



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 04:12 AM EST

PDB ID : 7UWL
EMDB ID : EMD-26835
Title : Structure of the IL-25-IL-17RB-IL-17RA ternary complex
Authors : Wilson, S.C.; Caveney, N.A.; Jude, K.M.; Garcia, K.C.
Deposited on : 2022-05-03
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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

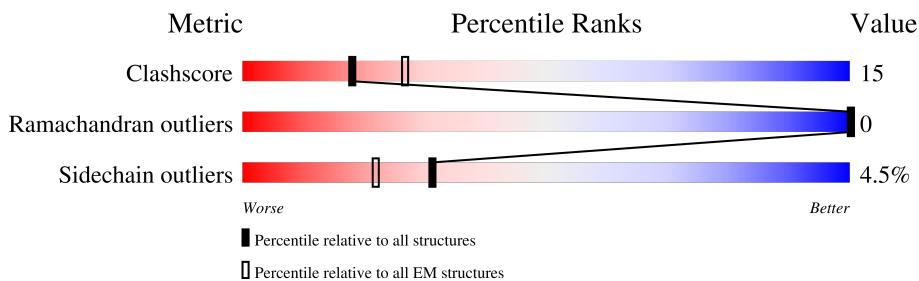
1 Overall quality at a glance i

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.




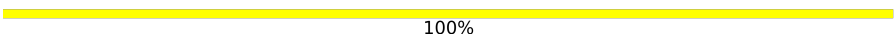
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	188	
1	B	188	
2	C	305	
2	D	305	
3	E	319	
3	F	319	
4	G	2	
4	H	2	

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Mol	Chain	Length	Quality of chain
4	I	2	 50% 50%
4	J	2	 100%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10100 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 Interleukin-25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	96	774	475	154	136	9	0	0
1	B	96	774	475	154	136	9	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ASP	-	expression tag	UNP Q9H293
A	27	ALA	-	expression tag	UNP Q9H293
A	28	SER	-	expression tag	UNP Q9H293
A	29	ALA	-	expression tag	UNP Q9H293
A	178	ALA	-	expression tag	UNP Q9H293
A	179	PRO	-	expression tag	UNP Q9H293
A	180	ALA	-	expression tag	UNP Q9H293
A	181	ALA	-	expression tag	UNP Q9H293
A	182	LEU	-	expression tag	UNP Q9H293
A	183	GLU	-	expression tag	UNP Q9H293
A	184	VAL	-	expression tag	UNP Q9H293
A	185	LEU	-	expression tag	UNP Q9H293
A	186	PHE	-	expression tag	UNP Q9H293
A	187	GLN	-	expression tag	UNP Q9H293
A	188	GLY	-	expression tag	UNP Q9H293
A	189	PRO	-	expression tag	UNP Q9H293
A	190	GLY	-	expression tag	UNP Q9H293
A	191	ALA	-	expression tag	UNP Q9H293
A	192	ALA	-	expression tag	UNP Q9H293
A	193	GLY	-	expression tag	UNP Q9H293
A	194	LEU	-	expression tag	UNP Q9H293
A	195	ASN	-	expression tag	UNP Q9H293
A	196	ASP	-	expression tag	UNP Q9H293
A	197	ILE	-	expression tag	UNP Q9H293
A	198	PHE	-	expression tag	UNP Q9H293
A	199	GLU	-	expression tag	UNP Q9H293

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Chain	Residue	Modelled	Actual	Comment	Reference
A	200	ALA	-	expression tag	UNP Q9H293
A	201	GLN	-	expression tag	UNP Q9H293
A	202	LYS	-	expression tag	UNP Q9H293
A	203	ILE	-	expression tag	UNP Q9H293
A	204	GLU	-	expression tag	UNP Q9H293
A	205	TRP	-	expression tag	UNP Q9H293
A	206	HIS	-	expression tag	UNP Q9H293
A	207	GLU	-	expression tag	UNP Q9H293
A	208	HIS	-	expression tag	UNP Q9H293
A	209	HIS	-	expression tag	UNP Q9H293
A	210	HIS	-	expression tag	UNP Q9H293
A	211	HIS	-	expression tag	UNP Q9H293
A	212	HIS	-	expression tag	UNP Q9H293
A	213	HIS	-	expression tag	UNP Q9H293
B	26	ASP	-	expression tag	UNP Q9H293
B	27	ALA	-	expression tag	UNP Q9H293
B	28	SER	-	expression tag	UNP Q9H293
B	29	ALA	-	expression tag	UNP Q9H293
B	178	ALA	-	expression tag	UNP Q9H293
B	179	PRO	-	expression tag	UNP Q9H293
B	180	ALA	-	expression tag	UNP Q9H293
B	181	ALA	-	expression tag	UNP Q9H293
B	182	LEU	-	expression tag	UNP Q9H293
B	183	GLU	-	expression tag	UNP Q9H293
B	184	VAL	-	expression tag	UNP Q9H293
B	185	LEU	-	expression tag	UNP Q9H293
B	186	PHE	-	expression tag	UNP Q9H293
B	187	GLN	-	expression tag	UNP Q9H293
B	188	GLY	-	expression tag	UNP Q9H293
B	189	PRO	-	expression tag	UNP Q9H293
B	190	GLY	-	expression tag	UNP Q9H293
B	191	ALA	-	expression tag	UNP Q9H293
B	192	ALA	-	expression tag	UNP Q9H293
B	193	GLY	-	expression tag	UNP Q9H293
B	194	LEU	-	expression tag	UNP Q9H293
B	195	ASN	-	expression tag	UNP Q9H293
B	196	ASP	-	expression tag	UNP Q9H293
B	197	ILE	-	expression tag	UNP Q9H293
B	198	PHE	-	expression tag	UNP Q9H293
B	199	GLU	-	expression tag	UNP Q9H293
B	200	ALA	-	expression tag	UNP Q9H293
B	201	GLN	-	expression tag	UNP Q9H293

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Chain	Residue	Modelled	Actual	Comment	Reference
B	202	LYS	-	expression tag	UNP Q9H293
B	203	ILE	-	expression tag	UNP Q9H293
B	204	GLU	-	expression tag	UNP Q9H293
B	205	TRP	-	expression tag	UNP Q9H293
B	206	HIS	-	expression tag	UNP Q9H293
B	207	GLU	-	expression tag	UNP Q9H293
B	208	HIS	-	expression tag	UNP Q9H293
B	209	HIS	-	expression tag	UNP Q9H293
B	210	HIS	-	expression tag	UNP Q9H293
B	211	HIS	-	expression tag	UNP Q9H293
B	212	HIS	-	expression tag	UNP Q9H293
B	213	HIS	-	expression tag	UNP Q9H293

- Molecule 2 is a protein called Interleukin-17 receptor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	250	1931	1222	329	364	16	0	0
2	D	252	1947	1231	332	368	16	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	289	ALA	-	expression tag	UNP Q9NRM6
C	290	ALA	-	expression tag	UNP Q9NRM6
C	291	ALA	-	expression tag	UNP Q9NRM6
C	292	LEU	-	expression tag	UNP Q9NRM6
C	293	GLU	-	expression tag	UNP Q9NRM6
C	294	VAL	-	expression tag	UNP Q9NRM6
C	295	LEU	-	expression tag	UNP Q9NRM6
C	296	PHE	-	expression tag	UNP Q9NRM6
C	297	GLN	-	expression tag	UNP Q9NRM6
C	298	GLY	-	expression tag	UNP Q9NRM6
C	299	PRO	-	expression tag	UNP Q9NRM6
C	300	GLY	-	expression tag	UNP Q9NRM6
C	301	ALA	-	expression tag	UNP Q9NRM6
C	302	ALA	-	expression tag	UNP Q9NRM6
C	303	GLU	-	expression tag	UNP Q9NRM6
C	304	ASP	-	expression tag	UNP Q9NRM6
C	305	GLN	-	expression tag	UNP Q9NRM6
C	306	VAL	-	expression tag	UNP Q9NRM6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	307	ASP	-	expression tag	UNP Q9NRM6
C	308	PRO	-	expression tag	UNP Q9NRM6
C	309	ARG	-	expression tag	UNP Q9NRM6
C	310	LEU	-	expression tag	UNP Q9NRM6
C	311	ILE	-	expression tag	UNP Q9NRM6
C	312	ASP	-	expression tag	UNP Q9NRM6
C	313	GLY	-	expression tag	UNP Q9NRM6
C	314	LYS	-	expression tag	UNP Q9NRM6
C	315	HIS	-	expression tag	UNP Q9NRM6
C	316	HIS	-	expression tag	UNP Q9NRM6
C	317	HIS	-	expression tag	UNP Q9NRM6
C	318	HIS	-	expression tag	UNP Q9NRM6
C	319	HIS	-	expression tag	UNP Q9NRM6
C	320	HIS	-	expression tag	UNP Q9NRM6
C	321	HIS	-	expression tag	UNP Q9NRM6
C	322	HIS	-	expression tag	UNP Q9NRM6
D	289	ALA	-	expression tag	UNP Q9NRM6
D	290	ALA	-	expression tag	UNP Q9NRM6
D	291	ALA	-	expression tag	UNP Q9NRM6
D	292	LEU	-	expression tag	UNP Q9NRM6
D	293	GLU	-	expression tag	UNP Q9NRM6
D	294	VAL	-	expression tag	UNP Q9NRM6
D	295	LEU	-	expression tag	UNP Q9NRM6
D	296	PHE	-	expression tag	UNP Q9NRM6
D	297	GLN	-	expression tag	UNP Q9NRM6
D	298	GLY	-	expression tag	UNP Q9NRM6
D	299	PRO	-	expression tag	UNP Q9NRM6
D	300	GLY	-	expression tag	UNP Q9NRM6
D	301	ALA	-	expression tag	UNP Q9NRM6
D	302	ALA	-	expression tag	UNP Q9NRM6
D	303	GLU	-	expression tag	UNP Q9NRM6
D	304	ASP	-	expression tag	UNP Q9NRM6
D	305	GLN	-	expression tag	UNP Q9NRM6
D	306	VAL	-	expression tag	UNP Q9NRM6
D	307	ASP	-	expression tag	UNP Q9NRM6
D	308	PRO	-	expression tag	UNP Q9NRM6
D	309	ARG	-	expression tag	UNP Q9NRM6
D	310	LEU	-	expression tag	UNP Q9NRM6
D	311	ILE	-	expression tag	UNP Q9NRM6
D	312	ASP	-	expression tag	UNP Q9NRM6
D	313	GLY	-	expression tag	UNP Q9NRM6
D	314	LYS	-	expression tag	UNP Q9NRM6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	315	HIS	-	expression tag	UNP Q9NRM6
D	316	HIS	-	expression tag	UNP Q9NRM6
D	317	HIS	-	expression tag	UNP Q9NRM6
D	318	HIS	-	expression tag	UNP Q9NRM6
D	319	HIS	-	expression tag	UNP Q9NRM6
D	320	HIS	-	expression tag	UNP Q9NRM6
D	321	HIS	-	expression tag	UNP Q9NRM6
D	322	HIS	-	expression tag	UNP Q9NRM6

- Molecule 3 is a protein called Interleukin-17 receptor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	271	Total	C	N	O	S	0	0
			2180	1372	399	394	15		
3	F	271	Total	C	N	O	S	0	0
			2186	1375	402	394	15		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	318	SER	-	expression tag	UNP Q96F46
E	319	ALA	-	expression tag	UNP Q96F46
E	320	ALA	-	expression tag	UNP Q96F46
E	321	LEU	-	expression tag	UNP Q96F46
E	322	GLU	-	expression tag	UNP Q96F46
E	323	VAL	-	expression tag	UNP Q96F46
E	324	LEU	-	expression tag	UNP Q96F46
E	325	PHE	-	expression tag	UNP Q96F46
E	326	GLN	-	expression tag	UNP Q96F46
E	327	GLY	-	expression tag	UNP Q96F46
E	328	PRO	-	expression tag	UNP Q96F46
E	329	GLY	-	expression tag	UNP Q96F46
E	330	ALA	-	expression tag	UNP Q96F46
E	331	ALA	-	expression tag	UNP Q96F46
E	332	GLU	-	expression tag	UNP Q96F46
E	333	ASP	-	expression tag	UNP Q96F46
E	334	GLN	-	expression tag	UNP Q96F46
E	335	VAL	-	expression tag	UNP Q96F46
E	336	ASP	-	expression tag	UNP Q96F46
E	337	PRO	-	expression tag	UNP Q96F46
E	338	ARG	-	expression tag	UNP Q96F46
E	339	LEU	-	expression tag	UNP Q96F46

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Chain	Residue	Modelled	Actual	Comment	Reference
E	340	ILE	-	expression tag	UNP Q96F46
E	341	ASP	-	expression tag	UNP Q96F46
E	342	GLY	-	expression tag	UNP Q96F46
E	343	LYS	-	expression tag	UNP Q96F46
E	344	HIS	-	expression tag	UNP Q96F46
E	345	HIS	-	expression tag	UNP Q96F46
E	346	HIS	-	expression tag	UNP Q96F46
E	347	HIS	-	expression tag	UNP Q96F46
E	348	HIS	-	expression tag	UNP Q96F46
E	349	HIS	-	expression tag	UNP Q96F46
E	350	HIS	-	expression tag	UNP Q96F46
E	351	HIS	-	expression tag	UNP Q96F46
F	318	SER	-	expression tag	UNP Q96F46
F	319	ALA	-	expression tag	UNP Q96F46
F	320	ALA	-	expression tag	UNP Q96F46
F	321	LEU	-	expression tag	UNP Q96F46
F	322	GLU	-	expression tag	UNP Q96F46
F	323	VAL	-	expression tag	UNP Q96F46
F	324	LEU	-	expression tag	UNP Q96F46
F	325	PHE	-	expression tag	UNP Q96F46
F	326	GLN	-	expression tag	UNP Q96F46
F	327	GLY	-	expression tag	UNP Q96F46
F	328	PRO	-	expression tag	UNP Q96F46
F	329	GLY	-	expression tag	UNP Q96F46
F	330	ALA	-	expression tag	UNP Q96F46
F	331	ALA	-	expression tag	UNP Q96F46
F	332	GLU	-	expression tag	UNP Q96F46
F	333	ASP	-	expression tag	UNP Q96F46
F	334	GLN	-	expression tag	UNP Q96F46
F	335	VAL	-	expression tag	UNP Q96F46
F	336	ASP	-	expression tag	UNP Q96F46
F	337	PRO	-	expression tag	UNP Q96F46
F	338	ARG	-	expression tag	UNP Q96F46
F	339	LEU	-	expression tag	UNP Q96F46
F	340	ILE	-	expression tag	UNP Q96F46
F	341	ASP	-	expression tag	UNP Q96F46
F	342	GLY	-	expression tag	UNP Q96F46
F	343	LYS	-	expression tag	UNP Q96F46
F	344	HIS	-	expression tag	UNP Q96F46
F	345	HIS	-	expression tag	UNP Q96F46
F	346	HIS	-	expression tag	UNP Q96F46
F	347	HIS	-	expression tag	UNP Q96F46

