



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:18 PM UTC

PDB ID : 6XCM / pdb_00006xcm
EMDB ID : EMD-22127
Title : Structure of the SARS-CoV-2 spike glycoprotein in complex with the C105 neutralizing antibody Fab fragment (state 1)
Authors : Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2020-06-08
Resolution : 3.42 Å(reported)
Based on initial model : 6VYB

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

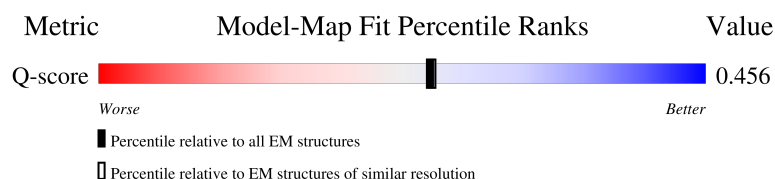
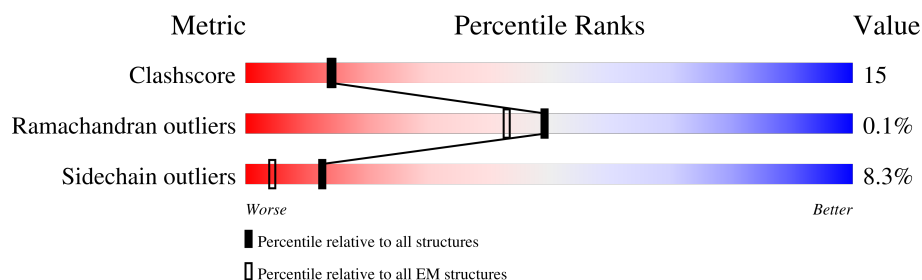
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 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	13959 (2.92 - 3.92)

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	1259	
1	B	1259	
1	C	1259	
2	H	230	

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Mol	Chain	Length	Quality of chain
2	N	230	
3	L	217	
3	S	217	
4	D	2	
4	E	2	
4	G	2	
4	I	2	
4	K	2	
4	M	2	
4	O	2	
4	P	2	
4	R	2	
5	F	2	
6	J	3	
6	T	3	
7	Q	3	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26772 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	966	Total	C	N	O	S	0	0
			7393	4741	1235	1385	32		
1	B	985	Total	C	N	O	S	2	0
			7587	4857	1259	1437	34		
1	C	985	Total	C	N	O	S	1	0
			7581	4854	1258	1435	34		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	607	GLU	GLN	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	607	GLU	GLN	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
C	607	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 C105 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	116	Total	C	N	O	S	0	0
			890	562	150	174	4		
2	N	116	Total	C	N	O	S	0	0
			890	562	150	174	4		

- Molecule 3 is a protein called C105 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total	C	N	O	S	0	0
			810	504	134	169	3		
3	S	111	Total	C	N	O	S	0	0
			810	504	134	169	3		

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



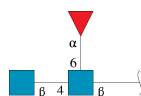
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		

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



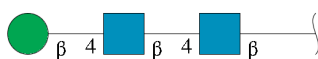
Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	2	Total	C	N	O	0	0
			24	14	1	9		

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



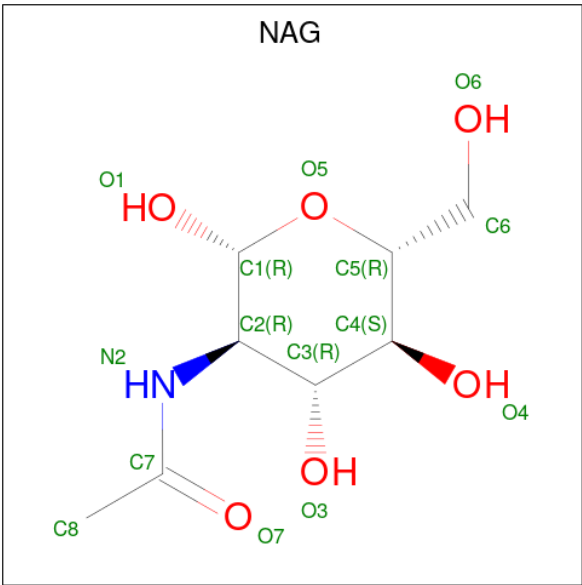
Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	3	Total	C	N	O	0	0
			38	22	2	14		
6	T	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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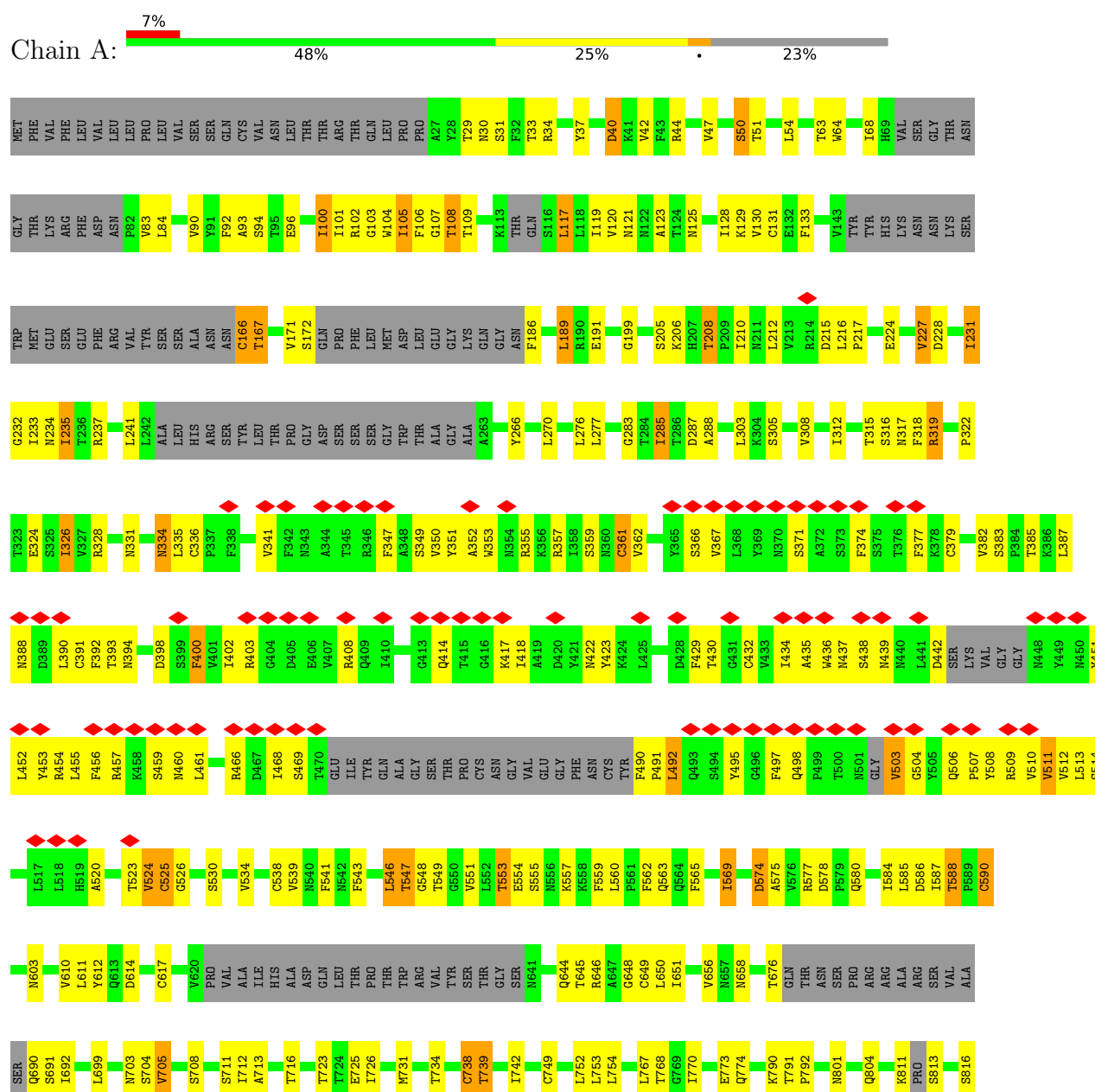
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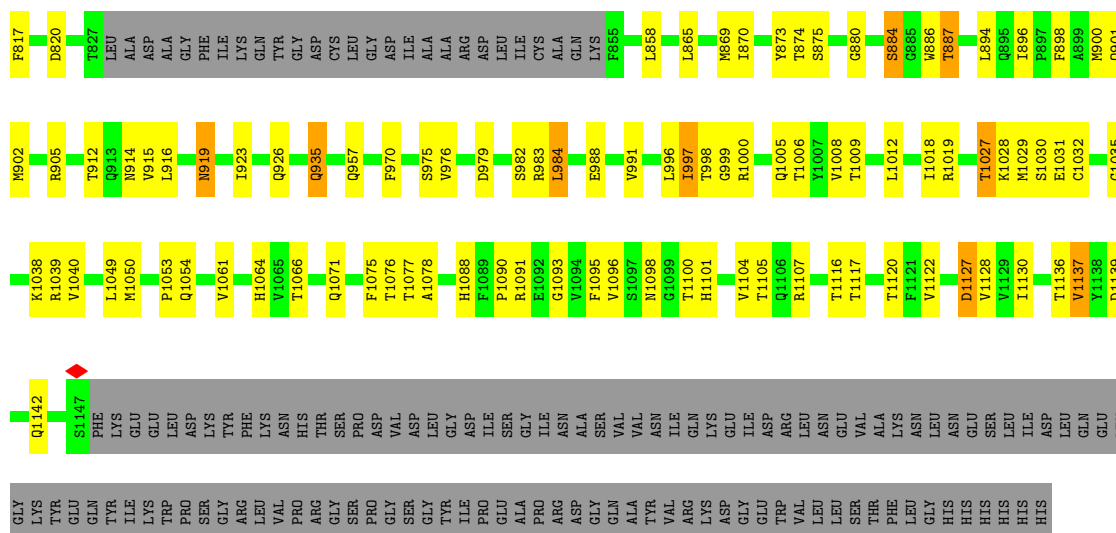
Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8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

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.

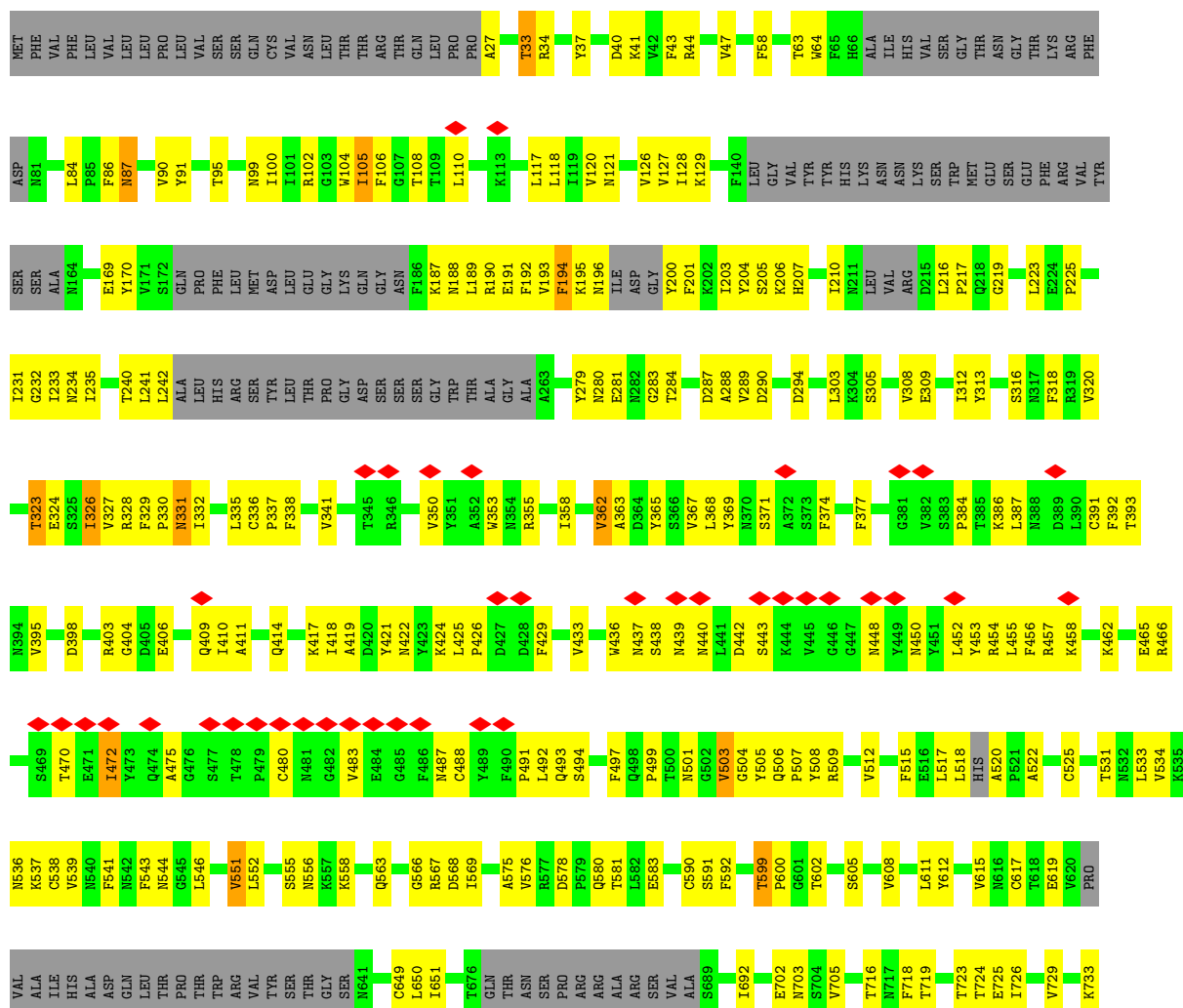
• Molecule 1: Spike glycoprotein



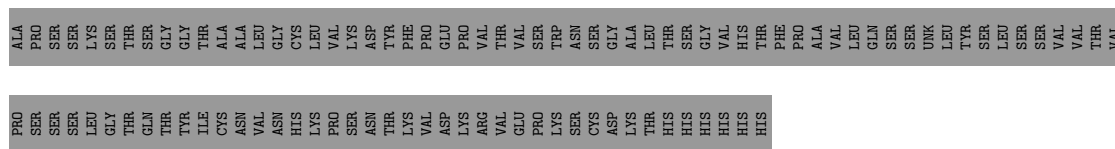


• Molecule 1: Spike glycoprotein

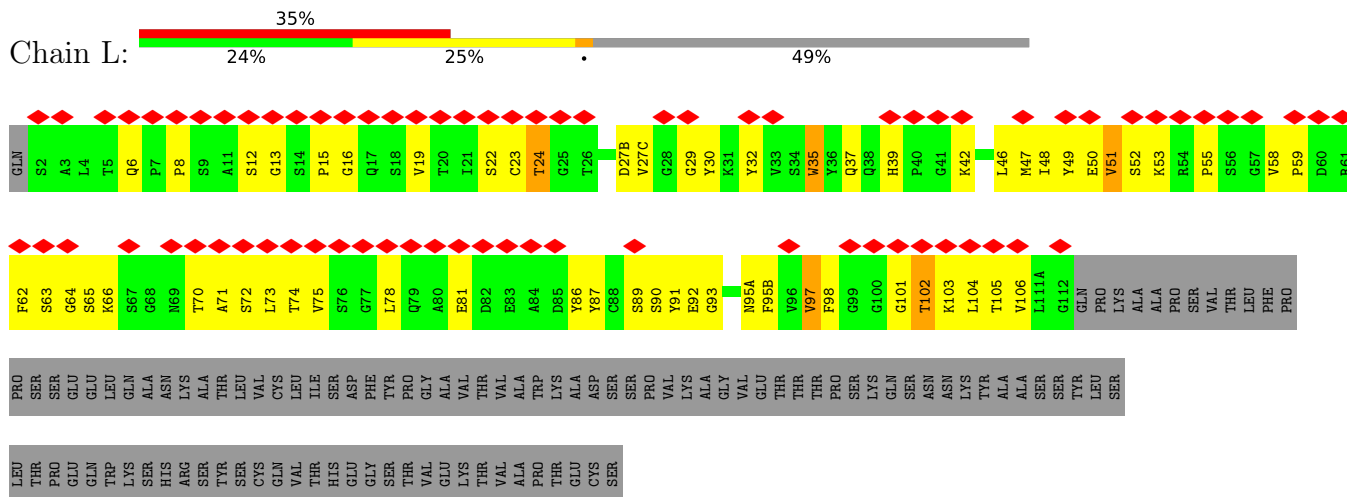
Chain B: 51% 26% 22%



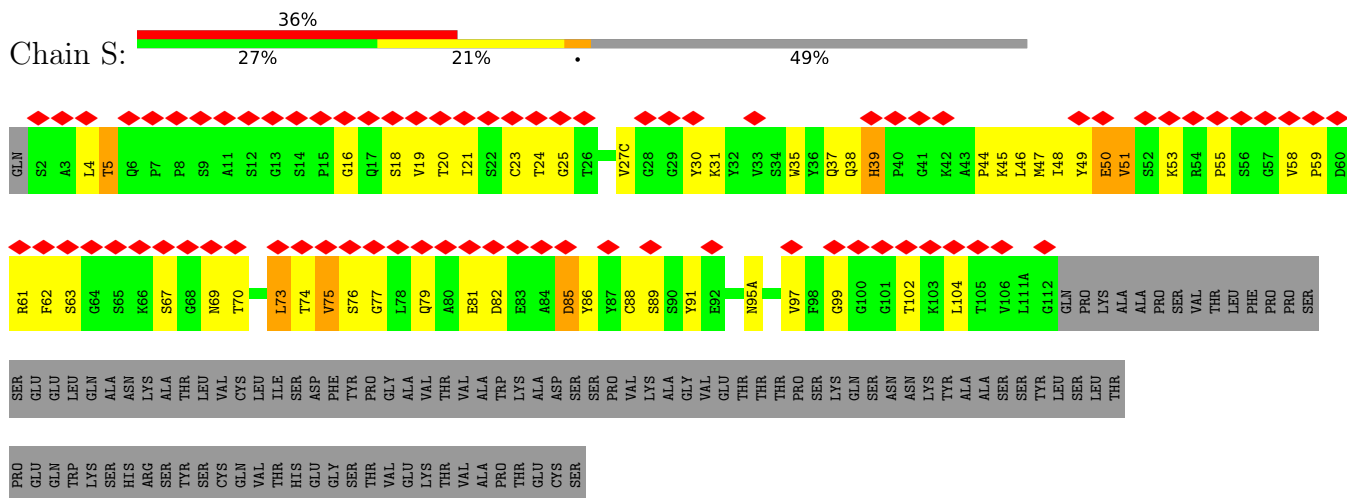




- Molecule 3: C105 Fab Light Chain



- Molecule 3: C105 Fab Light Chain



- 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

Chain G:  50% 50%



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

Chain I:  100%



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

Chain K:  50% 50%



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

Chain M:  50% 50%



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

Chain O:  100%



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

Chain P:  50% 50%



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

Chain R:  100%

NAG1
NAG2

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

Chain F:  100%

NAG1
FUC2

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

Chain J:  67%
100%

NAG1
NAG2
FUC3

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

Chain T:  33%
67%

NAG1
NAG2
FUC3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  33%
100%

NAG1
NAG2
MAN3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58873	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	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.701	Depositor
Minimum map value	-0.289	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	294.272, 294.272, 294.272	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/7554	0.45	0/10291
1	B	0.35	0/7758	0.44	0/10564
1	C	0.37	0/7752	0.44	1/10556 (0.0%)
2	H	0.15	0/911	0.37	0/1237
2	N	0.13	0/911	0.35	0/1237
3	L	0.17	0/829	0.44	0/1125
3	S	0.14	0/829	0.38	0/1125
All	All	0.34	0/26544	0.44	1/36135 (0.0%)

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	2
3	S	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	CYS	CA-CB-SG	6.10	128.43	114.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	CYS	Peptide
1	A	617	CYS	Peptide
3	S	50	GLU	Peptide

