



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 11:03 AM UTC

PDB ID : 7YR3 / pdb_00007yr3
EMDB ID : EMD-34044
Title : SARS-CoV-2 BA.2.75 S Trimer in complex with ACE2(state2)
Authors : Wang, L.
Deposited on : 2022-08-08
Resolution : 3.52 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

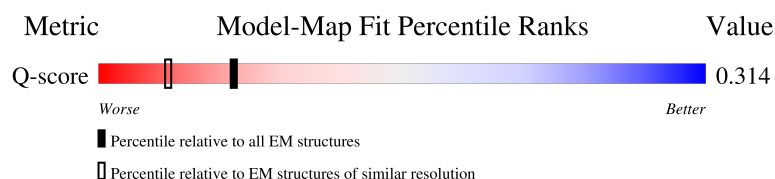
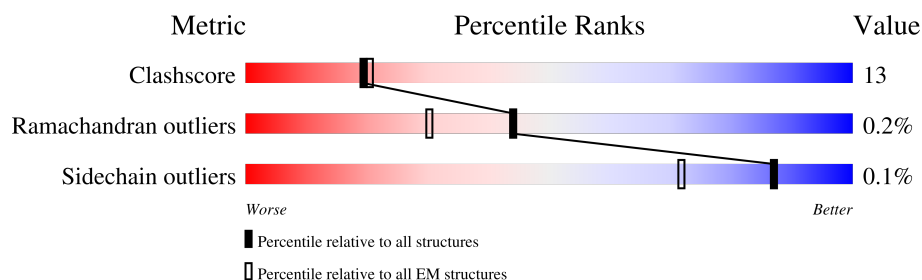
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.52 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	13017 (3.02 - 4.02)

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	B	1270	
1	C	1270	
1	F	1270	
2	D	603	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	603	83% 69% 30%
3	A	2	50% 50%
3	E	2	50% 50%
3	H	2	50% 100%
3	I	2	100%
3	J	2	100%
3	K	2	50% 50%
3	L	2	100%
3	M	2	100%
3	N	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	G	902	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35899 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	B	1058	Total	C	N	O	S	0	0
			8258	5271	1380	1571	36		
1	C	1080	Total	C	N	O	S	0	0
			8426	5380	1407	1603	36		
1	F	1068	Total	C	N	O	S	0	0
			8335	5323	1392	1583	37		

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	147	GLU	LYS	variant	UNP P0DTC2
B	152	ARG	TRP	variant	UNP P0DTC2
B	157	LEU	PHE	variant	UNP P0DTC2
B	210	VAL	ILE	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	257	SER	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	engineered mutation	UNP P0DTC2
B	685	ALA	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	147	GLU	LYS	variant	UNP P0DTC2
C	152	ARG	TRP	variant	UNP P0DTC2
C	157	LEU	PHE	variant	UNP P0DTC2
C	210	VAL	ILE	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	257	SER	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	engineered mutation	UNP P0DTC2
C	685	ALA	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
F	22	ILE	THR	variant	UNP P0DTC2
F	?	-	LEU	deletion	UNP P0DTC2
F	?	-	PRO	deletion	UNP P0DTC2
F	?	-	PRO	deletion	UNP P0DTC2
F	27	SER	ALA	variant	UNP P0DTC2
F	142	ASP	GLY	variant	UNP P0DTC2
F	147	GLU	LYS	variant	UNP P0DTC2
F	152	ARG	TRP	variant	UNP P0DTC2
F	157	LEU	PHE	variant	UNP P0DTC2
F	210	VAL	ILE	variant	UNP P0DTC2
F	213	GLY	VAL	variant	UNP P0DTC2
F	257	SER	GLY	variant	UNP P0DTC2
F	339	HIS	GLY	variant	UNP P0DTC2
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	376	ALA	THR	variant	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	446	SER	GLY	variant	UNP P0DTC2
F	460	LYS	ASN	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2
F	478	LYS	THR	variant	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	498	ARG	GLN	variant	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	variant	UNP P0DTC2
F	614	GLY	ASP	variant	UNP P0DTC2
F	655	TYR	HIS	variant	UNP P0DTC2
F	679	LYS	ASN	variant	UNP P0DTC2
F	681	HIS	PRO	variant	UNP P0DTC2
F	683	ALA	ARG	engineered mutation	UNP P0DTC2
F	685	ALA	ARG	engineered mutation	UNP P0DTC2
F	764	LYS	ASN	variant	UNP P0DTC2
F	796	TYR	ASP	variant	UNP P0DTC2
F	817	PRO	PHE	engineered mutation	UNP P0DTC2
F	892	PRO	ALA	engineered mutation	UNP P0DTC2
F	899	PRO	ALA	engineered mutation	UNP P0DTC2
F	942	PRO	ALA	engineered mutation	UNP P0DTC2
F	954	HIS	GLN	variant	UNP P0DTC2
F	969	LYS	ASN	variant	UNP P0DTC2
F	986	PRO	LYS	engineered mutation	UNP P0DTC2
F	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	G	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1
G	616	HIS	-	expression tag	UNP Q9BYF1
G	617	HIS	-	expression tag	UNP Q9BYF1
G	618	HIS	-	expression tag	UNP Q9BYF1
G	619	HIS	-	expression tag	UNP Q9BYF1
G	620	HIS	-	expression tag	UNP Q9BYF1
G	621	HIS	-	expression tag	UNP Q9BYF1

- Molecule 3 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
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Cl	0
			1	1	
6	G	1	Total	Cl	0
			1	1	

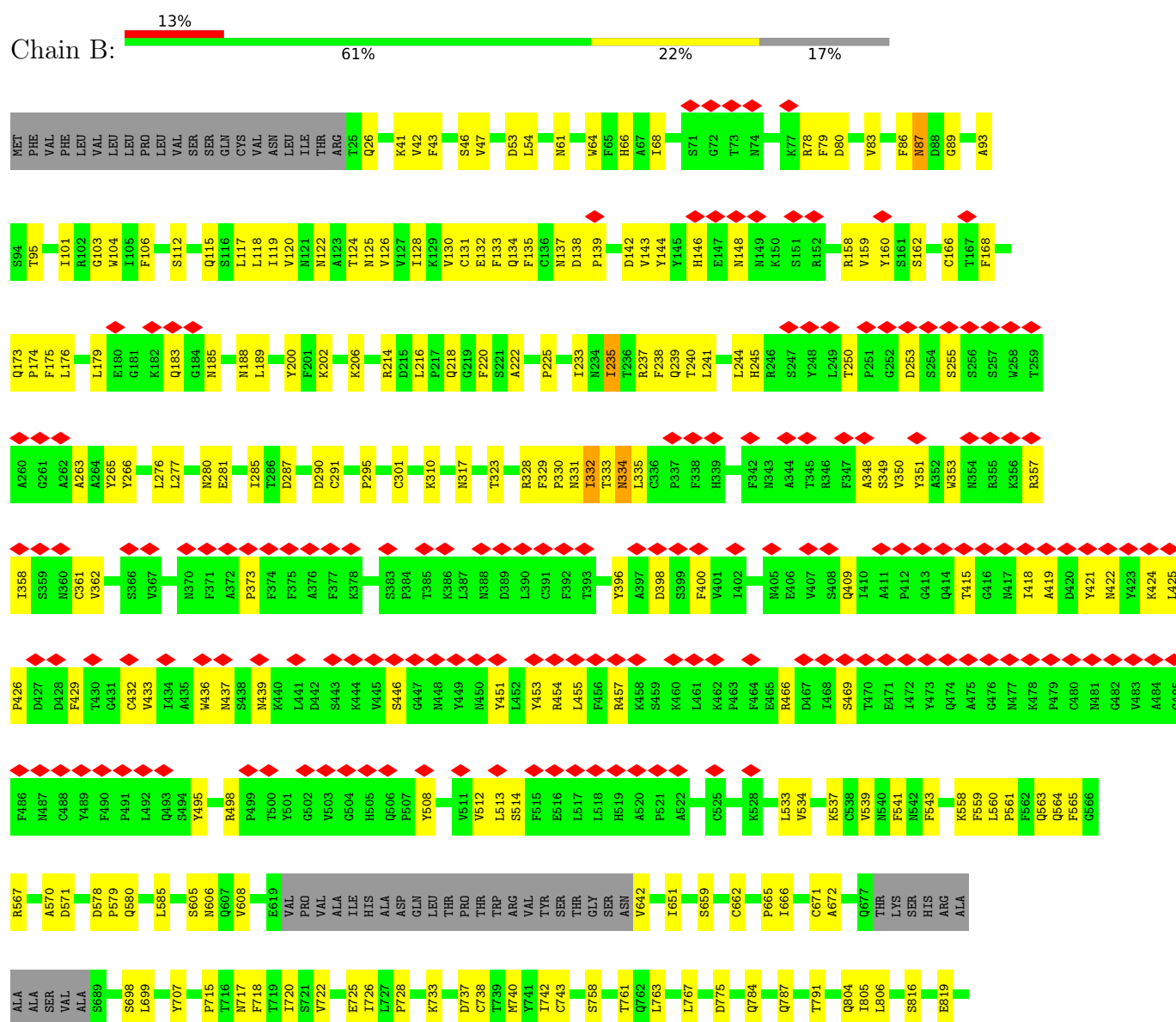
- Molecule 7 is water.

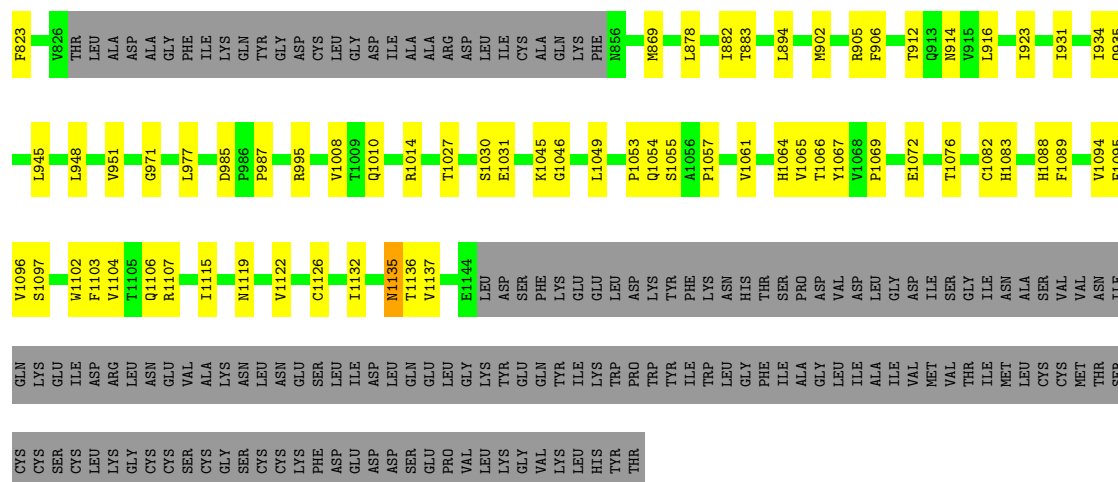
Mol	Chain	Residues	Atoms		AltConf
7	D	71	Total	O	0
			71	71	
7	G	71	Total	O	0
			71	71	

3 Residue-property plots

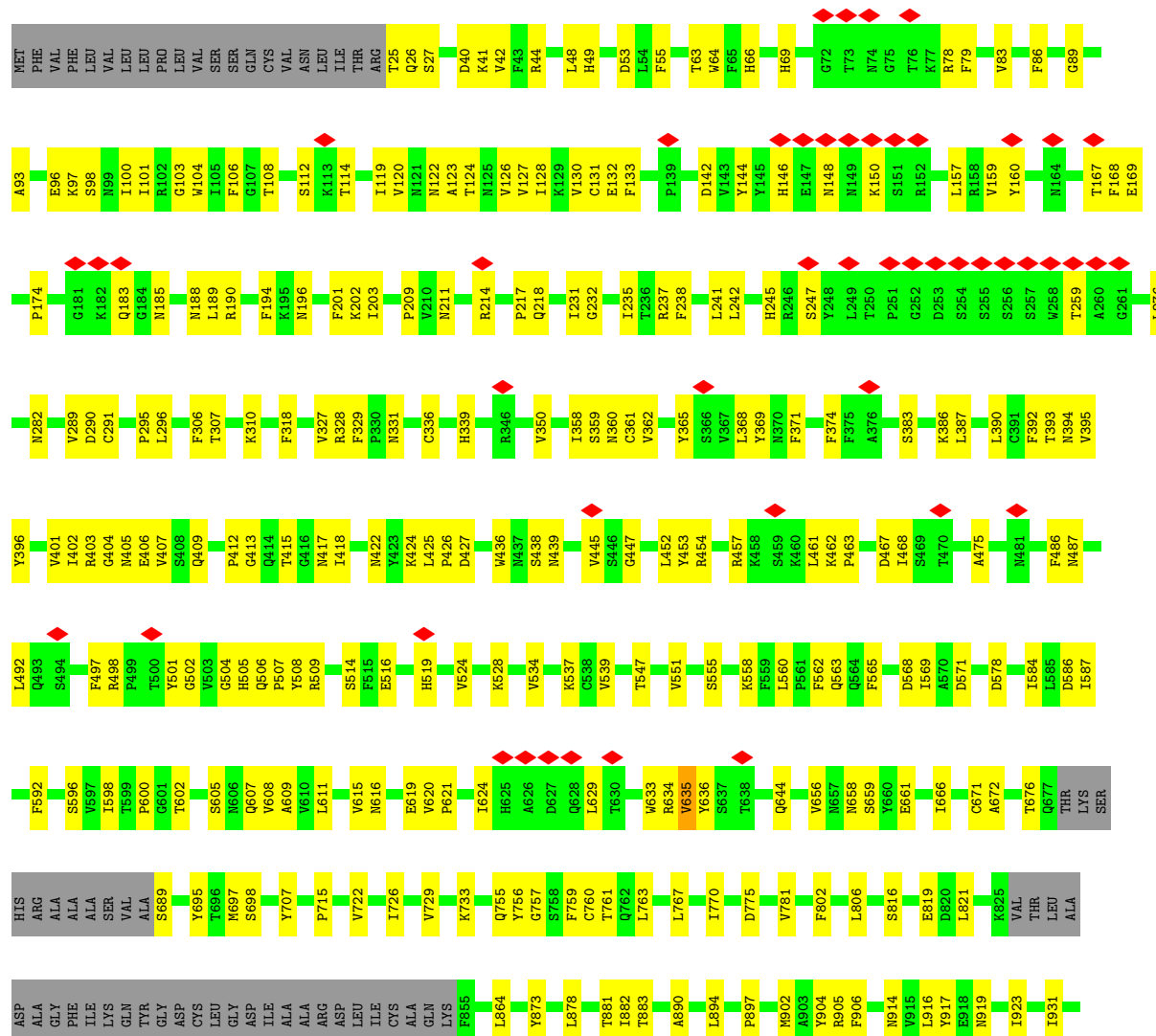
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

