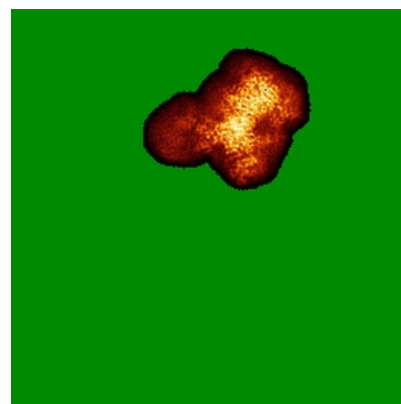
6.4.1 Primary map



X

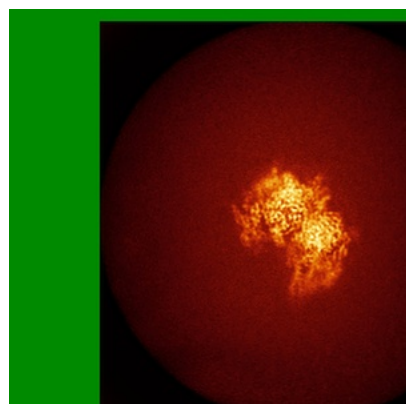


Y

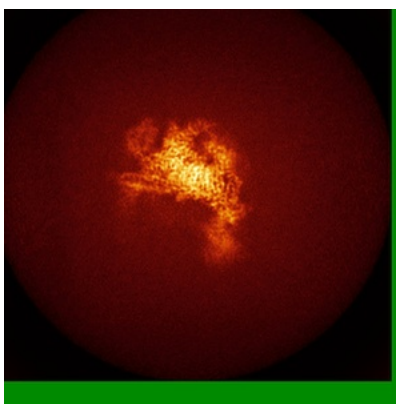


Z

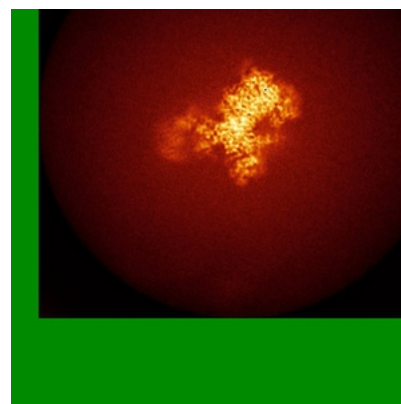
6.4.2 Raw map



X



Y

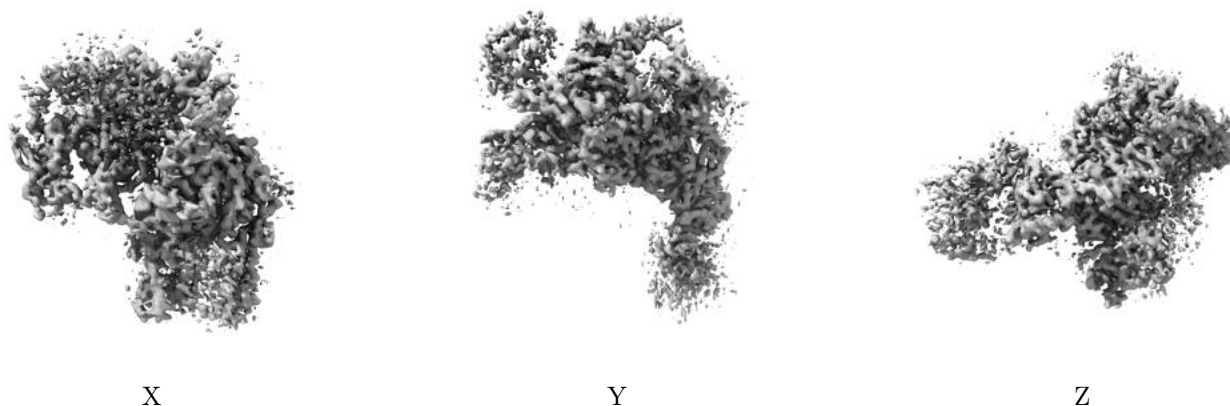


Z

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.

