



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 10:59 AM EST

PDB ID : 7TB8  
EMDB ID : EMD-25794  
Title : Cryo-EM structure of SARS-CoV-2 spike in complex with antibodies B1-182.1 and A19-61.1  
Authors : Zhou, T.; Tsybovsky, T.; Kwong, P.D.  
Deposited on : 2021-12-21  
Resolution : 2.83 Å(reported)  
Based on initial model : 7MM0

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

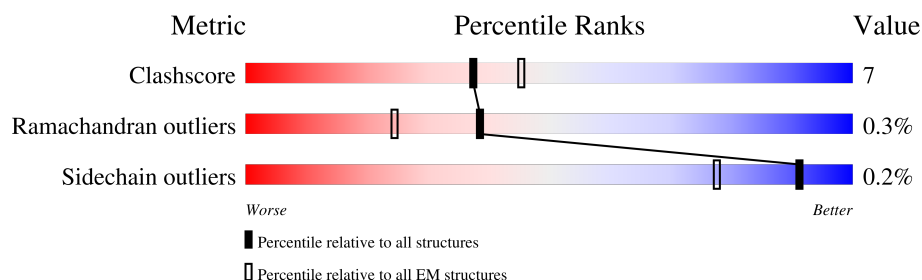
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.83 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1195	
1	B	1195	
1	C	1195	
2	D	127	
2	F	127	
2	J	127	
3	E	107	
3	G	107	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	K	107	 96% 10%
4	H	123	 87% 25%
5	L	108	 98% 18%
6	I	2	 50% 50%
6	N	2	 50% 50%
6	O	2	 100%
6	P	2	 100%
6	Q	2	 50% 50%
6	R	2	 100%
6	S	2	 100%
6	T	2	 100%
7	M	2	 100%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 33230 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	1085	Total	C	N	O	S	0	0
			8492	5421	1418	1615	38		
1	B	1088	Total	C	N	O	S	0	0
			8513	5434	1421	1620	38		
1	C	1088	Total	C	N	O	S	0	0
			8514	5436	1421	1619	38		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called The heavy chain of SARS-CoV-2 antibody A19-61.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	126	Total	C	N	O	S	0	0
			973	614	169	186	4		
2	F	126	Total	C	N	O	S	0	0
			973	614	169	186	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	126	Total	C	N	O	S	0	0
			973	614	169	186	4		

- Molecule 3 is a protein called The light chain of SARS-COV-2 antibody A19-61.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	107	Total	C	N	O	S	0	0
			813	512	136	162	3		
3	G	107	Total	C	N	O	S	0	0
			813	512	136	162	3		
3	K	107	Total	C	N	O	S	0	0
			813	512	136	162	3		

- Molecule 4 is a protein called The heavy chain of SARS-CoV-2 antibody B1-182.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	122	Total	C	N	O	S	1	0
			932	584	159	181	8		

- Molecule 5 is a protein called The light chain of SARS-COV-2 antibody B1-182.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	107	Total	C	N	O	S	1	0
			819	516	138	163	2		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



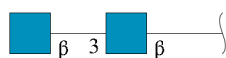
Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	O	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		

*Continued on next page...*

Continued from previous page...

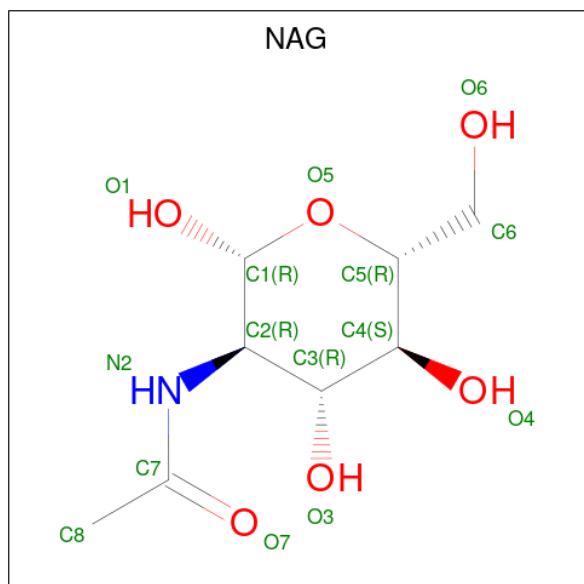
Mol	Chain	Residues	Atoms				AltConf	Trace
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