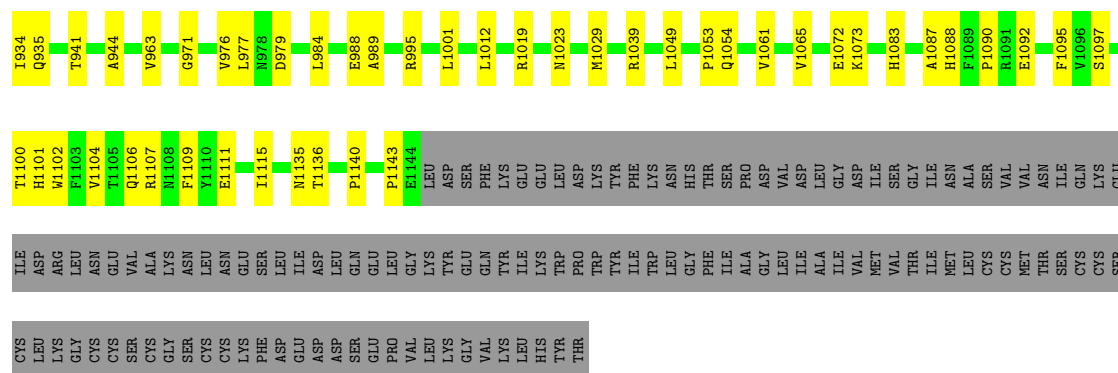
• Molecule 1: Spike glycoprotein



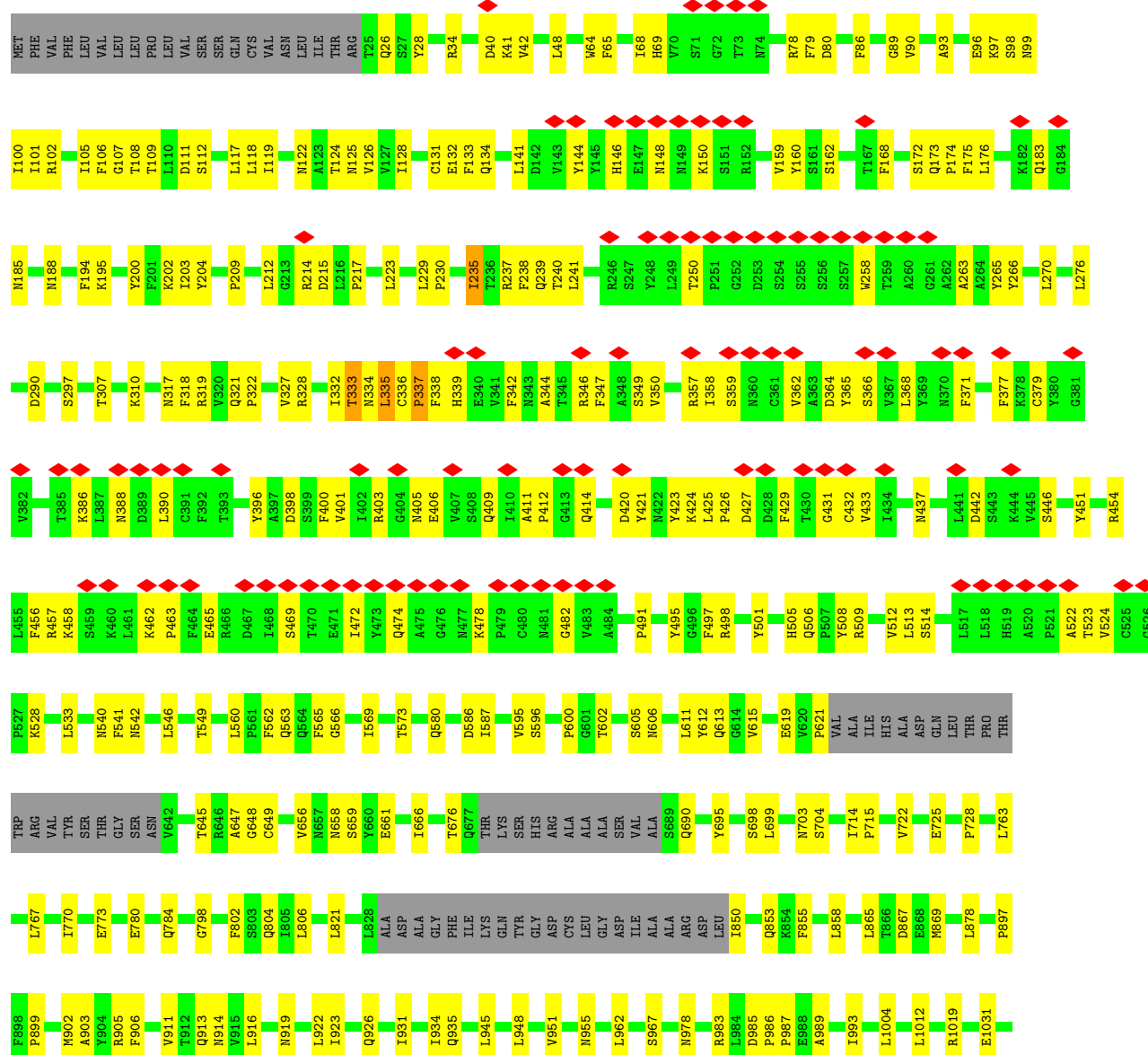


• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein



L1049	L1050	S1051	F1052	P1053	Q1054	H1064	V1065	E1072	F1075	I1081	K1086	F1089	G1093	V1096	S1097	W1102	F1103	R1107	V1122	V1133	N1134	N1135	D1139	E1144	LEU	ASP	ASP	PHE	GLY	GLU	GLU	LEU	ASP	TRP	TYR	PHE	LYS	TRP	LYS	ASN	HIS	THR	SER	PRO	ASP	VAL	ASP								
ALA	ILE	VAL	MET	VAL	THR	ILE	ASN	ALA	VAL	THR	ASN	ILE	GLN	LYS	SER	GLU	ARG	LYS	GLY	CYS	CYS	ASN	VAL	ALA	LYS	ASN	LEU	ASP	ASP	GLU	GLN	GLY	VAL	LYS	ILE	GLU	LEU	TRP	PRO	THR	LYS	TRP	ILE	LYS	TRP	GLY	PHE	THR	ILE	ALA	GLY	LEU	VAL	ASP	ILE

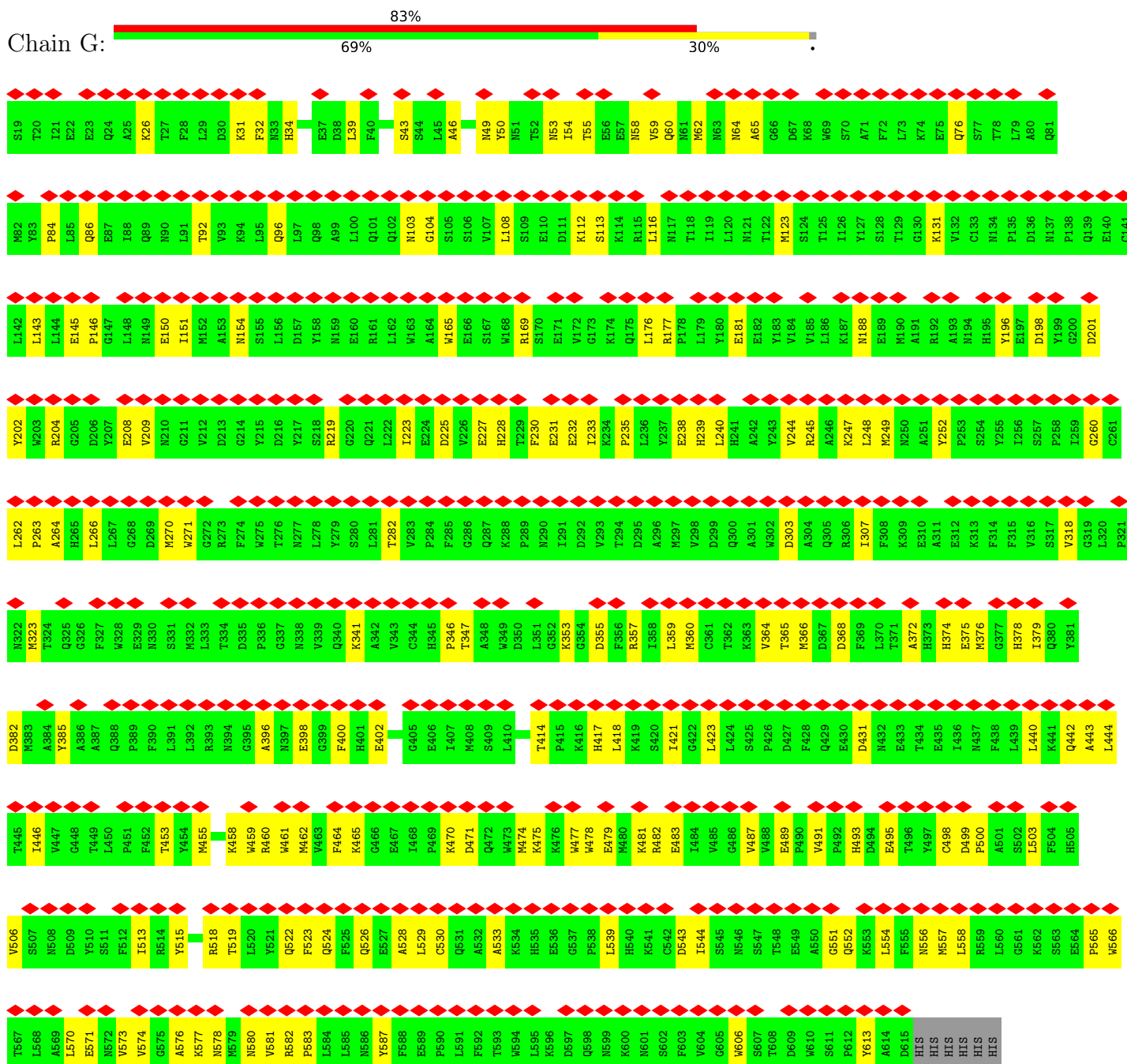
ALA	ILE	VAL	MET	VAL	THR	ILE	ASN	ALA	VAL	THR	ASN	ILE	GLN	LYS	SER	GLU	ARG	LYS	GLY	CYS	CYS	ASN	VAL	ALA	LYS	ASN	LEU	ASP	ASP	GLU	GLN	GLY	VAL	LYS	ILE	GLU	LEU	TRP	PRO	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 2: Angiotensin-converting enzyme 2