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	7131	220	0
1	B	7587	0	7310	234	0
1	C	7581	0	7305	227	0
2	H	890	0	851	39	0
2	N	890	0	851	45	0
3	L	810	0	769	48	0
3	S	810	0	769	45	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	G	28	0	25	0	0
4	I	28	0	25	3	0
4	K	28	0	25	1	0
4	M	28	0	25	1	0
4	O	28	0	25	0	0
4	P	28	0	25	1	0
4	R	28	0	24	0	0
5	F	24	0	22	0	0
6	J	38	0	34	0	0
6	T	38	0	34	1	0
7	Q	39	0	34	0	0
8	A	140	0	130	2	0
8	B	154	0	141	4	0
8	C	126	0	117	0	0
All	All	26772	0	25722	811	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 (811) 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:A:107:GLY:H	1:A:235:ILE:HG23	1.41	0.85
1:C:131:CYS:HA	1:C:166:CYS:HB3	1.57	0.85
1:A:738:CYS:SG	1:A:739:THR:N	2.55	0.79
2:H:28:THR:OG1	2:H:32:ASN:ND2	2.17	0.78
1:C:502:GLY:H	3:L:29:GLY:HA2	1.49	0.78
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.18	0.77
1:B:536:ASN:HA	1:B:551:VAL:HG23	1.66	0.76
1:A:437:ASN:HD21	1:A:439:ASN:HB2	1.50	0.76
1:C:676:THR:OG1	1:C:690:GLN:NE2	2.17	0.75
3:L:64:GLY:HA3	3:L:73:LEU:HA	1.67	0.75
1:C:475:ALA:HB1	2:H:32:ASN:HD21	1.52	0.75
1:C:326:ILE:HG22	1:C:541:PHE:HA	1.69	0.74
1:A:326:ILE:HD11	1:A:534:VAL:H	1.52	0.74
2:N:50:VAL:HG12	2:N:58:TYR:HB2	1.69	0.74
1:B:303:LEU:HD12	1:B:308:VAL:HG12	1.69	0.73
3:S:48:ILE:HD11	3:S:62:PHE:HB3	1.71	0.73
1:C:108:THR:OG1	1:C:234:ASN:O	2.07	0.73
1:B:456:PHE:HB2	1:B:491:PRO:HA	1.70	0.72
1:C:131:CYS:CA	1:C:166:CYS:HB3	2.18	0.72
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.20	0.72
1:C:81:ASN:N	1:C:265:TYR:HH	1.87	0.72
1:C:81:ASN:N	1:C:265:TYR:OH	2.23	0.72
1:C:422:ASN:HD21	1:C:454:ARG:H	1.38	0.71
2:N:14:PRO:HA	2:N:111:VAL:HB	1.73	0.71
1:C:738:CYS:SG	1:C:739:THR:N	2.63	0.70
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.55	0.70
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.24	0.70
1:A:984:LEU:HD13	1:A:988:GLU:HB3	1.72	0.70
1:B:716:THR:HG21	1:B:1073:LYS:HE3	1.72	0.70
3:L:92:GLU:HG3	3:L:93:GLY:H	1.56	0.70
2:N:29:VAL:HG23	2:N:71:ARG:HH11	1.57	0.70
1:A:382:VAL:HG21	1:A:387:LEU:HD11	1.75	0.68
1:C:644:GLN:NE2	1:C:645:THR:O	2.27	0.68
1:C:226:LEU:HG	1:C:227:VAL:HG23	1.74	0.67
1:B:100:ILE:HG22	1:B:242:LEU:HD22	1.76	0.67
1:C:644:GLN:NE2	1:C:648:GLY:O	2.27	0.67
1:A:456:PHE:HB2	1:A:491:PRO:HB3	1.77	0.67
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.28	0.67
1:C:323:THR:OG1	1:C:324:GLU:OE1	2.12	0.67
1:B:475:ALA:HB1	2:N:32:ASN:HD21	1.61	0.66
2:N:68:THR:HB	2:N:81:GLN:HB3	1.77	0.66
2:N:71:ARG:HH22	2:N:73:ASN:HB3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:50:GLU:O	3:L:53:LYS:N	2.28	0.66
1:A:96:GLU:OE2	1:A:101:ILE:N	2.29	0.66
1:B:916:LEU:HD12	1:B:923:ILE:HD12	1.78	0.66
3:L:6:GLN:HG2	3:L:23:CYS:HA	1.77	0.66
1:A:350:VAL:HG22	1:A:422:ASN:HD21	1.60	0.66
3:S:38:GLN:HB3	3:S:85:ASP:HB2	1.78	0.66
3:L:23:CYS:HB3	3:L:71:ALA:HB3	1.78	0.65
1:B:205:SER:OG	1:B:206:LYS:N	2.29	0.65
1:C:90:VAL:HG13	1:C:92:PHE:H	1.61	0.65
1:A:352:ALA:HA	1:A:468:ILE:HD12	1.78	0.65
1:C:29:THR:HG22	1:C:30:ASN:H	1.62	0.65
1:C:784:GLN:NE2	1:C:1030:SER:OG	2.29	0.65
1:C:326:ILE:HD11	1:C:533:LEU:HA	1.76	0.65
3:S:91:TYR:HE1	3:S:95(A):ASN:HA	1.62	0.65
1:A:303:LEU:HD12	1:A:308:VAL:HG22	1.79	0.65
1:B:398:ASP:HB2	1:B:512:VAL:HB	1.78	0.65
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.27	0.64
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.79	0.64
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.79	0.64
1:B:555:SER:OG	1:B:556:ASN:N	2.29	0.64
1:C:106:PHE:HD2	1:C:235:ILE:HG21	1.63	0.64
1:A:560:LEU:HD12	1:A:562:PHE:HE2	1.63	0.64
1:C:615:VAL:HG23	1:C:617:CYS:H	1.62	0.64
3:S:51:VAL:O	3:S:63:SER:OG	2.15	0.64
1:A:317:ASN:ND2	1:B:737:ASP:OD2	2.31	0.64
1:A:1093:GLY:O	1:A:1107:ARG:NH2	2.29	0.64
1:A:328:ARG:NH1	1:A:578:ASP:OD2	2.31	0.64
1:C:357:ARG:NH1	1:C:394:ASN:OD1	2.30	0.64
1:C:560:LEU:HB2	1:C:563:GLN:HE21	1.62	0.64
1:B:414:GLN:O	1:B:424:LYS:NZ	2.30	0.64
1:B:501:ASN:O	1:B:506:GLN:NE2	2.32	0.63
1:B:1011:GLN:OE1	1:B:1014:ARG:NH1	2.31	0.63
1:C:555:SER:OG	1:C:556:ASN:N	2.29	0.63
1:A:1005:GLN:NE2	1:C:1006:THR:OG1	2.32	0.63
1:B:91:TYR:HE1	1:B:191:GLU:HG2	1.64	0.63
1:C:461:LEU:HB3	1:C:465:GLU:HB3	1.78	0.63
1:B:566:GLY:N	1:B:575:ALA:O	2.32	0.63
1:B:1091:ARG:NH1	1:B:1120:THR:O	2.32	0.63
1:B:206:LYS:HB2	1:B:223:LEU:HD23	1.81	0.63
1:C:420:ASP:OD2	1:C:460:ASN:ND2	2.29	0.63
1:A:466:ARG:HG2	1:A:468:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:O	1:B:117:LEU:N	2.31	0.62
1:A:438:SER:O	1:A:442:ASP:N	2.33	0.62
1:A:434:ILE:HB	1:A:511:VAL:HG13	1.81	0.62
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.81	0.62
1:B:337:PRO:HG2	1:B:358:ILE:HD12	1.81	0.62
1:B:702:GLU:OE1	1:C:790:LYS:NZ	2.26	0.62
3:S:38:GLN:N	3:S:85:ASP:O	2.32	0.62
1:B:518:LEU:O	1:B:520:ALA:N	2.32	0.62
3:L:35:TRP:O	3:L:47:MET:N	2.27	0.62
1:A:29:THR:HG22	1:A:30:ASN:H	1.63	0.62
1:A:227:VAL:HG12	1:A:228:ASP:H	1.65	0.62
1:C:442:ASP:O	1:C:448:ASN:ND2	2.33	0.62
1:A:555:SER:HB2	1:A:586:ASP:N	2.15	0.61
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.81	0.61
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.82	0.61
1:A:898:PHE:HZ	1:A:1050:MET:HE1	1.64	0.61
3:L:32:TYR:HE1	3:L:49:TYR:HB2	1.66	0.61
1:A:106:PHE:HB2	1:A:117:LEU:HB2	1.83	0.61
1:B:280:ASN:OD1	1:B:284:THR:N	2.31	0.61
1:B:1028:LYS:O	1:B:1032:CYS:HB2	2.01	0.61
3:L:15:PRO:HA	3:L:78:LEU:HB3	1.83	0.61
3:S:18:SER:HA	3:S:76:SER:HA	1.81	0.61
1:B:455:LEU:O	2:N:33:TYR:OH	2.19	0.61
2:N:38:ARG:NH1	2:N:86:ASP:OD1	2.34	0.61
4:K:1:NAG:H83	4:K:1:NAG:H3	1.82	0.61
1:B:393:THR:HA	1:B:522:ALA:HA	1.83	0.60
1:C:309:GLU:O	1:C:313:TYR:OH	2.12	0.60
3:S:37:GLN:HE22	3:S:39:HIS:HD2	1.48	0.60
2:N:37:VAL:HG22	2:N:47:TRP:HA	1.82	0.60
4:I:1:NAG:H62	4:I:2:NAG:H82	1.83	0.60
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.82	0.60
1:A:530:SER:OG	1:A:580:GLN:NE2	2.35	0.60
1:A:92:PHE:CE2	1:A:94:SER:HB3	2.36	0.60
1:B:367:VAL:O	1:B:371:SER:OG	2.19	0.60
1:B:331:ASN:ND2	4:I:1:NAG:O7	2.35	0.60
1:B:336:CYS:N	1:B:362:VAL:O	2.34	0.60
1:A:645:THR:OG1	1:A:646:ARG:N	2.33	0.60
1:C:560:LEU:HB2	1:C:563:GLN:HG3	1.84	0.60
1:A:454:ARG:NH1	1:A:469:SER:O	2.35	0.59
1:A:1107:ARG:HD3	1:B:904:TYR:CZ	2.37	0.59
1:A:104:TRP:HB3	1:A:106:PHE:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG12	1:A:172:SER:H	1.66	0.59
1:B:129:LYS:HB3	1:B:169:GLU:HG2	1.82	0.59
8:B:1308:NAG:H3	8:B:1308:NAG:H83	1.84	0.59
1:A:353:TRP:CZ2	1:A:466:ARG:HA	2.38	0.59
1:C:455:LEU:HD22	1:C:493:GLN:HB2	1.84	0.59
1:A:553:THR:O	1:A:586:ASP:N	2.32	0.59
1:A:31:SER:O	1:A:31:SER:OG	2.20	0.59
1:A:383:SER:OG	1:B:985:ASP:N	2.35	0.59
1:A:557:LYS:HD3	1:A:575:ALA:HB2	1.83	0.59
2:H:7:SER:HG	2:H:21:SER:HG	1.48	0.59
1:B:475:ALA:HB3	1:B:487:ASN:HA	1.84	0.59
1:B:417:LYS:HE3	2:N:98:TRP:HZ2	1.68	0.59
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.23	0.59
1:A:121:ASN:O	1:A:123:ALA:N	2.33	0.59
1:B:108:THR:OG1	1:B:234:ASN:O	2.21	0.59
1:C:949:GLN:NE2	1:C:953:ASN:OD1	2.35	0.59
1:A:357:ARG:NH2	1:A:359:SER:OG	2.35	0.59
1:A:716:THR:N	1:A:1071:GLN:O	2.31	0.59
1:C:339:GLY:HA2	4:P:1:NAG:H83	1.83	0.59
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.36	0.59
1:A:50:SER:HB2	1:A:276:LEU:HD12	1.86	0.58
1:B:43:PHE:HE1	1:B:283:GLY:HA3	1.67	0.58
1:A:894:LEU:HD13	1:C:715:PRO:HD3	1.86	0.58
1:B:426:PRO:HD2	1:B:429:PHE:HB2	1.84	0.58
1:B:326:ILE:HD11	1:B:533:LEU:HA	1.84	0.58
1:A:676:THR:HA	1:A:690:GLN:HA	1.85	0.58
1:B:599:THR:HB	1:B:608:VAL:HG12	1.85	0.58
1:A:167:THR:O	1:A:167:THR:OG1	2.19	0.58
1:C:1091:ARG:NH1	1:C:1120:THR:O	2.37	0.58
1:C:104:TRP:O	1:C:105:ILE:HG13	2.04	0.58
2:N:93:ALA:HB1	2:N:100(B):TYR:HB3	1.86	0.58
3:S:86:TYR:HB2	3:S:102:THR:HB	1.85	0.58
1:A:92:PHE:HE2	1:A:94:SER:HB3	1.69	0.58
1:A:703:ASN:ND2	1:B:787:GLN:OE1	2.36	0.58
1:B:105:ILE:HG23	1:B:241:LEU:HD11	1.86	0.57
2:N:27:PHE:O	2:N:76:ASN:ND2	2.24	0.57
1:B:281:GLU:HB2	8:B:1310:NAG:H82	1.86	0.57
1:C:559:PHE:HB2	1:C:577:ARG:HH21	1.69	0.57
1:B:403:ARG:HB2	1:B:505:TYR:HA	1.84	0.57
1:B:599:THR:OG1	1:B:600:PRO:O	2.22	0.57
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:5:THR:N	3:S:24:THR:O	2.28	0.57
1:C:898:PHE:HZ	1:C:1050:MET:HE1	1.70	0.57
1:A:1077:THR:OG1	1:A:1078:ALA:N	2.35	0.57
1:B:1039:ARG:NH2	1:C:1031:GLU:OE2	2.38	0.57
1:B:91:TYR:CE1	1:B:191:GLU:HG2	2.39	0.57
1:A:40:ASP:OD1	1:A:40:ASP:N	2.37	0.57
1:A:316:SER:OG	1:A:317:ASN:N	2.37	0.57
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.85	0.57
1:B:323:THR:OG1	1:B:324:GLU:N	2.37	0.57
1:C:128:ILE:HD13	1:C:229:LEU:HD11	1.87	0.57
1:A:557:LYS:NZ	1:A:574:ASP:OD2	2.25	0.56
2:H:20:LEU:HD11	2:H:90:TYR:HD1	1.70	0.56
2:H:52:TYR:OH	3:L:95(A):ASN:OD1	2.23	0.56
2:N:34:MET:HA	2:N:94:ARG:HA	1.87	0.56
1:A:773:GLU:OE2	1:A:1019:ARG:NH1	2.35	0.56
1:A:976:VAL:HB	1:A:979:ASP:HB2	1.87	0.56
1:B:318:PHE:HE2	1:B:615:VAL:HG11	1.70	0.56
1:C:89:GLY:HA3	1:C:270:LEU:HG	1.87	0.56
3:L:48:ILE:HG13	3:L:63:SER:HA	1.87	0.56
3:S:25:GLY:H	3:S:27(C):VAL:HG21	1.70	0.56
1:C:466:ARG:HG2	1:C:468:ILE:HD11	1.87	0.56
3:L:22:SER:HA	3:L:72:SER:HA	1.86	0.56
1:A:105:ILE:HG13	1:A:241:LEU:HD11	1.86	0.56
1:B:902:MET:HE1	1:B:1049:LEU:HD13	1.87	0.56
1:C:430:THR:HG22	1:C:515:PHE:HD2	1.68	0.56
1:B:193:VAL:HG21	1:B:223:LEU:HD13	1.87	0.56
1:C:880:GLY:O	1:C:884:SER:OG	2.20	0.56
1:C:393:THR:HG23	1:C:517:LEU:HD12	1.87	0.56
1:B:1043:CYS:HB3	1:B:1048:HIS:ND1	2.20	0.56
1:A:1091:ARG:NH1	1:A:1120:THR:O	2.38	0.56
1:A:1098:ASN:ND2	1:A:1100:THR:OG1	2.39	0.56
1:C:716:THR:N	1:C:1071:GLN:O	2.34	0.56
1:A:1139:ASP:OD2	1:A:1142:GLN:NE2	2.39	0.56
1:C:1051:SER:OG	1:C:1064:HIS:ND1	2.36	0.56
2:N:20:LEU:HD13	2:N:82:MET:HE2	1.86	0.55
3:L:92:GLU:HB3	3:L:95(B):PHE:HB3	1.87	0.55
3:S:21:ILE:HD12	3:S:102:THR:HG21	1.88	0.55
1:A:1035:GLY:HA3	1:C:1040:VAL:HG21	1.89	0.55
1:B:398:ASP:O	1:B:512:VAL:N	2.34	0.55
1:A:131:CYS:O	1:A:133:PHE:N	2.39	0.55
1:A:186:PHE:N	1:A:212:LEU:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:MET:HE1	1:C:1094:VAL:HG23	1.88	0.55
1:B:436:TRP:NE1	1:B:438:SER:OG	2.38	0.55
1:C:902:MET:HE1	1:C:1049:LEU:HD13	1.88	0.55
1:C:969:ASN:OD1	1:C:975:SER:OG	2.23	0.55
1:A:614:ASP:H	1:A:648:GLY:HA2	1.72	0.55
1:A:362:VAL:HG13	1:A:526:GLY:HA2	1.88	0.55
1:B:377:PHE:HE2	1:B:384:PRO:HB3	1.72	0.55
1:C:437:ASN:HD21	1:C:439:ASN:HB2	1.71	0.55
1:A:189:LEU:HD23	1:A:208:THR:HG23	1.88	0.55
1:A:503:VAL:HA	1:A:506:GLN:HE21	1.72	0.55
1:A:898:PHE:CZ	1:A:1050:MET:HE1	2.41	0.55
1:B:294:ASP:N	1:B:294:ASP:OD1	2.38	0.55
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.06	0.55
1:C:107:GLY:H	1:C:235:ILE:HG23	1.72	0.55
1:A:770:ILE:O	1:A:774:GLN:HG2	2.07	0.55
1:C:1077:THR:OG1	1:C:1078:ALA:N	2.40	0.55
3:S:91:TYR:CE1	3:S:95(A):ASN:HA	2.42	0.55
1:A:128:ILE:HG22	1:A:129:LYS:H	1.72	0.55
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.18	0.55
1:A:1030:SER:OG	1:C:1041:ASP:HB2	2.06	0.55
1:C:415:THR:O	2:H:58:TYR:OH	2.24	0.55
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.31	0.54
1:A:367:VAL:O	1:A:371:SER:HB3	2.08	0.54
1:B:188:ASN:OD1	1:B:190:ARG:NH1	2.40	0.54
2:H:38:ARG:HD3	2:H:90:TYR:CE2	2.42	0.54
1:B:335:LEU:HA	1:B:362:VAL:HG13	1.90	0.54
3:L:92:GLU:HG3	3:L:93:GLY:N	2.22	0.54
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.88	0.54
1:C:437:ASN:HB2	1:C:508:TYR:CZ	2.43	0.54
1:A:503:VAL:HA	1:A:506:GLN:HG3	1.89	0.54
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.88	0.54
1:B:619:GLU:N	1:B:619:GLU:OE1	2.40	0.54
1:C:544:ASN:OD1	1:C:545:GLY:N	2.41	0.54
4:I:2:NAG:H3	4:I:2:NAG:H83	1.89	0.54
1:A:328:ARG:NH2	1:A:580:GLN:OE1	2.33	0.54
1:B:58:PHE:HD2	1:B:290:ASP:HB2	1.72	0.53
2:N:72:ASP:HB2	2:N:79:TYR:HD2	1.74	0.53
1:A:334:ASN:OD1	1:A:334:ASN:N	2.28	0.53
1:B:475:ALA:N	1:B:487:ASN:O	2.29	0.53
1:C:1081:ILE:HD11	1:C:1115:ILE:HG21	1.90	0.53
1:A:656:VAL:HG12	1:A:658:ASN:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:21:ILE:N	3:S:73:LEU:O	2.23	0.53
1:B:803:SER:OG	1:B:804:GLN:NE2	2.42	0.53
1:A:451:TYR:HB2	1:A:495:TYR:HB2	1.91	0.53
3:S:50:GLU:O	3:S:53:LYS:N	2.38	0.53
1:C:366:SER:HA	1:C:369:TYR:HB3	1.88	0.53
1:C:192:PHE:O	1:C:193:VAL:HG23	2.08	0.53
1:C:393:THR:HG21	1:C:518:LEU:H	1.73	0.53
1:B:1104:VAL:HG11	1:B:1119:ASN:HB3	1.91	0.53
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.90	0.53
1:C:33:THR:HG23	1:C:58:PHE:HE2	1.74	0.53
1:C:398:ASP:N	1:C:398:ASP:OD1	2.41	0.53
3:L:50:GLU:O	3:L:52:SER:N	2.42	0.53
1:A:547:THR:OG1	1:A:548:GLY:N	2.41	0.53
2:H:38:ARG:HH12	2:H:86:ASP:HB3	1.73	0.53
3:L:16:GLY:N	3:L:78:LEU:O	2.42	0.53
1:A:199:GLY:HA2	1:A:232:GLY:HA2	1.90	0.52
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.90	0.52
1:C:406:GLU:OE1	1:C:495:TYR:OH	2.27	0.52
1:C:619:GLU:N	1:C:619:GLU:OE1	2.42	0.52
1:C:620:VAL:HG21	1:C:651:ILE:HD11	1.89	0.52
2:H:29:VAL:HG22	2:H:75:LYS:HA	1.91	0.52
2:N:12:ILE:HD11	2:N:82(C):LEU:HD13	1.91	0.52
3:S:37:GLN:HG3	3:S:45:LYS:HB3	1.91	0.52
1:B:403:ARG:HG2	1:B:406:GLU:CD	2.34	0.52
1:B:433:VAL:HG12	1:B:512:VAL:HG22	1.89	0.52
2:H:59:TYR:HB3	2:H:63:VAL:HG23	1.92	0.52
3:L:37:GLN:HE22	3:L:42:LYS:HZ3	1.57	0.52
1:A:350:VAL:HG22	1:A:422:ASN:ND2	2.24	0.52
1:C:599:THR:HB	1:C:608:VAL:HG12	1.92	0.52
2:H:62:SER:O	2:H:66:ARG:NH2	2.28	0.52
2:N:28:THR:HG23	2:N:31:SER:HB2	1.92	0.52
1:B:391:CYS:CB	1:B:525:CYS:HA	2.40	0.52
1:A:403:ARG:NE	1:A:504:GLY:O	2.36	0.52
1:A:418:ILE:HA	1:A:422:ASN:HB3	1.92	0.52
1:A:813:SER:O	1:A:813:SER:OG	2.24	0.52
1:A:1075:PHE:HB3	1:A:1096:VAL:HB	1.90	0.52
1:B:204:TYR:HA	1:B:225:PRO:HA	1.91	0.52
1:B:392:PHE:HB3	1:B:517:LEU:HB3	1.91	0.52
1:B:567:ARG:HG3	1:B:568:ASP:H	1.75	0.52
1:B:393:THR:HG23	1:B:517:LEU:HB2	1.92	0.52
1:A:210:ILE:HG21	1:A:217:PRO:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1083:HIS:HB2	1:C:1137:VAL:HG23	1.92	0.52
3:L:90:SER:O	3:L:97:VAL:N	2.34	0.52
1:B:194:PHE:HD2	1:B:203:ILE:HG12	1.74	0.51
1:B:358:ILE:HB	1:B:395:VAL:HG13	1.93	0.51
1:C:380:TYR:HD1	1:C:429:PHE:HE2	1.58	0.51
1:C:383:SER:OG	1:C:385:THR:O	2.28	0.51
3:L:39:HIS:H	3:L:42:LYS:HE2	1.74	0.51
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.39	0.51
1:B:99:ASN:OD1	1:B:190:ARG:NH2	2.43	0.51
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.35	0.51
3:S:16:GLY:HA2	3:S:77:GLY:HA2	1.93	0.51
1:B:417:LYS:HG2	2:N:52:TYR:HE2	1.75	0.51
1:C:1120:THR:OG1	1:C:1121:PHE:N	2.44	0.51
3:S:61:ARG:NE	3:S:76:SER:O	2.30	0.51
1:A:436:TRP:O	1:A:509:ARG:N	2.34	0.51
1:A:901:GLN:O	1:A:905:ARG:HG2	2.11	0.51
1:B:1081:ILE:HD11	1:B:1115:ILE:HG21	1.92	0.51
1:B:453:TYR:N	1:B:493:GLN:O	2.44	0.51
1:C:393:THR:O	1:C:394:ASN:ND2	2.44	0.51
1:A:452:LEU:HD23	1:A:453:TYR:N	2.25	0.51
1:A:957:GLN:OE1	1:B:765:ARG:NH1	2.44	0.51
1:B:1084:ASP:HB2	1:B:1086:LYS:HE3	1.93	0.51
2:H:52:TYR:HB2	2:H:56:SER:HB3	1.92	0.51
1:A:34:ARG:NH1	1:A:217:PRO:O	2.43	0.51
1:B:58:PHE:CD2	1:B:290:ASP:HB2	2.45	0.51
1:C:91:TYR:CG	1:C:91:TYR:O	2.63	0.51
1:A:277:LEU:HD13	1:A:285:ILE:HD11	1.93	0.50
1:A:366:SER:N	1:A:388:ASN:HD21	2.09	0.50
2:N:35:SER:N	2:N:93:ALA:O	2.40	0.50
2:N:59:TYR:CD1	2:N:63:VAL:HG13	2.47	0.50
1:B:439:ASN:O	1:B:443:SER:OG	2.14	0.50
1:C:50:SER:O	1:C:50:SER:OG	2.28	0.50
3:L:89:SER:HB2	3:L:98:PHE:CE1	2.46	0.50
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.93	0.50
2:H:28:THR:HG22	2:H:75:LYS:HD2	1.92	0.50
3:L:32:TYR:CE1	3:L:49:TYR:HB2	2.46	0.50
1:C:127:VAL:HG12	1:C:171:VAL:HG22	1.93	0.50
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.45	0.50
3:L:66:LYS:HA	3:L:71:ALA:HA	1.93	0.50
1:A:459:SER:OG	1:A:460:ASN:N	2.45	0.50
1:B:190:ARG:O	1:B:191:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:924:ALA:O	1:B:928:ASN:ND2	2.44	0.50
2:N:3:GLN:NE2	2:N:23:ALA:O	2.43	0.50
1:A:804:GLN:HB3	1:A:935:GLN:HE21	1.77	0.50
1:B:546:LEU:HD11	1:B:576:VAL:HG11	1.94	0.50
2:N:19:ARG:HD2	2:N:79:TYR:HE1	1.76	0.50
1:C:403:ARG:HG2	1:C:406:GLU:CD	2.37	0.50
2:N:47:TRP:NE1	2:N:49:SER:O	2.45	0.50
1:B:392:PHE:CD2	1:B:515:PHE:HB3	2.47	0.50
1:B:458:LYS:NZ	2:N:30:SER:O	2.36	0.50
1:B:870:ILE:O	1:B:874:THR:HG23	2.12	0.50
1:C:34:ARG:HB3	1:C:34:ARG:HH11	1.77	0.50
1:C:327:VAL:HG22	1:C:542:ASN:HB3	1.93	0.50
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.94	0.50
1:A:106:PHE:HD2	1:A:235:ILE:HG21	1.77	0.50
1:B:287:ASP:OD1	1:B:288:ALA:N	2.45	0.50
1:B:898:PHE:HZ	1:B:1050:MET:HE1	1.77	0.50
2:N:100(A):PRO:HG3	3:S:49:TYR:CG	2.47	0.50
3:S:35:TRP:CD1	3:S:48:ILE:HB	2.47	0.50
3:S:37:GLN:HG2	3:S:47:MET:HE2	1.94	0.50
1:A:403:ARG:HB3	1:A:497:PHE:HZ	1.77	0.49
1:B:326:ILE:HG22	1:B:541:PHE:HA	1.94	0.49
1:C:341:VAL:HG21	1:C:397:ALA:HB1	1.94	0.49
1:C:423:TYR:CE2	1:C:512:VAL:HG11	2.47	0.49
1:A:460:ASN:OD1	1:A:461:LEU:N	2.45	0.49
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.94	0.49
1:A:699:LEU:HD21	1:B:869:MET:HG2	1.94	0.49
1:B:581:THR:O	1:B:583:GLU:N	2.43	0.49
2:H:87:THR:OG1	2:H:111:VAL:O	2.25	0.49
2:H:101:ASP:HA	3:L:46:LEU:HD22	1.94	0.49
3:L:65:SER:OG	3:L:66:LYS:N	2.45	0.49
1:C:299:THR:HG22	1:C:308:VAL:HG11	1.94	0.49
1:A:215:ASP:N	1:A:215:ASP:OD1	2.44	0.49
1:B:969:ASN:OD1	1:B:975:SER:OG	2.26	0.49
1:A:324:GLU:HG3	1:A:534:VAL:HG21	1.95	0.49
1:C:60:SER:OG	1:C:61:ASN:N	2.45	0.49
1:A:108:THR:OG1	1:A:234:ASN:O	2.30	0.49
1:A:870:ILE:O	1:A:874:THR:HG23	2.13	0.49
1:B:703:ASN:ND2	1:C:787:GLN:OE1	2.45	0.49
1:B:897:PRO:HB2	1:B:900:MET:HG3	1.94	0.49
3:L:8:PRO:HA	3:L:102:THR:HA	1.94	0.49
1:A:1039:ARG:NH2	1:B:1031:GLU:OE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:O	1:B:102:ARG:HG2	2.13	0.49
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.95	0.49
1:A:125:ASN:ND2	1:A:125:ASN:O	2.46	0.49
1:A:1127:ASP:N	1:A:1127:ASP:OD1	2.46	0.49
1:C:438:SER:OG	1:C:438:SER:O	2.30	0.49
1:B:448:ASN:ND2	1:B:450:ASN:OD1	2.46	0.48
1:B:454:ARG:HH22	1:B:470:THR:HG23	1.78	0.48
2:H:12:ILE:HD11	2:H:18:LEU:HD21	1.93	0.48
2:N:39:GLN:HB2	2:N:45:LEU:HG	1.95	0.48
3:L:55:PRO:HG2	3:L:58:VAL:HB	1.95	0.48
1:B:44:ARG:HD2	1:B:279:TYR:CE1	2.48	0.48
1:B:338:PHE:HE2	1:B:363:ALA:HB1	1.78	0.48
1:B:421:TYR:HH	2:N:53:SER:HG	1.42	0.48
1:B:536:ASN:O	1:B:537:LYS:HG3	2.13	0.48
1:C:323:THR:OG1	1:C:324:GLU:N	2.47	0.48
1:C:454:ARG:HH11	1:C:457:ARG:HG2	1.78	0.48
3:L:37:GLN:HA	3:L:86:TYR:HA	1.94	0.48
3:S:21:ILE:O	3:S:73:LEU:N	2.44	0.48
3:L:95(A):ASN:O	3:L:95(A):ASN:ND2	2.46	0.48
1:A:331:ASN:HD22	8:A:1306:NAG:C7	2.26	0.48
1:A:816:SER:OG	1:A:817:PHE:N	2.44	0.48
1:A:1088:HIS:CE1	1:A:1137:VAL:HG11	2.48	0.48
1:B:63:THR:HG22	1:B:64:TRP:H	1.77	0.48
1:C:321:GLN:OE1	1:C:322:PRO:HD2	2.13	0.48
1:C:455:LEU:N	1:C:491:PRO:O	2.45	0.48
1:C:480:CYS:O	1:C:483:VAL:HG12	2.14	0.48
1:A:379:CYS:HA	1:A:432:CYS:HA	1.94	0.48
1:A:988:GLU:O	1:A:991:VAL:HG12	2.14	0.48
1:C:802:PHE:HD2	1:C:805:ILE:HD11	1.78	0.48
2:N:29:VAL:HG12	2:N:34:MET:HE1	1.96	0.48
1:A:457:ARG:NH1	1:A:459:SER:O	2.38	0.48
1:B:33:THR:OG1	1:B:219:GLY:O	2.25	0.48