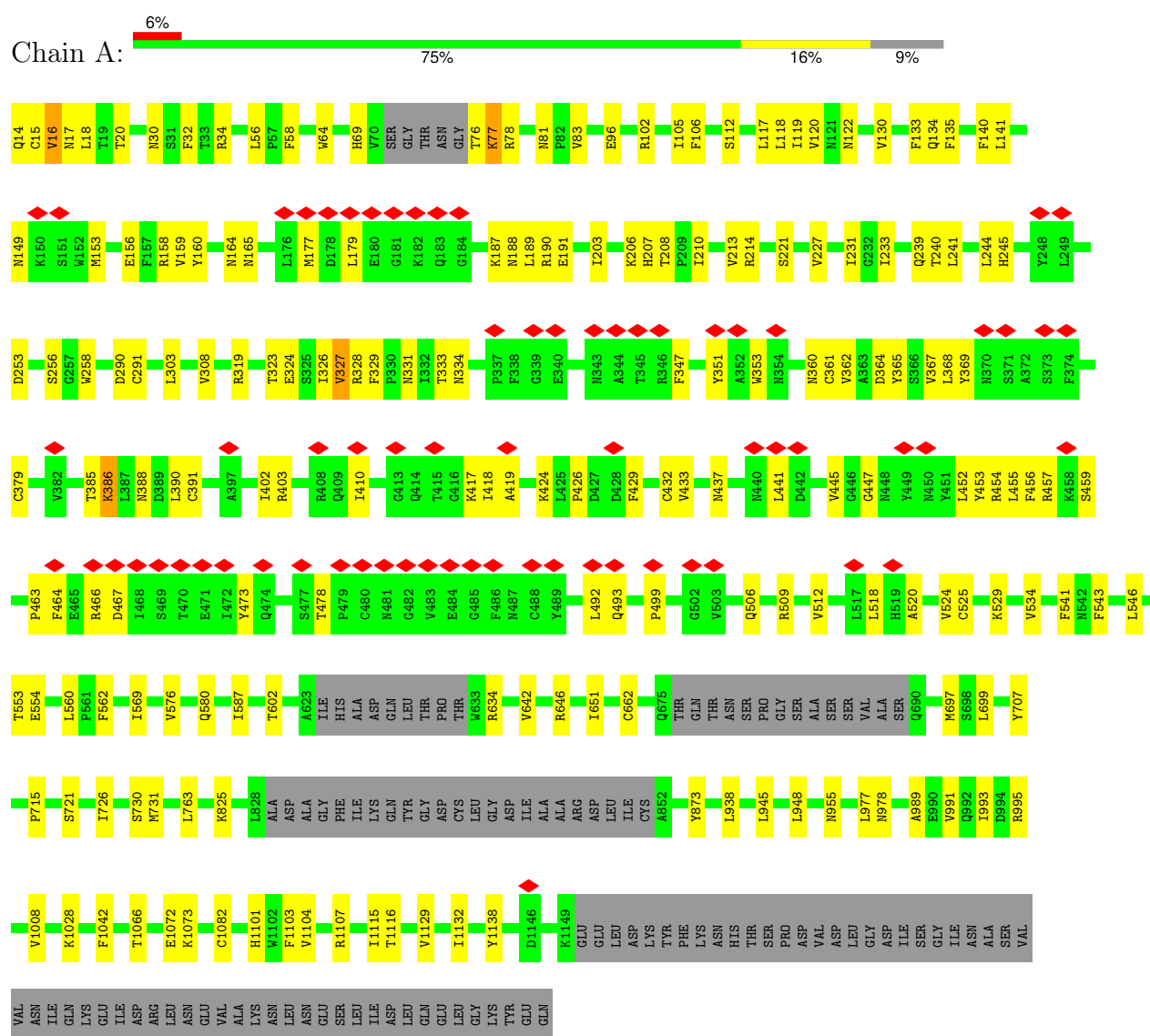
Mol	Chain	Residues	Atoms				AltConf
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	



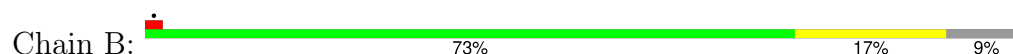
### 3 Residue-property plots

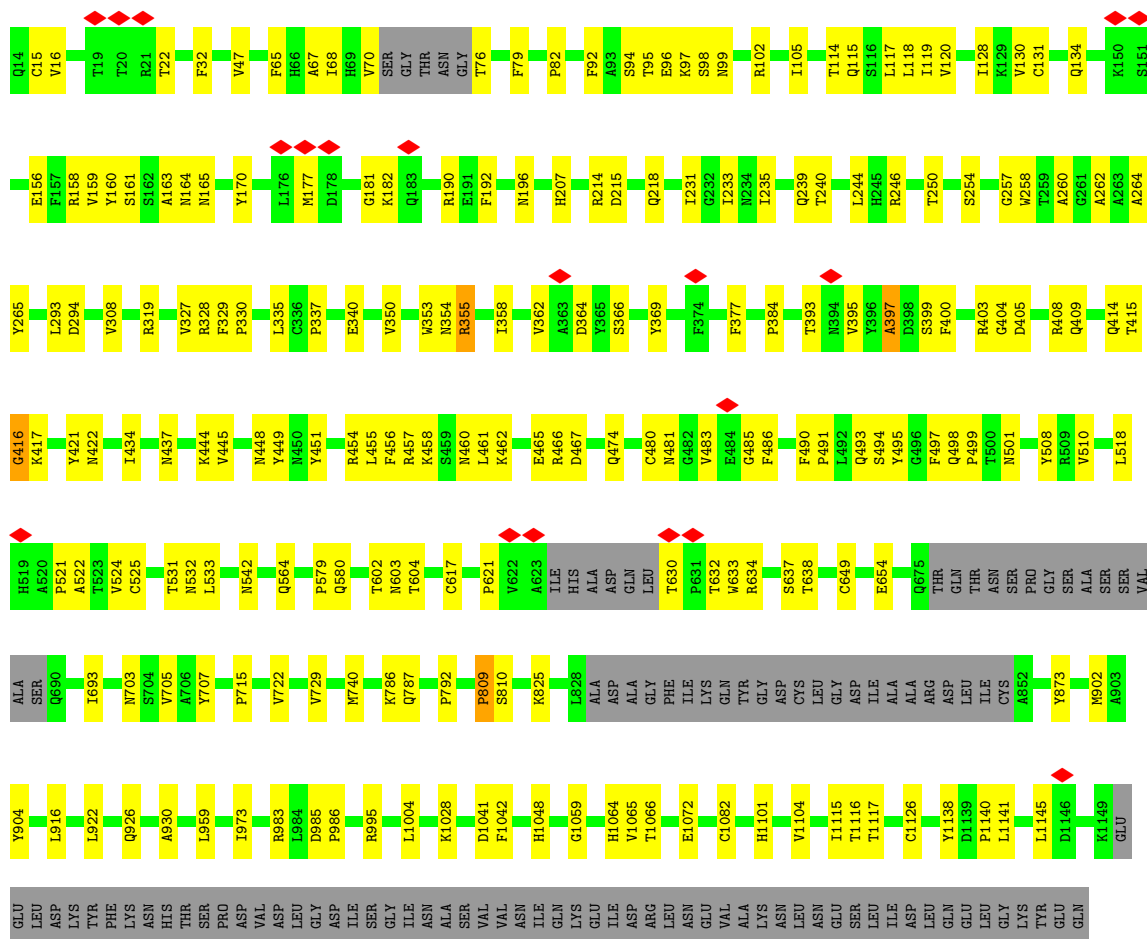
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Spike glycoprotein