HIS	S19	L79	Q139	Y199	I259	G319	T379	L439	D499	R559	S599	L599	HIS
	T20	A80	E140	G200	G260	L320	Q380	L440	P500	L560	P500	L560	HIS
	I21	Q81	C141	D201	C261	P321	Y381	K441	A501	G561	A501	G561	HIS
HIS	E22	M82	L142	Y202	L262	M322	D382	Q442	S502	K562	S502	K562	HIS
	E23	Y83	L143	W203	P263	M323	M383	A443	L503	S563	L503	S563	
	Q24	P84	L144	R204	A264	T324	A384	L444	F504	E564	F504	E564	
HIS	K26	L85	E145	G205	L265	Q325	Y385	T445	H505	P565	H505	P565	HIS
	A25	Q86	P146	D206	L266	G326	A386	I446	V506	W566	V506	W566	
	T27	E87	G147	Y207	L267	F327	A387	V447	S507	T567	T567	S507	
HIS	F28	I88	L148	E208	G268	W328	Q388	G448	N508	L568	N508	G448	HIS
	L29	Q89	N149	V209	D269	E329	P389	T449	D509	A569	D509	T449	
	D30	N90	E150	W210	M270	N330	F390	L450	Y510	L570	L570	A569	
HIS	K31	L91	I151	G211	W271	S331	L391	P451	S511	E571	S511	P451	HIS
	F32	T92	M152	V212	G272	M332	L392	F452	F512	N572	N572	F452	
	N93	V93	A153	D213	R273	L333	R393	T453	I513	V573	V573	I513	
HIS	H34	K94	N154	G214	W275	T334	N394	Y454	R514	V574	R514	Y454	HIS
	E35	L95	S155	Y215	G275	D335	G395	M455	Y515	G575	G575	M455	
	A36	Q96	L156	D216	T276	P336	A396	L456	Y516	A576	A576	L456	
HIS	E37	L97	D157	Y217	N277	G337	N397	E457	T517	K577	K577	E457	HIS
	D38	Q98	Y158	S218	L278	N338	E398	K458	R518	N578	N578	K458	
	L39	A99	N159	R219	Y279	V339	G399	W459	T519	M579	M579	W459	
HIS	F40	L100	E160	G220	S280	Q340	F400	R460	Y520	N580	N580	R460	HIS
	Y41	Q101	R161	Q221	L281	K341	H401	W461	Y521	V581	V581	W461	
	Q42	Q102	L162	L222	T282	A342	E402	M462	Q522	R582	R582	M462	
HIS	S43	N103	W163	I223	V283	V343	A403	V463	F523	P583	P583	V463	HIS
	S44	G104	A164	E224	P284	C344	G405	F464	Q524	L584	L584	G405	
	L45	S105	W165	D225	G285	H345	E406	K465	F525	L585	L585	K465	
HIS	A46	S106	E166	V226	Q286	P346	E406	G466	G526	N586	N586	G466	HIS
	S47	V107	S167	E227	Q287	T347	I407	E467	E527	Y587	Y587	I407	
	W48	L108	G168	H228	K288	A348	M408	L468	A528	F588	F588	A348	
HIS	Y49	N49	R169	T229	P289	W349	S409	P469	L529	E588	E588	W349	HIS
	Y50	E110	S170	T230	N290	D350	L410	K470	C530	P590	P590	D350	
	N51	K111	E171	E231	L291	L351	A412	D471	Q531	L591	L591	A412	
HIS	T52	S113	V172	E232	D292	G352	A413	Q472	A532	F592	F592	Q472	HIS
	N53	K114	G173	I233	V293	K353	T414	W473	A533	T593	T593	W473	
	I54	R115	K174	K234	T294	D354	T415	M474	L415	W594	W594	T415	
HIS	T55	L116	Q175	P235	D295	D355	K416	K475	H535	L595	L595	K475	HIS
	E56	N117	L176	L236	A296	F356	R416	K476	E536	K596	K596	R416	
	E57	T118	R177	Y237	M297	R357	L418	H417	G537	D597	D597	H417	
HIS	N58	I119	P178	E238	K288	I358	K419	W478	P538	Q598	Q598	W478	HIS
	V59	L120	L179	H239	P289	L359	S420	E479	L539	N599	N599	L359	
	Q60	M121	Y180	L240	Q300	M360	I421	M480	K481	H540	H540	M360	
HIS	N61	T122	E181	H241	A301	C361	L421	K481	C541	N601	N601	C361	HIS
	M62	M123	E182	A242	W302	T362	G422	R482	C542	S602	S602	T362	
	N63	S124	Y183	Y243	D303	K363	L423	E483	D543	F603	F603	E483	
HIS	N64	T125	V184	V244	A304	V364	L424	I484	I544	V604	V604	V364	HIS
	A65	I126	Y185	R245	Q305	T365	S425	V485	S645	G605	G605	T365	
	G66	Y127	L186	A246	R306	M366	P426	G486	N546	W606	W606	M366	
HIS	D67	S128	K187	K247	I307	D367	D427	V487	S647	S607	S607	D367	HIS
	K68	T129	E188	L248	F308	D368	F428	W487	T548	T608	T608	F308	
	W69	G130	E189	M249	E309	F369	Q429	V488	E489	D609	D609	Q429	
HIS	S70	K131	M190	H250	E310	L370	E430	P490	W550	W610	W610	L370	HIS
	A71	V132	A191	A251	A311	T371	D431	V491	G551	S611	S611	D431	
	F72	C133	R192	Y252	E312	H373	A372	P492	K552	P612	P612	H373	
HIS	L73	N134	A193	P253	K313	H374	T434	H493	K553	Y613	Y613	T434	HIS
	K74	P135	N194	S254	F314	E375	E435	D494	L554	A614	A614	E375	
	E75	D136	H195	Y255	F315	E375	M376	E495	F555	A614	A614	M376	
HIS	Q76	N137	Y196	I256	V316	G377	I436	T496	N556	D615	D615	G377	HIS
	S77	P138	E197	L256	S317	H378	M437	Y497	M557	HIS	HIS	H378	
	T78	D198	S257	P258	V318	H378	F438	C498	L558	HIS	HIS	H378	

- Molecule 2: Angiotensin-converting enzyme 2



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 

MA01
MA02

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 100%

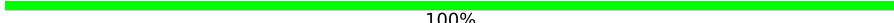


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

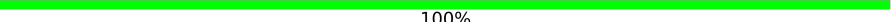


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	313740	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.894	Depositor
Minimum map value	-0.423	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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, ZN, CL

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	B	0.16	0/8455	0.34	1/11509 (0.0%)
1	C	0.16	0/8631	0.35	0/11756
1	F	0.16	0/8534	0.34	0/11617
2	D	0.12	0/5007	0.31	0/6803
2	G	0.11	0/5007	0.29	0/6803
All	All	0.15	0/35634	0.33	1/48488 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1135	ASN	CB-CA-C	-5.21	109.59	115.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8258	0	8044	204	0
1	C	8426	0	8195	239	0
1	F	8335	0	8129	232	0
2	D	4870	0	4639	109	0
2	G	4870	0	4639	139	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	25	2	0
3	E	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
4	B	210	0	192	7	0
4	C	238	0	221	3	0
4	D	56	0	52	0	0
4	F	182	0	169	3	0
4	G	56	0	52	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	2	0
7	D	71	0	0	8	0
7	G	71	0	0	13	0
All	All	35899	0	34557	883	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 13.

The worst 5 of 883 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:332:ILE:HG23	1:B:334:ASN:H	1.26	0.98
1:F:335:LEU:HG	1:F:338:PHE:HB2	1.47	0.97
1:B:740:MET:HE1	1:F:319:ARG:HE	1.44	0.82
1:B:331:ASN:HD21	4:B:1308:NAG:HN2	1.28	0.80
1:C:89:GLY:HA2	1:C:194:PHE:O	1.82	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1050/1270 (83%)	934 (89%)	113 (11%)	3 (0%)	36	66
1	C	1074/1270 (85%)	976 (91%)	96 (9%)	2 (0%)	43	74
1	F	1060/1270 (84%)	964 (91%)	94 (9%)	2 (0%)	43	74
2	D	595/603 (99%)	578 (97%)	17 (3%)	0	100	100
2	G	595/603 (99%)	573 (96%)	22 (4%)	0	100	100
All	All	4374/5016 (87%)	4025 (92%)	342 (8%)	7 (0%)	44	74

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	635	VAL
1	F	337	PRO
1	B	332	ILE
1	C	756	TYR
1	B	334	ASN

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	B	921/1111 (83%)	918 (100%)	3 (0%)	86	83
1	C	939/1111 (84%)	939 (100%)	0	100	100
1	F	930/1111 (84%)	928 (100%)	2 (0%)	87	85
2	D	527/533 (99%)	527 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	527/533 (99%)	527 (100%)	0	100	100
All	All	3844/4399 (87%)	3839 (100%)	5 (0%)	87	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	B	335	LEU
1	B	439	ASN
1	F	333	THR
1	F	335	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	345	HIS
2	G	345	HIS
1	F	165	ASN
2	G	290	ASN
2	G	60	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 ⓘ

18 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	$\# Z > 2$
3	NAG	A	1	3	14,14,15	0.17	0	17,19,21	0.46	0
3	NAG	A	2	3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	E	1	3	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	E	2	3	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
3	NAG	H	1	3,1	14,14,15	0.38	0	17,19,21	0.63	0
3	NAG	H	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	I	1	3,1	14,14,15	0.23	0	17,19,21	0.56	0
3	NAG	I	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	J	1	3	14,14,15	0.17	0	17,19,21	0.60	0
3	NAG	J	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	K	1	3,1	14,14,15	0.87	1 (7%)	17,19,21	1.27	1 (5%)
3	NAG	K	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	L	1	3	14,14,15	0.32	0	17,19,21	0.41	0
3	NAG	L	2	3	14,14,15	0.18	0	17,19,21	0.47	0
3	NAG	M	1	3	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	N	1	3,1	14,14,15	0.88	1 (7%)	17,19,21	1.27	1 (5%)
3	NAG	N	2	3	14,14,15	0.22	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	3	-	1/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	NAG	O5-C1	3.06	1.48	1.43
3	K	1	NAG	O5-C1	2.95	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C1-O5-C5	4.77	118.58	112.19
3	K	1	NAG	C1-O5-C5	4.77	118.58	112.19
3	E	2	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

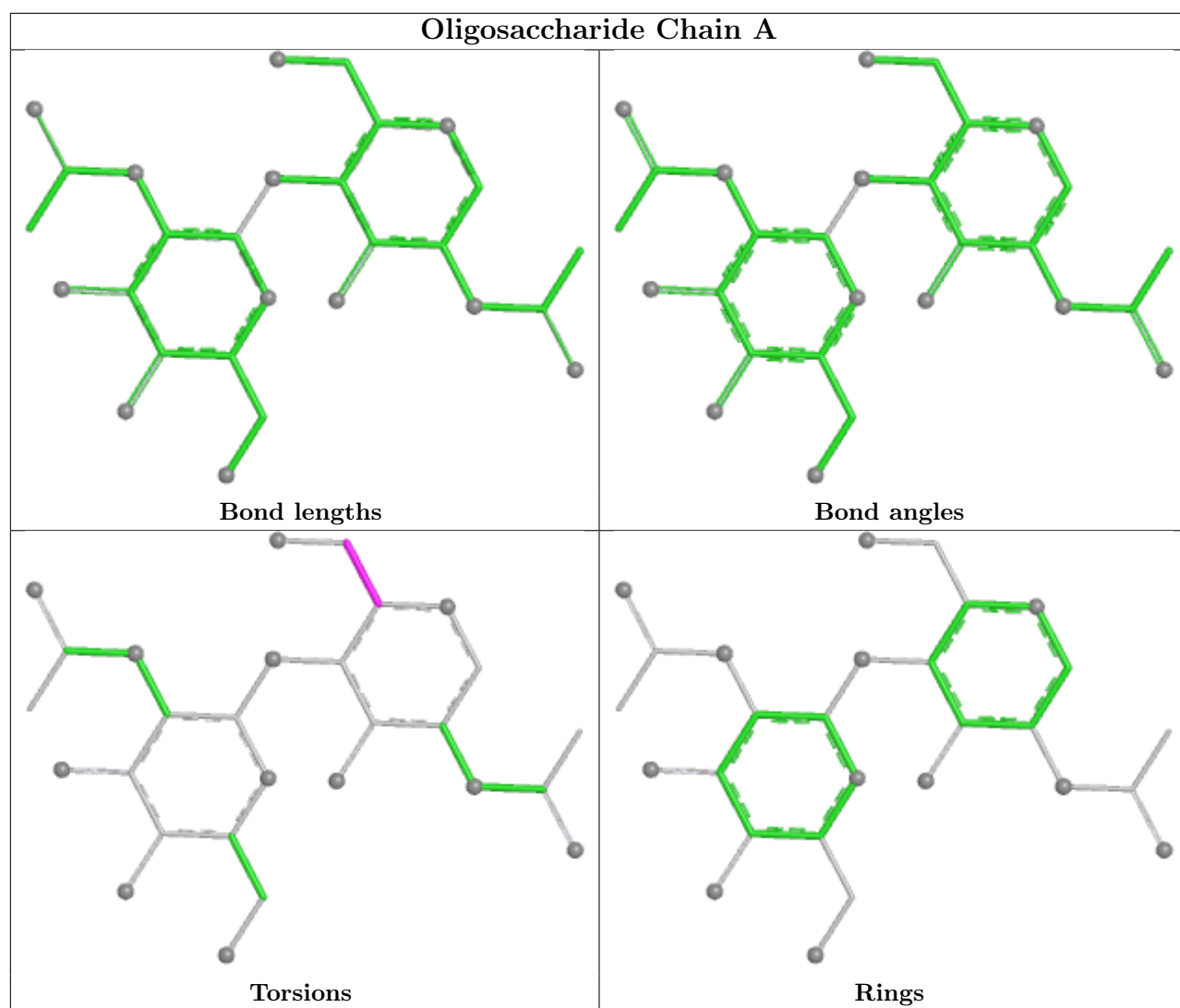
Mol	Chain	Res	Type	Atoms
3	K	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6

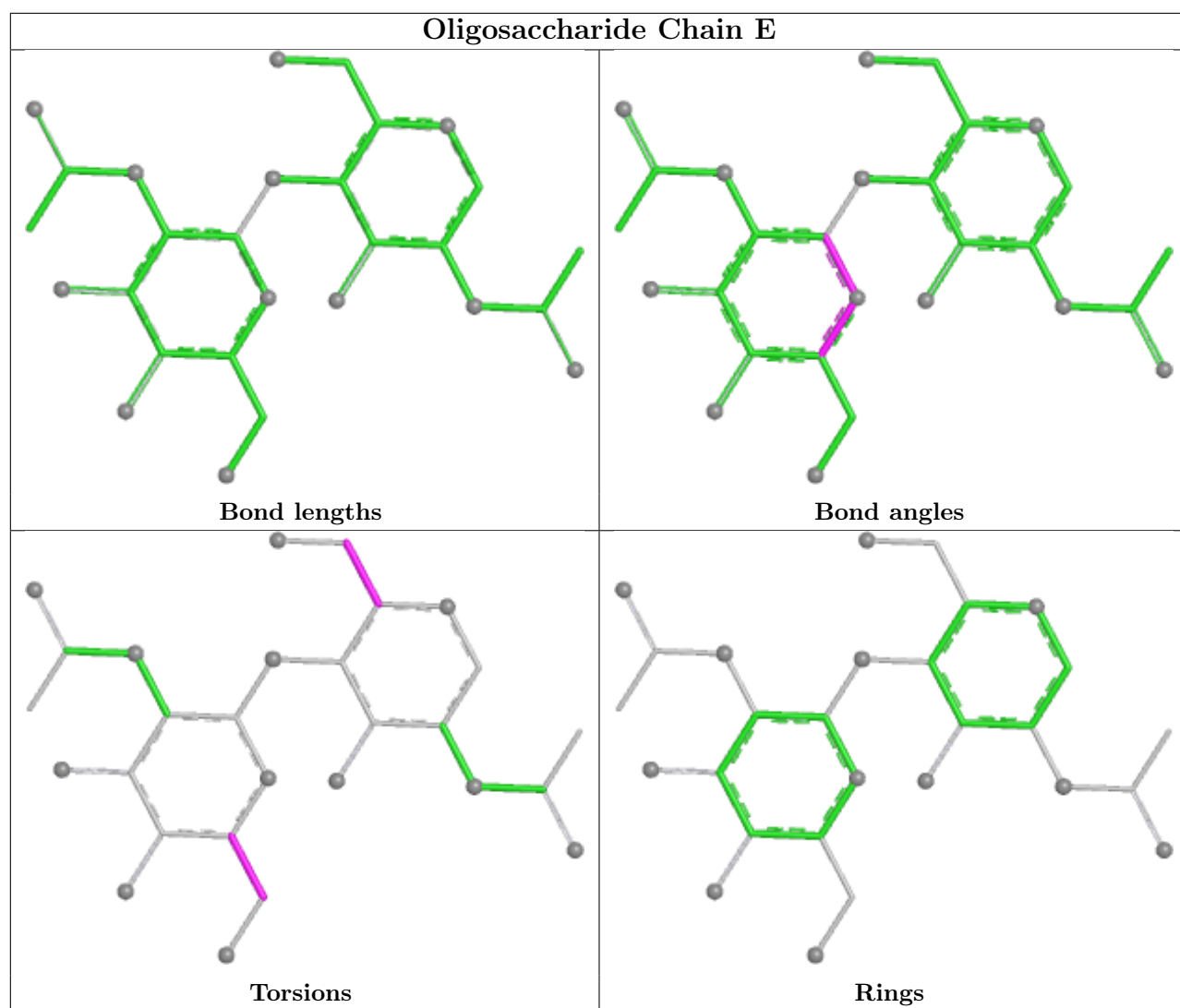
There are no ring outliers.

