



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 06:50 PM JST

PDB ID : 7WGY
EMDB ID : EMD-32492
Title : SARS-CoV-2 spike glycoprotein trimer in Intermediate state
Authors : Zhu, Y.; Tai, L.; Yin, G.; Sun, F.
Deposited on : 2021-12-29
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

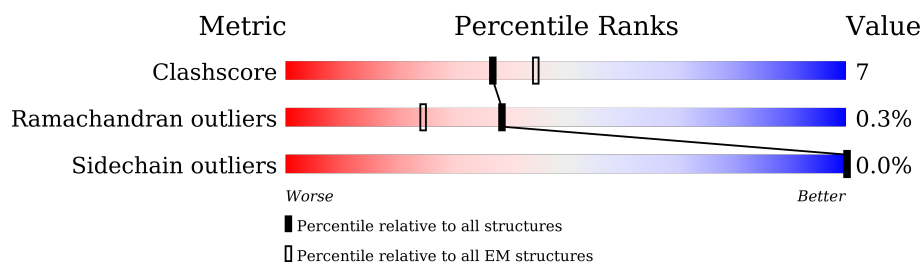
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1204	<div> <div>9%</div> <div>71%</div> <div>15%</div> <div>14%</div> </div>
1	B	1204	<div> <div>9%</div> <div>55%</div> <div>13%</div> <div>32%</div> </div>
1	C	1204	<div> <div>11%</div> <div>70%</div> <div>15%</div> <div>15%</div> </div>
2	D	2	<div> <div>100%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div>50%</div> <div>100%</div> </div>
2	G	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>
2	H	2	<div> <div>50%</div> <div>100%</div> </div>

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22914 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	1033	Total	C	N	O	S	0	0
			8078	5160	1344	1537	37		
1	B	821	Total	C	N	O	S	0	0
			6393	4083	1057	1225	28		
1	C	1025	Total	C	N	O	S	0	0
			8009	5117	1331	1525	36		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2

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



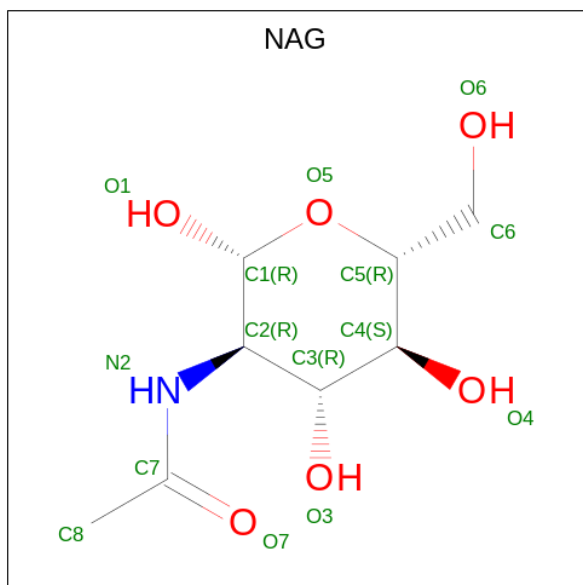
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16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

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

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



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

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

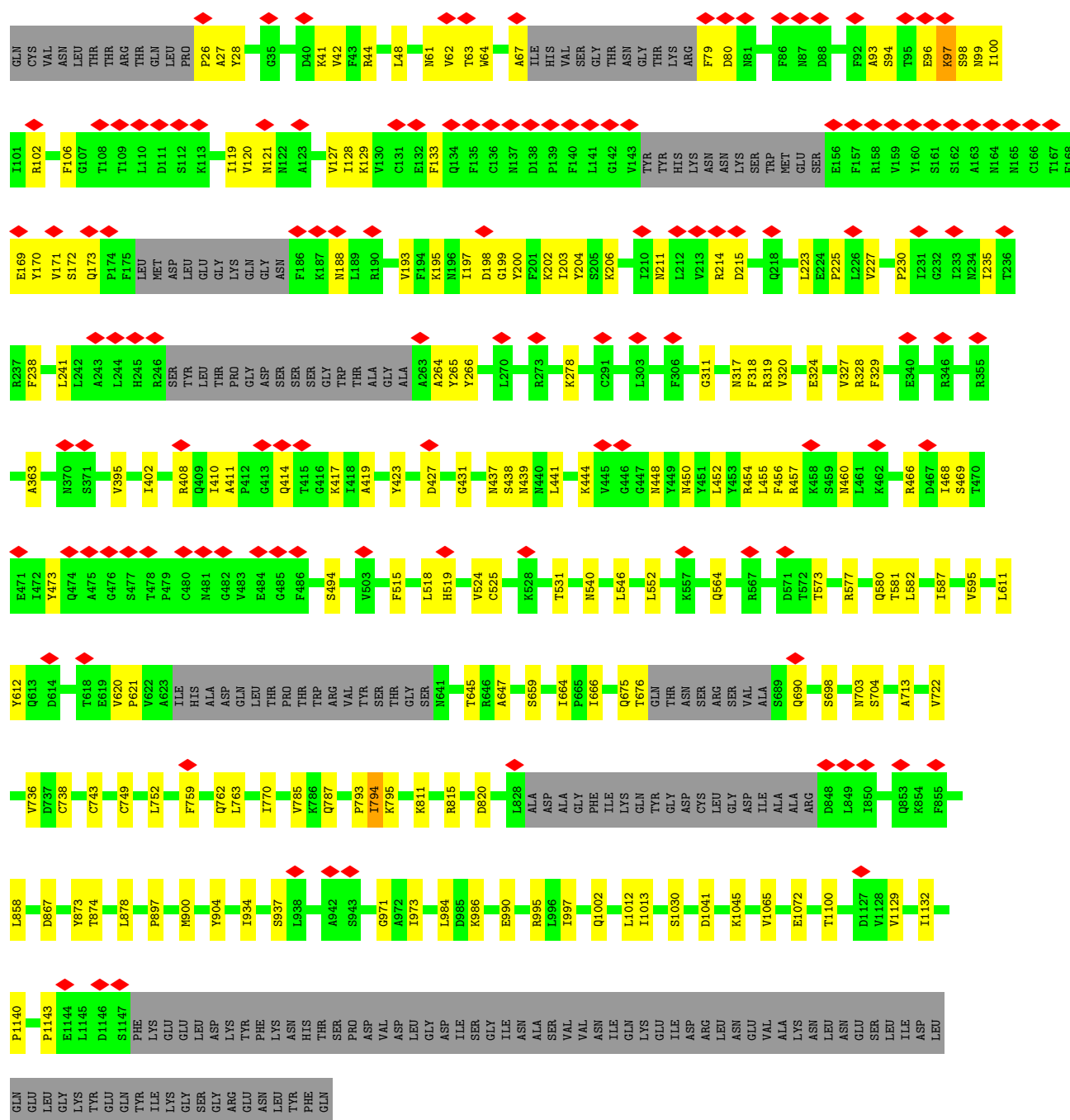
- Molecule 1: Spike glycoprotein

R1091	G1092	G1093	F906	N703	L582	GLY	LYS	PRO	E324	L226	S161	F92	GLN
G1092	G1093	G1093	N807	S704	E583	TYR	VAL	THR	S325	V227	S162	A93	CYS
H1101	L916	L585	G908	I726	I594	PRO	GLY	LYS	T326	I231	S161	E96	VAL
L1105	D936	D586	L916	M740	L585	TYR	TYR	ASN	N327	G232	A163	K97	THR
L1115	S939	S591	D936	S746	D586	VAL	TYR	LEU	R328	I233	N164	S98	THR
D1118	S940	F592	S939	C749	S591	VAL	LEU	PHE	F329	I234	N165	N99	ARG
N1134	A942	T616	S940	Q755	F592	LEU	ARG	ASN	ASN	I235	C166	I100	GLN
Q1142	S943	E619	A942	Q755	E619	GLY	PHE	VAL	THR	I236	T167	I101	LEU
L1145	A944	V620	S943	F759	V620	LEU	ASN	TYR	LEU	I237	F168	R102	PRO
L1145	L948	V622	A944	L763	V622	LEU	LYS	ASP	CYS	Q239	E169	I105	P96
D1146	Q949	A623	L948	V785	A623	ALA	LEU	PHE	GLY	Q240	Q173	F106	A27
S1147	D950	HIS	Q949	Q786	HIS	PRO	LEU	VAL	GLY	T240	P174	G107	S31
PHE	V951	ALA	D950	Q787	ALA	THR	PRO	ILE	VAL	L241	F175	T108	R34
LYS	A958	GLN	V951	I794	THR	VAL	PHE	GLY	ASN	L242	LEU	T109	V86
GLY	A958	LEU	A958	I794	CYS	VAL	PHE	GLY	GLY	A243	ASP	L110	Y37
LEU	T961	THR	T961	F812	GLY	GLY	ARG	THR	THR	HIS	GLU	D111	D40
ASP	N969	PRO	T961	F817	PRO	PRO	ASP	VAL	ARG	A244	GLY	S112	K41
LYS	S975	THR	N969	F817	LYS	LYS	ILE	ARG	ALA	L244	GLN	T114	S46
TYR	S975	TRP	S975	L821	THR	THR	GLU	ILE	SER	A245	PRO	Q115	
PHE	T980	VAL	S975	L821	ARG	TYR	THR	ALA	VAL	F186	ASN	S116	
LYS	T980	TYR	T980	T827	VAL	TYR	ILE	PRO	ALA	K187	ASP	L117	T51
HIS	L981	SER	T980	T827	TYR	GLN	TYR	GLN	TRP	N188	SER	M122	Q52
THR	L984	THR	L984	L828	GLY	ALA	GLY	ALA	ASN	L189	SER	A123	D53
SER	D985	GLY	D985	ALA	N544	GLY	GLY	THR	ARG	G190	GLY	T124	L54
PRO	K986	ASP	K986	ASP	G545	SER	THR	GLY	LYS	E191	LYS	N125	L56
VAL	V987	GLY	V987	PHE	L546	THR	THR	ILE	ARG	T192	THR	K129	S80
ASP	E988	ILE	E988	ILE	T547	PRO	PRO	ALA	ILE	V193	GLY	V130	
LEU	E990	LYS	A989	GLN	L552	ASN	CYS	ASP	CYS	F194	ASP	C131	
GLY	V991	TYR	A989	TYR	T553	TYR	GLY	TYR	ASN	K195	VAL	E132	M64
ILE	D994	GLY	D994	GLY	E554	ASN	GLY	ASN	VAL	N196	ASP	F133	A67
SER	R995	ASP	R995	ASP	K557	GLY	PHE	PRO	TYR	Z265	D198	Q134	ILE
GLY	S1003	CYS	R995	CYS	L560	ASN	ASN	ASP	VAL	T274	G199	C136	HIS
ILE	V1008	GLY	S1003	GLY	P561	TYR	TYR	PHE	THR	L277	ASN	D138	VAL
SER	S1030	ILE	V1008	ILE	F562	PHE	PHE	THR	GLY	N280	SER	F139	GLY
VAL	L1034	ALA	S1030	ALA	Q564	PRO	PRO	GLY	SER	T274	GLY	P140	ASN
VAL	L1034	ALA	L1034	ALA	Q564	GLN	GLN	VAL	ALA	A288	VAL	V143	LYS
ILE	K1038	ARG	L1034	ARG	R567	SER	SER	ILE	PHE	T302	T208	TVR	THR
GLN	D1041	VAL	K1038	VAL	D568	THR	GLY	TRP	THR	L303	T209	TVR	ARG
LYS	Q857	ALA	D1041	ALA	A570	ASN	ASN	ASN	PHE	K304	M211	HIS	F79
ILE	T866	S											

VAL
ALA
LYS
ASN
LEU
ASN
GLU
SER
LEU
ILE
ASP
LEU
GLN
GLU
GLY
LYS
TYR
GLU
GLN
TYR
ILE
LYS
GLY
SER
GLY
GLY
ARG
GLU
ASN
LEU
TYR
PHE
GLN

• Molecule 1: Spike glycoprotein

Chain C: 



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

Chain D: 



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



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



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



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



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



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





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

Chain K:

100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21045	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.706	Depositor
Minimum map value	-0.696	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.506	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/8260	0.51	0/11236
1	B	0.31	0/6525	0.51	0/8874
1	C	0.30	0/8189	0.50	0/11141
All	All	0.31	0/22974	0.51	0/31251

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	620	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8078	0	7912	114	0
1	B	6393	0	6299	102	0
1	C	8009	0	7848	129	0
2	D	28	0	25	1	0
2	E	28	0	25	2	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	1	0
2	I	28	0	25	1	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
3	A	70	0	65	2	0
3	B	70	0	65	2	0
3	C	70	0	63	1	0
All	All	22914	0	22452	334	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 7.