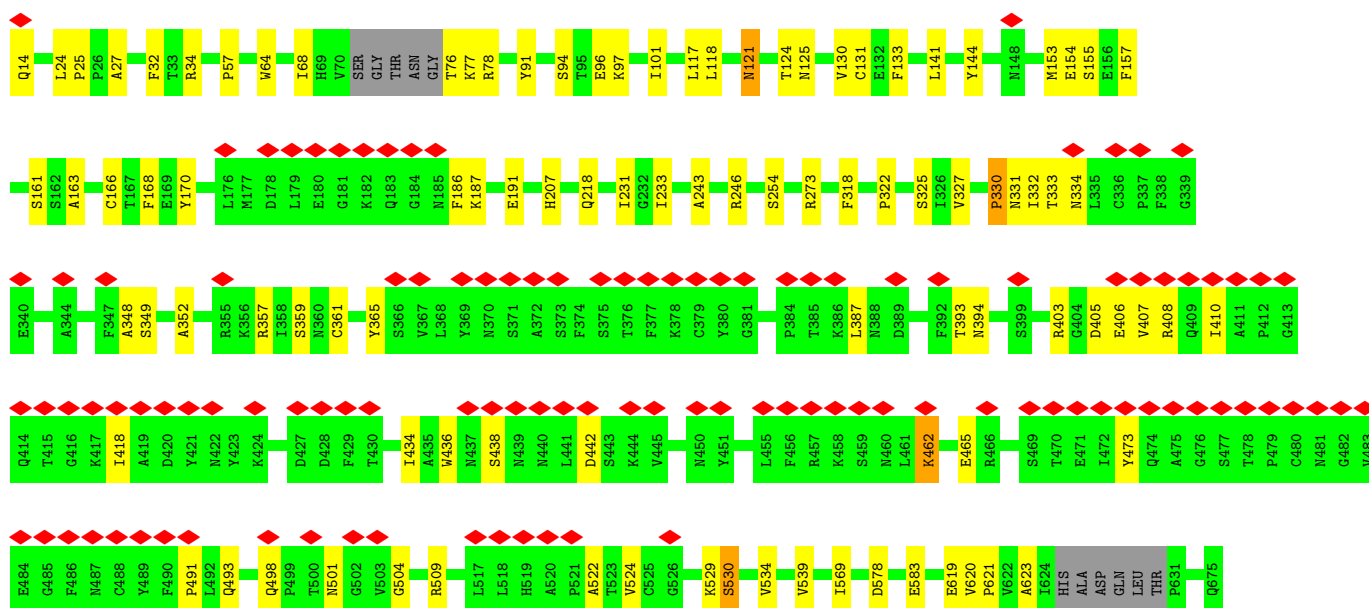
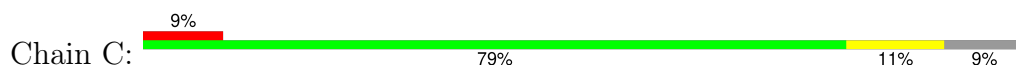