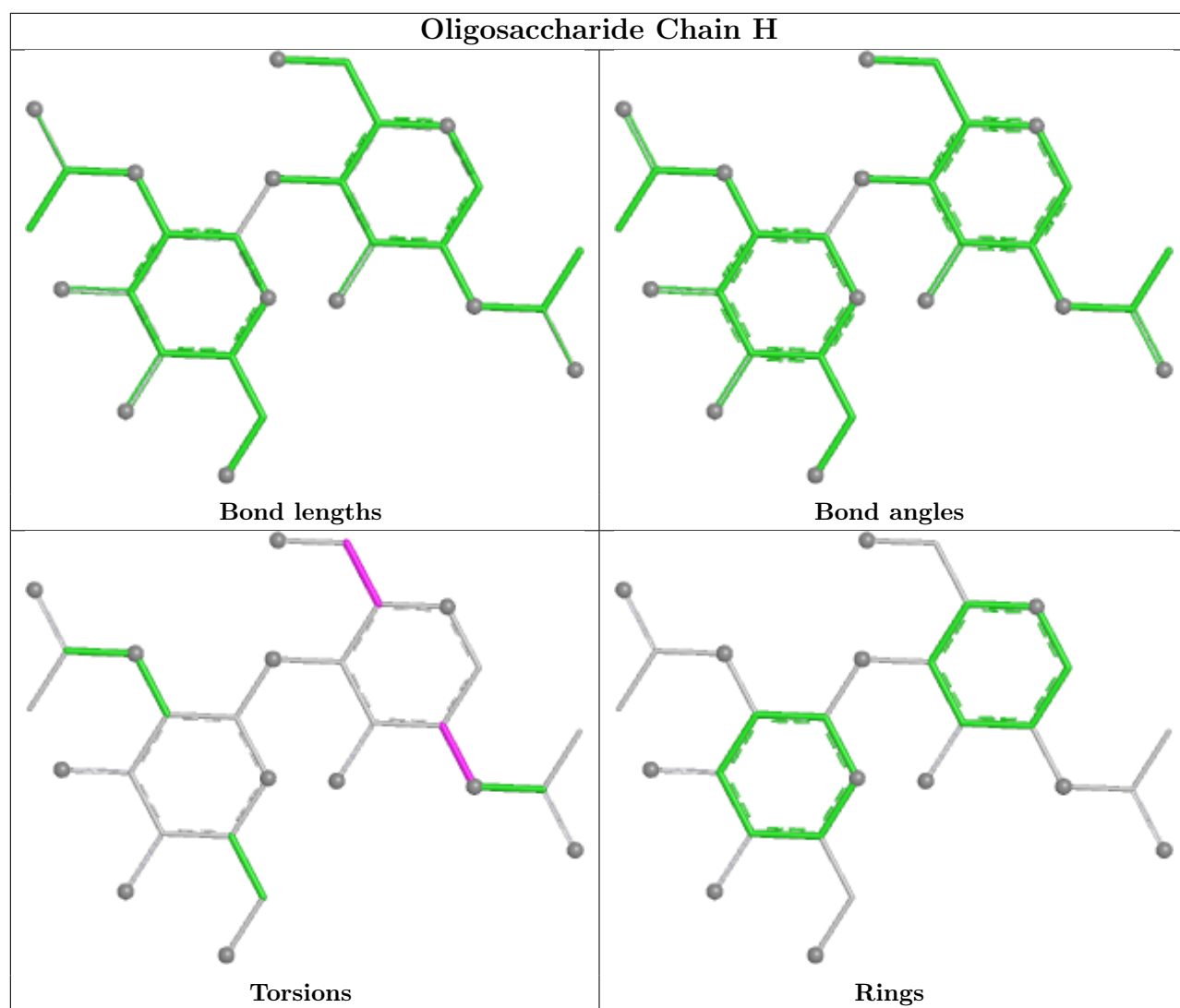
1 monomer is involved in 2 short contacts:

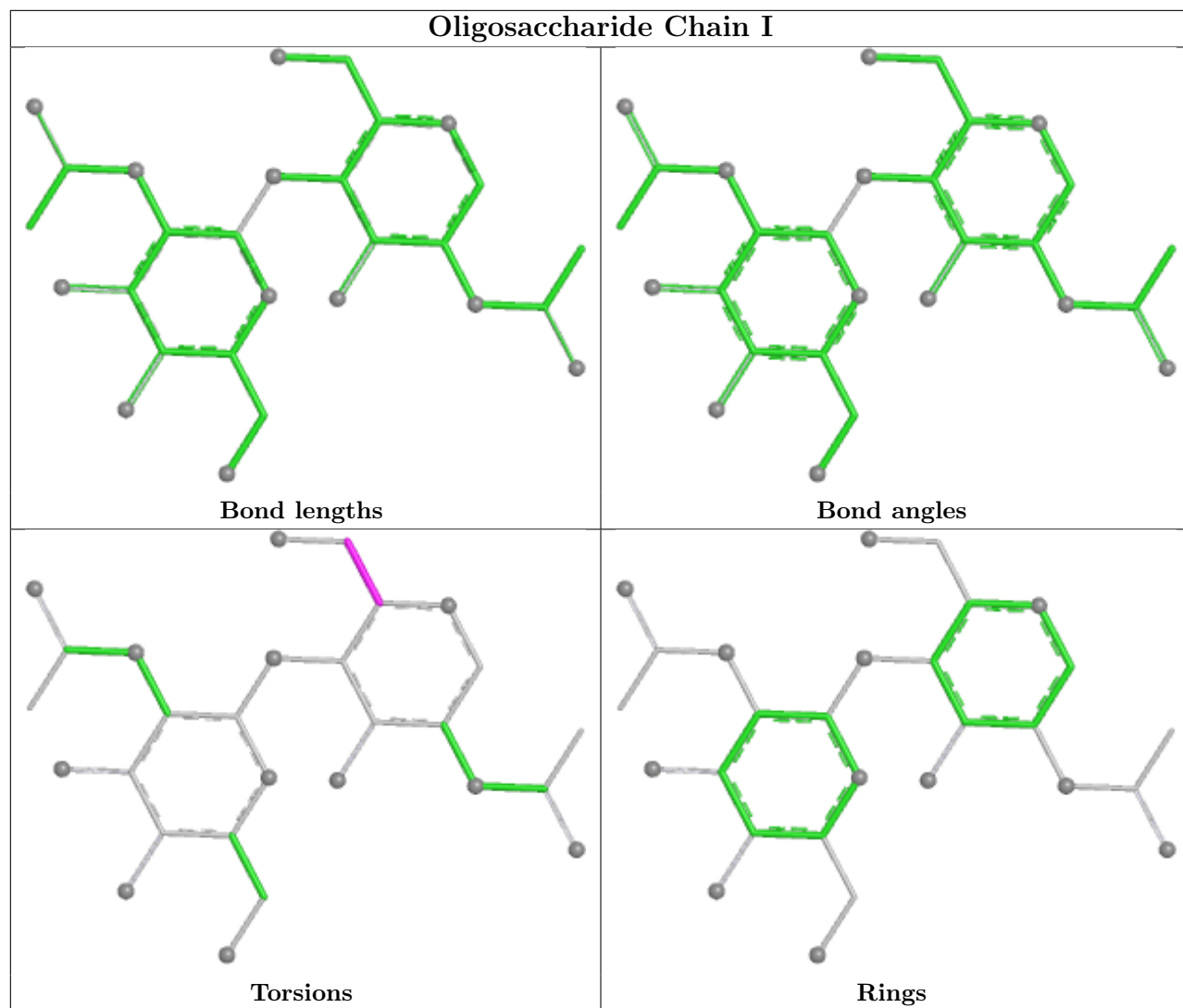
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NAG	2	0

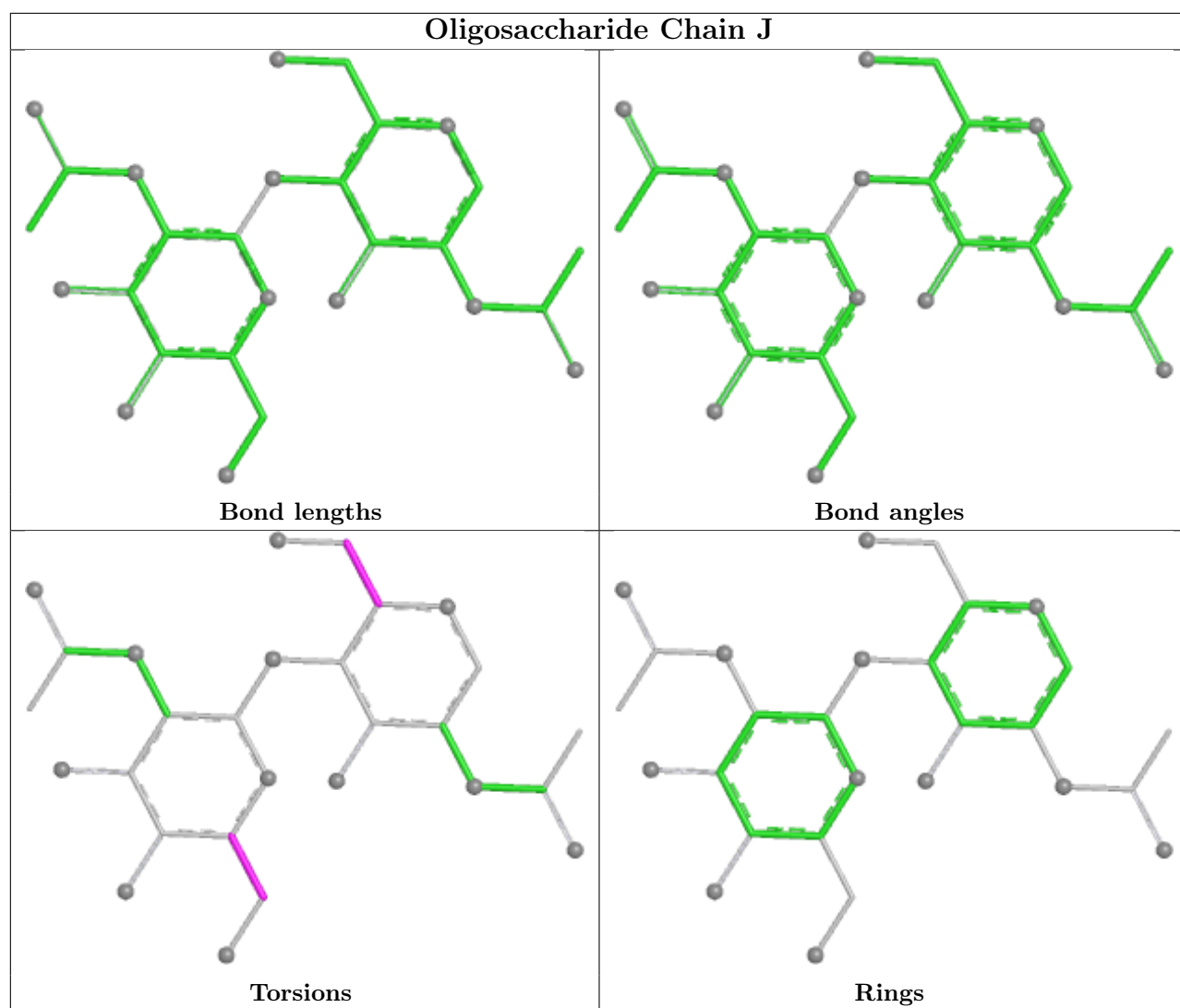
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