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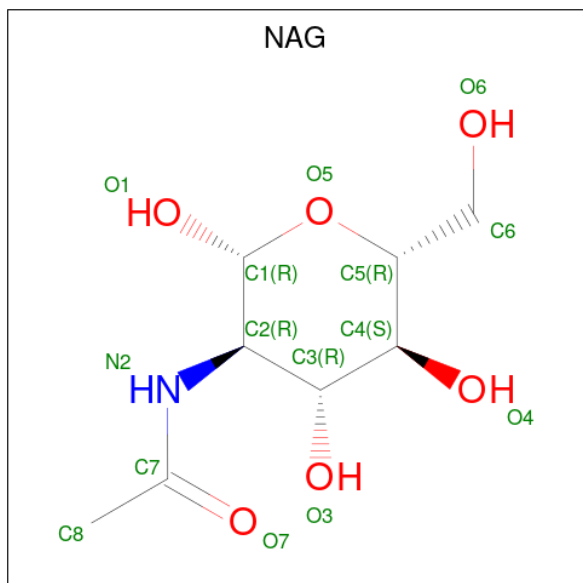
Chain	Residue	Modelled	Actual	Comment	Reference
F	348	HIS	-	expression tag	UNP Q96F46
F	349	HIS	-	expression tag	UNP Q96F46
F	350	HIS	-	expression tag	UNP Q96F46
F	351	HIS	-	expression tag	UNP Q96F46

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	G	2	Total 28	C 16	N 2	O 10	0	0
4	H	2	Total 28	C 16	N 2	O 10	0	0
4	I	2	Total 28	C 16	N 2	O 10	0	0
4	J	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).




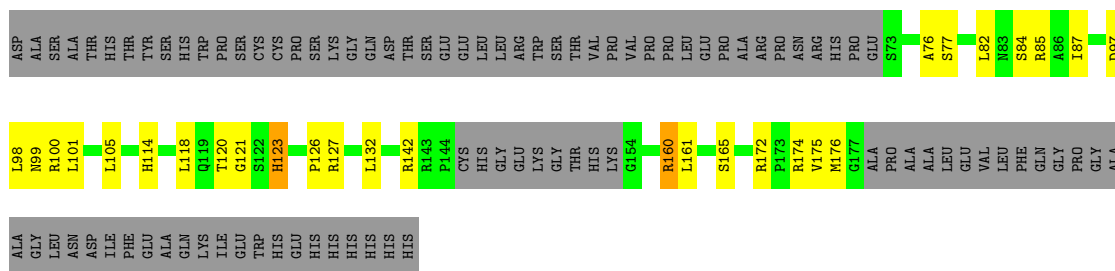
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			42	24	3	15	
5	C	1	Total	C	N	O	0
			42	24	3	15	
5	C	1	Total	C	N	O	0
			42	24	3	15	
5	D	1	Total	C	N	O	0
			42	24	3	15	
5	D	1	Total	C	N	O	0
			42	24	3	15	
5	D	1	Total	C	N	O	0
			42	24	3	15	
5	E	1	Total	C	N	O	0
			42	24	3	15	
5	E	1	Total	C	N	O	0
			42	24	3	15	
5	E	1	Total	C	N	O	0
			42	24	3	15	
5	F	1	Total	C	N	O	0
			42	24	3	15	
5	F	1	Total	C	N	O	0
			42	24	3	15	
5	F	1	Total	C	N	O	0
			42	24	3	15	

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.

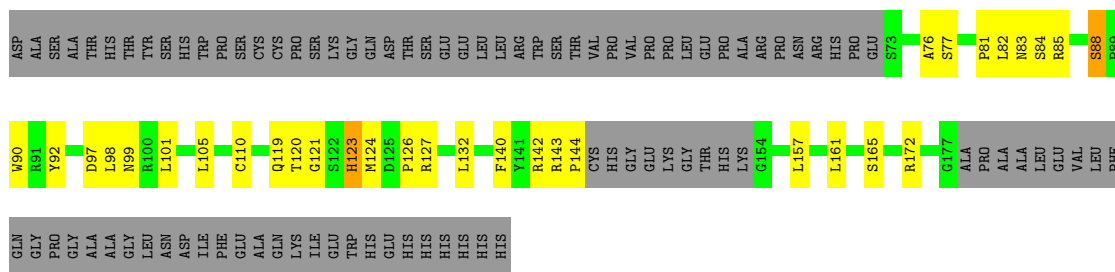
- Molecule 1: Interleukin-25

Chain A: 



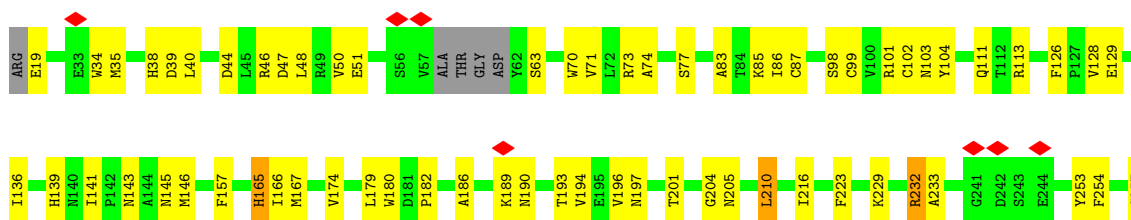
- Molecule 1: Interleukin-25

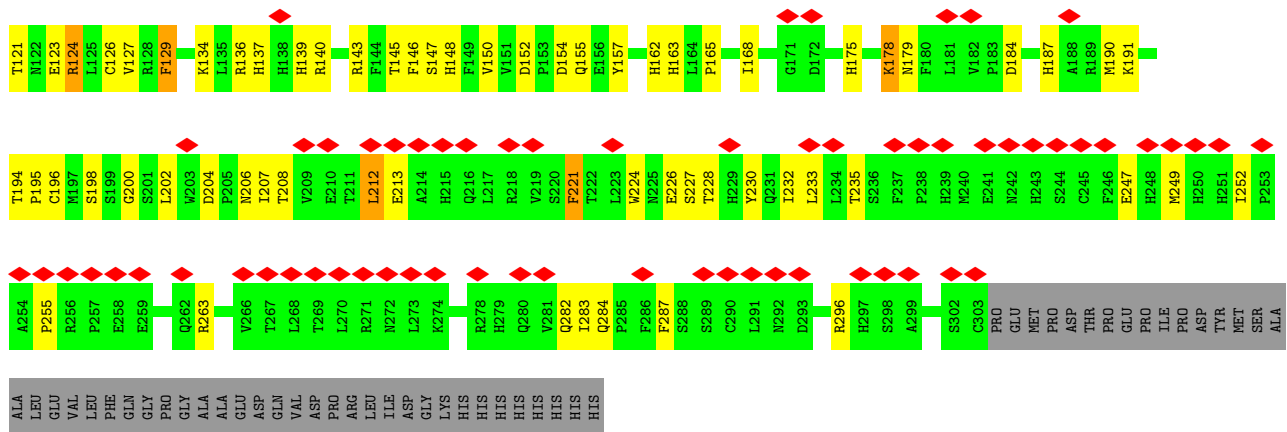
Chain B: 



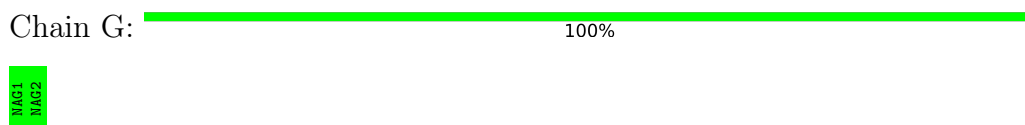
- Molecule 2: Interleukin-17 receptor B

Chain C: 





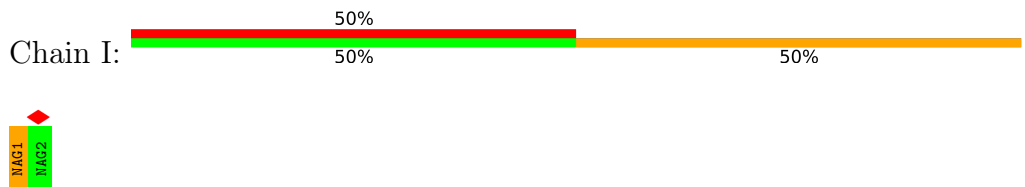
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



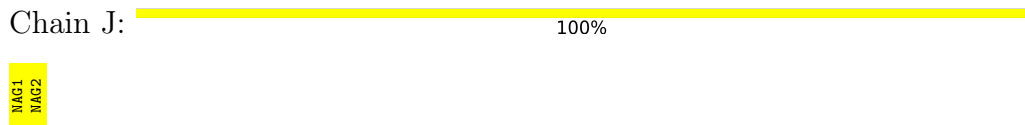
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	1287497	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.940	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	327.20642, 327.20642, 327.20642	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8521001, 0.8521001, 0.8521001	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: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/791	0.63	0/1069
1	B	0.29	0/791	0.59	0/1069
2	C	0.29	0/1978	0.54	0/2692
2	D	0.30	0/1994	0.55	0/2714
3	E	0.29	0/2245	0.54	0/3062
3	F	0.28	0/2251	0.55	0/3069
All	All	0.29	0/10050	0.56	0/13675

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	774	0	747	22	0
1	B	774	0	747	26	0
2	C	1931	0	1889	48	0
2	D	1947	0	1904	62	0
3	E	2180	0	2058	70	0
3	F	2186	0	2069	82	0
4	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	1	0
4	I	28	0	25	2	0
4	J	28	0	25	3	0
5	A	14	0	13	1	0
5	B	14	0	13	1	0
5	C	42	0	39	1	0
5	D	42	0	39	1	0
5	E	42	0	39	0	0
5	F	42	0	39	1	0
All	All	10100	0	9696	292	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 15.