1:B:440:ASN:OD1	1:B:440:ASN:N	2.40	0.48
1:C:127:VAL:O	1:C:127:VAL:HG23	2.14	0.48
1:C:490:PHE:HD2	1:C:492:LEU:H	1.60	0.48
3:L:16:GLY:H	3:L:78:LEU:HB3	1.79	0.48
2:N:48:VAL:HA	2:N:60:ALA:HB2	1.96	0.48
1:A:128:ILE:HG22	1:A:129:LYS:N	2.28	0.48
1:A:349:SER:HB3	1:A:352:ALA:HB3	1.96	0.48
1:C:364:ASP:HB2	1:C:367:VAL:HG13	1.96	0.48
3:S:63:SER:H	3:S:73:LEU:HD13	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.73	0.47
1:A:171:VAL:HG12	1:A:172:SER:N	2.30	0.47
1:A:873:TYR:CZ	1:C:699:LEU:HD22	2.50	0.47
1:A:919:ASN:OD1	1:A:919:ASN:N	2.47	0.47
3:L:24:THR:HB	3:L:70:THR:HG22	1.95	0.47
1:A:902:MET:HE1	1:A:1049:LEU:HD13	1.95	0.47
1:B:189:LEU:HD13	1:B:210:ILE:HD13	1.95	0.47
1:B:1080:ALA:HB3	1:B:1132:ILE:HD12	1.96	0.47
1:C:31:SER:HB3	1:C:62:VAL:HG13	1.95	0.47
1:C:353:TRP:HE1	1:C:466:ARG:HA	1.79	0.47
1:C:612:TYR:HE1	1:C:651:ILE:HD12	1.79	0.47
1:A:880:GLY:O	1:A:884:SER:OG	2.30	0.47
1:C:726:ILE:HD13	1:C:945:LEU:HG	1.97	0.47
1:C:1102:TRP:CH2	1:C:1133:VAL:HG21	2.50	0.47
3:S:67:SER:O	3:S:67:SER:OG	2.32	0.47
1:A:984:LEU:HD23	1:A:984:LEU:HA	1.66	0.47
1:B:231:ILE:HG13	1:B:232:GLY:H	1.78	0.47
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.15	0.47
1:C:884:SER:O	1:C:887:THR:OG1	2.31	0.47
3:S:19:VAL:O	3:S:75:VAL:N	2.42	0.47
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.96	0.47
1:B:480:CYS:HB2	1:B:483:VAL:HG12	1.97	0.47
1:B:497:PHE:HB3	1:B:507:PRO:HD3	1.96	0.47
1:C:439:ASN:HA	1:C:443:SER:OG	2.15	0.47
3:S:55:PRO:HD2	3:S:58:VAL:HG21	1.96	0.47
1:B:538:CYS:HB2	1:B:590:CYS:HB3	1.48	0.47
1:C:86:PHE:CE1	1:C:106:PHE:HE2	2.33	0.47
1:C:126:VAL:HG23	1:C:126:VAL:O	2.15	0.47
1:C:455:LEU:HG	1:C:456:PHE:CE2	2.50	0.47
1:A:886:TRP:HZ3	1:A:905:ARG:HD3	1.80	0.47
1:A:1027:THR:O	1:A:1031:GLU:HG3	2.15	0.47
1:B:189:LEU:HD22	1:B:210:ILE:HG21	1.96	0.47
1:B:821:LEU:O	1:B:825:LYS:HG2	2.15	0.47
1:C:353:TRP:NE1	1:C:466:ARG:HA	2.30	0.47
1:C:357:ARG:HB2	1:C:396:TYR:HE1	1.79	0.47
1:B:943:SER:O	1:B:943:SER:OG	2.28	0.47
1:A:205:SER:OG	1:A:206:LYS:N	2.46	0.47
1:C:870:ILE:O	1:C:874:THR:HG23	2.15	0.47
3:L:39:HIS:CD2	3:L:42:LYS:HZ3	2.33	0.47
1:A:563:GLN:HA	1:B:41:LYS:HB3	1.97	0.46
1:B:472:ILE:HD11	1:B:488:CYS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:TRP:CZ2	1:B:1133:VAL:HG21	2.50	0.46
1:C:361:CYS:O	1:C:524:VAL:HA	2.15	0.46
1:B:329:PHE:O	1:B:580:GLN:NE2	2.46	0.46
1:B:617:CYS:HB2	1:B:649:CYS:HB2	1.68	0.46
1:B:718:PHE:HE1	1:B:923:ILE:HG12	1.81	0.46
1:C:435:ALA:HB2	1:C:510:VAL:HG23	1.98	0.46
1:C:1097:SER:HB2	1:C:1102:TRP:CE3	2.50	0.46
3:L:27(C):VAL:HA	3:L:30:TYR:CZ	2.50	0.46
1:B:801:ASN:OD1	4:M:1:NAG:N2	2.49	0.46
1:C:612:TYR:CE1	1:C:651:ILE:HD12	2.51	0.46
1:A:37:TYR:OH	1:A:54:LEU:O	2.16	0.46
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.79	0.46
1:C:364:ASP:OD1	1:C:364:ASP:N	2.36	0.46
1:C:438:SER:N	1:C:507:PRO:O	2.36	0.46
1:C:475:ALA:HB3	1:C:487:ASN:O	2.16	0.46
1:C:770:ILE:HD11	1:C:1012:LEU:HA	1.98	0.46
1:A:970:PHE:CG	1:A:999:GLY:HA3	2.51	0.46
1:C:879:ALA:O	1:C:883:THR:OG1	2.31	0.46
3:S:89:SER:HA	3:S:97:VAL:O	2.15	0.46
1:B:195:LYS:O	1:B:201:PHE:HA	2.15	0.46
1:B:409:GLN:OE1	1:B:419:ALA:N	2.33	0.46
1:B:959:LEU:HA	1:B:959:LEU:HD23	1.68	0.46
1:C:971:GLY:O	1:C:995:ARG:NH1	2.48	0.46
2:H:6:GLU:HB2	2:H:105:GLN:HE22	1.80	0.46
3:L:27(B):ASP:HB2	3:L:30:TYR:HE1	1.81	0.46
3:L:37:GLN:HB3	3:L:47:MET:SD	2.56	0.46
1:A:215:ASP:HA	1:A:266:TYR:OH	2.16	0.46
1:A:577:ARG:NE	1:A:584:ILE:HD11	2.30	0.46
1:A:704:SER:OG	1:A:705:VAL:N	2.49	0.46
1:C:644:GLN:HE21	1:C:645:THR:N	2.14	0.46
2:H:69:ILE:HG13	2:H:79:TYR:O	2.16	0.46
2:N:49:SER:OG	2:N:69:ILE:HD13	2.16	0.46
1:A:452:LEU:HD21	1:A:492:LEU:HB3	1.97	0.46
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.15	0.46
1:A:914:ASN:OD1	1:A:915:VAL:N	2.48	0.46
1:B:1073:LYS:HB2	1:B:1075:PHE:CE1	2.50	0.46
1:C:996:LEU:HD23	1:C:996:LEU:HA	1.81	0.46
1:A:93:ALA:HA	1:A:191:GLU:HA	1.97	0.46
1:B:404:GLY:N	1:B:504:GLY:O	2.49	0.46
2:H:98:TRP:H	2:H:98:TRP:HE3	1.58	0.46
2:N:72:ASP:HB3	2:N:77:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:880:GLY:O	1:B:884:SER:OG	2.31	0.45
1:B:1103:PHE:HZ	8:B:1320:NAG:H62	1.79	0.45
1:C:704:SER:O	1:C:704:SER:OG	2.34	0.45
1:C:816:SER:OG	1:C:819:GLU:OE1	2.24	0.45
1:C:1097:SER:OG	1:C:1101:HIS:O	2.21	0.45
2:N:72:ASP:N	2:N:77:THR:O	2.49	0.45
3:S:38:GLN:O	3:S:85:ASP:N	2.41	0.45
1:A:131:CYS:HA	1:A:166:CYS:N	2.32	0.45
1:A:691:SER:OG	1:A:692:ILE:N	2.48	0.45
1:A:901:GLN:NE2	1:A:905:ARG:HH21	2.14	0.45
1:C:90:VAL:CG1	1:C:92:PHE:H	2.27	0.45
2:N:19:ARG:HD2	2:N:79:TYR:CE1	2.51	0.45
2:N:98:TRP:HB3	3:S:91:TYR:HB2	1.97	0.45
1:A:982:SER:OG	1:A:983:ARG:N	2.49	0.45
1:C:45:SER:OG	1:C:281:GLU:O	2.27	0.45
1:C:742:ILE:HG22	1:C:743:CYS:SG	2.56	0.45
2:N:18:LEU:HD12	2:N:19:ARG:H	1.81	0.45
1:A:63:THR:HG22	1:A:64:TRP:H	1.81	0.45
1:A:357:ARG:HE	1:A:394:ASN:HD21	1.63	0.45
1:A:408:ARG:O	1:A:414:GLN:NE2	2.37	0.45
3:L:8:PRO:O	3:L:103:LYS:N	2.50	0.45
3:S:61:ARG:HB2	3:S:76:SER:H	1.82	0.45
1:A:541:PHE:HB2	1:A:543:PHE:CE1	2.52	0.45
1:C:379:CYS:HA	1:C:432:CYS:HA	1.97	0.45
1:B:327:VAL:O	1:B:531:THR:N	2.50	0.45
1:B:985:ASP:HB2	1:B:987:PRO:HD2	1.98	0.45
1:B:1028:LYS:O	1:B:1032:CYS:CB	2.64	0.45
1:C:455:LEU:HG	1:C:456:PHE:CD2	2.52	0.45
6:T:1:NAG:H61	6:T:2:NAG:C7	2.47	0.45
1:A:44:ARG:O	1:A:283:GLY:HA2	2.16	0.45
1:B:921:LYS:HD2	1:B:921:LYS:HA	1.81	0.45
1:C:934:ILE:HD13	1:C:934:ILE:HA	1.68	0.45
1:C:90:VAL:HG13	1:C:92:PHE:N	2.28	0.45
1:C:1073:LYS:HB2	1:C:1075:PHE:CE1	2.51	0.45
1:A:392:PHE:HB2	1:A:524:VAL:HG13	1.98	0.45
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.52	0.45
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.78	0.45
1:C:294:ASP:OD1	1:C:294:ASP:N	2.46	0.45
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.80	0.45
1:C:1086:LYS:HA	1:C:1125:ASN:HA	1.99	0.45
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:CYS:HB2	1:A:361:CYS:HB3	1.72	0.45
1:A:1031:GLU:OE2	1:C:1039:ARG:NH2	2.50	0.45
1:B:558:LYS:HA	1:B:558:LYS:HD3	1.58	0.45
3:S:59:PRO:HB2	3:S:61:ARG:HG2	1.98	0.45
3:S:88:CYS:O	3:S:99:GLY:N	2.49	0.45
1:B:169:GLU:OE1	1:B:170:TYR:N	2.50	0.44
1:B:393:THR:OG1	1:B:517:LEU:HA	2.16	0.44
3:L:87:TYR:CD1	3:L:101:GLY:HA2	2.51	0.44
3:S:61:ARG:HG3	3:S:62:PHE:CD2	2.53	0.44
1:A:347:PHE:CZ	1:A:509:ARG:HB3	2.52	0.44
1:A:402:ILE:HG12	1:A:510:VAL:HG21	1.99	0.44
1:C:31:SER:O	1:C:31:SER:OG	2.31	0.44
1:C:393:THR:HG23	1:C:517:LEU:HA	2.00	0.44
1:C:584:ILE:HD12	1:C:584:ILE:H	1.81	0.44
2:N:48:VAL:O	2:N:60:ALA:N	2.50	0.44
1:A:708:SER:OG	1:A:711:SER:N	2.49	0.44
1:A:869:MET:HE1	1:C:697:MET:HG3	1.98	0.44
1:B:200:TYR:HB2	1:B:201:PHE:H	1.61	0.44
1:B:452:LEU:HD13	1:B:494:SER:HB2	1.98	0.44
2:H:100(A):PRO:HG3	3:L:32:TYR:CE1	2.52	0.44
1:A:439:ASN:OD1	1:A:507:PRO:HD2	2.17	0.44
1:A:557:LYS:HB3	1:A:559:PHE:CE1	2.51	0.44
1:B:117:LEU:HD23	1:B:118:LEU:N	2.32	0.44
1:B:980:ILE:HD13	1:B:992:GLN:HB3	1.99	0.44
1:B:986:PRO:HB2	1:B:987:PRO:HD3	2.00	0.44
1:B:404:GLY:HA3	1:B:503:VAL:O	2.17	0.44
1:B:409:GLN:HB3	1:B:419:ALA:HB2	1.98	0.44
1:C:298:GLU:OE1	1:C:316:SER:OG	2.34	0.44
1:C:326:ILE:HD12	1:C:534:VAL:HG22	1.98	0.44
3:S:25:GLY:O	3:S:69:ASN:ND2	2.32	0.44
1:A:103:GLY:HA2	1:A:119:ILE:O	2.17	0.44
1:B:190:ARG:HB3	1:B:192:PHE:CE1	2.52	0.44
1:B:309:GLU:O	1:B:313:TYR:OH	2.18	0.44
1:B:386:LYS:HB3	1:B:386:LYS:HE2	1.65	0.44
1:B:410:ILE:HG23	1:B:425:LEU:HD11	2.00	0.44
1:C:431:GLY:HA3	1:C:513:LEU:O	2.18	0.44
2:H:41:PRO:HD3	2:H:88:ALA:HA	2.00	0.44
1:A:644:GLN:HG3	1:A:645:THR:N	2.33	0.44
1:A:1038:LYS:HB3	1:A:1038:LYS:HE2	1.74	0.44
1:B:126:VAL:HG12	1:B:128:ILE:HG13	2.00	0.44
1:B:190:ARG:HD3	1:B:192:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:CYS:HB3	1:B:525:CYS:HA	2.00	0.44
1:B:392:PHE:HD1	1:B:517:LEU:HD13	1.82	0.44
1:B:1083:HIS:CG	1:B:1137:VAL:H	2.36	0.44
1:C:398:ASP:O	1:C:511:VAL:HA	2.18	0.44
3:L:78:LEU:HD11	3:L:106:VAL:HG22	2.00	0.44
3:S:82:ASP:O	3:S:104:LEU:HB2	2.18	0.44
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.36	0.44
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.53	0.44
1:B:320:VAL:HG23	1:B:591:SER:O	2.17	0.44
1:B:754:LEU:HA	1:B:754:LEU:HD23	1.74	0.44
1:C:375:SER:OG	1:C:435:ALA:O	2.28	0.44
2:H:20:LEU:O	2:H:79:TYR:HA	2.18	0.44
1:A:315:THR:OG1	1:A:316:SER:N	2.51	0.43
1:B:541:PHE:HD1	1:B:543:PHE:HD1	1.65	0.43
1:B:612:TYR:HE1	1:B:651:ILE:HD12	1.83	0.43
1:B:976:VAL:HB	1:B:979:ASP:HB2	2.00	0.43
1:C:359:SER:OG	1:C:360:ASN:N	2.51	0.43
1:C:977:LEU:HD12	1:C:977:LEU:HA	1.67	0.43
2:H:38:ARG:HG2	2:H:48:VAL:HG11	2.00	0.43
2:N:67:PHE:HB3	2:N:80:LEU:HD11	1.99	0.43
1:B:86:PHE:HE2	1:B:196:ASN:HD21	1.66	0.43
1:B:187:LYS:HA	1:B:210:ILE:HG13	1.99	0.43
1:B:556:ASN:N	1:B:556:ASN:OD1	2.51	0.43
1:B:1072:GLU:N	1:B:1072:GLU:OE1	2.50	0.43
1:C:169:GLU:HG2	1:C:170:TYR:H	1.83	0.43
1:C:749:CYS:SG	1:C:977:LEU:HD21	2.58	0.43
1:A:900:MET:HE2	1:A:900:MET:HB3	1.76	0.43
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.99	0.43
1:B:1029:MET:HE3	1:B:1029:MET:HB2	1.91	0.43
1:C:501:ASN:HD22	1:C:505:TYR:HB3	1.83	0.43
2:N:47:TRP:HE1	2:N:50:VAL:HB	1.83	0.43
1:A:451:TYR:HD1	1:A:497:PHE:HB2	1.84	0.43
1:A:753:LEU:HB2	1:A:997:ILE:HD13	2.00	0.43
1:B:600:PRO:HD3	1:B:692:ILE:HD11	2.01	0.43
1:C:58:PHE:HE1	1:C:275:PHE:CE2	2.36	0.43
1:A:417:LYS:H	1:A:417:LYS:HG3	1.59	0.43
1:B:563:GLN:CD	1:C:43:PHE:HB2	2.44	0.43
3:L:90:SER:OG	3:L:91:TYR:N	2.51	0.43
1:A:713:ALA:HB3	1:B:894:LEU:HB3	2.00	0.43
1:B:95:THR:O	1:B:95:THR:OG1	2.35	0.43
1:A:357:ARG:HE	1:A:394:ASN:ND2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:VAL:HG21	1:B:1035:GLY:HA3	1.99	0.43
1:B:363:ALA:HB3	1:B:365:TYR:CZ	2.53	0.43
3:L:53:LYS:HE3	3:L:53:LYS:HB2	1.77	0.43
1:A:167:THR:HB	1:C:357:ARG:NH1	2.33	0.43
1:A:603:ASN:ND2	8:A:1308:NAG:O7	2.52	0.43
1:A:712:ILE:HG12	1:A:713:ALA:H	1.84	0.43
1:B:505:TYR:OH	3:S:30:TYR:HB3	2.19	0.43
1:B:568:ASP:OD1	1:B:569:ILE:N	2.42	0.43
1:C:411:ALA:HB3	1:C:414:GLN:CG	2.49	0.43
1:C:1037:SER:H	1:C:1048:HIS:HD2	1.66	0.43
1:C:1055:SER:OG	1:C:1056:ALA:N	2.51	0.43
1:A:216:LEU:HG	1:A:266:TYR:CD1	2.54	0.43
1:A:586:ASP:O	1:A:587:ILE:HG13	2.19	0.43
1:B:442:ASP:HB3	1:B:507:PRO:HG3	2.00	0.43
1:B:719:THR:HA	1:B:926:GLN:HE22	1.84	0.43
1:C:977:LEU:HD11	1:C:993:ILE:HG12	1.99	0.43
1:A:569:ILE:H	1:A:569:ILE:HG12	1.60	0.43
1:A:1064:HIS:O	1:A:1066:THR:HG23	2.19	0.43
1:B:169:GLU:CD	1:B:170:TYR:H	2.26	0.43
1:B:421:TYR:CE1	1:B:457:ARG:HB3	2.54	0.43
1:C:392:PHE:HA	1:C:517:LEU:HD13	2.00	0.43
1:C:416:GLY:N	1:C:420:ASP:OD1	2.38	0.43
1:A:353:TRP:CE2	1:A:466:ARG:HG3	2.54	0.42
1:B:1083:HIS:HB2	1:B:1137:VAL:HG23	2.01	0.42
2:N:98:TRP:H	2:N:98:TRP:CD1	2.38	0.42
1:A:353:TRP:HB3	1:A:400:PHE:HD2	1.84	0.42
1:B:368:LEU:HD21	8:B:1311:NAG:H83	2.01	0.42
1:B:403:ARG:NE	1:B:504:GLY:O	2.38	0.42
1:B:856:ASN:OD1	1:B:856:ASN:N	2.52	0.42
1:C:65:PHE:CE1	1:C:84:LEU:HD21	2.54	0.42
1:C:959:LEU:HA	1:C:959:LEU:HD23	1.74	0.42
3:L:59:PRO:HG2	3:L:62:PHE:CE2	2.53	0.42
3:S:46:LEU:HD11	3:S:49:TYR:HD2	1.83	0.42
1:B:87:ASN:ND2	1:B:87:ASN:H	2.16	0.42
1:B:1100:THR:OG1	1:B:1101:HIS:ND1	2.34	0.42
2:H:11:LEU:O	2:H:12:ILE:HD13	2.19	0.42
2:H:75:LYS:H	2:H:75:LYS:HG2	1.70	0.42
1:A:231:ILE:H	1:A:231:ILE:HG12	1.66	0.42
1:A:324:GLU:HB2	1:A:539:VAL:HG23	2.01	0.42
1:A:538:CYS:HB2	1:A:590:CYS:HB3	1.40	0.42
1:A:752:LEU:HD23	1:A:752:LEU:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:PRO:HG3	1:A:1095:PHE:CE2	2.54	0.42
1:C:240:THR:HG22	1:C:241:LEU:O	2.20	0.42
1:C:759:PHE:O	1:C:763:LEU:HG	2.19	0.42
2:H:33:TYR:CD1	2:H:96:GLU:HG2	2.53	0.42
2:H:100(A):PRO:HG2	3:L:49:TYR:CD2	2.55	0.42
1:A:790:LYS:HB3	1:A:790:LYS:HE2	1.57	0.42
1:B:418:ILE:HG23	1:B:422:ASN:HB2	2.01	0.42
1:C:102:ARG:HA	1:C:102:ARG:HD3	1.81	0.42
1:C:782:PHE:O	1:C:784:GLN:N	2.50	0.42
2:H:20:LEU:HD11	2:H:90:TYR:CD1	2.54	0.42
2:N:14:PRO:HD3	2:N:112:SER:C	2.44	0.42
3:L:12:SER:OG	3:L:105:THR:O	2.34	0.42
1:A:429:PHE:HE1	1:A:514:SER:HB3	1.84	0.42
1:A:557:LYS:O	1:A:559:PHE:N	2.53	0.42
1:A:1029:MET:HE3	1:A:1029:MET:HB2	1.75	0.42
1:B:37:TYR:HB3	1:B:223:LEU:HB2	2.01	0.42
1:C:901:GLN:O	1:C:905:ARG:HG2	2.19	0.42
3:S:37:GLN:HE21	3:S:45:LYS:HD3	1.84	0.42
1:A:355:ARG:HB3	1:A:398:ASP:OD1	2.19	0.42
1:B:330:PRO:HD3	1:B:544:ASN:OD1	2.20	0.42
1:B:437:ASN:HA	1:B:508:TYR:CE1	2.54	0.42
1:B:453:TYR:HE2	1:B:455:LEU:HD13	1.85	0.42
1:C:231:ILE:HG13	1:C:233:ILE:HG22	2.02	0.42
1:C:396:TYR:O	1:C:513:LEU:HA	2.19	0.42
1:C:1074:ASN:OD1	1:C:1074:ASN:N	2.51	0.42
1:A:916:LEU:HD12	1:A:923:ILE:HD12	2.01	0.42
1:B:207:HIS:C	1:B:207:HIS:CD2	2.97	0.42
1:A:767:LEU:HA	1:A:767:LEU:HD23	1.84	0.42
1:B:386:LYS:O	1:B:386:LYS:HG2	2.20	0.42
1:C:168:PHE:CE1	1:C:230:PRO:HD2	2.55	0.42
2:H:38:ARG:HD2	2:H:88:ALA:HB3	2.02	0.42
1:A:902:MET:HE3	1:A:902:MET:HB3	1.95	0.42
1:B:369:TYR:CD2	1:B:384:PRO:HB2	2.55	0.42
1:B:602:THR:HA	1:B:605:SER:O	2.19	0.42
2:H:98:TRP:HB2	3:L:32:TYR:CE2	2.55	0.42
3:S:79:GLN:NE2	3:S:81:GLU:OE1	2.53	0.42
1:A:287:ASP:OD1	1:A:288:ALA:N	2.49	0.41
1:B:353:TRP:CZ2	1:B:466:ARG:HB2	2.55	0.41
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.85	0.41
1:C:131:CYS:O	1:C:133:PHE:N	2.52	0.41
1:C:437:ASN:HA	1:C:508:TYR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:19:VAL:HG11	3:S:104:LEU:HD22	2.02	0.41
3:S:20:THR:HA	3:S:74:THR:HA	2.02	0.41
1:A:130:VAL:HG12	1:A:130:VAL:O	2.19	0.41
1:A:453:TYR:CE2	1:A:455:LEU:HD11	2.55	0.41
1:A:560:LEU:O	1:A:562:PHE:N	2.52	0.41
1:B:1043:CYS:HB3	1:B:1048:HIS:CE1	2.55	0.41
1:C:120:VAL:HG22	1:C:241:LEU:HD11	2.02	0.41
1:C:543:PHE:O	1:C:544:ASN:C	2.63	0.41
1:C:1086:LYS:HE2	1:C:1086:LYS:HB3	1.84	0.41
2:H:36:TRP:CG	2:H:80:LEU:HD22	2.55	0.41
1:A:551:VAL:HB	1:A:588:THR:HG23	2.02	0.41
1:A:887:THR:HG21	1:A:894:LEU:HD12	2.02	0.41
1:B:452:LEU:HD12	1:B:492:LEU:HG	2.03	0.41
1:B:534:VAL:HG21	1:B:539:VAL:HG11	2.02	0.41
1:C:34:ARG:HB3	1:C:34:ARG:NH1	2.34	0.41
1:C:95:THR:HG23	1:C:95:THR:O	2.20	0.41
1:C:170:TYR:O	1:C:171:VAL:HG23	2.19	0.41
1:A:100:ILE:O	1:A:102:ARG:HG3	2.21	0.41
1:A:319:ARG:NH1	1:B:740:MET:SD	2.94	0.41
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.61	0.41
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.25	0.41
1:B:338:PHE:CE2	1:B:363:ALA:HB1	2.55	0.41
1:B:592:PHE:HE1	1:C:857:GLY:HA2	1.85	0.41
1:C:406:GLU:HA	1:C:409:GLN:HB2	2.03	0.41
1:C:438:SER:OG	1:C:442:ASP:N	2.51	0.41
1:C:444:LYS:HB3	1:C:444:LYS:HE3	1.61	0.41
1:C:517:LEU:HD12	1:C:517:LEU:HA	1.88	0.41
3:L:78:LEU:HD21	3:L:106:VAL:HG21	2.02	0.41
3:L:103:LYS:HG3	3:L:105:THR:HG22	2.03	0.41
1:A:131:CYS:HB2	1:A:166:CYS:HB3	1.71	0.41
1:C:276:LEU:O	1:C:288:ALA:HA	2.21	0.41
1:C:825:LYS:HA	1:C:825:LYS:HD3	1.72	0.41
2:N:100(A):PRO:HG2	3:S:46:LEU:HD22	2.03	0.41
1:A:650:LEU:HD12	1:A:650:LEU:HA	1.90	0.41
1:B:503:VAL:HA	1:B:506:GLN:HB2	2.02	0.41
1:C:792:PRO:O	1:C:795:LYS:NZ	2.53	0.41
1:A:437:ASN:HA	1:A:508:TYR:HA	2.01	0.41
1:A:731:MET:HG3	1:A:1018:ILE:HG13	2.03	0.41
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.02	0.41
1:B:1094:VAL:HG13	1:C:904:TYR:OH	2.20	0.41
2:N:34:MET:SD	2:N:78:LEU:HD22	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:67:PHE:CE1	2:N:82(C):LEU:HG	2.55	0.41
3:S:61:ARG:HD3	3:S:75:VAL:HG12	2.02	0.41
1:A:901:GLN:HE21	1:A:905:ARG:HH21	1.69	0.41
1:C:442:ASP:OD1	1:C:448:ASN:ND2	2.53	0.41
1:C:938:LEU:HD23	1:C:938:LEU:HA	1.92	0.41
1:A:84:LEU:O	1:A:237:ARG:HG2	2.20	0.41
1:A:335:LEU:HD12	1:A:335:LEU:HA	1.95	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.79	0.41
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.55	0.41
1:A:870:ILE:HD13	1:A:870:ILE:HA	1.76	0.41
1:B:33:THR:HA	1:B:58:PHE:CD1	2.55	0.41
1:B:438:SER:HB2	1:B:509:ARG:H	1.86	0.41
1:B:443:SER:HB2	1:B:499:PRO:HD3	2.02	0.41
1:B:534:VAL:CG2	1:B:539:VAL:HG11	2.51	0.41
1:B:1125:ASN:OD1	1:B:1126:CYS:N	2.54	0.41
1:C:189:LEU:HB2	1:C:210:ILE:HD13	2.03	0.41
1:C:538:CYS:HB2	1:C:590:CYS:HB2	1.94	0.41
3:L:13:GLY:HA3	3:L:19:VAL:HG22	2.03	0.41
1:A:435:ALA:HA	1:A:509:ARG:O	2.21	0.41
1:A:865:LEU:HD23	1:A:865:LEU:HA	1.78	0.41
1:B:456:PHE:CE1	2:N:100:LEU:HD11	2.56	0.41
1:B:462:LYS:O	1:B:465:GLU:HB2	2.21	0.41
1:B:649:CYS:SG	1:B:650:LEU:N	2.94	0.41
1:B:1128:VAL:HG23	1:B:1129:VAL:HG13	2.03	0.41
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.56	0.41
1:C:787:GLN:O	1:C:788:ILE:HD13	2.21	0.41
1:C:906:PHE:O	1:C:909:ILE:HG12	2.21	0.41
1:C:980:ILE:HD13	1:C:992:GLN:HB3	2.03	0.41
1:A:322:PRO:HA	1:A:538:CYS:O	2.22	0.40
1:A:385:THR:HG22	1:A:385:THR:O	2.21	0.40
1:B:328:ARG:HH21	1:B:578:ASP:CG	2.30	0.40
1:C:392:PHE:CD1	1:C:515:PHE:HB3	2.55	0.40
1:C:450:ASN:OD1	1:C:450:ASN:N	2.35	0.40
1:C:721:SER:OG	1:C:1066:THR:OG1	2.39	0.40
1:C:856:ASN:OD1	1:C:856:ASN:N	2.53	0.40
2:H:82(C):LEU:HB3	2:H:111:VAL:HG11	2.02	0.40
1:B:592:PHE:CE1	1:C:857:GLY:HA2	2.56	0.40
1:B:966:LEU:HA	1:B:966:LEU:HD23	1.69	0.40
1:B:981:LEU:HD23	1:B:981:LEU:HA	1.81	0.40
1:C:116:SER:O	1:C:116:SER:OG	2.32	0.40
1:C:329:PHE:CD2	1:C:544:ASN:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:ASN:HD21	1:C:454:ARG:N	2.12	0.40
1:C:457:ARG:HA	1:C:457:ARG:HD2	1.67	0.40
2:H:74:SER:OG	2:H:76:ASN:ND2	2.54	0.40
2:H:82:MET:HG3	2:H:82(C):LEU:HD21	2.02	0.40
2:H:98:TRP:HB3	3:L:91:TYR:HB2	2.02	0.40
2:N:103:TRP:NE1	3:S:44:PRO:O	2.54	0.40
3:S:23:CYS:HB2	3:S:35:TRP:CZ3	2.56	0.40
1:A:120:VAL:HG12	1:A:121:ASN:N	2.36	0.40
1:A:543:PHE:O	1:A:546:LEU:HB3	2.21	0.40
1:B:825:LYS:HA	1:B:825:LYS:HD3	1.80	0.40
1:B:1083:HIS:CD2	1:B:1137:VAL:HB	2.56	0.40
1:C:106:PHE:HB2	1:C:117:LEU:HB3	2.02	0.40
1:C:474:GLN:H	1:C:474:GLN:HG3	1.73	0.40
1:C:534:VAL:HG21	1:C:539:VAL:HG11	2.02	0.40
1:C:708:SER:OG	1:C:709:ASN:N	2.54	0.40
1:C:731:MET:HB2	1:C:731:MET:HE2	1.80	0.40
1:C:733:LYS:HE3	1:C:771:ALA:O	2.22	0.40
1:C:794:ILE:O	1:C:795:LYS:NZ	2.41	0.40
2:H:12:ILE:HG22	2:H:13:GLN:O	2.21	0.40
2:H:33:TYR:HB3	2:H:96:GLU:HB2	2.02	0.40
1:B:120:VAL:HG12	1:B:121:ASN:N	2.36	0.40
1:C:206:LYS:HG3	1:C:207:HIS:N	2.36	0.40
2:H:11:LEU:HA	2:H:110:THR:O	2.21	0.40
1:A:383:SER:N	1:B:983:ARG:O	2.53	0.40
1:B:365:TYR:CD2	1:B:387:LEU:HG	2.57	0.40
1:B:501:ASN:HD21	3:S:31:LYS:H	1.68	0.40
1:C:228:ASP:OD1	1:C:229:LEU:N	2.55	0.40
1:C:703:ASN:OD1	1:C:704:SER:N	2.55	0.40
1:C:731:MET:N	1:C:774:GLN:OE1	2.49	0.40
1:C:821:LEU:O	1:C:825:LYS:HG2	2.22	0.40
2:H:82(B):SER:OG	2:H:83:ARG:NH2	2.55	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	436/1259 (35%)	373 (86%)	63 (14%)	0	100	100
1	B	963/1259 (76%)	847 (88%)	114 (12%)	2 (0%)	43	71
1	C	962/1259 (76%)	857 (89%)	105 (11%)	0	100	100
2	H	114/230 (50%)	100 (88%)	14 (12%)	0	100	100
2	N	114/230 (50%)	108 (95%)	6 (5%)	0	100	100
3	L	109/217 (50%)	89 (82%)	19 (17%)	1 (1%)	14	41
3	S	109/217 (50%)	95 (87%)	14 (13%)	0	100	100
All	All	2807/4671 (60%)	2469 (88%)	335 (12%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	331	ASN
1	B	332	ILE
3	L	51	VAL

