



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:59 AM UTC

PDB ID : 7WGY / pdb_00007wgy
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:

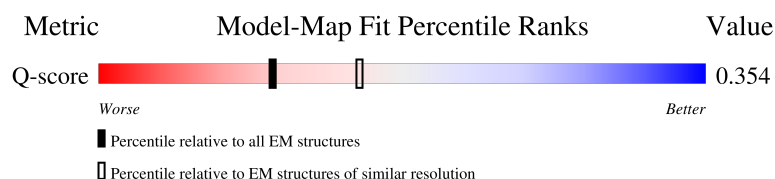
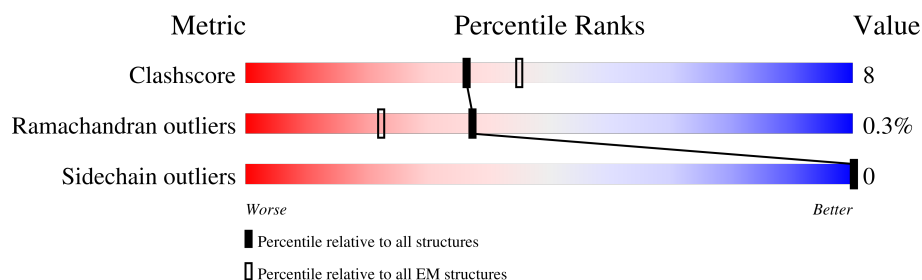
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	9% 70% 15% 14%
1	B	1204	9% 55% 14% 32%
1	C	1204	11% 69% 15% 15%
2	D	2	100%

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Mol	Chain	Length	Quality of chain
2	E	2	50% 50%
2	F	2	50% 100%
2	G	2	50% 50%
2	H	2	50% 100%
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:

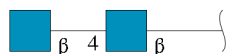
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression 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.



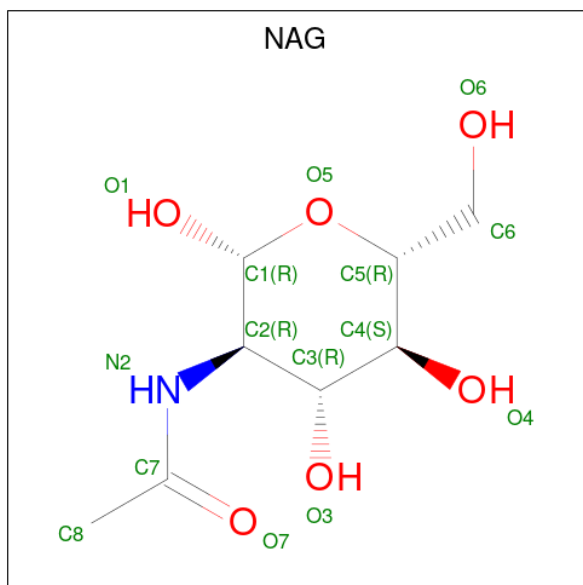
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	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 (CCD ID: 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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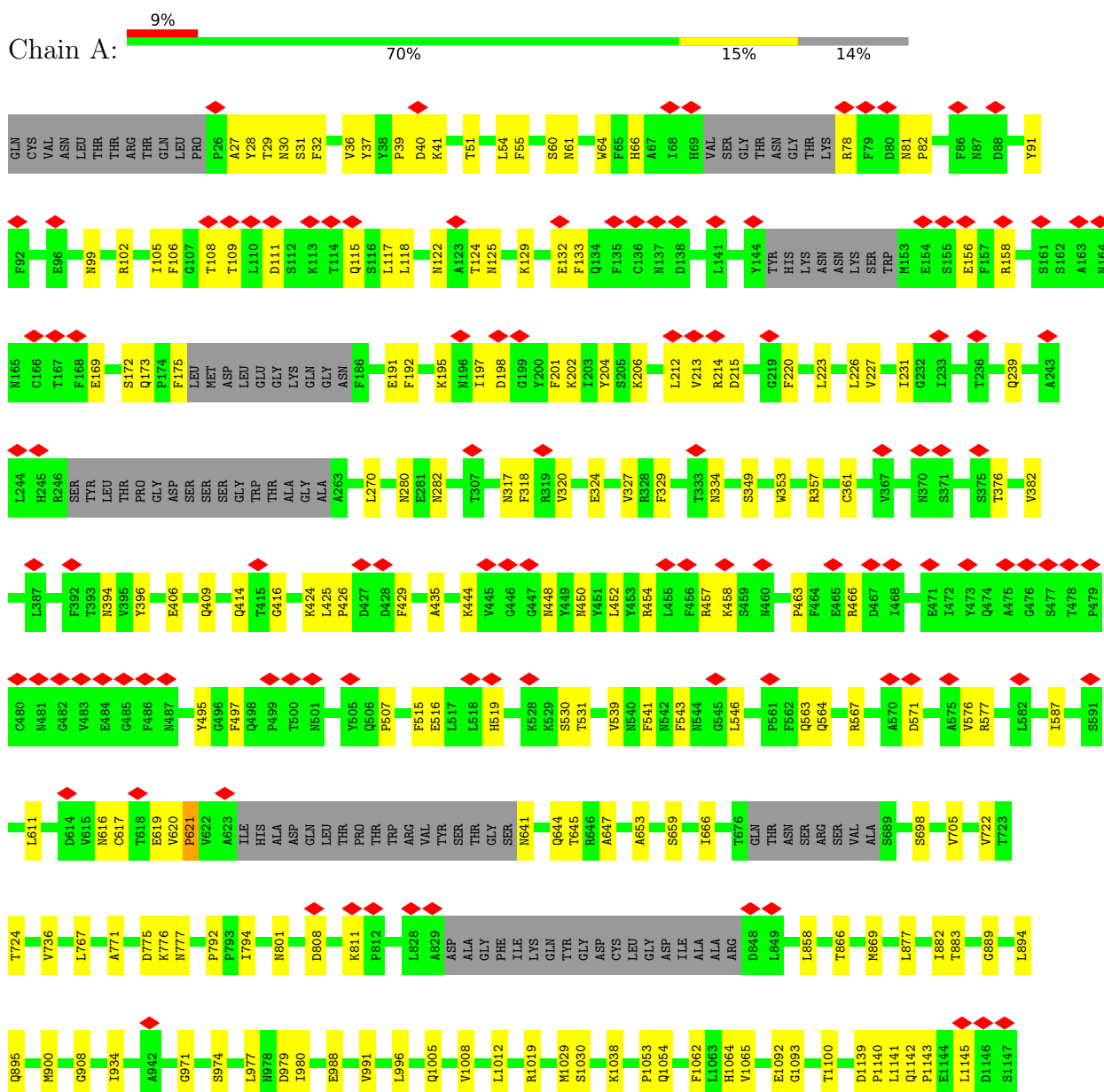
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Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

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



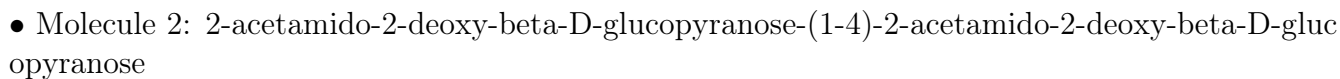
PHE	LYS	GLU	ASN	LEU	ASP	LYS	TYR	PHE	LYS	ASN	LEU	HIS	THR	SER	PRO	ASP	VAL	ASP	LEU	GLY	ASP	ILE	SER	GLY	ILE	ASN	ALA	SER	VAL	VAL	ASN	ILE	GLN	LYS	GLU	ILE	ASP	ARG	LEU	ASN	GLU	VAL	VAL	ALA	LYS	ASN	LEU	ASN	GLU	ASP	GLY	LYS	TYR	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
GLN	TYR	ILE	LYS	GLY	SER	GLY	ARG	GLU	ASN	GLN	LEU	TYR	PHE	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				</

● Molecule 1: Spike glycoprotein



GLN	CYS	VAL	ASN	THR	THR	THR	ARG	THR	GLN	LEU	PRO	P26	A27	S31	R34	G35	Y37	D40	K41	S46	T51	Q52	D53	L54	F55	L56	S60	W64	A67	ILE	HIS	VAL	SER	GLY	THR	ASN	GLY	THR	LYS	ARG	F79	D80	N81	P82	W83	L84	P85	F86	N87	D88						
		F92	A93			E96	K97	S98	N99	I100	R102	I105	F106	G107	T108	T109	L110	D111	S112	K113	T114	Q115	S116	L117	M122	A123	T124	M125	K129	V130	C131	E132	F133	Q134	F135	C136	M137	D138	P139	F140	V143	TYR	TYR	HIS	LYS	ASN	ASN	LYS	SER	TRP	MET	E156	F157	R158		
		S161	S162	A163	N164	N165	C166	T167	F168	E169		Q173	P174	F175	LEU	MET	ASP	LEU	GLU	GLY	LYS	GLN	GLY	ASN	F186	K187	N188	L189	R190	E191	F192	V193	F194	K195	N196	I197	D198	G199	Y200	F201	Y204	S205	T208	P209	T210	N211	L212	V213	R214	D215	L216	P217	F220	L223	E224	P225
		L226	V227			T231	G232	I233	N234	T235	T236	R237	Q238	T239	L240	L241	L242	A243	HIS	ARG	SER	TYR	LEU	THR	PRO	GLN	GLY	ASP	SER	ALA	A264	Y265		Y269	T274	L277	N280	A288	T302	L303	K304	K310	R319	Q321	P322	T323										
E324	S325	I326	R328	F329	PRO	ASN	ILE	THR	ASN	LEU	CYS	PRO	PHE	GLY	GLU	VAL	PHE	ASN	ALA	THR	THR	PHE	ALA	VAL	TYR	TRP	ASN	GLY	LYS	ARG	ILE	ILE	ASN	VAL	VAL	ASP	TYR	VAL	LEU	TYR	ASN	ALA	PHE	THR	THR	LYS	CYS	TYR	GLY	VAL	SER					
PRO	THR	LYS	LEU	ASN	ASP	LEU	CYS	PHE	THR	VAL	TYR	ALA	ASP	SER	PHE	VAL	ILE	ARG	GLY	ASP	GLU	ASP	VAL	ARG	ILE	GLN	SER	THR	ILE	ALA	VAL	TYR	PRO	GLY	GLN	THR	GLY	VAL	ILE	ALA	TRP	ASN	PHE	GLN	SER	ASN	ASN	LEU	ASP	SER						
LYS	VAL	GLY	GLY	TYR	ASN	VAL	VAL	LEU	THR	ARG	PHE	GLU	LEU	ALA	PRO	LYS	THR	PRO	PHE	GLN	ASP	ARG	ILE	SER	THR	GLU	ILE	TYR	GLY	VAL	PRO	CYS	ASN	GLY	GLY	PHE	ASN	CYS	ASP	GLN	SER	THR	THR	THR	THR	THR	THR	VAL								
GLY	TYR	GLN	PRO	ARG	VAL	VAL	VAL	SER	PHE	GLU	LEU	LEU	HIS	PRO	ALA	ALA	ALA	THR	VAL	VAL	CYS	GLY	GLY	PRO	LYS	THR	ILE	GLY	VAL	TYR	N540	L552	T553	E554	K557	L560	P561	F562	Q563	Q564	R567	D568	I569	A570	D571	T572	T573	D574	A575	V576	R577					
T581	L582	E583	I584	L585	D586	S591	F592	T618	E619	V620	P621	V622	A623	ILE	HIS	ALA	ALA	ASP	GLN	GLU	LEU	THR	PRO	THR	THR	TRP	ARG	VAL	TYR	N641	Q644	G648	A653	C662	D663	I664	T676	GLN	THR	ASN	THR	ARG	SER	VAL	ALA	ALA	D571	T572	T573	A575	V576	R577				
M703	S704	I726	M731	M740	S746	C749	Q755	F759	L763	V785	K786	Q787	I794	D808	P809	S810	K811	P812	F817	L821	T827	L828	ALA	ASP	D985	K986	V987	E988	E989	E990	V991	D994	R995	V1008	A1015	M1029	S1030	L1034	K1038																	
T866	M869	Q895	F906	G907	G908	L916	D936	S939	S940	T941	A942	S943	A944	L948	Q949	D950	V951	A958	T961	N969	S975	T980	L981	L984	D985	K986	V987	E988	E989	E990	V991	D994	R995	V1008	A1015	M1029	S1030	L1034	K1038																	
D1041	P1053	Q1054	V1061	P1079	R1091	E1092	G1093	H1101	T1105	I1115	D1118	N1134	Q1142	L1145	D1146	S1147	PHE	LYS	GLU	GLU	LEU	ASP	LYS	THR	PHE	LYS	ASN	HIS	THR	PRO	ASP	VAL	LEU	ASP	GLY	ILE	SER	GLY	ILE	ASN	ALA	SER	SER	VAL	VAL	ASN										