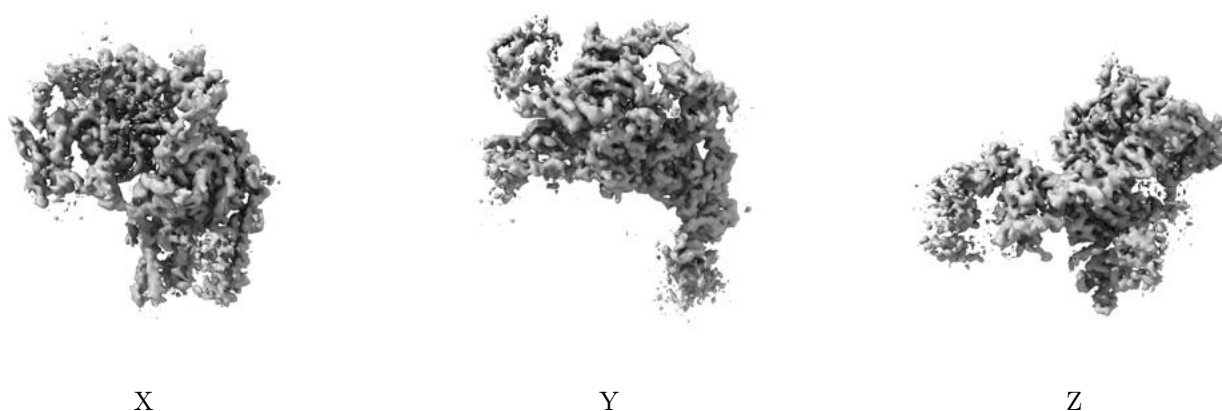
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.029. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

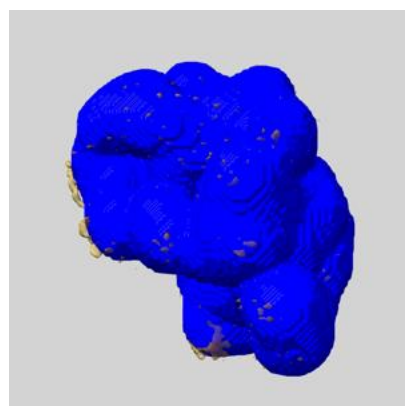
6.6 Mask visualisation [i](#)

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

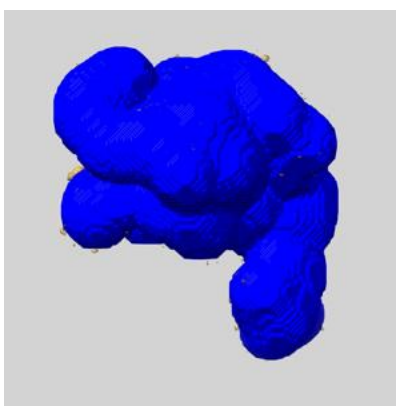
A mask typically either:

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

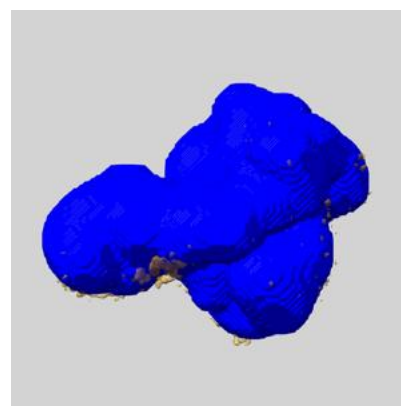
6.6.1 emd_36701_msk_1.map [i](#)