All (334) 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:B:54:LEU:HB2	1:B:195:LYS:HZ2	1.41	0.84
1:A:1012:LEU:HD21	1:C:1013:ILE:HG21	1.64	0.79
1:A:659:SER:HB3	1:A:698:SER:HB2	1.65	0.78
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.16	0.77
1:C:206:LYS:HB2	1:C:223:LEU:HG	1.66	0.76
1:B:1093:GLY:HA3	1:B:1105:THR:O	1.85	0.75
1:B:81:ASN:O	1:B:239:GLN:NE2	2.22	0.73
1:B:193:VAL:HG12	1:B:204:TYR:HB2	1.71	0.72
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.55	0.72
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.23	0.71
1:A:1100:THR:HG21	3:A:1303:NAG:HN2	1.55	0.71
1:B:620:VAL:O	1:B:622:VAL:N	2.23	0.70
1:C:214:ARG:HG3	1:C:215:ASP:H	1.55	0.70
1:A:801:ASN:ND2	2:E:1:NAG:O5	2.24	0.70
1:A:37:TYR:OH	1:A:54:LEU:O	2.10	0.69
1:A:775:ASP:OD1	1:A:776:LYS:N	2.25	0.69
1:B:37:TYR:HB3	1:B:223:LEU:HB3	1.75	0.69
1:B:560:LEU:HB2	1:B:563:GLN:HG3	1.73	0.69
1:B:763:LEU:HD12	1:B:1008:VAL:HG21	1.75	0.68
1:C:752:LEU:HD11	1:C:990:GLU:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:GLY:O	1:C:1045:LYS:NZ	2.21	0.68
1:C:934:ILE:O	1:C:937:SER:HB3	1.94	0.66
1:A:324:GLU:HB3	1:A:539:VAL:HG12	1.78	0.66
1:C:738:CYS:HB2	1:C:763:LEU:HD11	1.77	0.65
1:C:454:ARG:NH2	1:C:469:SER:O	2.27	0.65
1:A:317:ASN:OD1	1:A:318:PHE:N	2.30	0.64
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.30	0.64
1:A:66:HIS:HB2	1:A:78:ARG:HB3	1.79	0.64
1:C:67:ALA:HA	1:C:79:PHE:HA	1.79	0.63
1:B:1091:ARG:NH2	1:B:1118:ASP:O	2.23	0.63
1:C:759:PHE:HA	1:C:762:GLN:HE22	1.64	0.63
1:C:204:TYR:CD1	1:C:225:PRO:HA	2.35	0.62
1:A:908:GLY:O	1:A:1038:LYS:NZ	2.32	0.62
1:B:641:ASN:N	1:B:653:ALA:O	2.33	0.61
1:A:1005:GLN:OE1	1:C:1002:GLN:NE2	2.34	0.61
1:C:444:LYS:HE2	1:C:448:ASN:HA	1.82	0.61
1:A:777:ASN:OD1	1:A:1019:ARG:NH1	2.32	0.60
1:C:1100:THR:HG21	3:C:1303:NAG:HN2	1.66	0.60
1:B:827:THR:O	1:B:949:GLN:NE2	2.35	0.59
1:A:115:GLN:HA	1:A:132:GLU:HA	1.84	0.59
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.85	0.59
1:C:96:GLU:OE2	1:C:100:ILE:N	2.34	0.59
1:C:127:VAL:HG22	1:C:171:VAL:HG12	1.84	0.59
1:B:1142:GLN:HA	1:B:1145:LEU:HD23	1.84	0.59
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.36	0.59
1:C:97:LYS:O	1:C:188:ASN:ND2	2.36	0.58
1:C:203:ILE:HB	1:C:227:VAL:HB	1.86	0.58
1:C:97:LYS:HE3	1:C:100:ILE:HD11	1.84	0.58
1:A:424:LYS:HB3	1:A:463:PRO:HA	1.86	0.58
1:B:662:CYS:HB2	1:B:697:MET:SD	2.44	0.57
1:C:193:VAL:HG23	1:C:223:LEU:HD22	1.87	0.57
1:B:302:THR:O	1:B:304:LYS:NZ	2.25	0.57
1:A:576:VAL:HB	1:A:587:ILE:HD11	1.86	0.57
1:A:195:LYS:HE2	1:A:202:LYS:HD2	1.87	0.57
1:B:785:VAL:HG22	1:B:787:GLN:H	1.69	0.57
1:B:52:GLN:OE1	1:B:274:THR:OG1	2.21	0.57
1:A:641:ASN:N	1:A:653:ALA:O	2.38	0.56
1:C:99:ASN:O	1:C:102:ARG:NH2	2.27	0.56
1:B:746:SER:HB2	1:B:981:LEU:HD11	1.87	0.56
1:C:193:VAL:HB	1:C:204:TYR:HB2	1.88	0.56
1:C:736:VAL:HG22	1:C:858:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:LYS:HZ1	1:C:455:LEU:HA	1.70	0.56
1:C:546:LEU:HD21	1:C:573:THR:HG21	1.88	0.56
1:C:897:PRO:HB2	1:C:900:MET:HG2	1.87	0.56
1:A:327:VAL:O	1:A:531:THR:N	2.39	0.55
1:A:567:ARG:NH1	1:A:571:ASP:O	2.39	0.55
1:B:213:VAL:HG13	1:B:214:ARG:H	1.71	0.55
1:C:129:LYS:HG2	1:C:169:GLU:HA	1.87	0.55
1:A:156:GLU:OE2	1:A:158:ARG:NE	2.40	0.55
1:A:394:ASN:O	1:A:515:PHE:HA	2.06	0.55
1:B:984:LEU:HD13	1:B:988:GLU:HB3	1.89	0.54
1:B:100:ILE:HG23	1:B:243:ALA:HB3	1.89	0.54
1:C:42:VAL:HB	1:C:44:ARG:HH12	1.71	0.54
1:C:437:ASN:OD1	1:C:439:ASN:N	2.38	0.54
1:C:815:ARG:NH2	1:C:867:ASP:OD2	2.35	0.54
1:A:109:THR:OG1	1:A:111:ASP:OD1	2.21	0.54
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.88	0.54
1:B:620:VAL:C	1:B:622:VAL:H	2.10	0.54
1:A:454:ARG:HD3	1:A:457:ARG:HB2	1.90	0.54
1:A:30:ASN:HB2	1:A:32:PHE:CE1	2.43	0.54
1:B:99:ASN:O	1:B:102:ARG:NE	2.36	0.53
1:C:317:ASN:O	1:C:319:ARG:NH1	2.42	0.53
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.91	0.53
1:C:324:GLU:O	1:C:540:ASN:ND2	2.42	0.53
1:A:108:THR:HG23	1:A:109:THR:HG23	1.90	0.53
1:A:353:TRP:O	1:A:466:ARG:NH1	2.42	0.53
1:B:994:ASP:OD1	1:B:995:ARG:N	2.41	0.53
1:A:376:THR:HB	1:A:435:ALA:HB3	1.91	0.53
1:A:971:GLY:N	1:B:755:GLN:OE1	2.42	0.53
1:B:105:ILE:HG22	1:B:110:LEU:HD22	1.89	0.53
1:A:563:GLN:O	1:A:577:ARG:NH2	2.38	0.53
1:B:619:GLU:C	1:B:621:PRO:HD2	2.30	0.53
1:A:894:LEU:HD22	1:C:1072:GLU:HG2	1.90	0.53
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.90	0.53
1:C:311:GLY:HA2	1:C:664:ILE:HD12	1.90	0.52
1:C:564:GLN:NE2	1:C:577:ARG:O	2.42	0.52
1:A:988:GLU:O	1:A:991:VAL:HG22	2.10	0.52
1:C:456:PHE:HB3	1:C:473:TYR:CG	2.44	0.52
1:C:452:LEU:HD23	1:C:494:SER:HA	1.91	0.52
1:A:882:ILE:HG23	1:A:883:THR:HG23	1.91	0.52
1:A:81:ASN:O	1:A:239:GLN:NE2	2.31	0.51
1:A:425:LEU:HD12	1:A:426:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HG	1:A:227:VAL:HG23	1.92	0.51
1:A:201:PHE:CD2	1:A:231:ILE:HD11	2.46	0.51
1:C:793:PRO:O	1:C:794:ILE:HG22	2.10	0.51
1:B:568:ASP:N	1:B:572:THR:O	2.31	0.51
1:C:577:ARG:HH11	1:C:582:LEU:HB2	1.76	0.51
1:A:129:LYS:NZ	1:A:169:GLU:OE1	2.43	0.51
1:B:562:PHE:HB2	1:C:41:LYS:HD3	1.92	0.51
1:A:334:ASN:HB2	1:A:361:CYS:HA	1.93	0.51
1:C:327:VAL:O	1:C:531:THR:N	2.44	0.51
1:B:948:LEU:O	1:B:951:VAL:HB	2.10	0.50
1:A:767:LEU:HD21	1:A:1008:VAL:HG22	1.92	0.50
1:B:866:THR:H	1:B:869:MET:HE3	1.76	0.50
1:B:986:LYS:NZ	1:B:990:GLU:OE2	2.41	0.50
1:C:62:VAL:HG22	1:C:63:THR:H	1.76	0.50
1:C:417:LYS:NZ	1:C:455:LEU:HA	2.26	0.50
1:C:195:LYS:HG3	1:C:202:LYS:HE2	1.92	0.50
1:C:448:ASN:OD1	1:C:450:ASN:ND2	2.41	0.50
1:C:676:THR:HA	1:C:690:GLN:HA	1.93	0.50
1:B:130:VAL:O	1:B:167:THR:OG1	2.25	0.50
1:B:194:PHE:HB3	1:B:201:PHE:CE1	2.47	0.50
1:B:96:GLU:OE2	1:B:98:SER:N	2.45	0.50
1:B:212:LEU:HD11	1:B:215:ASP:O	2.11	0.50
1:A:206:LYS:HB2	1:A:223:LEU:HD13	1.94	0.49
1:B:34:ARG:NH1	1:B:220:PHE:O	2.45	0.49
1:B:92:PHE:CE1	1:B:265:TYR:HB2	2.47	0.49
1:A:213:VAL:HG22	1:A:214:ARG:HG3	1.94	0.49
1:A:724:THR:HA	1:A:1062:PHE:O	2.12	0.49
1:C:438:SER:HB2	1:C:441:LEU:HB2	1.94	0.49
1:C:785:VAL:HG22	1:C:787:GLN:H	1.78	0.49
1:A:99:ASN:O	1:A:102:ARG:NE	2.39	0.49
1:A:1092:GLU:OE2	1:A:1093:GLY:N	2.46	0.49
1:C:411:ALA:HB3	1:C:414:GLN:HE22	1.78	0.49
1:B:34:ARG:O	1:B:56:LEU:HD23	2.12	0.49
1:B:703:ASN:OD1	1:B:704:SER:N	2.45	0.49
1:A:36:VAL:HB	1:A:220:PHE:CZ	2.48	0.48
1:B:328:ARG:NH1	1:B:531:THR:O	2.45	0.48
1:B:620:VAL:N	1:B:621:PRO:HD2	2.28	0.48
1:B:1134:ASN:OD1	3:B:1304:NAG:N2	2.47	0.48
1:C:197:ILE:O	1:C:199:GLY:N	2.46	0.48
1:C:518:LEU:O	1:C:519:HIS:ND1	2.46	0.48
1:A:406:GLU:OE1	1:A:495:TYR:OH	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:950:ASP:OD1	1:B:951:VAL:N	2.47	0.48
1:C:749:CYS:SG	1:C:997:ILE:HD11	2.53	0.48
1:A:564:GLN:NE2	1:A:577:ARG:HB3	2.29	0.48
1:B:310:LYS:HG3	1:B:664:ILE:HD11	1.95	0.48
1:C:26:PRO:HA	1:C:64:TRP:O	2.13	0.48
1:C:427:ASP:OD1	1:C:427:ASP:N	2.45	0.48
2:D:1:NAG:H61	2:D:2:NAG:N2	2.28	0.48
1:B:35:GLY:HA3	1:B:56:LEU:HB3	1.95	0.48
1:A:124:THR:O	1:A:175:PHE:N	2.47	0.48
1:A:329:PHE:HB3	1:A:530:SER:HB3	1.95	0.48
1:C:703:ASN:OD1	1:C:704:SER:N	2.47	0.48
1:A:767:LEU:O	1:A:771:ALA:N	2.43	0.48
1:A:979:ASP:OD1	1:A:979:ASP:N	2.47	0.48
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.95	0.48
1:C:64:TRP:HD1	1:C:265:TYR:O	1.97	0.48
1:A:564:GLN:HE22	1:A:577:ARG:HB3	1.78	0.47
1:C:106:PHE:CE2	1:C:238:PHE:HB2	2.49	0.47
1:C:329:PHE:O	1:C:580:GLN:NE2	2.43	0.47
1:B:644:GLN:NE2	1:B:648:GLY:O	2.47	0.47
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.96	0.47
1:B:567:ARG:HA	1:B:573:THR:HA	1.96	0.47
1:A:516:GLU:OE2	1:A:519:HIS:ND1	2.47	0.47
1:B:93:ALA:HB1	1:B:189:LEU:HD11	1.95	0.47
1:A:122:ASN:OD1	1:A:125:ASN:N	2.43	0.47
1:B:27:ALA:HB3	1:B:64:TRP:HB3	1.97	0.47
1:C:97:LYS:HD2	1:C:98:SER:N	2.30	0.47
1:A:448:ASN:OD1	1:A:450:ASN:ND2	2.47	0.46
1:A:1141:LEU:HG	1:A:1145:LEU:HD23	1.95	0.46
1:B:988:GLU:HA	1:B:991:VAL:HG12	1.96	0.46
1:C:611:LEU:HD22	1:C:666:ILE:HG23	1.97	0.46
1:B:567:ARG:NH1	1:B:571:ASP:O	2.48	0.46
1:A:280:ASN:HB3	1:A:282:ASN:O	2.14	0.46
1:B:213:VAL:HG13	1:B:214:ARG:N	2.29	0.46
1:B:557:LYS:NZ	1:B:574:ASP:OD2	2.46	0.46
1:C:329:PHE:CE2	1:C:525:CYS:HB3	2.51	0.46
1:A:617:CYS:N	1:A:644:GLN:OE1	2.46	0.46
1:C:329:PHE:HE2	1:C:525:CYS:HB3	1.81	0.46
1:C:794:ILE:C	1:C:795:LYS:HD2	2.36	0.46
1:C:102:ARG:N	1:C:241:LEU:O	2.48	0.46
2:H:1:NAG:O6	2:H:2:NAG:N2	2.49	0.46
1:A:1100:THR:HG21	3:A:1303:NAG:N2	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:TRP:HZ2	1:B:214:ARG:HG2	1.81	0.46
1:B:231:ILE:HG13	1:B:232:GLY:N	2.31	0.46
1:C:94:SER:OG	1:C:96:GLU:OE1	2.26	0.46
1:A:382:VAL:HG11	1:A:515:PHE:HZ	1.80	0.45
1:B:190:ARG:HB3	1:B:192:PHE:HE1	1.81	0.45
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.98	0.45
1:A:212:LEU:HD13	1:A:215:ASP:H	1.81	0.45
1:A:974:SER:HB3	1:A:980:ILE:HG13	1.97	0.45
1:C:106:PHE:HB3	1:C:235:ILE:HG21	1.99	0.45
1:B:37:TYR:CB	1:B:223:LEU:HB3	2.44	0.45
1:A:1030:SER:OG	1:C:1041:ASP:HB3	2.16	0.45
1:A:31:SER:OG	1:A:60:SER:N	2.49	0.45
1:A:541:PHE:HB2	1:A:543:PHE:HE1	1.82	0.45
1:B:326:ILE:N	1:B:540:ASN:O	2.49	0.45
1:C:64:TRP:CD1	1:C:266:TYR:CD1	3.04	0.45
1:C:120:VAL:HG22	1:C:121:ASN:H	1.81	0.45
1:A:563:GLN:HA	1:B:41:LYS:HB3	1.98	0.45
1:A:895:GLN:NE2	1:C:713:ALA:HB2	2.32	0.45
1:C:317:ASN:OD1	1:C:318:PHE:N	2.50	0.45
1:A:192:PHE:HA	1:A:204:TYR:O	2.16	0.45
1:C:129:LYS:HE2	1:C:133:PHE:HZ	1.81	0.45
1:C:328:ARG:NH2	1:C:580:GLN:OE1	2.50	0.45
1:B:31:SER:OG	1:B:60:SER:N	2.50	0.44
1:C:214:ARG:HG3	1:C:215:ASP:N	2.27	0.44
1:C:675:GLN:O	1:C:690:GLN:HA	2.17	0.44
1:C:1140:PRO:O	1:C:1143:PRO:HD2	2.17	0.44
1:A:122:ASN:HD22	2:G:1:NAG:HN2	1.65	0.44
1:A:620:VAL:N	1:A:621:PRO:HD2	2.32	0.44
1:B:936:ASP:HA	1:B:939:SER:HB3	2.00	0.44
1:A:543:PHE:O	1:A:546:LEU:HB3	2.17	0.44
1:C:363:ALA:HB2	1:C:524:VAL:HG12	2.00	0.44
1:C:874:THR:O	1:C:878:LEU:HD23	2.17	0.44
1:A:81:ASN:N	1:A:82:PRO:HD3	2.33	0.44
1:C:198:ASP:OD1	1:C:198:ASP:N	2.50	0.44
1:C:200:TYR:HA	1:C:230:PRO:HA	1.98	0.44
1:C:402:ILE:HD13	1:C:410:ILE:HD13	1.99	0.44
1:A:444:LYS:HG2	1:A:448:ASN:HB2	1.99	0.44
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.98	0.44
1:B:1003:SER:HG	1:C:759:PHE:HZ	1.65	0.44
1:C:27:ALA:HB3	1:C:64:TRP:CE3	2.52	0.44
1:C:64:TRP:NE1	1:C:264:ALA:HB1	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ALA:HA	1:C:423:TYR:O	2.17	0.44
1:C:1129:VAL:HG11	1:C:1132:ILE:HD12	1.99	0.44
1:A:1142:GLN:HA	1:A:1145:LEU:HG	1.99	0.44
1:C:119:ILE:HG23	1:C:128:ILE:HG13	2.00	0.44
1:C:172:SER:OG	1:C:173:GLN:OE1	2.36	0.44
1:A:357:ARG:HD3	1:A:396:TYR:CZ	2.53	0.44
1:B:100:ILE:O	1:B:102:ARG:HG2	2.16	0.44
1:B:205:SER:O	1:B:224:GLU:HB2	2.18	0.44
1:C:431:GLY:HA2	1:C:515:PHE:CE2	2.52	0.44
1:A:801:ASN:HD21	2:E:1:NAG:C1	2.30	0.44
1:B:969:ASN:OD1	1:B:975:SER:HB3	2.18	0.44
1:B:304:LYS:HE2	1:B:304:LYS:HB2	1.80	0.43
1:B:746:SER:OG	1:B:746:SER:O	2.36	0.43
1:C:28:TYR:HB3	1:C:61:ASN:OD1	2.18	0.43
1:C:408:ARG:O	1:C:414:GLN:NE2	2.51	0.43
1:A:349:SER:HB3	1:A:452:LEU:O	2.18	0.43
1:A:156:GLU:HG3	1:A:158:ARG:HG2	2.00	0.43
1:B:568:ASP:OD2	1:B:574:ASP:HB3	2.18	0.43
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.54	0.43
1:B:1093:GLY:CA	1:B:1105:THR:O	2.62	0.43
1:A:409:GLN:HA	1:A:414:GLN:HG2	2.01	0.43
1:A:1140:PRO:O	1:A:1143:PRO:HD2	2.19	0.43
1:C:42:VAL:O	1:C:44:ARG:NH1	2.51	0.43
1:A:736:VAL:HG22	1:A:858:LEU:HD13	1.99	0.43
1:C:214:ARG:CG	1:C:215:ASP:H	2.29	0.43
1:C:395:VAL:HG21	1:C:524:VAL:HG21	2.00	0.43
1:A:426:PRO:HG2	1:A:429:PHE:HB2	2.00	0.43
1:A:792:PRO:HG3	1:A:883:THR:HG21	2.00	0.43
1:B:676:THR:HA	1:B:690:GLN:HA	2.01	0.43
1:C:411:ALA:HB3	1:C:414:GLN:NE2	2.34	0.43
1:C:206:LYS:HD2	1:C:206:LYS:HA	1.82	0.43
1:B:37:TYR:HB3	1:B:223:LEU:HD23	2.00	0.43
1:B:96:GLU:OE2	1:B:100:ILE:HG12	2.18	0.43
1:C:27:ALA:HB3	1:C:64:TRP:HE3	1.83	0.43
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.53	0.42
1:B:1093:GLY:O	1:C:904:TYR:OH	2.37	0.42
1:B:122:ASN:OD1	1:B:125:ASN:N	2.49	0.42
1:B:699:LEU:HD22	1:C:873:TYR:CZ	2.54	0.42
1:C:457:ARG:NH2	1:C:460:ASN:O	2.43	0.42
1:C:986:LYS:HA	1:C:986:LYS:HD3	1.81	0.42
1:A:877:LEU:HD23	1:A:877:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:SER:HB3	1:C:698:SER:HB2	2.01	0.42
1:C:743:CYS:HA	1:C:749:CYS:SG	2.59	0.42
1:A:172:SER:OG	1:A:173:GLN:N	2.53	0.42
1:A:645:THR:HG23	1:A:647:ALA:H	1.84	0.42
1:B:105:ILE:HG13	1:B:241:LEU:HD11	2.01	0.42
1:B:129:LYS:HE2	1:B:133:PHE:HZ	1.83	0.42
1:C:759:PHE:HD1	1:C:762:GLN:HE22	1.67	0.42
2:I:1:NAG:O6	2:I:2:NAG:H2	2.18	0.42
1:A:27:ALA:HB3	1:A:64:TRP:O	2.20	0.42
1:B:53:ASP:OD1	1:B:54:LEU:N	2.45	0.42
1:A:105:ILE:HD11	1:A:118:LEU:HD13	2.02	0.42
1:B:277:LEU:HD13	1:B:288:ALA:HB2	2.02	0.42
1:C:170:TYR:CE2	1:C:172:SER:HB2	2.55	0.42
1:C:759:PHE:HA	1:C:762:GLN:NE2	2.34	0.42
1:A:29:THR:HG22	1:A:30:ASN:N	2.35	0.42
1:A:616:ASN:HB2	1:A:619:GLU:OE1	2.19	0.42
1:B:759:PHE:O	1:B:763:LEU:HD23	2.20	0.42
1:A:28:TYR:HB3	1:A:61:ASN:OD1	2.19	0.42
1:B:564:GLN:NE2	1:B:577:ARG:O	2.48	0.42
1:C:64:TRP:CD1	1:C:266:TYR:HD1	2.37	0.42
1:C:172:SER:HG	1:C:173:GLN:H	1.68	0.41
1:C:202:LYS:HE2	1:C:202:LYS:HB2	1.87	0.41
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.55	0.41
1:B:740:MET:SD	1:B:857:GLY:HA3	2.60	0.41
1:C:971:GLY:C	1:C:995:ARG:HH21	2.24	0.41
1:C:973:ILE:HD11	1:C:984:LEU:HD21	2.02	0.41
1:A:197:ILE:HG22	1:A:198:ASP:OD1	2.21	0.41
1:A:977:LEU:HD21	1:A:996:LEU:HD23	2.01	0.41
1:B:1030:SER:O	1:B:1034:LEU:HB2	2.21	0.41
1:B:1101:HIS:CE1	3:B:1303:NAG:H3	2.55	0.41
1:C:417:LYS:HZ1	1:C:455:LEU:HD12	1.86	0.41
1:B:208:THR:HG23	1:B:210:ILE:HG12	2.02	0.41
1:C:552:LEU:HD22	1:C:587:ILE:HG12	2.03	0.41
1:C:645:THR:HG23	1:C:647:ALA:H	1.85	0.41
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	2.01	0.41
1:A:40:ASP:OD1	1:A:41:LYS:N	2.45	0.41
1:A:1139:ASP:HB3	1:A:1142:GLN:HG2	2.03	0.41
1:B:204:TYR:CD1	1:B:225:PRO:HA	2.55	0.41
1:B:817:PHE:O	1:B:821:LEU:HG	2.21	0.41
1:C:188:ASN:HA	1:C:211:ASN:HD22	1.85	0.41
1:A:705:VAL:HG12	1:B:895:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:SER:OG	1:C:173:GLN:N	2.54	0.41
1:A:808:ASP:HB3	1:A:811:LYS:HE2	2.02	0.41
1:A:106:PHE:CD1	1:A:117:LEU:HD23	2.55	0.41
1:A:129:LYS:HB3	1:A:133:PHE:HZ	1.86	0.41
1:A:934:ILE:HD13	1:A:934:ILE:HA	1.91	0.41
1:A:1062:PHE:HB3	1:A:1064:HIS:CE1	2.56	0.41
1:C:48:LEU:HG	1:C:278:LYS:HG3	2.03	0.41
1:B:1041:ASP:HB3	1:C:1030:SER:OG	2.20	0.41
1:C:581:THR:O	1:C:582:LEU:HG	2.21	0.41
1:C:595:VAL:HG22	1:C:612:TYR:CD1	2.55	0.41
1:A:353:TRP:CZ2	1:A:466:ARG:HB2	2.56	0.41
1:C:80:ASP:O	1:C:265:TYR:OH	2.24	0.41
1:B:46:SER:N	1:B:280:ASN:O	2.52	0.40
1:A:448:ASN:HB3	1:A:497:PHE:HB2	2.02	0.40
1:A:611:LEU:HD22	1:A:666:ILE:HG23	2.02	0.40
1:B:958:ALA:O	1:B:961:THR:HB	2.21	0.40
1:A:55:PHE:O	1:A:270:LEU:HA	2.21	0.40
1:A:457:ARG:NH1	1:A:458:LYS:HB2	2.35	0.40
1:A:977:LEU:HD23	1:A:977:LEU:HA	1.83	0.40
1:B:216:LEU:HG	1:B:217:PRO:HD2	2.03	0.40
1:B:1115:ILE:H	1:B:1115:ILE:HD12	1.86	0.40
1:C:195:LYS:CG	1:C:202:LYS:HB2	2.51	0.40
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	2.03	0.40
1:A:996:LEU:HD12	1:A:996:LEU:HA	1.88	0.40
1:B:746:SER:O	1:B:749:CYS:N	2.48	0.40
1:B:980:ILE:H	1:B:980:ILE:HD12	1.87	0.40
1:C:466:ARG:HG3	1:C:468:ILE:HG23	2.02	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	1017/1204 (84%)	958 (94%)	56 (6%)	3 (0%)	37	71
1	B	803/1204 (67%)	754 (94%)	46 (6%)	3 (0%)	30	66
1	C	1009/1204 (84%)	952 (94%)	54 (5%)	3 (0%)	37	71
All	All	2829/3612 (78%)	2664 (94%)	156 (6%)	9 (0%)	38	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	621	PRO
1	B	621	PRO
1	C	621	PRO
1	C	794	ILE
1	A	794	ILE
1	C	320	VAL
1	A	320	VAL
1	B	320	VAL
1	B	794	ILE

