



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:16 AM UTC

PDB ID : 7UAR / pdb_00007uar
EMDB ID : EMD-26431
Title : Structure of the SARS-CoV-2 S 6P trimer in complex with the neutralizing antibody Fab fragment, C1717
Authors : Barnes, C.O.
Deposited on : 2022-03-13
Resolution : 3.50 Å(reported)
Based on initial model : 6XKL

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

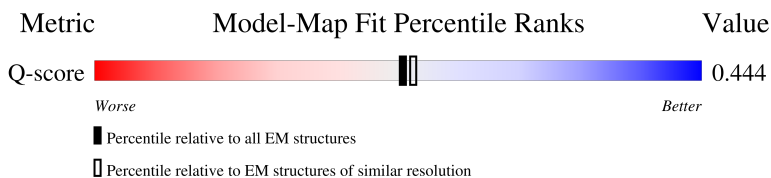
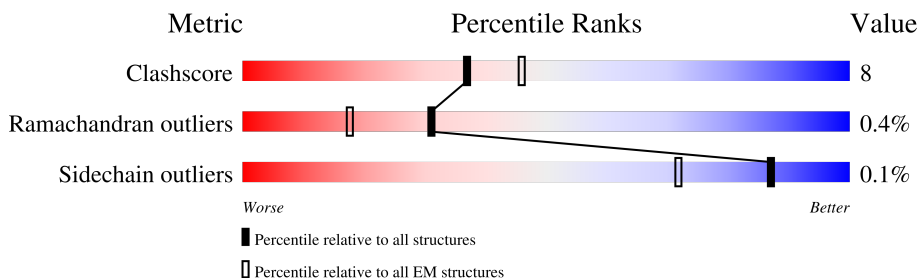
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	1256	9% 64% 12% 23%
1	B	1256	6% 65% 12% 22%
1	C	1256	64% 14% 22%
2	D	227	8% 40% 13% 48%

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Mol	Chain	Length	Quality of chain
2	F	227	
2	H	227	
3	E	216	
3	G	216	
3	L	216	
4	I	2	
4	J	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
5	K	4	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 27996 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	968	Total	C	N	O	S	0	0
			7393	4729	1230	1401	33		
1	B	983	Total	C	N	O	S	0	0
			7505	4797	1244	1430	34		
1	C	976	Total	C	N	O	S	0	0
			7355	4702	1217	1402	34		

There are 165 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	VAL	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	SER	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	ILE	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	PRO	-	expression tag	UNP P0DTC2
B	1233	ARG	-	expression tag	UNP P0DTC2
B	1234	ASP	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	GLN	-	expression tag	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP P0DTC2
B	1238	TYR	-	expression tag	UNP P0DTC2
B	1239	VAL	-	expression tag	UNP P0DTC2
B	1240	ARG	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	GLU	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	THR	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	LEU	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	VAL	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	SER	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	ILE	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	PRO	-	expression tag	UNP P0DTC2
C	1233	ARG	-	expression tag	UNP P0DTC2
C	1234	ASP	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	GLN	-	expression tag	UNP P0DTC2
C	1237	ALA	-	expression tag	UNP P0DTC2
C	1238	TYR	-	expression tag	UNP P0DTC2
C	1239	VAL	-	expression tag	UNP P0DTC2
C	1240	ARG	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1245	TRP	-	expression tag	UNP P0DTC2
C	1246	VAL	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	THR	-	expression tag	UNP P0DTC2
C	1251	PHE	-	expression tag	UNP P0DTC2
C	1252	LEU	-	expression tag	UNP P0DTC2
C	1253	GLY	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called C1717 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	119	Total	C	N	O	S	1	0
			918	582	156	176	4		
2	D	119	Total	C	N	O	S	1	0
			918	582	156	176	4		
2	F	119	Total	C	N	O	S	1	0
			918	582	156	176	4		

- Molecule 3 is a protein called C1717 Fab Light Chain.

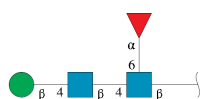
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	110	Total	C	N	O	S	0	0
			798	488	141	166	3		
3	E	110	Total	C	N	O	S	0	0
			798	488	141	166	3		
3	G	110	Total	C	N	O	S	0	0
			798	488	141	166	3		

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



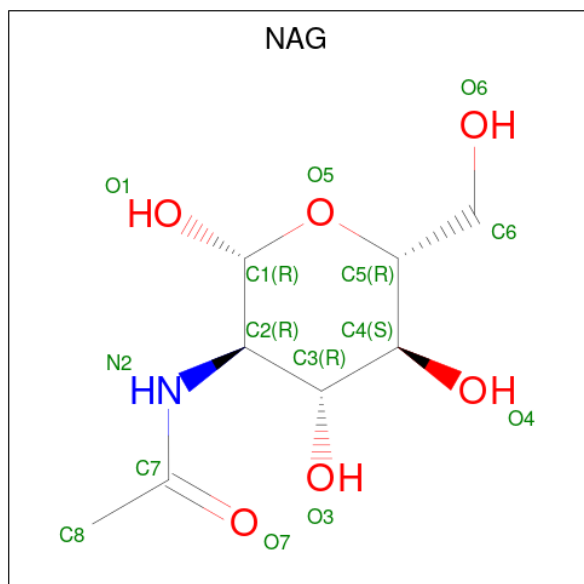
Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

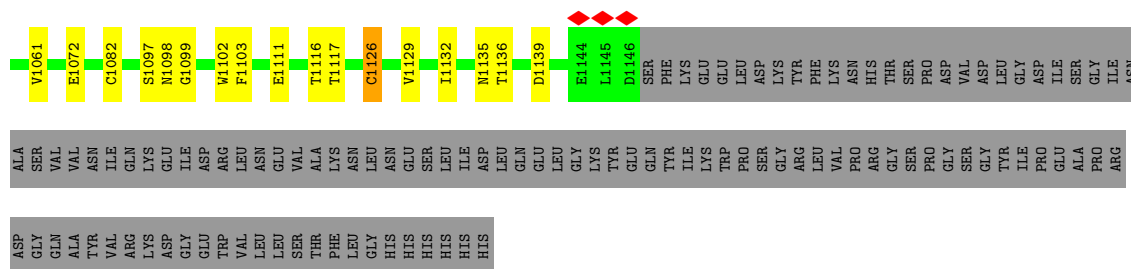


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6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

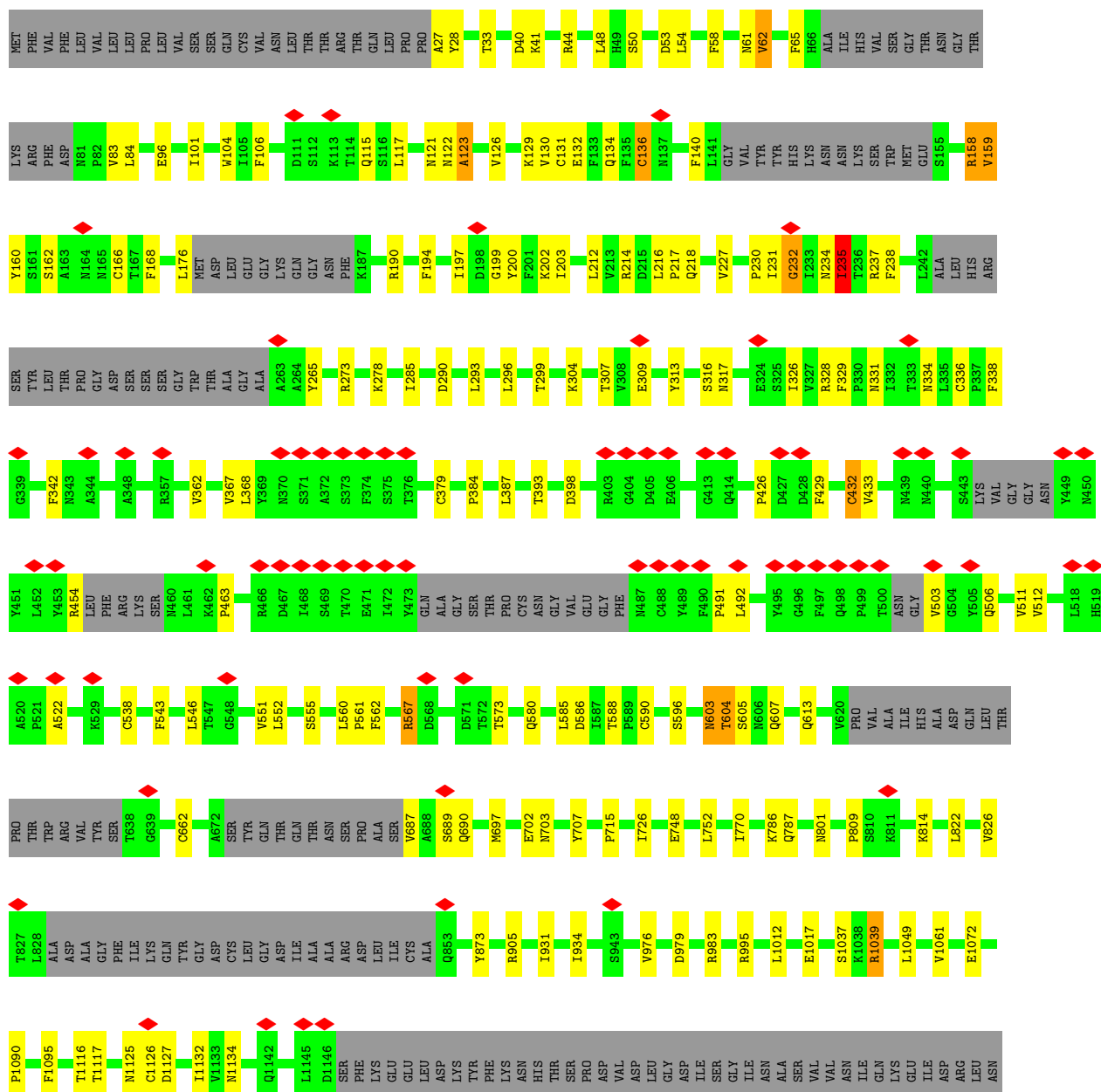
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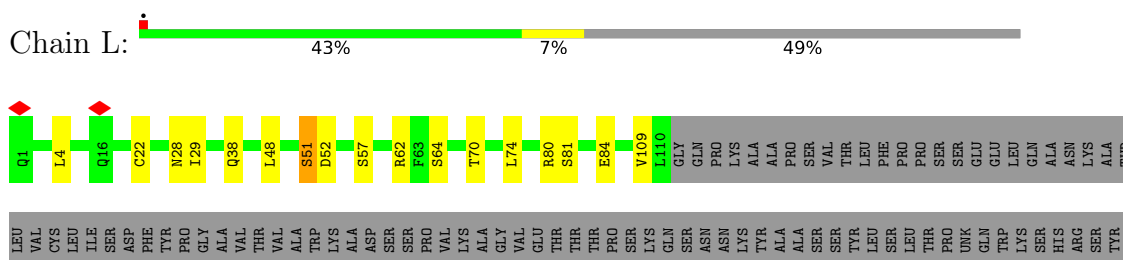
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	



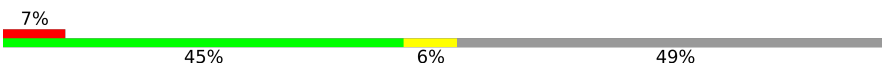
• Molecule 1: Spike glycoprotein





SER CYS GLN VAL THR HIS GLU GLY SER THR VAL GLU LYS THR VAL ALA ALA PRO THR GLU CYS SER

• Molecule 3: C1717 Fab Light Chain

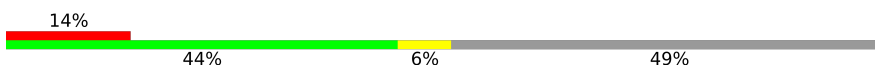
Chain E: 

Q1 A10 S11 G12 T13 P14 G15 Q16 N28 I29 V34 N35 W36 Y37 Q38 G42 T43 L47 L48 M49 D52 R55 P56 S57 G58 V59 F60 A61 R62 G78 S81 E82 D83 E84 R95 L110 GLN PRO LYS ALA ALA PRO SER VAL THR PRO

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

LEU THR PRO UNK TRP LYS SER HIS ARG SER TYR SER CYS GLN VAL THR HIS GLU GLY SER THR VAL LYS THR VAL ALA PRO THR CYS SER

• Molecule 3: C1717 Fab Light Chain

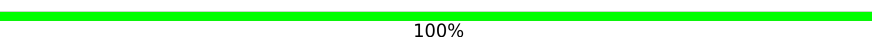
Chain G: 

Q1 L4 F7 A10 S11 G12 T13 P14 G15 Q16 R17 V18 T19 I20 S21 Q38 R39 L40 P41 Q42 T43 L48 S51 R62 F63 S64 G65 S66 R67 S73 L74 A75 I76 S77 G78 L79 R80 S81 E82 D83 E84 A85 D93 D94 R95 L96 K106 L110 GLY

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

SER ASN ASN LYS TYR ALA ALA SER SER TYR LEU SER LEU THR PRO UNK GLN TRP LYS SER HIS ARG SER TYR SER CYS GLN VAL THR GLY GLU LYS THR VAL THR CYS SER

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

Chain I: 

NAG1
NAG2

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

Chain J: 

NAG1
NAG2

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

Chain M: 



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



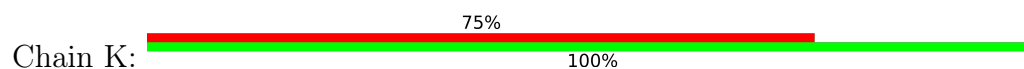
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	636528	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.951	Depositor
Minimum map value	-2.023	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.262	Depositor
Map size (Å)	368.064, 368.064, 368.064	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.852, 0.852, 0.852	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FUC, 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	0.24	0/7557	0.65	9/10304 (0.1%)
1	B	0.25	0/7669	0.75	18/10455 (0.2%)
1	C	0.25	0/7515	0.65	5/10257 (0.0%)
2	D	0.15	0/940	0.40	0/1278
2	F	0.15	0/940	0.41	0/1278
2	H	0.17	0/940	0.39	0/1278
3	E	0.13	0/814	0.38	0/1107
3	G	0.15	0/814	0.44	0/1107
3	L	0.18	0/814	0.49	2/1107 (0.2%)
All	All	0.23	0/28003	0.65	34/38171 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	1
All	All	0	5

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	432	CYS	CA-CB-SG	9.71	136.73	114.40
1	C	662	CYS	CA-CB-SG	8.40	133.72	114.40
1	B	604	THR	N-CA-C	8.01	122.98	112.72
1	B	234	ASN	CB-CA-C	-7.92	94.65	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	CYS	CA-CB-SG	7.85	132.46	114.40
1	A	717	ASN	N-CA-CB	7.84	123.53	111.46
1	A	283	GLY	N-CA-C	7.73	126.76	115.32
1	C	61	ASN	CB-CA-C	7.62	122.27	109.84
1	A	282	ASN	CB-CA-C	7.59	122.86	109.65
1	B	234	ASN	CA-CB-CG	7.35	119.95	112.60
1	A	1097	SER	CA-C-N	-5.94	113.46	121.71
1	A	1097	SER	C-N-CA	-5.94	113.46	121.71
1	A	538	CYS	CA-CB-SG	5.88	127.93	114.40
1	C	61	ASN	N-CA-CB	-5.81	100.95	109.95
1	B	232	GLY	N-CA-C	5.78	122.83	114.10
3	L	51	SER	CA-C-N	5.77	132.56	121.54
3	L	51	SER	C-N-CA	5.77	132.56	121.54
1	B	463	PRO	CA-N-CD	-5.64	104.10	112.00
1	B	234	ASN	CA-C-N	5.57	132.00	121.97
1	B	234	ASN	C-N-CA	5.57	132.00	121.97
1	B	136	CYS	CA-C-N	5.46	127.59	120.28
1	B	136	CYS	C-N-CA	5.46	127.59	120.28
1	A	602	THR	N-CA-C	5.39	119.48	113.01
1	B	158	ARG	N-CA-C	5.35	115.09	108.19
1	B	603	ASN	CA-C-N	-5.34	112.84	122.46
1	B	603	ASN	C-N-CA	-5.34	112.84	122.46
1	B	123	ALA	CA-C-N	-5.16	113.24	121.44
1	B	123	ALA	C-N-CA	-5.16	113.24	121.44
1	B	158	ARG	CA-C-N	5.10	131.16	121.97
1	B	158	ARG	C-N-CA	5.10	131.16	121.97
1	A	590	CYS	CA-CB-SG	5.07	126.06	114.40
1	A	1126	CYS	CA-CB-SG	5.07	126.07	114.40
1	C	62	VAL	N-CA-C	5.06	115.77	108.48
1	B	235	ILE	N-CA-C	-5.04	98.85	109.34