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	801/1096 (73%)	701 (88%)	100 (12%)	4	17
1	B	831/1096 (76%)	780 (94%)	51 (6%)	17	42
1	C	830/1096 (76%)	773 (93%)	57 (7%)	14	39
2	H	94/194 (48%)	90 (96%)	4 (4%)	26	50
2	N	94/194 (48%)	88 (94%)	6 (6%)	16	41
3	L	90/182 (50%)	81 (90%)	9 (10%)	7	25
3	S	90/182 (50%)	82 (91%)	8 (9%)	9	30
All	All	2830/4040 (70%)	2595 (92%)	235 (8%)	12	34

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	40	ASP
1	A	42	VAL
1	A	47	VAL
1	A	50	SER
1	A	51	THR
1	A	68	ILE
1	A	83	VAL
1	A	90	VAL
1	A	100	ILE
1	A	105	ILE
1	A	108	THR
1	A	109	THR
1	A	117	LEU
1	A	166	CYS
1	A	167	THR
1	A	189	LEU
1	A	208	THR
1	A	224	GLU
1	A	227	VAL
1	A	231	ILE
1	A	233	ILE
1	A	235	ILE
1	A	270	LEU
1	A	285	ILE
1	A	305	SER
1	A	312	ILE
1	A	318	PHE
1	A	319	ARG
1	A	326	ILE
1	A	334	ASN
1	A	341	VAL
1	A	351	TYR
1	A	377	PHE
1	A	390	LEU
1	A	400	PHE
1	A	430	THR
1	A	492	LEU
1	A	498	GLN
1	A	503	VAL
1	A	511	VAL
1	A	512	VAL

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Mol	Chain	Res	Type
1	A	523	THR
1	A	524	VAL
1	A	525	CYS
1	A	546	LEU
1	A	547	THR
1	A	549	THR
1	A	553	THR
1	A	554	GLU
1	A	565	PHE
1	A	569	ILE
1	A	574	ASP
1	A	585	LEU
1	A	588	THR
1	A	590	CYS
1	A	610	VAL
1	A	611	LEU
1	A	649	CYS
1	A	705	VAL
1	A	723	THR
1	A	734	THR
1	A	738	CYS
1	A	739	THR
1	A	754	LEU
1	A	768	THR
1	A	791	THR
1	A	801	ASN
1	A	858	LEU
1	A	875	SER
1	A	884	SER
1	A	887	THR
1	A	896	ILE
1	A	912	THR
1	A	919	ASN
1	A	926	GLN
1	A	935	GLN
1	A	975	SER
1	A	984	LEU
1	A	996	LEU
1	A	997	ILE
1	A	998	THR
1	A	1006	THR
1	A	1008	VAL

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Mol	Chain	Res	Type
1	A	1009	THR
1	A	1012	LEU
1	A	1027	THR
1	A	1032	CYS
1	A	1076	THR
1	A	1101	HIS
1	A	1104	VAL
1	A	1105	THR
1	A	1116	THR
1	A	1117	THR
1	A	1122	VAL
1	A	1127	ASP
1	A	1128	VAL
1	A	1130	ILE
1	A	1136	THR
1	A	1137	VAL
1	B	33	THR
1	B	40	ASP
1	B	47	VAL
1	B	84	LEU
1	B	87	ASN
1	B	90	VAL
1	B	105	ILE
1	B	110	LEU
1	B	127	VAL
1	B	194	PHE
1	B	233	ILE
1	B	240	THR
1	B	289	VAL
1	B	305	SER
1	B	312	ILE
1	B	316	SER
1	B	323	THR
1	B	326	ILE
1	B	341	VAL
1	B	362	VAL
1	B	472	ILE
1	B	503	VAL
1	B	551	VAL
1	B	552	LEU
1	B	599	THR
1	B	611	LEU

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Mol	Chain	Res	Type
1	B	705	VAL
1	B	723	THR
1	B	724	THR
1	B	729	VAL
1	B	760	CYS
1	B	768	THR
1	B	778	THR
1	B	821	LEU
1	B	823	PHE
1	B	856	ASN
1	B	869	MET
1	B	873	TYR
1	B	887	THR
1	B	912	THR
1	B	916	LEU
1	B	941	THR
1	B	951	VAL
1	B	961	THR
1	B	963	VAL
1	B	998	THR
1	B	1006	THR
1	B	1021	SER
1	B	1027	THR
1	B	1094	VAL
1	B	1116	THR
1	C	34	ARG
1	C	40	ASP
1	C	43	PHE
1	C	51	THR
1	C	83	VAL
1	C	90	VAL
1	C	99	ASN
1	C	118	LEU
1	C	165	ASN
1	C	193	VAL
1	C	195	LYS
1	C	208	THR
1	C	226	LEU
1	C	231	ILE
1	C	235	ILE
1	C	285	ILE
1	C	303	LEU