All (292) 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)
3:F:178:LYS:HE3	3:F:179:ASN:H	1.20	1.07
3:F:39:ARG:HD3	3:F:40:ALA:N	1.79	0.97
3:E:212:LEU:HD13	3:E:213:GLU:H	1.30	0.94
3:F:39:ARG:HD3	3:F:40:ALA:H	1.31	0.92
3:E:99:THR:HG22	3:E:143:ARG:HH12	1.35	0.91
3:E:284:GLN:HG2	3:E:296:ARG:HG2	1.55	0.89
3:F:178:LYS:HE3	3:F:179:ASN:N	1.92	0.85
3:E:212:LEU:CD1	3:E:213:GLU:H	1.91	0.84
1:A:127:ARG:HH22	2:D:216:ILE:HG13	1.45	0.81
2:C:83:ALA:HB1	2:C:102:CYS:O	1.80	0.80
1:B:101:LEU:HD23	1:B:140:PHE:HB2	1.63	0.80
3:F:57:CYS:SG	3:F:124:ARG:NH1	2.56	0.79
3:F:230:TYR:HB3	3:F:283:ILE:HD11	1.64	0.79
1:B:83:ASN:HD22	1:B:92:TYR:HE2	1.31	0.79
1:A:97:ASP:OD1	1:A:98:LEU:N	2.17	0.78
1:B:127:ARG:HH22	2:C:216:ILE:HG13	1.48	0.78
3:E:231:GLN:HE21	3:E:284:GLN:CD	1.86	0.78
3:E:231:GLN:NE2	3:E:284:GLN:OE1	2.17	0.77
3:F:187:HIS:HB3	3:F:190:MET:HB2	1.64	0.77
2:C:87:CYS:HA	2:C:99:CYS:HB3	1.67	0.76
2:D:167:MET:HE1	2:D:170:LYS:HD3	1.67	0.75
1:B:99:ASN:HA	2:D:34:TRP:HZ2	1.51	0.75
3:E:231:GLN:NE2	3:E:284:GLN:CD	2.41	0.74
3:E:139:HIS:CE1	3:E:141:ARG:HB3	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:65:PRO:C	3:F:66:ARG:HD3	2.09	0.73
3:E:139:HIS:HE1	3:E:141:ARG:HB3	1.54	0.73
2:C:85:LYS:HG3	2:C:141:ILE:HD11	1.71	0.72
2:D:87:CYS:HA	2:D:99:CYS:HB2	1.70	0.72
3:E:34:ARG:HH12	3:E:36:LEU:HD13	1.55	0.71
3:F:45:GLN:NE2	3:F:143:ARG:O	2.24	0.71
2:C:165:HIS:CE1	2:C:166:ILE:HG12	2.26	0.71
3:E:123:GLU:OE1	3:E:124:ARG:N	2.25	0.70
3:F:284:GLN:HB3	3:F:296:ARG:HG2	1.73	0.70
2:D:46:ARG:HG3	2:D:73:ARG:HA	1.75	0.69
3:E:233:LEU:HD12	3:E:284:GLN:OE1	1.92	0.69
1:B:132:LEU:HD22	1:B:165:SER:HB2	1.73	0.69
2:D:20:PRO:HD2	2:D:113:ARG:HH12	1.58	0.68
1:A:132:LEU:HD22	1:A:165:SER:HB2	1.75	0.68
3:F:155:GLN:HB2	3:F:157:TYR:CE1	2.28	0.67
2:D:73:ARG:HB3	2:D:78:ILE:HD11	1.76	0.67
3:E:197:MET:SD	3:E:202:LEU:HD13	2.34	0.67
3:F:39:ARG:HH11	3:F:40:ALA:H	1.43	0.67
3:F:87:GLN:NE2	3:F:89:ASP:HB2	2.09	0.67
1:B:97:ASP:OD1	1:B:98:LEU:N	2.27	0.66
3:E:212:LEU:HD13	3:E:213:GLU:N	2.08	0.66
3:F:33:LEU:N	3:F:150:VAL:O	2.29	0.65
3:F:85:THR:OG1	3:F:89:ASP:O	2.14	0.65
3:F:228:THR:HG21	3:F:287:PHE:HA	1.78	0.65
3:E:231:GLN:HE21	3:E:284:GLN:CG	2.09	0.65
2:C:262:ILE:HD12	2:C:262:ILE:H	1.61	0.65
3:F:121:THR:HG23	3:F:123:GLU:H	1.61	0.65
1:A:87:ILE:HD11	1:A:118:LEU:HD23	1.79	0.65
1:B:161:LEU:HD21	5:B:301:NAG:H2	1.78	0.65
3:E:84:HIS:HA	3:E:90:LEU:HA	1.77	0.65
3:F:155:GLN:HB2	3:F:157:TYR:CZ	2.32	0.65
3:F:97:GLU:HB2	3:F:145:THR:HG22	1.79	0.64
1:A:99:ASN:HA	2:C:34:TRP:HZ2	1.63	0.64
3:F:65:PRO:O	3:F:66:ARG:HD3	1.98	0.64
3:E:41:LEU:HD13	3:E:146:PHE:HZ	1.62	0.63
3:F:41:LEU:HD13	3:F:146:PHE:HZ	1.63	0.63
3:F:124:ARG:NH1	3:F:126:CYS:SG	2.71	0.63
3:E:33:LEU:N	3:E:150:VAL:O	2.32	0.63
1:B:143:ARG:HH11	1:B:144:PRO:HD2	1.63	0.63
3:F:53:LYS:NZ	3:F:54:ASN:O	2.31	0.62
2:C:139:HIS:ND1	2:C:143:ASN:OD1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:284:GLN:HG2	3:E:296:ARG:CG	2.29	0.61
2:D:22:VAL:CG2	2:D:102:CYS:SG	2.88	0.61
2:C:197:ASN:HB3	2:C:232:ARG:HE	1.66	0.61
2:D:201:THR:HG23	2:D:204:GLY:H	1.64	0.61
1:B:76:ALA:N	1:B:121:GLY:O	2.34	0.61
3:F:67:ASN:OD1	5:F:401:NAG:N2	2.34	0.61
2:C:39:ASP:OD1	2:C:40:LEU:N	2.34	0.60
1:A:76:ALA:N	1:A:121:GLY:O	2.34	0.60
2:C:46:ARG:HH21	2:C:73:ARG:HH21	1.48	0.60
3:F:65:PRO:HB3	3:F:168:ILE:HA	1.83	0.60
3:F:152:ASP:N	3:F:157:TYR:OH	2.33	0.60
1:A:100:ARG:HH12	1:A:105:LEU:HB2	1.66	0.60
3:E:235:THR:HG22	3:E:247:GLU:HG3	1.84	0.59
1:A:120:THR:HG21	1:A:123:HIS:HE1	1.66	0.59
2:C:197:ASN:HA	2:C:233:ALA:HB3	1.84	0.59
3:E:191:LYS:HG3	3:E:202:LEU:HG	1.84	0.59
3:F:120:ASN:OD1	3:F:121:THR:N	2.35	0.59
2:C:48:LEU:HD13	2:C:70:TRP:HB3	1.85	0.59
2:D:262:ILE:HD12	2:D:262:ILE:H	1.67	0.59
1:B:90:TRP:HA	1:B:110:CYS:HA	1.84	0.59
3:E:191:LYS:O	3:E:202:LEU:HD11	2.02	0.59
3:F:64:HIS:HB3	3:F:66:ARG:NH2	2.17	0.59
3:F:73:PRO:HG3	3:F:163:HIS:CD2	2.38	0.59
3:F:87:GLN:HE22	3:F:89:ASP:HB2	1.68	0.59
3:E:45:GLN:NE2	3:E:143:ARG:O	2.36	0.58
2:D:174:VAL:HG22	2:D:179:LEU:HD23	1.85	0.58
3:F:58:LEU:H	3:F:124:ARG:HH12	1.50	0.58
3:E:91:PHE:HD1	3:E:195:PRO:HD3	1.69	0.58
1:A:85:ARG:NH2	1:B:172:ARG:O	2.34	0.58
3:E:90:LEU:N	3:E:194:THR:OG1	2.36	0.58
1:A:99:ASN:HB3	1:A:142:ARG:HG2	1.86	0.57
2:C:86:ILE:O	2:C:99:CYS:HB2	2.05	0.57
2:D:189:LYS:HD2	2:D:195:GLU:HB2	1.87	0.57
3:E:121:THR:HG23	3:E:123:GLU:H	1.70	0.56
3:F:232:ILE:HD11	3:F:252:ILE:HD11	1.87	0.56
3:F:235:THR:HG22	3:F:247:GLU:HG3	1.85	0.56
3:F:118:GLN:HE22	3:F:157:TYR:HD2	1.52	0.56
2:D:95:GLN:OE1	2:D:95:GLN:N	2.39	0.56
3:E:89:ASP:HB3	3:E:194:THR:HG21	1.88	0.56
3:F:95:HIS:HA	3:F:147:SER:HB2	1.88	0.55
3:F:195:PRO:O	3:F:198:SER:OG	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:202:LEU:HD12	3:F:202:LEU:H	1.71	0.55
4:I:1:NAG:H83	4:I:1:NAG:H3	1.88	0.55
2:D:113:ARG:HB3	2:D:116:GLY:H	1.72	0.55
3:F:226:GLU:HG2	3:F:228:THR:HG23	1.89	0.55
3:E:91:PHE:CD1	3:E:195:PRO:HD3	2.41	0.55
3:E:152:ASP:N	3:E:157:TYR:OH	2.31	0.55
3:E:208:THR:OG1	3:E:263:ARG:NH2	2.39	0.55
3:F:82:PHE:HB3	3:F:90:LEU:HD11	1.89	0.55
2:D:20:PRO:HD2	2:D:113:ARG:NH1	2.22	0.55
3:F:152:ASP:HB2	3:F:157:TYR:OH	2.07	0.55
3:E:148:HIS:O	3:E:148:HIS:CD2	2.60	0.55
3:E:155:GLN:HB2	3:E:157:TYR:HE1	1.71	0.54
3:E:139:HIS:CE1	3:E:141:ARG:O	2.60	0.54
2:D:184:ILE:HG22	2:D:198:PHE:HB3	1.89	0.54
2:D:198:PHE:H	2:D:233:ALA:HB3	1.73	0.54
2:D:232:ARG:NH2	4:J:1:NAG:O6	2.41	0.54
2:C:189:LYS:H	2:C:194:VAL:HA	1.73	0.53
3:F:196:CYS:O	3:F:200:GLY:HA2	2.08	0.53
2:C:83:ALA:HB3	2:C:141:ILE:HD12	1.89	0.53
2:D:85:LYS:HD3	2:D:139:HIS:CE1	2.43	0.53
3:F:39:ARG:HA	3:F:39:ARG:NH1	2.24	0.53
1:B:82:LEU:HD11	2:D:93:ASN:HB2	1.91	0.52
3:E:73:PRO:HG3	3:E:163:HIS:CD2	2.45	0.52
1:A:114:HIS:NE2	2:D:208:MET:HE1	2.23	0.52
3:E:199:SER:OG	3:E:294:CYS:SG	2.65	0.52
3:E:109:LEU:HD21	3:E:163:HIS:HE1	1.75	0.52
3:F:233:LEU:HB2	3:F:282:GLN:HG2	1.92	0.51
3:E:67:ASN:HB3	3:E:68:LEU:HD12	1.92	0.51
1:A:127:ARG:NH2	2:D:216:ILE:HG13	2.21	0.51
3:E:206:ASN:OD1	3:E:263:ARG:NH1	2.44	0.51
3:F:89:ASP:OD1	3:F:194:THR:OG1	2.16	0.51
2:C:128:VAL:HG22	2:C:129:GLU:O	2.11	0.51
2:D:167:MET:HE3	2:D:169:TYR:H	1.75	0.51
2:D:188:LYS:HA	2:D:194:VAL:HG22	1.92	0.51
3:F:178:LYS:HE3	3:F:178:LYS:CA	2.40	0.51
2:C:38:HIS:O	2:C:145:ASN:ND2	2.41	0.51
2:D:72:LEU:HD21	2:D:78:ILE:HG21	1.93	0.51
1:B:101:LEU:HD21	2:D:34:TRP:HZ3	1.75	0.50
2:D:83:ALA:HB3	2:D:141:ILE:HD12	1.92	0.50
3:E:178:LYS:HE2	3:E:179:ASN:H	1.76	0.50
3:F:35:LEU:HD12	3:F:35:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:141:ARG:NH1	3:E:141:ARG:HA	2.26	0.50
1:B:88:SER:O	1:B:88:SER:OG	2.22	0.50
2:C:87:CYS:HA	2:C:99:CYS:CB	2.39	0.50
3:E:158:GLU:OE2	3:E:160:THR:OG1	2.30	0.50
2:C:232:ARG:HD3	4:H:1:NAG:H62	1.94	0.49
3:F:90:LEU:O	3:F:194:THR:OG1	2.29	0.49
1:B:119:GLN:NE2	2:D:214:SER:O	2.34	0.49
2:C:197:ASN:HD22	2:C:232:ARG:HG3	1.77	0.49
3:E:79:GLN:O	3:E:95:HIS:N	2.29	0.49
1:B:127:ARG:NH2	2:C:216:ILE:HG13	2.22	0.49
2:D:167:MET:HE1	2:D:170:LYS:CD	2.39	0.49
2:C:254:PHE:HB2	2:C:257:CYS:SG	2.53	0.49
1:A:175:VAL:HG22	2:D:265:LYS:HG2	1.93	0.49
3:E:109:LEU:HD11	3:E:163:HIS:ND1	2.27	0.48
2:C:190:ASN:ND2	2:C:193:THR:OG1	2.46	0.48
3:E:45:GLN:HE21	3:E:142:TRP:HZ3	1.61	0.48
2:C:197:ASN:ND2	2:C:232:ARG:HG3	2.28	0.48
3:E:146:PHE:CE2	3:E:148:HIS:HB3	2.49	0.48
3:F:48:LEU:HD12	3:F:49:ASN:N	2.27	0.48
1:B:142:ARG:NH2	1:B:157:LEU:HA	2.29	0.48
1:B:77:SER:OG	1:B:84:SER:O	2.25	0.48
3:F:79:GLN:O	3:F:95:HIS:N	2.30	0.48
2:D:28:THR:HG22	2:D:99:CYS:H	1.79	0.48
3:E:174:ASN:OD1	3:E:174:ASN:N	2.46	0.48
3:F:34:ARG:O	3:F:150:VAL:HG12	2.14	0.48
1:B:126:PRO:HB2	2:C:210:LEU:HD21	1.96	0.48
1:A:172:ARG:O	1:B:85:ARG:NH2	2.45	0.48
2:C:205:ASN:OD1	2:C:205:ASN:N	2.46	0.47
2:D:184:ILE:HD11	2:D:265:LYS:O	2.14	0.47
3:F:84:HIS:CE1	3:F:88:GLY:HA2	2.49	0.47
2:C:99:CYS:HA	2:C:126:PHE:HZ	1.78	0.47
3:F:137:HIS:NE2	3:F:140:ARG:HA	2.30	0.47
3:F:155:GLN:HB2	3:F:157:TYR:OH	2.14	0.47
2:D:88:VAL:HG22	2:D:136:ILE:HG13	1.96	0.47
3:F:184:ASP:OD1	3:F:184:ASP:N	2.47	0.47
2:D:51:GLU:O	2:D:67:ASN:N	2.39	0.47
2:C:19:GLU:OE2	2:C:113:ARG:NH2	2.46	0.47
2:C:73:ARG:HG3	2:C:74:ALA:N	2.30	0.47
2:D:70:TRP:NE1	2:D:104:TYR:OH	2.46	0.47
2:D:51:GLU:HG2	2:D:67:ASN:HB3	1.96	0.47
2:D:87:CYS:HA	2:D:99:CYS:CB	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:116:VAL:O	3:F:124:ARG:HG2	2.14	0.47
3:F:66:ARG:HD3	3:F:66:ARG:N	2.30	0.47
3:F:79:GLN:N	3:F:95:HIS:O	2.29	0.47
3:F:212:LEU:HD23	3:F:213:GLU:H	1.79	0.47
2:C:174:VAL:HG13	2:C:179:LEU:HB3	1.97	0.46
2:D:50:VAL:HG22	2:D:68:VAL:HG23	1.98	0.46
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.80	0.46
2:C:73:ARG:HG2	2:C:77:SER:HB2	1.97	0.46
3:E:215:HIS:O	3:E:270:LEU:N	2.40	0.46
2:C:180:TRP:CH2	2:C:182:PRO:HB3	2.51	0.46
3:F:178:LYS:CE	3:F:179:ASN:H	2.08	0.46
3:F:73:PRO:HG3	3:F:163:HIS:HD2	1.79	0.46
2:D:72:LEU:HD23	2:D:73:ARG:O	2.16	0.46
2:D:103:ASN:OD1	5:D:401:NAG:N2	2.49	0.46
3:E:114:LEU:HB2	3:E:127:VAL:HB	1.98	0.46
3:E:197:MET:SD	3:E:202:LEU:HB2	2.55	0.46
2:C:87:CYS:CA	2:C:99:CYS:HB3	2.37	0.46
2:D:86:ILE:O	2:D:99:CYS:HB2	2.16	0.45
2:C:70:TRP:HZ2	2:C:104:TYR:HH	1.63	0.45
2:C:201:THR:HG23	2:C:204:GLY:H	1.80	0.45
2:C:99:CYS:HA	2:C:126:PHE:CZ	2.50	0.45
2:C:167:MET:HA	2:C:167:MET:CE	2.47	0.45
3:F:34:ARG:HG2	3:F:35:LEU:O	2.17	0.45
3:F:114:LEU:HB2	3:F:127:VAL:HG13	1.98	0.45
3:E:231:GLN:O	3:E:283:ILE:HD12	2.17	0.45
3:F:70:PRO:HG2	3:F:109:LEU:HA	1.99	0.45
3:F:52:VAL:HG22	3:F:129:PHE:HE1	1.82	0.44
1:A:101:LEU:HD21	2:C:34:TRP:HZ3	1.82	0.44
1:A:161:LEU:HD21	5:A:301:NAG:H2	1.99	0.44
3:E:109:LEU:HD21	3:E:163:HIS:CE1	2.53	0.44
2:C:46:ARG:HH21	2:C:73:ARG:NH2	2.15	0.44
3:F:208:THR:OG1	3:F:263:ARG:NH2	2.51	0.44
2:D:64:ILE:C	2:D:65:LEU:HD23	2.38	0.44
3:F:70:PRO:HD2	3:F:165:PRO:HD2	1.99	0.44
2:C:47:ASP:HB3	2:C:71:VAL:HB	1.99	0.44
2:C:186:ALA:HB2	2:C:196:VAL:HG13	1.98	0.44
3:F:81:HIS:HB3	3:F:93:VAL:HG23	1.99	0.44
3:F:118:GLN:NE2	3:F:157:TYR:CD2	2.83	0.44
3:E:155:GLN:HB2	3:E:157:TYR:CE1	2.52	0.44
3:F:109:LEU:HD21	3:F:163:HIS:HE1	1.83	0.44
2:D:175:LYS:HB3	2:D:256:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:84:HIS:ND1	3:E:90:LEU:HB2	2.33	0.44
3:F:224:TRP:HB3	3:F:287:PHE:HZ	1.82	0.44
1:A:114:HIS:CD2	1:A:126:PRO:HA	2.53	0.43
2:C:50:VAL:HG11	2:C:136:ILE:HD12	2.00	0.43
2:D:22:VAL:HG22	2:D:102:CYS:SG	2.56	0.43
3:E:95:HIS:ND1	3:E:147:SER:OG	2.46	0.43
1:B:120:THR:HG21	1:B:123:HIS:HE1	1.83	0.43
3:E:168:ILE:HG12	3:E:169:PRO:HD2	2.00	0.43
4:J:1:NAG:H61	4:J:2:NAG:C7	2.48	0.43
2:D:25:GLY:O	2:D:100:VAL:HB	2.19	0.43
3:E:178:LYS:HE2	3:E:178:LYS:HA	2.01	0.43
1:A:77:SER:OG	1:A:84:SER:O	2.25	0.43
2:C:229:LYS:H	2:C:229:LYS:HG2	1.54	0.43
3:F:89:ASP:HA	3:F:194:THR:HG21	2.00	0.43
3:F:194:THR:N	3:F:195:PRO:HD2	2.33	0.43
1:A:99:ASN:HA	2:C:34:TRP:CZ2	2.49	0.43
1:B:101:LEU:HD21	2:D:34:TRP:CZ3	2.54	0.43
2:D:164:ASP:OD1	2:D:164:ASP:N	2.43	0.42
1:B:99:ASN:HA	2:D:34:TRP:CZ2	2.41	0.42
2:D:167:MET:HE2	2:D:170:LYS:HG2	2.00	0.42
3:E:231:GLN:HE21	3:E:284:GLN:HG3	1.84	0.42
3:E:280:GLN:HG2	3:E:300:THR:HG22	2.02	0.42
2:C:83:ALA:HB2	2:C:103:ASN:HA	2.02	0.42
2:D:64:ILE:O	2:D:65:LEU:HD23	2.20	0.42
3:E:41:LEU:HD21	3:E:148:HIS:CE1	2.55	0.42
3:F:227:SER:HA	3:F:255:PRO:HD2	2.01	0.42
2:C:111:GLN:OE1	3:E:68:LEU:HA	2.19	0.42
2:D:251:THR:HG23	2:D:263:ARG:HG2	2.01	0.42
3:E:84:HIS:CE1	3:E:90:LEU:HB2	2.55	0.42
3:F:146:PHE:CZ	3:F:148:HIS:ND1	2.87	0.42
2:C:51:GLU:OE2	5:C:402:NAG:O6	2.26	0.42
2:D:129:GLU:HA	2:D:129:GLU:OE2	2.19	0.42
3:E:197:MET:SD	3:E:202:LEU:CD1	3.04	0.42
2:D:197:ASN:HD22	2:D:232:ARG:HG3	1.85	0.41
3:E:123:GLU:OE1	3:E:124:ARG:C	2.58	0.41
3:F:154:ASP:OD2	3:F:184:ASP:HB3	2.19	0.41
3:E:74:LYS:HB2	3:E:101:GLN:HG3	2.01	0.41
3:F:81:HIS:CE1	3:F:82:PHE:O	2.73	0.41
3:E:82:PHE:HB3	3:E:90:LEU:HD11	2.02	0.41
3:F:206:ASN:OD1	3:F:263:ARG:NH1	2.54	0.41
3:F:207:ILE:HD13	3:F:221:PHE:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:HD2	1:A:161:LEU:O	2.20	0.41
2:D:75:ASP:HA	2:D:111:GLN:HG3	2.03	0.41
3:F:191:LYS:HE3	3:F:202:LEU:HA	2.01	0.41
3:E:227:SER:HA	3:E:255:PRO:HD2	2.02	0.41
3:F:134:LYS:HB2	3:F:136:ARG:HH21	1.86	0.41
1:B:81:PRO:HG2	1:B:83:ASN:OD1	2.21	0.41
2:D:113:ARG:HD2	2:D:113:ARG:HA	1.82	0.41
2:D:234:SER:OG	4:I:1:NAG:O6	2.34	0.41
3:E:69:THR:HG21	3:E:167:PRO:HA	2.03	0.41
3:E:185:CYS:SG	3:E:191:LYS:HA	2.61	0.41
3:F:93:VAL:HG12	3:F:150:VAL:HA	2.02	0.41
2:D:165:HIS:ND1	2:D:166:ILE:N	2.69	0.41
1:B:83:ASN:ND2	1:B:92:TYR:HE2	2.09	0.40
3:E:157:TYR:HB2	3:E:180:PHE:HB3	2.04	0.40
2:D:254:PHE:HB2	2:D:257:CYS:SG	2.61	0.40
3:E:80:LEU:HD12	3:E:81:HIS:N	2.36	0.40
4:J:1:NAG:H61	4:J:2:NAG:N2	2.36	0.40
1:A:175:VAL:CG2	2:D:265:LYS:HG2	2.50	0.40
2:D:47:ASP:HB3	2:D:71:VAL:HB	2.04	0.40
1:A:127:ARG:HH12	2:D:216:ILE:HD11	1.86	0.40
2:D:92:SER:C	2:D:94:PHE:H	2.25	0.40
3:F:58:LEU:N	3:F:124:ARG:HH12	2.18	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/188 (49%)	91 (99%)	1 (1%)	0	100	100
1	B	92/188 (49%)	89 (97%)	3 (3%)	0	100	100
2	C	246/305 (81%)	225 (92%)	21 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	248/305 (81%)	231 (93%)	17 (7%)	0	100	100
3	E	269/319 (84%)	248 (92%)	21 (8%)	0	100	100
3	F	269/319 (84%)	246 (91%)	23 (9%)	0	100	100
All	All	1216/1624 (75%)	1130 (93%)	86 (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	A	86/164 (52%)	81 (94%)	5 (6%)	20	52
1	B	86/164 (52%)	83 (96%)	3 (4%)	36	63
2	C	220/265 (83%)	207 (94%)	13 (6%)	19	51
2	D	222/265 (84%)	214 (96%)	8 (4%)	35	63
3	E	247/297 (83%)	241 (98%)	6 (2%)	49	71
3	F	248/297 (84%)	233 (94%)	15 (6%)	19	50
All	All	1109/1452 (76%)	1059 (96%)	50 (4%)	31	57