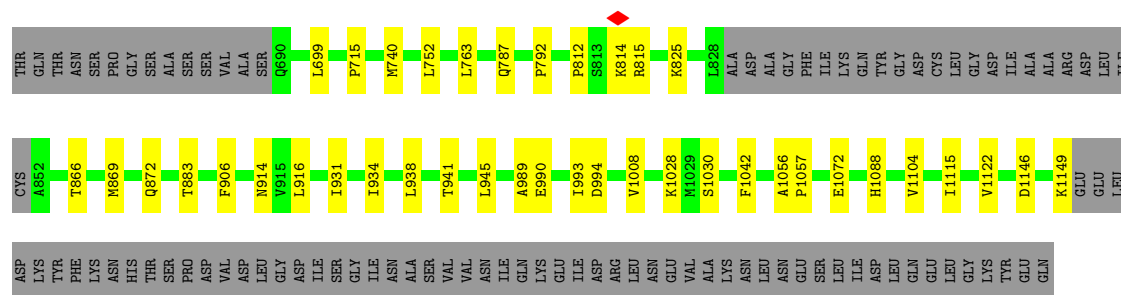
#### • Molecule 1: Spike glycoprotein





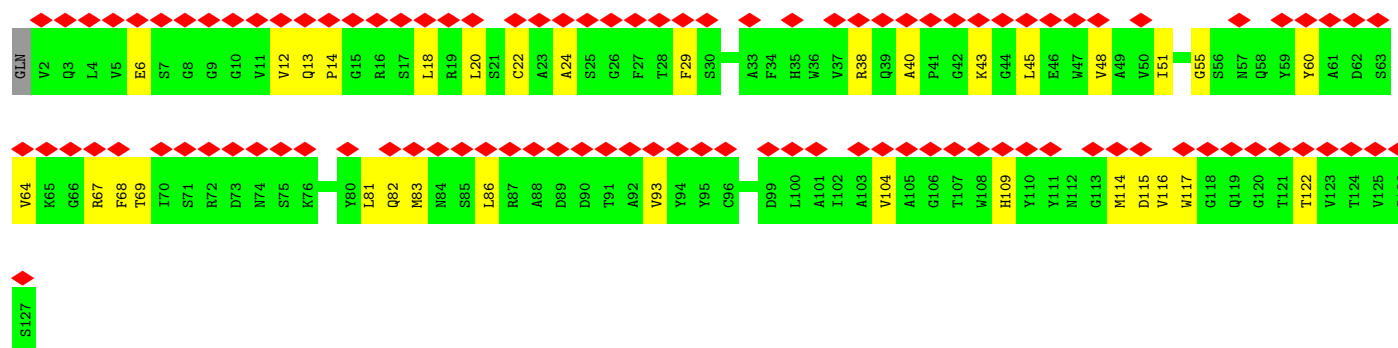
• Molecule 1: Spike glycoprotein





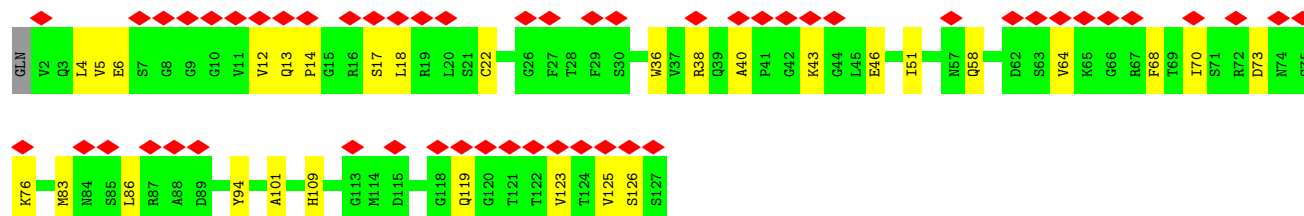
- Molecule 2: The heavy chain of SARS-CoV-2 antibody A19-61.1

Chain D: 81%  
73% 26%



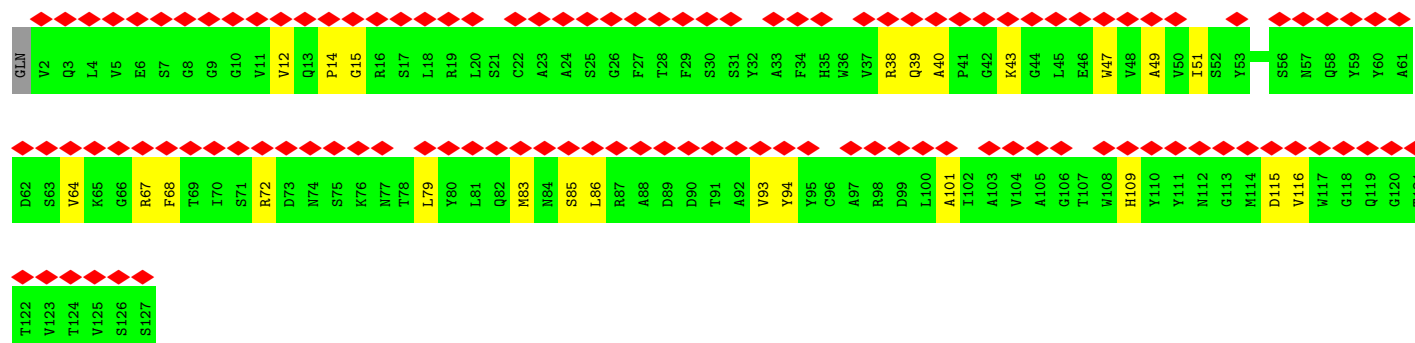
- Molecule 2: The heavy chain of SARS-CoV-2 antibody A19-61.1