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Mol	Chain	Res	Type
1	C	305	SER
1	C	326	ILE
1	C	332	ILE
1	C	341	VAL
1	C	358	ILE
1	C	361	CYS
1	C	364	ASP
1	C	398	ASP
1	C	444	LYS
1	C	450	ASN
1	C	472	ILE
1	C	500	THR
1	C	512	VAL
1	C	523	THR
1	C	531	THR
1	C	553	THR
1	C	587	ILE
1	C	607	GLU
1	C	611	LEU
1	C	656	VAL
1	C	705	VAL
1	C	723	THR
1	C	724	THR
1	C	768	THR
1	C	856	ASN
1	C	858	LEU
1	C	883	THR
1	C	886	TRP
1	C	913	GLN
1	C	919	ASN
1	C	934	ILE
1	C	959	LEU
1	C	969	ASN
1	C	1004	LEU
1	C	1006	THR
1	C	1040	VAL
1	C	1074	ASN
1	C	1082	CYS
1	C	1105	THR
1	C	1116	THR
2	H	49	SER
2	H	89	VAL

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Mol	Chain	Res	Type
2	H	101	ASP
2	H	107	THR
2	N	28	THR
2	N	61	ASP
2	N	77	THR
2	N	79	TYR
2	N	107	THR
2	N	111	VAL
3	L	24	THR
3	L	35	TRP
3	L	51	VAL
3	L	74	THR
3	L	75	VAL
3	L	81	GLU
3	L	97	VAL
3	L	102	THR
3	L	104	LEU
3	S	4	LEU
3	S	5	THR
3	S	39	HIS
3	S	51	VAL
3	S	70	THR
3	S	73	LEU
3	S	75	VAL
3	S	85	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	125	ASN
1	A	207	HIS
1	A	317	ASN
1	A	422	ASN
1	A	437	ASN
1	A	544	ASN
1	A	675	GLN
1	A	751	ASN
1	A	762	GLN
1	A	804	GLN
1	A	901	GLN
1	A	935	GLN

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Mol	Chain	Res	Type
1	A	1002	GLN
1	A	1005	GLN
1	A	1088	HIS
1	B	196	ASN
1	B	207	HIS
1	B	394	ASN
1	B	437	ASN
1	B	474	GLN
1	B	675	GLN
1	B	784	GLN
1	B	926	GLN
1	B	1005	GLN
1	B	1054	GLN
1	B	1071	GLN
1	C	49	HIS
1	C	207	HIS
1	C	317	ASN
1	C	388	ASN
1	C	422	ASN
1	C	437	ASN
1	C	580	GLN
1	C	644	GLN
1	C	690	GLN
1	C	784	GLN
1	C	949	GLN
1	C	953	ASN
1	C	1071	GLN
1	C	1106	GLN
1	C	1125	ASN
2	H	32	ASN
2	H	76	ASN
2	N	32	ASN
2	N	39	GLN
2	N	81	GLN
3	L	6	GLN
3	L	37	GLN
3	L	39	HIS
3	S	37	GLN
3	S	39	HIS

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 ⓘ

29 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	D	1	4,1	14,14,15	0.67	1 (7%)	17,19,21	0.61	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.36	0
4	NAG	E	1	4,1	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
4	NAG	E	2	4	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	F	1	5,1	14,14,15	0.28	0	17,19,21	0.39	0
5	FUC	F	2	5	10,10,11	0.59	0	14,14,16	0.80	0
4	NAG	G	1	4,1	14,14,15	0.19	0	17,19,21	0.50	0
4	NAG	G	2	4	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
4	NAG	I	1	4,1	14,14,15	0.65	1 (7%)	17,19,21	0.55	0
4	NAG	I	2	4	14,14,15	0.28	0	17,19,21	1.38	2 (11%)
6	NAG	J	1	6,1	14,14,15	0.27	0	17,19,21	0.55	0
6	NAG	J	2	6	14,14,15	0.28	0	17,19,21	0.53	0
6	FUC	J	3	6	10,10,11	0.45	0	14,14,16	0.79	0
4	NAG	K	1	4,1	14,14,15	0.48	0	17,19,21	1.36	2 (11%)
4	NAG	K	2	4	14,14,15	0.23	0	17,19,21	0.53	0
4	NAG	M	1	4,1	14,14,15	0.39	0	17,19,21	0.49	0
4	NAG	M	2	4	14,14,15	0.18	0	17,19,21	0.42	0
4	NAG	O	1	4,1	14,14,15	0.62	1 (7%)	17,19,21	0.53	0
4	NAG	O	2	4	14,14,15	0.66	1 (7%)	17,19,21	0.88	1 (5%)
4	NAG	P	1	4,1	14,14,15	0.26	0	17,19,21	0.60	0
4	NAG	P	2	4	14,14,15	0.24	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	Q	1	7,1	14,14,15	0.46	0	17,19,21	0.53	0
7	NAG	Q	2	7	14,14,15	0.20	0	17,19,21	0.49	0
7	BMA	Q	3	7	11,11,12	0.56	0	15,15,17	0.72	0
4	NAG	R	1	4,1	14,14,15	0.39	0	17,19,21	0.49	0
4	NAG	R	2	4	14,14,15	0.23	0	17,19,21	0.52	0
6	NAG	T	1	6,1	14,14,15	0.41	0	17,19,21	0.54	0
6	NAG	T	2	6	14,14,15	0.27	0	17,19,21	0.56	0
6	FUC	T	3	6	10,10,11	0.75	0	14,14,16	0.62	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	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	5,1	-	2/6/23/26	0/1/1/1
5	FUC	F	2	5	-	-	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	I	2	4	-	6/6/23/26	0/1/1/1
6	NAG	J	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	FUC	J	3	6	-	-	0/1/1/1
4	NAG	K	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
7	NAG	Q	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	R	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	4/6/23/26	0/1/1/1
6	FUC	T	3	6	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	-2.43	1.39	1.43
4	I	1	NAG	O5-C1	-2.36	1.39	1.43
4	O	1	NAG	O5-C1	-2.25	1.39	1.43
4	O	2	NAG	O5-C1	-2.19	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	C2-N2-C7	4.65	129.13	122.90
4	K	1	NAG	C2-N2-C7	4.46	128.88	122.90
4	I	2	NAG	C1-C2-N2	2.33	114.11	110.43
4	K	1	NAG	C1-C2-N2	2.21	113.91	110.43
4	O	2	NAG	C2-N2-C7	2.15	125.78	122.90
4	G	2	NAG	C1-O5-C5	2.07	114.97	112.19
4	E	1	NAG	C1-O5-C5	2.07	114.96	112.19

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	2	NAG	C1-C2-N2-C7
4	G	1	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	P	2	NAG	C4-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
7	Q	2	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
7	Q	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C1-C2-N2-C7
4	P	1	NAG	C1-C2-N2-C7
4	R	1	NAG	C1-C2-N2-C7
6	T	2	NAG	C1-C2-N2-C7
7	Q	3	BMA	C4-C5-C6-O6
4	E	1	NAG	C3-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
4	K	2	NAG	C3-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7
6	T	2	NAG	C3-C2-N2-C7
4	E	1	NAG	C1-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7
4	I	1	NAG	C1-C2-N2-C7

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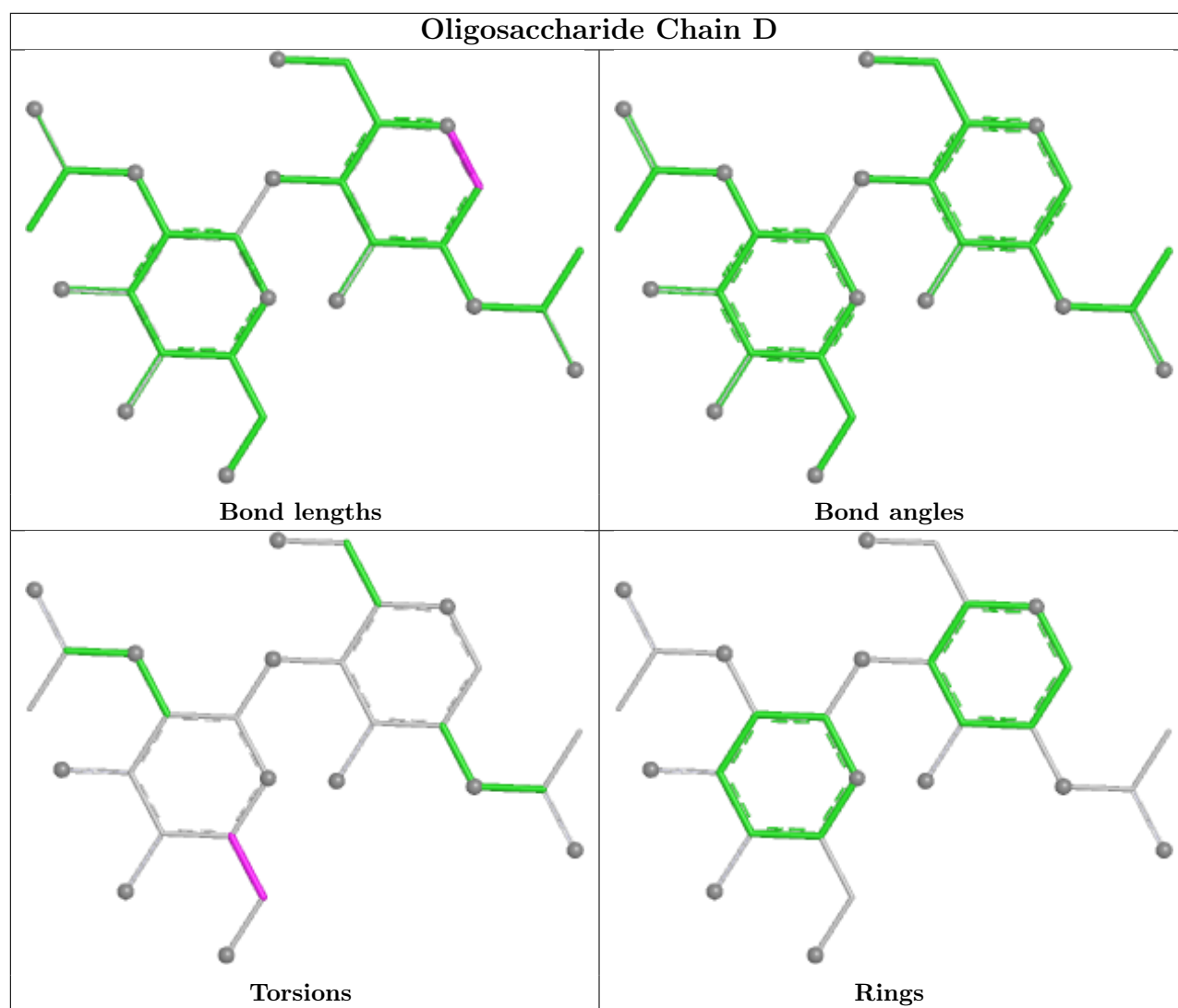
Mol	Chain	Res	Type	Atoms
4	I	2	NAG	C1-C2-N2-C7
4	K	1	NAG	C1-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7
4	P	1	NAG	C3-C2-N2-C7
5	F	1	NAG	C3-C2-N2-C7
4	K	1	NAG	C4-C5-C6-O6

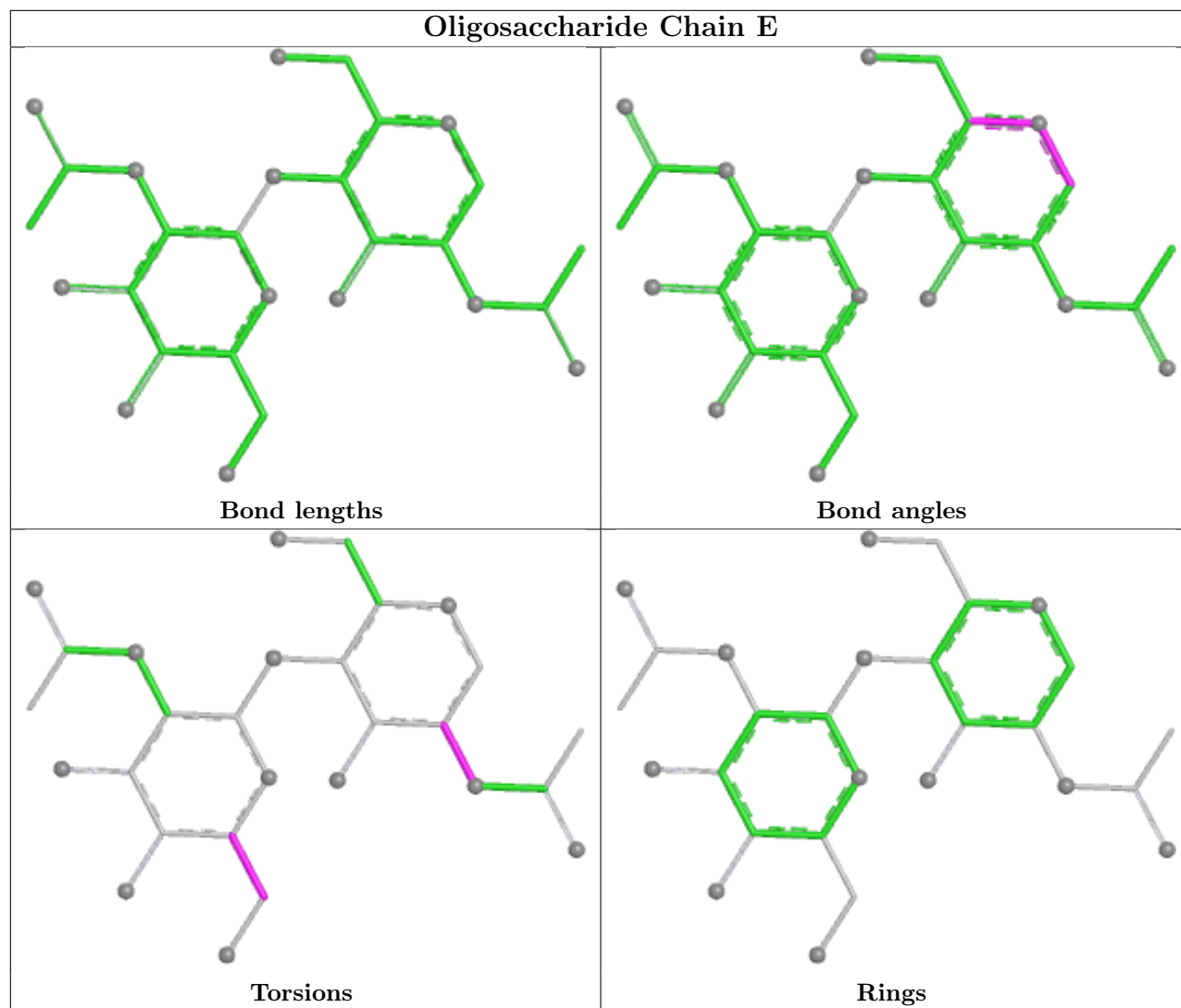
There are no ring outliers.

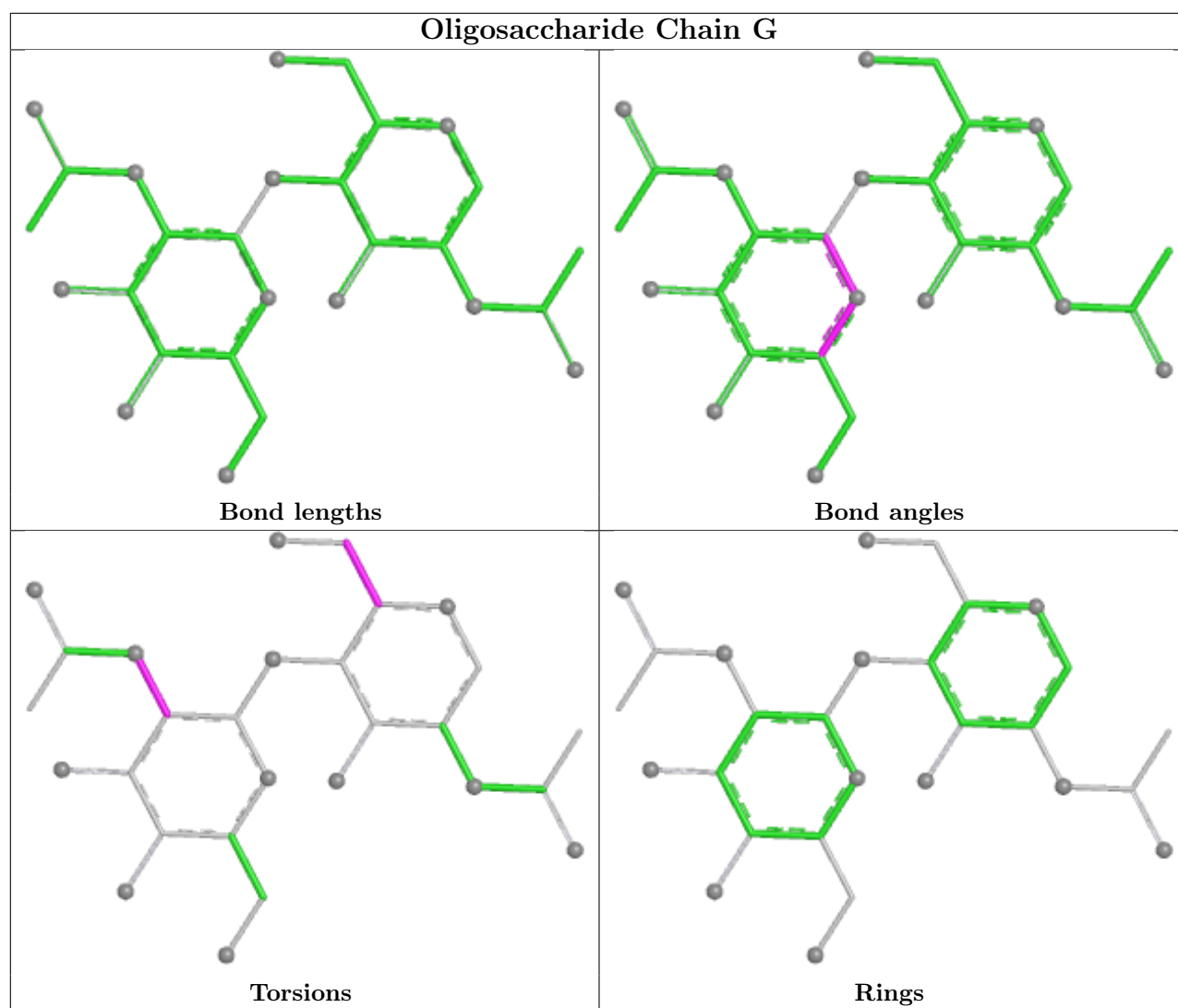
7 monomers are involved in 7 short contacts:

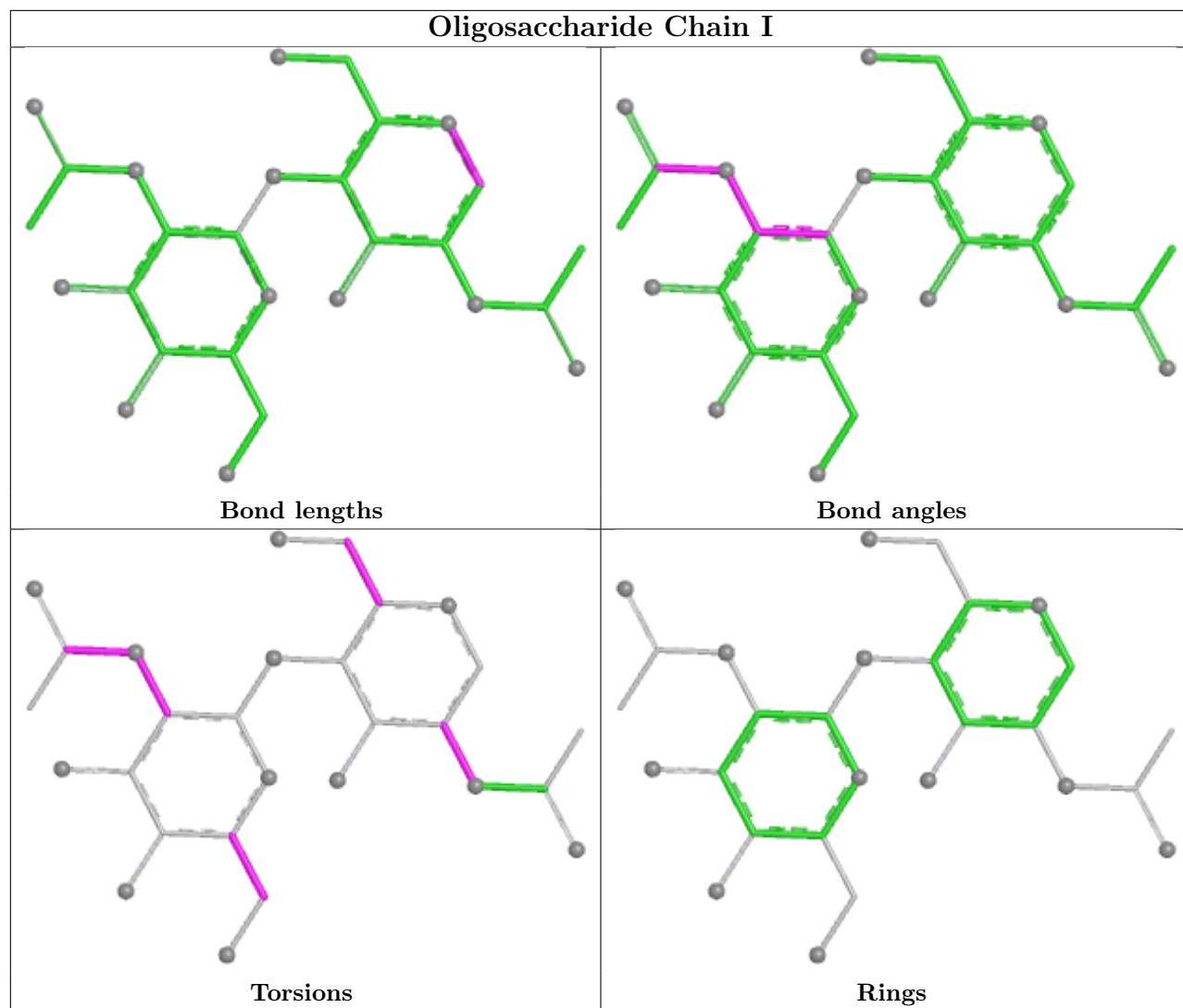
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	2	0
4	M	1	NAG	1	0
4	K	1	NAG	1	0
4	I	2	NAG	2	0
6	T	2	NAG	1	0
4	P	1	NAG	1	0
6	T	1	NAG	1	0