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	123	HIS
1	A	160	ARG
1	A	174	ARG
1	A	176	MET
1	B	88	SER
1	B	123	HIS
1	B	124	MET
2	C	35	MET
2	C	44	ASP

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Mol	Chain	Res	Type
2	C	63	SER
2	C	98	SER
2	C	101	ARG
2	C	146	MET
2	C	157	PHE
2	C	165	HIS
2	C	210	LEU
2	C	223	PHE
2	C	232	ARG
2	C	253	TYR
2	C	265	LYS
2	D	40	LEU
2	D	94	PHE
2	D	99	CYS
2	D	146	MET
2	D	159	SER
2	D	165	HIS
2	D	223	PHE
2	D	229	LYS
3	E	34	ARG
3	E	50	CYS
3	E	139	HIS
3	E	178	LYS
3	E	206	ASN
3	E	249	MET
3	F	35	LEU
3	F	39	ARG
3	F	50	CYS
3	F	69	THR
3	F	87	GLN
3	F	124	ARG
3	F	129	PHE
3	F	139	HIS
3	F	162	HIS
3	F	175	HIS
3	F	178	LYS
3	F	204	ASP
3	F	212	LEU
3	F	221	PHE
3	F	249	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	139	HIS
3	E	231	GLN
3	F	163	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](#)

8 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
4	NAG	G	1	2,4	14,14,15	0.27	0	17,19,21	0.52	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	H	1	2,4	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	H	2	4	14,14,15	0.32	0	17,19,21	0.44	0
4	NAG	I	1	2,4	14,14,15	0.37	0	17,19,21	1.30	2 (11%)
4	NAG	I	2	4	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	J	1	2,4	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.48	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
4	NAG	G	1	2,4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	2,4	-	5/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C2-N2-C7	4.36	129.12	122.90
4	I	1	NAG	C1-C2-N2	2.05	113.98	110.49

There are no chirality outliers.

All (20) torsion outliers are listed below:

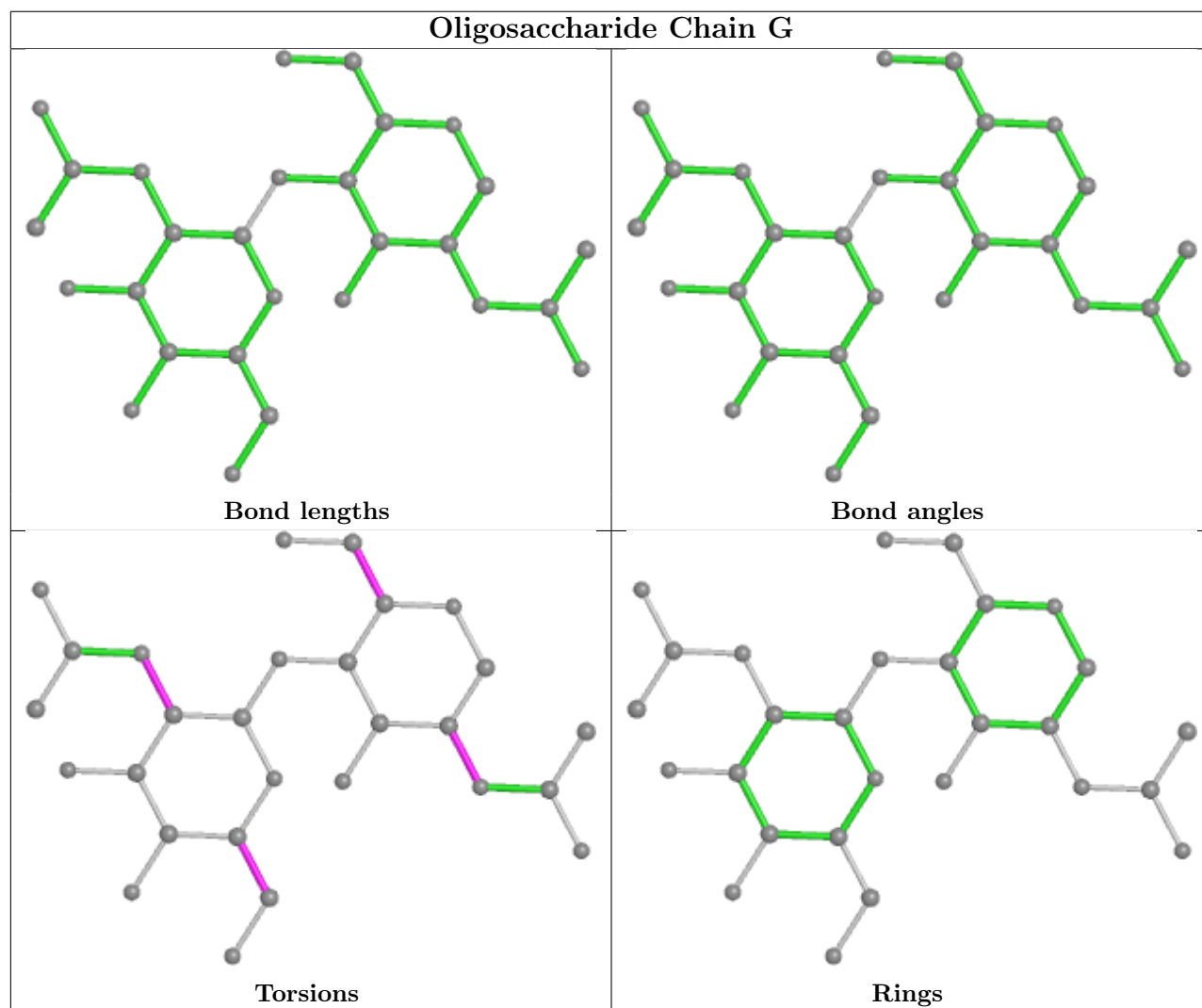
Mol	Chain	Res	Type	Atoms
4	G	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	G	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7
4	J	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
4	I	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C1-C2-N2-C7