Chain F: 42%  
76% 24%

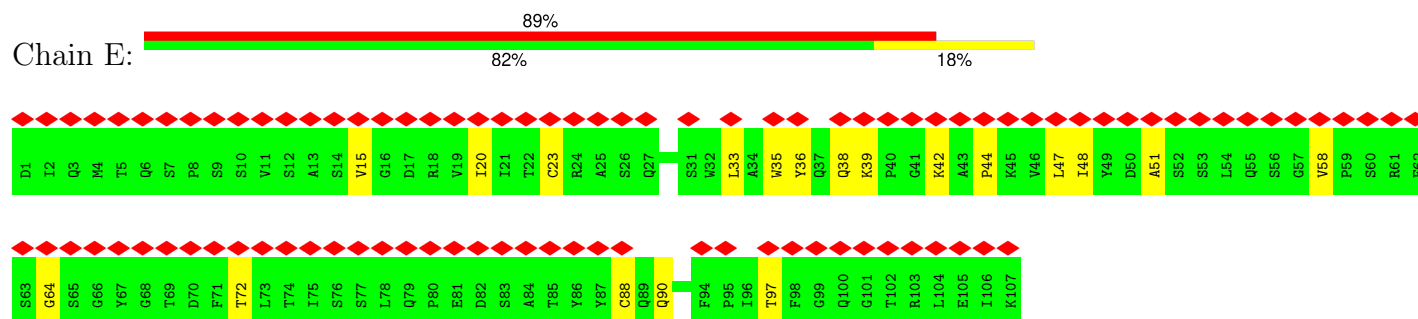


- Molecule 2: The heavy chain of SARS-CoV-2 antibody A19-61.1

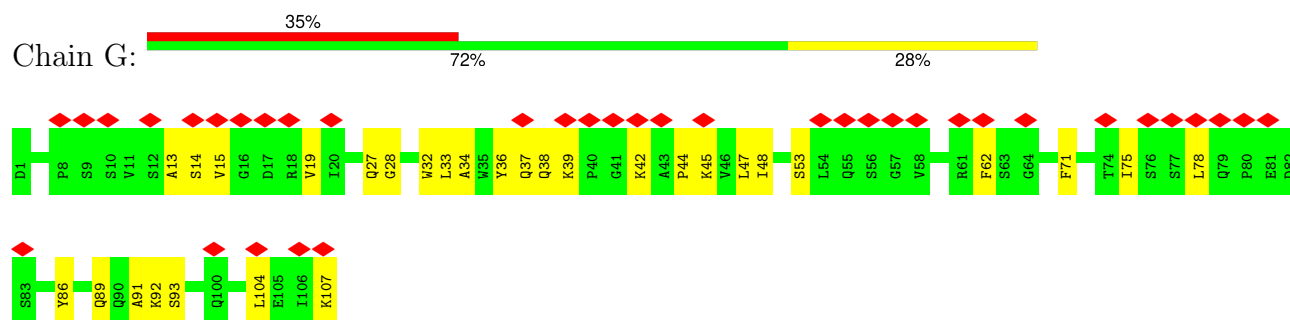
Chain J: 91%  
80% 19%



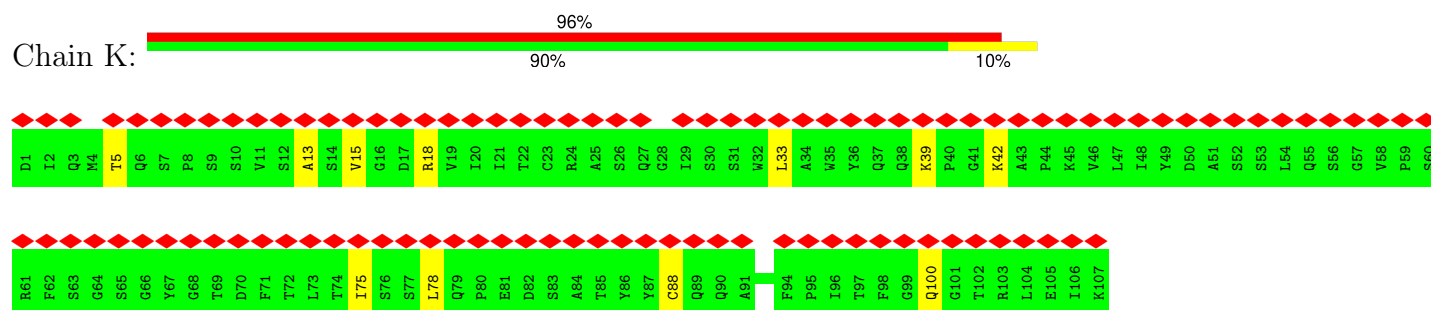
- Molecule 3: The light chain of SARS-COV-2 antibody A19-61.1



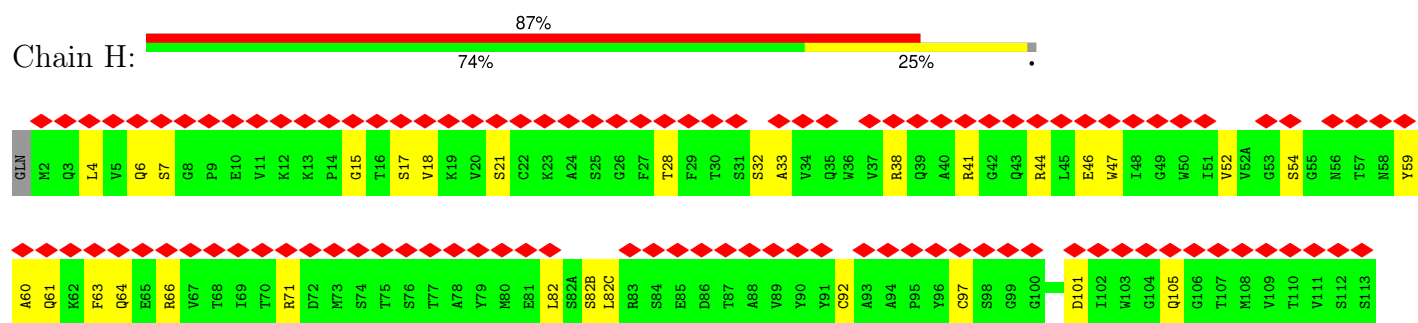
- Molecule 3: The light chain of SARS-COV-2 antibody A19-61.1