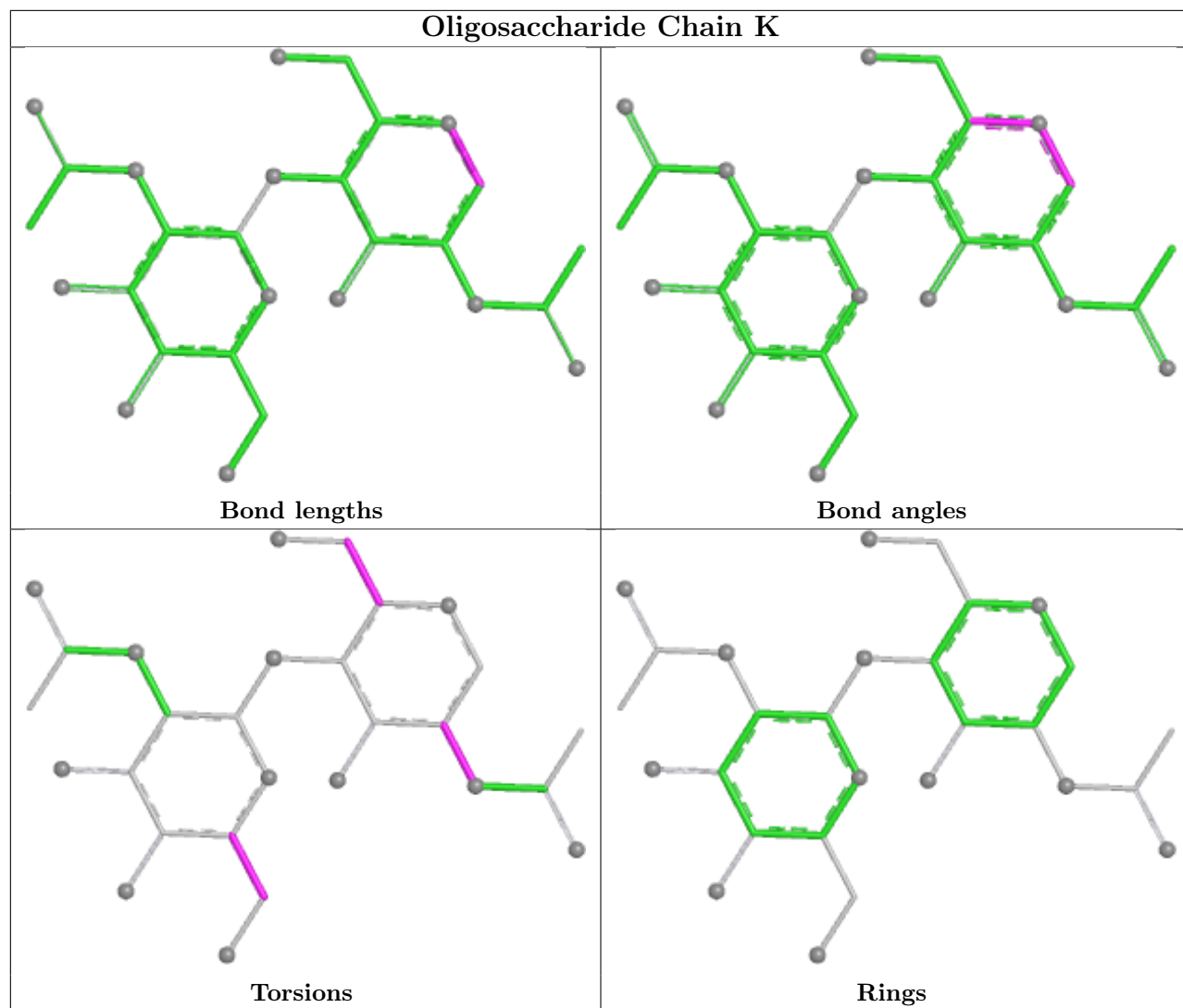


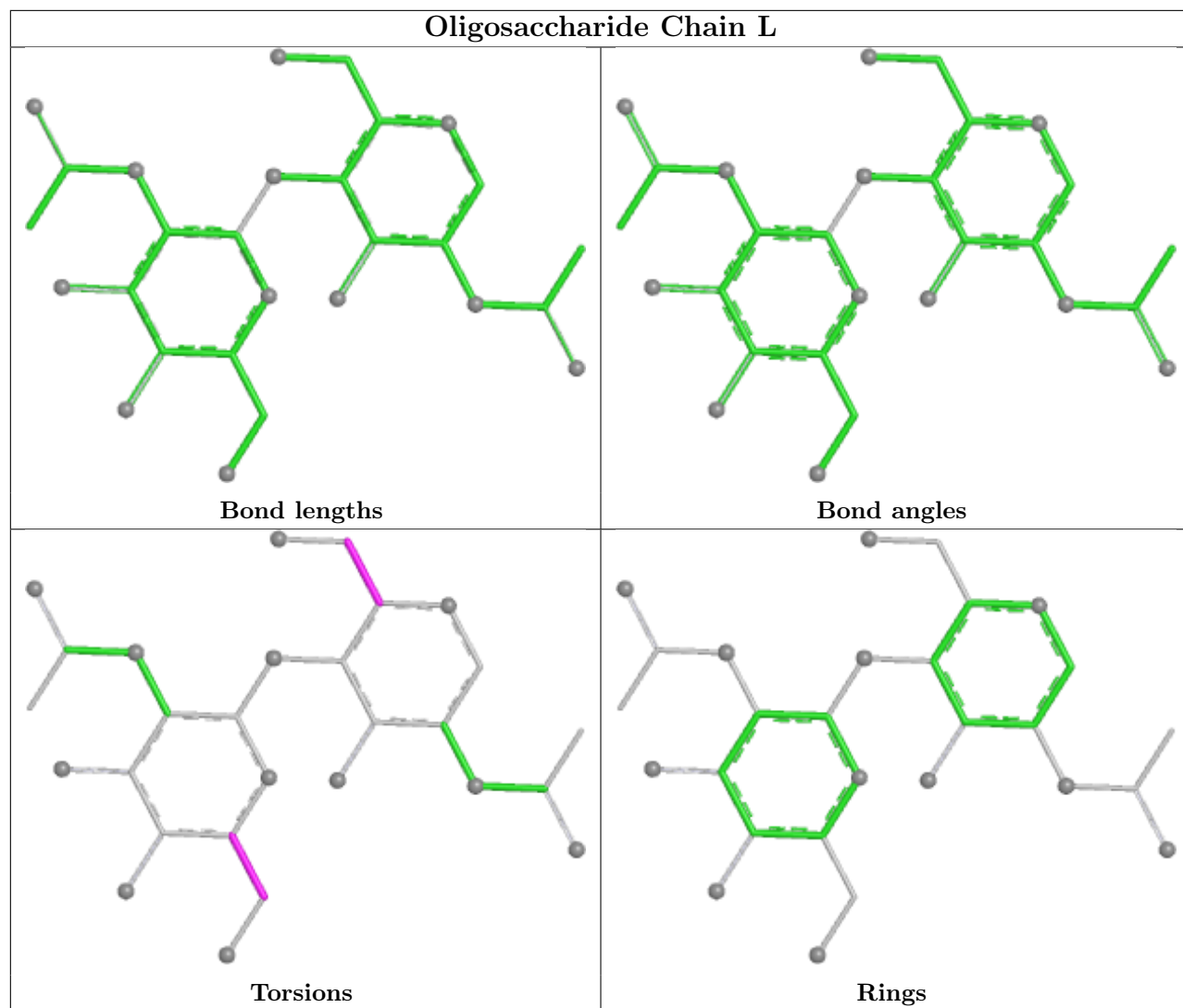


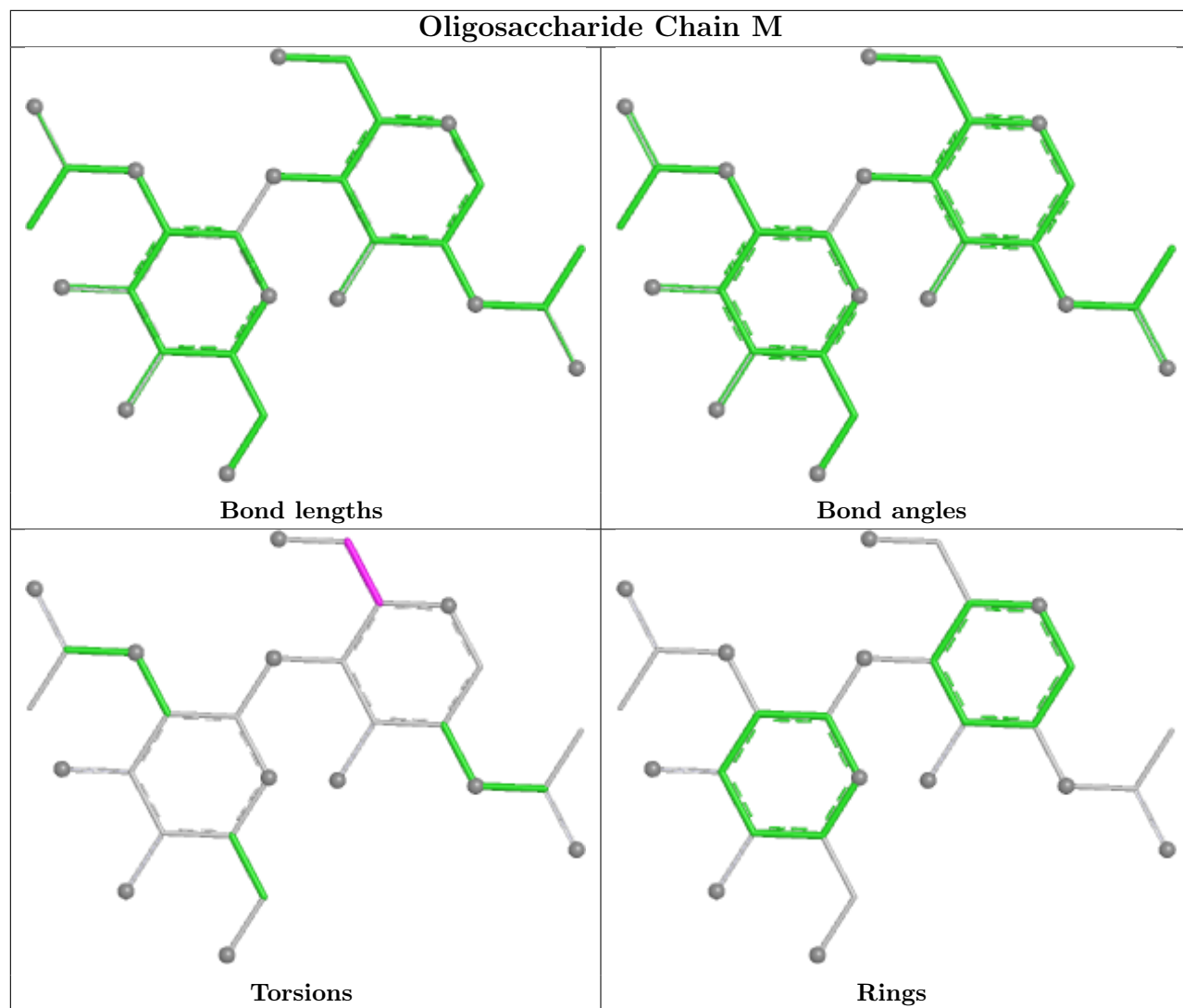


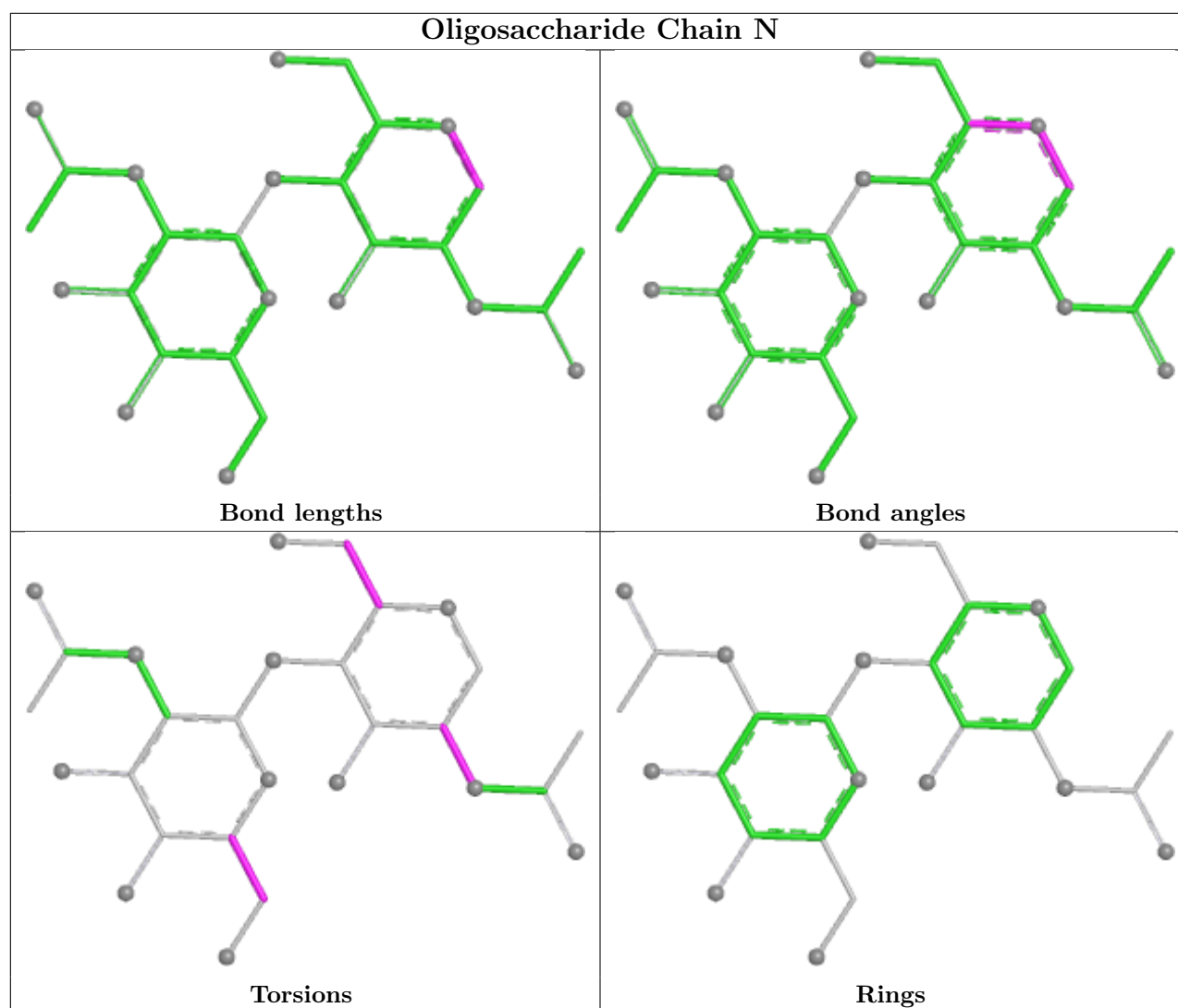












5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 4 are monoatomic - leaving 53 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	F	1305	-	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	G	906	2	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	1303	-	14,14,15	0.23	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	1304	-	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	C	1307	-	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	C	1311	1	14,14,15	0.22	0	17,19,21	0.38	0
4	NAG	B	1307	-	14,14,15	0.44	0	17,19,21	0.78	1 (5%)
4	NAG	D	905	2	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	C	1312	1	14,14,15	0.47	0	17,19,21	1.35	2 (11%)
4	NAG	C	1315	1	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	B	1314	-	14,14,15	0.22	0	17,19,21	0.56	0
4	NAG	B	1303	-	14,14,15	0.28	0	17,19,21	0.43	0
4	NAG	F	1302	-	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	C	1313	1	14,14,15	0.18	0	17,19,21	0.44	0
4	NAG	B	1305	-	14,14,15	0.27	0	17,19,21	0.57	0
4	NAG	C	1308	-	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	F	1308	-	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	F	1304	-	14,14,15	0.21	0	17,19,21	0.59	0
4	NAG	C	1306	-	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	B	1302	-	14,14,15	0.19	0	17,19,21	0.47	0
4	NAG	B	1315	-	14,14,15	0.19	0	17,19,21	0.47	0
4	NAG	B	1313	1	14,14,15	0.18	0	17,19,21	0.44	0
4	NAG	B	1301	-	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	B	1311	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	F	1303	-	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	F	1311	1	14,14,15	0.18	0	17,19,21	0.42	0
4	NAG	B	1304	-	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	G	905	2	14,14,15	0.25	0	17,19,21	0.41	0
4	NAG	B	1306	-	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	F	1312	-	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	F	1309	1	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	C	1310	1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	F	1313	1	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	F	1306	-	14,14,15	0.60	0	17,19,21	1.04	2 (11%)
4	NAG	C	1317	-	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	D	903	2	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	C	1305	-	14,14,15	0.24	0	17,19,21	0.56	0
4	NAG	D	904	2	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	B	1312	1	14,14,15	0.42	0	17,19,21	1.34	2 (11%)
4	NAG	G	904	2	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	B	1310	1	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	C	1316	-	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	D	906	2	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	B	1309	-	14,14,15	0.37	0	17,19,21	0.66	0
4	NAG	F	1307	-	14,14,15	0.29	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1314	-	14,14,15	0.22	0	17,19,21	0.54	0
4	NAG	G	903	2	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	C	1301	-	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	F	1301	-	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	F	1310	-	14,14,15	0.44	0	17,19,21	1.35	2 (11%)
4	NAG	C	1309	-	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	C	1302	-	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	B	1308	-	14,14,15	0.21	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1305	-	-	3/6/23/26	0/1/1/1
4	NAG	G	906	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1307	-	-	4/6/23/26	0/1/1/1
4	NAG	D	905	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1315	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1314	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	0/6/23/26	0/1/1/1