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	983	ARG	Sidechain
1	B	1039	ARG	Sidechain
1	B	567	ARG	Sidechain
1	B	995	ARG	Sidechain
1	C	567	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7393	0	7101	114	0
1	B	7505	0	7203	115	0
1	C	7355	0	6980	123	0
2	D	918	0	891	17	0
2	F	918	0	891	25	0
2	H	918	0	891	18	0
3	E	798	0	769	8	0
3	G	798	0	769	9	0
3	L	798	0	769	13	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	M	28	0	25	1	0
4	N	28	0	25	3	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
5	K	49	0	43	0	0
6	A	140	0	130	6	0
6	B	112	0	104	4	0
6	C	126	0	117	3	0
All	All	27996	0	26808	419	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 (419) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:SER:HG	2:F:2:VAL:N	1.61	0.98
1:A:226:LEU:HD23	1:A:227:VAL:HG23	1.48	0.95
1:B:379:CYS:HA	1:B:432:CYS:HB3	1.48	0.95
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.51	0.93
1:C:1134:ASN:HB3	6:C:1309:NAG:HN2	1.41	0.85
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.10	0.83
1:B:604:THR:HG21	1:B:687:VAL:HG11	1.61	0.82
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.61	0.82
1:B:203:ILE:HG12	1:B:227:VAL:HG22	1.63	0.80
1:C:216:LEU:HD11	1:C:266:TYR:HE2	1.46	0.79
1:B:158:ARG:O	1:B:160:TYR:N	2.17	0.76
1:C:1129:VAL:HG13	1:C:1132:ILE:HG21	1.67	0.76
1:A:788:ILE:HD12	1:A:872:GLN:HE22	1.51	0.75
3:E:38:GLN:HG2	3:E:48:LEU:HD11	1.69	0.74
1:C:650:LEU:HD21	1:C:653:ALA:HB3	1.69	0.74
1:C:517:LEU:HG	1:C:518:LEU:HG	1.67	0.74
1:A:603:ASN:OD1	6:A:1306:NAG:N2	2.22	0.73
1:C:34:ARG:NH2	1:C:191:GLU:OE2	2.21	0.73
1:C:918:GLU:N	1:C:918:GLU:OE1	2.21	0.73
1:B:104:TRP:HD1	1:B:238:PHE:HZ	1.37	0.73
1:A:436:TRP:HE1	1:A:509:ARG:HH21	1.34	0.72
1:A:1129:VAL:HB	1:A:1132:ILE:HD11	1.71	0.72
1:B:379:CYS:HA	1:B:432:CYS:CB	2.18	0.72
1:A:229:LEU:HD22	1:A:231:ILE:HB	1.72	0.72
1:C:378:LYS:NZ	1:C:380:TYR:OH	2.22	0.72
1:B:293:LEU:HD23	2:H:102:ALA:HB2	1.70	0.71
1:B:130:VAL:HG11	1:B:231:ILE:HG23	1.73	0.71
1:B:801:ASN:OD1	6:B:1306:NAG:N2	2.23	0.71
1:B:61:ASN:O	1:B:62:VAL:HG22	1.91	0.70
1:C:293:LEU:HD23	2:F:102:ALA:HB2	1.72	0.70
1:A:596:SER:OG	1:A:613:GLN:NE2	2.23	0.70
1:C:216:LEU:HD11	1:C:266:TYR:CE2	2.27	0.70
1:C:90:VAL:HG13	1:C:267:VAL:HG13	1.75	0.69
2:F:62:GLN:O	2:F:65:GLN:NE2	2.25	0.69
1:B:96:GLU:OE2	1:B:190:ARG:NH1	2.25	0.69
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.74	0.69
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.57	0.69
1:A:604:THR:O	2:D:2:VAL:N	2.25	0.69
1:A:122:ASN:OD1	1:A:125:ASN:N	2.24	0.68
1:B:384:PRO:HA	1:B:387:LEU:HD23	1.75	0.68
1:C:278:LYS:NZ	3:G:51:SER:OG	2.20	0.68
1:A:596:SER:HG	1:A:613:GLN:HE21	1.38	0.67
1:A:293:LEU:HD23	2:D:102:ALA:HB2	1.76	0.67
1:B:134:GLN:HE21	1:B:162:SER:HB3	1.60	0.67
1:B:367:VAL:HG23	1:B:368:LEU:HD12	1.78	0.66
1:A:606:ASN:HD21	2:D:28:THR:HA	1.60	0.66
1:B:605:SER:HG	2:H:2:VAL:N	1.94	0.66
1:C:560:LEU:HG	1:C:561:PRO:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:SER:OG	2:F:2:VAL:N	2.29	0.65
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.28	0.65
1:B:1017:GLU:HG2	1:C:1019:ARG:HH22	1.62	0.65
1:C:931:ILE:O	1:C:934:ILE:HG22	1.97	0.64
1:B:931:ILE:O	1:B:934:ILE:HG22	1.98	0.64
1:B:433:VAL:HG23	1:B:512:VAL:HG12	1.80	0.63
1:B:129:LYS:HA	1:B:168:PHE:O	1.98	0.63
1:B:1134:ASN:OD1	6:B:1308:NAG:N2	2.30	0.63
1:C:439:ASN:OD1	1:C:443:SER:OG	2.14	0.63
1:B:689:SER:O	1:B:690:GLN:HG3	1.99	0.63
1:A:497:PHE:O	1:A:498:GLN:C	2.40	0.63
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.80	0.63
2:H:12:LYS:NZ	2:H:17:SER:O	2.32	0.63
1:C:654:GLU:OE2	1:C:691:SER:OG	2.17	0.62
1:C:568:ASP:OD1	1:C:569:ILE:N	2.32	0.62
1:C:231:ILE:HG12	1:C:233:ILE:HG23	1.80	0.62
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.81	0.62
2:F:19:LYS:HD2	2:F:80:TYR:HB3	1.82	0.62
1:C:738:CYS:SG	1:C:739:THR:N	2.73	0.61
1:B:278:LYS:NZ	3:L:51:SER:OG	2.26	0.61
1:C:324:GLU:O	1:C:539:VAL:HG13	1.99	0.61
1:A:770:ILE:HD11	1:A:1015:ALA:HB2	1.82	0.61
1:A:671:CYS:SG	1:A:697:MET:HE2	2.41	0.61
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.83	0.61
1:A:1098:ASN:OD1	1:A:1099:GLY:N	2.31	0.61
1:C:383:SER:OG	1:C:386:LYS:HG3	2.01	0.61
1:A:117:LEU:HD12	1:A:231:ILE:HD13	1.81	0.60
1:B:140:PHE:O	1:B:158:ARG:NH1	2.35	0.60
2:F:99:HIS:CD2	2:F:100:HIS:H	2.18	0.60
1:A:355:ARG:HG2	1:A:357:ARG:NH1	2.17	0.60
1:A:498:GLN:CB	1:A:499:PRO:HD3	2.31	0.60
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.35	0.60
4:N:1:NAG:O3	4:N:2:NAG:O5	2.17	0.60
6:A:1303:NAG:H83	6:A:1303:NAG:H3	1.83	0.59
1:B:976:VAL:HG23	1:B:979:ASP:HB2	1.84	0.59
1:A:1103:PHE:HZ	6:A:1309:NAG:H62	1.66	0.59
1:C:64:TRP:CD1	1:C:266:TYR:HE1	2.21	0.59
1:C:811:LYS:HG3	1:C:812:PRO:HD2	1.84	0.59
1:B:53:ASP:OD1	1:B:54:LEU:N	2.33	0.59
1:C:495:TYR:OH	1:C:505:TYR:O	2.22	0.58
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:41:PRO:HD3	2:F:92:ALA:HA	1.86	0.58
1:A:122:ASN:HD21	1:A:125:ASN:HB2	1.69	0.58
4:M:1:NAG:H83	4:M:1:NAG:H3	1.85	0.58
1:B:555:SER:OG	1:B:586:ASP:HB2	2.04	0.58
1:A:449:TYR:HE1	1:A:496:GLY:HA2	1.68	0.57
1:C:379:CYS:HA	1:C:432:CYS:CB	2.31	0.57
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.87	0.57
1:A:45:SER:OG	1:A:281:GLU:O	2.20	0.56
1:C:231:ILE:HG23	1:C:233:ILE:HG12	1.87	0.56
2:D:86:LEU:HD21	2:D:119:VAL:HG21	1.87	0.56
1:A:777:ASN:OD1	1:A:1019:ARG:NH1	2.38	0.56
6:A:1305:NAG:H83	6:A:1305:NAG:H3	1.88	0.56
2:D:109:ASP:OD1	2:D:110:TYR:N	2.39	0.56
1:C:34:ARG:HH22	1:C:189:LEU:HD11	1.71	0.56
3:L:84:GLU:OE2	3:L:109:VAL:N	2.37	0.56
1:C:299:THR:HG22	1:C:308:VAL:HG11	1.88	0.56
1:B:115:GLN:HA	1:B:132:GLU:HG3	1.88	0.56
1:C:328:ARG:O	1:C:329:PHE:HD1	1.89	0.55
1:C:1134:ASN:OD1	1:C:1135:ASN:N	2.39	0.55
1:C:84:LEU:HD12	1:C:85:PRO:HD2	1.87	0.55
1:A:506:GLN:OE1	1:A:507:PRO:HD2	2.06	0.55
1:B:331:ASN:HB3	6:B:1304:NAG:N2	2.22	0.55
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.39	0.55
1:C:664:ILE:O	1:C:672:ALA:N	2.35	0.55
1:A:303:LEU:HD23	1:A:308:VAL:HG12	1.88	0.54
1:C:1126:CYS:HB2	1:C:1132:ILE:HD11	1.89	0.54
1:A:503:VAL:HG13	1:A:505:TYR:CE1	2.43	0.54
1:B:809:PRO:HA	1:B:814:LYS:HD3	1.89	0.54
1:A:402:ILE:HD11	1:A:510:VAL:HG21	1.89	0.54
1:C:367:VAL:HG23	1:C:368:LEU:HD22	1.89	0.54
1:A:506:GLN:CD	1:A:507:PRO:HD2	2.33	0.54
1:C:336:CYS:SG	1:C:358:ILE:HG23	2.48	0.54
1:C:604:THR:O	2:F:2:VAL:N	2.41	0.54
1:A:31:SER:OG	1:A:60:SER:N	2.41	0.54
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.40	0.53
1:A:433:VAL:HG23	1:A:512:VAL:HG22	1.91	0.53
1:B:296:LEU:O	1:B:299:THR:HG22	2.08	0.53
1:C:656:VAL:HG11	1:C:693:ILE:HD12	1.90	0.53
2:F:40:ALA:HA	2:F:92:ALA:HA	1.89	0.53
1:A:393:THR:HA	1:A:522:ALA:HA	1.89	0.53
1:C:28:TYR:HD2	6:C:1301:NAG:O5	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:THR:O	2:H:2:VAL:N	2.41	0.53
1:C:761:THR:HG22	1:C:765:ARG:NH1	2.23	0.53
1:A:503:VAL:C	1:A:505:TYR:H	2.16	0.53
1:B:334:ASN:O	1:B:362:VAL:HG12	2.07	0.53
1:B:596:SER:OG	1:B:613:GLN:OE1	2.21	0.53
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.32	0.53
2:F:33:ALA:HB3	2:F:99:HIS:HB3	1.90	0.53
1:A:877:LEU:HD13	1:A:1029:MET:HE2	1.91	0.53
1:B:1017:GLU:HG2	1:C:1019:ARG:NH2	2.23	0.53
1:C:130:VAL:HG12	1:C:168:PHE:HB3	1.90	0.53
1:C:170:TYR:CE2	1:C:172:SER:HB2	2.44	0.53
1:C:231:ILE:HD13	1:C:233:ILE:HD13	1.91	0.52
1:C:1129:VAL:HG13	1:C:1132:ILE:CG2	2.39	0.52
1:C:741:TYR:CE1	1:C:966:LEU:HD11	2.45	0.52
1:A:800:PHE:HE1	1:A:924:ALA:HA	1.73	0.52
6:A:1302:NAG:H3	6:A:1302:NAG:H83	1.91	0.52
1:A:280:ASN:OD1	1:A:281:GLU:N	2.40	0.52
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.43	0.52
2:F:36:TRP:HB3	2:F:48:MET:HE3	1.92	0.52
1:A:287:ASP:OD2	2:D:104:ALA:HB3	2.10	0.51
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.92	0.51
1:B:560:LEU:HB3	1:B:561:PRO:HD2	1.92	0.51
1:C:715:PRO:HA	1:C:1071:GLN:O	2.10	0.51
1:B:199:GLY:HA2	1:B:232:GLY:HA2	1.92	0.51
1:B:552:LEU:HD23	1:B:585:LEU:HD13	1.92	0.51
1:B:707:TYR:HD1	1:C:883:THR:HG23	1.76	0.51
1:C:816:SER:OG	1:C:819:GLU:HG2	2.10	0.51
1:A:130:VAL:HG12	1:A:130:VAL:O	2.11	0.51
1:A:393:THR:OG1	1:A:516:GLU:O	2.27	0.51
1:B:393:THR:HA	1:B:522:ALA:HA	1.92	0.51
1:B:492:LEU:H	1:B:492:LEU:HD23	1.75	0.51
1:B:1125:ASN:ND2	1:B:1127:ASP:OD2	2.44	0.51
1:A:396:TYR:HB2	1:A:514:SER:OG	2.11	0.51
1:C:334:ASN:O	1:C:362:VAL:HG12	2.11	0.51
1:A:503:VAL:O	1:A:505:TYR:N	2.42	0.51
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.44	0.51
1:A:1103:PHE:CZ	6:A:1309:NAG:H62	2.45	0.51
1:C:87:ASN:OD1	1:C:88:ASP:N	2.43	0.51
1:B:748:GLU:O	1:B:752:LEU:HD12	2.11	0.51
1:B:983:ARG:HH11	1:B:983:ARG:CB	2.23	0.51
1:B:316:SER:OG	1:B:317:ASN:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:LYS:HE3	1:A:1019:ARG:HH22	1.76	0.50
1:A:1139:ASP:OD1	1:A:1139:ASP:N	2.43	0.50
3:L:28:ASN:OD1	3:L:29:ILE:N	2.44	0.50
3:E:55:ARG:NH1	3:E:59:VAL:O	2.44	0.50
1:A:357:ARG:HH21	1:A:396:TYR:HA	1.77	0.50
1:A:907:ASN:HD22	1:A:913:GLN:HE21	1.59	0.50
1:C:662:CYS:SG	1:C:697:MET:HE3	2.51	0.50
1:C:1014:ARG:O	1:C:1017:GLU:HG2	2.12	0.50
2:F:87:THR:N	2:F:90:ASP:OD2	2.36	0.50
2:F:6:GLN:NE2	2:F:114:GLY:H	2.09	0.50
1:A:355:ARG:HG2	1:A:357:ARG:HH12	1.75	0.50
1:A:495:TYR:HB3	1:A:497:PHE:CE1	2.47	0.50
1:B:214:ARG:H	1:B:214:ARG:HD3	1.76	0.50
1:B:331:ASN:HB3	6:B:1304:NAG:C7	2.42	0.50
2:H:54:VAL:HG13	2:H:55:LEU:HD13	1.93	0.50
3:L:4:LEU:HD21	3:L:29:ILE:HD11	1.94	0.50
3:L:80:ARG:HG2	3:L:81:SER:H	1.76	0.50
1:B:117:LEU:HD13	1:B:231:ILE:HD13	1.94	0.49
1:A:355:ARG:C	1:A:357:ARG:HH12	2.20	0.49
1:B:662:CYS:HB2	1:B:697:MET:HB3	1.95	0.49
1:B:200:TYR:HE2	1:B:230:PRO:HB3	1.77	0.49
1:C:200:TYR:CE1	1:C:230:PRO:HB3	2.47	0.49
1:A:449:TYR:CE1	1:A:496:GLY:HA2	2.45	0.49
1:C:1090:PRO:HG3	1:C:1095:PHE:CE2	2.48	0.49
1:A:562:PHE:O	1:B:41:LYS:NZ	2.41	0.49
1:A:645:THR:OG1	1:A:648:GLY:O	2.20	0.49
1:B:983:ARG:HH11	1:B:983:ARG:HB3	1.77	0.49
3:L:4:LEU:HD23	3:L:22:CYS:SG	2.52	0.49
2:F:6:GLN:HE21	2:F:114:GLY:H	1.61	0.49
1:C:1126:CYS:HB2	1:C:1132:ILE:CD1	2.43	0.49
1:C:743:CYS:SG	1:C:750:SER:N	2.85	0.48
2:F:38:ARG:O	2:F:46:GLU:N	2.40	0.48
1:B:328:ARG:HG3	1:B:543:PHE:HE1	1.79	0.48
1:C:853:GLN:O	1:C:854:LYS:HE2	2.13	0.48