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	903/1049 (86%)	903 (100%)	0	100	100
1	B	720/1049 (69%)	720 (100%)	0	100	100
1	C	896/1049 (85%)	895 (100%)	1 (0%)	92	94
All	All	2519/3147 (80%)	2518 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	1005	GLN
1	A	1048	HIS
1	C	1002	GLN

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
2	NAG	D	1	1,2	14,14,15	1.94	4 (28%)	17,19,21	1.21	2 (11%)
2	NAG	D	2	2	14,14,15	2.02	3 (21%)	17,19,21	1.01	1 (5%)
2	NAG	E	1	2	14,14,15	1.94	3 (21%)	17,19,21	1.50	5 (29%)
2	NAG	E	2	2	14,14,15	2.02	3 (21%)	17,19,21	1.13	2 (11%)
2	NAG	F	1	1,2	14,14,15	2.02	4 (28%)	17,19,21	1.60	4 (23%)
2	NAG	F	2	2	14,14,15	2.05	3 (21%)	17,19,21	1.15	2 (11%)
2	NAG	G	1	2	14,14,15	2.01	3 (21%)	17,19,21	1.10	2 (11%)
2	NAG	G	2	2	14,14,15	2.03	3 (21%)	17,19,21	1.14	2 (11%)
2	NAG	H	1	1,2	14,14,15	1.99	4 (28%)	17,19,21	1.24	2 (11%)
2	NAG	H	2	2	14,14,15	2.08	3 (21%)	17,19,21	1.34	3 (17%)
2	NAG	I	1	1,2	14,14,15	2.01	3 (21%)	17,19,21	1.60	3 (17%)
2	NAG	I	2	2	14,14,15	2.13	4 (28%)	17,19,21	1.18	3 (17%)
2	NAG	J	1	1,2	14,14,15	1.95	3 (21%)	17,19,21	1.05	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	J	2	2	14,14,15	1.99	3 (21%)	17,19,21	1.08	1 (5%)
2	NAG	K	1	1,2	14,14,15	2.04	5 (35%)	17,19,21	2.12	5 (29%)
2	NAG	K	2	2	14,14,15	2.00	3 (21%)	17,19,21	1.16	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	O5-C1	5.61	1.52	1.43
2	H	2	NAG	O5-C1	5.45	1.52	1.43
2	F	2	NAG	O5-C1	5.41	1.52	1.43
2	G	2	NAG	O5-C1	5.32	1.52	1.43
2	K	2	NAG	O5-C1	5.28	1.52	1.43
2	K	1	NAG	O5-C1	5.27	1.52	1.43
2	F	1	NAG	O5-C1	5.26	1.52	1.43
2	J	2	NAG	O5-C1	5.25	1.52	1.43
2	I	1	NAG	O5-C1	5.24	1.52	1.43
2	G	1	NAG	O5-C1	5.23	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	O5-C1	5.19	1.52	1.43
2	J	1	NAG	O5-C1	5.18	1.52	1.43
2	D	2	NAG	O5-C1	5.17	1.52	1.43
2	H	1	NAG	O5-C1	5.16	1.52	1.43
2	E	1	NAG	O5-C1	4.93	1.51	1.43
2	D	1	NAG	O5-C1	4.85	1.51	1.43
2	I	2	NAG	C7-N2	3.27	1.45	1.34
2	D	2	NAG	C7-N2	3.26	1.45	1.34
2	H	2	NAG	C7-N2	3.25	1.45	1.34
2	I	1	NAG	C7-N2	3.24	1.45	1.34
2	E	2	NAG	C7-N2	3.20	1.45	1.34
2	F	2	NAG	C7-N2	3.16	1.45	1.34
2	J	2	NAG	C7-N2	3.16	1.45	1.34
2	G	1	NAG	C7-N2	3.14	1.45	1.34
2	G	2	NAG	C7-N2	3.14	1.45	1.34
2	D	1	NAG	C7-N2	3.13	1.45	1.34
2	K	1	NAG	C7-N2	3.12	1.45	1.34
2	H	1	NAG	C7-N2	3.12	1.45	1.34
2	E	1	NAG	C7-N2	3.10	1.45	1.34
2	K	2	NAG	C7-N2	3.07	1.44	1.34
2	F	1	NAG	C7-N2	3.06	1.44	1.34
2	I	2	NAG	C2-N2	2.99	1.51	1.46
2	J	1	NAG	C7-N2	2.97	1.44	1.34
2	D	2	NAG	C2-N2	2.95	1.51	1.46
2	H	2	NAG	C2-N2	2.93	1.51	1.46
2	E	2	NAG	C2-N2	2.87	1.51	1.46
2	F	2	NAG	C2-N2	2.86	1.51	1.46
2	J	2	NAG	C2-N2	2.81	1.51	1.46
2	G	1	NAG	C2-N2	2.80	1.51	1.46
2	G	2	NAG	C2-N2	2.80	1.51	1.46
2	I	1	NAG	C2-N2	2.75	1.51	1.46
2	E	1	NAG	C2-N2	2.70	1.50	1.46
2	D	1	NAG	C2-N2	2.60	1.50	1.46
2	K	2	NAG	C2-N2	2.57	1.50	1.46
2	F	1	NAG	C2-N2	2.56	1.50	1.46
2	K	1	NAG	C2-N2	2.56	1.50	1.46
2	J	1	NAG	C2-N2	2.45	1.50	1.46
2	H	1	NAG	C2-N2	2.44	1.50	1.46
2	I	2	NAG	O5-C5	2.25	1.48	1.43
2	H	1	NAG	C3-C2	-2.13	1.48	1.52
2	K	1	NAG	C3-C2	-2.12	1.48	1.52
2	D	1	NAG	C3-C2	-2.08	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C3-C2	-2.04	1.48	1.52
2	K	1	NAG	O5-C5	2.03	1.47	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	C2-N2-C7	-4.68	116.24	122.90
2	K	1	NAG	C1-O5-C5	4.64	118.48	112.19
2	I	1	NAG	C1-O5-C5	4.01	117.62	112.19
2	F	1	NAG	C1-O5-C5	3.75	117.28	112.19
2	K	1	NAG	C6-C5-C4	-3.12	105.70	113.00
2	D	1	NAG	C2-N2-C7	-2.81	118.90	122.90
2	E	1	NAG	C4-C3-C2	2.73	115.01	111.02
2	F	1	NAG	C2-N2-C7	-2.72	119.03	122.90
2	H	2	NAG	C1-O5-C5	2.71	115.87	112.19
2	E	1	NAG	C3-C4-C5	2.69	115.03	110.24
2	K	2	NAG	C2-N2-C7	-2.58	119.23	122.90
2	K	1	NAG	C8-C7-N2	2.50	120.32	116.10
2	G	1	NAG	C2-N2-C7	-2.50	119.35	122.90
2	H	2	NAG	C8-C7-N2	2.49	120.32	116.10
2	D	1	NAG	C8-C7-N2	2.45	120.24	116.10
2	F	2	NAG	C8-C7-N2	2.41	120.19	116.10
2	F	2	NAG	C2-N2-C7	-2.40	119.49	122.90
2	G	2	NAG	C2-N2-C7	-2.39	119.50	122.90
2	H	2	NAG	C2-N2-C7	-2.38	119.51	122.90
2	F	1	NAG	C8-C7-N2	2.37	120.12	116.10
2	G	2	NAG	C8-C7-N2	2.36	120.10	116.10
2	G	1	NAG	C8-C7-N2	2.36	120.09	116.10
2	D	2	NAG	C8-C7-N2	2.34	120.07	116.10
2	I	1	NAG	C8-C7-N2	2.33	120.04	116.10
2	E	2	NAG	C8-C7-N2	2.32	120.03	116.10
2	J	2	NAG	C8-C7-N2	2.32	120.03	116.10
2	K	2	NAG	C8-C7-N2	2.29	119.98	116.10
2	E	1	NAG	C6-C5-C4	-2.29	107.64	113.00
2	I	1	NAG	C6-C5-C4	-2.27	107.68	113.00
2	J	1	NAG	C8-C7-N2	2.27	119.94	116.10
2	E	1	NAG	C8-C7-N2	2.21	119.84	116.10
2	I	2	NAG	C1-O5-C5	2.18	115.14	112.19
2	F	1	NAG	C6-C5-C4	-2.15	107.97	113.00
2	I	2	NAG	C8-C7-N2	2.14	119.73	116.10
2	H	1	NAG	C6-C5-C4	-2.10	108.08	113.00
2	J	1	NAG	C2-N2-C7	-2.09	119.93	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C8-C7-N2	2.08	119.61	116.10
2	E	2	NAG	C2-N2-C7	-2.07	119.96	122.90
2	K	1	NAG	O5-C5-C4	2.06	115.84	110.83
2	E	1	NAG	C2-N2-C7	-2.05	119.98	122.90
2	I	2	NAG	O5-C5-C6	2.02	110.37	107.20