4	NAG	F	1302	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1308	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1308	-	-	1/6/23/26	0/1/1/1
4	NAG	F	1304	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1315	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1303	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	-	-	3/6/23/26	0/1/1/1
4	NAG	G	905	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1312	-	-	3/6/23/26	0/1/1/1
4	NAG	F	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	F	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	F	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1317	-	-	2/6/23/26	0/1/1/1
4	NAG	D	903	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	-	-	3/6/23/26	0/1/1/1
4	NAG	D	904	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	6/6/23/26	0/1/1/1
4	NAG	G	904	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1316	-	-	2/6/23/26	0/1/1/1
4	NAG	D	906	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1307	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1314	-	-	4/6/23/26	0/1/1/1
4	NAG	G	903	2	-	3/6/23/26	0/1/1/1
4	NAG	C	1301	-	-	1/6/23/26	0/1/1/1
4	NAG	F	1301	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1310	-	-	6/6/23/26	0/1/1/1
4	NAG	C	1309	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1312	NAG	C2-N2-C7	4.61	129.07	122.90
4	C	1312	NAG	C2-N2-C7	4.59	129.06	122.90
4	F	1310	NAG	C2-N2-C7	4.57	129.02	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1306	NAG	C1-O5-C5	3.02	116.24	112.19
4	B	1307	NAG	C1-O5-C5	2.89	116.06	112.19

There are no chirality outliers.

5 of 112 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1302	NAG	C4-C5-C6-O6
4	C	1315	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	B	1312	NAG	C4-C5-C6-O6
4	C	1317	NAG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1305	NAG	1	0
4	C	1307	NAG	1	0
4	C	1312	NAG	1	0
4	C	1308	NAG	1	0
4	B	1301	NAG	1	0
4	B	1312	NAG	1	0
4	B	1309	NAG	2	0
4	F	1307	NAG	1	0
4	F	1310	NAG	1	0
4	B	1308	NAG	3	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.

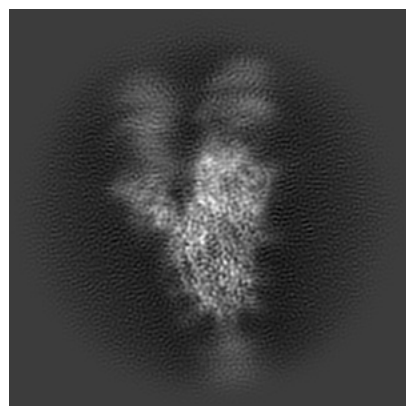
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34044. These allow visual inspection of the internal detail of the map and identification of artifacts.

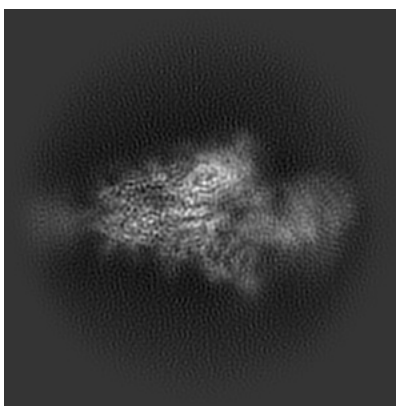
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

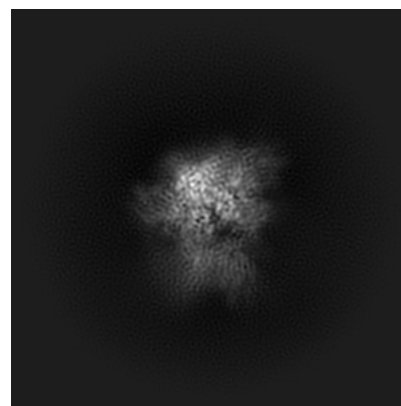
6.1.1 Primary map



X

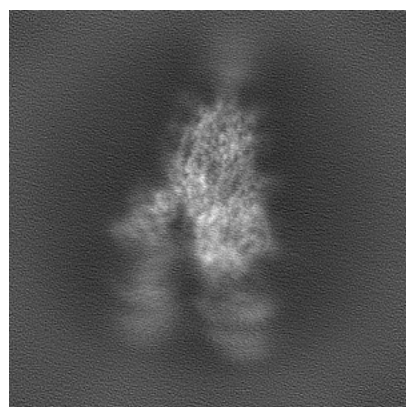


Y

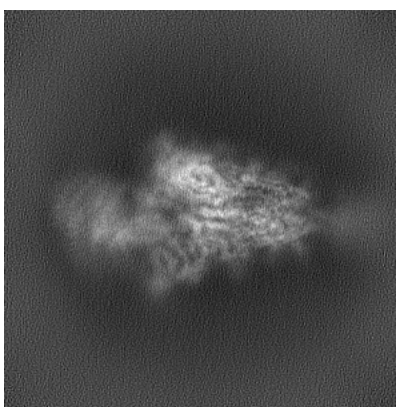


Z

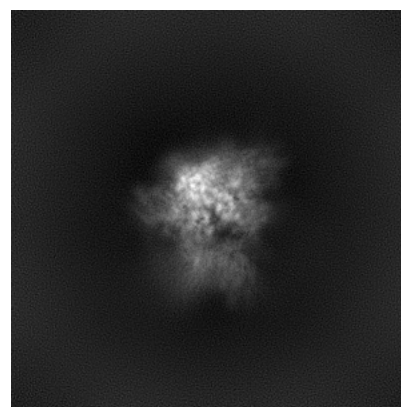
6.1.2 Raw map



X



Y

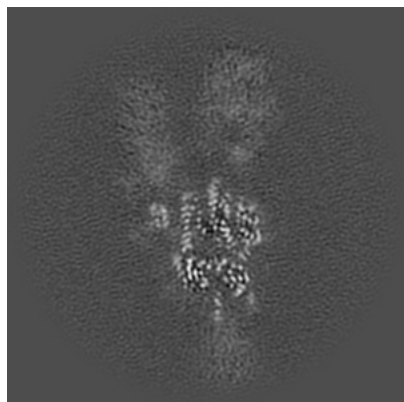


Z

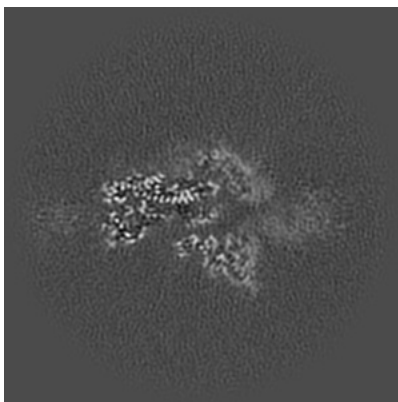
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

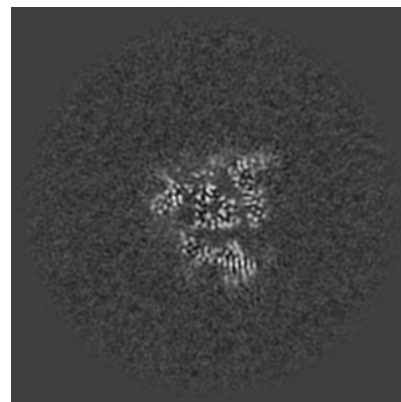
6.2.1 Primary map



X Index: 160

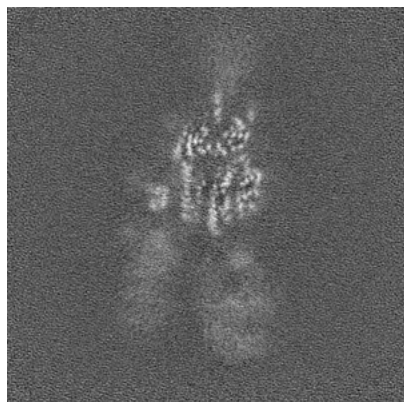


Y Index: 160

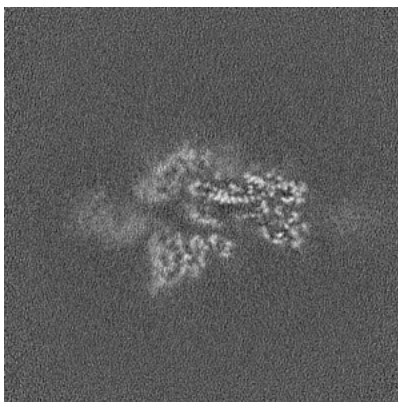


Z Index: 160

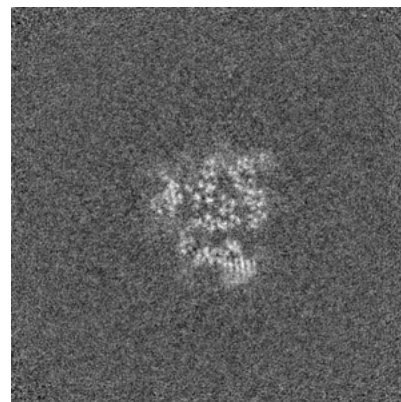
6.2.2 Raw map



X Index: 160



Y Index: 160

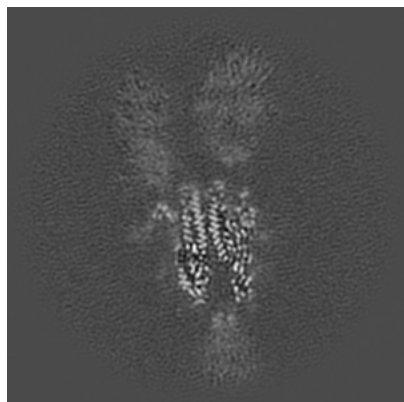


Z Index: 160

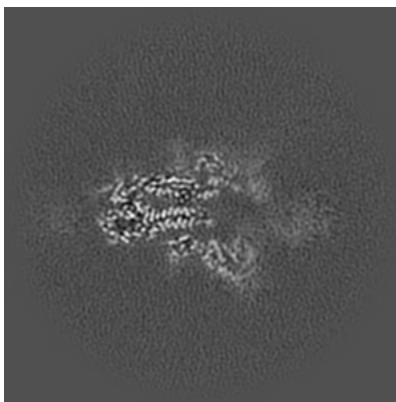
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

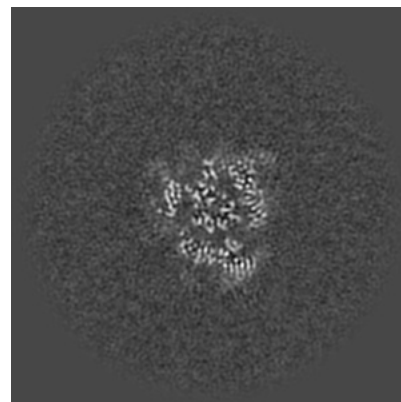
6.3.1 Primary map



X Index: 156

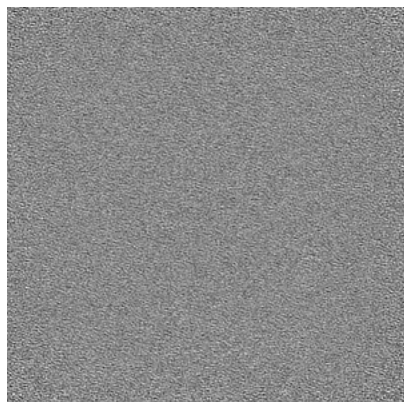


Y Index: 155

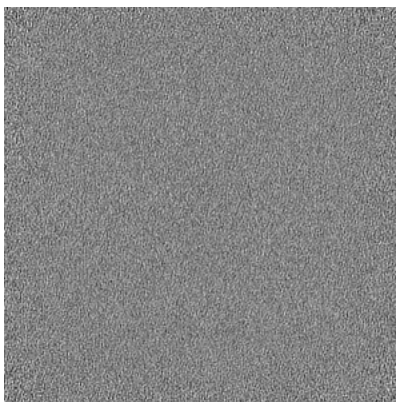


Z Index: 158

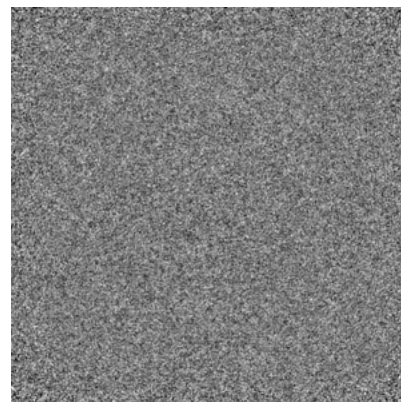
6.3.2 Raw map



X Index: 0



Y Index: 0

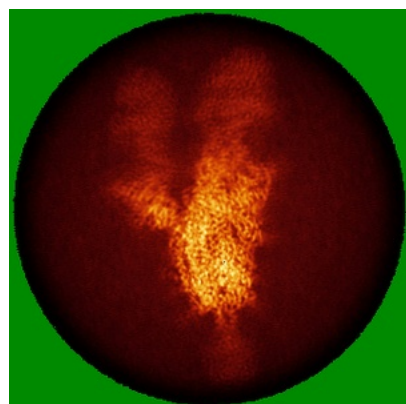


Z Index: 0

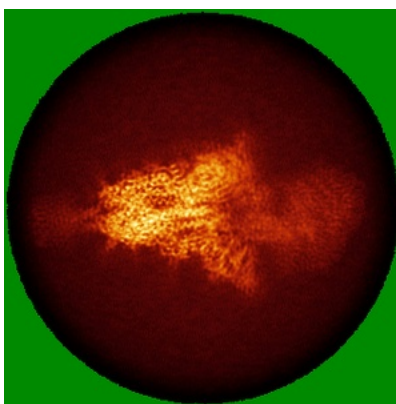
The images above show the largest variance slices of the map in three orthogonal directions.