X



Y

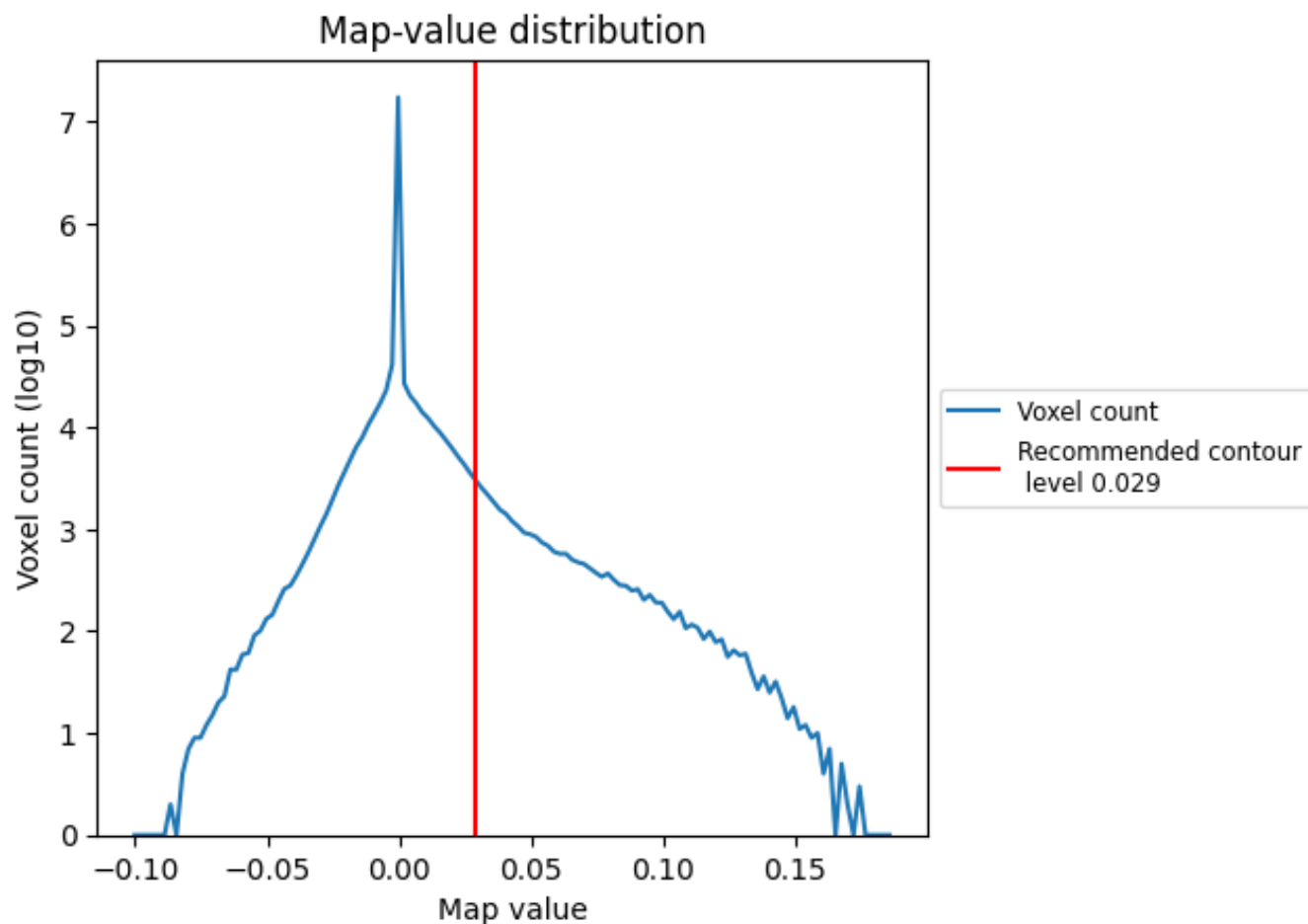


Z

7 Map analysis [i](#)