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C1-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C3-C2-N2-C7
2	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 6 short contacts:

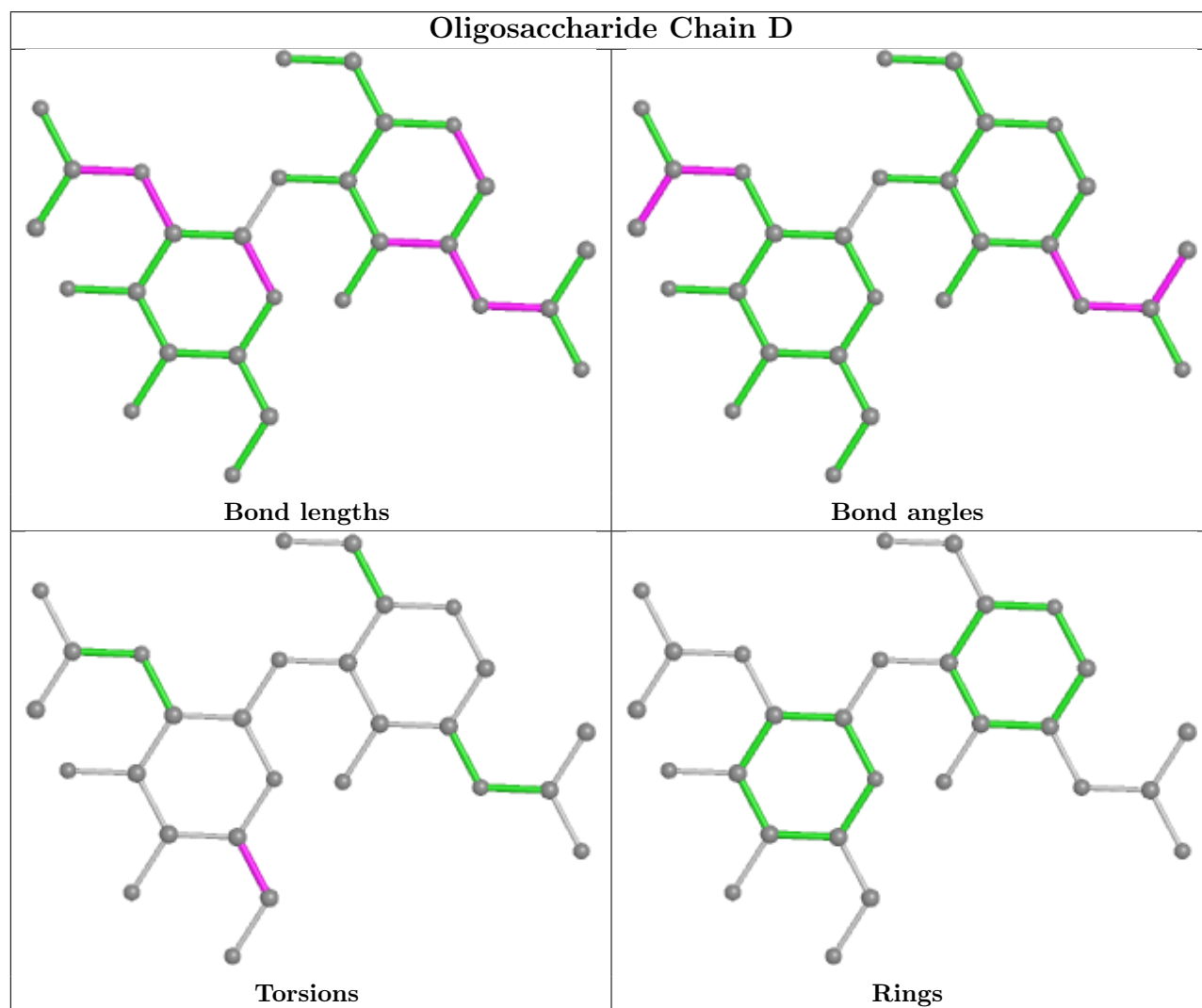
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	1	0
2	I	1	NAG	1	0
2	E	1	NAG	2	0
2	D	2	NAG	1	0
2	D	1	NAG	1	0

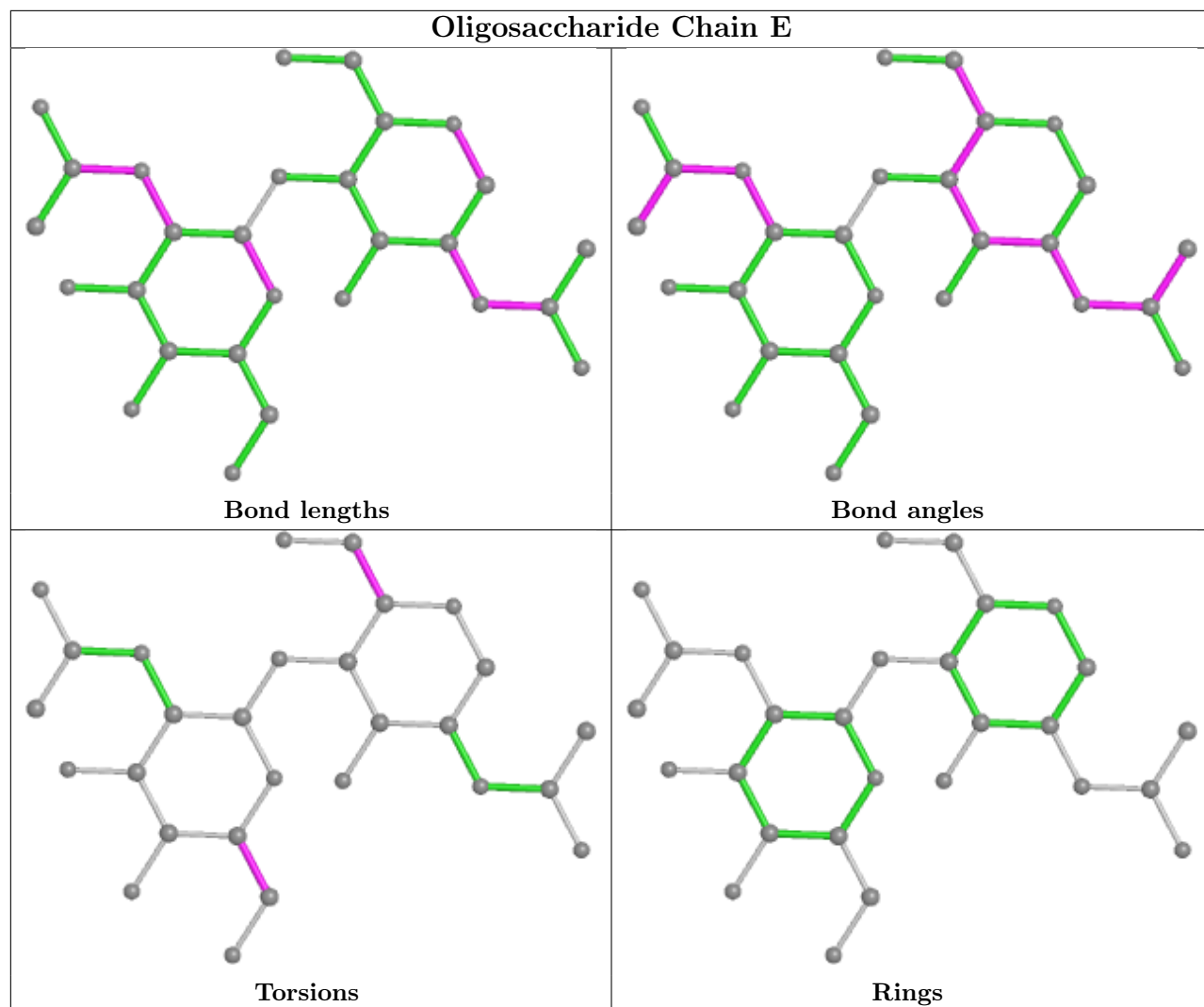
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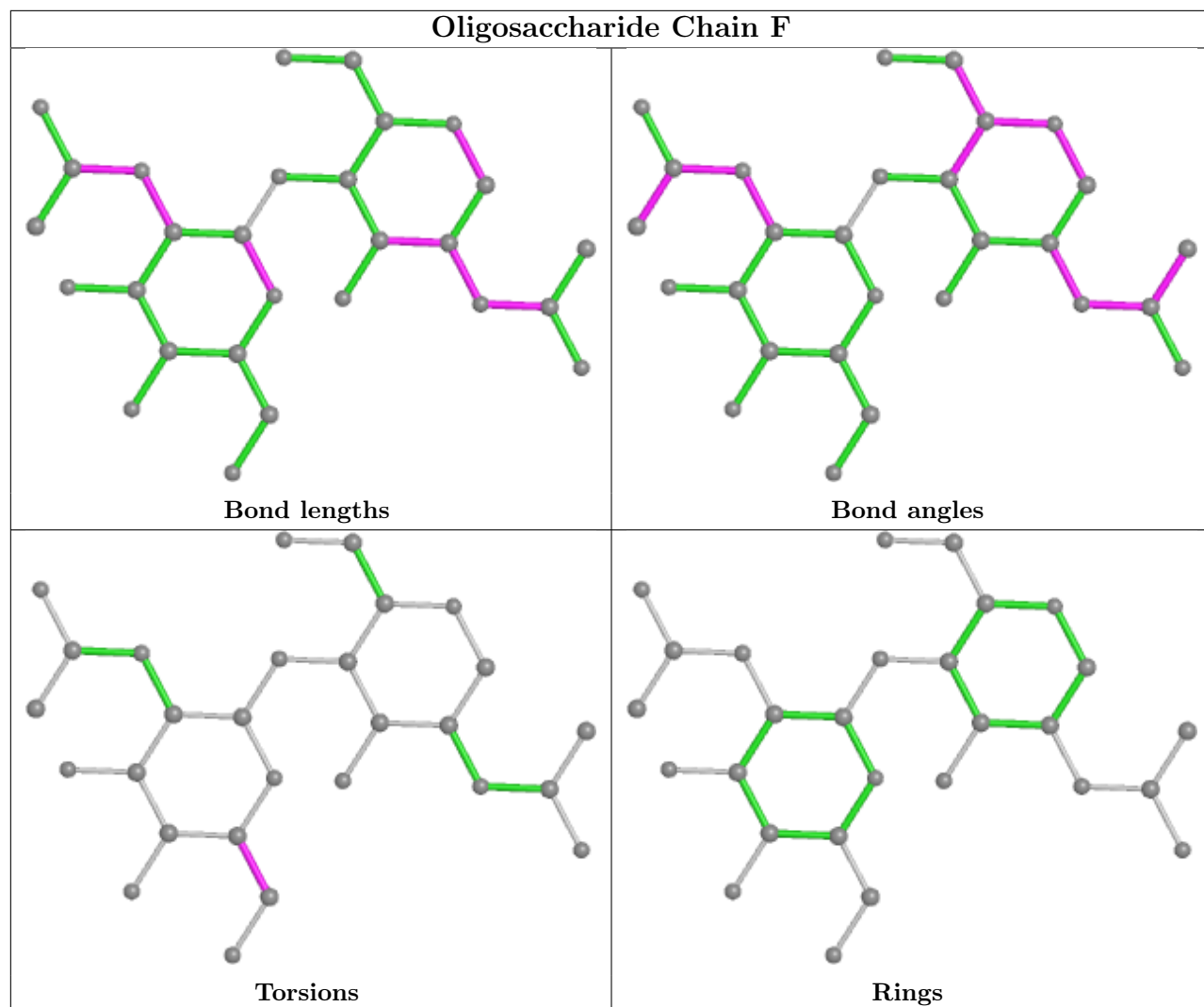
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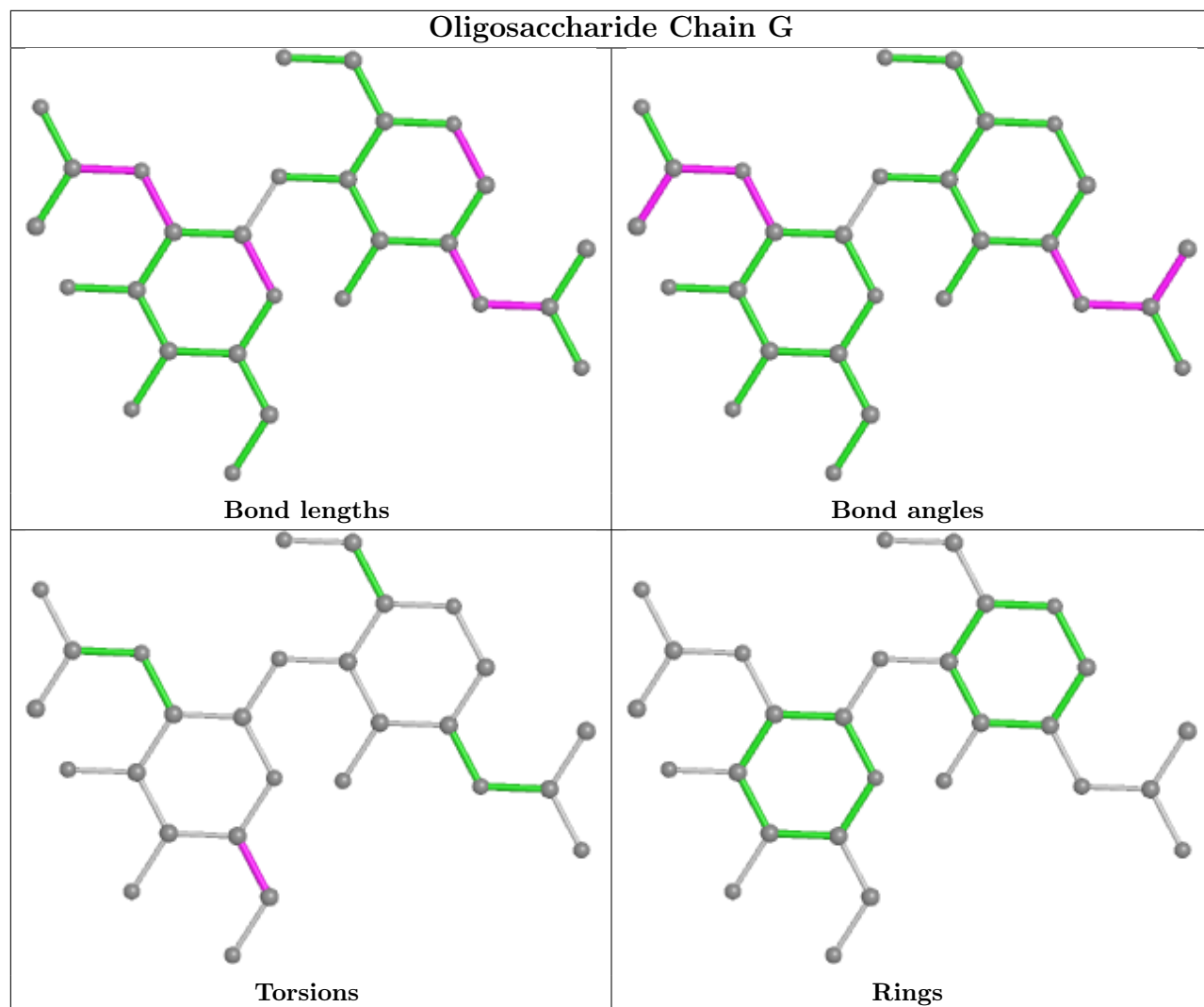
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	G	1	NAG	1	0
2	I	2	NAG	1	0