1:C:912:THR:OG1	1:C:914:ASN:OD1	2.17	0.48
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.95	0.48
3:E:28:ASN:OD1	3:E:29:ILE:HG12	2.13	0.48
1:C:595:VAL:HG22	1:C:612:TYR:HD1	1.79	0.48
1:C:1077:THR:HG22	1:C:1078:ALA:N	2.29	0.48
1:C:814:LYS:HG3	1:C:814:LYS:O	2.14	0.48
1:B:83:VAL:HG21	1:B:237:ARG:HH21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:HB3	1:B:235:ILE:HG23	1.96	0.47
1:B:1116:THR:HG22	1:B:1117:THR:N	2.29	0.47
1:C:560:LEU:HD23	1:C:562:PHE:CE2	2.49	0.47
1:C:1105:THR:HG22	1:C:1112:PRO:HA	1.96	0.47
2:D:25:SER:OG	2:D:26:GLY:N	2.48	0.47
3:G:66:SER:OG	3:G:73:SER:OG	2.32	0.47
1:B:212:LEU:HD12	1:B:212:LEU:O	2.14	0.47
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.96	0.47
1:C:646:ARG:HG3	1:C:646:ARG:O	2.13	0.47
1:B:131:CYS:CB	1:B:166:CYS:HA	2.44	0.47
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.48	0.47
1:B:176:LEU:HG	1:B:190:ARG:HD2	1.96	0.47
1:C:344:ALA:HB3	1:C:347:PHE:HE2	1.78	0.47
3:G:13:THR:HG23	3:G:16:GLN:OE1	2.13	0.47
1:A:646:ARG:HD2	1:A:646:ARG:O	2.15	0.47
1:A:921:LYS:HB2	1:A:921:LYS:HE2	1.65	0.47
1:B:329:PHE:O	1:B:580:GLN:NE2	2.45	0.47
1:C:36:VAL:HG11	1:C:220:PHE:CE2	2.50	0.47
2:F:25:SER:OG	2:F:26:GLY:N	2.47	0.47
3:G:93:ASP:OD2	3:G:96:LEU:N	2.41	0.47
1:C:551:VAL:HG22	1:C:588:THR:O	2.15	0.47
2:F:6:GLN:HE22	2:F:112:GLY:HA3	1.79	0.47
1:B:40:ASP:OD1	1:B:40:ASP:N	2.47	0.46
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.97	0.46
3:E:36:TRP:HD1	3:E:49:MET:HB2	1.80	0.46
1:B:203:ILE:CG1	1:B:227:VAL:HG22	2.41	0.46
2:H:29:PHE:HE2	2:H:77:SER:HA	1.80	0.46
1:A:102:ARG:HG3	1:A:102:ARG:HH11	1.81	0.46
1:B:567:ARG:HH11	1:B:567:ARG:HB2	1.80	0.46
1:B:707:TYR:CD1	1:C:883:THR:HG23	2.50	0.46
1:A:517:LEU:HD23	1:A:517:LEU:H	1.79	0.46
2:H:25:SER:OG	2:H:26:GLY:N	2.47	0.46
3:G:38:GLN:HB3	3:G:48:LEU:HD11	1.97	0.46
1:B:551:VAL:HG22	1:B:588:THR:O	2.16	0.46
1:A:819:GLU:OE2	1:A:1055:SER:OG	2.27	0.46
1:B:786:LYS:HG3	1:B:787:GLN:HG3	1.97	0.46
1:C:617:CYS:HB3	1:C:649:CYS:HB3	1.90	0.46
1:C:736:VAL:HG22	1:C:858:LEU:HD23	1.97	0.46
1:A:971:GLY:C	1:A:995:ARG:HH11	2.24	0.46
1:B:309:GLU:HG2	1:B:313:TYR:OH	2.16	0.46
1:A:350:VAL:O	1:A:353:TRP:HE3	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:HD12	1:B:873:TYR:CZ	2.51	0.46
2:D:54:VAL:HG13	2:D:55:LEU:HG	1.97	0.46
1:A:497:PHE:CZ	1:A:507:PRO:HD3	2.51	0.45
1:B:1037:SER:OG	1:B:1039:ARG:HG2	2.16	0.45
1:C:973:ILE:HG23	1:C:992:GLN:OE1	2.15	0.45
1:A:617:CYS:HB3	1:A:649:CYS:HB3	1.92	0.45
1:C:391:CYS:HB3	1:C:524:VAL:O	2.17	0.45
1:C:867:ASP:OD1	1:C:868:GLU:N	2.50	0.45
1:C:36:VAL:HG11	1:C:220:PHE:CZ	2.51	0.45
6:C:1309:NAG:O7	6:C:1309:NAG:O3	2.29	0.45
1:A:409:GLN:NE2	1:A:415:THR:O	2.30	0.45
1:C:328:ARG:C	1:C:329:PHE:HD1	2.25	0.45
1:C:200:TYR:HE1	1:C:230:PRO:HB3	1.82	0.45
1:C:523:THR:HG23	1:C:524:VAL:HG23	1.99	0.45
1:C:531:THR:HG22	1:C:532:ASN:N	2.32	0.45
2:D:108:PHE:O	3:E:47:LEU:HD21	2.16	0.45
1:A:533:LEU:HD11	1:A:535:LYS:HE3	1.97	0.45
1:C:568:ASP:HB2	1:C:574:ASP:HB2	1.98	0.45
1:C:170:TYR:HE2	1:C:172:SER:HB2	1.81	0.45
1:C:338:PHE:CE2	1:C:358:ILE:HD13	2.51	0.45
1:C:662:CYS:HB3	1:C:671:CYS:HB2	1.81	0.45
1:B:121:ASN:OD1	1:B:126:VAL:HG12	2.17	0.44
1:C:28:TYR:CD1	1:C:63:THR:HA	2.52	0.44
2:H:48:MET:SD	2:H:81:MET:HE1	2.56	0.44
1:A:538:CYS:HB3	1:A:590:CYS:HB3	1.81	0.44
1:A:979:ASP:OD1	1:A:980:ILE:N	2.51	0.44
1:C:94:SER:OG	1:C:101:ILE:HG13	2.17	0.44
1:A:30:ASN:HD21	1:A:59:PHE:HD1	1.63	0.44
1:C:48:LEU:HD21	1:C:278:LYS:HG3	1.99	0.44
1:C:205:SER:OG	1:C:226:LEU:HD22	2.17	0.44
2:F:18:VAL:HG12	2:F:83:LEU:HB2	2.00	0.44
1:A:1116:THR:HG22	1:A:1117:THR:N	2.32	0.44
1:B:273:ARG:NH2	1:B:290:ASP:OD1	2.51	0.44
1:C:948:LEU:O	1:C:951:VAL:HG22	2.17	0.44
1:A:168:PHE:CE2	1:A:229:LEU:HD21	2.52	0.44
1:A:724:THR:OG1	1:A:934:ILE:HD11	2.18	0.44
1:A:811:LYS:HE2	1:A:811:LYS:HB2	1.74	0.44
1:B:40:ASP:OD2	1:B:44:ARG:NH1	2.42	0.44
1:A:100:ILE:HG22	1:A:242:LEU:HB2	1.99	0.44
1:A:391:CYS:SG	1:A:392:PHE:N	2.90	0.44
1:C:541:PHE:CZ	1:C:587:ILE:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:GLN:OE1	1:C:699:LEU:HD13	2.18	0.44
2:H:50:ARG:NH1	2:H:52:ILE:HD11	2.33	0.44
1:A:523:THR:HG23	1:A:524:VAL:HG13	2.00	0.44
1:B:58:PHE:CE2	1:B:290:ASP:HB2	2.53	0.44
1:B:136:CYS:SG	1:B:159:VAL:HA	2.58	0.44
1:B:605:SER:HB3	1:B:607:GLN:OE1	2.18	0.44
1:C:342:PHE:HE2	1:C:511:VAL:HG21	1.83	0.44
1:C:533:LEU:HD23	1:C:533:LEU:H	1.83	0.44
2:F:83:LEU:HD23	2:F:83:LEU:HA	1.90	0.44
3:G:18:VAL:HG22	3:G:79:LEU:HD11	1.99	0.44
2:D:76:THR:O	2:D:77:SER:OG	2.34	0.43
1:B:546:LEU:HD21	1:B:573:THR:HG21	2.00	0.43
3:L:64:SER:O	3:L:74:LEU:HD12	2.19	0.43
1:A:64:TRP:CD1	1:A:266:TYR:HE1	2.37	0.43
1:B:27:ALA:O	1:B:28:TYR:HD1	2.02	0.43
1:B:503:VAL:HA	1:B:506:GLN:NE2	2.32	0.43
1:C:914:ASN:O	1:C:918:GLU:OE1	2.37	0.43
1:B:65:PHE:CE2	1:B:84:LEU:HD21	2.54	0.43
1:B:101:ILE:HD12	1:B:265:TYR:OH	2.19	0.43
3:E:38:GLN:CG	3:E:48:LEU:HD11	2.44	0.43
1:A:375:SER:HB2	1:A:436:TRP:HA	2.00	0.43
1:C:124:THR:CG2	1:C:174:PRO:HG3	2.49	0.43
1:C:344:ALA:HB3	1:C:347:PHE:CE2	2.53	0.43
1:A:931:ILE:O	1:A:934:ILE:HG22	2.18	0.43
1:B:130:VAL:O	1:B:130:VAL:HG13	2.18	0.43
2:H:30:ASN:HA	2:H:54:VAL:HB	2.01	0.43
2:H:76:THR:O	2:H:77:SER:OG	2.34	0.43
2:D:103:VAL:HG21	2:D:107:TYR:HE1	1.82	0.43
1:A:106:PHE:HB2	1:A:117:LEU:HB3	2.01	0.43
1:A:307:THR:HB	3:E:57:SER:HB2	2.01	0.43
2:D:5:VAL:HG23	2:D:23:LYS:HB3	2.00	0.43
1:B:194:PHE:HD1	1:B:203:ILE:HG22	1.83	0.43
2:H:16:SER:O	2:H:86:LEU:HD23	2.18	0.43
1:A:30:ASN:OD1	1:A:59:PHE:HA	2.18	0.43
1:A:814:LYS:HE3	1:A:814:LYS:HB2	1.82	0.43
1:B:58:PHE:CD2	1:B:290:ASP:HB2	2.54	0.43
1:B:562:PHE:O	1:C:41:LYS:NZ	2.41	0.43
1:C:559:PHE:HB3	1:C:577:ARG:NH2	2.34	0.43
2:D:68:ILE:HD11	2:D:81:MET:HE3	2.00	0.43
1:A:226:LEU:HD23	1:A:227:VAL:CG2	2.34	0.43
1:A:240:THR:HG22	1:A:241:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ARG:HA	1:B:491:PRO:O	2.19	0.43
1:A:125:ASN:O	1:A:174:PRO:HG3	2.19	0.42
1:A:273:ARG:HE	1:A:292:ALA:HB3	1.84	0.42
1:B:702:GLU:OE2	1:C:790:LYS:NZ	2.52	0.42
1:C:124:THR:HG22	1:C:174:PRO:HG3	2.01	0.42
1:C:709:ASN:OD1	1:C:709:ASN:O	2.37	0.42
1:A:1082:CYS:HB2	1:A:1126:CYS:HB2	1.88	0.42
1:B:131:CYS:HB2	1:B:166:CYS:HA	2.02	0.42
1:B:326:ILE:O	1:B:326:ILE:HG13	2.19	0.42
1:A:326:ILE:O	1:A:326:ILE:HG13	2.19	0.42
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	2.00	0.42
1:C:662:CYS:HB2	1:C:671:CYS:HB3	1.63	0.42
1:A:531:THR:HG22	1:A:532:ASN:N	2.34	0.42
1:A:822:LEU:HD21	1:A:938:LEU:HD21	2.01	0.42
1:C:56:LEU:HD12	1:C:57:PRO:HD2	2.00	0.42
2:F:88:SER:HA	2:F:119:VAL:HG11	2.02	0.42
1:A:350:VAL:HB	1:A:401:VAL:O	2.19	0.42
1:B:197:ILE:HD11	1:B:202:LYS:NZ	2.33	0.42
1:A:567:ARG:HD3	1:A:571:ASP:HA	2.02	0.42
1:C:379:CYS:CA	1:C:432:CYS:HB3	2.25	0.42
2:H:32:PHE:HD1	2:H:99:HIS:O	2.02	0.42
2:H:40:ALA:HB3	2:H:43:GLN:HB2	2.02	0.42
1:C:303:LEU:HD23	1:C:308:VAL:HG12	2.02	0.42
1:C:341:VAL:HG23	1:C:342:PHE:CD2	2.55	0.42
1:C:559:PHE:O	1:C:577:ARG:NH2	2.51	0.42
1:A:907:ASN:ND2	1:A:913:GLN:HE21	2.18	0.42
1:B:336:CYS:HB2	1:B:338:PHE:CE2	2.54	0.42
1:B:48:LEU:CD2	1:B:278:LYS:HG3	2.50	0.42
1:B:200:TYR:CE2	1:B:230:PRO:HB3	2.54	0.42
1:C:618:THR:O	1:C:618:THR:HG22	2.19	0.42
1:A:825:LYS:HA	1:A:825:LYS:HD3	1.83	0.41
1:B:121:ASN:OD1	1:B:122:ASN:N	2.53	0.41
1:B:216:LEU:HA	1:B:217:PRO:HD3	1.76	0.41
1:B:307:THR:HB	3:L:57:SER:HB2	2.02	0.41
1:B:334:ASN:O	1:B:362:VAL:N	2.41	0.41
1:C:361:CYS:O	1:C:524:VAL:HG13	2.19	0.41
2:F:10:GLU:HG3	2:F:18:VAL:HG21	2.01	0.41
2:F:72:ALA:HA	2:F:79:ALA:HA	2.02	0.41
2:F:103:VAL:HG11	2:F:107:TYR:HE1	1.85	0.41
3:G:95:ARG:HA	3:G:95:ARG:HD2	1.89	0.41
1:B:342:PHE:HE1	1:B:511:VAL:HG11	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:811:LYS:HG3	1:C:812:PRO:CD	2.49	0.41
1:B:603:ASN:OD1	4:N:1:NAG:H2	2.21	0.41
3:L:28:ASN:OD1	3:L:29:ILE:HG12	2.19	0.41
1:A:503:VAL:C	1:A:505:TYR:N	2.79	0.41
1:A:1031:GLU:OE1	1:C:1039:ARG:HB3	2.20	0.41
1:B:50:SER:OG	1:B:304:LYS:NZ	2.54	0.41
1:B:278:LYS:NZ	3:L:51:SER:O	2.53	0.41
1:B:603:ASN:OD1	4:N:1:NAG:H4	2.21	0.41
2:D:19:LYS:NZ	2:D:21:SER:HB3	2.35	0.41
1:B:1090:PRO:HG3	1:B:1095:PHE:CE2	2.55	0.41
3:G:13:THR:HA	3:G:14:PRO:HD3	1.95	0.41
1:A:201:PHE:HE2	1:A:203:ILE:HD11	1.85	0.41
1:A:418:ILE:HD12	1:A:418:ILE:H	1.85	0.41
1:B:328:ARG:HG3	1:B:543:PHE:CE1	2.56	0.41
1:B:398:ASP:HB2	1:B:512:VAL:CG2	2.50	0.41
2:H:13:LYS:HD2	2:H:14:PRO:HD2	2.02	0.41
2:D:99:HIS:NE2	2:D:106:PRO:HA	2.35	0.41
2:D:37:VAL:C	2:D:48:MET:HE1	2.45	0.41
1:A:1111:GLU:OE1	1:A:1111:GLU:HA	2.20	0.41
1:C:462:LYS:HE3	1:C:462:LYS:HB2	1.67	0.41
3:L:51:SER:O	3:L:52:ASP:OD1	2.39	0.41
1:A:776:LYS:HE2	1:A:1019:ARG:HH12	1.86	0.41
2:H:91:THR:HB	2:H:119:VAL:HG22	2.03	0.41
1:A:190:ARG:HG2	1:A:207:HIS:ND1	2.36	0.41
1:A:555:SER:HB3	1:A:586:ASP:CG	2.46	0.41
2:H:29:PHE:CE2	2:H:77:SER:HA	2.55	0.40
2:D:40:ALA:HB3	2:D:43:GLN:HB2	2.02	0.40
1:A:604:THR:HG22	1:A:605:SER:OG	2.21	0.40
1:A:736:VAL:HG22	1:A:858:LEU:HG	2.03	0.40
1:B:33:THR:HA	1:B:58:PHE:CD1	2.56	0.40
1:B:703:ASN:OD1	1:B:703:ASN:C	2.64	0.40
1:B:1072:GLU:H	1:B:1072:GLU:CD	2.28	0.40
3:L:70:THR:O	3:L:70:THR:HG22	2.22	0.40
1:A:328:ARG:HH21	1:A:533:LEU:HD23	1.86	0.40
1:B:822:LEU:O	1:B:826:VAL:HG12	2.22	0.40
3:E:34:VAL:HG22	3:E:52:ASP:OD1	2.22	0.40
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.37	0.40
1:B:538:CYS:HB2	1:B:590:CYS:HB3	1.89	0.40
1:C:211:ASN:HB2	3:G:95:ARG:NH1	2.36	0.40
2:H:69:THR:HB	2:H:82:GLU:OE1	2.22	0.40
2:F:68:ILE:HG12	2:F:83:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:99:HIS:NE2	2:F:106:PRO:HA	2.37	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	A	944/1256 (75%)	895 (95%)	44 (5%)	5 (0%)	24	57
1	B	959/1256 (76%)	901 (94%)	52 (5%)	6 (1%)	21	54
1	C	950/1256 (76%)	913 (96%)	37 (4%)	0	100	100
2	D	118/227 (52%)	111 (94%)	7 (6%)	0	100	100
2	F	118/227 (52%)	113 (96%)	5 (4%)	0	100	100
2	H	118/227 (52%)	112 (95%)	6 (5%)	0	100	100
3	E	108/216 (50%)	102 (94%)	5 (5%)	1 (1%)	14	47
3	G	108/216 (50%)	100 (93%)	7 (6%)	1 (1%)	14	47
3	L	108/216 (50%)	101 (94%)	6 (6%)	1 (1%)	14	47
All	All	3531/5097 (69%)	3348 (95%)	169 (5%)	14 (0%)	31	62