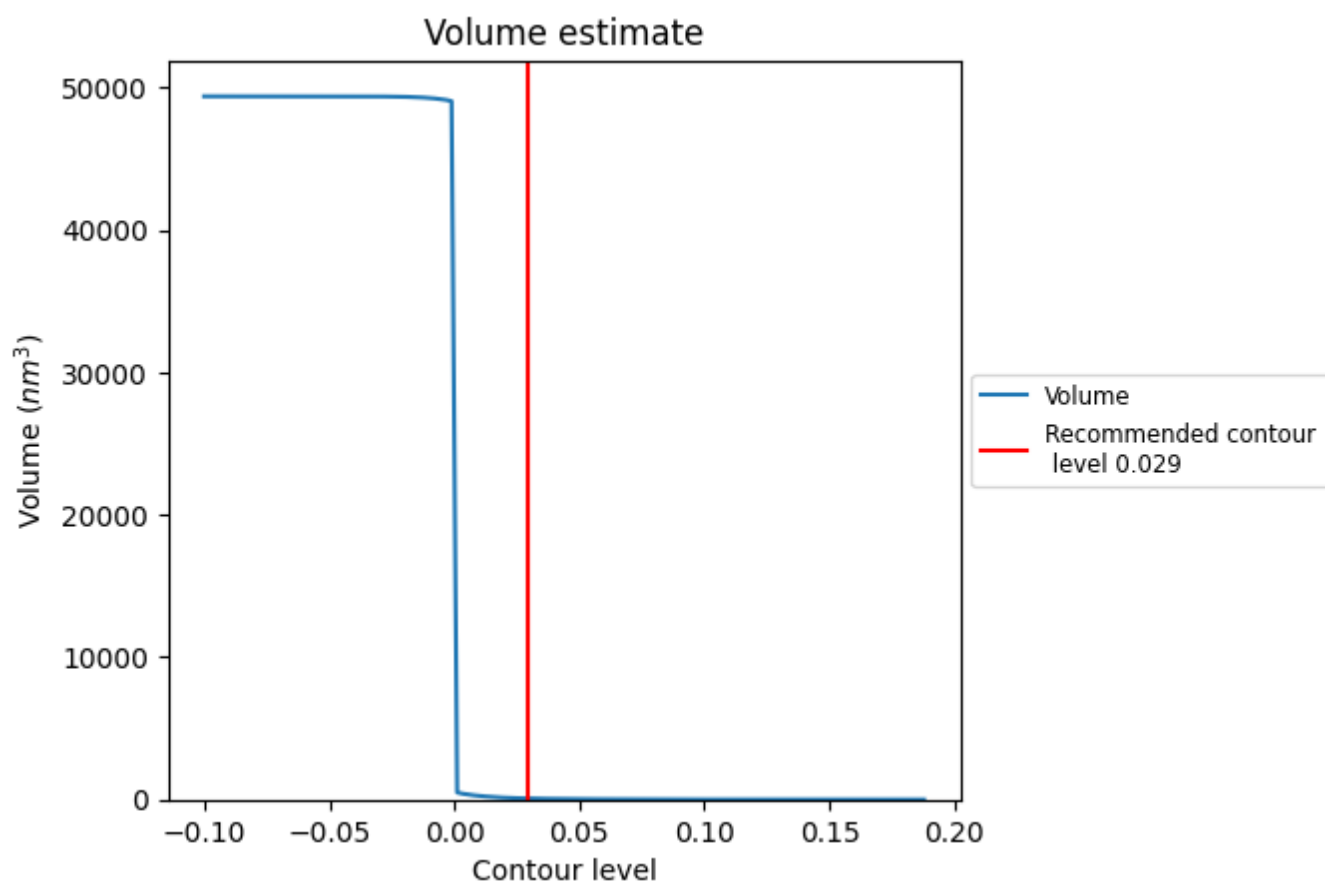
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