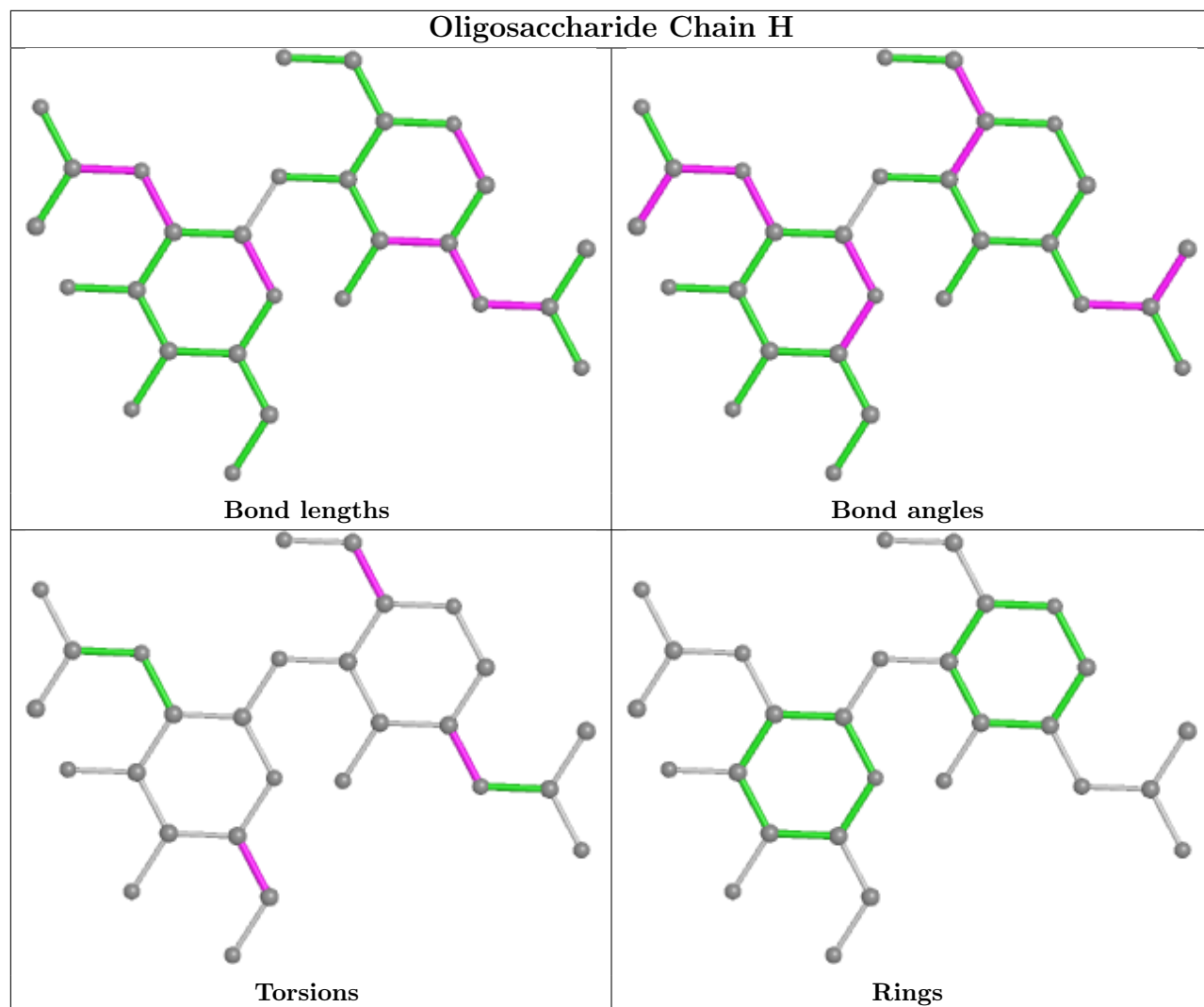
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