Chain C:



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	0.21	0/8260	0.39	0/11236
1	B	0.21	0/6525	0.39	0/8874
1	C	0.20	0/8189	0.40	0/11141
All	All	0.21	0/22974	0.39	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	120	0
1	B	6393	0	6299	109	0
1	C	8009	0	7848	134	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	350	0

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

All (350) 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:C:417:LYS:HZ1	1:C:455:LEU:HA	1.47	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:A:889:GLY:O	1:C:1045:LYS:NZ	2.21	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:1079:PRO:HA	1:C:900:MET:HE1	1.80	0.63
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:B:620:VAL:C	1:B:622:VAL:H	2.10	0.58
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:A:109:THR:OG1	1:A:111:ASP:OD1	2.21	0.57
1:B:619:GLU:C	1:B:621:PRO:HD2	2.30	0.57
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:900:MET:HE1	1:C:1079:PRO:HA	1.87	0.56
1:C:736:VAL:HG22	1:C:858:LEU:HD13	1.88	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:C:93:ALA:HB3	1:C:266:TYR:HB2	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:794:ILE:C	1:C:795:LYS:HD2	2.36	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:986:LYS:NZ	1:B:990:GLU:OE2	2.41	0.50
1:B:581:THR:OG1	1:B:583:GLU:OE1	2.23	0.50
1:C:62:VAL:HG22	1:C:63:THR:H	1.76	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:A:900:MET:HE1	1:C:1079:PRO:CA	2.42	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:296:LEU:O	1:C:299:THR:OG1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:866:THR:H	1:B:869:MET:HE3	1.78	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: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:B:557:LYS:NZ	1:B:574:ASP:OD2	2.46	0.47
1:B:808:ASP:CG	1:B:810:SER:HG	2.21	0.47
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:B:731:MET:HE3	1:B:1015:ALA:HA	1.97	0.47
1:C:439:ASN:O	1:C:443:SER:OG	2.29	0.47
1:B:34:ARG:HH21	1:B:217:PRO:C	2.23	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:866:THR:H	1:A:869:MET:HE2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:329:PHE:CE2	1:C:525:CYS:HB3	2.51	0.46
1:C:971:GLY:C	1:C:995:ARG:HH21	2.24	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: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
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:B:1029:MET:HE3	1:B:1029:MET:HB3	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:419:ALA:HA	1:C:423:TYR:O	2.17	0.44
1:A:1029:MET:HE2	1:A:1029:MET:HB2	1.93	0.44
1:C:1129:VAL:HG11	1:C:1132:ILE:HD12	1.99	0.44
1:A:979:ASP:OD1	1:A:979:ASP:N	2.47	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:O	1:B:746:SER:OG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:353:TRP:CD1	1:C:353:TRP:H	2.36	0.42
1:C:620:VAL:O	1:C:621:PRO:C	2.62	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
1:B:96:GLU:CD	1:B:100:ILE:H	2.28	0.42
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:B:620:VAL:C	1:B:622:VAL:N	2.74	0.42
1:C:748:GLU:CD	1:C:748:GLU:H	2.28	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: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:902:MET:HE1	1:C:1050:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:409:GLN:CD	1:A:416:GLY:HA3	2.46	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:914:ASN:O	1:C:915:VAL:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	70
1	B	803/1204 (67%)	754 (94%)	46 (6%)	3 (0%)	30	65
1	C	1009/1204 (84%)	952 (94%)	54 (5%)	3 (0%)	36	70
All	All	2829/3612 (78%)	2664 (94%)	156 (6%)	9 (0%)	37	70

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 [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	211/1049 (20%)	211 (100%)	0	100	100
1	B	53/1049 (5%)	53 (100%)	0	100	100
1	C	896/1049 (85%)	896 (100%)	0	100	100
All	All	1160/3147 (37%)	1160 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	C	439	ASN
1	C	481	ASN
1	C	764	ASN
1	C	901	GLN
1	C	913	GLN
1	C	949	GLN
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	2,1	14,14,15	1.95	4 (28%)	17,19,21	1.24	2 (11%)
2	NAG	D	2	2	14,14,15	2.03	3 (21%)	17,19,21	0.99	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	4 (28%)	17,19,21	1.12	2 (11%)
2	NAG	F	1	2,1	14,14,15	2.02	5 (35%)	17,19,21	1.62	4 (23%)
2	NAG	F	2	2	14,14,15	2.04	3 (21%)	17,19,21	1.17	2 (11%)
2	NAG	G	1	2	14,14,15	2.01	4 (28%)	17,19,21	1.12	2 (11%)
2	NAG	G	2	2	14,14,15	2.02	3 (21%)	17,19,21	1.15	2 (11%)
2	NAG	H	1	2,1	14,14,15	1.98	4 (28%)	17,19,21	1.24	3 (17%)
2	NAG	H	2	2	14,14,15	2.08	3 (21%)	17,19,21	1.37	3 (17%)
2	NAG	I	1	2,1	14,14,15	2.01	3 (21%)	17,19,21	1.61	3 (17%)
2	NAG	I	2	2	14,14,15	2.13	4 (28%)	17,19,21	1.14	2 (11%)
2	NAG	J	1	2,1	14,14,15	1.95	3 (21%)	17,19,21	1.04	2 (11%)
2	NAG	J	2	2	14,14,15	1.99	3 (21%)	17,19,21	1.08	2 (11%)
2	NAG	K	1	2,1	14,14,15	2.04	5 (35%)	17,19,21	2.16	5 (29%)
2	NAG	K	2	2	14,14,15	2.00	3 (21%)	17,19,21	1.17	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	2,1	-	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	2,1	-	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	2,1	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	2,1	-	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	2,1	-	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	O5-C1	5.34	1.52	1.43
2	H	2	NAG	O5-C1	5.19	1.52	1.43
2	F	2	NAG	O5-C1	5.15	1.52	1.43
2	G	2	NAG	O5-C1	5.07	1.52	1.43
2	K	2	NAG	O5-C1	5.04	1.52	1.43
2	K	1	NAG	O5-C1	5.03	1.52	1.43
2	F	1	NAG	O5-C1	5.01	1.52	1.43
2	J	2	NAG	O5-C1	5.01	1.52	1.43
2	I	1	NAG	O5-C1	5.00	1.52	1.43
2	G	1	NAG	O5-C1	4.98	1.52	1.43
2	E	2	NAG	O5-C1	4.95	1.52	1.43
2	J	1	NAG	O5-C1	4.93	1.52	1.43
2	D	2	NAG	O5-C1	4.93	1.52	1.43
2	H	1	NAG	O5-C1	4.92	1.52	1.43
2	E	1	NAG	O5-C1	4.70	1.51	1.43
2	D	1	NAG	O5-C1	4.62	1.51	1.43
2	I	2	NAG	C7-N2	3.48	1.45	1.34
2	D	2	NAG	C7-N2	3.48	1.45	1.34
2	H	2	NAG	C7-N2	3.47	1.45	1.34
2	I	1	NAG	C7-N2	3.45	1.45	1.34
2	E	2	NAG	C7-N2	3.41	1.45	1.34
2	F	2	NAG	C7-N2	3.37	1.45	1.34
2	J	2	NAG	C7-N2	3.36	1.45	1.34
2	G	1	NAG	C7-N2	3.35	1.45	1.34
2	G	2	NAG	C7-N2	3.35	1.45	1.34
2	D	1	NAG	C7-N2	3.34	1.45	1.34
2	K	1	NAG	C7-N2	3.33	1.45	1.34
2	H	1	NAG	C7-N2	3.32	1.45	1.34
2	E	1	NAG	C7-N2	3.30	1.45	1.34
2	K	2	NAG	C7-N2	3.27	1.44	1.34
2	F	1	NAG	C7-N2	3.26	1.44	1.34
2	J	1	NAG	C7-N2	3.17	1.44	1.34
2	I	2	NAG	C2-N2	3.10	1.51	1.46
2	D	2	NAG	C2-N2	3.06	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	NAG	C2-N2	3.05	1.51	1.46
2	E	2	NAG	C2-N2	2.98	1.51	1.46
2	F	2	NAG	C2-N2	2.97	1.51	1.46
2	J	2	NAG	C2-N2	2.92	1.51	1.46
2	G	1	NAG	C2-N2	2.91	1.51	1.46
2	G	2	NAG	C2-N2	2.91	1.51	1.46
2	I	1	NAG	C2-N2	2.86	1.51	1.46
2	E	1	NAG	C2-N2	2.80	1.50	1.46
2	D	1	NAG	C2-N2	2.70	1.50	1.46
2	K	2	NAG	C2-N2	2.68	1.50	1.46
2	F	1	NAG	C2-N2	2.67	1.50	1.46
2	K	1	NAG	C2-N2	2.67	1.50	1.46
2	J	1	NAG	C2-N2	2.55	1.50	1.46
2	H	1	NAG	C2-N2	2.55	1.50	1.46
2	I	2	NAG	O5-C5	2.35	1.48	1.43
2	H	1	NAG	C3-C2	-2.16	1.48	1.52
2	K	1	NAG	C3-C2	-2.15	1.48	1.52
2	K	1	NAG	O5-C5	2.11	1.47	1.43
2	D	1	NAG	C3-C2	-2.11	1.48	1.52
2	E	2	NAG	O5-C5	2.08	1.47	1.43
2	F	1	NAG	O5-C5	2.08	1.47	1.43
2	F	1	NAG	C3-C2	-2.07	1.48	1.52
2	G	1	NAG	O5-C5	2.04	1.47	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	C2-N2-C7	-4.97	116.24	122.90
2	K	1	NAG	C1-O5-C5	4.69	118.48	112.19
2	I	1	NAG	C1-O5-C5	4.06	117.62	112.19
2	F	1	NAG	C1-O5-C5	3.80	117.28	112.19
2	K	1	NAG	C6-C5-C4	-2.98	105.70	113.02
2	D	1	NAG	C2-N2-C7	-2.98	118.90	122.90
2	F	1	NAG	C2-N2-C7	-2.89	119.03	122.90
2	H	2	NAG	C1-O5-C5	2.75	115.87	112.19
2	K	2	NAG	C2-N2-C7	-2.74	119.23	122.90
2	E	1	NAG	C4-C3-C2	2.73	115.01	111.02
2	G	1	NAG	C2-N2-C7	-2.65	119.35	122.90
2	E	1	NAG	C3-C4-C5	2.65	115.03	110.23
2	F	2	NAG	C2-N2-C7	-2.55	119.49	122.90
2	G	2	NAG	C2-N2-C7	-2.54	119.50	122.90
2	K	1	NAG	C8-C7-N2	2.54	120.32	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	NAG	C8-C7-N2	2.53	120.32	116.12
2	H	2	NAG	C2-N2-C7	-2.53	119.51	122.90
2	D	1	NAG	C8-C7-N2	2.49	120.24	116.12
2	F	2	NAG	C8-C7-N2	2.45	120.19	116.12
2	F	1	NAG	C8-C7-N2	2.41	120.12	116.12
2	G	2	NAG	C8-C7-N2	2.40	120.10	116.12
2	G	1	NAG	C8-C7-N2	2.39	120.09	116.12
2	D	2	NAG	C8-C7-N2	2.38	120.07	116.12
2	I	1	NAG	C8-C7-N2	2.36	120.04	116.12
2	E	2	NAG	C8-C7-N2	2.36	120.03	116.12
2	J	2	NAG	C8-C7-N2	2.36	120.03	116.12
2	K	2	NAG	C8-C7-N2	2.33	119.98	116.12
2	J	1	NAG	C8-C7-N2	2.30	119.94	116.12
2	E	1	NAG	C8-C7-N2	2.25	119.84	116.12
2	J	1	NAG	C2-N2-C7	-2.22	119.93	122.90
2	I	2	NAG	C1-O5-C5	2.21	115.14	112.19
2	E	2	NAG	C2-N2-C7	-2.19	119.96	122.90
2	E	1	NAG	C6-C5-C4	-2.19	107.64	113.02
2	E	1	NAG	C2-N2-C7	-2.18	119.98	122.90
2	I	2	NAG	C8-C7-N2	2.18	119.73	116.12
2	I	1	NAG	C6-C5-C4	-2.17	107.68	113.02
2	H	1	NAG	C2-N2-C7	-2.11	120.08	122.90
2	H	1	NAG	C8-C7-N2	2.11	119.61	116.12
2	K	1	NAG	O5-C5-C4	2.06	115.84	110.83
2	F	1	NAG	C6-C5-C4	-2.06	107.97	113.02
2	J	2	NAG	C2-N2-C7	-2.02	120.19	122.90
2	H	1	NAG	C6-C5-C4	-2.01	108.08	113.02