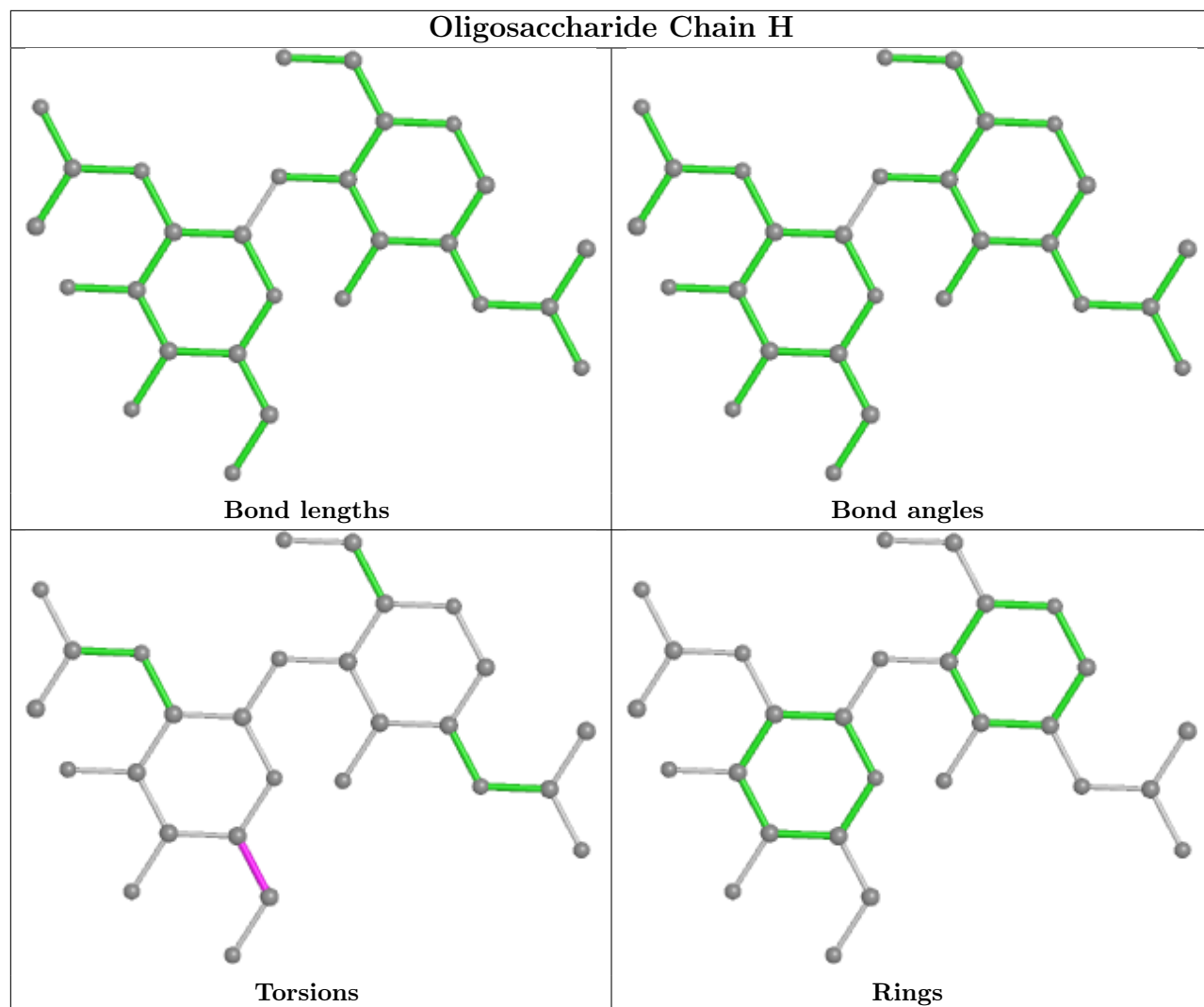
There are no ring outliers.

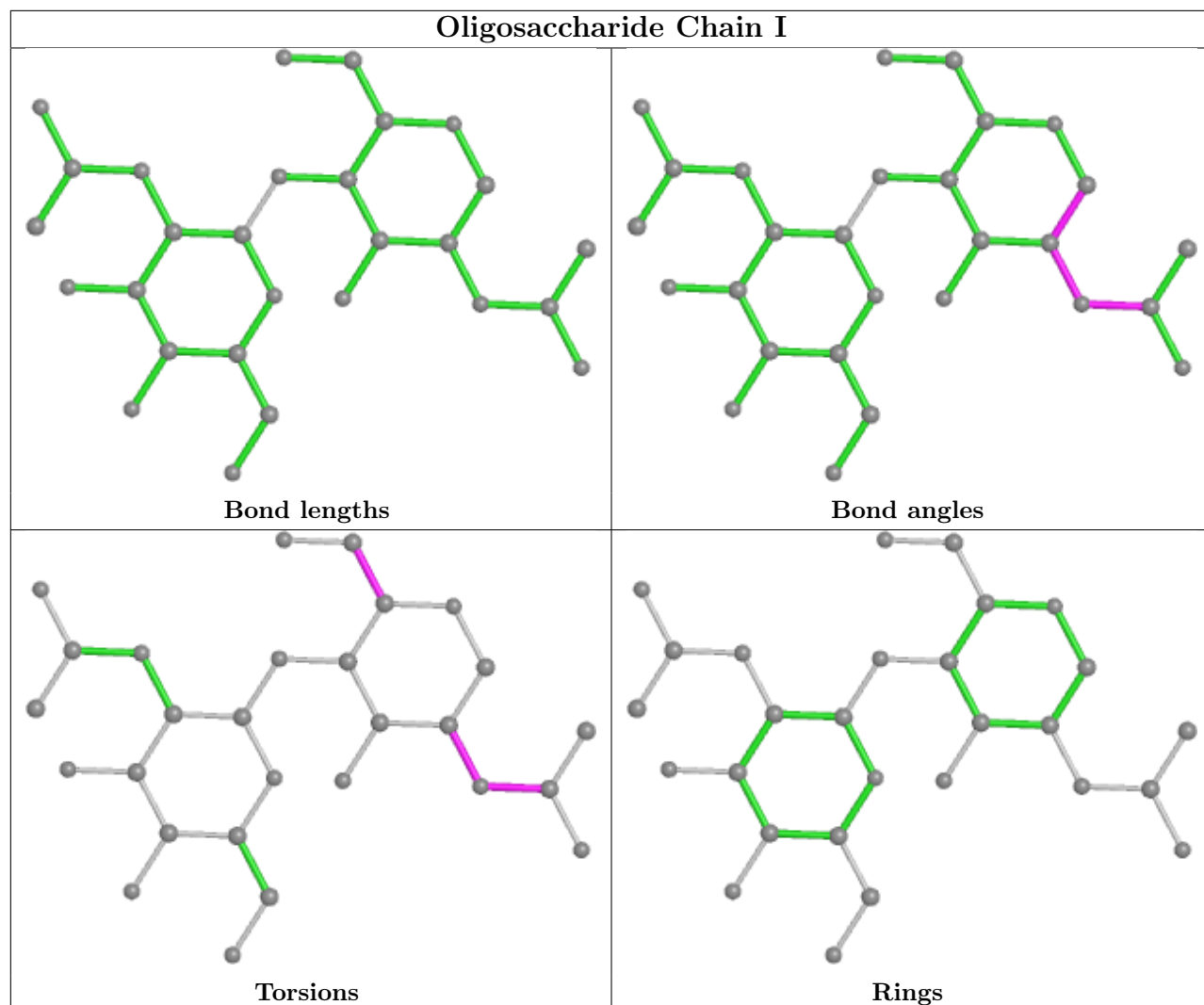
4 monomers are involved in 6 short contacts:

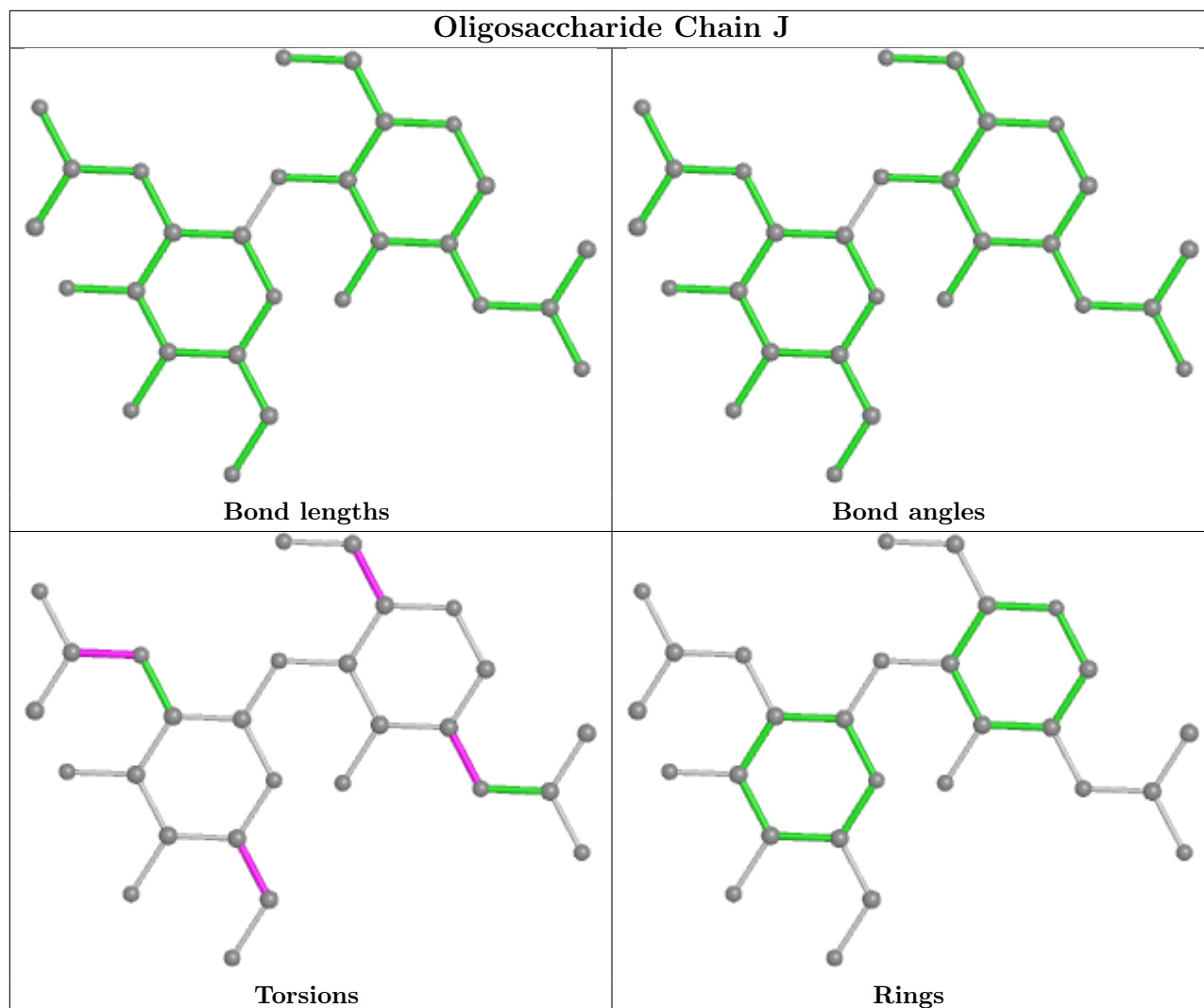
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0
4	J	1	NAG	3	0
4	J	2	NAG	2	0
4	I	1	NAG	2	0

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









5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
5	NAG	B	301	1	14,14,15	0.28	0	17,19,21	0.52	0
5	NAG	A	301	1	14,14,15	0.26	0	17,19,21	0.51	0
5	NAG	D	402	2	14,14,15	0.16	0	17,19,21	0.43	0
5	NAG	C	403	2	14,14,15	0.21	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	403	2	14,14,15	0.31	0	17,19,21	0.71	1 (5%)
5	NAG	E	403	3	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	F	402	3	14,14,15	0.98	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	C	402	2	14,14,15	0.32	0	17,19,21	0.64	0
5	NAG	E	402	3	14,14,15	0.17	0	17,19,21	0.40	0
5	NAG	F	401	3	14,14,15	0.34	0	17,19,21	0.53	0
5	NAG	D	401	2	14,14,15	0.43	0	17,19,21	0.59	0
5	NAG	F	403	3	14,14,15	0.15	0	17,19,21	0.42	0
5	NAG	C	401	2	14,14,15	0.44	0	17,19,21	0.89	1 (5%)
5	NAG	E	401	3	14,14,15	0.99	2 (14%)	17,19,21	0.98	1 (5%)