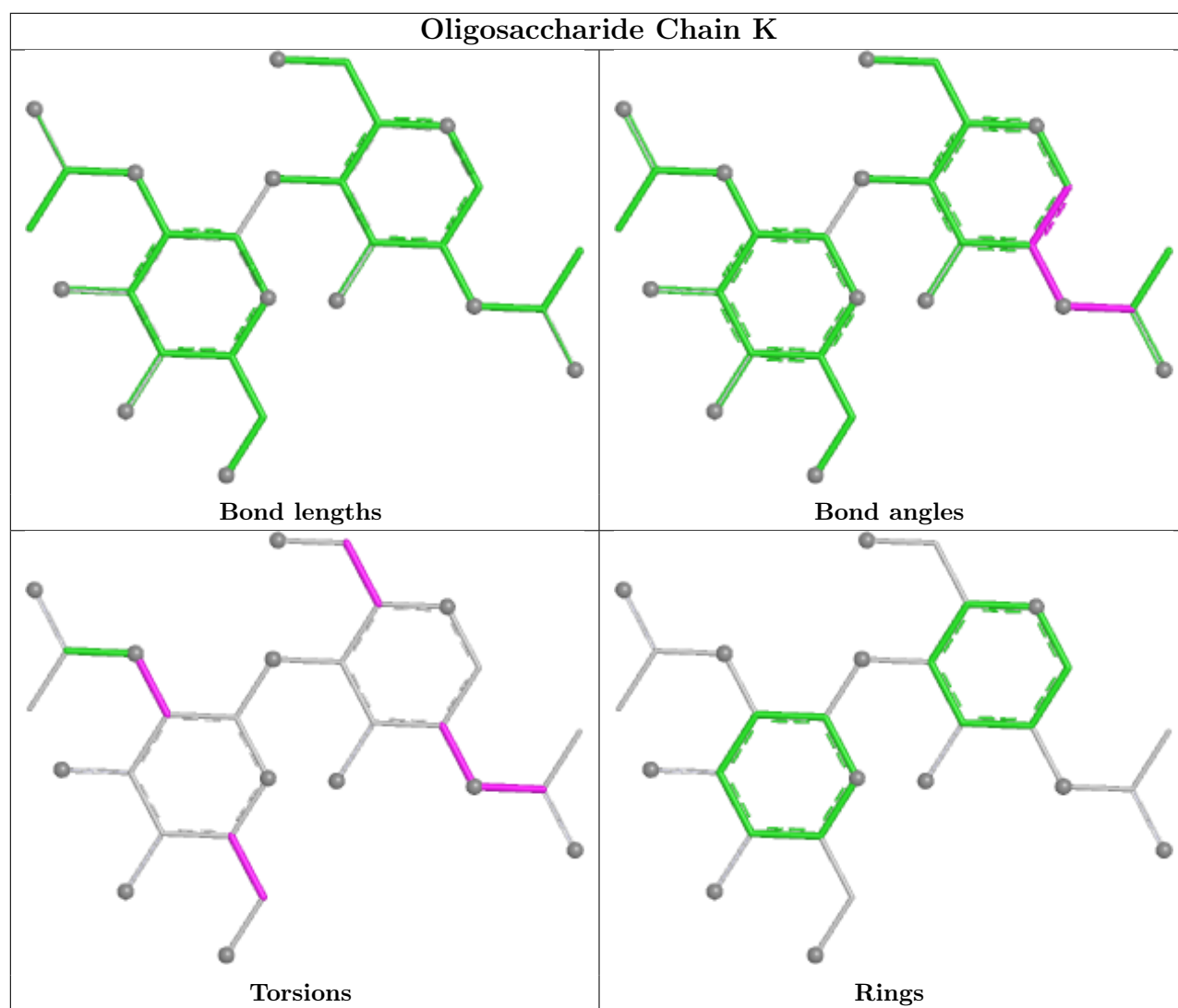
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