- Molecule 3: The light chain of SARS-COV-2 antibody A19-61.1



- Molecule 4: The heavy chain of SARS-CoV-2 antibody B1-182.1



- Molecule 5: The light chain of SARS-COV-2 antibody B1-182.1





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	358526	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.720	Depositor
Minimum map value	-0.203	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0838	Depositor
Map size ( $\text{\AA}$ )	453.96002, 453.96002, 453.96002	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.873, 0.873, 0.873	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.27	0/8690	0.50	0/11824
1	B	0.28	0/8714	0.52	1/11863 (0.0%)
1	C	0.28	0/8715	0.50	0/11863
2	D	0.24	0/997	0.51	0/1356
2	F	0.25	0/997	0.51	0/1356
2	J	0.24	0/997	0.52	0/1356
3	E	0.25	0/831	0.49	0/1127
3	G	0.25	0/831	0.48	0/1127
3	K	0.25	0/831	0.49	0/1127
4	H	0.24	0/952	0.52	0/1289
5	L	0.25	0/840	0.52	0/1142
All	All	0.27	0/33395	0.51	1/45430 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	809	PRO	CA-N-CD	-7.05	101.63	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	397	ALA	Peptide
1	B	416	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8492	0	8274	133	0
1	B	8513	0	8296	154	0
1	C	8514	0	8297	92	0
2	D	973	0	921	20	0
2	F	973	0	921	18	0
2	J	973	0	921	13	0
3	E	813	0	798	12	0
3	G	813	0	798	19	0
3	K	813	0	798	6	0
4	H	932	0	893	18	0
5	L	819	0	784	13	0
6	I	28	0	25	0	0
6	N	28	0	25	2	0
6	O	28	0	25	0	0
6	P	28	0	25	0	0
6	Q	28	0	25	1	0
6	R	28	0	25	0	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
7	M	28	0	25	0	0
8	A	98	0	91	0	0
8	B	70	0	65	0	0
8	C	182	0	169	0	0
All	All	33230	0	32251	475	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (475) 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:67:ALA:O	1:B:262:ALA:HA	1.64	0.96
1:B:65:PHE:HB2	1:B:265:TYR:HB3	1.54	0.89
1:C:408:ARG:HH12	1:C:504:GLY:HA2	1.44	0.81
1:C:131:CYS:HB2	1:C:166:CYS:HA	1.61	0.80
1:C:246:ARG:NH1	1:C:254:SER:O	2.18	0.76
2:J:40:ALA:HB3	2:J:43:LYS:HB2	1.66	0.75
1:A:333:THR:HG22	1:A:334:ASN:H	1.50	0.75
1:C:473:TYR:H	1:C:491:PRO:HD3	1.51	0.75
1:C:327:VAL:O	1:C:529:LYS:NZ	2.19	0.74
2:D:18:LEU:HB3	2:D:83:MET:HB3	1.69	0.74
2:F:12:VAL:HG22	2:F:14:PRO:HD3	1.69	0.73
1:C:121:ASN:O	1:C:121:ASN:ND2	2.17	0.73
1:B:329:PHE:O	1:B:580:GLN:NE2	2.21	0.73
2:D:12:VAL:HG22	2:D:14:PRO:HD3	1.71	0.72
3:G:34:ALA:HB3	3:G:89:GLN:HB3	1.70	0.72
1:B:22:THR:H	1:B:76:THR:HG23	1.56	0.71
1:A:410:ILE:HG21	1:A:433:VAL:HG11	1.74	0.70
1:B:190:ARG:HG2	1:B:192:PHE:HE1	1.57	0.70
3:E:39:LYS:HB2	3:E:42:LYS:HB2	1.73	0.69
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.74	0.69
1:B:353:TRP:O	1:B:466:ARG:NH1	2.26	0.69
1:C:866:THR:HG22	1:C:869:MET:HG3	1.74	0.69
1:B:455:LEU:N	1:B:491:PRO:O	2.26	0.68
1:A:452:LEU:HD13	1:A:492:LEU:HB3	1.75	0.68
1:A:16:VAL:HG11	1:A:140:PHE:HE1	1.58	0.68
1:B:128:ILE:HD13	1:B:170:TYR:HD2	1.58	0.68
1:B:498:GLN:H	1:B:501:ASN:HD21	1.42	0.68
1:B:498:GLN:O	1:B:501:ASN:ND2	2.28	0.67
1:A:15:CYS:O	1:A:17:ASN:N	2.28	0.67
2:F:101:ALA:HA	2:F:109:HIS:O	1.95	0.67
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.77	0.67
1:A:105:ILE:HD11	1:A:135:PHE:CE1	2.30	0.67
1:A:177:MET:HG3	1:A:179:LEU:H	1.59	0.66
1:B:703:ASN:ND2	1:C:787:GLN:OE1	2.28	0.66
1:B:22:THR:O	1:B:76:THR:N	2.29	0.66
1:B:444:LYS:HD2	3:G:92:LYS:HG3	1.78	0.65
1:A:1104:VAL:HG23	1:A:1115:ILE:HG12	1.78	0.65
1:B:337:PRO:HB2	1:B:340:GLU:HG3	1.78	0.65
1:B:483:VAL:HG12	1:B:485:GLY:H	1.59	0.65
1:B:393:THR:HA	1:B:522:ALA:HB3	1.78	0.65
1:B:1141:LEU:HD21	1:B:1145:LEU:HD22	1.79	0.65
1:B:246:ARG:HH21	1:B:254:SER:HA	1.61	0.65