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	498	GLN
1	A	499	PRO
1	B	159	VAL
1	B	285	ILE
1	A	32	PHE
1	A	110	LEU
1	A	504	GLY

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Mol	Chain	Res	Type
1	B	62	VAL
3	L	62	ARG
3	E	62	ARG
3	G	62	ARG
1	B	218	GLN
1	B	235	ILE
1	B	123	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	804/1096 (73%)	801 (100%)	3 (0%)	84	81
1	B	820/1096 (75%)	820 (100%)	0	100	100
1	C	788/1096 (72%)	788 (100%)	0	100	100
2	D	98/192 (51%)	98 (100%)	0	100	100
2	F	98/192 (51%)	98 (100%)	0	100	100
2	H	98/192 (51%)	98 (100%)	0	100	100
3	E	90/180 (50%)	90 (100%)	0	100	100
3	G	90/180 (50%)	90 (100%)	0	100	100
3	L	90/180 (50%)	90 (100%)	0	100	100
All	All	2976/4404 (68%)	2973 (100%)	3 (0%)	87	87

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

Mol	Chain	Res	Type
1	A	503	VAL
1	A	505	TYR
1	A	506	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	A	334	ASN
1	A	422	ASN
1	A	606	ASN
1	A	613	GLN
1	A	703	ASN
1	A	774	GLN
1	A	872	GLN
1	A	901	GLN
1	A	913	GLN
1	B	134	GLN
1	B	644	GLN
1	B	774	GLN
1	B	872	GLN
1	B	901	GLN
1	B	955	ASN
1	B	1010	GLN
1	C	1002	GLN
1	C	1005	GLN
1	C	1071	GLN
1	C	1088	HIS
1	C	1106	GLN
1	C	1108	ASN
3	L	16	GLN
3	L	35	ASN
3	E	16	GLN
3	E	35	ASN
3	E	39	HIS
3	E	54	GLN
2	F	6	GLN
2	F	62	GLN
2	F	99	HIS
3	G	35	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 ⓘ

16 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	I	1	4,1	14,14,15	0.38	0	17,19,21	0.55	0
4	NAG	I	2	4	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	J	1	4,1	14,14,15	1.11	1 (7%)	17,19,21	0.78	0
4	NAG	J	2	4	14,14,15	0.45	0	17,19,21	0.47	0
5	NAG	K	1	5,1	14,14,15	0.31	0	17,19,21	0.44	0
5	NAG	K	2	5	14,14,15	0.28	0	17,19,21	0.49	0
5	BMA	K	3	5	11,11,12	0.58	0	15,15,17	0.70	0
5	FUC	K	4	5	10,10,11	0.63	0	14,14,16	0.85	0
4	NAG	M	1	4,1	14,14,15	0.56	0	17,19,21	1.32	1 (5%)
4	NAG	M	2	4	14,14,15	0.26	0	17,19,21	0.38	0
4	NAG	N	1	4,1	14,14,15	1.19	2 (14%)	17,19,21	1.22	1 (5%)
4	NAG	N	2	4	14,14,15	0.42	0	17,19,21	0.68	1 (5%)
4	NAG	O	1	4,1	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	O	2	4	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	P	1	4,1	14,14,15	0.20	0	17,19,21	0.74	0
4	NAG	P	2	4	14,14,15	0.31	0	17,19,21	0.43	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	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	K	4	5	-	-	0/1/1/1
4	NAG	M	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	N	2	4	-	1/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	P	2	4	-	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)
4	J	1	NAG	O5-C1	-3.91	1.37	1.43
4	N	1	NAG	O5-C1	3.62	1.49	1.43
4	N	1	NAG	C1-C2	2.46	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1	NAG	C2-N2-C7	4.53	128.97	122.90
4	N	1	NAG	C1-O5-C5	4.51	118.23	112.19
4	N	2	NAG	C1-O5-C5	2.38	115.37	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	1	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
4	O	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6

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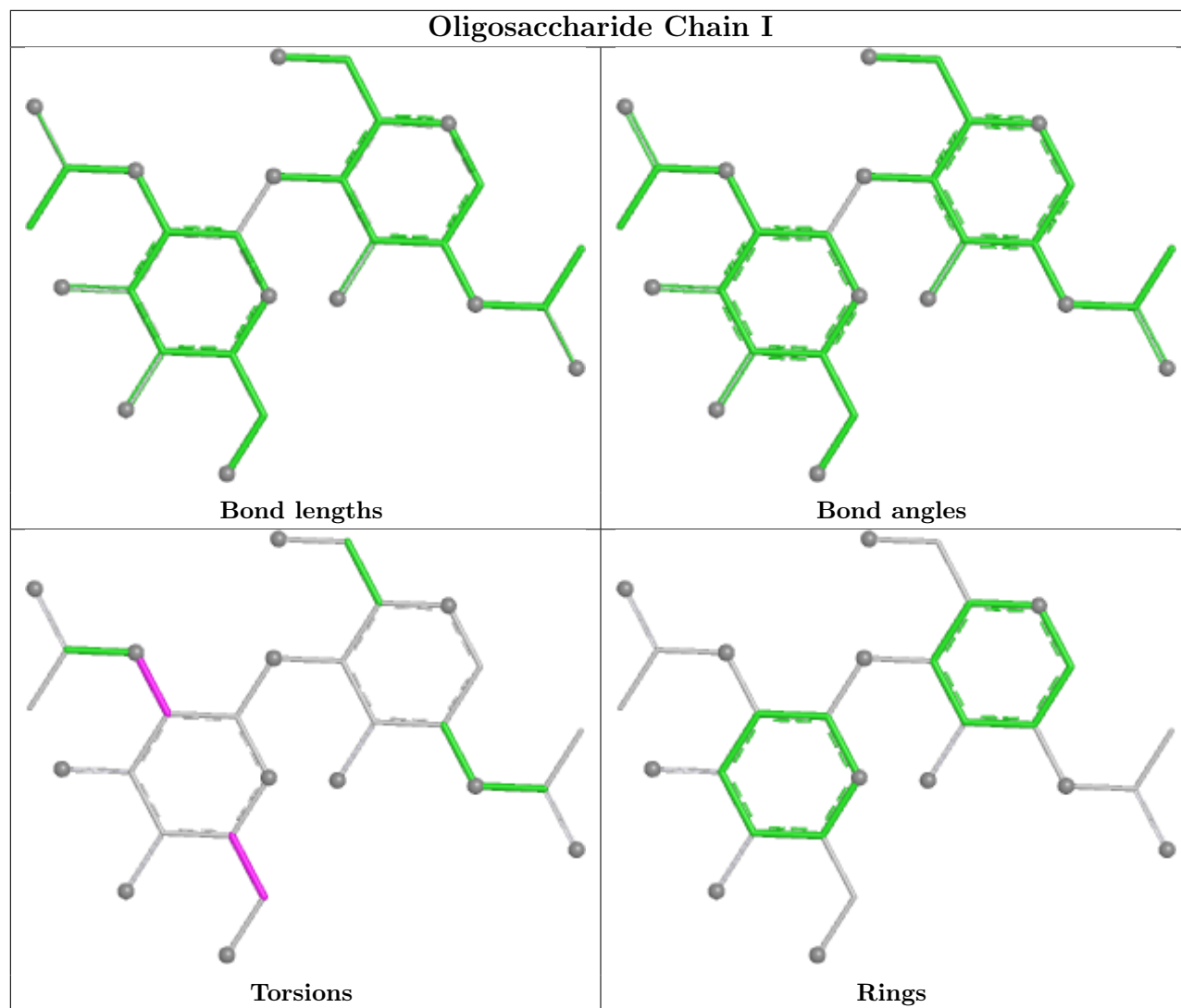
Mol	Chain	Res	Type	Atoms
4	P	1	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C1-C2-N2-C7
5	K	1	NAG	O5-C5-C6-O6
4	N	1	NAG	C3-C2-N2-C7
4	P	1	NAG	C3-C2-N2-C7
4	M	1	NAG	C1-C2-N2-C7
4	N	2	NAG	C1-C2-N2-C7
4	P	1	NAG	C1-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7
4	M	1	NAG	C3-C2-N2-C7

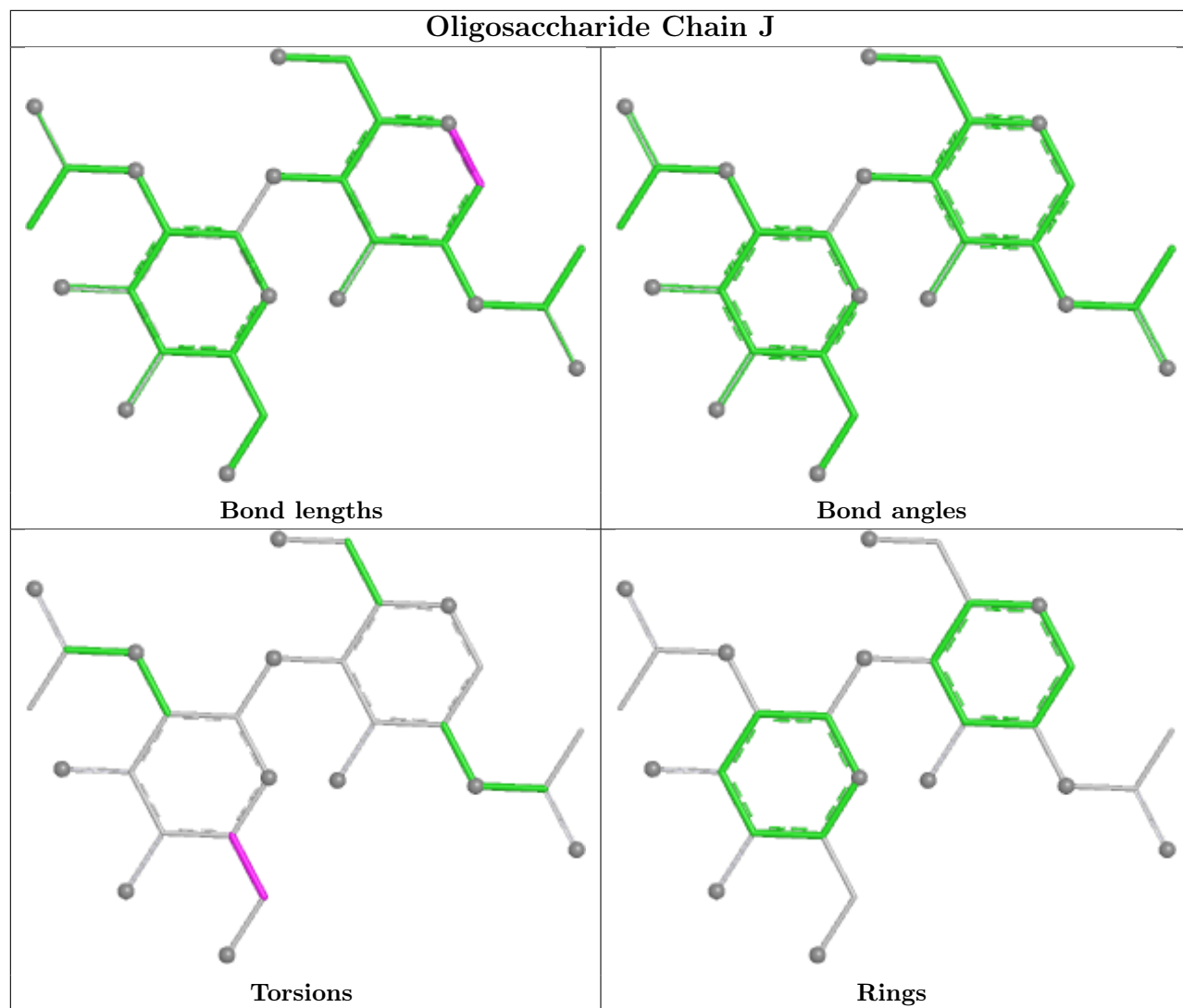
There are no ring outliers.