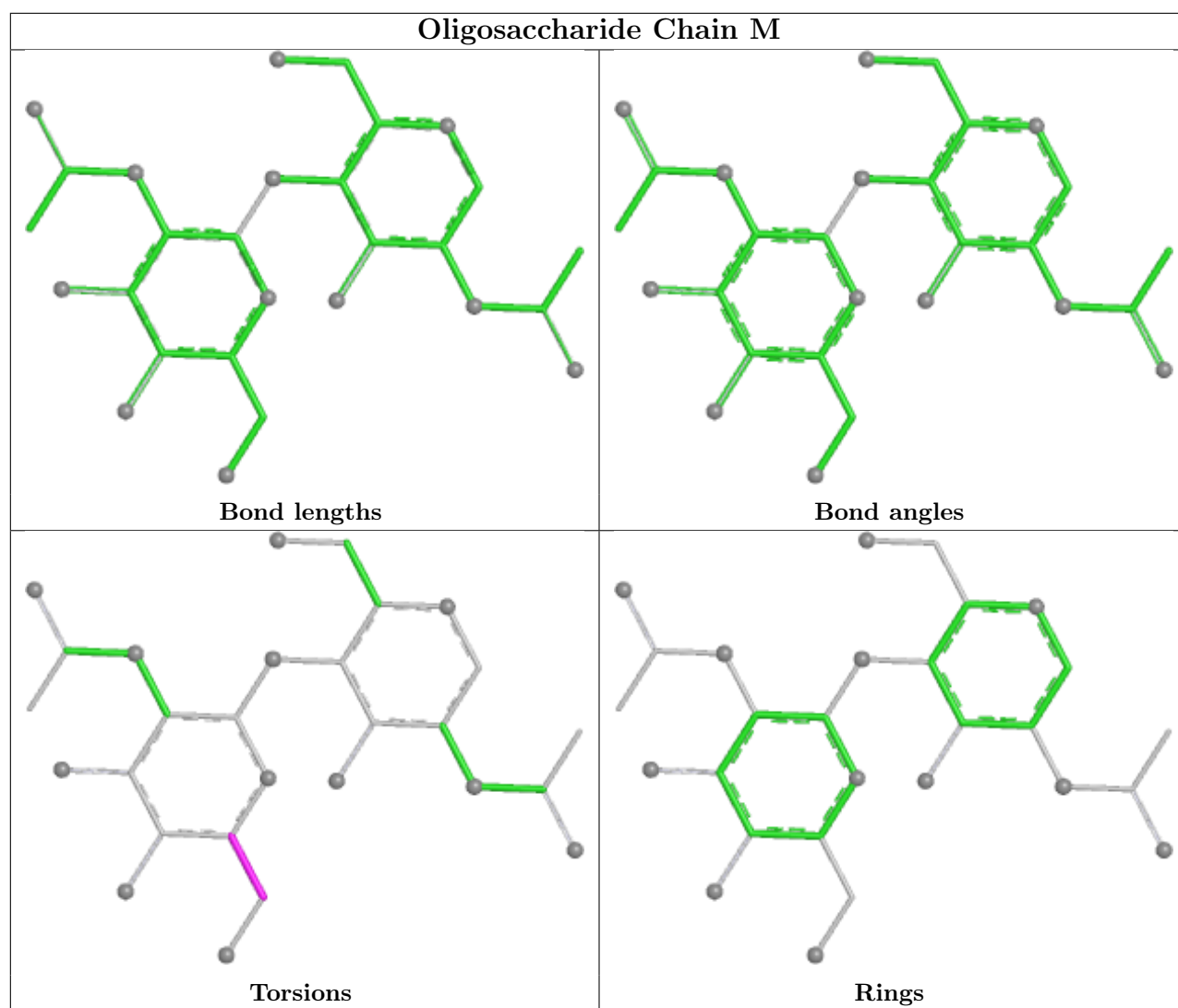


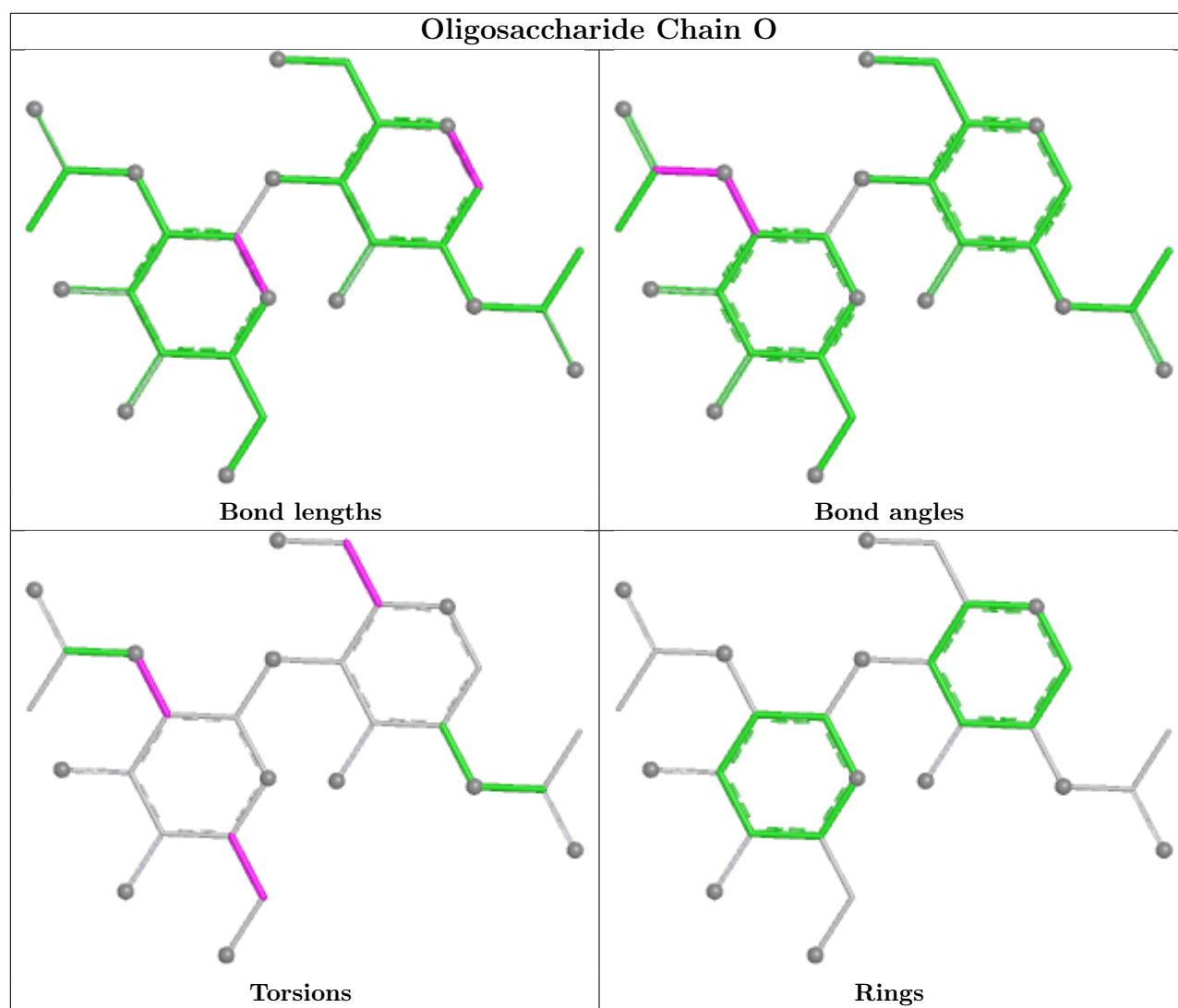


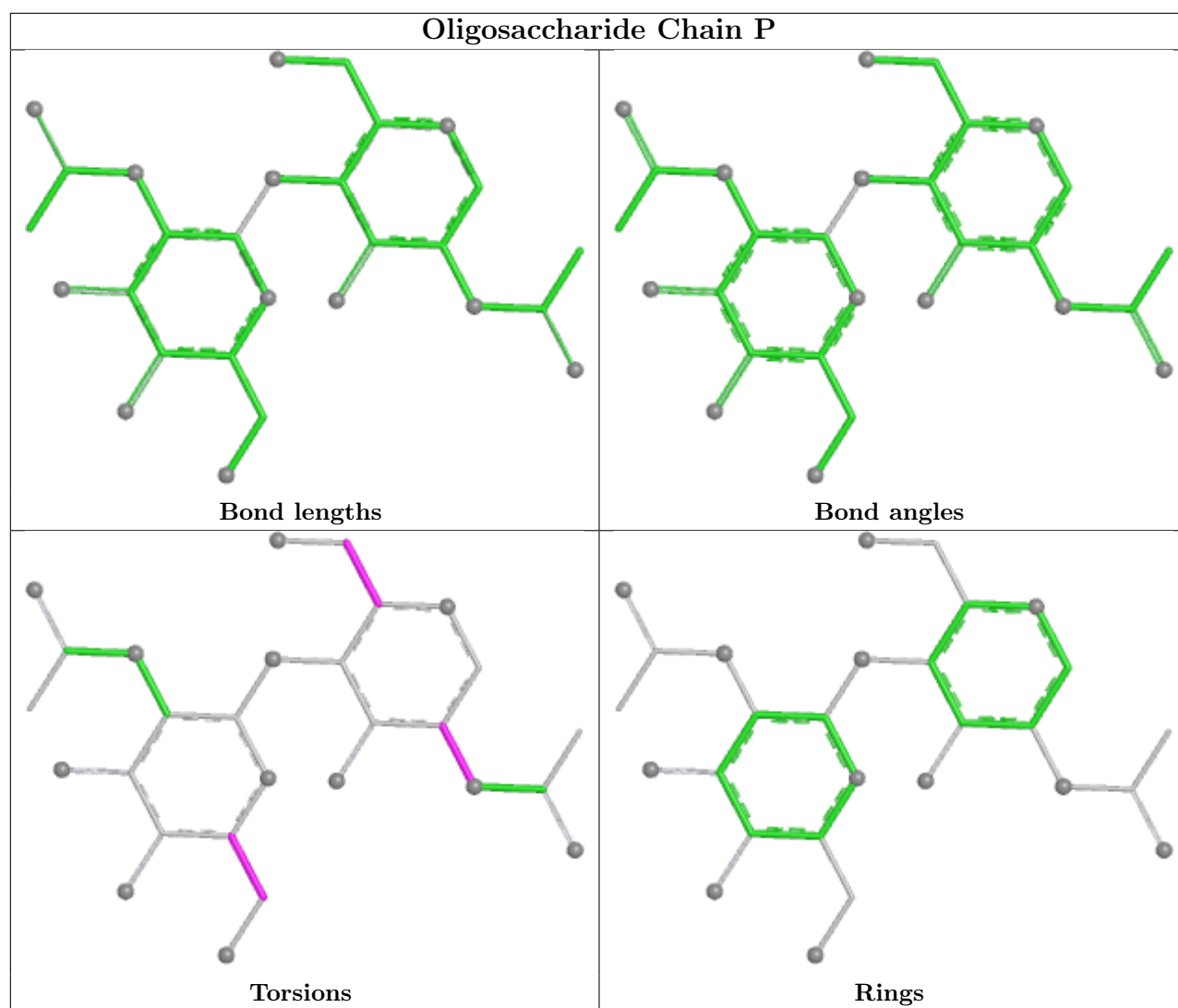


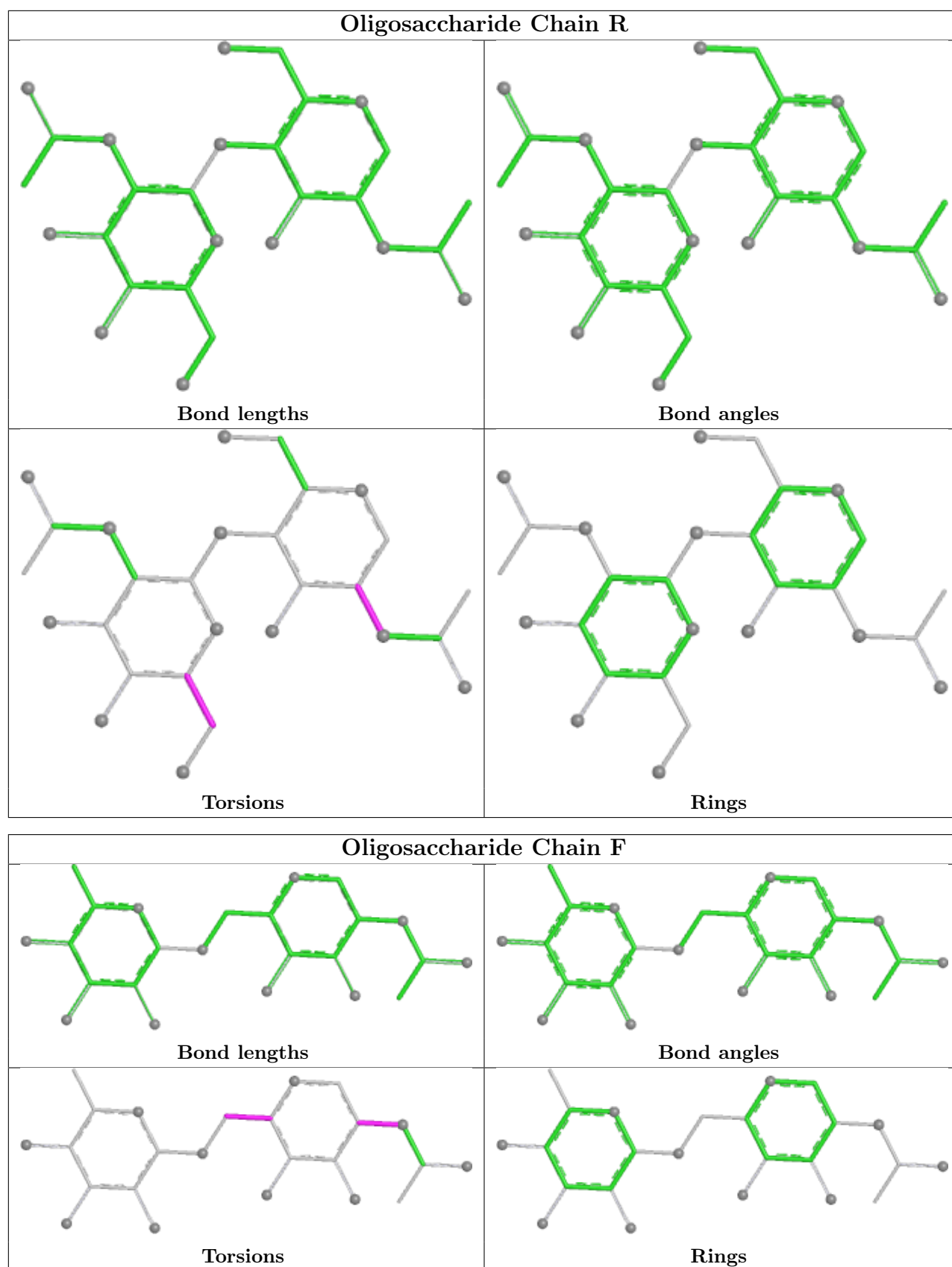


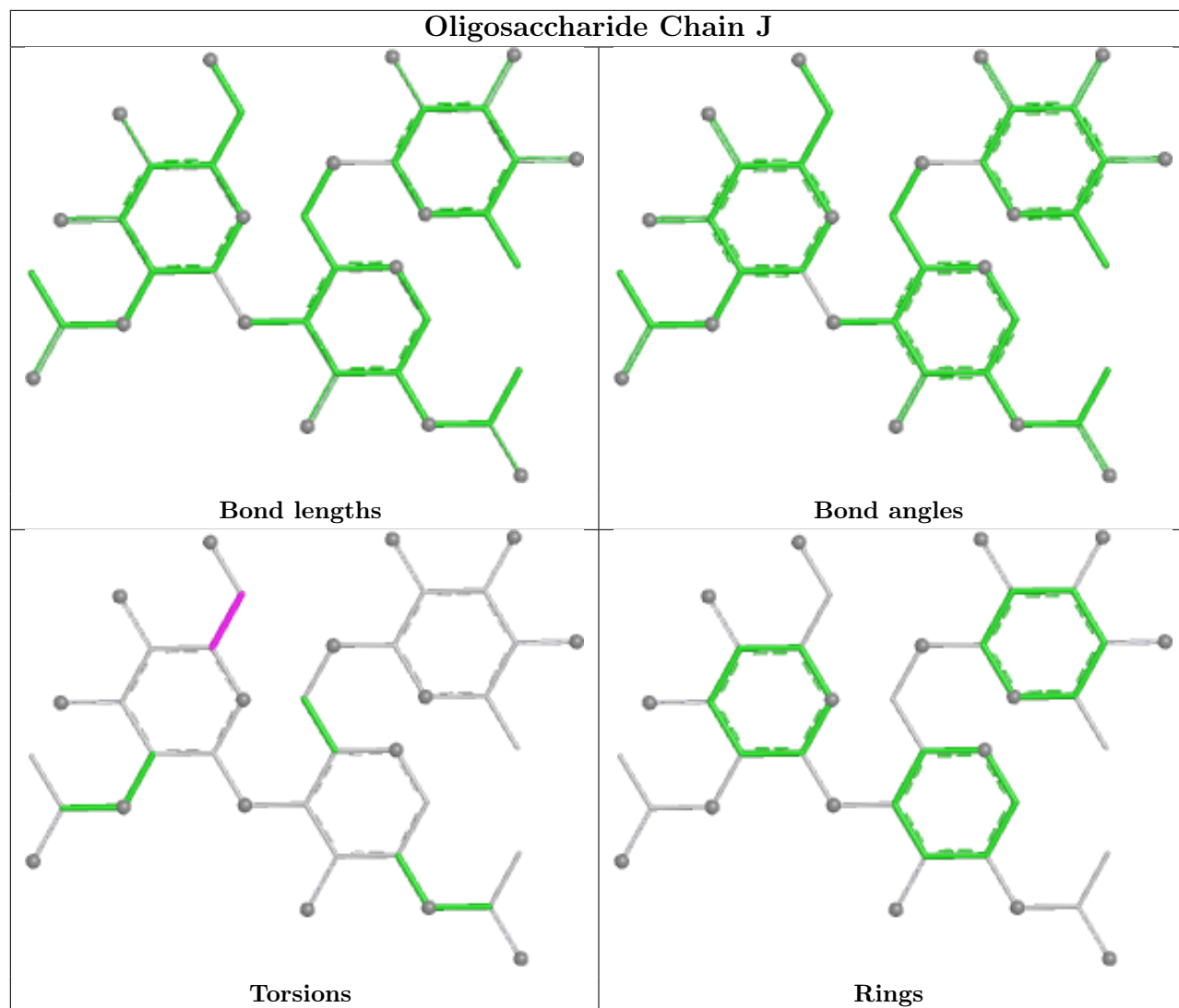


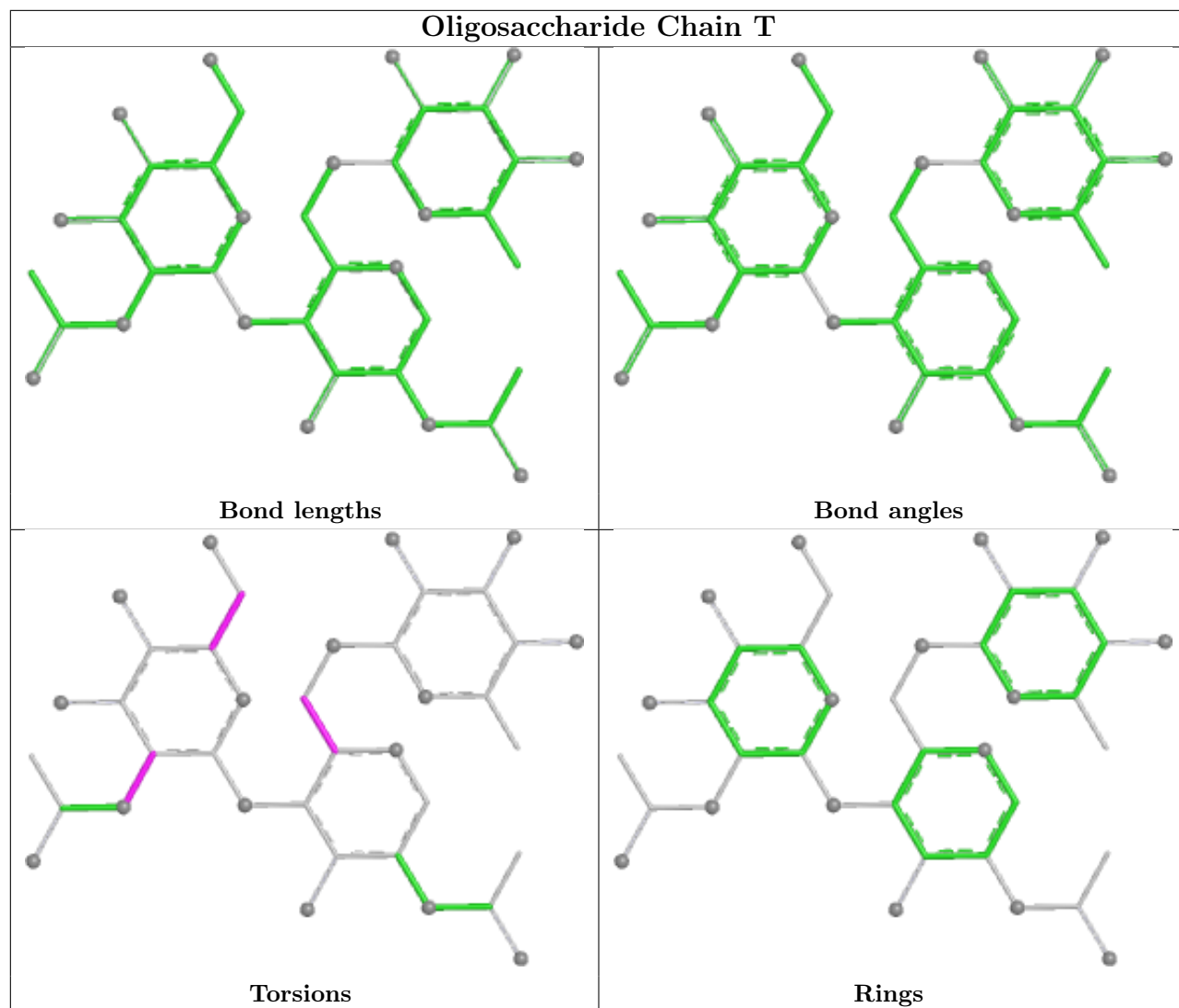


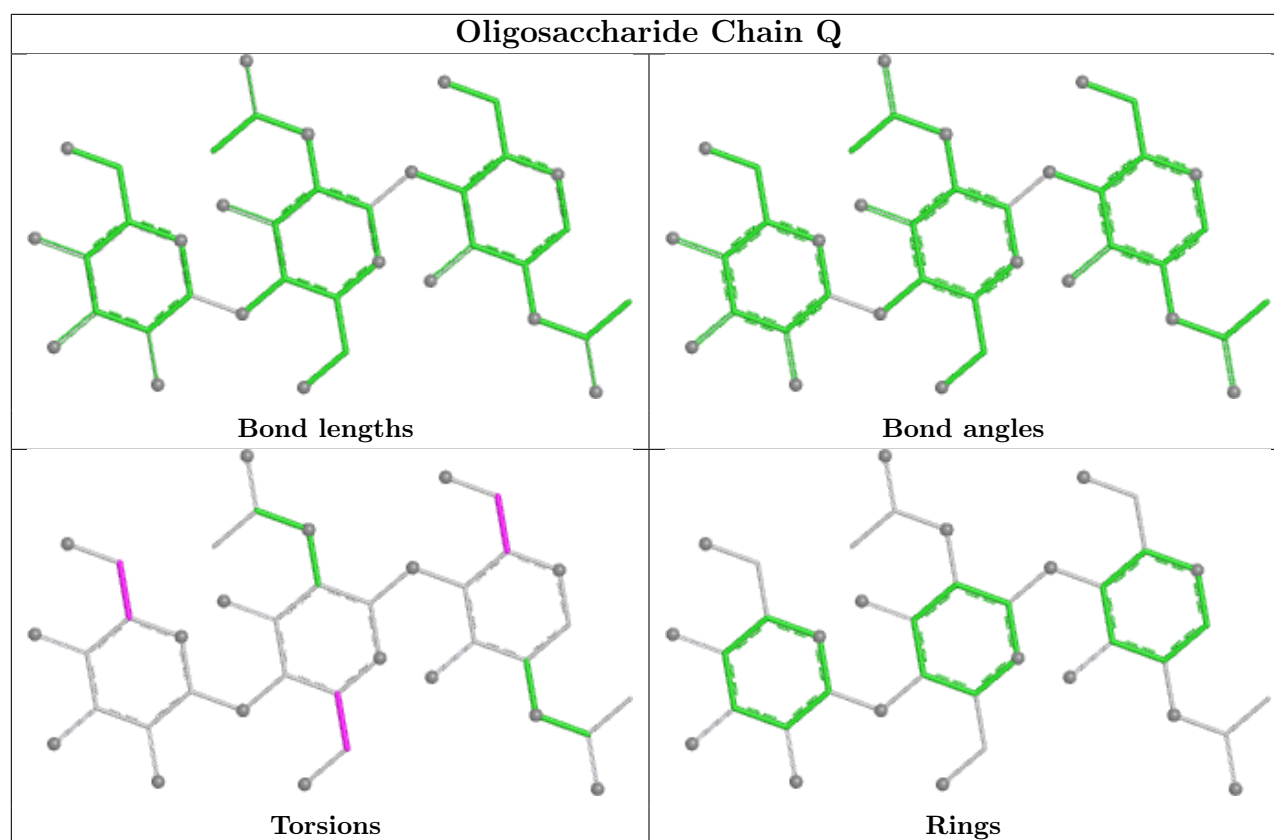












5.6 Ligand geometry [i](#)

30 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	$\# Z > 2$
8	NAG	C	1310	1	14,14,15	0.19	0	17,19,21	0.53	0
8	NAG	A	1308	1	14,14,15	0.29	0	17,19,21	0.42	0
8	NAG	C	1308	1	14,14,15	0.30	0	17,19,21	0.60	0
8	NAG	C	1311	1	14,14,15	0.39	0	17,19,21	0.60	0
8	NAG	B	1309	1	14,14,15	0.29	0	17,19,21	0.53	0
8	NAG	A	1307	1	14,14,15	0.22	0	17,19,21	0.39	0
8	NAG	A	1311	1	14,14,15	0.22	0	17,19,21	0.52	0
8	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.39	0
8	NAG	A	1310	1	14,14,15	0.27	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.56	0
8	NAG	C	1309	1	14,14,15	0.30	0	17,19,21	0.58	0
8	NAG	A	1316	1	14,14,15	0.30	0	17,19,21	0.41	0
8	NAG	B	1312	1	14,14,15	0.15	0	17,19,21	0.48	0
8	NAG	B	1320	1	14,14,15	0.20	0	17,19,21	0.65	0
8	NAG	A	1302	1	14,14,15	0.29	0	17,19,21	0.61	0
8	NAG	B	1307	1	14,14,15	0.27	0	17,19,21	0.43	0
8	NAG	C	1312	1	14,14,15	0.17	0	17,19,21	0.41	0
8	NAG	B	1311	1	14,14,15	0.21	0	17,19,21	0.41	0
8	NAG	B	1319	1	14,14,15	0.22	0	17,19,21	0.43	0
8	NAG	B	1313	1	14,14,15	0.32	0	17,19,21	0.61	1 (5%)
8	NAG	B	1303	1	14,14,15	0.28	0	17,19,21	0.35	0
8	NAG	C	1306	1	14,14,15	0.16	0	17,19,21	0.58	0
8	NAG	C	1307	1	14,14,15	0.21	0	17,19,21	0.39	0
8	NAG	B	1308	1	14,14,15	0.57	0	17,19,21	1.37	2 (11%)
8	NAG	A	1306	1	14,14,15	0.22	0	17,19,21	0.47	0
8	NAG	A	1309	1	14,14,15	0.23	0	17,19,21	0.58	0
8	NAG	B	1310	1	14,14,15	0.25	0	17,19,21	0.57	0
8	NAG	C	1305	1	14,14,15	0.34	0	17,19,21	0.57	0
8	NAG	C	1321	1	14,14,15	0.15	0	17,19,21	0.64	0
8	NAG	B	1314	1	14,14,15	0.23	0	17,19,21	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
8	NAG	A	1316	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1320	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
8	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1319	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1308	1	-	6/6/23/26	0/1/1/1
8	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1321	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1314	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1308	NAG	C2-N2-C7	4.55	129.00	122.90
8	B	1308	NAG	C1-C2-N2	2.18	113.87	110.43
8	B	1313	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1320	NAG	C4-C5-C6-O6
8	C	1312	NAG	C4-C5-C6-O6
8	B	1313	NAG	O5-C5-C6-O6
8	C	1310	NAG	O5-C5-C6-O6
8	B	1320	NAG	O5-C5-C6-O6
8	A	1301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	B	1303	NAG	C4-C5-C6-O6
8	A	1302	NAG	C4-C5-C6-O6
8	A	1306	NAG	C4-C5-C6-O6
8	B	1308	NAG	C4-C5-C6-O6
8	B	1309	NAG	C4-C5-C6-O6
8	B	1313	NAG	C4-C5-C6-O6
8	A	1303	NAG	O5-C5-C6-O6
8	B	1312	NAG	C4-C5-C6-O6
8	C	1312	NAG	O5-C5-C6-O6
8	B	1309	NAG	O5-C5-C6-O6
8	B	1312	NAG	O5-C5-C6-O6
8	C	1310	NAG	C4-C5-C6-O6
8	A	1301	NAG	O5-C5-C6-O6
8	A	1316	NAG	C4-C5-C6-O6
8	B	1303	NAG	O5-C5-C6-O6
8	A	1302	NAG	O5-C5-C6-O6
8	B	1311	NAG	O5-C5-C6-O6
8	B	1319	NAG	O5-C5-C6-O6
8	C	1307	NAG	C4-C5-C6-O6
8	B	1311	NAG	C4-C5-C6-O6
8	B	1319	NAG	C4-C5-C6-O6
8	B	1310	NAG	C4-C5-C6-O6
8	A	1316	NAG	O5-C5-C6-O6
8	B	1308	NAG	C8-C7-N2-C2
8	B	1308	NAG	O7-C7-N2-C2
8	A	1306	NAG	O5-C5-C6-O6
8	B	1308	NAG	O5-C5-C6-O6
8	C	1307	NAG	O5-C5-C6-O6
8	B	1310	NAG	O5-C5-C6-O6
8	A	1303	NAG	C4-C5-C6-O6
8	C	1309	NAG	O5-C5-C6-O6
8	B	1314	NAG	O5-C5-C6-O6
8	C	1311	NAG	O5-C5-C6-O6
8	A	1311	NAG	C1-C2-N2-C7
8	B	1314	NAG	C1-C2-N2-C7
8	C	1305	NAG	C1-C2-N2-C7
8	C	1321	NAG	C1-C2-N2-C7
8	A	1302	NAG	C3-C2-N2-C7
8	A	1311	NAG	C3-C2-N2-C7
8	B	1309	NAG	C3-C2-N2-C7
8	B	1314	NAG	C3-C2-N2-C7
8	B	1320	NAG	C3-C2-N2-C7

Continued on next page...

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Mol	Chain	Res	Type	Atoms
8	C	1305	NAG	C3-C2-N2-C7
8	C	1309	NAG	C3-C2-N2-C7
8	C	1321	NAG	C3-C2-N2-C7
8	C	1306	NAG	C4-C5-C6-O6
8	A	1308	NAG	C4-C5-C6-O6
8	A	1302	NAG	C1-C2-N2-C7
8	B	1308	NAG	C1-C2-N2-C7
8	B	1309	NAG	C1-C2-N2-C7
8	B	1320	NAG	C1-C2-N2-C7
8	C	1309	NAG	C1-C2-N2-C7
8	B	1308	NAG	C3-C2-N2-C7
8	C	1306	NAG	O5-C5-C6-O6
8	B	1314	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1308	NAG	1	0
8	B	1320	NAG	1	0
8	B	1311	NAG	1	0
8	B	1308	NAG	1	0
8	A	1306	NAG	1	0
8	B	1310	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.

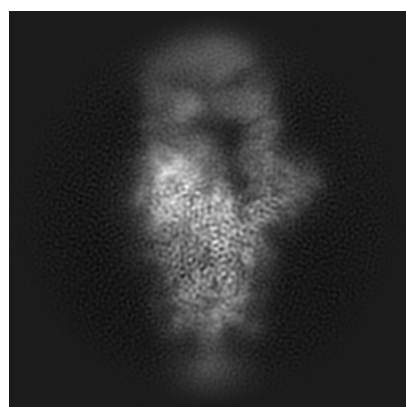
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22127. These allow visual inspection of the internal detail of the map and identification of artifacts.

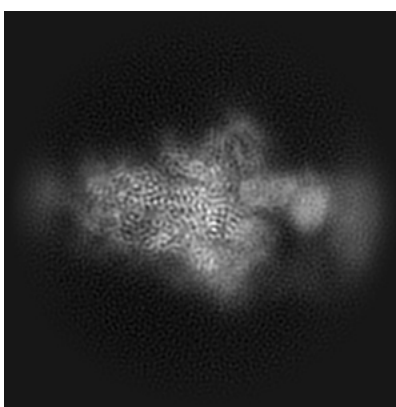
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

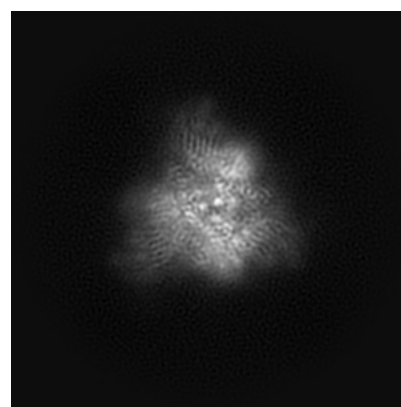
6.1.1 Primary map



X



Y

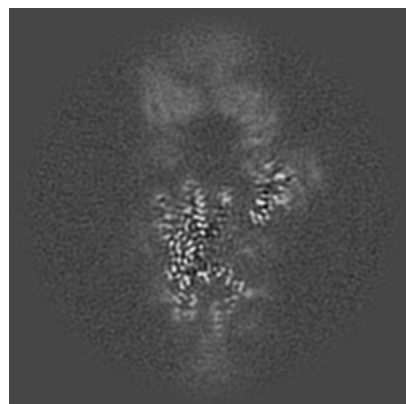


Z

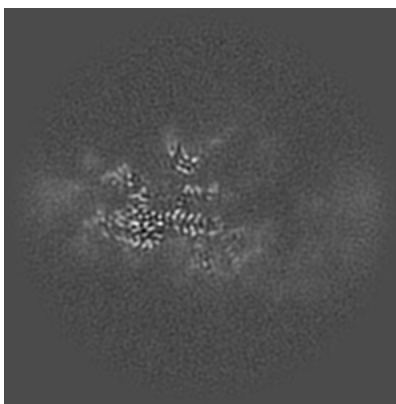
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

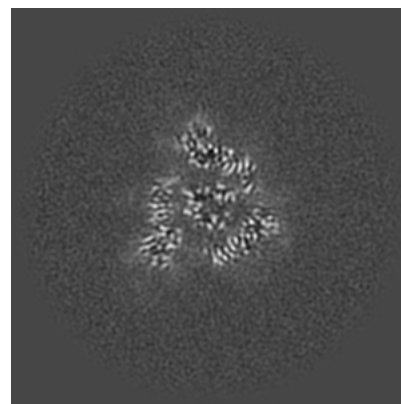
6.2.1 Primary map



X Index: 176



Y Index: 176

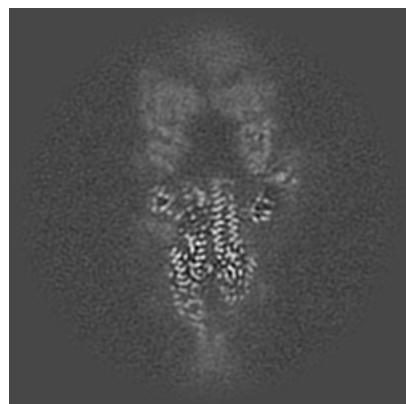


Z Index: 176

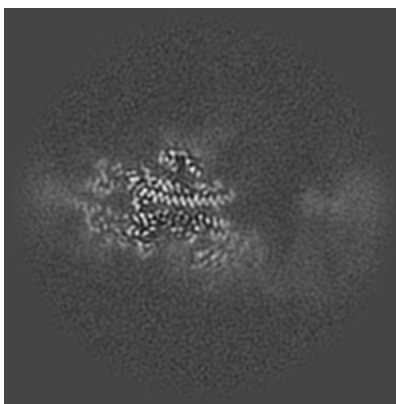
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

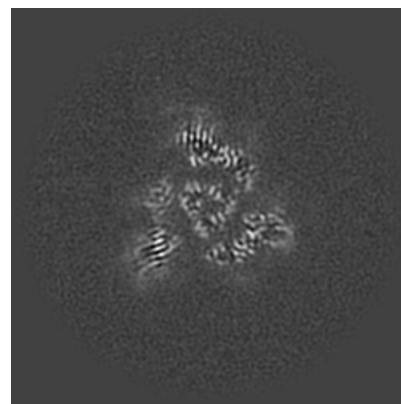
6.3.1 Primary map



X Index: 183



Y Index: 184

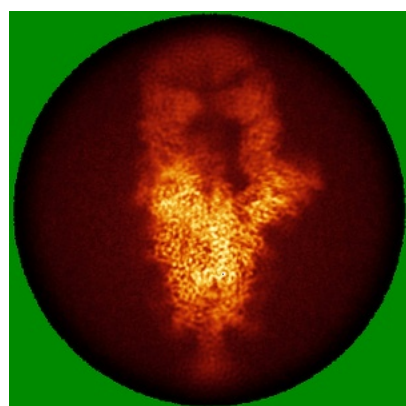


Z Index: 183

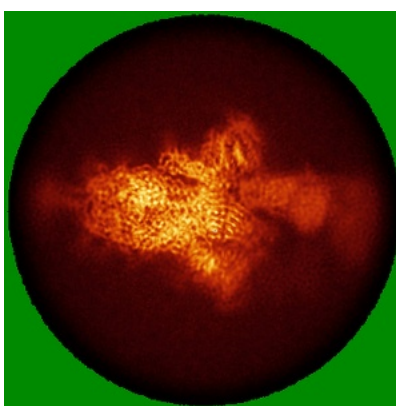
The images above show the largest variance slices of the map in three orthogonal directions.