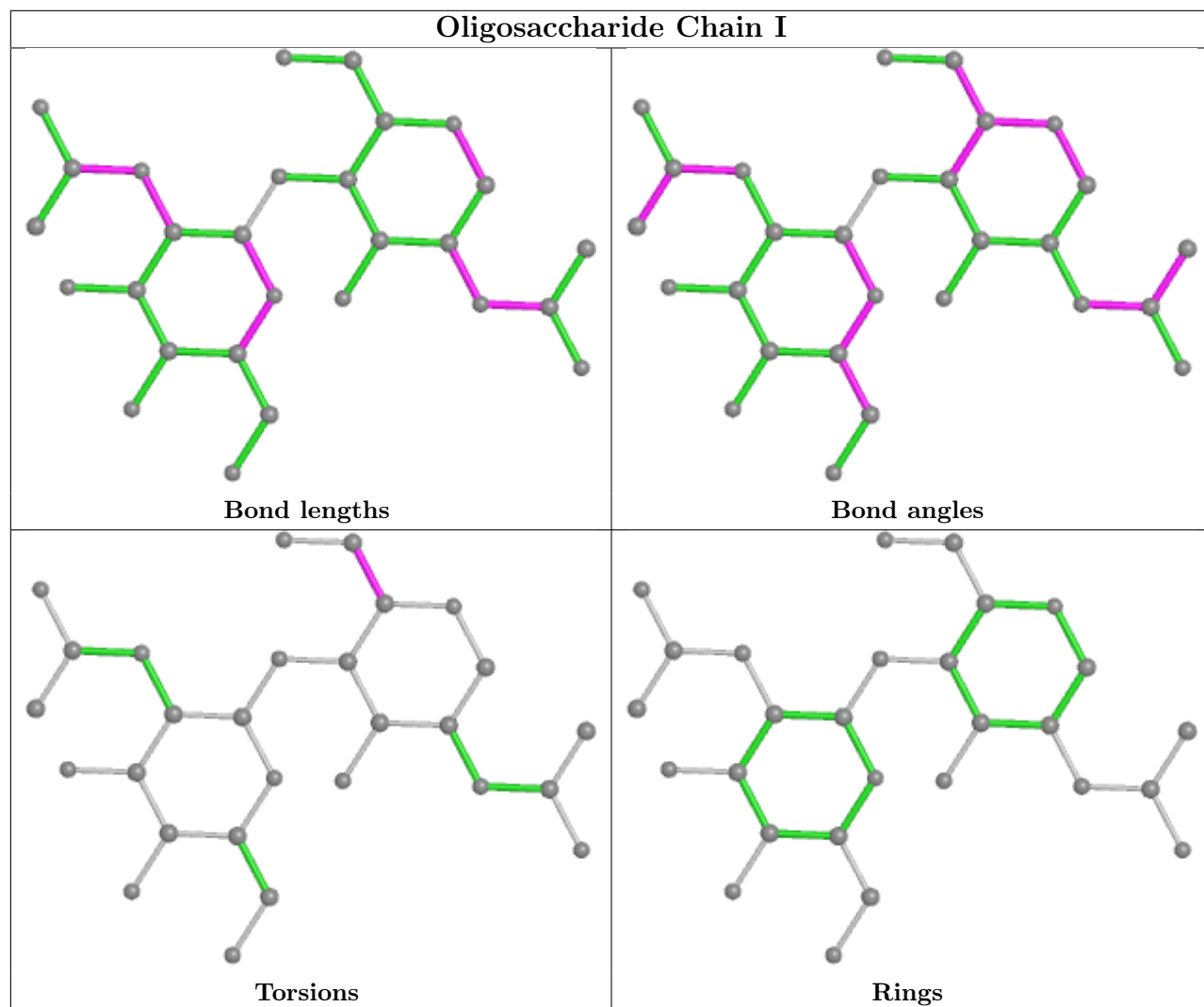


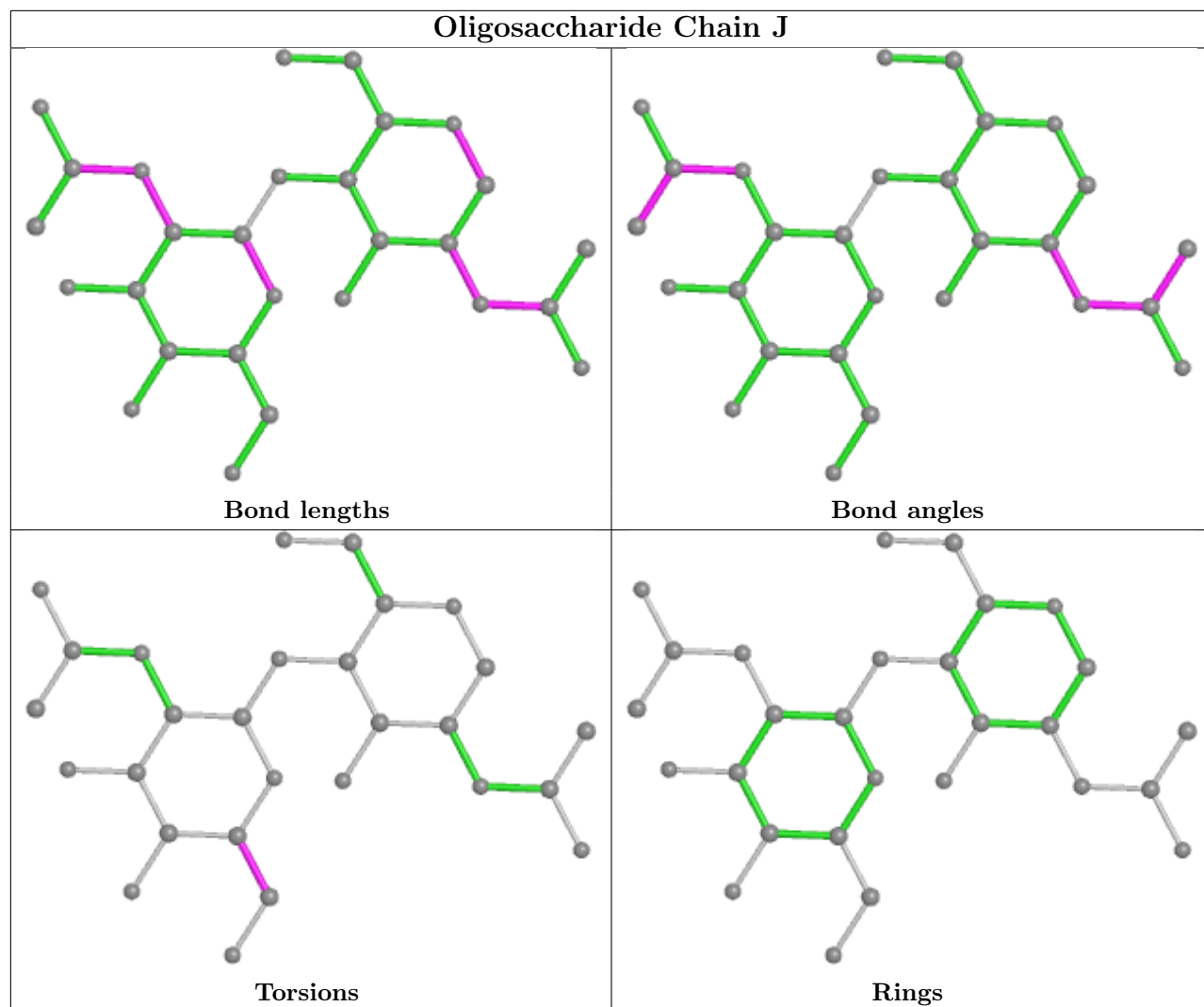


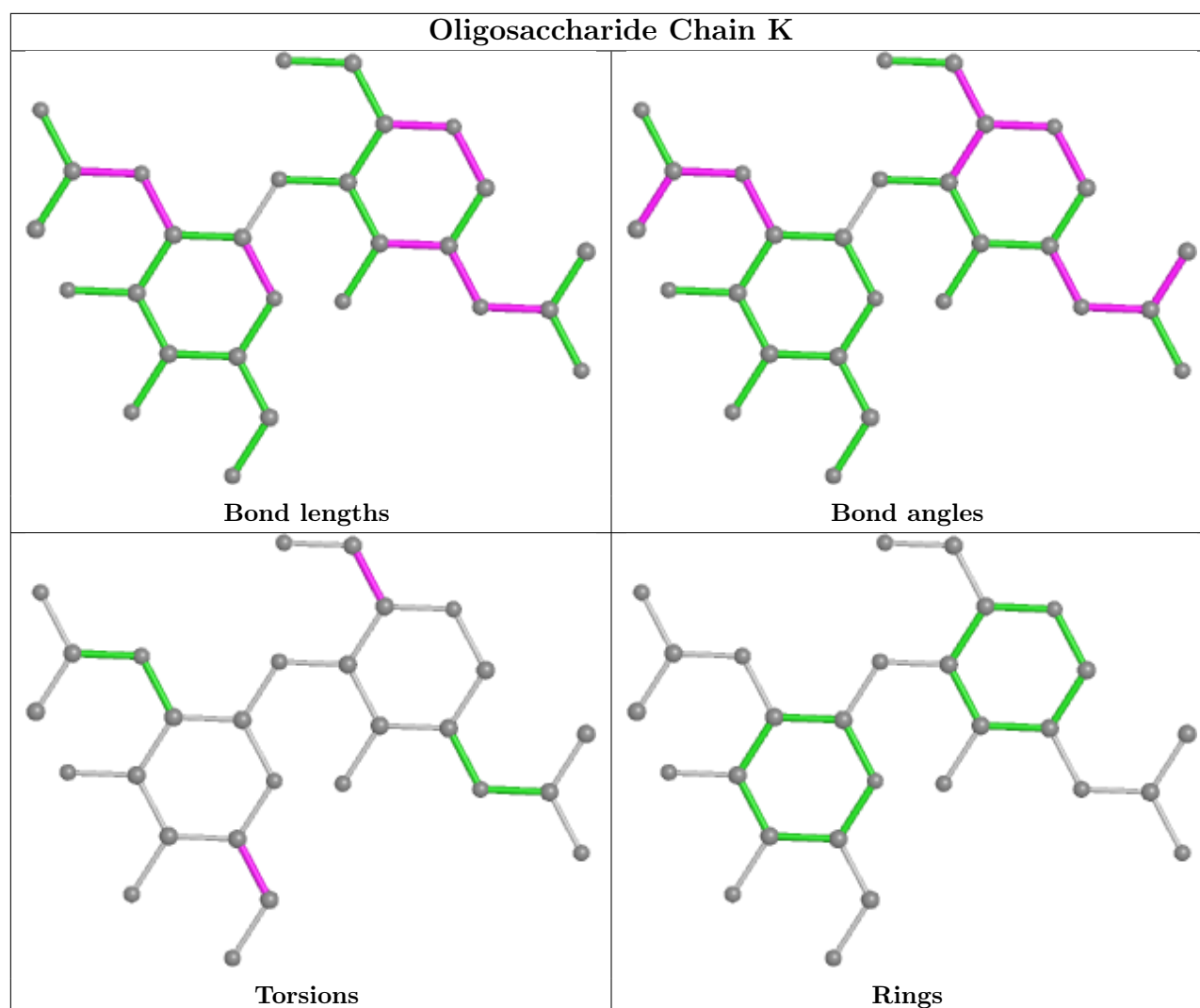












5.6 Ligand geometry [i](#)

15 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$
3	NAG	B	1303	-	14,14,15	2.00	5 (35%)	17,19,21	1.29	2 (11%)
3	NAG	C	1305	1	14,14,15	2.02	3 (21%)	17,19,21	1.14	1 (5%)
3	NAG	A	1303	-	14,14,15	2.00	4 (28%)	17,19,21	1.22	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1302	1	14,14,15	2.02	3 (21%)	17,19,21	1.19	1 (5%)
3	NAG	C	1304	-	14,14,15	1.99	3 (21%)	17,19,21	1.21	2 (11%)
3	NAG	B	1304	1	14,14,15	2.02	3 (21%)	17,19,21	1.20	3 (17%)
3	NAG	B	1301	1	14,14,15	1.96	3 (21%)	17,19,21	1.25	3 (17%)
3	NAG	C	1303	-	14,14,15	2.03	3 (21%)	17,19,21	1.18	2 (11%)
3	NAG	C	1301	1	14,14,15	1.99	3 (21%)	17,19,21	1.23	2 (11%)
3	NAG	A	1305	1	14,14,15	2.09	3 (21%)	17,19,21	1.45	4 (23%)
3	NAG	A	1301	1	14,14,15	1.92	3 (21%)	17,19,21	1.46	3 (17%)
3	NAG	B	1305	-	14,14,15	2.00	3 (21%)	17,19,21	1.21	3 (17%)
3	NAG	A	1304	1	14,14,15	2.06	3 (21%)	17,19,21	1.47	3 (17%)
3	NAG	B	1302	-	14,14,15	1.95	3 (21%)	17,19,21	1.16	2 (11%)
3	NAG	A	1302	1	14,14,15	2.06	3 (21%)	17,19,21	1.32	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1303	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1304	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1305	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1302	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1305	NAG	O5-C1	5.56	1.52	1.43
3	A	1302	NAG	O5-C1	5.53	1.52	1.43
3	C	1302	NAG	O5-C1	5.43	1.52	1.43
3	A	1304	NAG	O5-C1	5.42	1.52	1.43
3	B	1304	NAG	O5-C1	5.34	1.52	1.43
3	C	1305	NAG	O5-C1	5.32	1.52	1.43
3	C	1303	NAG	O5-C1	5.26	1.52	1.43
3	C	1301	NAG	O5-C1	5.22	1.52	1.43
3	B	1302	NAG	O5-C1	5.17	1.52	1.43
3	B	1305	NAG	O5-C1	5.10	1.51	1.43
3	B	1301	NAG	O5-C1	5.09	1.51	1.43
3	C	1304	NAG	O5-C1	5.08	1.51	1.43
3	A	1303	NAG	O5-C1	5.04	1.51	1.43
3	A	1301	NAG	O5-C1	5.00	1.51	1.43
3	B	1303	NAG	O5-C1	4.97	1.51	1.43
3	A	1304	NAG	C7-N2	3.41	1.46	1.34
3	B	1303	NAG	C7-N2	3.21	1.45	1.34
3	C	1302	NAG	C7-N2	3.20	1.45	1.34
3	A	1305	NAG	C7-N2	3.19	1.45	1.34
3	A	1304	NAG	C2-N2	3.19	1.51	1.46
3	C	1305	NAG	C7-N2	3.18	1.45	1.34
3	C	1303	NAG	C7-N2	3.17	1.45	1.34
3	A	1302	NAG	C7-N2	3.15	1.45	1.34
3	A	1303	NAG	C7-N2	3.15	1.45	1.34
3	B	1305	NAG	C7-N2	3.13	1.45	1.34
3	C	1304	NAG	C7-N2	3.11	1.45	1.34
3	B	1304	NAG	C7-N2	3.11	1.45	1.34
3	B	1301	NAG	C7-N2	3.11	1.45	1.34
3	C	1301	NAG	C7-N2	3.08	1.44	1.34
3	B	1302	NAG	C7-N2	3.05	1.44	1.34
3	A	1305	NAG	C2-N2	2.92	1.51	1.46
3	A	1301	NAG	C7-N2	2.92	1.44	1.34
3	C	1305	NAG	C2-N2	2.84	1.51	1.46
3	C	1302	NAG	C2-N2	2.83	1.51	1.46
3	C	1303	NAG	C2-N2	2.80	1.51	1.46
3	B	1305	NAG	C2-N2	2.77	1.51	1.46
3	B	1304	NAG	C2-N2	2.75	1.51	1.46
3	A	1303	NAG	C2-N2	2.72	1.50	1.46
3	B	1303	NAG	C2-N2	2.71	1.50	1.46
3	A	1302	NAG	C2-N2	2.70	1.50	1.46
3	C	1304	NAG	C2-N2	2.69	1.50	1.46
3	C	1301	NAG	C2-N2	2.62	1.50	1.46
3	B	1301	NAG	C2-N2	2.60	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	NAG	C2-N2	2.53	1.50	1.46
3	A	1301	NAG	C2-N2	2.33	1.50	1.46
3	A	1303	NAG	O5-C5	2.05	1.47	1.43
3	B	1303	NAG	C3-C2	-2.03	1.48	1.52
3	B	1303	NAG	O5-C5	2.01	1.47	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1304	NAG	C4-C3-C2	3.53	116.19	111.02
3	A	1305	NAG	C1-O5-C5	3.39	116.78	112.19
3	A	1301	NAG	C2-N2-C7	-3.08	118.51	122.90
3	A	1301	NAG	C1-C2-N2	-2.96	105.43	110.49
3	B	1303	NAG	C2-N2-C7	-2.93	118.73	122.90
3	C	1303	NAG	C2-N2-C7	-2.91	118.76	122.90
3	A	1304	NAG	C8-C7-N2	2.82	120.87	116.10
3	B	1305	NAG	C2-N2-C7	-2.70	119.06	122.90
3	B	1303	NAG	C8-C7-N2	2.69	120.65	116.10
3	C	1304	NAG	C2-N2-C7	-2.68	119.09	122.90
3	C	1303	NAG	C8-C7-N2	2.57	120.45	116.10
3	C	1301	NAG	C8-C7-N2	2.54	120.39	116.10
3	C	1301	NAG	C2-N2-C7	-2.49	119.36	122.90
3	A	1302	NAG	C1-O5-C5	2.46	115.53	112.19
3	B	1304	NAG	C2-N2-C7	-2.44	119.43	122.90
3	C	1304	NAG	C8-C7-N2	2.38	120.12	116.10
3	B	1304	NAG	C8-C7-N2	2.36	120.09	116.10
3	B	1305	NAG	C8-C7-N2	2.35	120.07	116.10
3	B	1302	NAG	C2-N2-C7	-2.34	119.58	122.90
3	A	1301	NAG	C8-C7-N2	2.33	120.05	116.10
3	A	1305	NAG	C8-C7-N2	2.33	120.04	116.10
3	A	1303	NAG	C2-N2-C7	-2.30	119.63	122.90
3	C	1305	NAG	C8-C7-N2	2.30	119.99	116.10
3	A	1303	NAG	C8-C7-N2	2.28	119.96	116.10
3	A	1305	NAG	O5-C1-C2	2.24	114.83	111.29
3	A	1302	NAG	C8-C7-N2	2.24	119.89	116.10
3	B	1301	NAG	C2-N2-C7	-2.23	119.72	122.90
3	C	1302	NAG	C8-C7-N2	2.23	119.87	116.10
3	B	1304	NAG	C6-C5-C4	-2.14	107.99	113.00
3	A	1303	NAG	C6-C5-C4	-2.10	108.08	113.00
3	B	1305	NAG	C6-C5-C4	-2.08	108.13	113.00
3	B	1301	NAG	C8-C7-N2	2.08	119.62	116.10
3	A	1302	NAG	O5-C1-C2	2.06	114.54	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1304	NAG	O7-C7-C8	-2.05	118.26	122.06
3	A	1305	NAG	C6-C5-C4	-2.05	108.21	113.00
3	B	1301	NAG	C1-C2-N2	-2.02	107.03	110.49
3	B	1302	NAG	C8-C7-N2	2.02	119.52	116.10

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1302	NAG	C4-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	A	1304	NAG	C1-C2-N2-C7
3	C	1303	NAG	C4-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	A	1304	NAG	C3-C2-N2-C7
3	C	1302	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1303	NAG	1	0
3	A	1303	NAG	2	0
3	B	1304	NAG	1	0
3	C	1303	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.

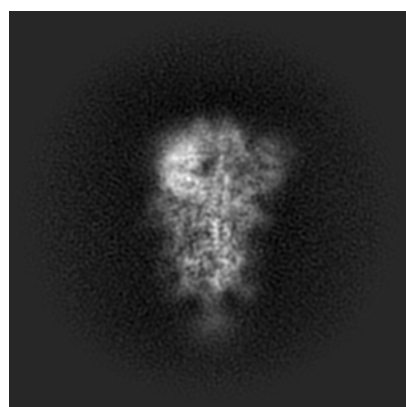
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32492. These allow visual inspection of the internal detail of the map and identification of artifacts.