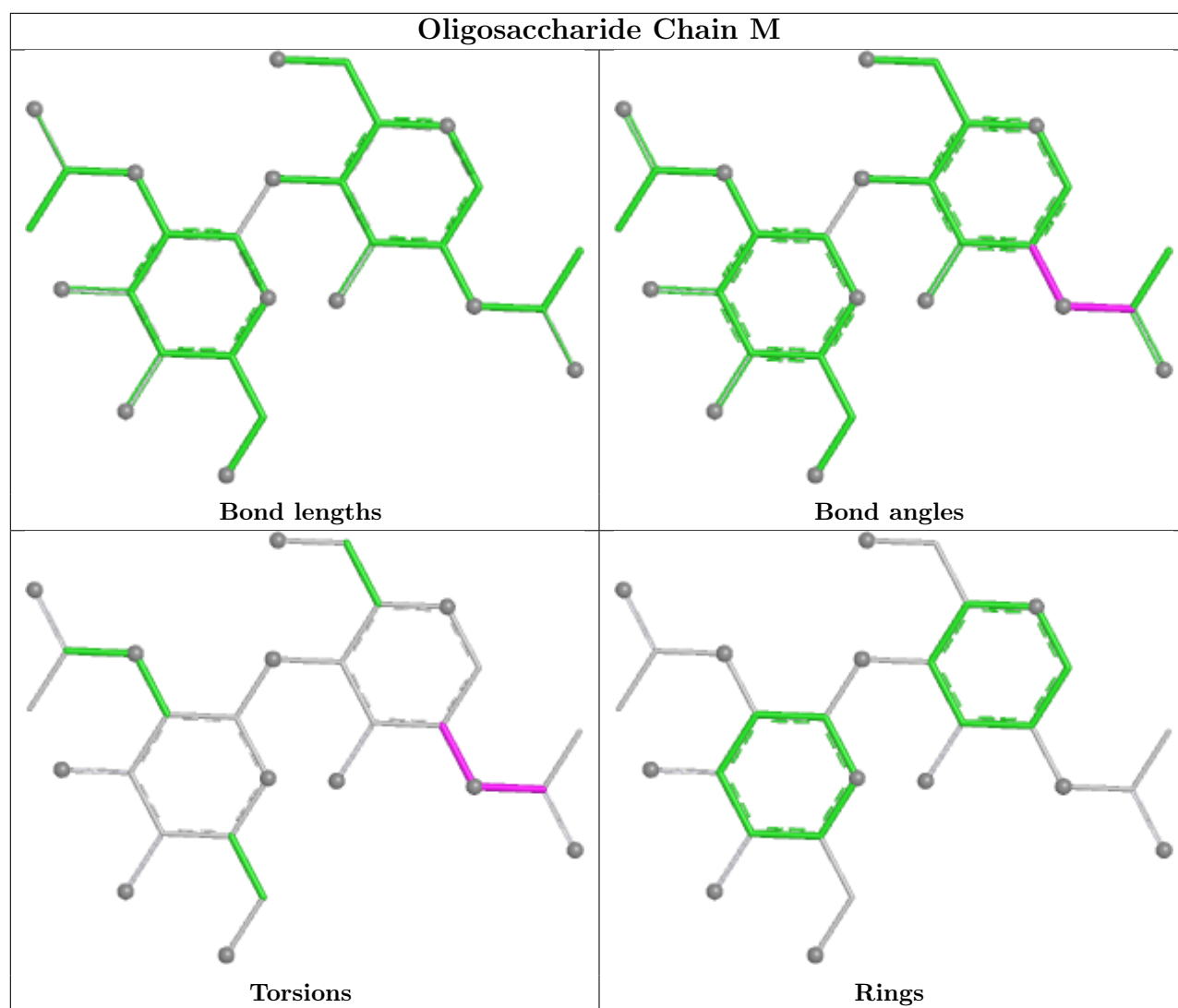
3 monomers are involved in 4 short contacts:

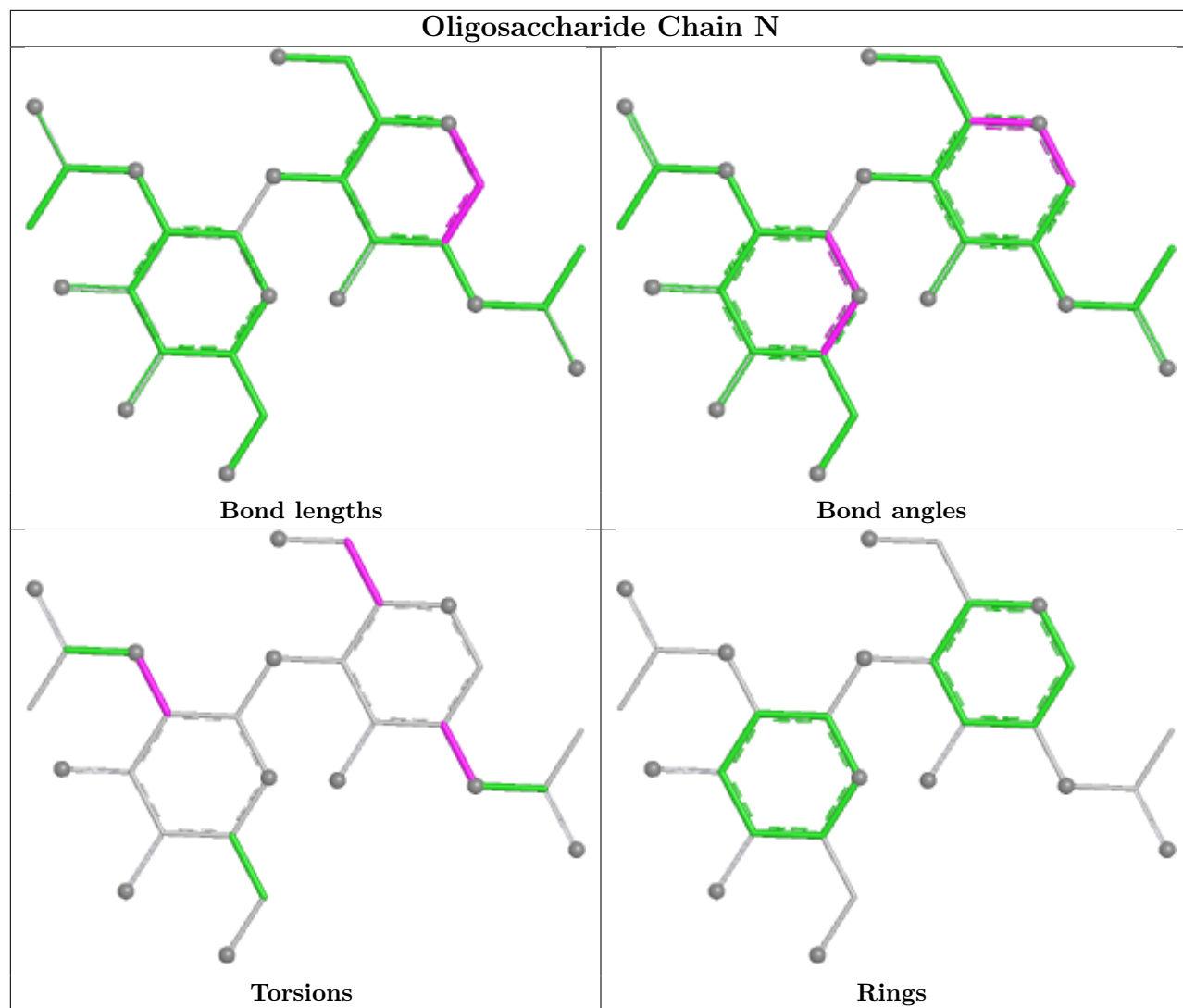
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	2	NAG	1	0
4	M	1	NAG	1	0
4	N	1	NAG	3	0

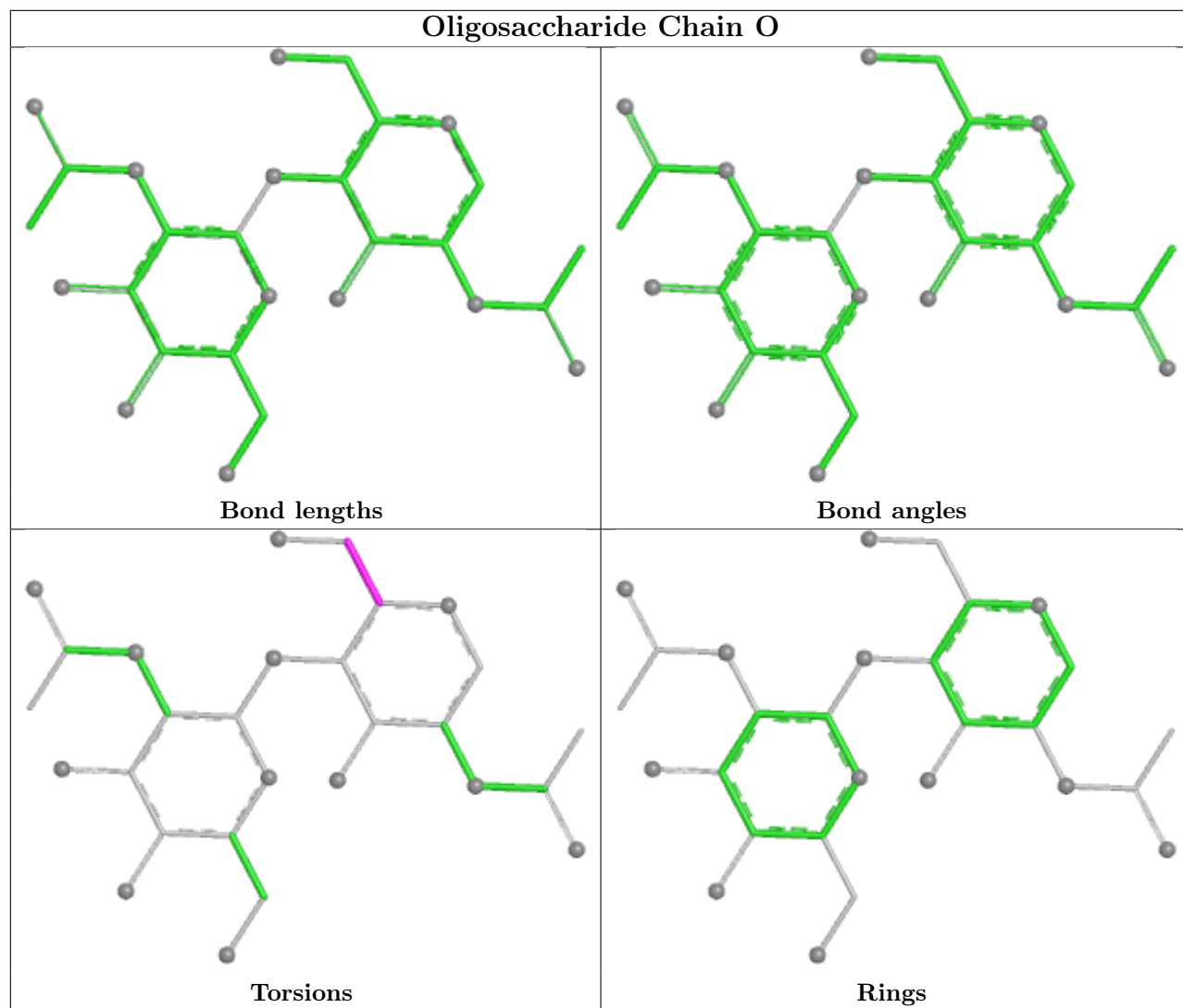
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