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

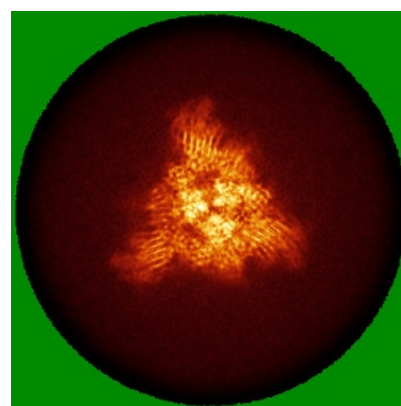
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

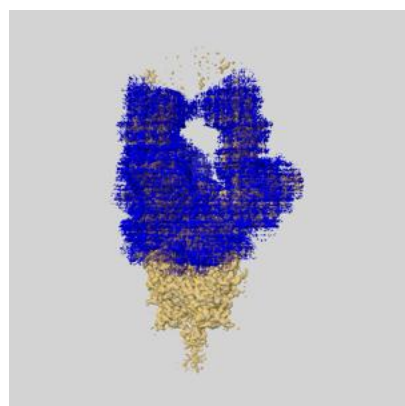
6.6 Mask visualisation [i](#)

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

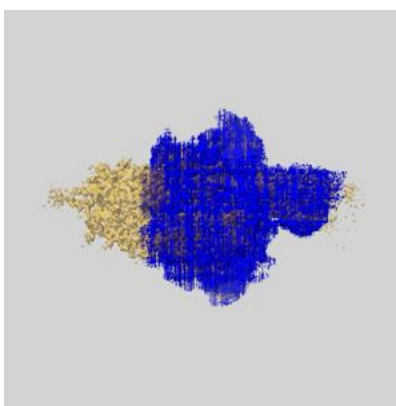
A mask typically either:

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

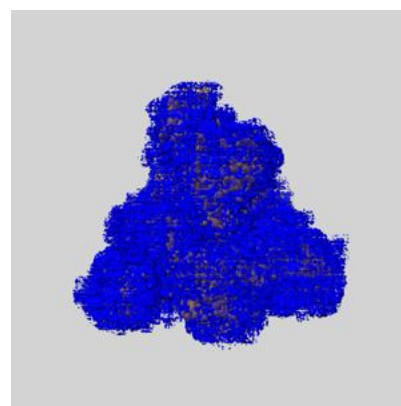
6.6.1 emd_22127_msk_1.map [i](#)



X



Y

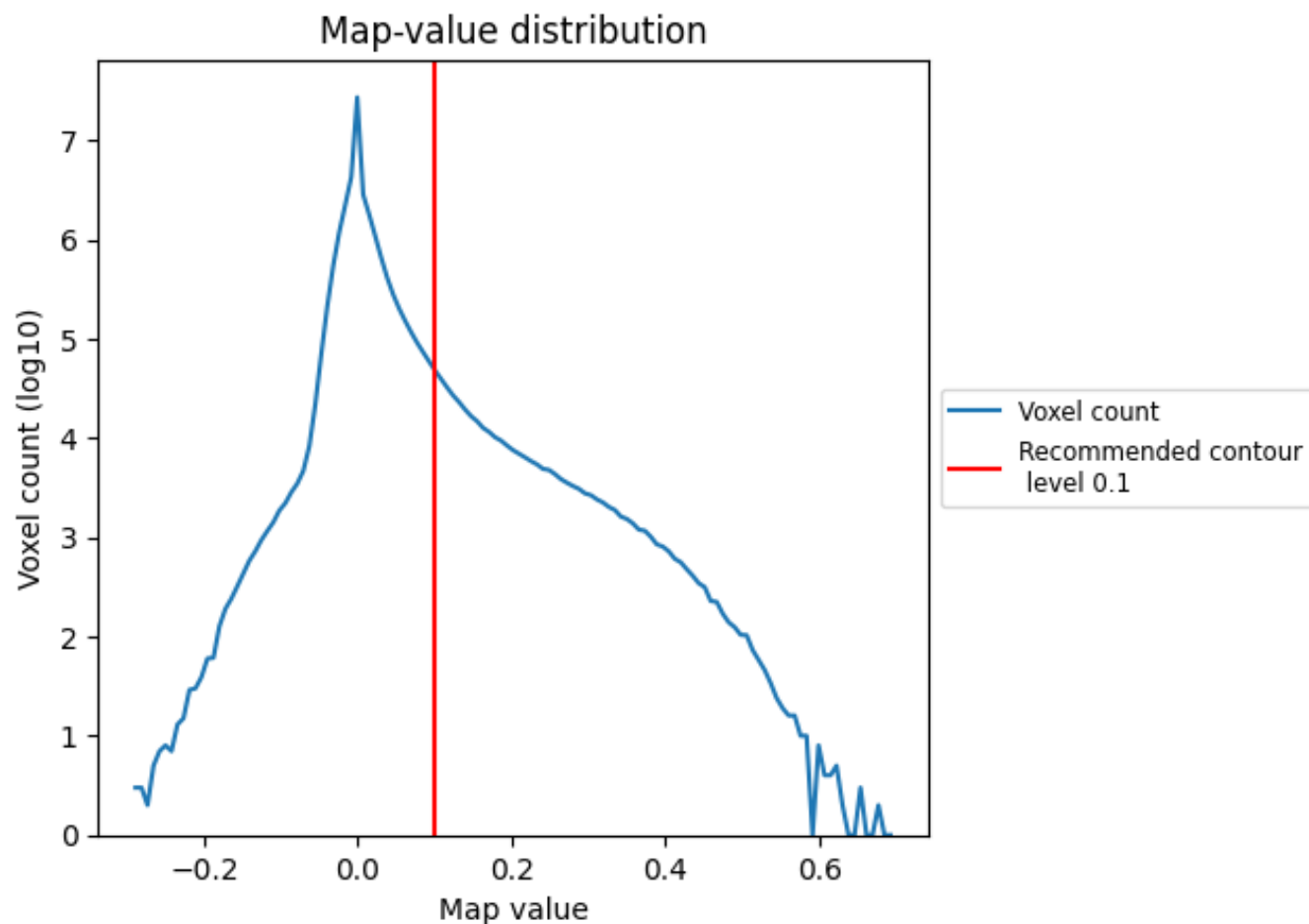


Z

7 Map analysis [i](#)

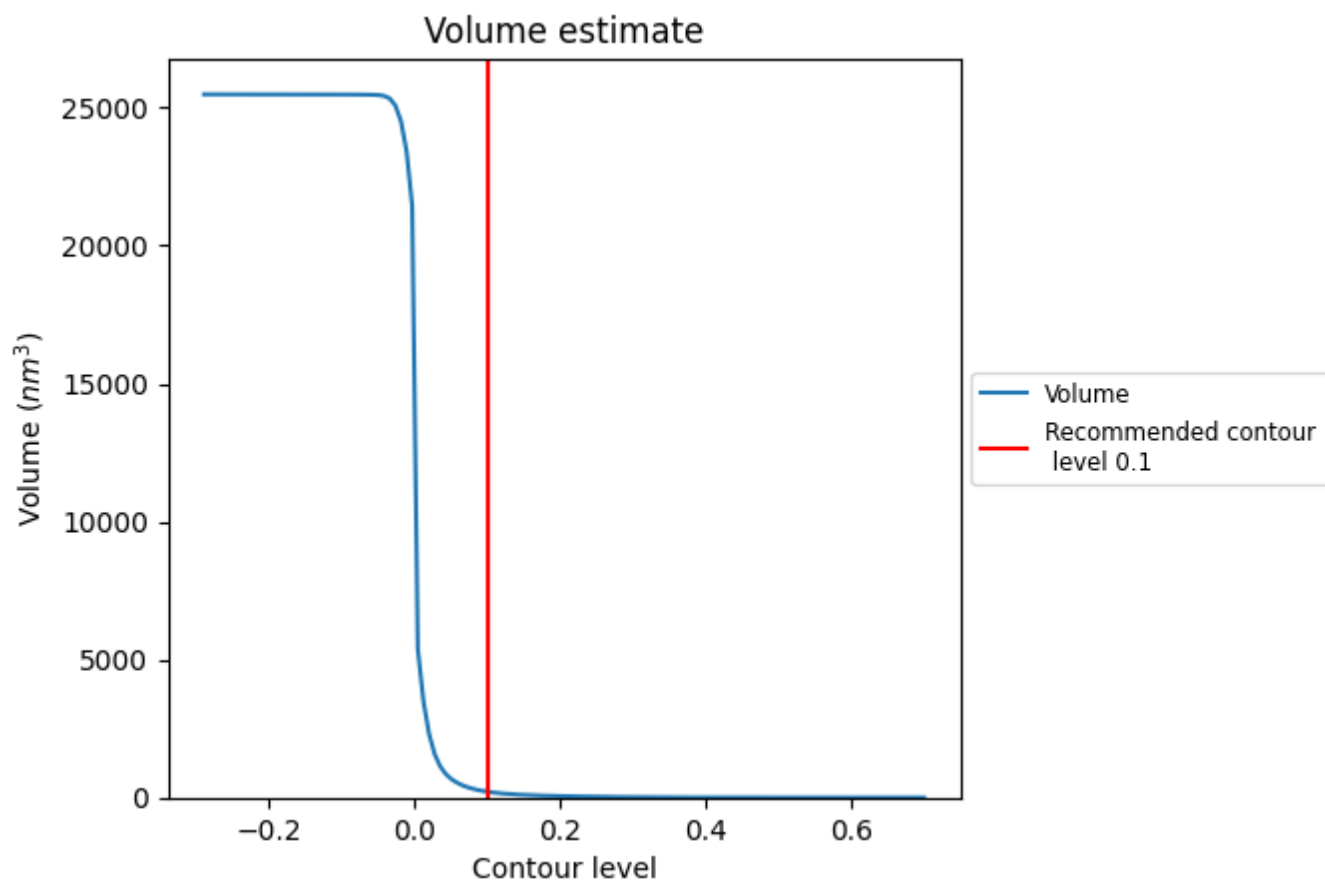
This section contains the results of statistical analysis of the map.

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.

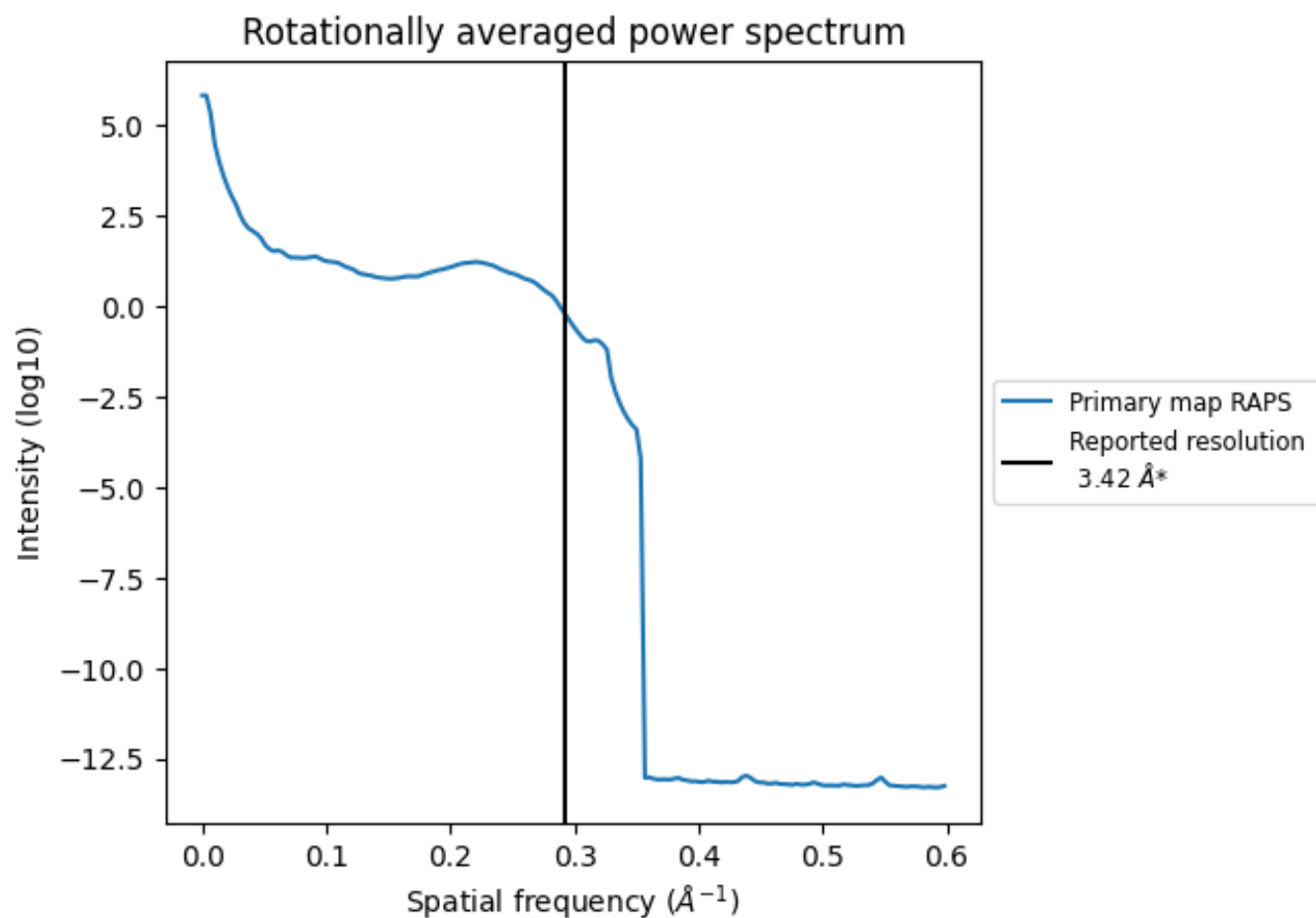
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm³; this corresponds to an approximate mass of 192 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 ⓘ

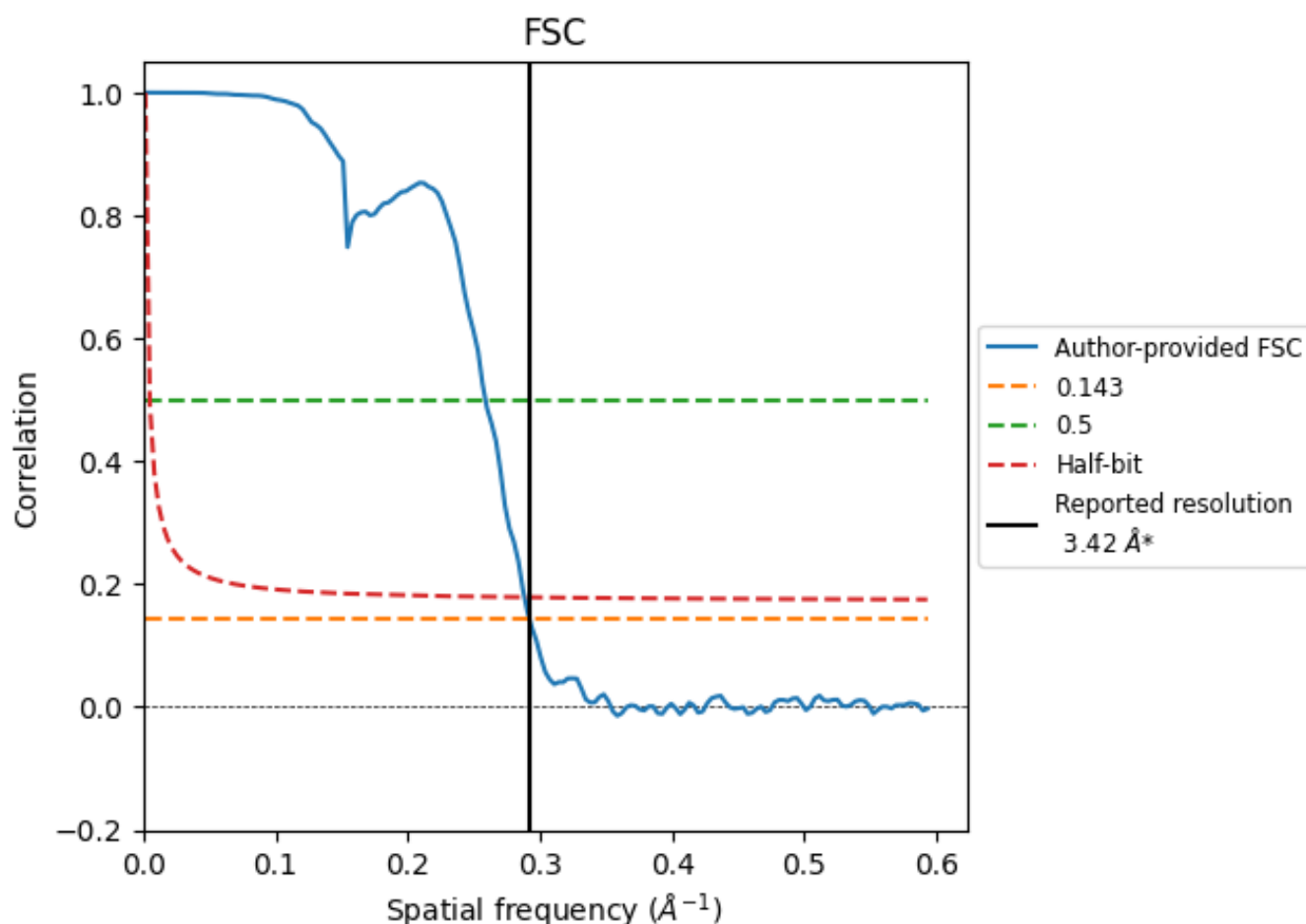


*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

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 0.292 Å⁻¹

8.2 Resolution estimates [i](#)

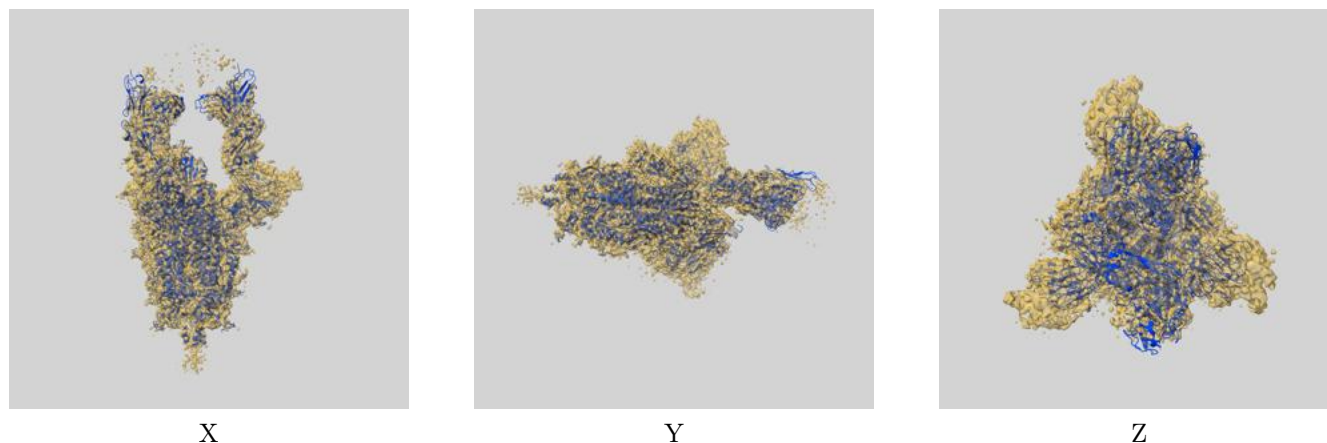
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	3.86	3.47
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

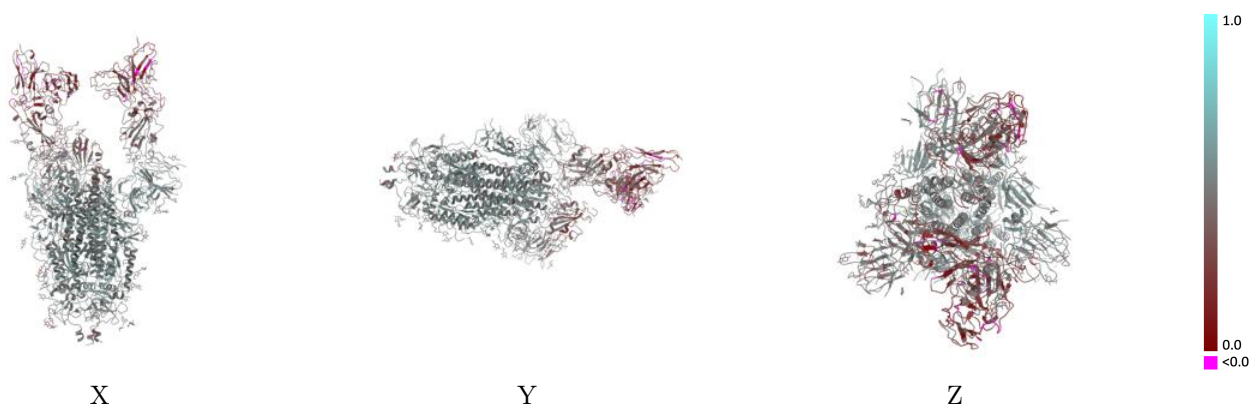
This section contains information regarding the fit between EMDB map EMD-22127 and PDB model 6XCM. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)



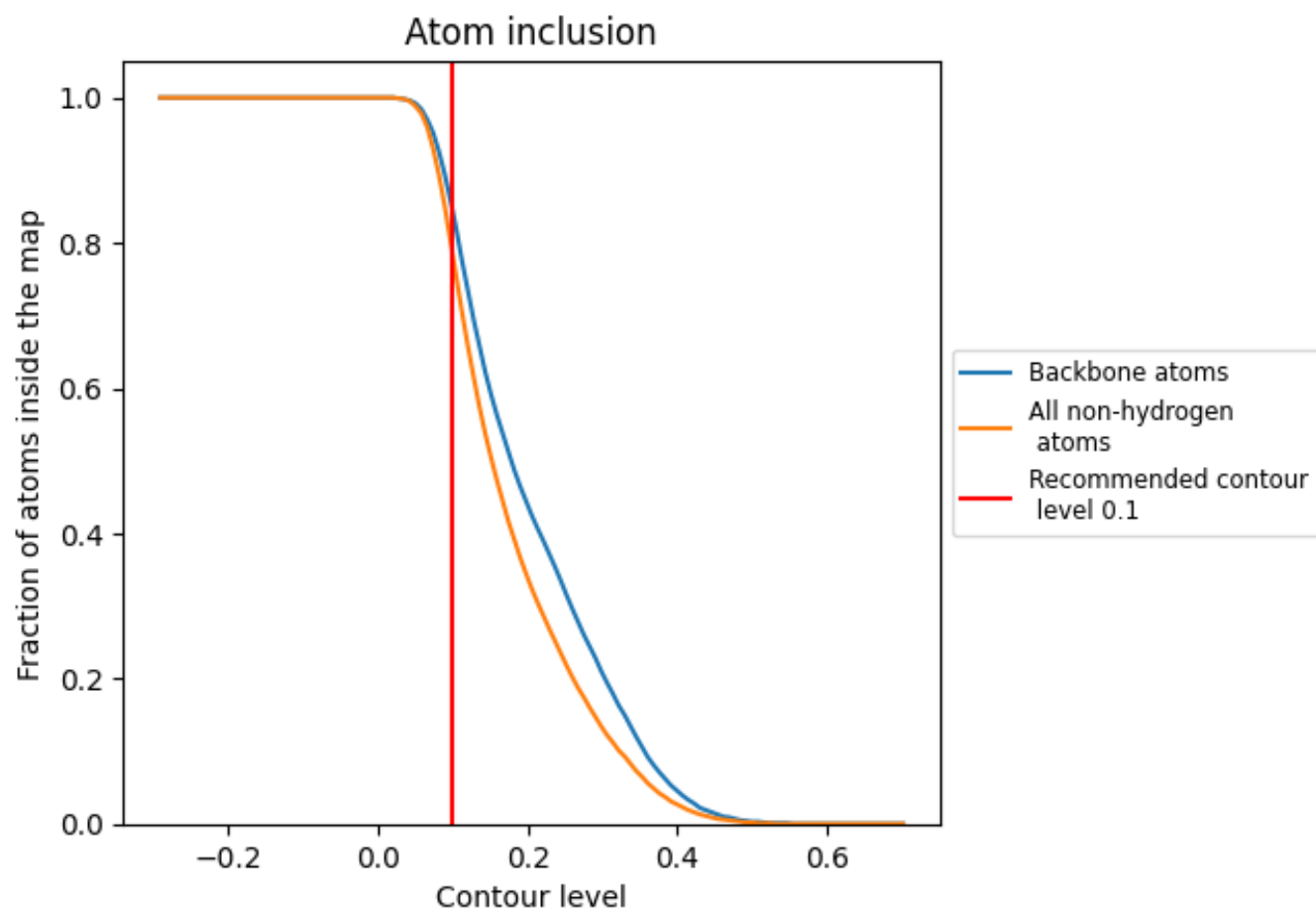
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 79% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7860	 0.4560
A	 0.8380	 0.4870
B	 0.8510	 0.4700
C	 0.8810	 0.4920
D	 0.7140	 0.4140
E	 0.6790	 0.4560
F	 0.7920	 0.4470
G	 0.6790	 0.4990
H	 0.3920	 0.3080
I	 0.8570	 0.4610
J	 0.5000	 0.3590
K	 0.8210	 0.4220
L	 0.2740	 0.2680
M	 0.7860	 0.4810
N	 0.3710	 0.2620
O	 0.9290	 0.4690
P	 0.4640	 0.3730
Q	 0.5900	 0.4820
R	 0.6790	 0.3500
S	 0.2320	 0.2590
T	 0.3950	 0.4070