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	B	301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	301	1	-	3/6/23/26	0/1/1/1
5	NAG	D	402	2	-	1/6/23/26	0/1/1/1
5	NAG	C	403	2	-	2/6/23/26	0/1/1/1
5	NAG	D	403	2	-	3/6/23/26	0/1/1/1
5	NAG	E	403	3	-	2/6/23/26	0/1/1/1
5	NAG	F	402	3	-	0/6/23/26	0/1/1/1
5	NAG	C	402	2	-	3/6/23/26	0/1/1/1
5	NAG	E	402	3	-	2/6/23/26	0/1/1/1
5	NAG	F	401	3	-	3/6/23/26	0/1/1/1
5	NAG	D	401	2	-	4/6/23/26	0/1/1/1
5	NAG	F	403	3	-	2/6/23/26	0/1/1/1
5	NAG	C	401	2	-	1/6/23/26	0/1/1/1
5	NAG	E	401	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	402	NAG	O5-C1	3.02	1.48	1.43
5	E	401	NAG	O5-C1	2.90	1.48	1.43
5	E	401	NAG	C1-C2	2.14	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	402	NAG	C1-O5-C5	4.10	117.75	112.19
5	E	401	NAG	C1-O5-C5	3.83	117.38	112.19
5	C	401	NAG	C1-O5-C5	2.81	115.99	112.19
5	D	403	NAG	C1-O5-C5	2.19	115.16	112.19

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	402	NAG	O5-C5-C6-O6
5	A	301	NAG	O5-C5-C6-O6
5	E	403	NAG	C4-C5-C6-O6
5	E	403	NAG	O5-C5-C6-O6
5	D	403	NAG	C4-C5-C6-O6
5	F	403	NAG	O5-C5-C6-O6
5	C	403	NAG	C8-C7-N2-C2
5	C	403	NAG	O7-C7-N2-C2
5	D	401	NAG	C8-C7-N2-C2
5	D	401	NAG	O7-C7-N2-C2
5	F	401	NAG	C8-C7-N2-C2
5	F	401	NAG	O7-C7-N2-C2
5	F	403	NAG	C4-C5-C6-O6
5	C	402	NAG	C4-C5-C6-O6
5	E	402	NAG	O5-C5-C6-O6
5	C	401	NAG	O5-C5-C6-O6
5	E	402	NAG	C4-C5-C6-O6
5	F	401	NAG	O5-C5-C6-O6
5	A	301	NAG	C4-C5-C6-O6
5	D	403	NAG	O5-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6
5	D	401	NAG	C4-C5-C6-O6
5	D	402	NAG	O5-C5-C6-O6
5	D	401	NAG	O5-C5-C6-O6
5	A	301	NAG	C3-C2-N2-C7
5	B	301	NAG	C3-C2-N2-C7
5	C	402	NAG	C3-C2-N2-C7
5	D	403	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	NAG	1	0
5	A	301	NAG	1	0
5	C	402	NAG	1	0
5	F	401	NAG	1	0
5	D	401	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.

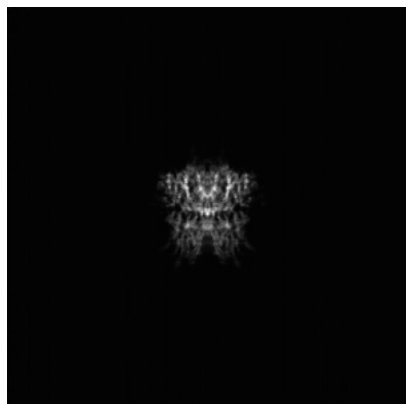
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26835. These allow visual inspection of the internal detail of the map and identification of artifacts.

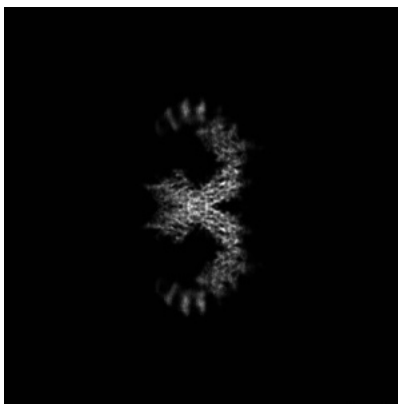
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

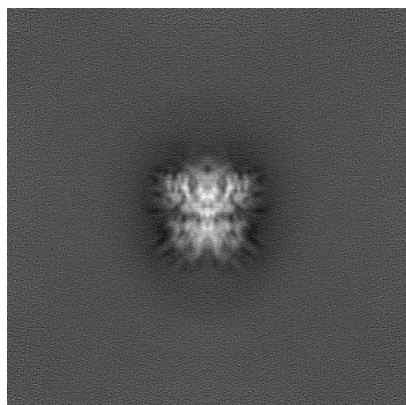


Y

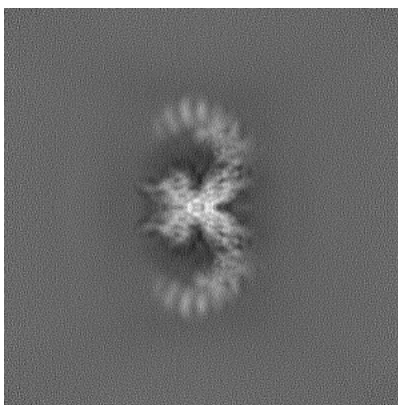


Z

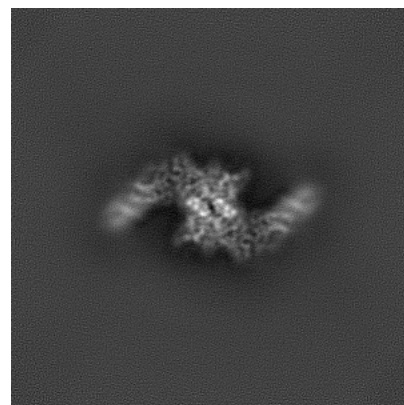
6.1.2 Raw map



X



Y

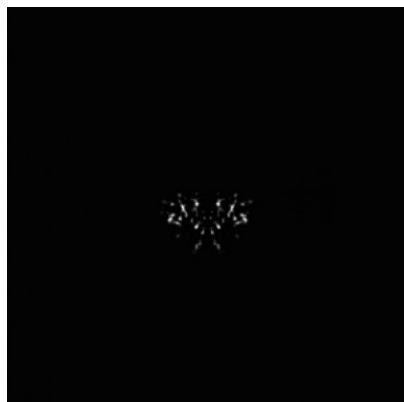


Z

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

6.2 Central slices [i](#)

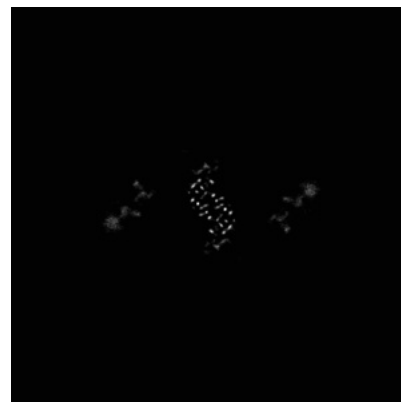
6.2.1 Primary map



X Index: 192

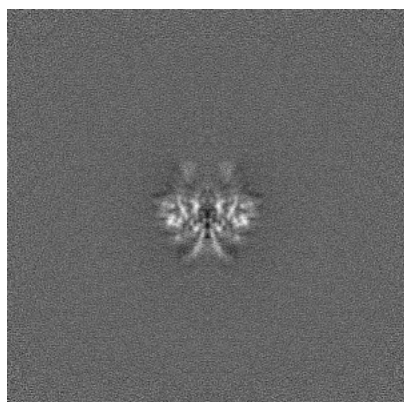


Y Index: 192

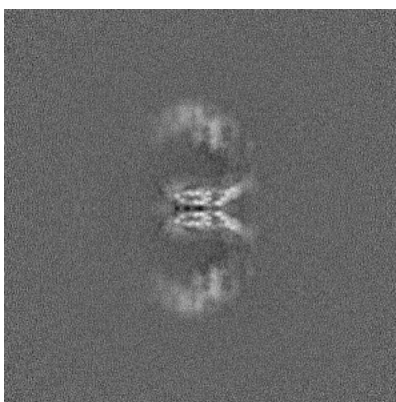


Z Index: 192

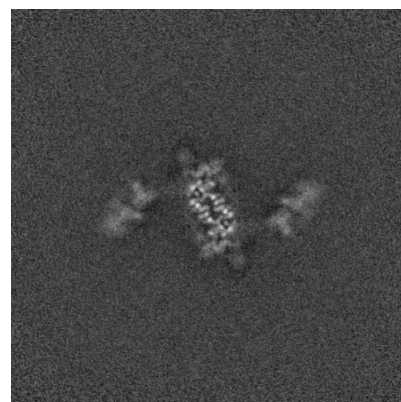
6.2.2 Raw map



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](#)

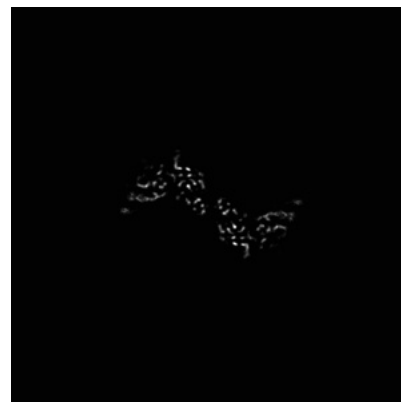
6.3.1 Primary map



X Index: 201

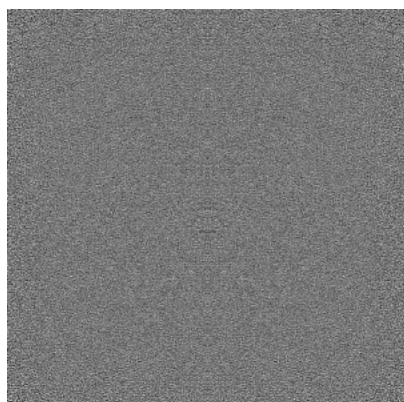


Y Index: 211

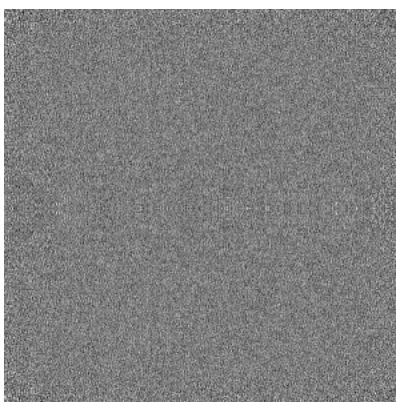


Z Index: 210

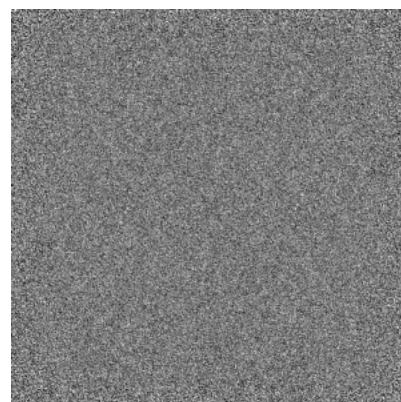
6.3.2 Raw map



X Index: 0



Y Index: 0

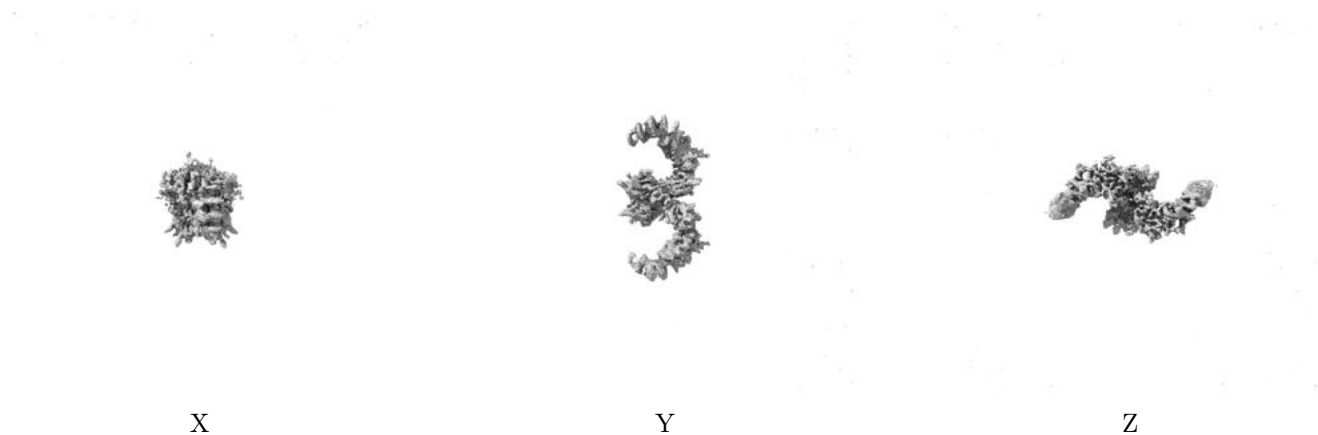


Z Index: 383

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

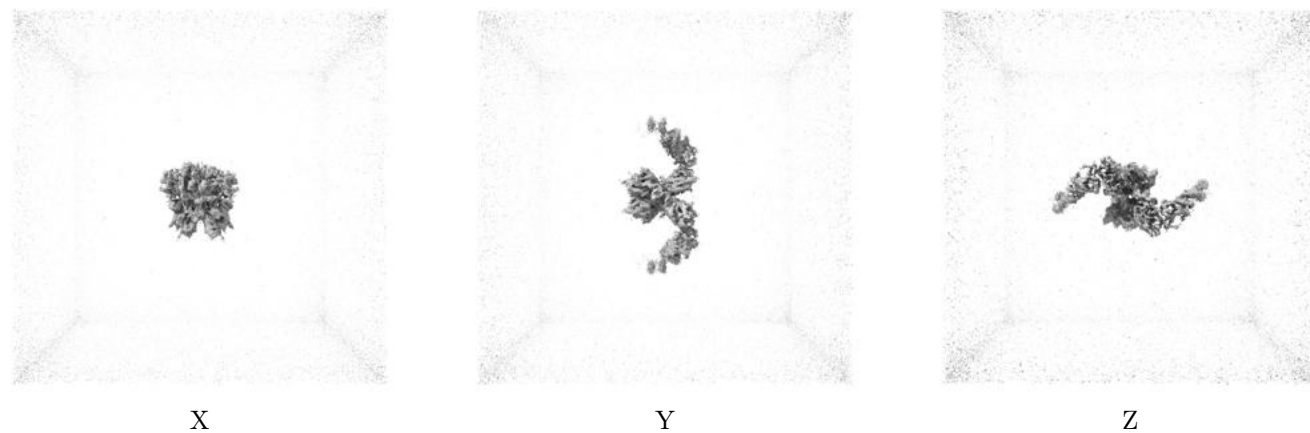
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