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	J	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6

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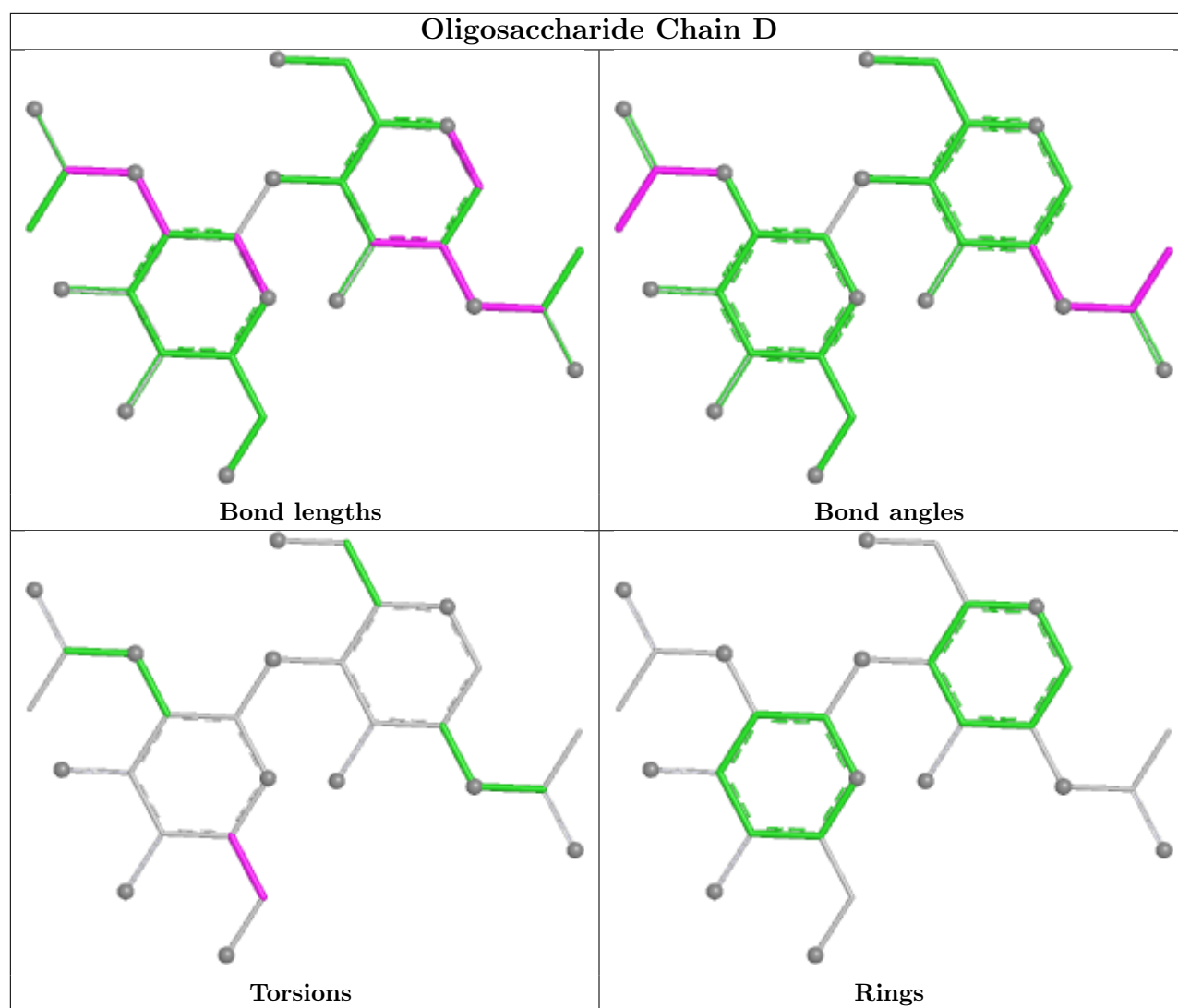
Mol	Chain	Res	Type	Atoms
2	K	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C1-C2-N2-C7
2	H	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

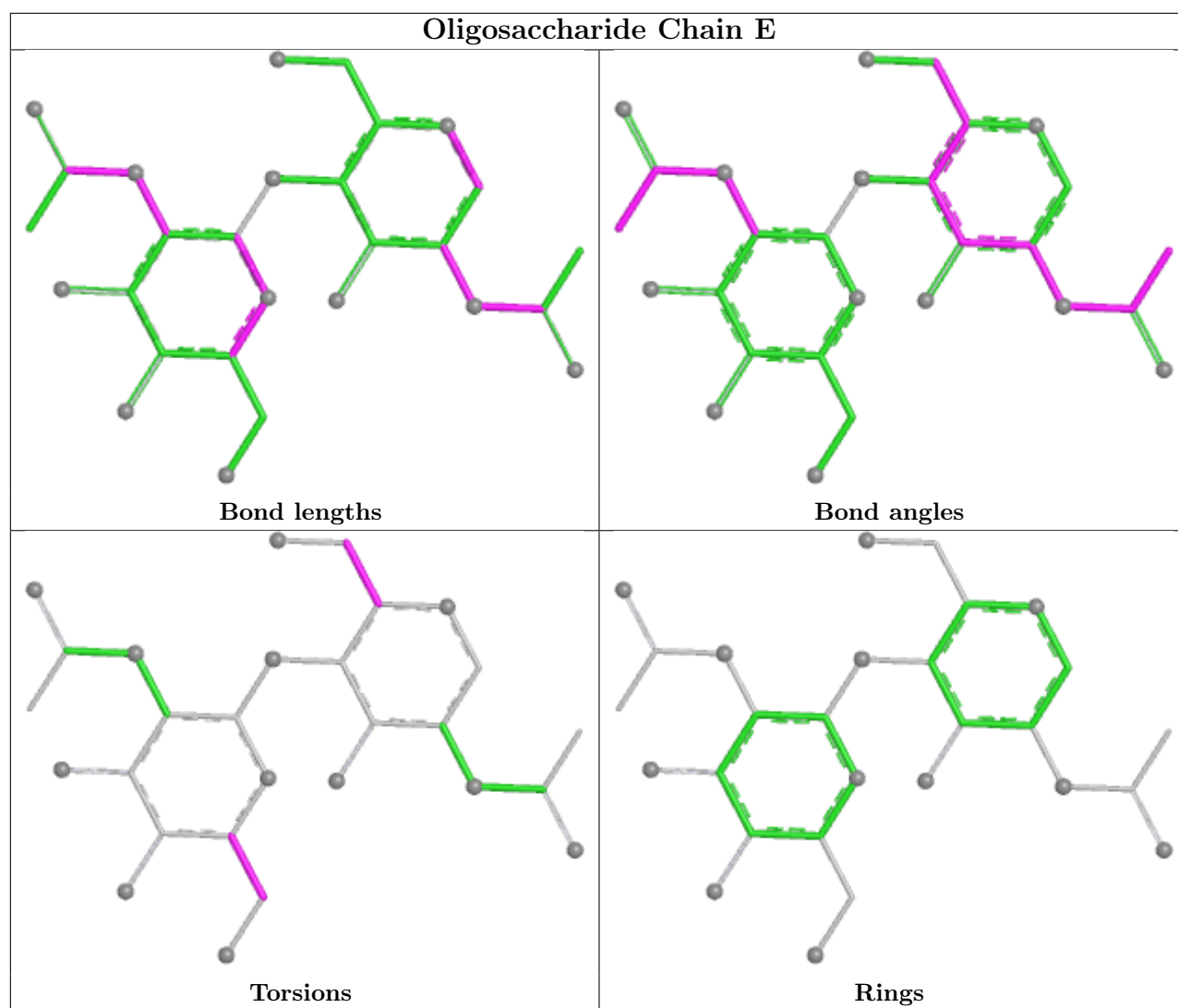
There are no ring outliers.

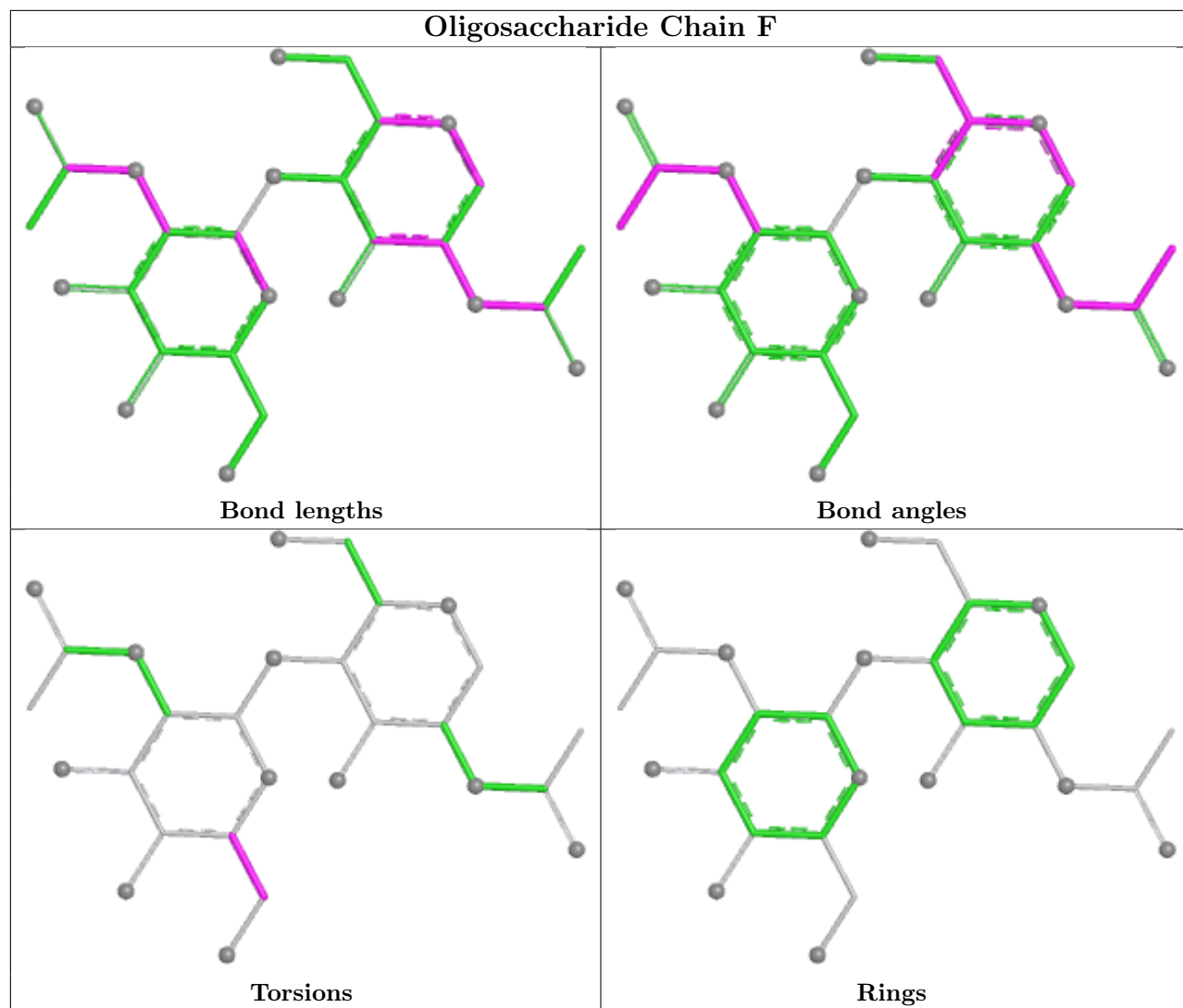
8 monomers are involved in 6 short contacts:

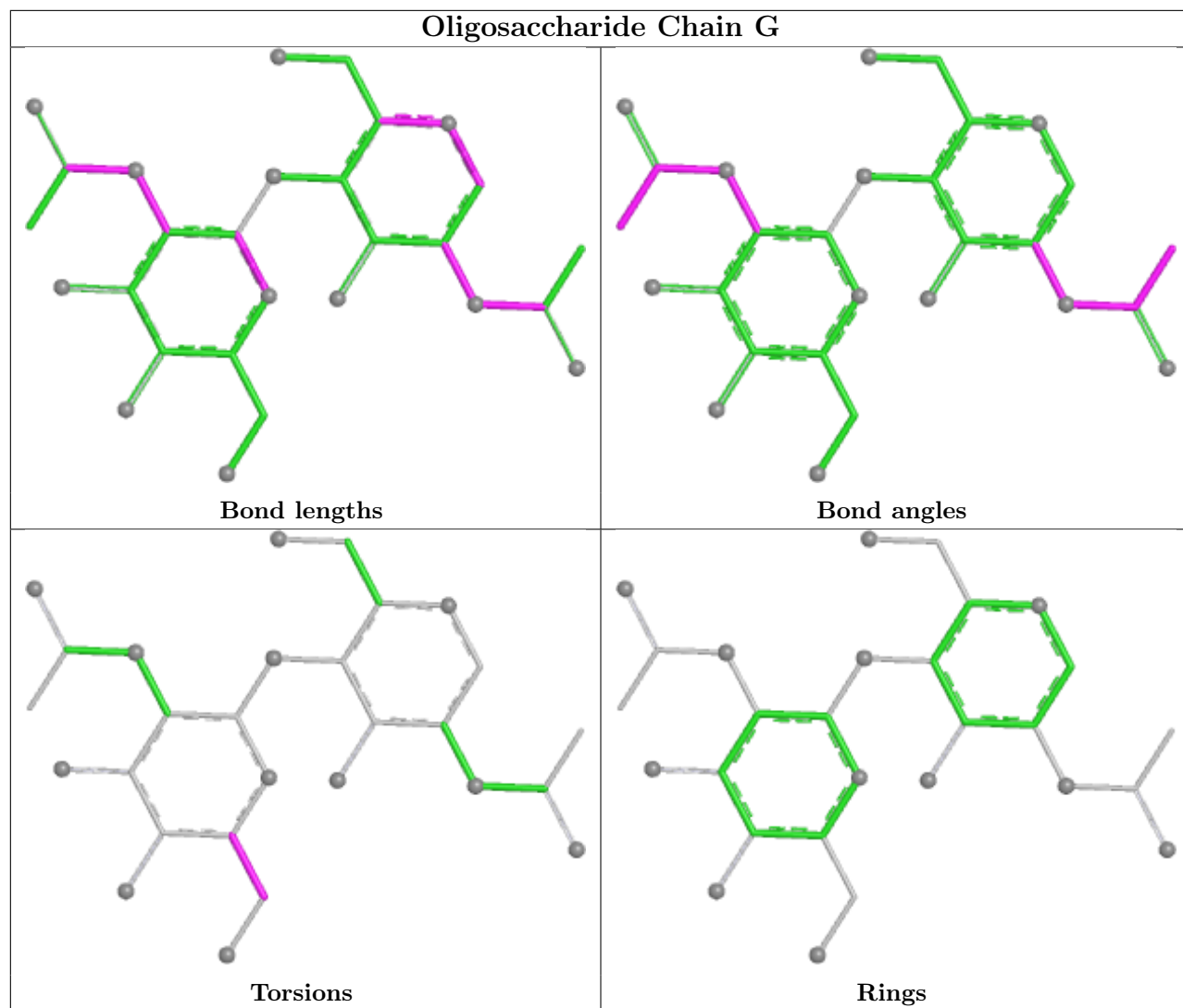
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	H	2	NAG	1	0
2	I	1	NAG	1	0
2	D	2	NAG	1	0
2	E	1	NAG	2	0
2	I	2	NAG	1	0
2	D	1	NAG	1	0
2	G	1	NAG	1	0

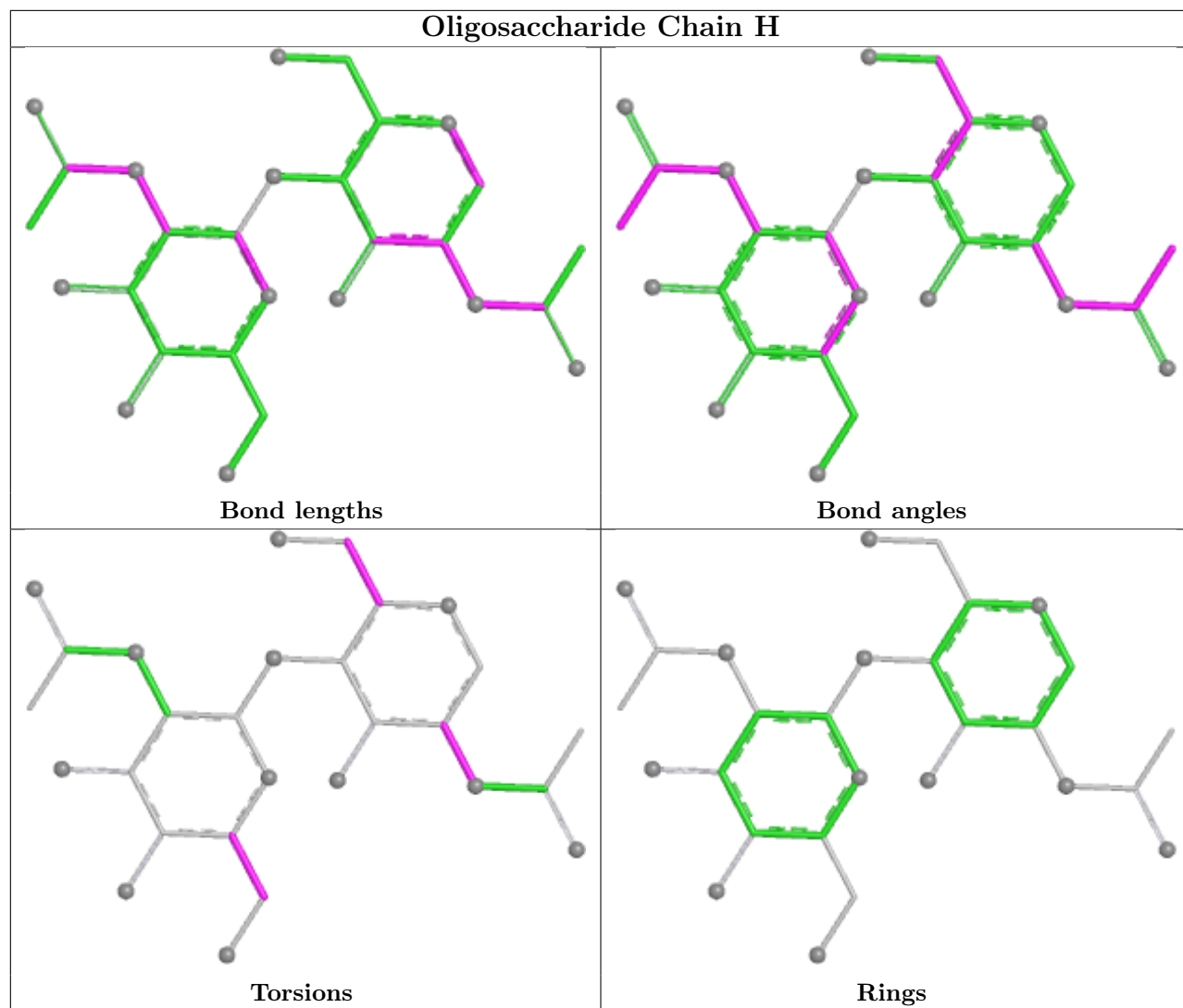
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