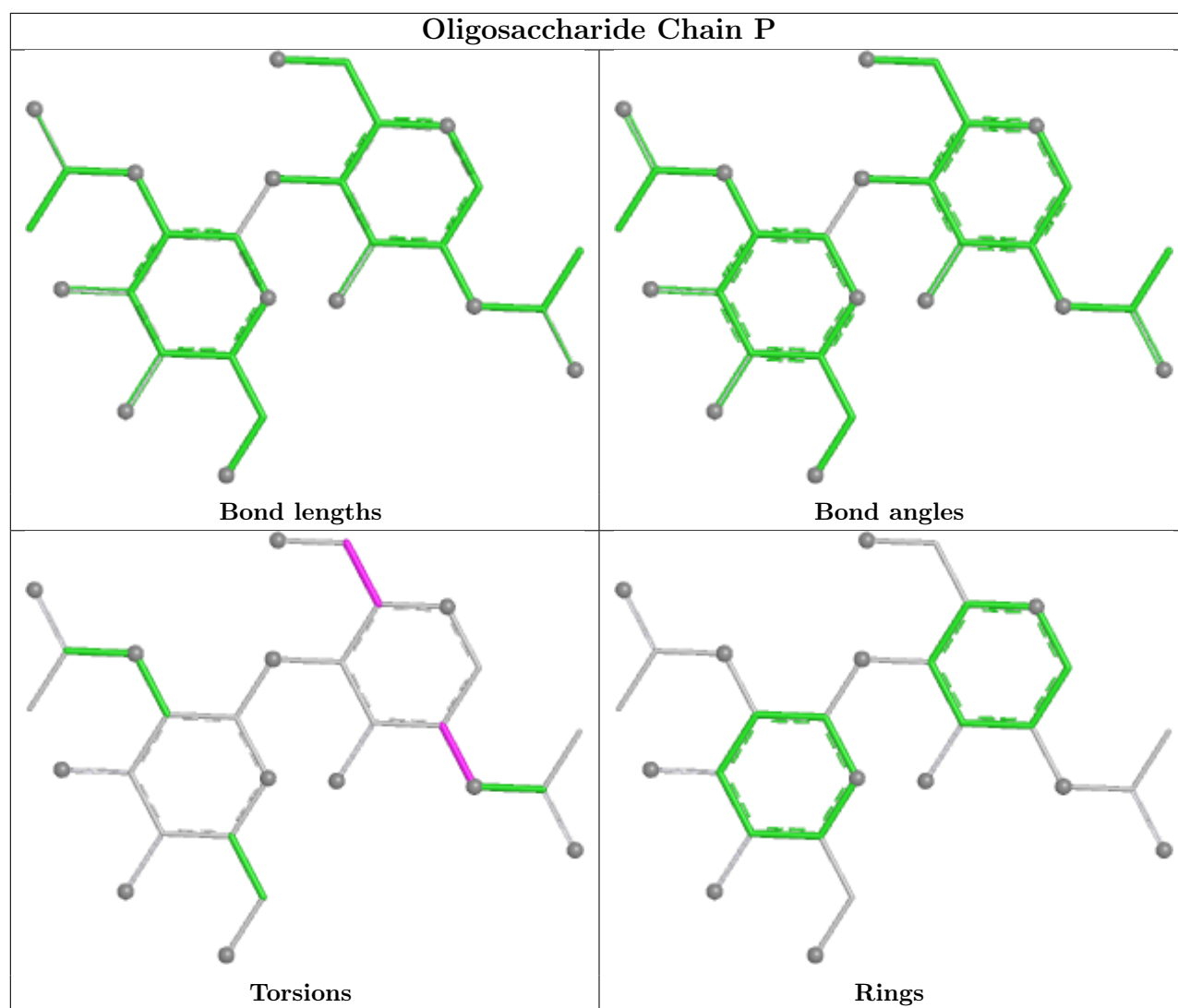


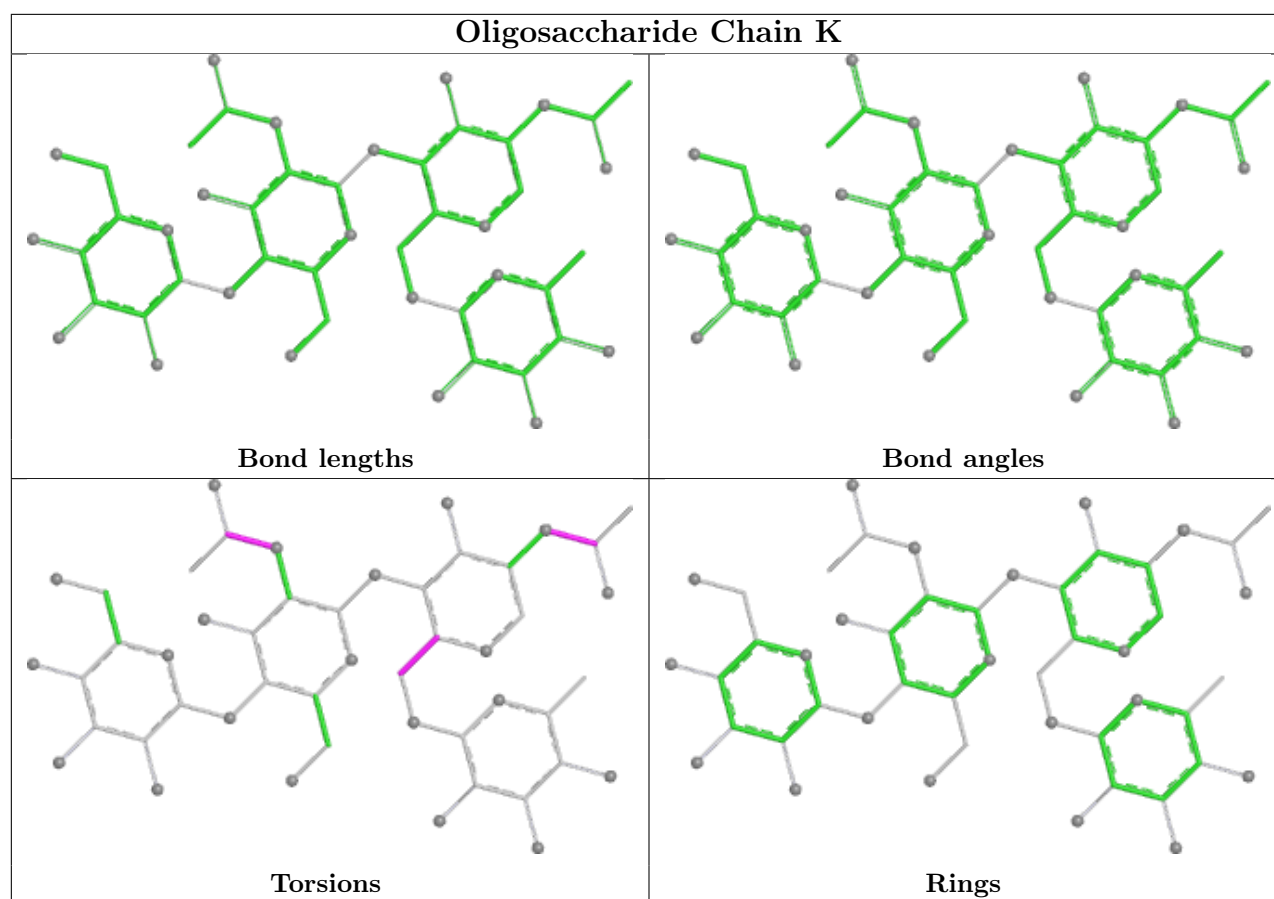












5.6 Ligand geometry [i](#)

27 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	$\# Z > 2$
6	NAG	B	1302	1	14,14,15	0.26	0	17,19,21	0.51	0
6	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.56	0
6	NAG	A	1307	1	14,14,15	0.24	0	17,19,21	0.56	0
6	NAG	B	1304	1	14,14,15	0.72	1 (7%)	17,19,21	0.77	1 (5%)
6	NAG	A	1304	1	14,14,15	0.30	0	17,19,21	0.82	1 (5%)
6	NAG	C	1309	1	14,14,15	0.54	0	17,19,21	0.56	0
6	NAG	A	1305	1	14,14,15	0.42	0	17,19,21	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	1305	1	14,14,15	0.28	0	17,19,21	0.47	0
6	NAG	B	1306	1	14,14,15	0.92	1 (7%)	17,19,21	0.65	1 (5%)
6	NAG	A	1309	1	14,14,15	0.28	0	17,19,21	0.55	0
6	NAG	C	1301	1	14,14,15	0.44	0	17,19,21	0.40	0
6	NAG	A	1310	1	14,14,15	0.23	0	17,19,21	0.51	0
6	NAG	B	1301	1	14,14,15	0.29	0	17,19,21	0.47	0
6	NAG	B	1307	1	14,14,15	0.23	0	17,19,21	0.56	0
6	NAG	C	1307	1	14,14,15	0.25	0	17,19,21	0.53	0
6	NAG	C	1308	1	14,14,15	0.48	0	17,19,21	0.66	0
6	NAG	C	1302	1	14,14,15	0.20	0	17,19,21	0.48	0
6	NAG	C	1304	1	14,14,15	0.24	0	17,19,21	0.41	0
6	NAG	B	1308	1	14,14,15	0.64	0	17,19,21	0.87	1 (5%)
6	NAG	B	1303	1	14,14,15	0.22	0	17,19,21	0.48	0
6	NAG	A	1308	1	14,14,15	0.25	0	17,19,21	0.52	0
6	NAG	A	1306	1	14,14,15	0.82	1 (7%)	17,19,21	0.61	0
6	NAG	A	1301	1	14,14,15	0.42	0	17,19,21	0.49	0
6	NAG	C	1306	1	14,14,15	0.44	0	17,19,21	0.61	0
6	NAG	A	1303	1	14,14,15	0.39	0	17,19,21	1.33	2 (11%)
6	NAG	C	1303	1	14,14,15	0.41	0	17,19,21	0.50	0
6	NAG	A	1302	1	14,14,15	0.63	1 (7%)	17,19,21	1.32	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	6/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1309	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1310	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	6/6/23/26	0/1/1/1
6	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1306	NAG	C1-C2	2.78	1.56	1.52
6	A	1306	NAG	C1-C2	2.62	1.55	1.52
6	B	1304	NAG	C1-C2	2.43	1.55	1.52
6	A	1302	NAG	C1-C2	2.15	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1305	NAG	C2-N2-C7	4.58	129.04	122.90
6	A	1303	NAG	C2-N2-C7	4.57	129.02	122.90
6	A	1302	NAG	C2-N2-C7	4.52	128.96	122.90
6	B	1308	NAG	C1-O5-C5	2.77	115.89	112.19
6	A	1304	NAG	C1-O5-C5	2.76	115.88	112.19
6	B	1304	NAG	C1-O5-C5	2.66	115.75	112.19
6	A	1302	NAG	C1-C2-N2	2.37	114.17	110.43
6	A	1303	NAG	C1-C2-N2	2.08	113.71	110.43
6	A	1305	NAG	C1-C2-N2	2.08	113.71	110.43
6	B	1306	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1306	NAG	C4-C5-C6-O6
6	C	1305	NAG	C4-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6
6	C	1305	NAG	O5-C5-C6-O6
6	A	1305	NAG	O5-C5-C6-O6
6	B	1306	NAG	O5-C5-C6-O6
6	C	1306	NAG	O5-C5-C6-O6
6	C	1309	NAG	O5-C5-C6-O6
6	A	1305	NAG	C4-C5-C6-O6
6	A	1310	NAG	O5-C5-C6-O6
6	B	1304	NAG	O5-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	C	1306	NAG	C4-C5-C6-O6
6	A	1306	NAG	O5-C5-C6-O6
6	B	1303	NAG	C4-C5-C6-O6
6	C	1302	NAG	O5-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
6	C	1304	NAG	C4-C5-C6-O6
6	C	1307	NAG	O5-C5-C6-O6
6	B	1306	NAG	C4-C5-C6-O6
6	C	1308	NAG	O5-C5-C6-O6
6	C	1309	NAG	C4-C5-C6-O6
6	A	1310	NAG	C4-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6
6	A	1302	NAG	C8-C7-N2-C2
6	A	1302	NAG	O7-C7-N2-C2
6	A	1303	NAG	C8-C7-N2-C2
6	A	1303	NAG	O7-C7-N2-C2
6	A	1305	NAG	C8-C7-N2-C2
6	A	1305	NAG	O7-C7-N2-C2
6	B	1304	NAG	C8-C7-N2-C2
6	B	1304	NAG	O7-C7-N2-C2
6	B	1304	NAG	C4-C5-C6-O6
6	A	1303	NAG	C4-C5-C6-O6
6	A	1304	NAG	O5-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6
6	C	1302	NAG	C4-C5-C6-O6
6	A	1309	NAG	C4-C5-C6-O6
6	A	1307	NAG	O5-C5-C6-O6
6	A	1308	NAG	O5-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	1301	NAG	O5-C5-C6-O6
6	B	1307	NAG	O5-C5-C6-O6
6	C	1307	NAG	C4-C5-C6-O6
6	A	1309	NAG	O5-C5-C6-O6
6	B	1303	NAG	C1-C2-N2-C7
6	C	1308	NAG	C4-C5-C6-O6
6	A	1302	NAG	C3-C2-N2-C7
6	A	1303	NAG	C3-C2-N2-C7
6	A	1307	NAG	C3-C2-N2-C7
6	A	1309	NAG	C3-C2-N2-C7
6	B	1303	NAG	C3-C2-N2-C7
6	B	1307	NAG	C3-C2-N2-C7
6	B	1308	NAG	C3-C2-N2-C7
6	C	1308	NAG	C3-C2-N2-C7
6	C	1309	NAG	C3-C2-N2-C7
6	A	1304	NAG	C4-C5-C6-O6
6	A	1302	NAG	C1-C2-N2-C7
6	A	1303	NAG	C1-C2-N2-C7
6	A	1305	NAG	C1-C2-N2-C7
6	A	1307	NAG	C1-C2-N2-C7
6	A	1309	NAG	C1-C2-N2-C7
6	B	1307	NAG	C1-C2-N2-C7
6	B	1308	NAG	C1-C2-N2-C7
6	C	1308	NAG	C1-C2-N2-C7
6	A	1305	NAG	C3-C2-N2-C7

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1304	NAG	2	0
6	C	1309	NAG	2	0
6	A	1305	NAG	1	0
6	B	1306	NAG	1	0
6	A	1309	NAG	2	0
6	C	1301	NAG	1	0
6	B	1308	NAG	1	0
6	A	1306	NAG	1	0
6	A	1303	NAG	1	0
6	A	1302	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

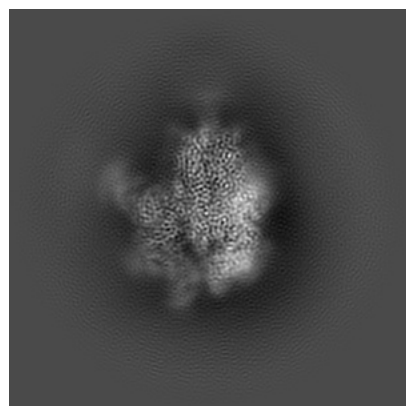
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26431. These allow visual inspection of the internal detail of the map and identification of artifacts.

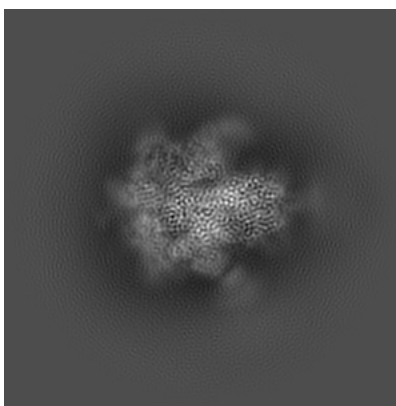
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

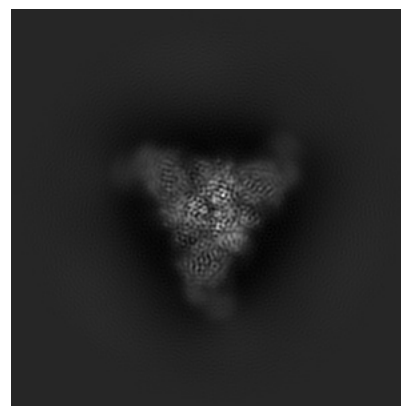
6.1.1 Primary map



X

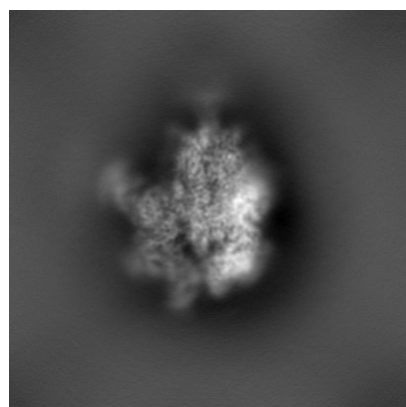


Y

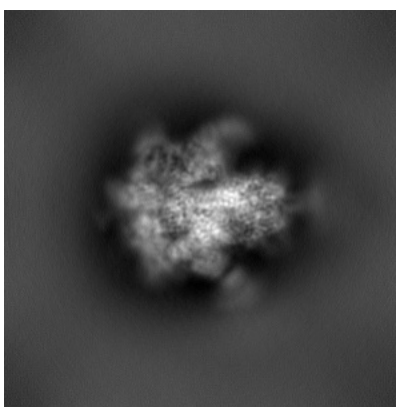


Z

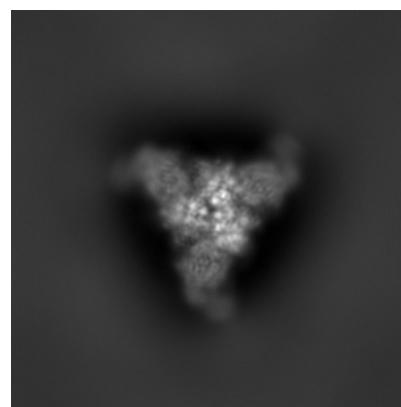
6.1.2 Raw map



X



Y

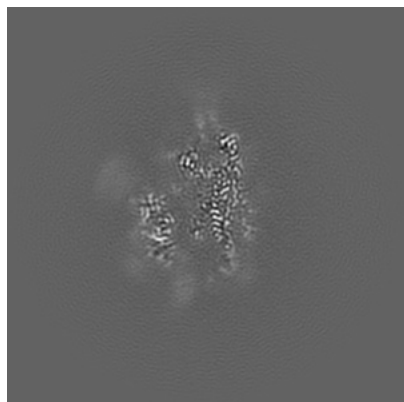


Z

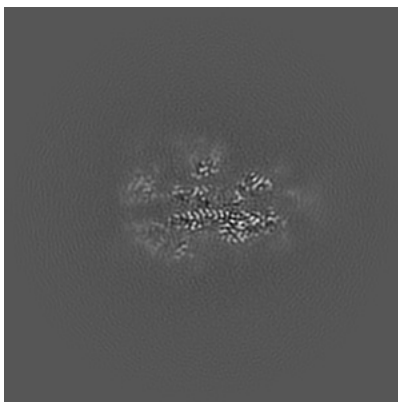
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