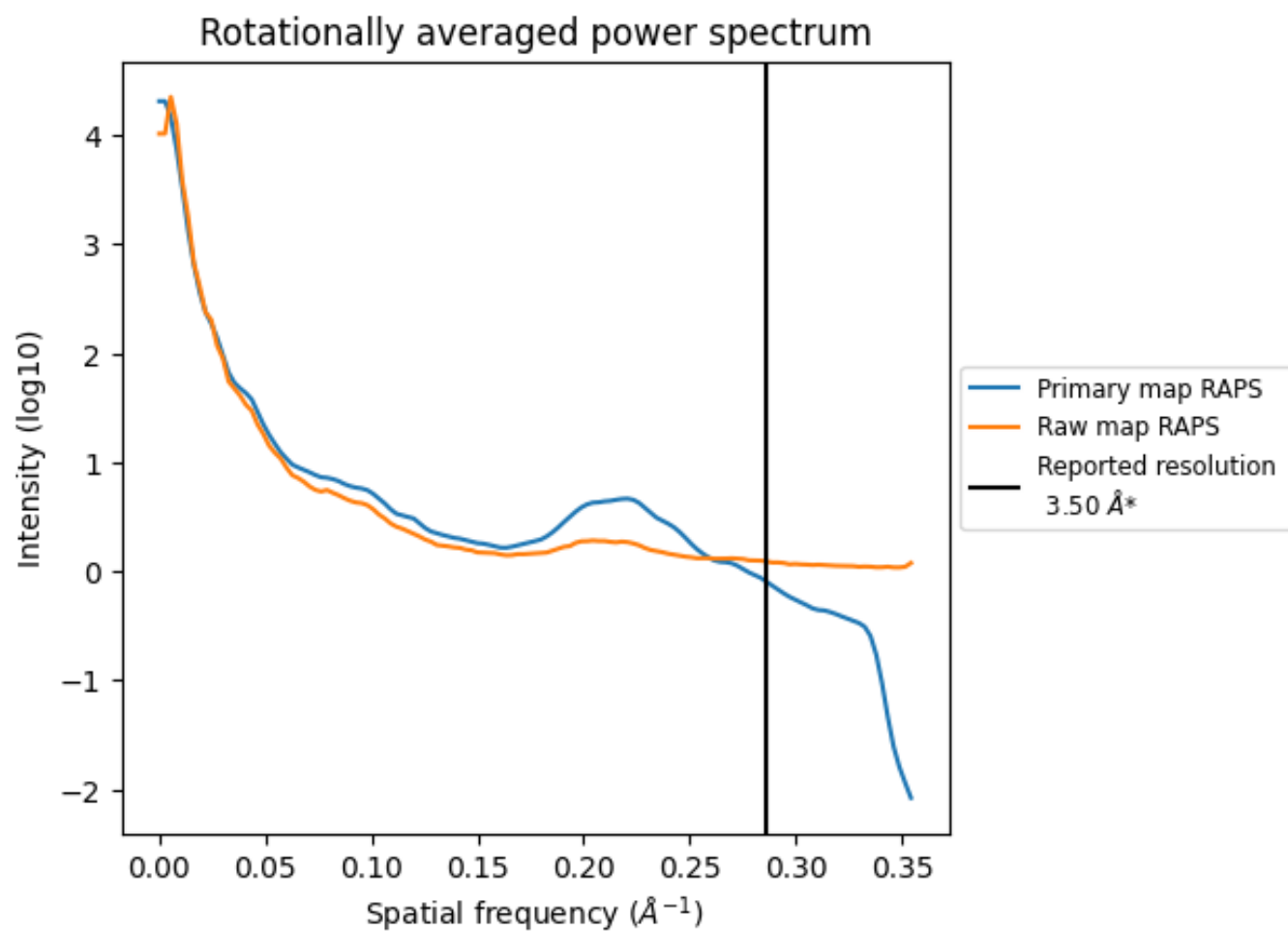
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm^3 ; this corresponds to an approximate mass of 70 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 ⓘ