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

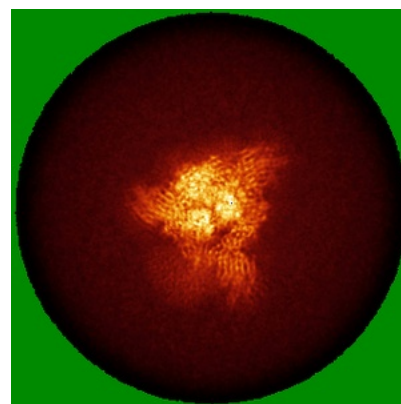
6.4.1 Primary map



X

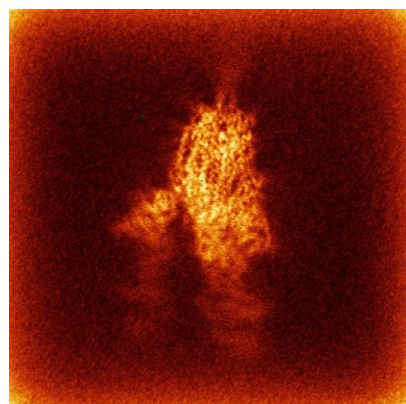


Y

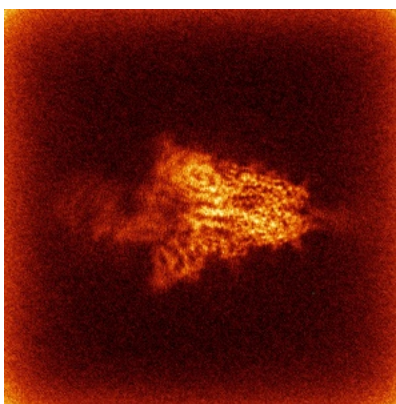


Z

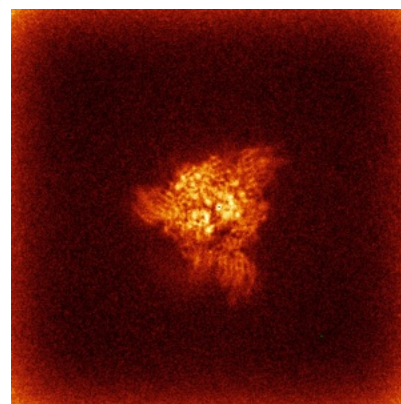
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



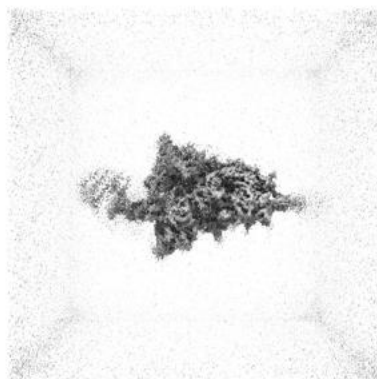
Z

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

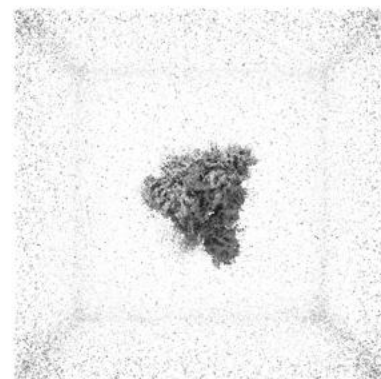
6.5.2 Raw map



X



Y



Z

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

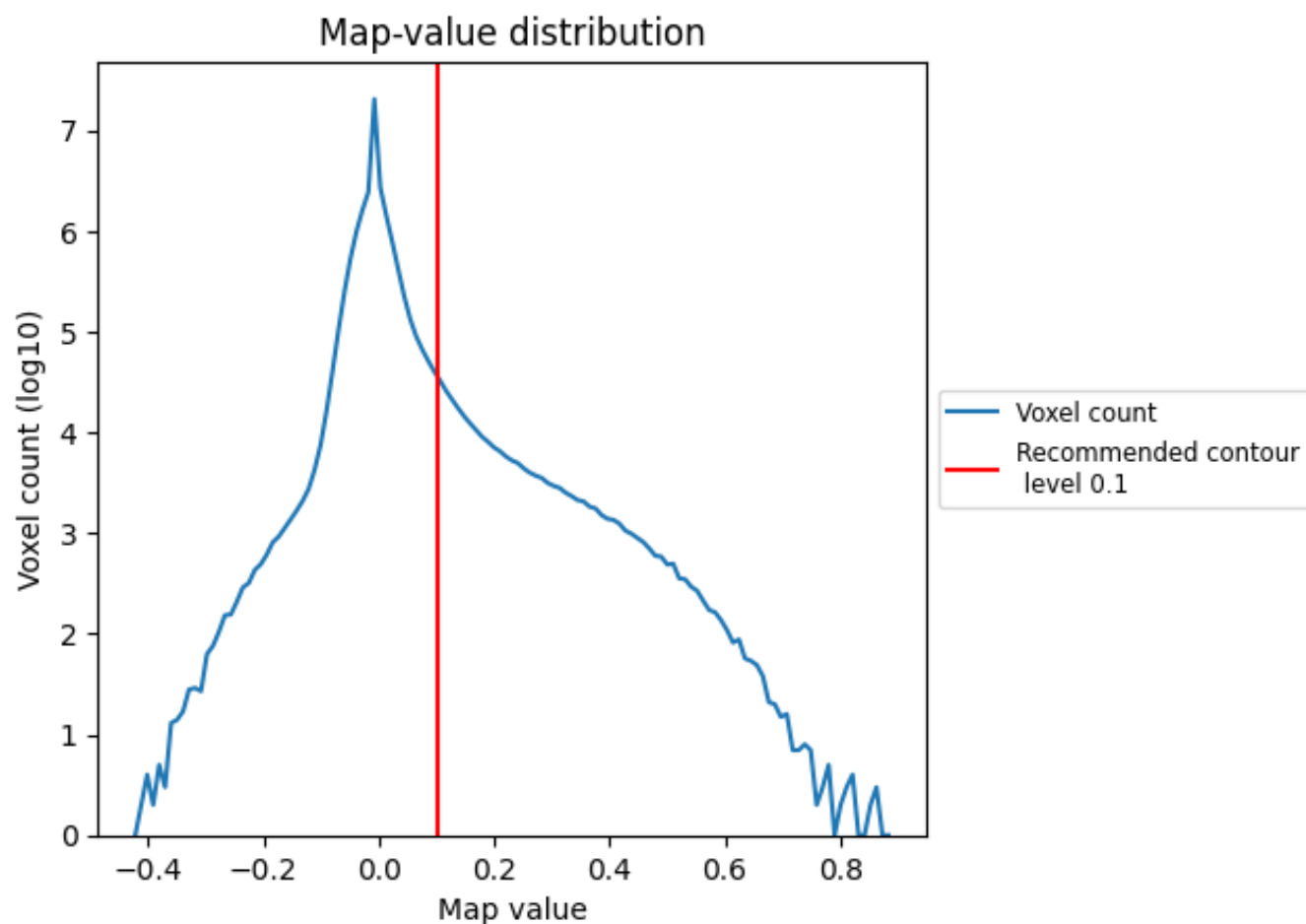
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

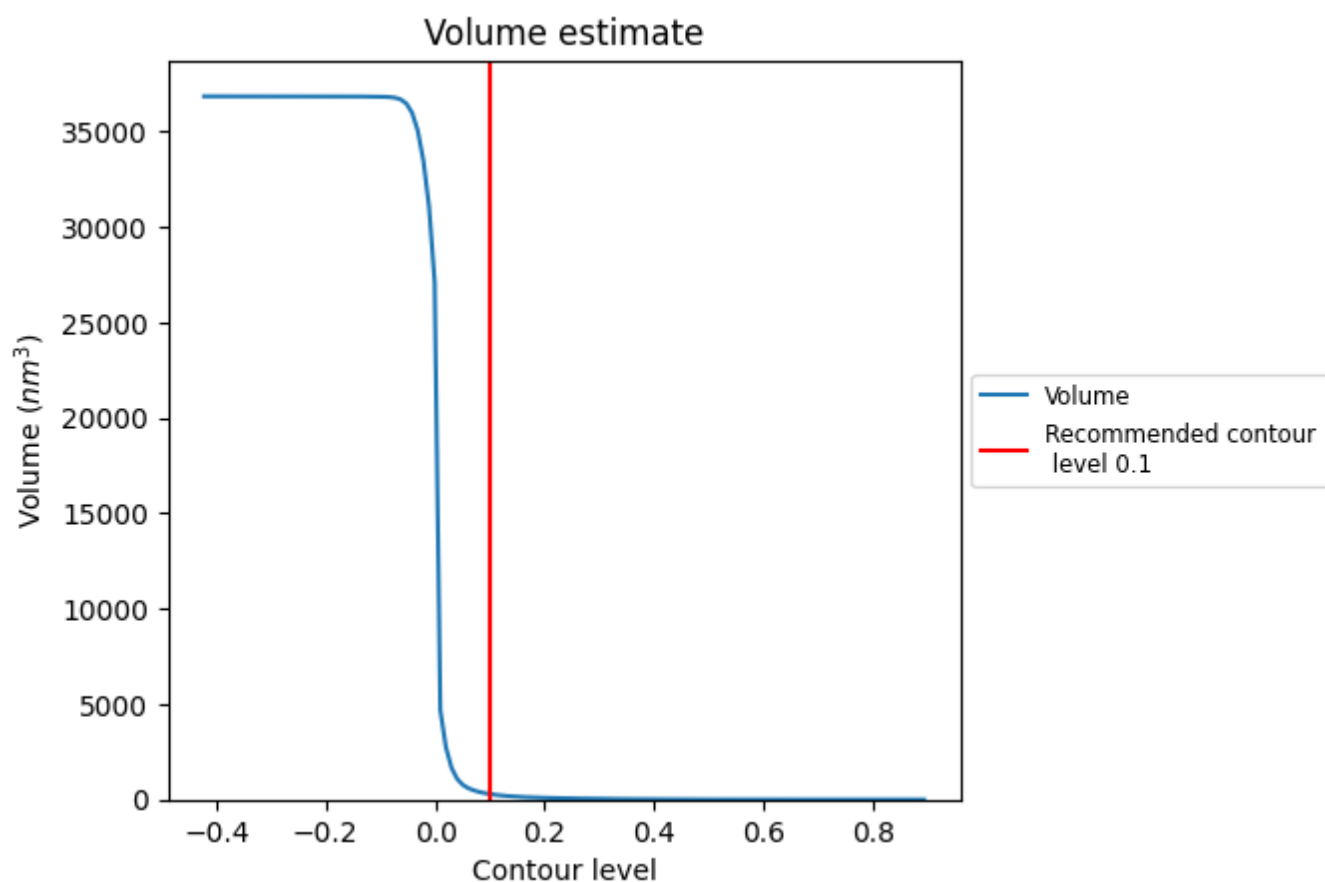
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