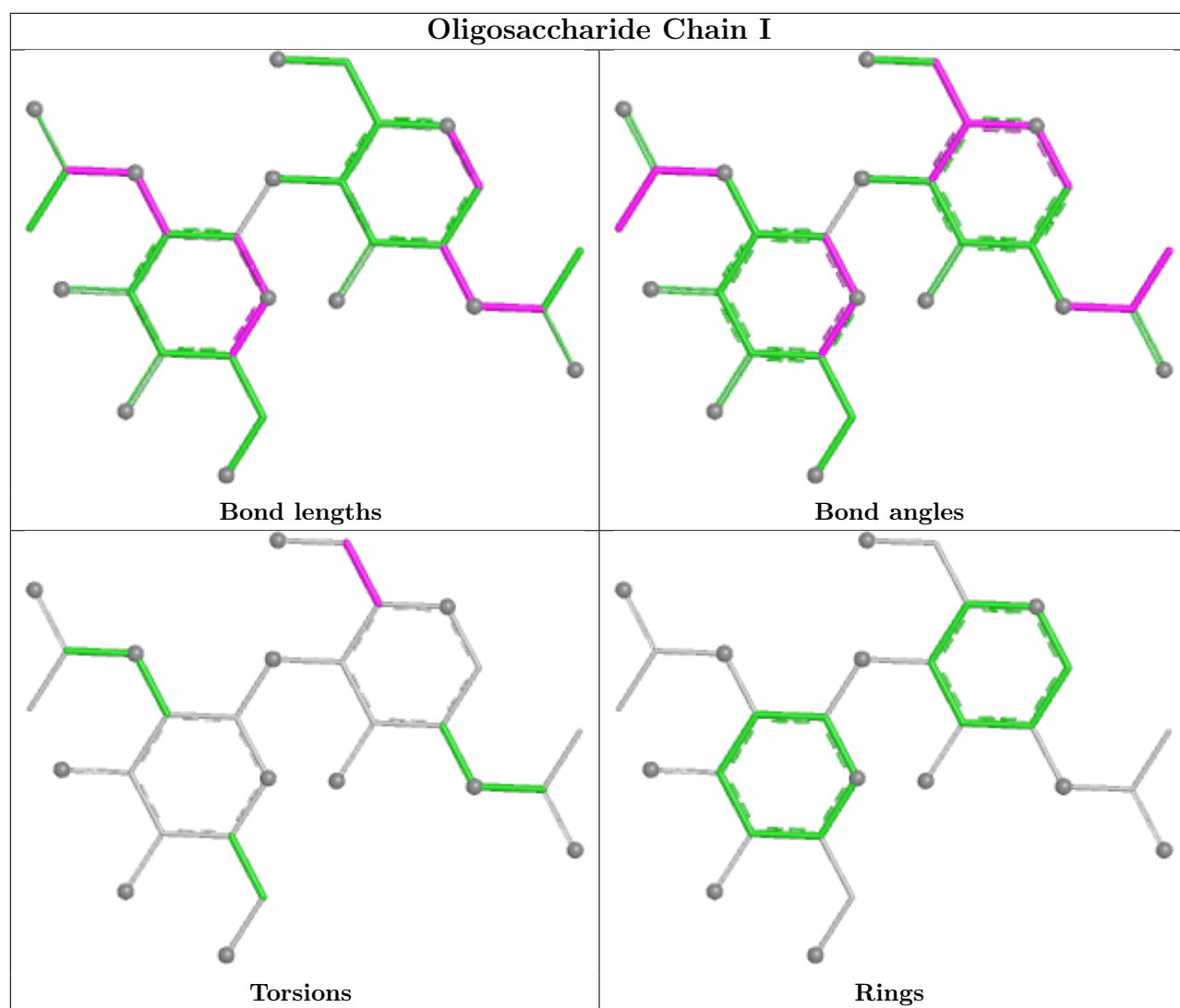


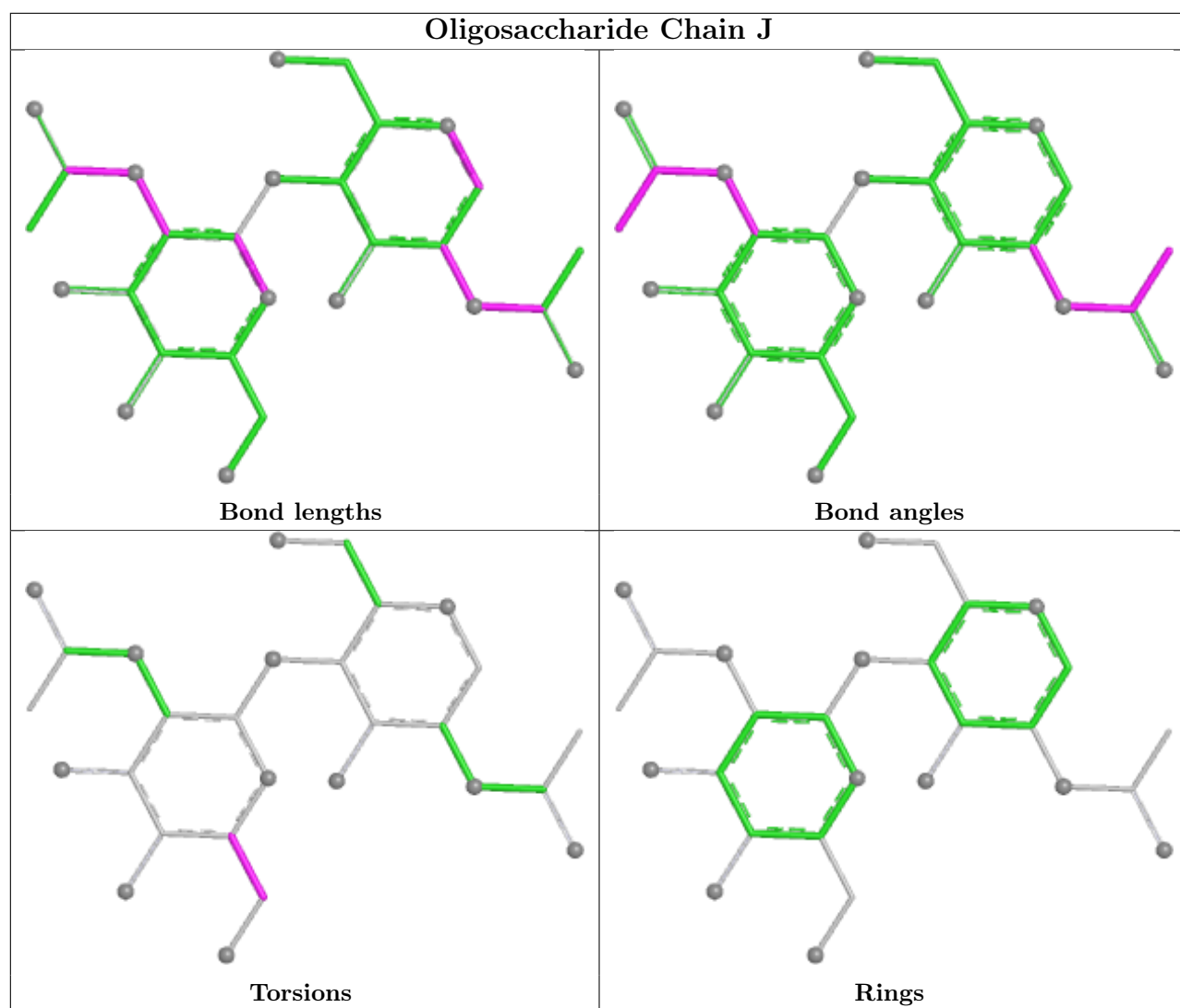


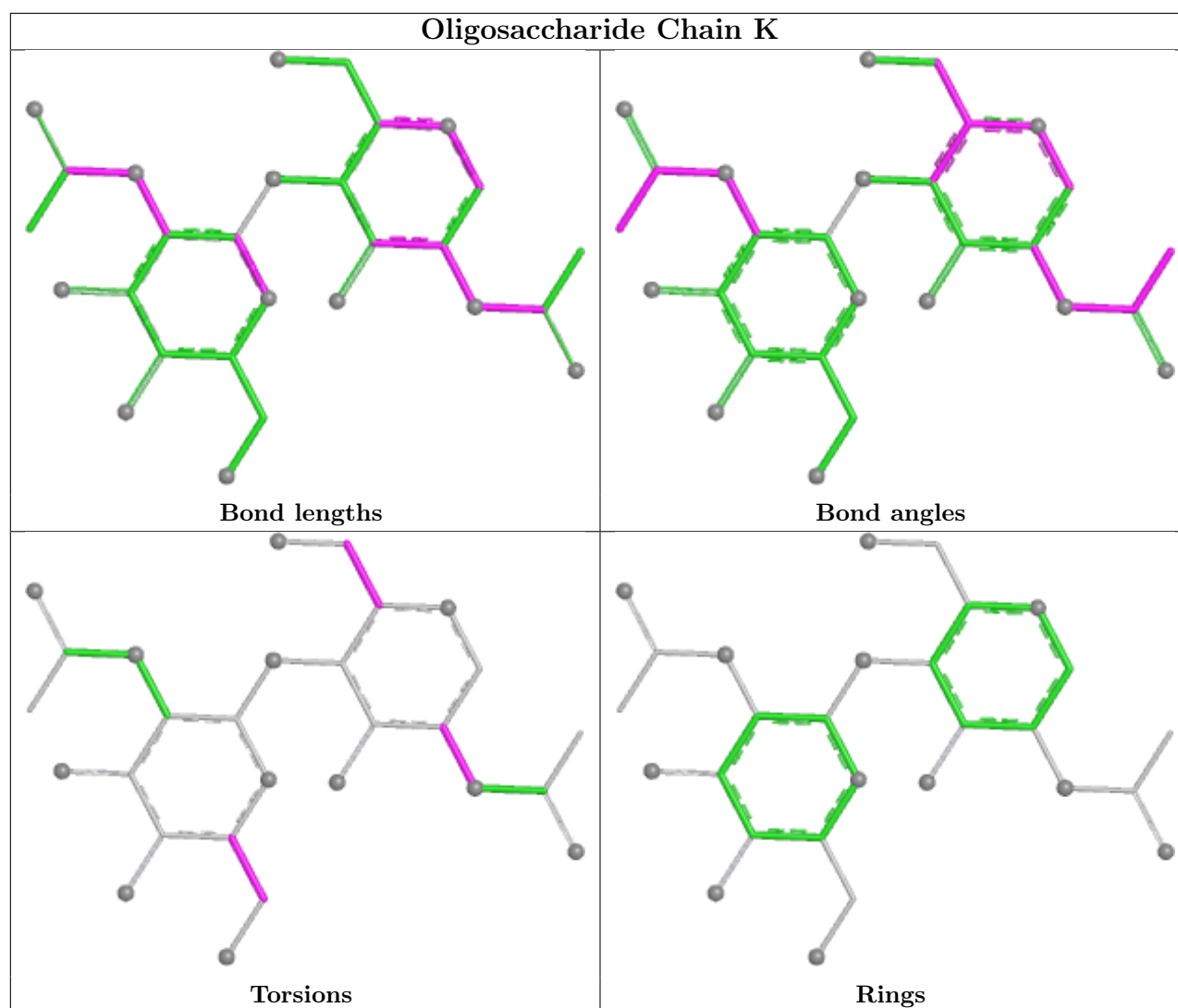












5.6 Ligand geometry [i](#)

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	2.01	5 (35%)	17,19,21	1.32	2 (11%)
3	NAG	B	1305	-	14,14,15	2.00	4 (28%)	17,19,21	1.23	2 (11%)
3	NAG	A	1302	1	14,14,15	2.05	3 (21%)	17,19,21	1.32	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1301	1	14,14,15	1.96	3 (21%)	17,19,21	1.26	3 (17%)
3	NAG	C	1302	1	14,14,15	2.02	3 (21%)	17,19,21	1.18	1 (5%)
3	NAG	C	1303	-	14,14,15	2.03	4 (28%)	17,19,21	1.19	2 (11%)
3	NAG	C	1305	1	14,14,15	2.02	3 (21%)	17,19,21	1.13	1 (5%)
3	NAG	B	1304	1	14,14,15	2.02	3 (21%)	17,19,21	1.21	3 (17%)
3	NAG	A	1301	1	14,14,15	1.92	3 (21%)	17,19,21	1.50	3 (17%)
3	NAG	A	1304	1	14,14,15	2.06	3 (21%)	17,19,21	1.45	3 (17%)
3	NAG	A	1305	1	14,14,15	2.09	4 (28%)	17,19,21	1.46	3 (17%)
3	NAG	A	1303	-	14,14,15	2.01	4 (28%)	17,19,21	1.23	3 (17%)
3	NAG	C	1304	-	14,14,15	1.99	3 (21%)	17,19,21	1.22	2 (11%)
3	NAG	B	1302	-	14,14,15	1.94	3 (21%)	17,19,21	1.15	2 (11%)
3	NAG	C	1301	1	14,14,15	1.98	3 (21%)	17,19,21	1.24	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
3	NAG	B	1303	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	-	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1305	NAG	O5-C1	5.30	1.52	1.43
3	A	1302	NAG	O5-C1	5.27	1.52	1.43
3	C	1302	NAG	O5-C1	5.17	1.52	1.43
3	A	1304	NAG	O5-C1	5.17	1.52	1.43
3	B	1304	NAG	O5-C1	5.09	1.52	1.43
3	C	1305	NAG	O5-C1	5.07	1.52	1.43
3	C	1303	NAG	O5-C1	5.01	1.52	1.43
3	C	1301	NAG	O5-C1	4.98	1.52	1.43
3	B	1302	NAG	O5-C1	4.93	1.52	1.43
3	B	1305	NAG	O5-C1	4.87	1.51	1.43
3	B	1301	NAG	O5-C1	4.85	1.51	1.43
3	C	1304	NAG	O5-C1	4.85	1.51	1.43
3	A	1303	NAG	O5-C1	4.81	1.51	1.43
3	A	1301	NAG	O5-C1	4.77	1.51	1.43
3	B	1303	NAG	O5-C1	4.74	1.51	1.43
3	A	1304	NAG	C7-N2	3.64	1.46	1.34
3	B	1303	NAG	C7-N2	3.42	1.45	1.34
3	C	1302	NAG	C7-N2	3.40	1.45	1.34
3	A	1305	NAG	C7-N2	3.40	1.45	1.34
3	C	1305	NAG	C7-N2	3.39	1.45	1.34
3	C	1303	NAG	C7-N2	3.38	1.45	1.34
3	A	1302	NAG	C7-N2	3.36	1.45	1.34
3	A	1303	NAG	C7-N2	3.36	1.45	1.34
3	B	1305	NAG	C7-N2	3.33	1.45	1.34
3	C	1304	NAG	C7-N2	3.32	1.45	1.34
3	B	1304	NAG	C7-N2	3.32	1.45	1.34
3	B	1301	NAG	C7-N2	3.31	1.45	1.34
3	A	1304	NAG	C2-N2	3.31	1.51	1.46
3	C	1301	NAG	C7-N2	3.28	1.44	1.34
3	B	1302	NAG	C7-N2	3.25	1.44	1.34
3	A	1301	NAG	C7-N2	3.11	1.44	1.34
3	A	1305	NAG	C2-N2	3.04	1.51	1.46
3	C	1305	NAG	C2-N2	2.96	1.51	1.46
3	C	1302	NAG	C2-N2	2.94	1.51	1.46
3	C	1303	NAG	C2-N2	2.91	1.51	1.46
3	B	1305	NAG	C2-N2	2.88	1.51	1.46
3	B	1304	NAG	C2-N2	2.86	1.51	1.46
3	A	1303	NAG	C2-N2	2.83	1.50	1.46
3	B	1303	NAG	C2-N2	2.82	1.50	1.46
3	A	1302	NAG	C2-N2	2.81	1.50	1.46
3	C	1304	NAG	C2-N2	2.80	1.50	1.46
3	C	1301	NAG	C2-N2	2.73	1.50	1.46
3	B	1301	NAG	C2-N2	2.71	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	NAG	C2-N2	2.64	1.50	1.46
3	A	1301	NAG	C2-N2	2.43	1.50	1.46
3	A	1303	NAG	O5-C5	2.14	1.47	1.43
3	B	1303	NAG	O5-C5	2.09	1.47	1.43
3	B	1303	NAG	C3-C2	-2.06	1.48	1.52
3	B	1305	NAG	O5-C5	2.04	1.47	1.43
3	C	1303	NAG	O5-C5	2.04	1.47	1.43
3	A	1305	NAG	O5-C5	2.03	1.47	1.43