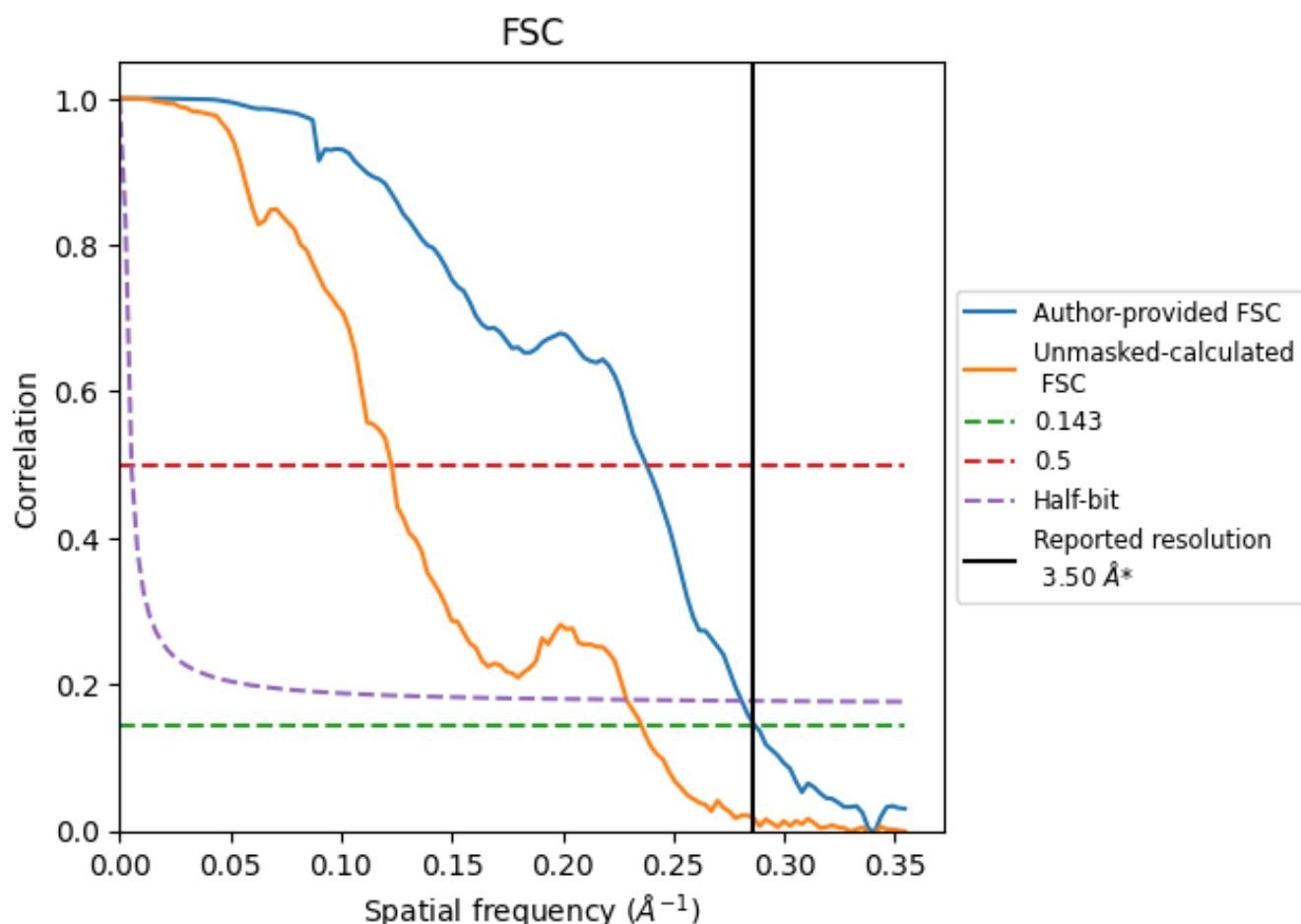


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

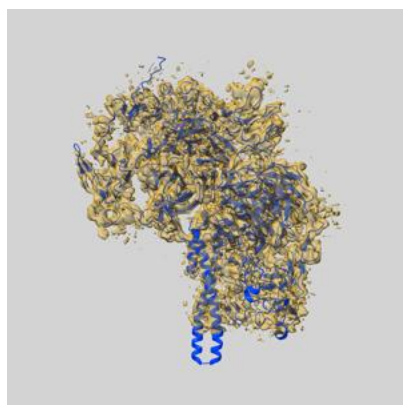
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.21	3.56
Unmasked-calculated*	4.24	8.15	4.37

*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 4.24 differs from the reported value 3.5 by more than 10 %

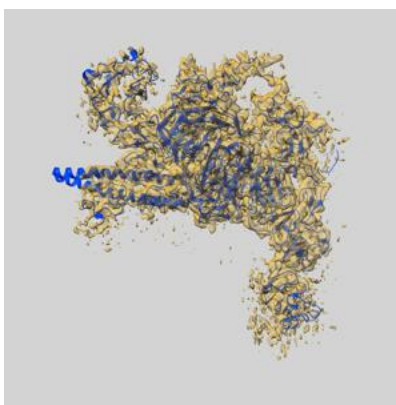
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36701 and PDB model 8JXH. Per-residue inclusion information can be found in section [3](#) on page [8](#).