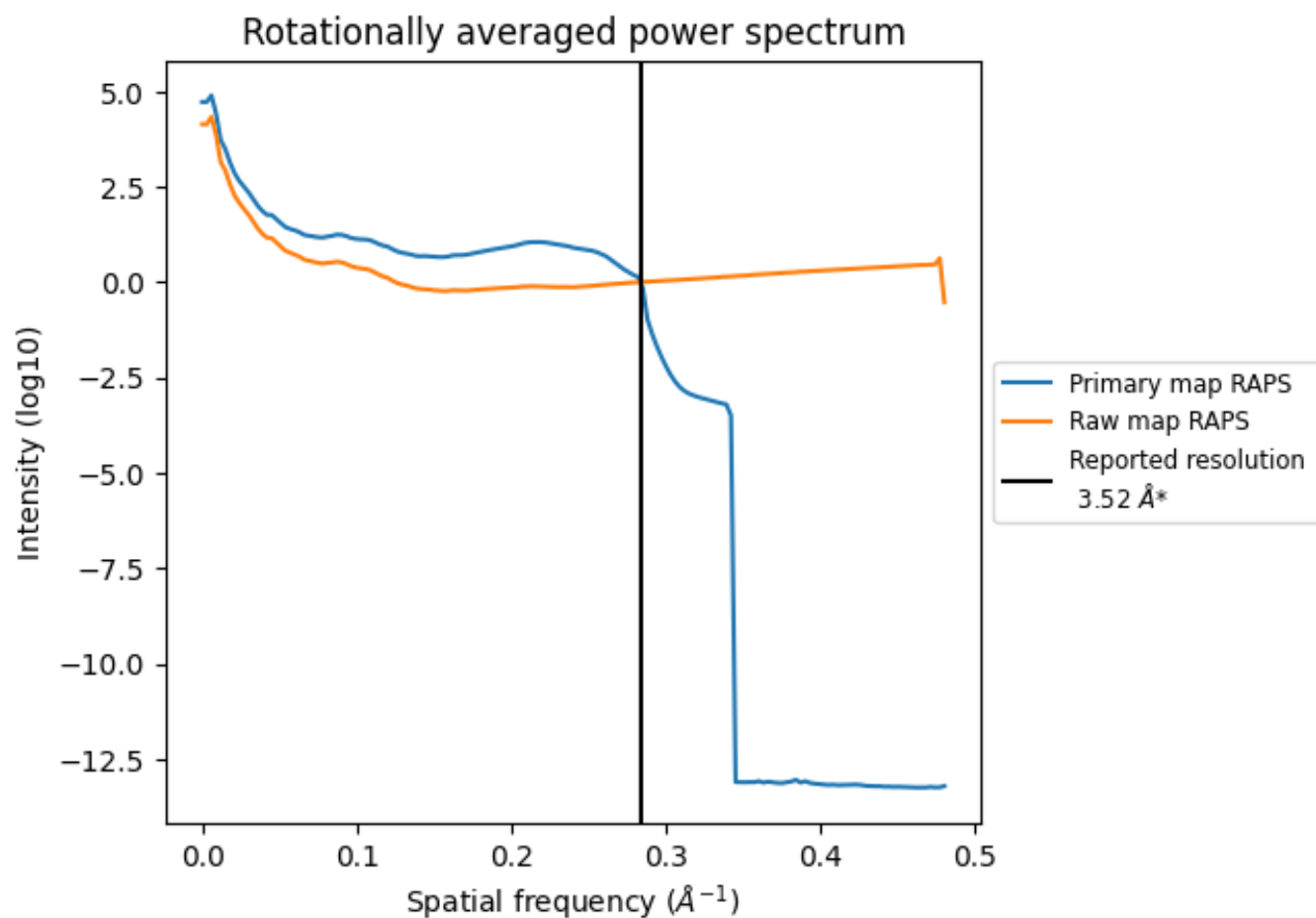
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290 nm³; this corresponds to an approximate mass of 262 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 ⓘ

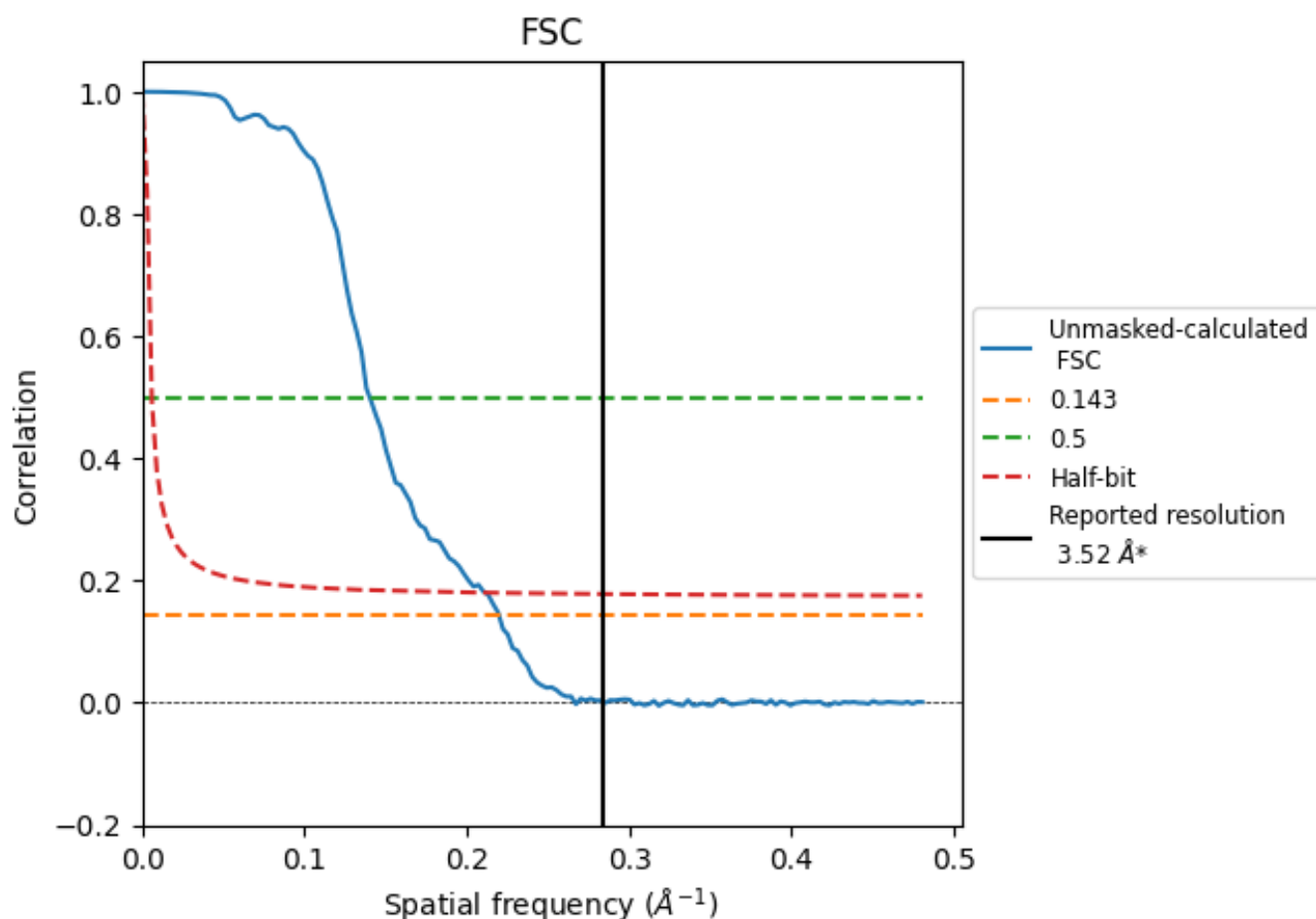


*Reported resolution corresponds to spatial frequency of 0.284 $\text{\AA}^{-1}$

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 0.284 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

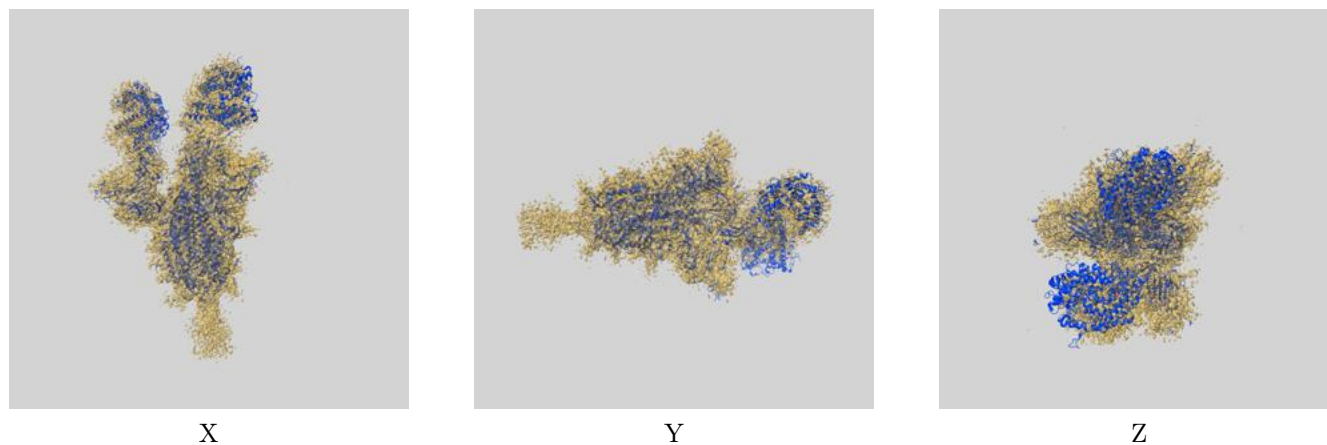
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.55	7.13	4.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.55 differs from the reported value 3.52 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34044 and PDB model 7YR3. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



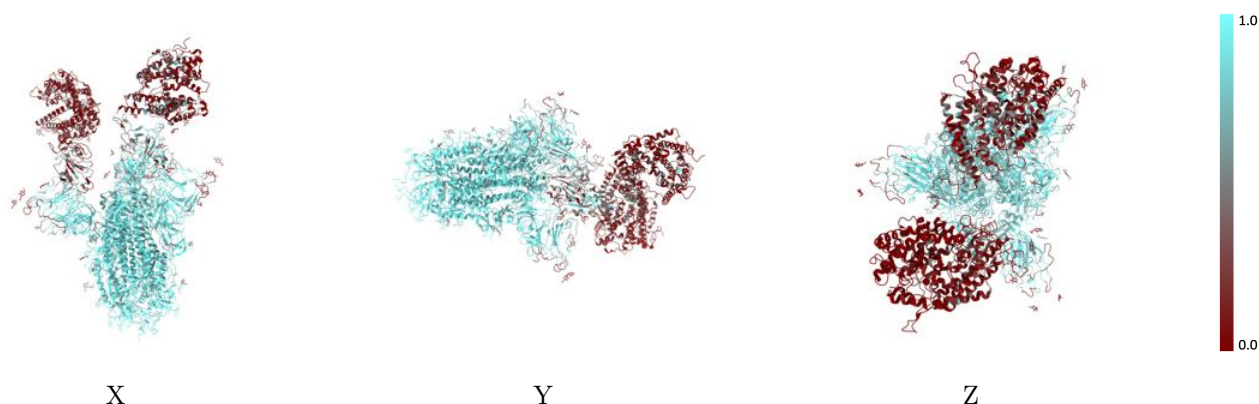
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



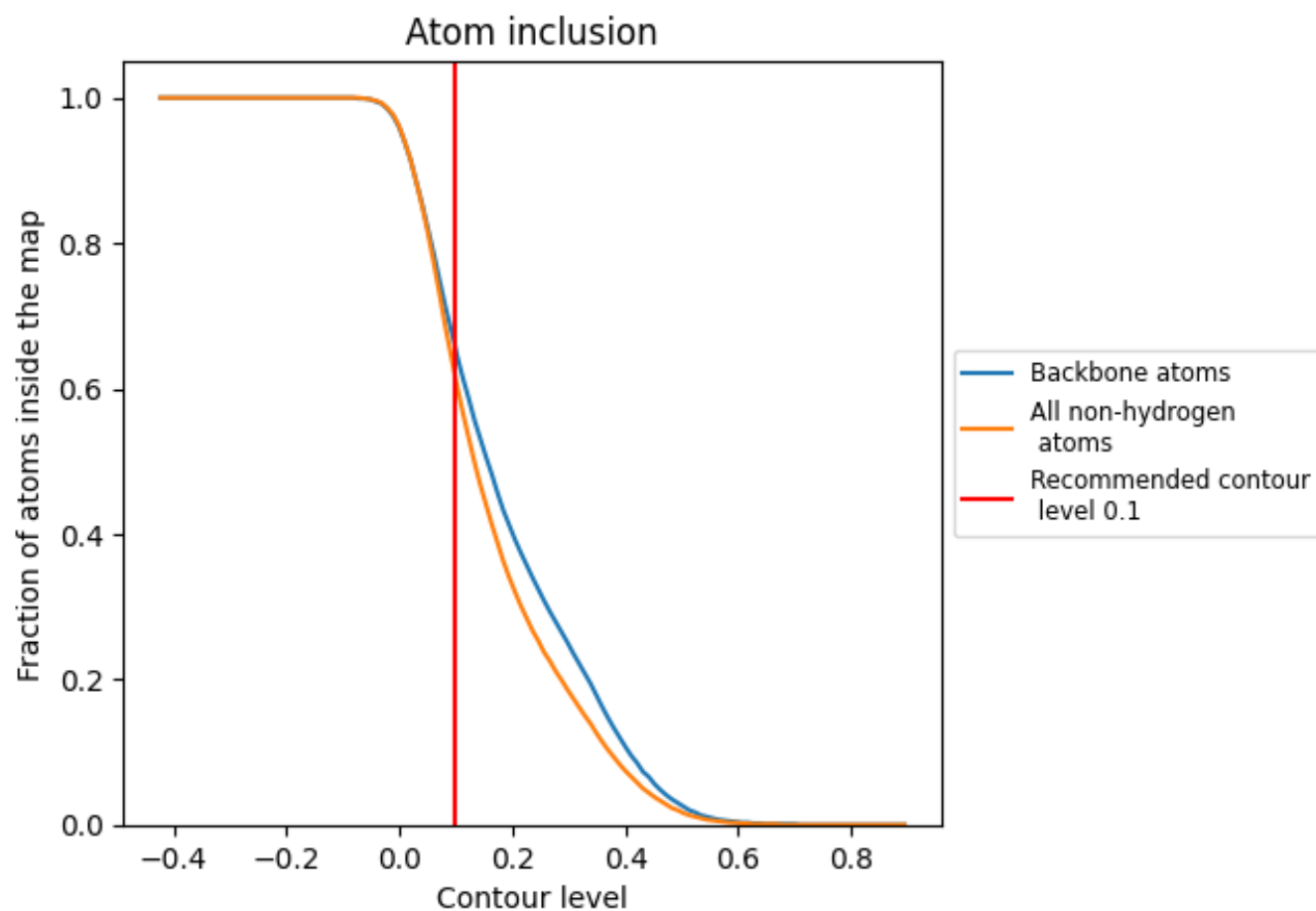
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6130	0.3140
A	0.8570	0.4270
B	0.7560	0.3810
C	0.8300	0.4090
D	0.0730	0.1000
E	0.7500	0.3650
F	0.7990	0.3860
G	0.1950	0.1130
H	0.6070	0.3760
I	0.8570	0.4830
J	0.6430	0.2910
K	0.6790	0.4300
L	0.8930	0.4500
M	0.5710	0.2810
N	0.6070	0.3400