All (35) 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	3.43	116.78	112.19
3	A	1301	NAG	C2-N2-C7	-3.27	118.51	122.90
3	A	1301	NAG	C1-C2-N2	-3.18	105.43	110.43
3	B	1303	NAG	C2-N2-C7	-3.11	118.73	122.90
3	C	1303	NAG	C2-N2-C7	-3.09	118.76	122.90
3	A	1304	NAG	C8-C7-N2	2.87	120.87	116.12
3	B	1305	NAG	C2-N2-C7	-2.87	119.06	122.90
3	C	1304	NAG	C2-N2-C7	-2.84	119.09	122.90
3	B	1303	NAG	C8-C7-N2	2.73	120.65	116.12
3	C	1301	NAG	C2-N2-C7	-2.64	119.36	122.90
3	C	1303	NAG	C8-C7-N2	2.62	120.45	116.12
3	B	1304	NAG	C2-N2-C7	-2.59	119.43	122.90
3	C	1301	NAG	C8-C7-N2	2.58	120.39	116.12
3	A	1302	NAG	C1-O5-C5	2.49	115.53	112.19
3	B	1302	NAG	C2-N2-C7	-2.48	119.58	122.90
3	A	1303	NAG	C2-N2-C7	-2.44	119.63	122.90
3	C	1304	NAG	C8-C7-N2	2.41	120.12	116.12
3	B	1304	NAG	C8-C7-N2	2.40	120.09	116.12
3	B	1305	NAG	C8-C7-N2	2.38	120.07	116.12
3	B	1301	NAG	C2-N2-C7	-2.37	119.72	122.90
3	A	1301	NAG	C8-C7-N2	2.37	120.05	116.12
3	A	1305	NAG	C8-C7-N2	2.36	120.04	116.12
3	C	1305	NAG	C8-C7-N2	2.33	119.99	116.12
3	A	1303	NAG	C8-C7-N2	2.32	119.96	116.12
3	A	1305	NAG	O5-C1-C2	2.29	114.83	111.29
3	A	1302	NAG	C8-C7-N2	2.28	119.89	116.12
3	C	1302	NAG	C8-C7-N2	2.26	119.87	116.12
3	B	1301	NAG	C1-C2-N2	-2.16	107.03	110.43
3	A	1304	NAG	O7-C7-C8	-2.13	118.26	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1301	NAG	C8-C7-N2	2.11	119.62	116.12
3	A	1302	NAG	O5-C1-C2	2.10	114.54	111.29
3	B	1302	NAG	C8-C7-N2	2.05	119.52	116.12
3	B	1304	NAG	C6-C5-C4	-2.05	107.99	113.02
3	A	1303	NAG	C6-C5-C4	-2.01	108.08	113.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1303	NAG	O5-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	A	1304	NAG	C3-C2-N2-C7
3	C	1302	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	A	1303	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	C	1303	NAG	1	0
3	B	1304	NAG	1	0
3	A	1303	NAG	2	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.

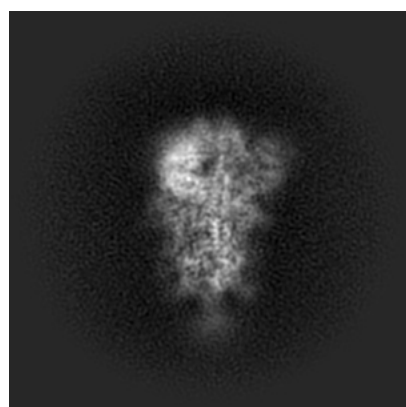
6 Map visualisation [i](#)

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.

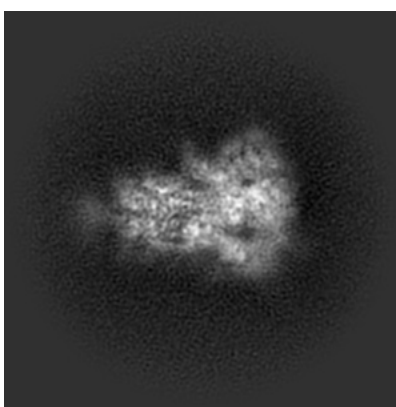
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

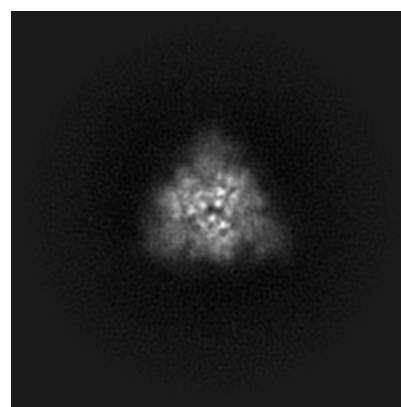
6.1.1 Primary map



X



Y

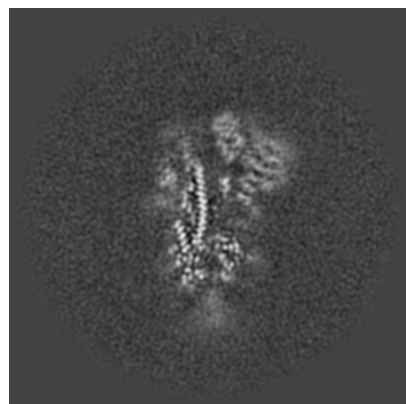


Z

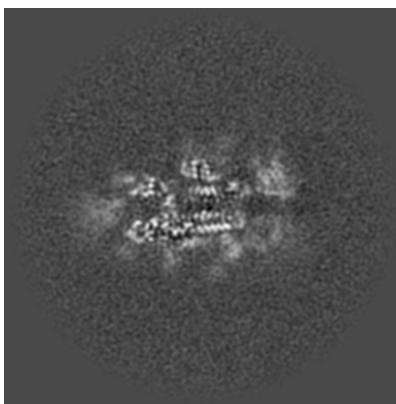
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

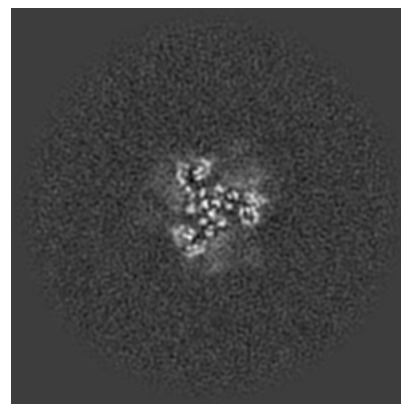
6.2.1 Primary map



X Index: 128



Y Index: 128

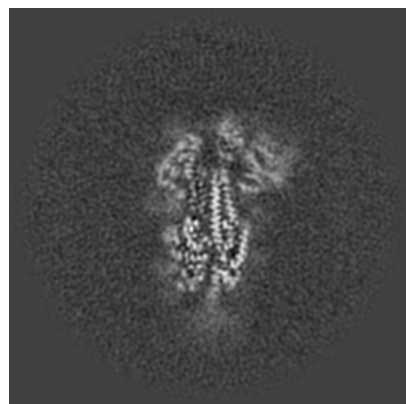


Z Index: 128

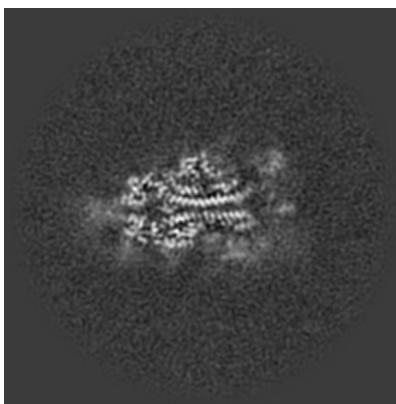
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

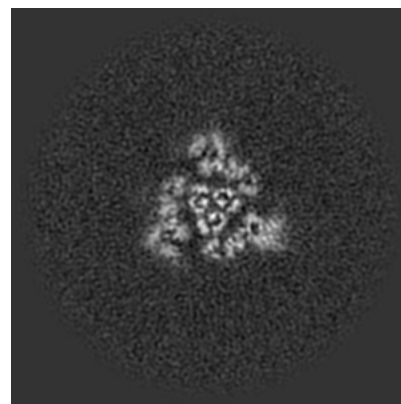
6.3.1 Primary map



X Index: 132



Y Index: 132

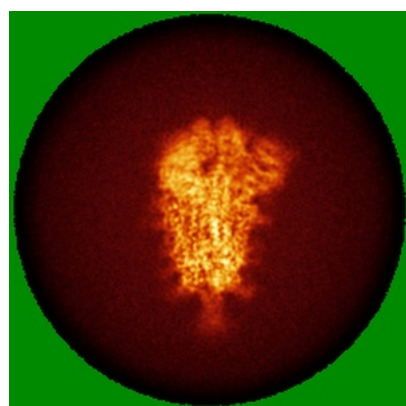


Z Index: 148

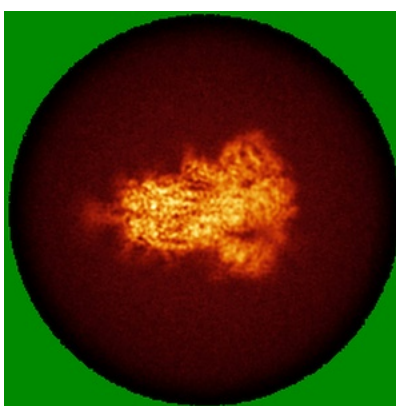
The images above show the largest variance slices of the map in three orthogonal directions.

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

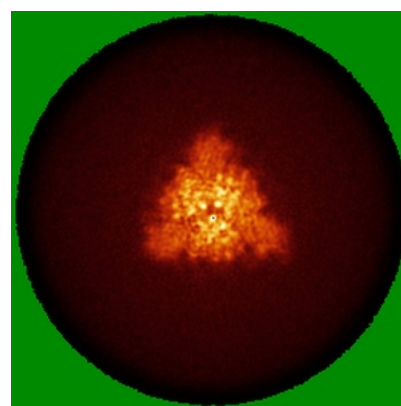
6.4.1 Primary map



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.