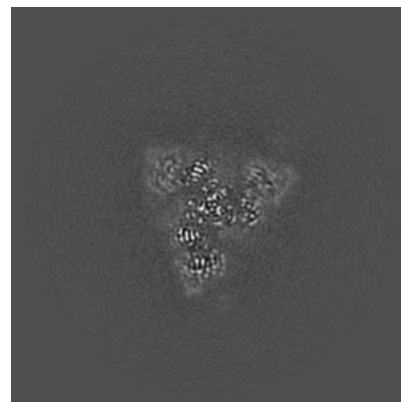
6.2.1 Primary map



X Index: 216

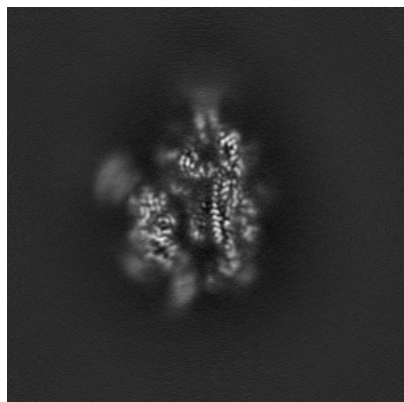


Y Index: 216

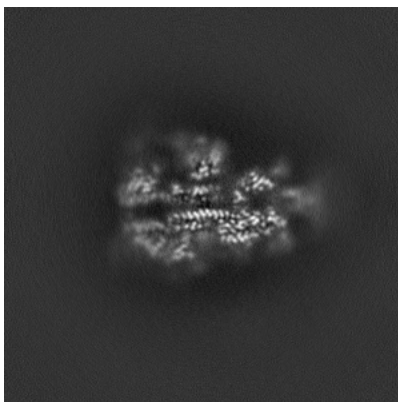


Z Index: 216

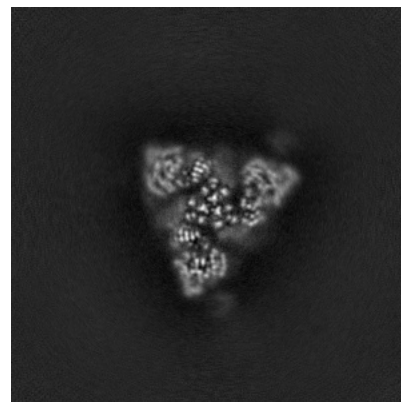
6.2.2 Raw map



X Index: 216



Y Index: 216

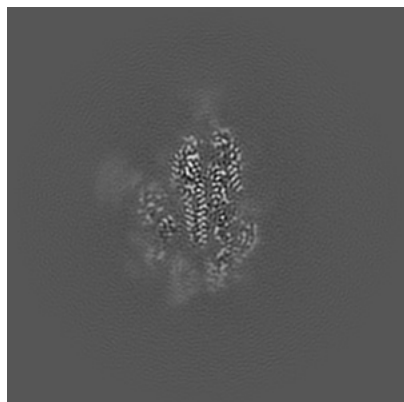


Z Index: 216

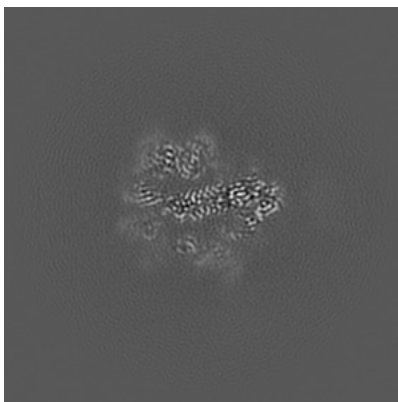
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

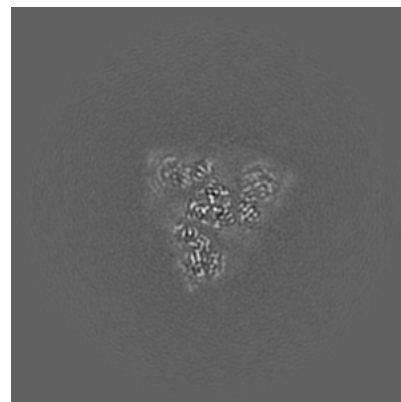
6.3.1 Primary map



X Index: 223

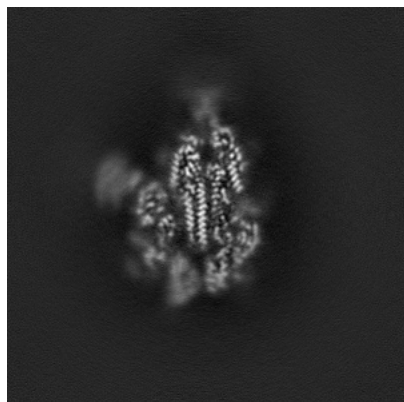


Y Index: 232

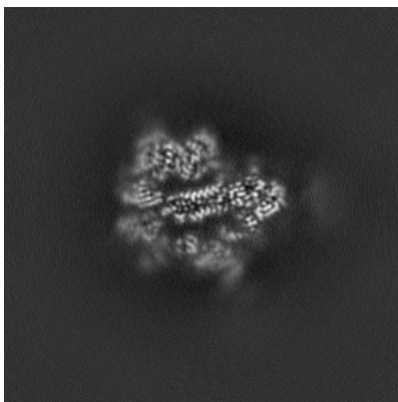


Z Index: 211

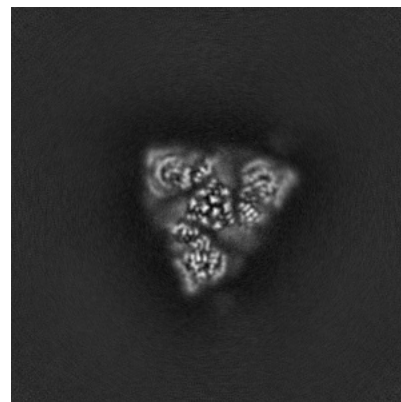
6.3.2 Raw map



X Index: 223



Y Index: 232

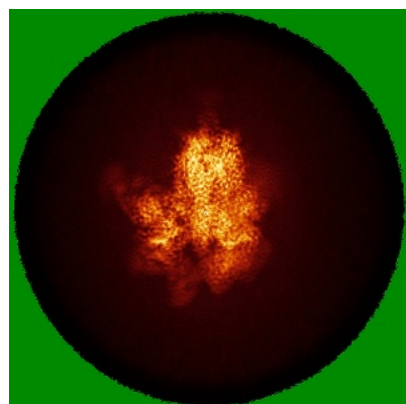


Z Index: 212

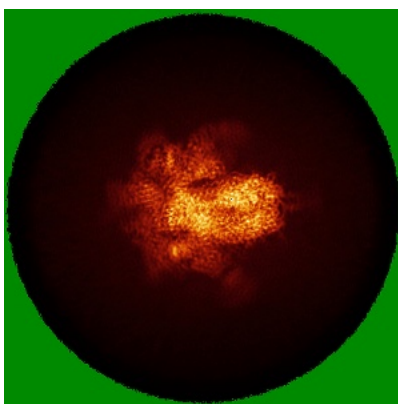
The images above show the largest variance slices of the map in three orthogonal directions.

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

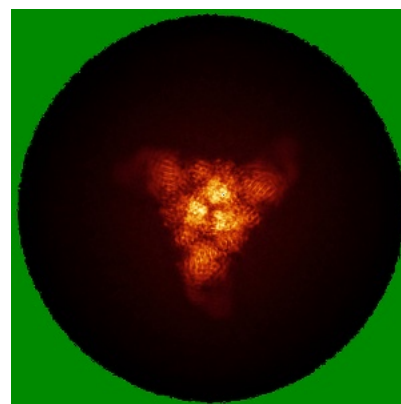
6.4.1 Primary map



X

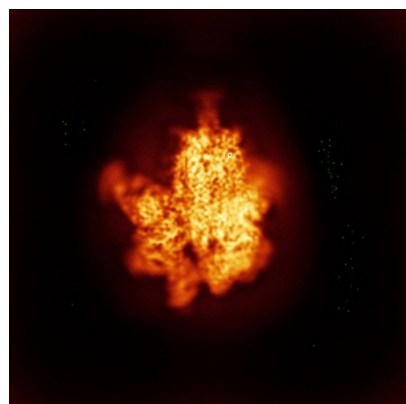


Y

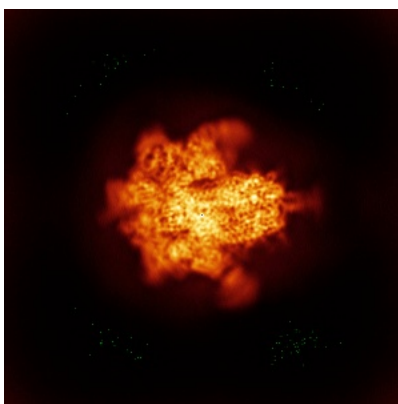


Z

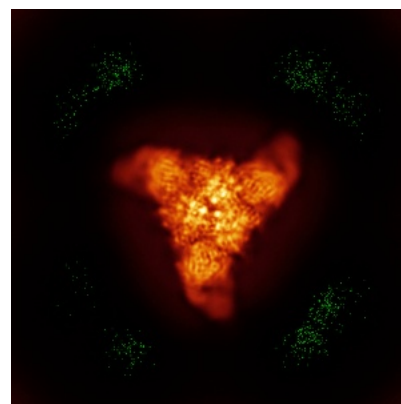
6.4.2 Raw map



X



Y

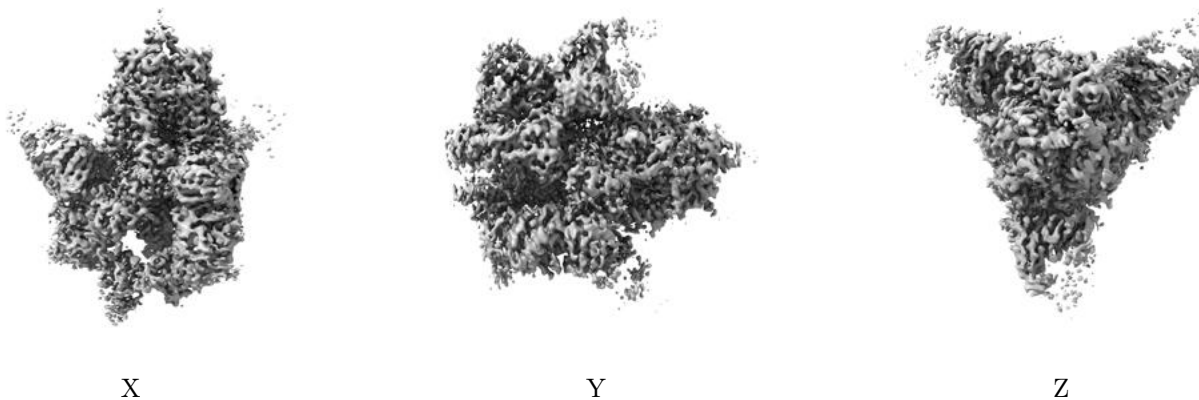


Z

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.

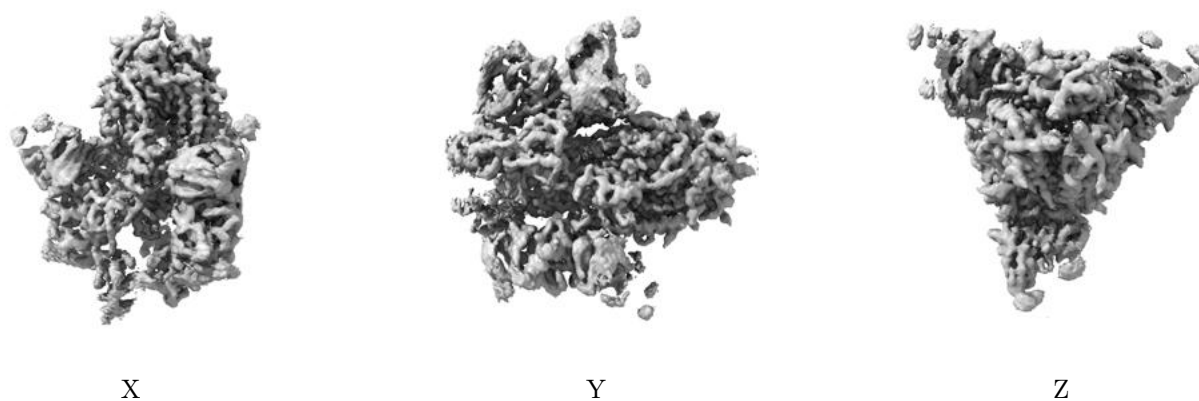
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.262. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

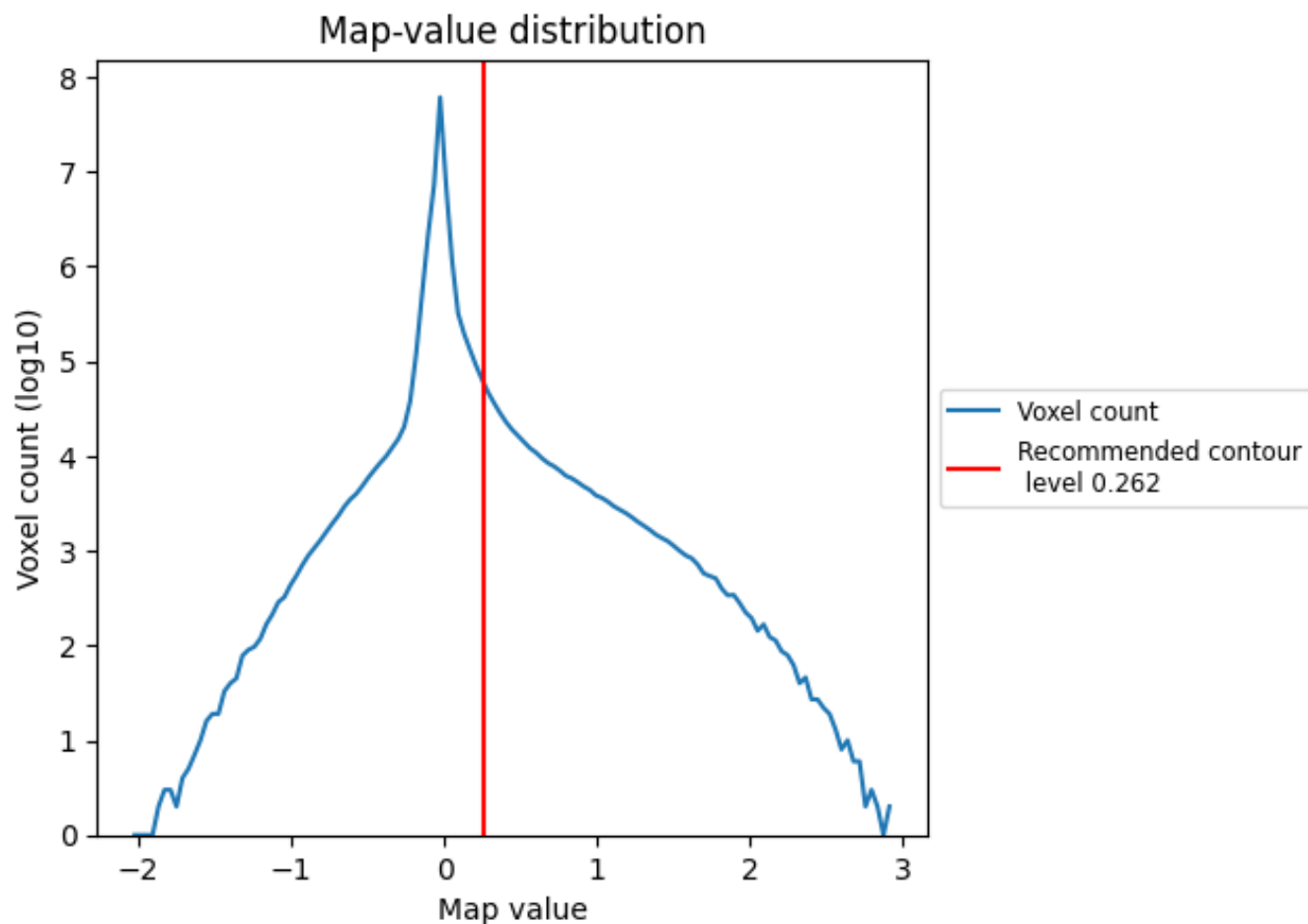
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