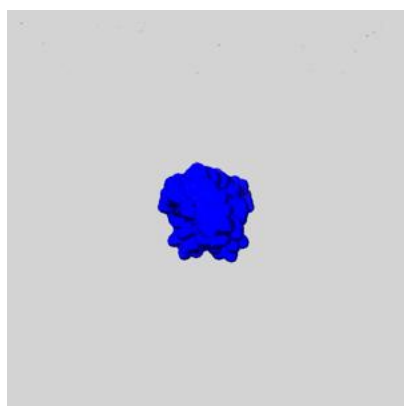
6.5 Mask visualisation [i](#)

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

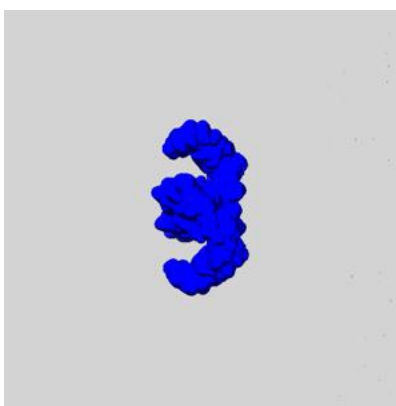
A mask typically either:

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

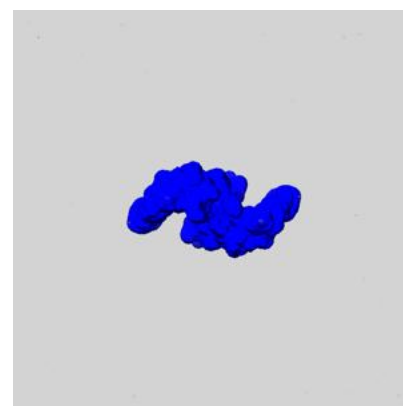
6.5.1 emd_26835_msk_1.map [i](#)



X



Y

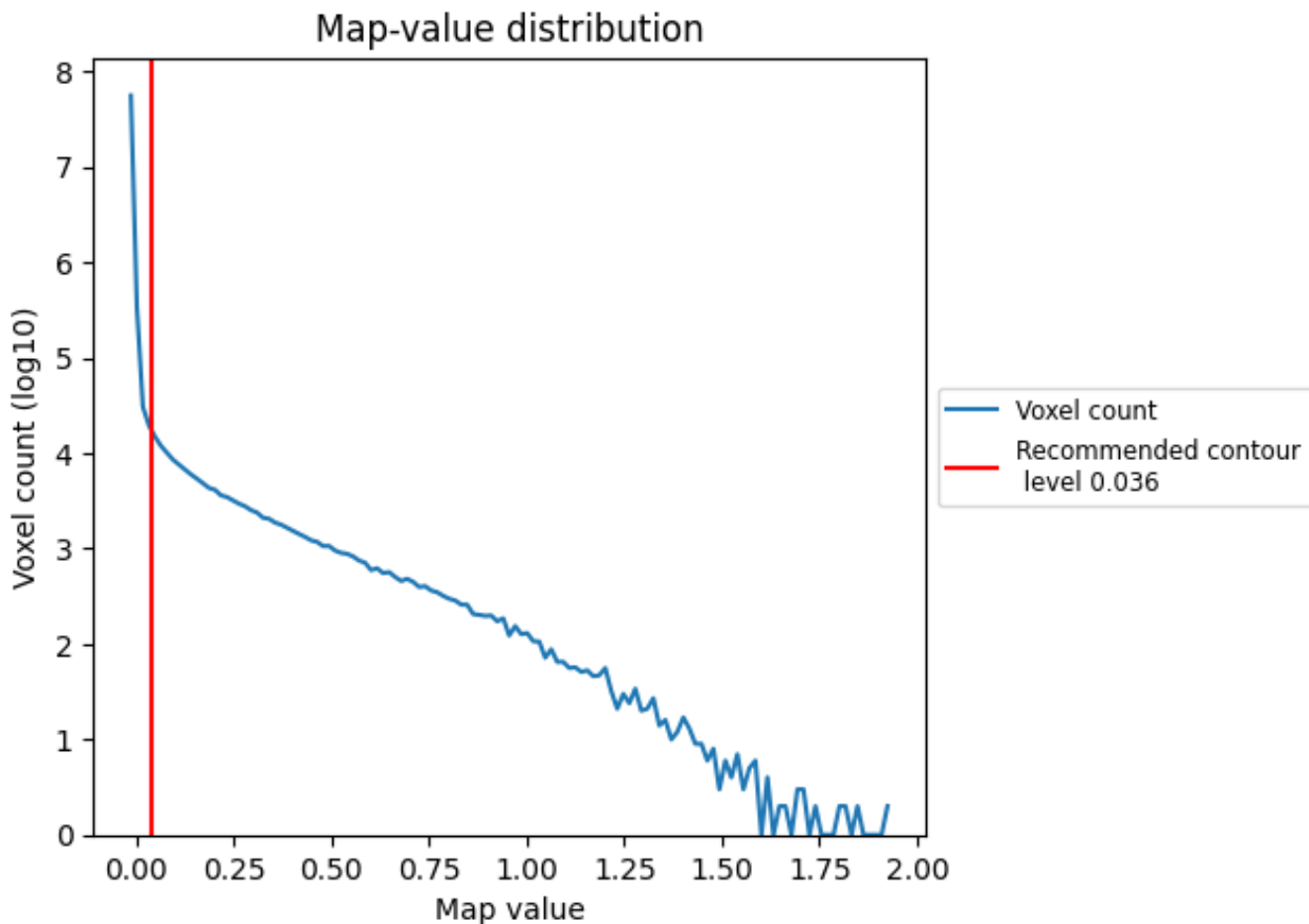


Z

7 Map analysis [i](#)

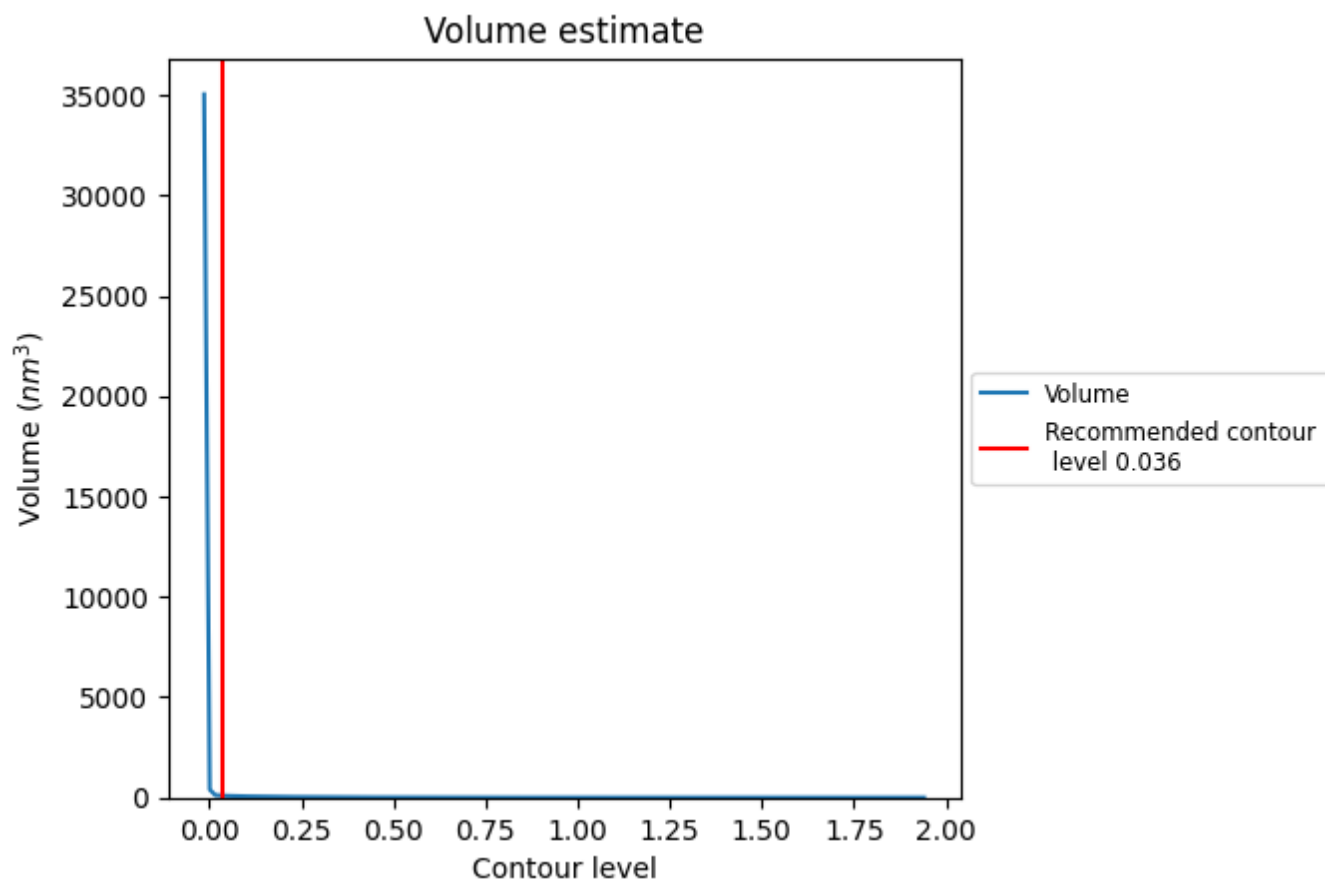
This section contains the results of statistical analysis of the map.

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.

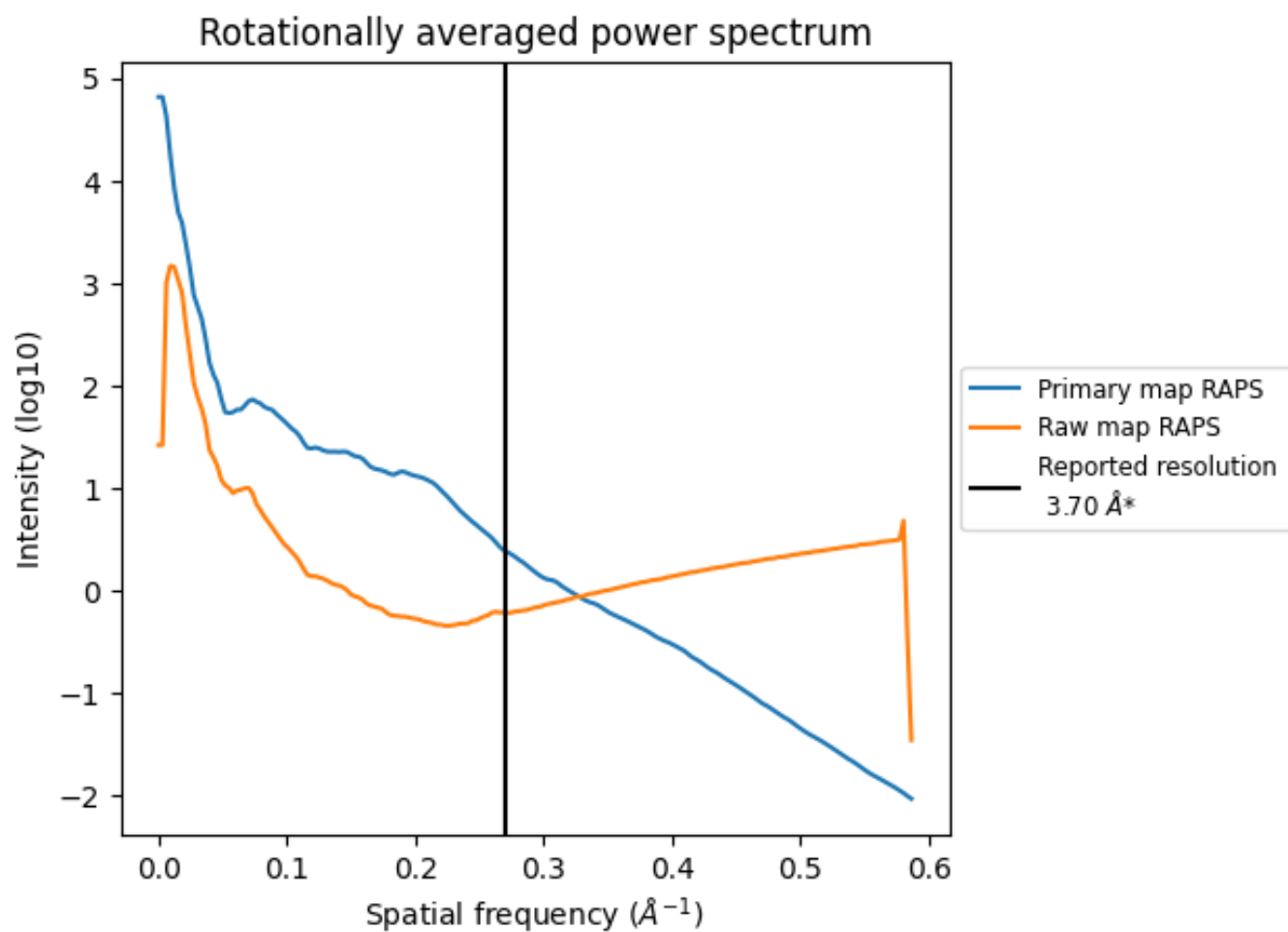
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm³; this corresponds to an approximate mass of 85 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 i