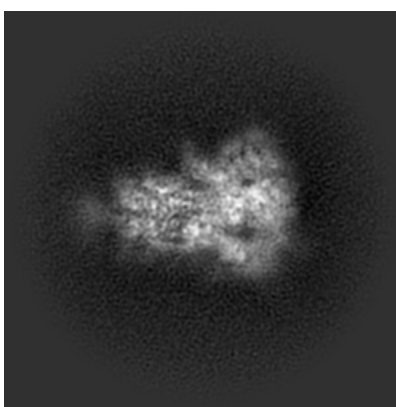
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

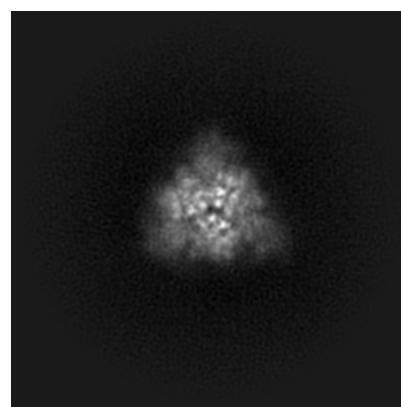
6.1.1 Primary map



X



Y

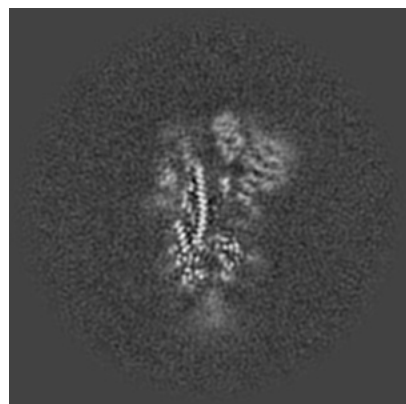


Z

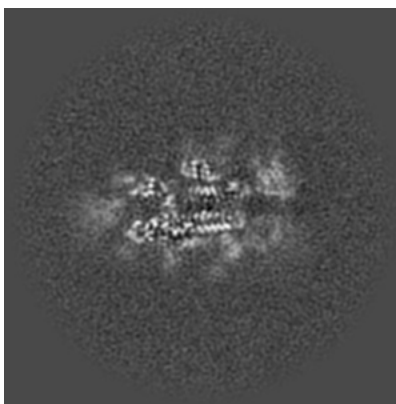
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

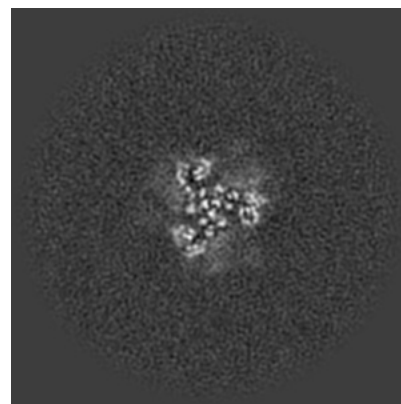
6.2.1 Primary map



X Index: 128



Y Index: 128

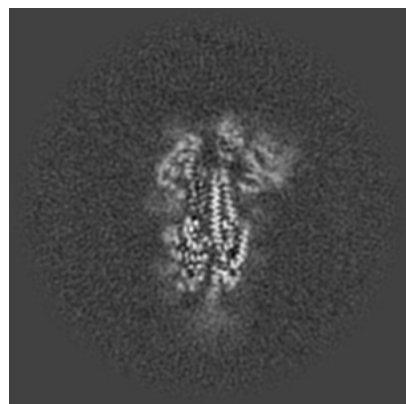


Z Index: 128

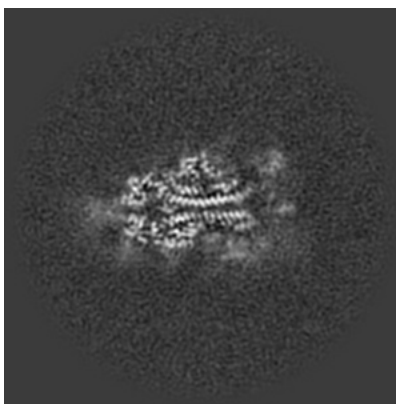
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

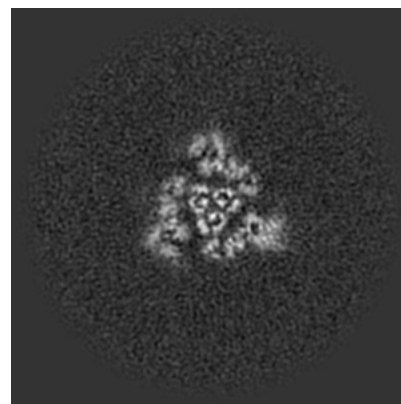
6.3.1 Primary map



X Index: 132



Y Index: 132

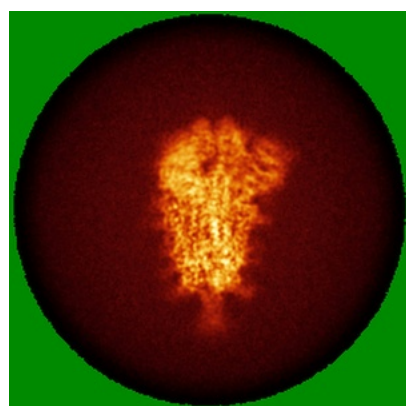


Z Index: 148

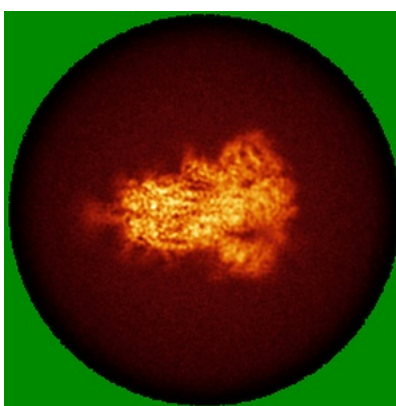
The images above show the largest variance slices of the map in three orthogonal directions.

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

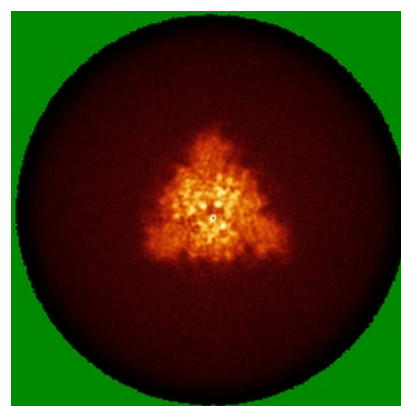
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.506. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

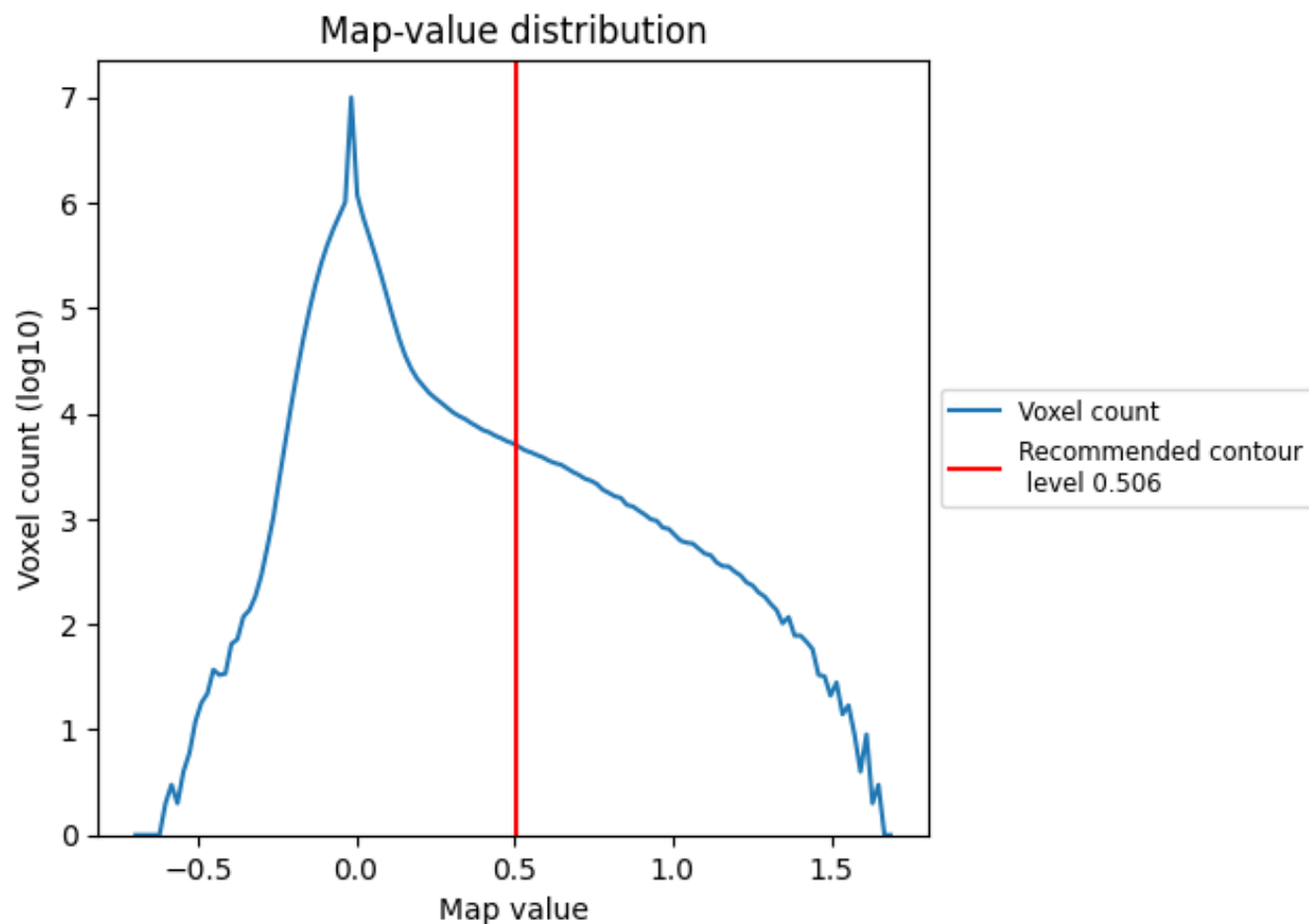
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

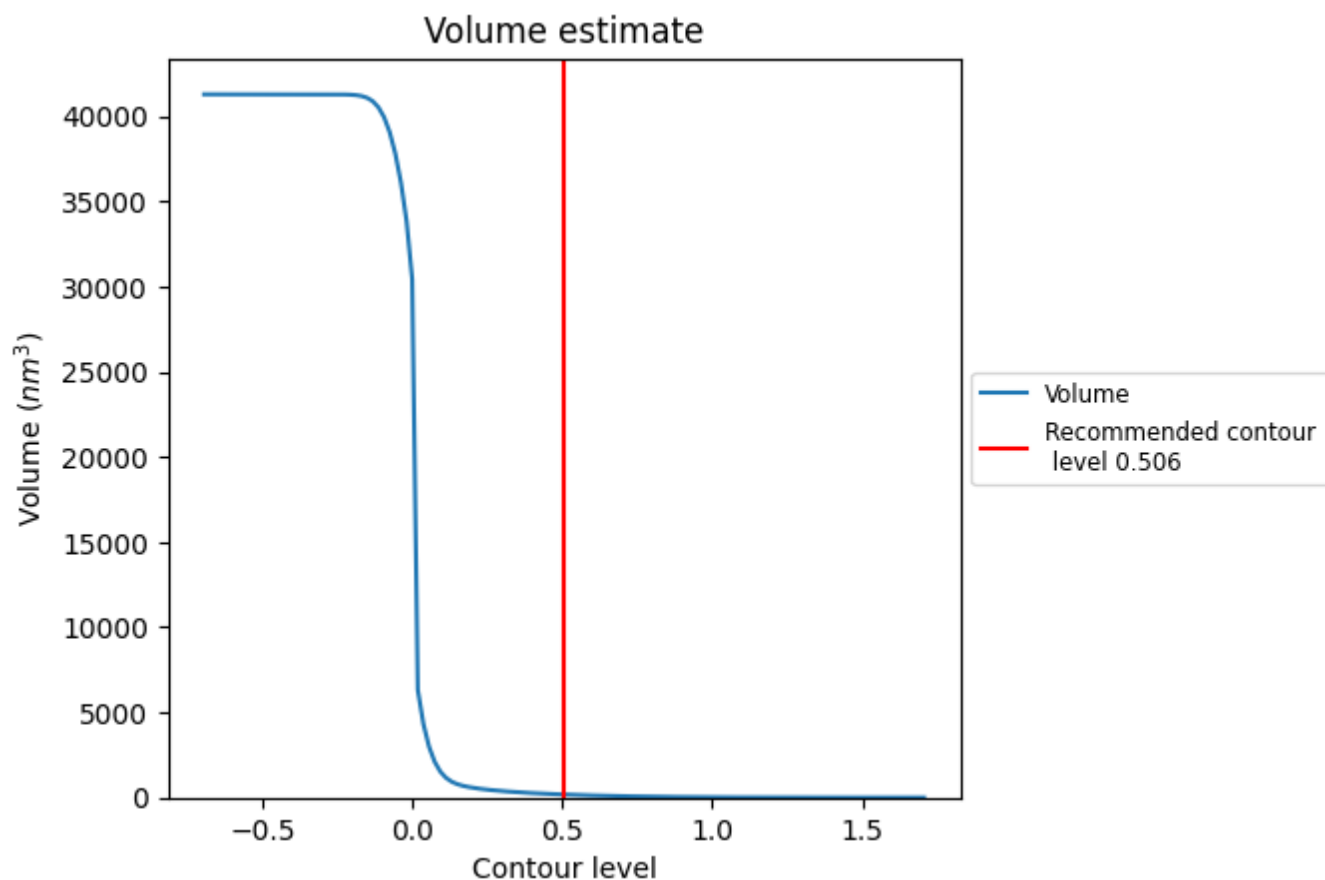
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

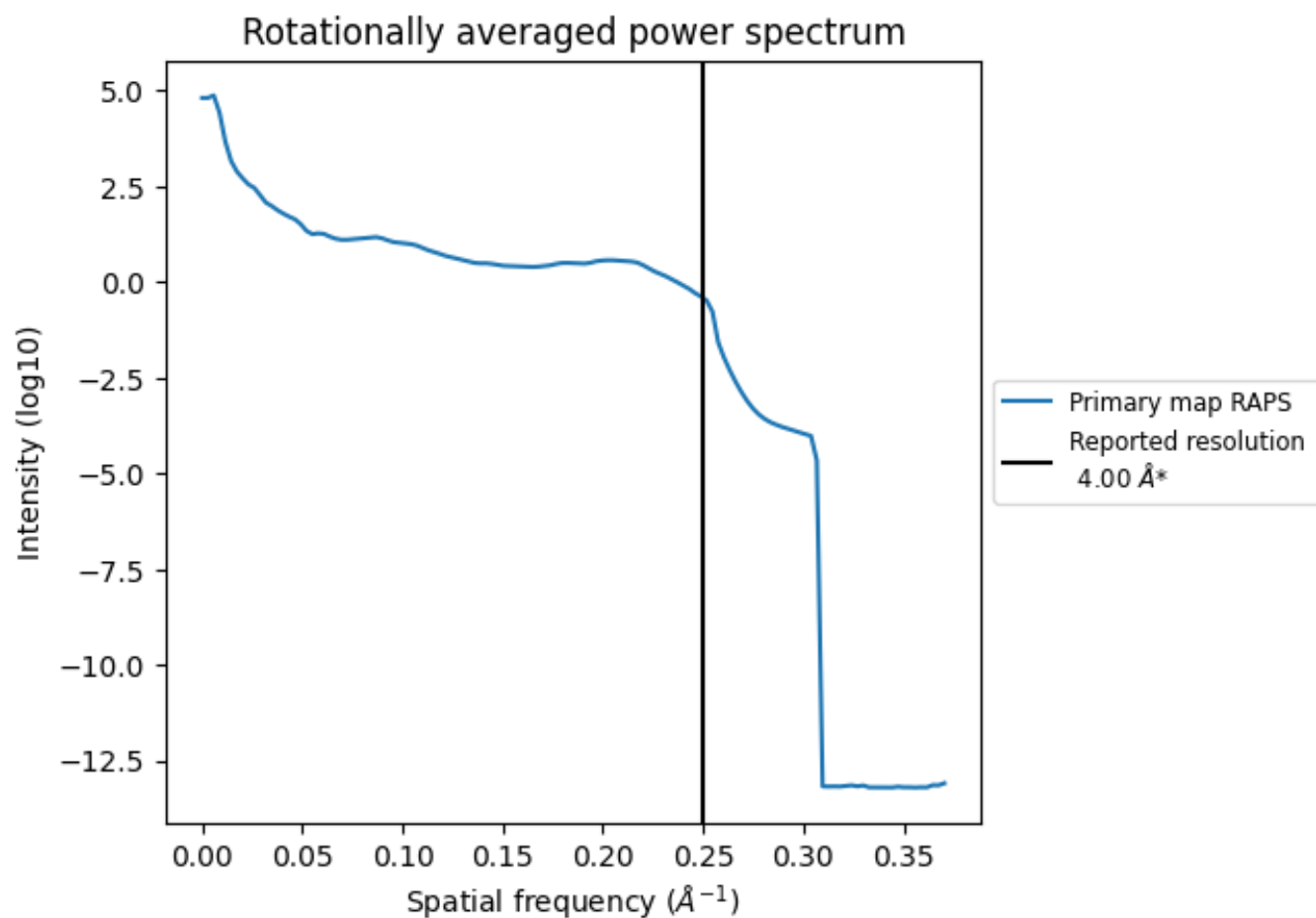
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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 ⓘ