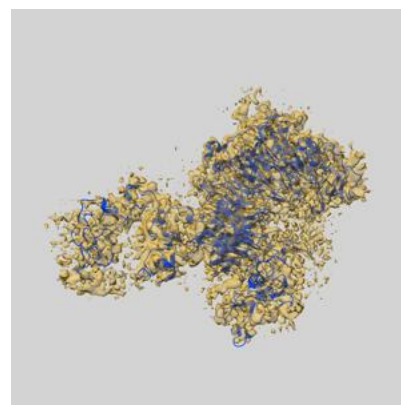
9.1 Map-model overlay [i](#)



X



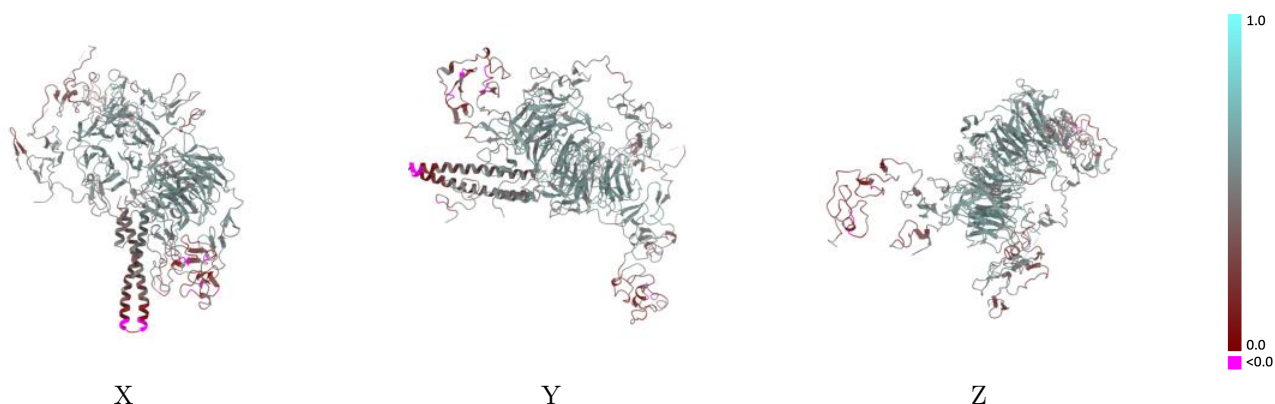
Y



Z

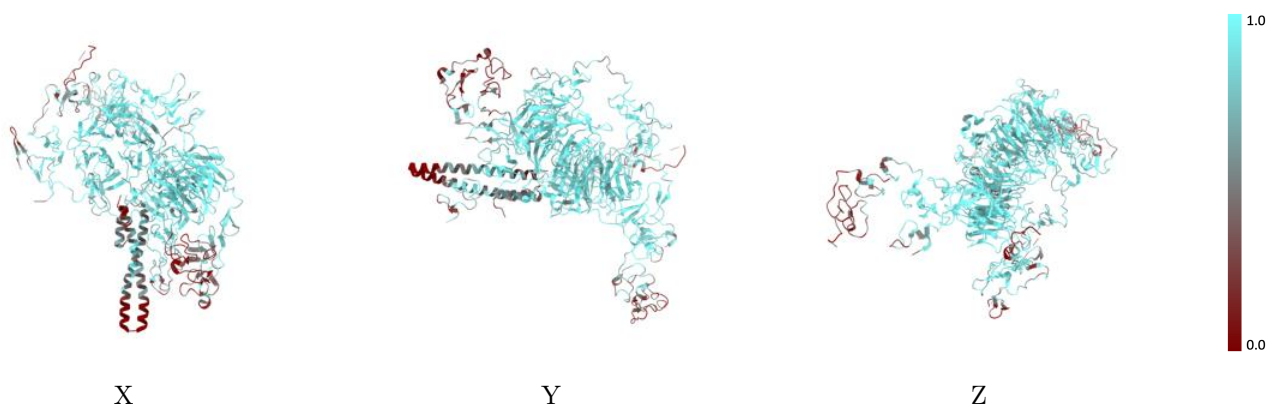
The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