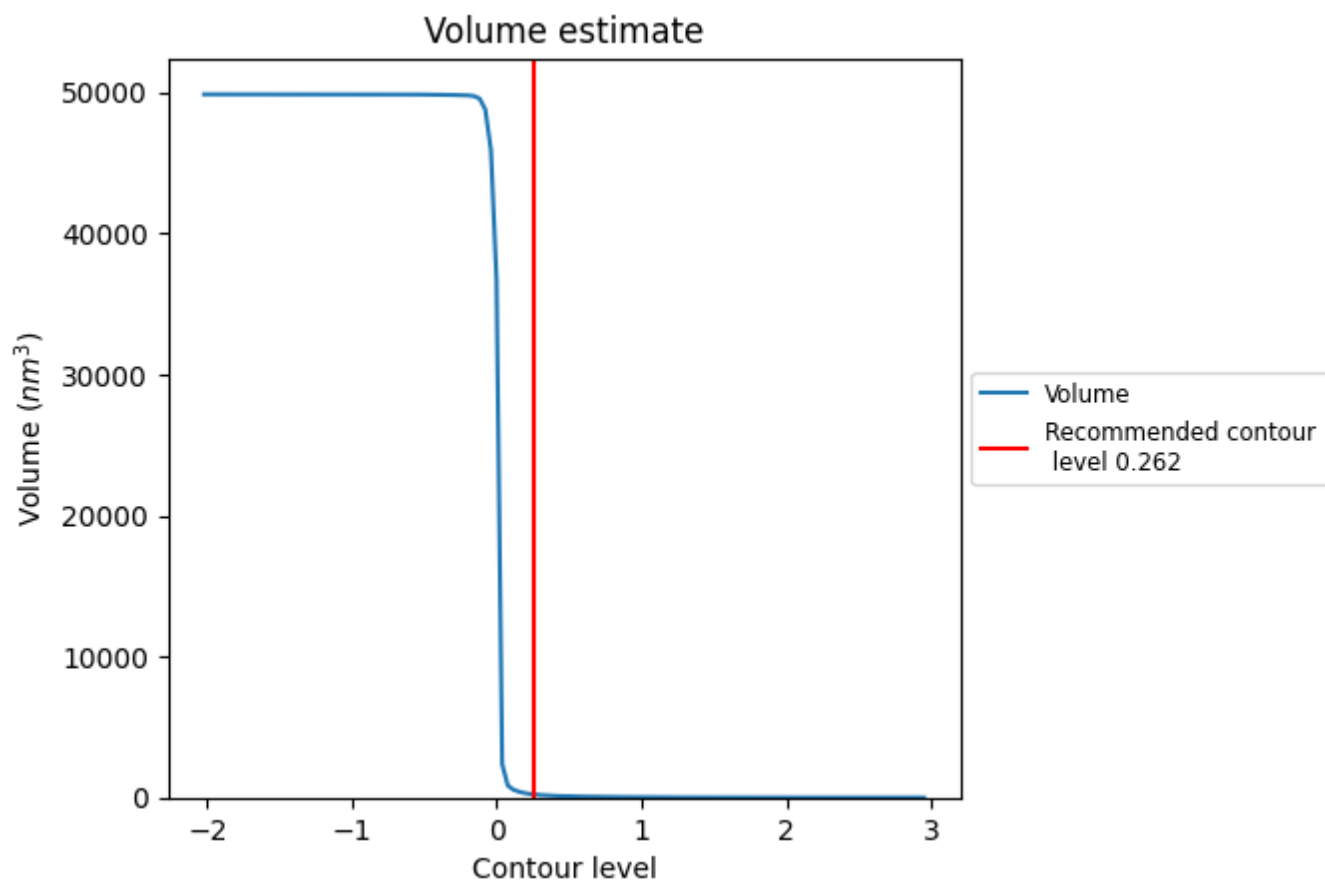
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

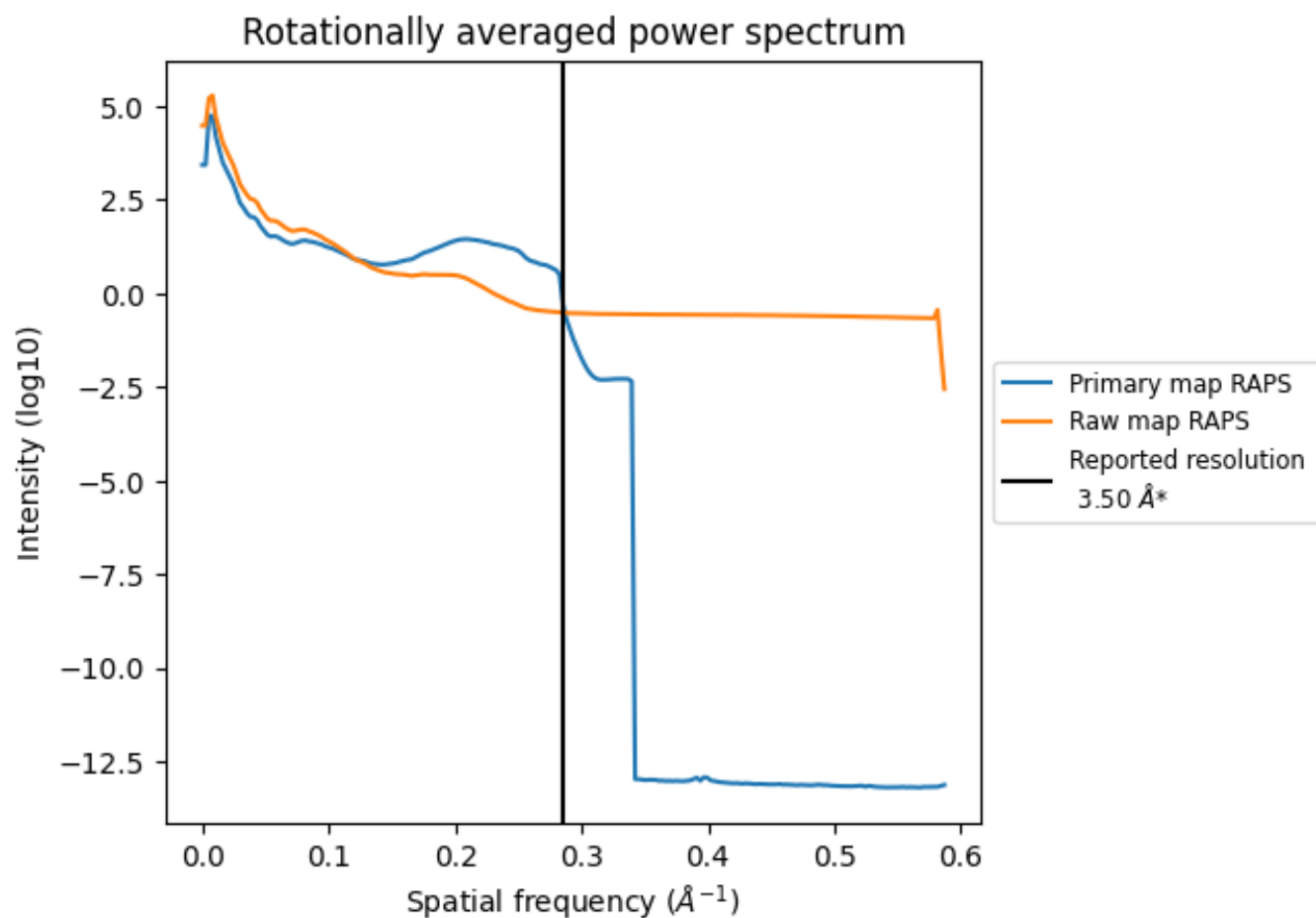
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm³; this corresponds to an approximate mass of 194 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 Å⁻¹

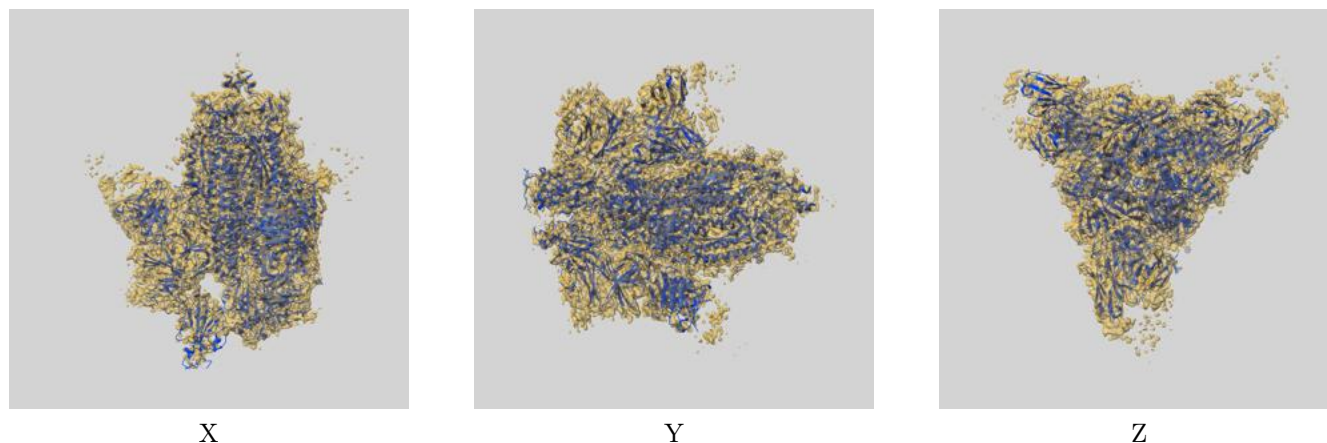
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

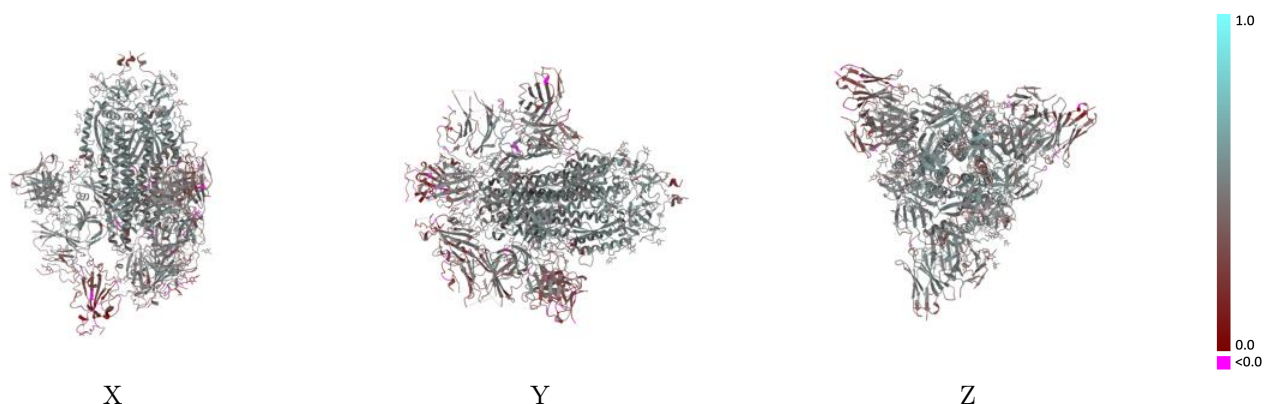
This section contains information regarding the fit between EMDB map EMD-26431 and PDB model 7UAR. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



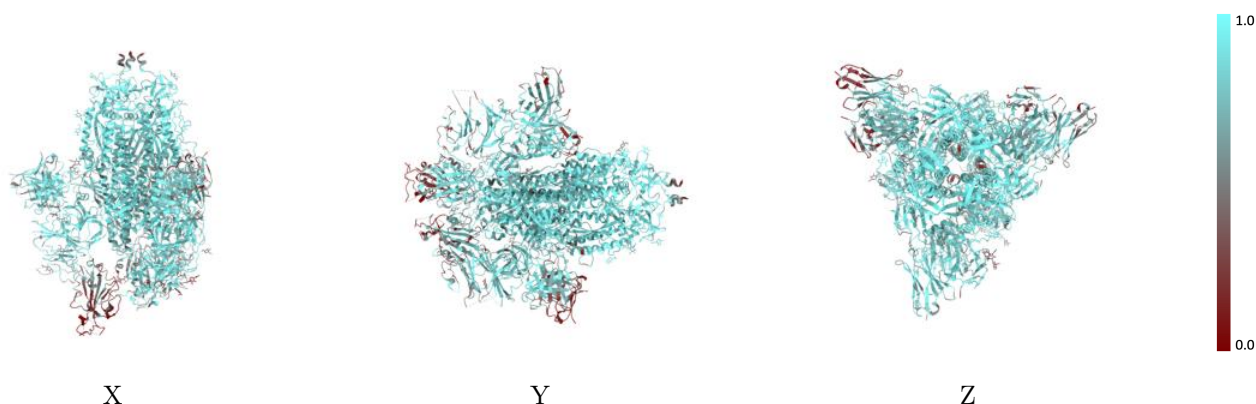
The images above show the 3D surface view of the map at the recommended contour level 0.262 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



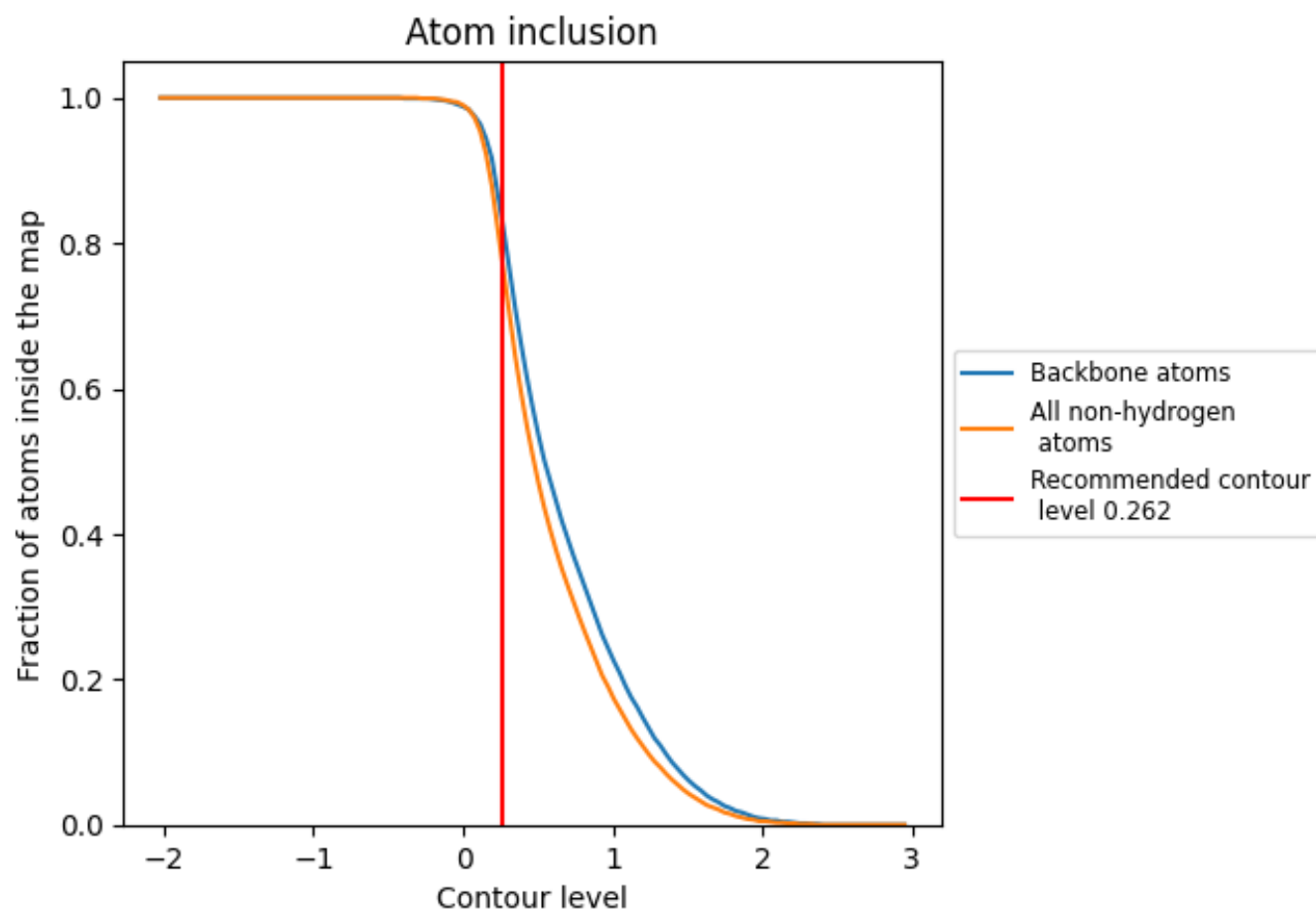
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.262).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.262) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.4440
A	 0.7640	 0.4370
B	 0.7960	 0.4600
C	 0.8180	 0.4620
D	 0.6910	 0.3980
E	 0.6860	 0.4010
F	 0.5920	 0.3420
G	 0.6030	 0.3660
H	 0.8360	 0.4870
I	 0.6430	 0.3850
J	 0.6430	 0.4080
K	 0.3670	 0.3680
L	 0.8170	 0.4610
M	 0.2140	 0.2350
N	 0.3930	 0.1960
O	 0.7500	 0.4670
P	 0.7860	 0.4450