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:12:VAL:HG22	2:J:14:PRO:HD3	1.80	0.64
1:A:20:THR:OG1	1:A:77:LYS:NZ	2.30	0.64
1:B:493:GLN:CD	1:B:494:SER:H	2.01	0.64
2:D:40:ALA:HB3	2:D:43:LYS:HB2	1.79	0.64
1:B:366:SER:H	1:B:369:TYR:HD2	1.46	0.64
1:A:379:CYS:HB2	1:A:432:CYS:HA	1.79	0.64
1:A:379:CYS:HB2	1:A:432:CYS:CA	2.28	0.64
1:C:357:ARG:NH1	1:C:394:ASN:OD1	2.31	0.63
4:H:60:ALA:O	4:H:64:GLN:NE2	2.31	0.63
5:L:88:CYS:O	5:L:99:GLY:N	2.31	0.63
4:H:17:SER:HA	4:H:82:LEU:O	1.98	0.63
4:H:61:GLN:HA	4:H:64:GLN:HE22	1.64	0.63
1:B:404:GLY:O	1:B:408:ARG:NH2	2.31	0.63
2:F:40:ALA:HB3	2:F:43:LYS:HB2	1.81	0.62
3:G:27:GLN:OE1	3:G:92:LYS:NZ	2.30	0.62
2:J:39:GLN:O	2:J:93:VAL:N	2.31	0.62
1:A:253:ASP:OD1	1:A:256:SER:OG	2.16	0.62
1:A:327:VAL:O	1:A:529:LYS:NZ	2.30	0.61
3:E:35:TRP:HB2	3:E:48:ILE:HB	1.80	0.61
1:B:15:CYS:HB3	1:B:158:ARG:HB3	1.82	0.61
1:C:24:LEU:HD12	1:C:25:PRO:HD2	1.82	0.61
3:K:13:ALA:HB3	3:K:78:LEU:HD12	1.81	0.61
1:B:377:PHE:HD1	1:B:434:ILE:HG12	1.66	0.61
1:C:57:PRO:HG3	1:C:273:ARG:HE	1.66	0.61
1:A:447:GLY:O	2:D:109:HIS:ND1	2.34	0.61
1:A:518:LEU:HG	1:A:520:ALA:H	1.64	0.61
1:B:294:ASP:OD1	1:B:632:THR:OG1	2.17	0.61
1:B:973:ILE:HD12	1:B:983:ARG:HH21	1.66	0.60
1:A:319:ARG:NH1	1:B:740:MET:SD	2.74	0.60
1:C:322:PRO:HB3	1:C:539:VAL:HA	1.83	0.60
1:A:361:CYS:H	1:A:524:VAL:HG21	1.66	0.60
1:B:729:VAL:HG22	1:B:1059:GLY:HA2	1.83	0.60
4:H:38:ARG:NH2	4:H:46:GLU:OE1	2.35	0.59
1:B:190:ARG:HG3	1:B:207:HIS:CD2	2.38	0.59
1:A:303:LEU:HD12	1:A:308:VAL:HG12	1.85	0.59
1:B:722:VAL:HG22	1:B:930:ALA:HB1	1.84	0.59
1:C:434:ILE:HG22	1:C:436:TRP:HD1	1.68	0.59
1:B:403:ARG:NH1	1:B:405:ASP:OD1	2.35	0.59
5:L:64:GLY:HA3	5:L:73:LEU:HA	1.84	0.59
1:A:206:LYS:HE2	1:A:221:SER:HB2	1.84	0.58
1:B:244:LEU:HD12	1:B:258:TRP:HB2	1.83	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD13	1:A:210:ILE:HG21	1.84	0.58
1:B:327:VAL:HG12	1:B:542:ASN:HB3	1.84	0.58
1:B:454:ARG:NH1	1:B:467:ASP:OD2	2.36	0.58
5:L:37:GLN:HE22	5:L:39:LYS:HE3	1.69	0.58
2:J:15:GLY:H	2:J:86:LEU:HB2	1.68	0.58
1:B:239:GLN:NE2	1:B:240:THR:O	2.36	0.58
1:B:786:LYS:HG3	1:B:787:GLN:HG3	1.84	0.58
1:B:366:SER:HA	1:B:369:TYR:HB2	1.86	0.57
1:B:495:TYR:CE2	1:B:497:PHE:HB2	2.39	0.57
1:C:825:LYS:NZ	1:C:941:THR:O	2.31	0.57
1:A:326:ILE:HG13	1:A:327:VAL:HG23	1.85	0.57
1:C:117:LEU:HD13	1:C:130:VAL:HG22	1.87	0.57
3:G:36:TYR:OH	3:G:89:GLN:OE1	2.10	0.57
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.38	0.57
1:A:133:PHE:HB2	1:A:135:PHE:CE1	2.39	0.57
1:B:68:ILE:HG23	1:B:70:VAL:HG23	1.87	0.57
1:C:407:VAL:HG23	1:C:408:ARG:HD3	1.87	0.56
1:A:726:ILE:HD13	1:A:945:LEU:HD13	1.85	0.56
1:C:752:LEU:HD11	1:C:990:GLU:HG3	1.87	0.56
3:G:14:SER:HB3	3:G:107:LYS:HB3	1.87	0.56
1:B:403:ARG:HD2	1:B:405:ASP:H	1.71	0.56
3:G:13:ALA:HB3	3:G:78:LEU:HD12	1.87	0.56
1:A:69:HIS:O	1:A:76:THR:N	2.38	0.56
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.39	0.56
1:B:130:VAL:HG12	1:B:130:VAL:O	2.06	0.56
2:F:4:LEU:O	2:F:119:GLN:NE2	2.39	0.56
2:D:6:GLU:HG2	2:D:22:CYS:HB3	1.88	0.56
1:A:244:LEU:HD11	1:A:258:TRP:HB2	1.86	0.56
1:B:190:ARG:HG2	1:B:192:PHE:CE1	2.38	0.56
1:C:34:ARG:NH2	1:C:191:GLU:OE2	2.38	0.56
1:B:134:GLN:O	1:B:161:SER:N	2.37	0.55
1:B:308:VAL:HG22	1:B:602:THR:HG23	1.89	0.55
1:C:357:ARG:NH2	1:C:359:SER:OG	2.40	0.55
1:A:825:LYS:NZ	1:A:938:LEU:O	2.40	0.55
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.88	0.55
1:A:117:LEU:HD21	1:A:119:ILE:HG13	1.89	0.55
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.87	0.55
1:B:330:PRO:HD3	1:B:579:PRO:HB3	1.89	0.55
1:B:809:PRO:HD2	1:B:810:SER:N	2.22	0.55
1:C:349:SER:HB3	1:C:352:ALA:HB3	1.89	0.55
1:B:92:PHE:HE1	1:B:94:SER:HB3	1.72	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLU:OE2	1:B:190:ARG:NH2	2.39	0.55
1:A:441:LEU:O	1:A:509:ARG:NH2	2.40	0.55
1:B:231:ILE:HG22	1:B:233:ILE:HG23	1.88	0.55
1:C:403:ARG:HD2	1:C:418:ILE:HG21	1.88	0.55
4:H:28:THR:OG1	4:H:97:CYS:O	2.24	0.54
5:L:66:GLY:HA3	5:L:72:THR:H	1.72	0.54
1:A:1129:VAL:HB	1:A:1132:ILE:HD11	1.88	0.54
1:C:131:CYS:CB	1:C:166:CYS:HA	2.37	0.54
2:J:67:ARG:NE	2:J:85:SER:OG	2.35	0.54
1:A:159:VAL:HG13	1:A:160:TYR:HD1	1.72	0.54