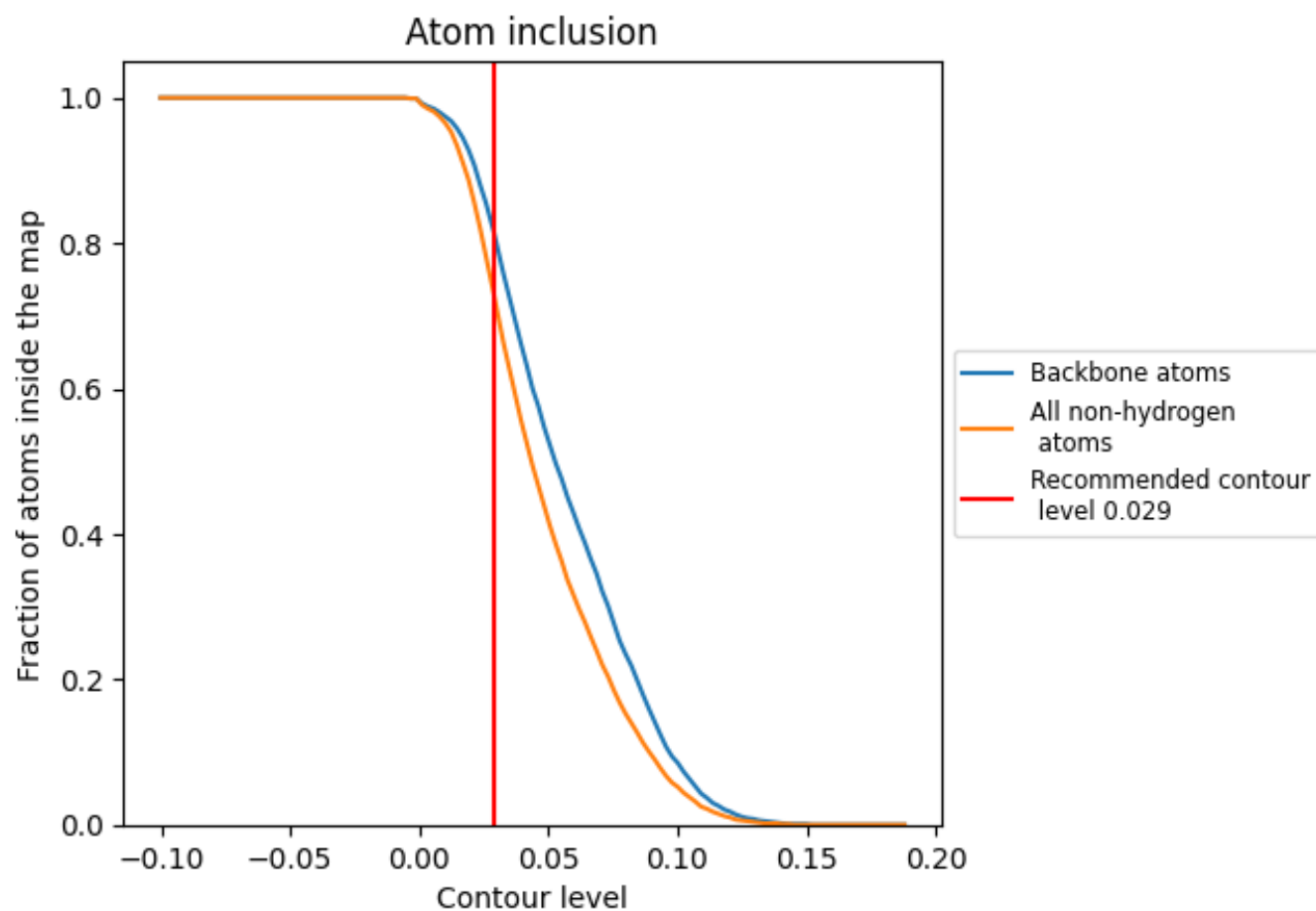
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.029).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7280	<div></div> 0.4720
A	<div></div> 0.5770	<div></div> 0.3550
B	<div></div> 0.7800	<div></div> 0.5000
C	<div></div> 0.5360	<div></div> 0.3450
D	<div></div> 0.4330	<div></div> 0.3610
E	<div></div> 0.6920	<div></div> 0.4500
F	<div></div> 0.1790	<div></div> 0.1630
G	<div></div> 0.3770	<div></div> 0.3750
Q	<div></div> 0.9000	<div></div> 0.5590
R	<div></div> 0.9290	<div></div> 0.5520

1.0

0.0

<0.0