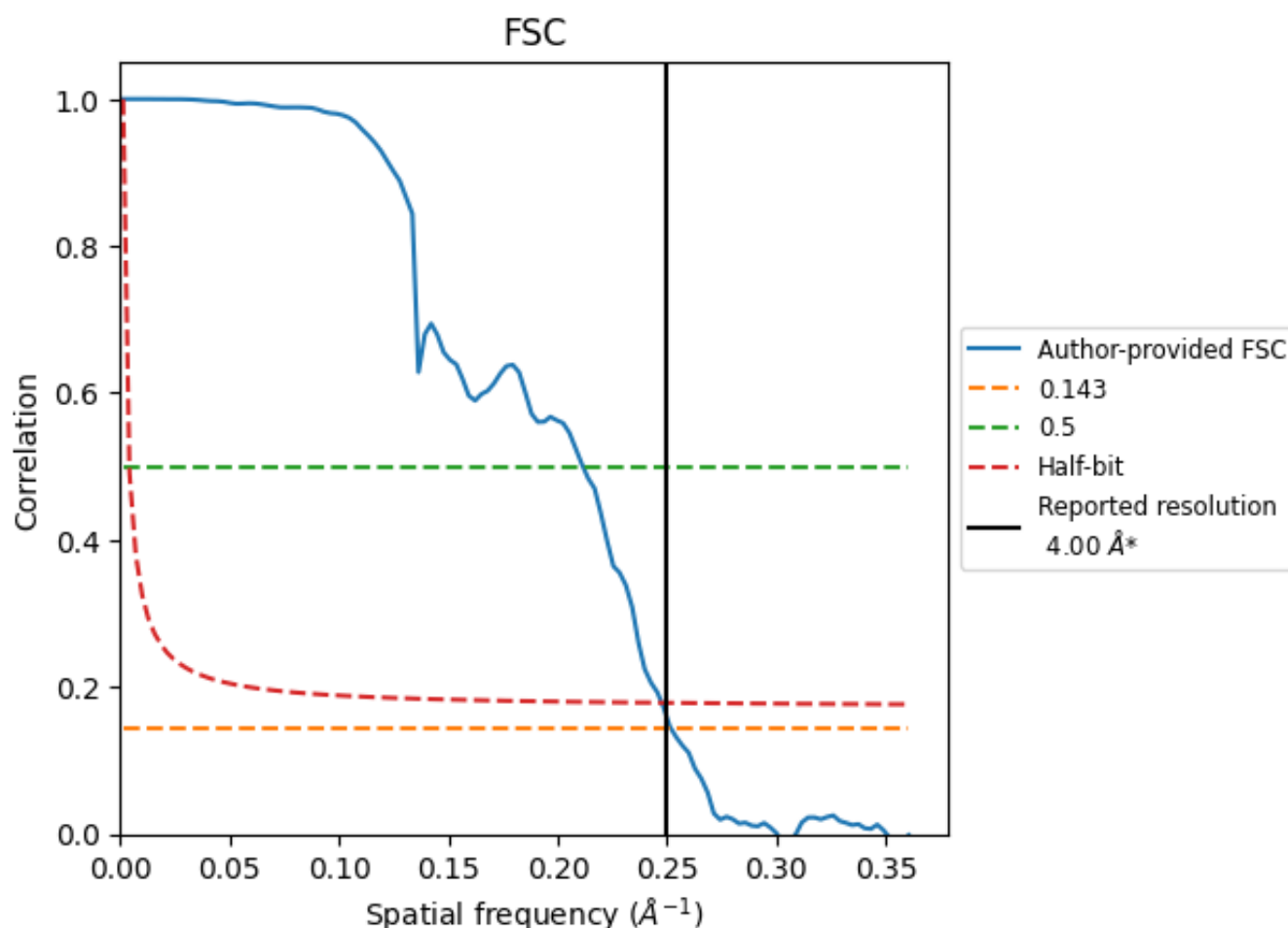


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

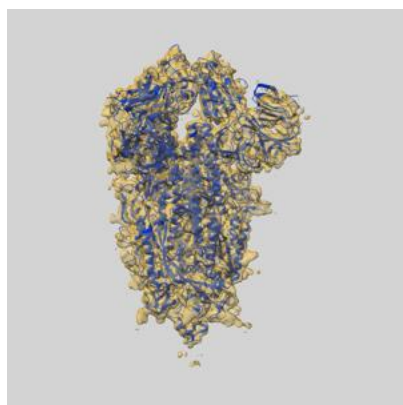
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.97	4.73	4.04
Unmasked-calculated*	-	-	-

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

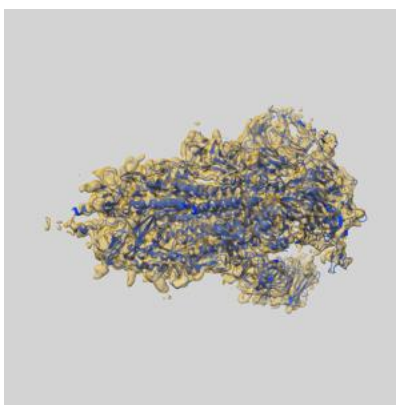
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32492 and PDB model 7WGY. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

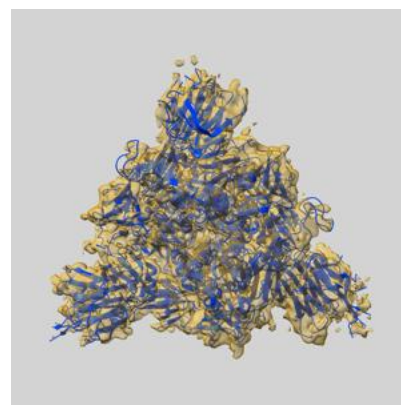
9.1 Map-model overlay [i](#)



X



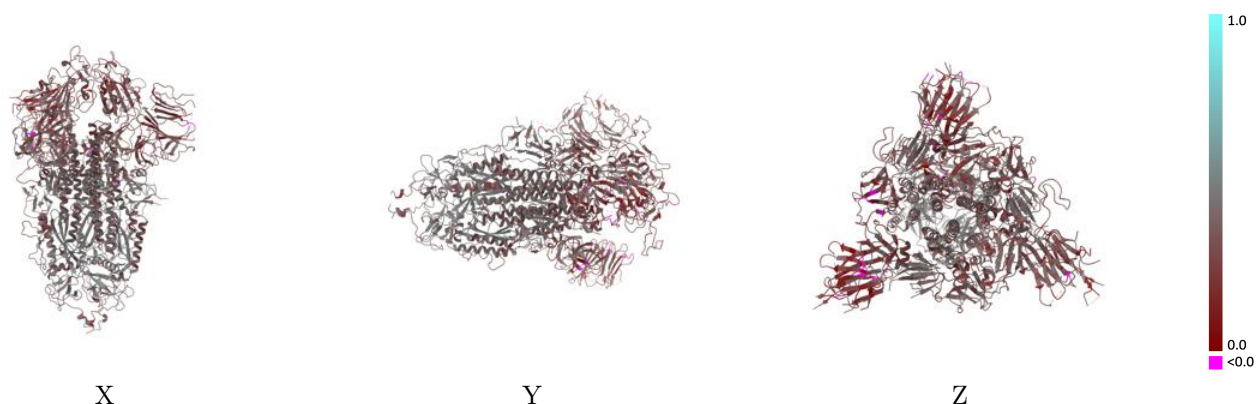
Y



Z

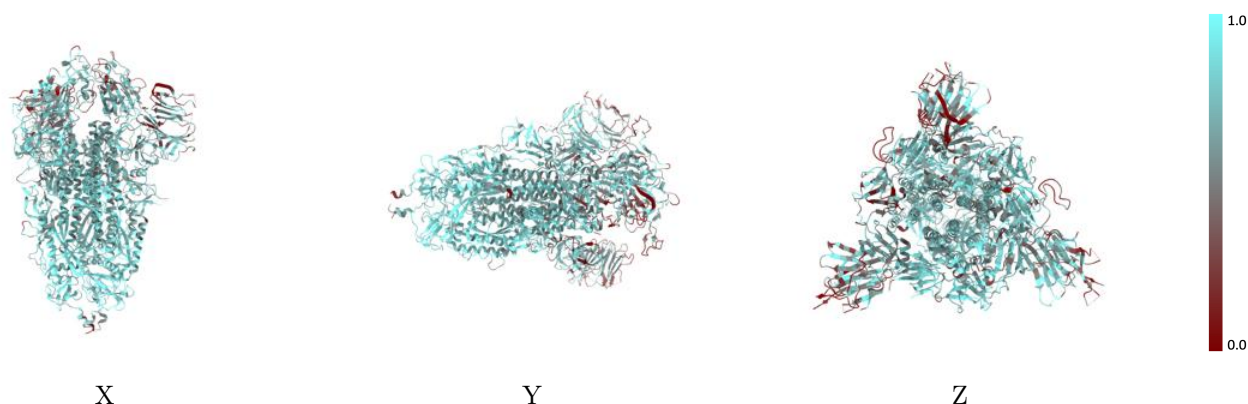
The images above show the 3D surface view of the map at the recommended contour level 0.506 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



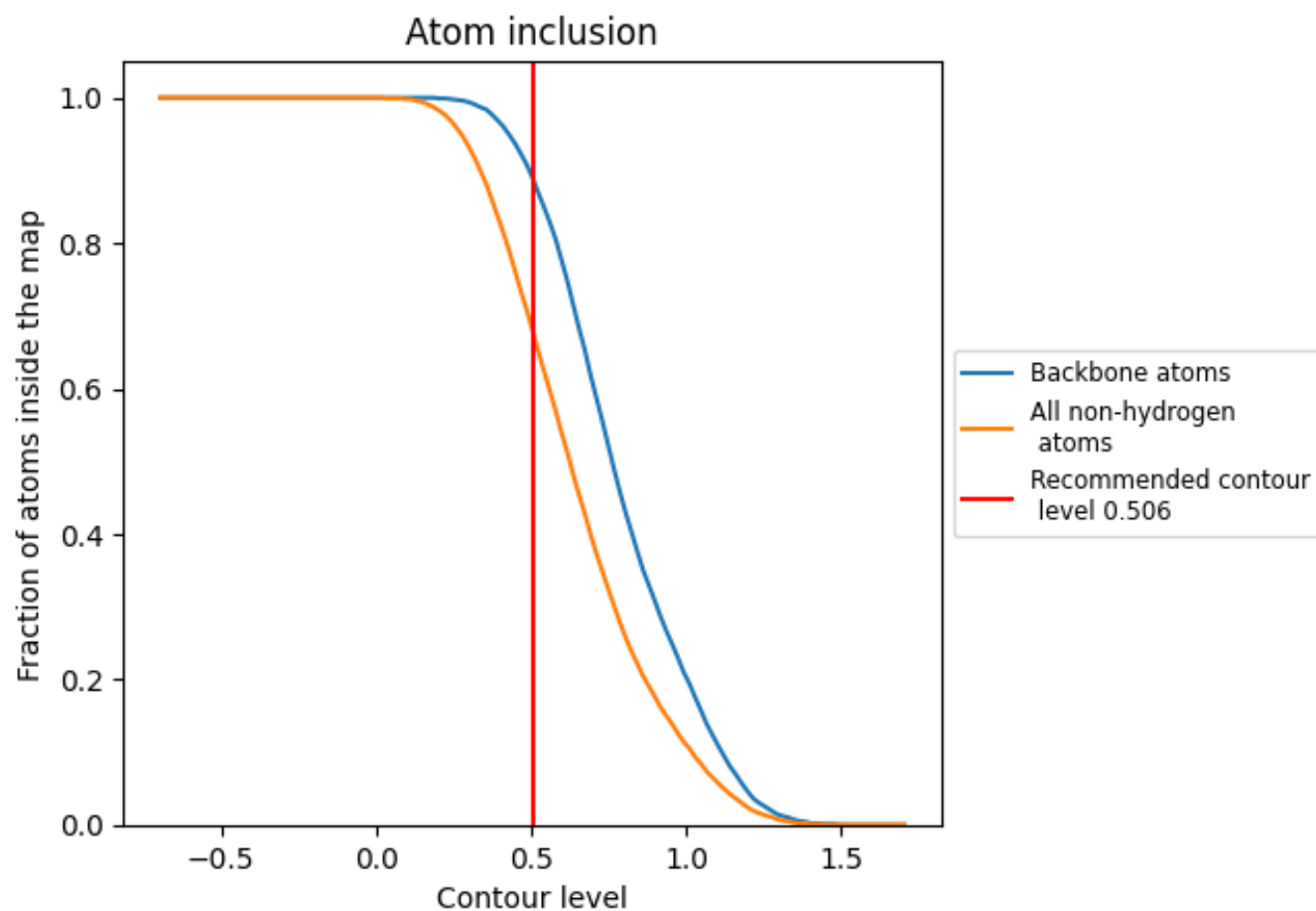
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.506).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 68% 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 (0.506) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6790	<div></div> 0.3540
A	<div></div> 0.6850	<div></div> 0.3580
B	<div></div> 0.6770	<div></div> 0.3570
C	<div></div> 0.6780	<div></div> 0.3480
D	<div></div> 0.6070	<div></div> 0.4030
E	<div></div> 0.5360	<div></div> 0.2760
F	<div></div> 0.5710	<div></div> 0.3250
G	<div></div> 0.2860	<div></div> 0.2600
H	<div></div> 0.5710	<div></div> 0.3370
I	<div></div> 0.5360	<div></div> 0.2650
J	<div></div> 0.6070	<div></div> 0.3470
K	<div></div> 0.6430	<div></div> 0.3380

1.0

0.0

<0.0