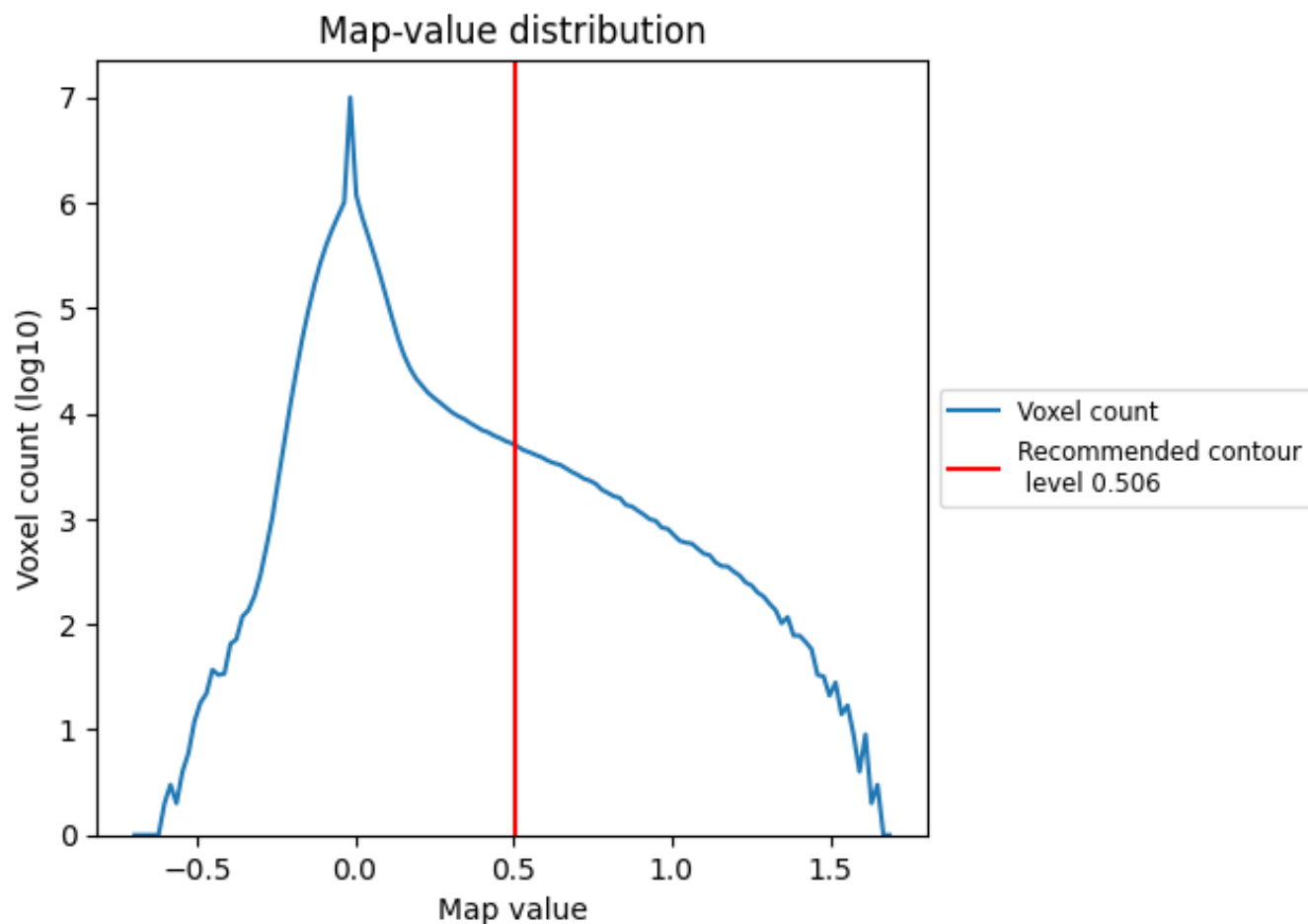
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

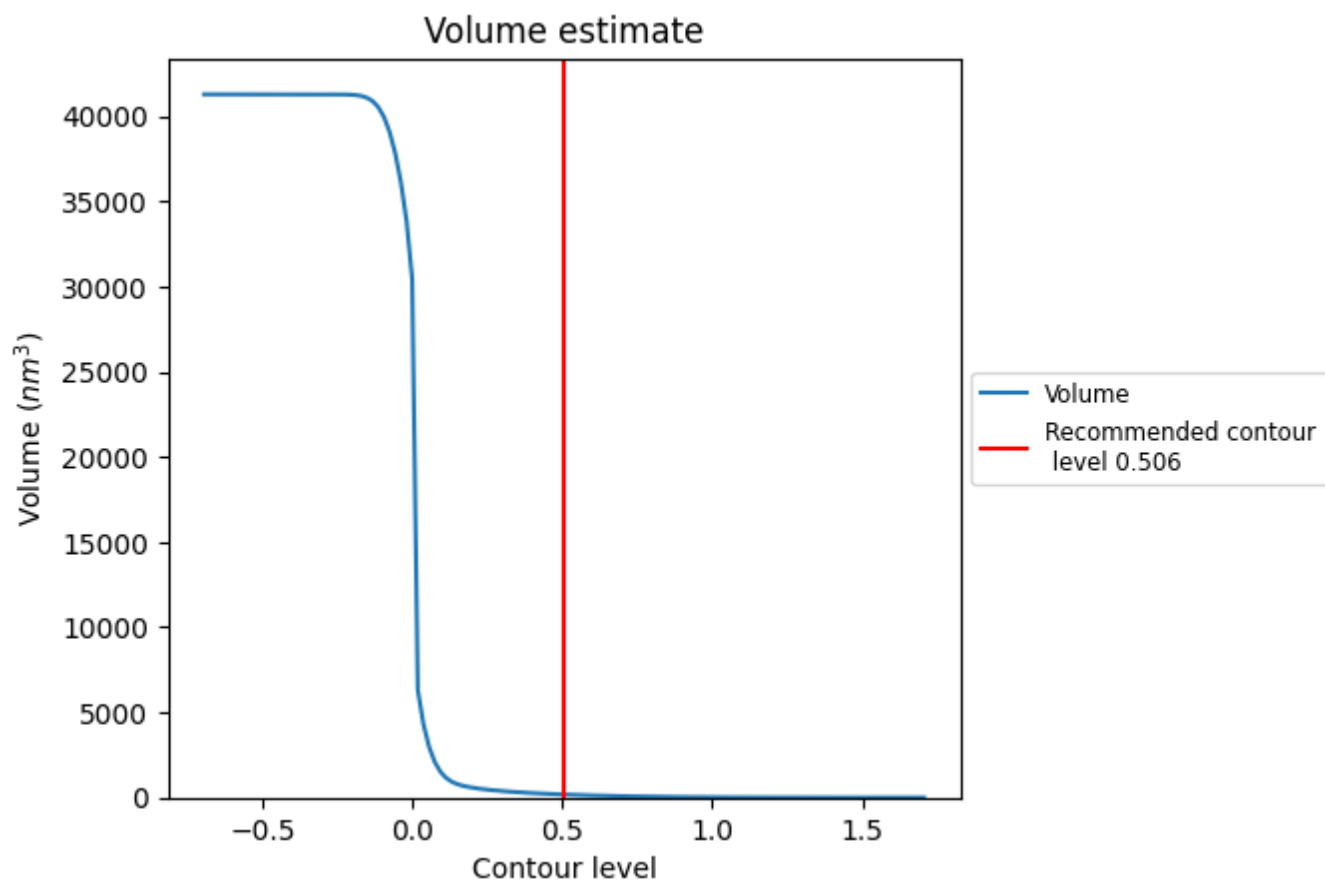
This section contains the results of statistical analysis of the map.

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.

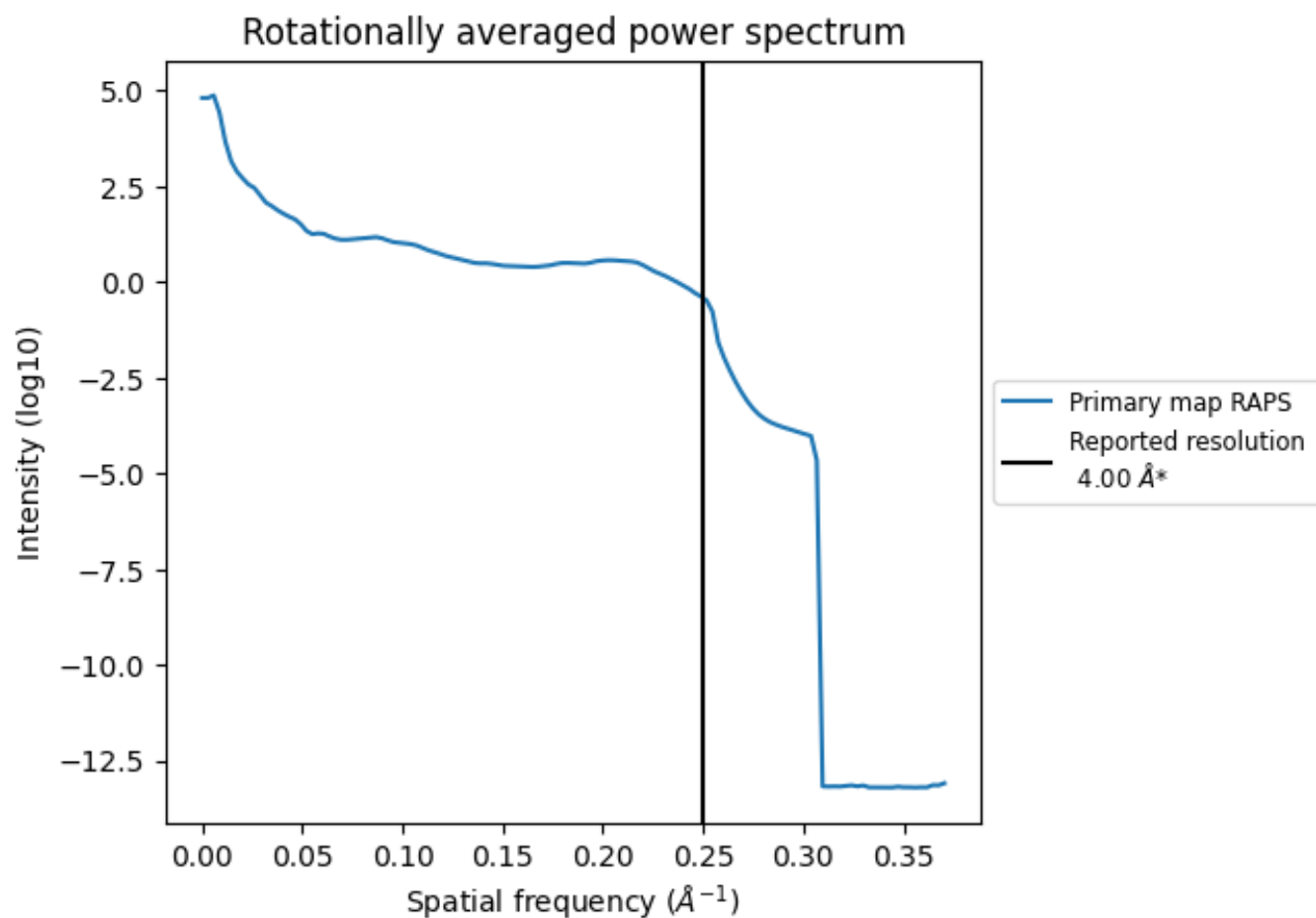
7.2 Volume estimate [i](#)