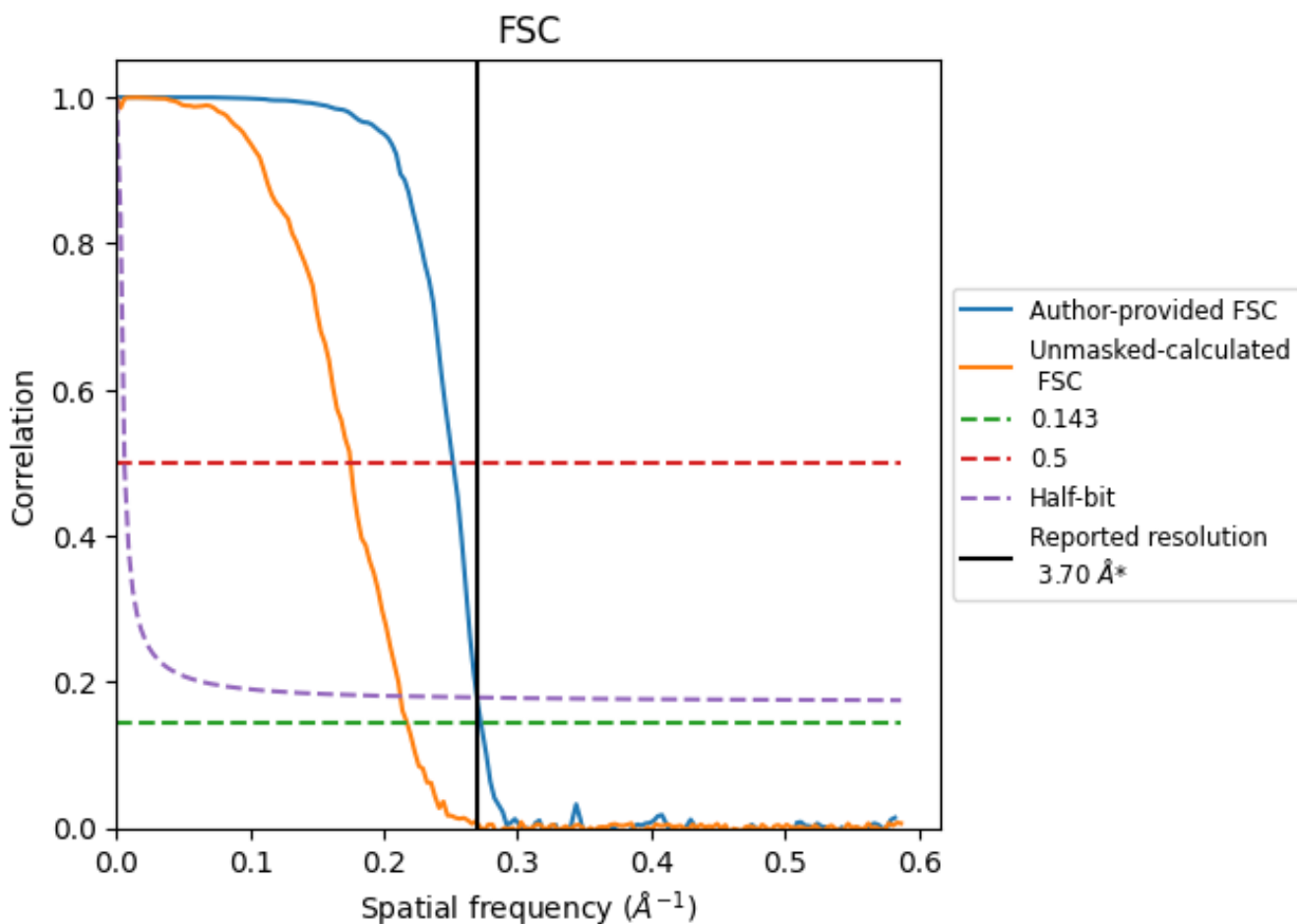


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

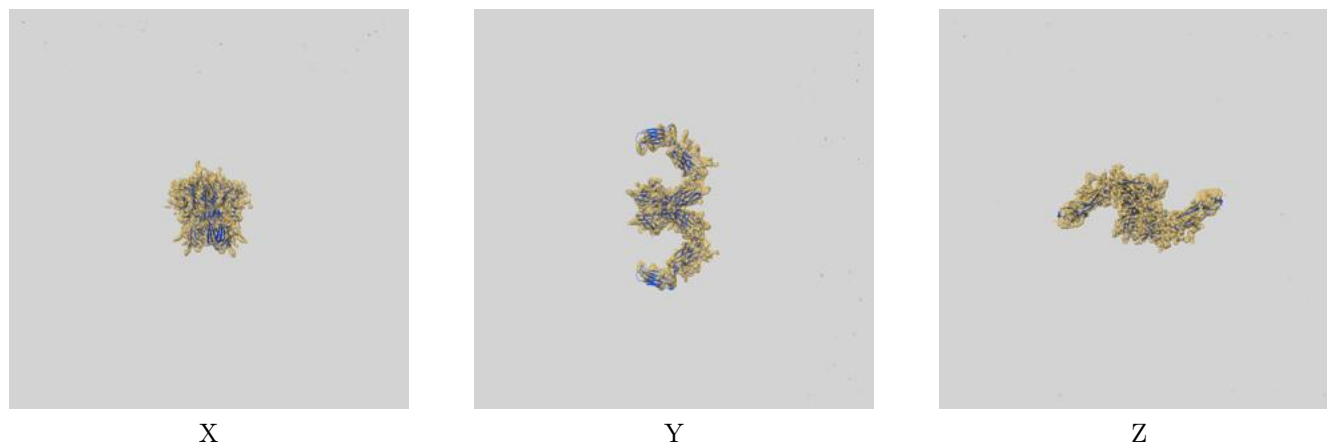
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	3.97	3.71
Unmasked-calculated*	4.60	5.71	4.71

*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 4.60 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

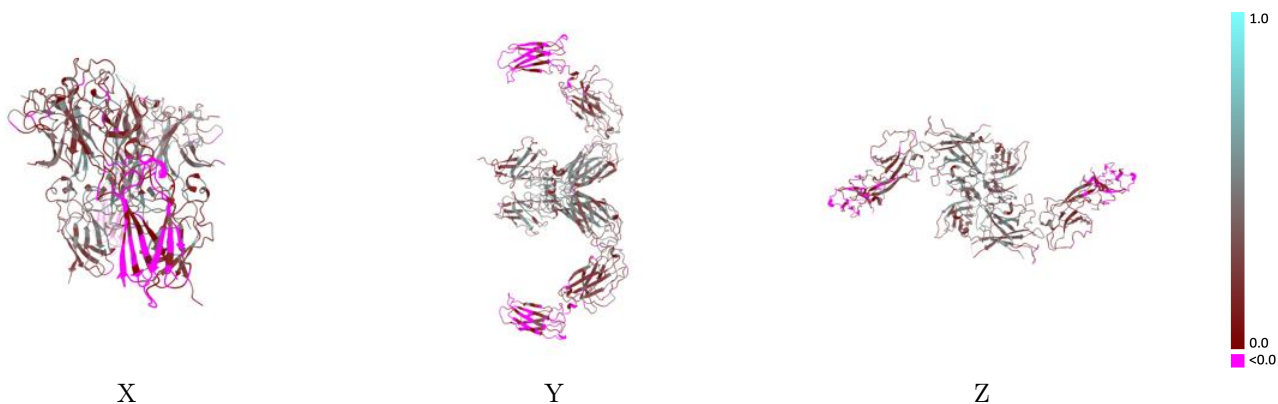
This section contains information regarding the fit between EMDB map EMD-26835 and PDB model 7UWL. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



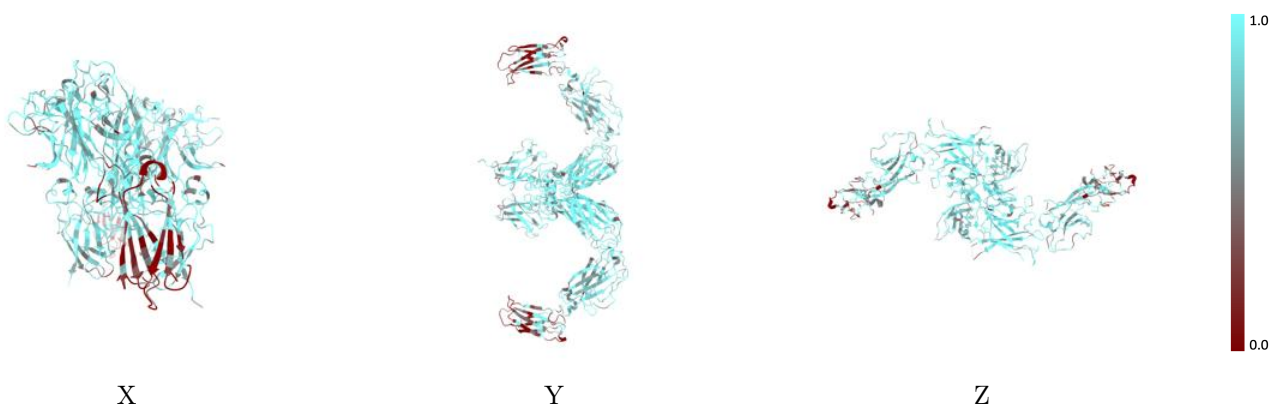
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



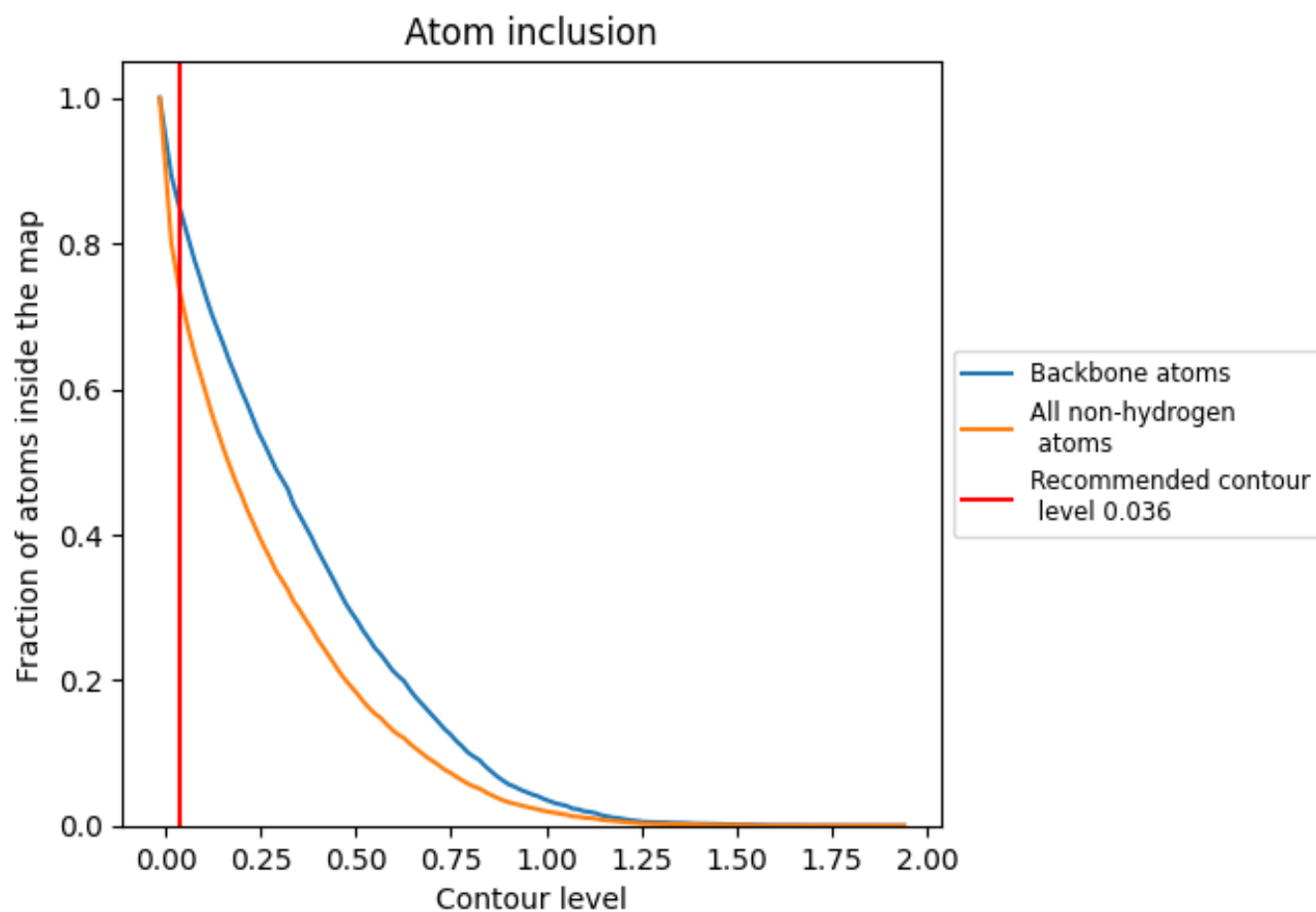
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).























9.4 Atom inclusion [i](#)



At the recommended contour level, 85% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7394	 0.2690
A	 0.8793	 0.4190
B	 0.8833	 0.4290
C	 0.8338	 0.3520
D	 0.8229	 0.3460
E	 0.6041	 0.1370
F	 0.6144	 0.1450
G	 0.8214	 0.4060
H	 0.9643	 0.4630
I	 0.5357	 0.2640
J	 0.9286	 0.3990