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 ⓘ

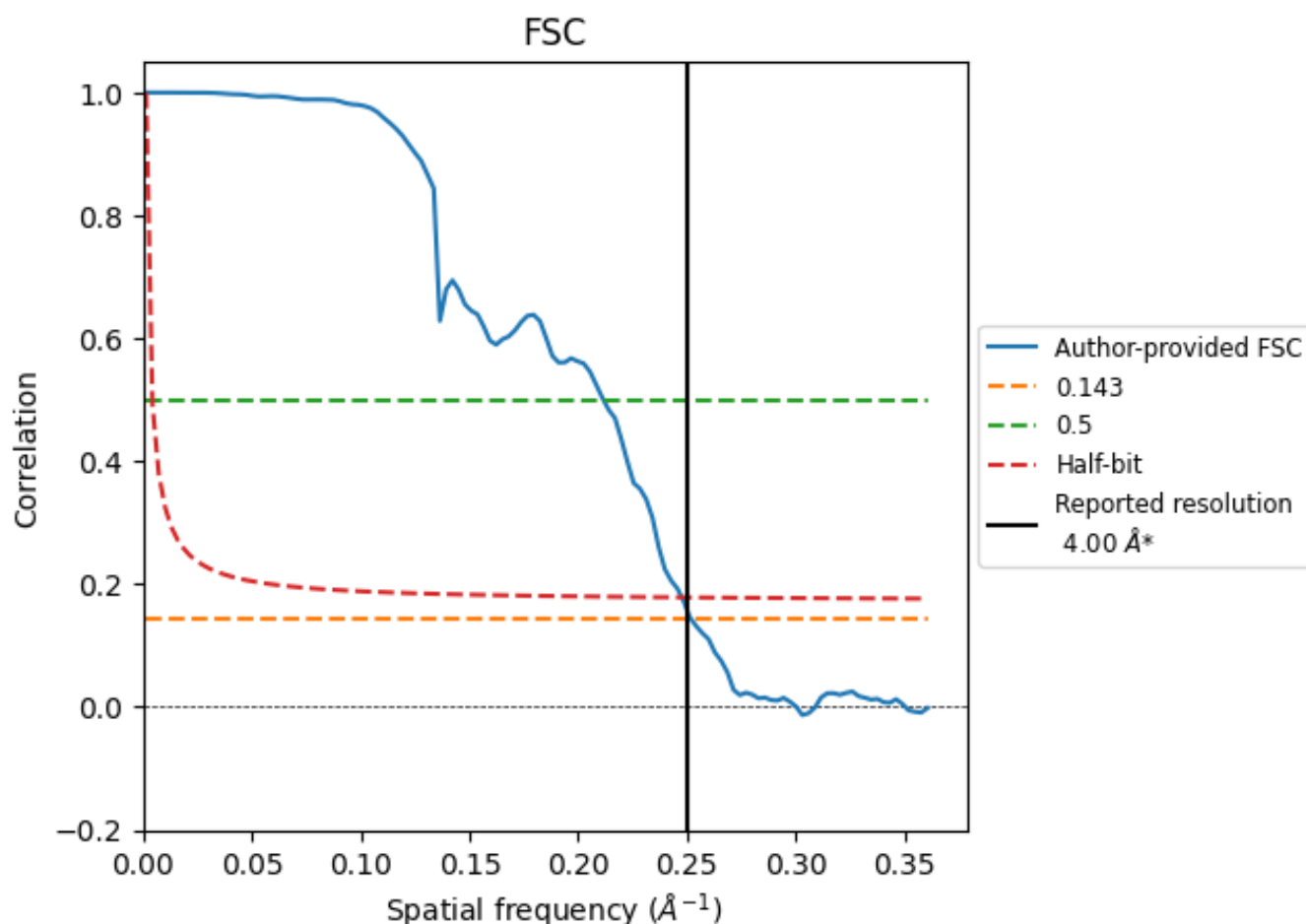


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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](#)

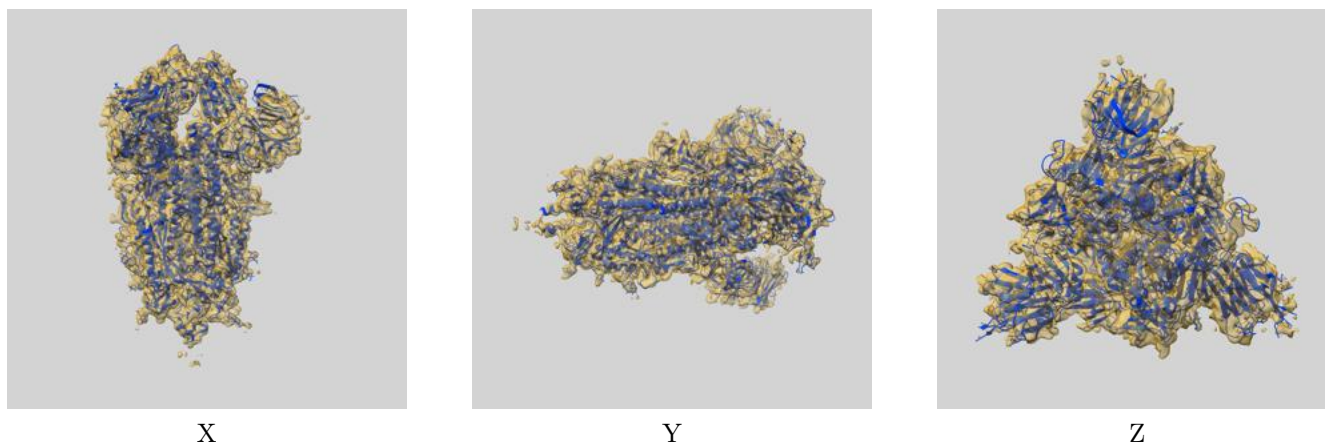
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.97	4.73	4.04
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

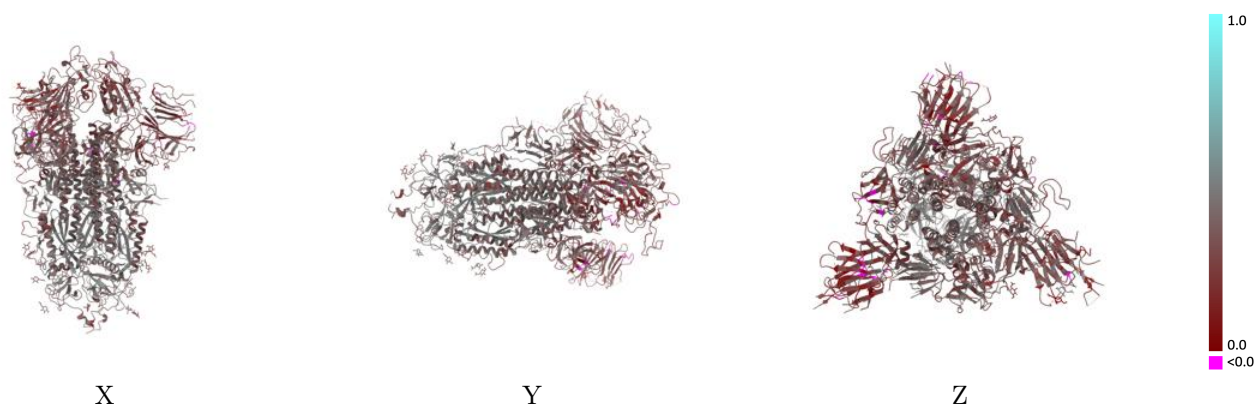
This section contains information regarding the fit between EMDB map EMD-32492 and PDB model 7WGY. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



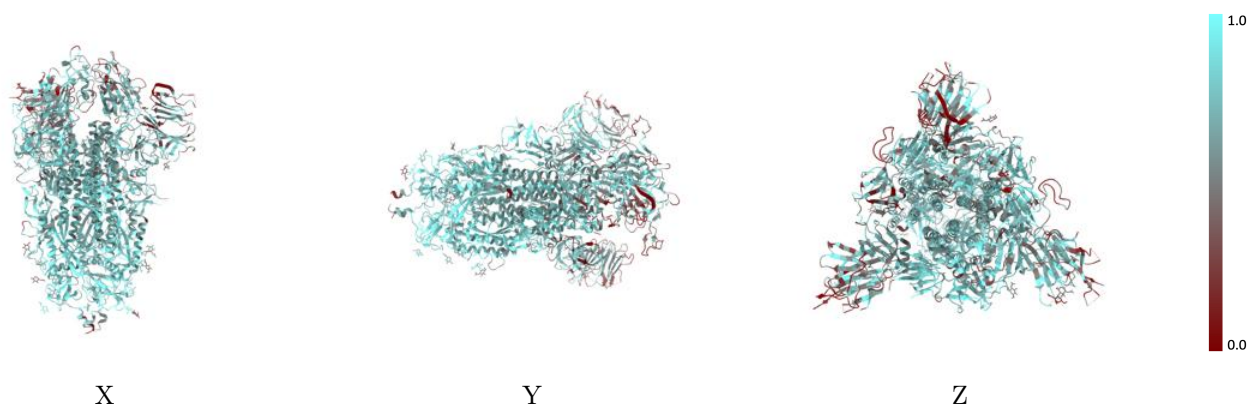
The images above show the 3D surface view of the map at the recommended contour level 0.506 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



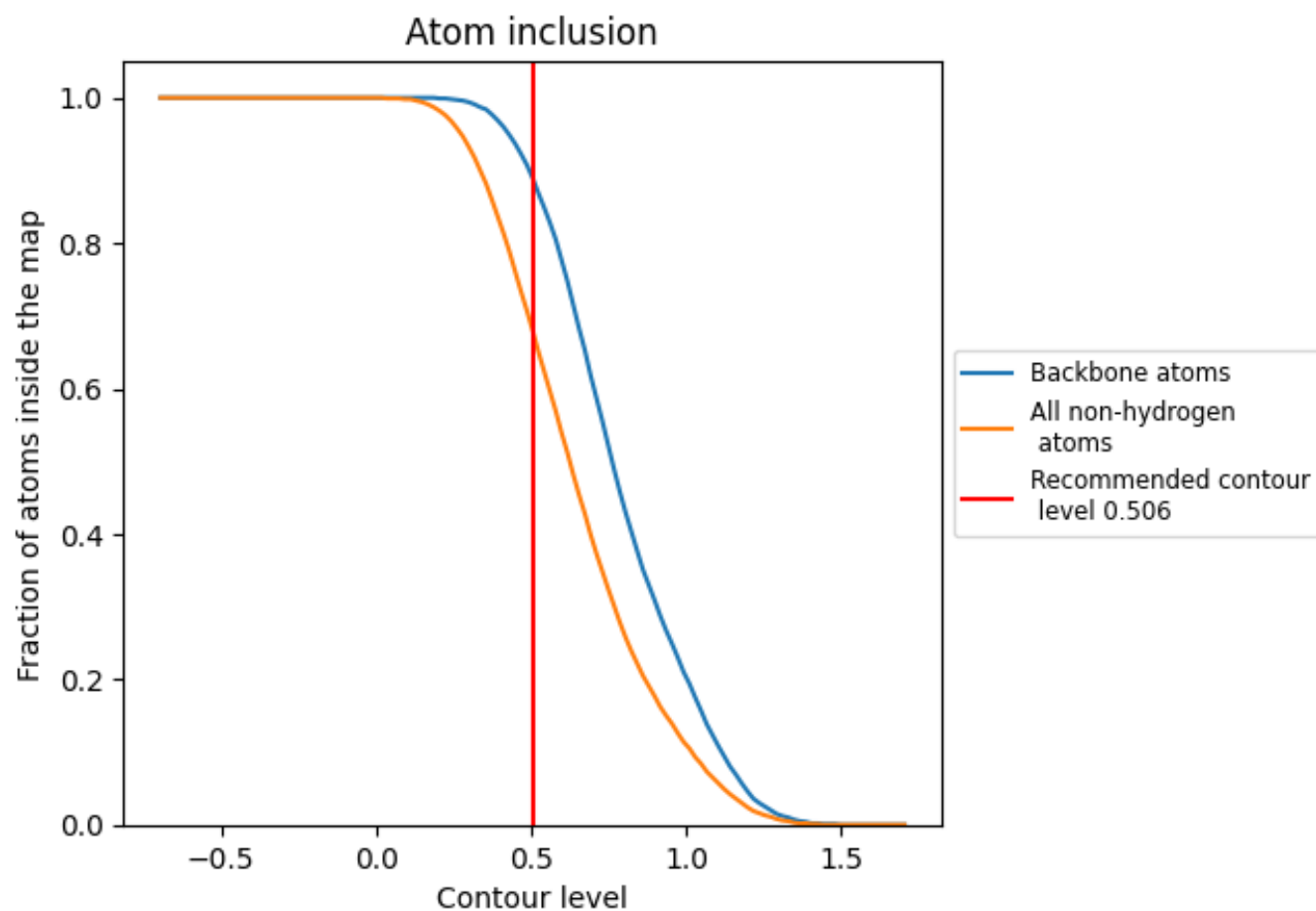
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.6790	0.3540
A	0.6850	0.3580
B	0.6770	0.3570
C	0.6780	0.3480
D	0.6070	0.4030
E	0.5360	0.2760
F	0.5710	0.3250
G	0.2860	0.2600
H	0.5710	0.3370
I	0.5360	0.2650
J	0.6070	0.3470
K	0.6430	0.3380

1.0

0.0

<0.0