1:A:419:ALA:HA	1:A:424:LYS:HA	1.90	0.54
1:A:426:PRO:HB3	1:A:463:PRO:HB3	1.90	0.54
2:D:60:TYR:HB3	2:D:64:VAL:HG12	1.89	0.54
1:B:355:ARG:HH21	1:B:400:PHE:HZ	1.55	0.54
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	1.88	0.54
1:B:422:ASN:OD1	1:B:454:ARG:HB3	2.08	0.54
1:A:149:ASN:HB2	1:A:153:MET:HE1	1.89	0.53
2:D:51:ILE:HD11	2:D:55:GLY:HA2	1.90	0.53
2:D:69:THR:HB	2:D:82:GLN:HB3	1.90	0.53
1:B:377:PHE:HE2	1:B:384:PRO:HB3	1.73	0.53
3:G:32:TRP:HB3	3:G:91:ALA:HB3	1.91	0.53
1:B:98:SER:HB3	1:B:181:GLY:HA2	1.91	0.53
2:J:47:TRP:NE1	2:J:49:ALA:O	2.42	0.53
1:B:461:LEU:HD12	1:B:465:GLU:HB2	1.90	0.53
1:B:809:PRO:HD2	1:B:810:SER:H	1.73	0.53
1:C:403:ARG:HB2	1:C:406:GLU:HB2	1.90	0.53
1:C:393:THR:HG22	1:C:522:ALA:HA	1.91	0.53
1:A:369:TYR:OH	1:A:388:ASN:OD1	2.24	0.52
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.90	0.52
1:B:214:ARG:HH11	1:B:215:ASP:H	1.57	0.52
1:A:323:THR:O	1:A:324:GLU:HG2	2.10	0.52
1:A:493:GLN:HE22	4:H:71:ARG:NH1	2.07	0.52
1:B:96:GLU:OE1	1:B:99:ASN:N	2.38	0.52
1:B:532:ASN:OD1	1:B:533:LEU:N	2.43	0.52
1:C:117:LEU:HD12	1:C:118:LEU:H	1.75	0.52
1:C:619:GLU:N	1:C:619:GLU:OE1	2.43	0.52
1:B:362:VAL:HG23	1:B:525:CYS:O	2.10	0.52
1:B:498:GLN:H	1:B:501:ASN:ND2	2.05	0.52
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.92	0.52
5:L:2:ILE:HG13	5:L:2:ILE:O	2.09	0.52
1:B:521:PRO:HB3	1:B:564:GLN:HG3	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:39:LYS:HB2	3:G:42:LYS:HB2	1.91	0.51
1:A:190:ARG:NH1	1:A:207:HIS:HB2	2.26	0.51
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.43	0.51
1:B:117:LEU:HD21	1:B:119:ILE:HD11	1.92	0.51
1:C:68:ILE:O	1:C:78:ARG:HB2	2.10	0.51
1:B:246:ARG:HG2	1:B:257:GLY:O	2.10	0.51
1:B:329:PHE:CD1	1:B:330:PRO:HD2	2.45	0.51
1:A:327:VAL:HG21	1:A:541:PHE:HB2	1.92	0.51
1:C:97:LYS:CE	1:C:187:LYS:H	2.23	0.51
1:B:722:VAL:HA	1:B:1064:HIS:O	2.11	0.51
1:C:931:ILE:O	1:C:934:ILE:HG22	2.11	0.51
2:F:17:SER:HA	2:F:83:MET:O	2.10	0.51
1:A:213:VAL:HG23	1:A:214:ARG:HG2	1.92	0.51
1:B:474:GLN:HG2	1:B:481:ASN:H	1.76	0.51
1:B:621:PRO:O	1:B:634:ARG:NH1	2.44	0.51
1:B:995:ARG:NH2	1:C:994:ASP:OD2	2.43	0.51
4:H:66:ARG:HD2	4:H:82(B):SER:HB2	1.92	0.51
4:H:59:TYR:HB3	4:H:63:PHE:HB2	1.93	0.51
1:A:14:GLN:HB2	1:A:158:ARG:HG2	1.92	0.50
1:A:120:VAL:HG12	1:A:122:ASN:H	1.76	0.50
1:C:348:ALA:H	1:C:509:ARG:HH12	1.60	0.50
1:C:498:GLN:H	1:C:501:ASN:HB2	1.75	0.50
5:L:20:THR:OG1	5:L:73:LEU:O	2.22	0.50
1:B:395:VAL:HG11	1:B:524:VAL:HG21	1.94	0.50
2:J:68:PHE:CE1	2:J:83:MET:HG2	2.46	0.50
1:A:81:ASN:ND2	1:A:240:THR:O	2.44	0.50
1:A:403:ARG:NH2	1:A:453:TYR:OH	2.42	0.50
3:K:18:ARG:HA	3:K:75:ILE:O	2.11	0.50
1:A:347:PHE:HD2	1:A:509:ARG:HH11	1.58	0.50
1:B:92:PHE:CE1	1:B:94:SER:HB3	2.47	0.50
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.92	0.50
1:A:365:TYR:O	1:A:368:LEU:HG	2.12	0.50
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.44	0.50
1:B:902:MET:HG3	1:B:916:LEU:HD11	1.91	0.50
1:A:105:ILE:HG23	1:A:239:GLN:HB2	1.94	0.50
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.94	0.49
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.94	0.49
5:L:33:LEU:H	5:L:50:GLY:HA2	1.77	0.49
1:A:361:CYS:N	1:A:524:VAL:HG21	2.26	0.49
1:C:76:THR:OG1	1:C:77:LYS:N	2.46	0.49
1:A:991:VAL:O	1:A:995:ARG:HG3	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ARG:NH1	1:C:740:MET:SD	2.83	0.49
1:B:722:VAL:HG12	1:B:1065:VAL:HG22	1.94	0.49
1:C:365:TYR:CE2	1:C:387:LEU:HD22	2.48	0.49
1:C:989:ALA:O	1:C:993:ILE:HG12	2.12	0.49
2:F:36:TRP:HD1	2:F:70:ILE:HD11	1.77	0.49
1:A:456:PHE:HB3	1:A:473:TYR:CG	2.48	0.49
1:A:334:ASN:O	1:A:362:VAL:N	2.42	0.49
1:C:825:LYS:NZ	1:C:938:LEU:O	2.43	0.49
1:C:133:PHE:HB3	1:C:163:ALA:HA	1.93	0.48
2:D:64:VAL:HG13	2:D:68:PHE:CD2	2.49	0.48
1:B:448:ASN:HA	3:G:32:TRP:CZ2	2.48	0.48
4:H:32:SER:OG	4:H:33:ALA:N	2.46	0.48
1:C:91:TYR:OH	1:C:191:GLU:OE1	2.26	0.48
1:C:168:PHE:HE1	1:C:170:TYR:HB2	1.79	0.48
1:C:96:GLU:C	1:C:97:LYS:HD2	2.32	0.48
1:A:457:ARG:HH12	1:A:467:ASP:CG	2.17	0.48
1:A:329:PHE:O	1:A:580:GLN:NE2	2.44	0.47
1:A:730:SER:OG	1:A:731:MET:N	2.47	0.47
1:A:16:VAL:HG13	1:A:17:ASN:H	1.80	0.47
1:B:415:THR:HG22	1:B:416:GLY:N	2.30	0.47
1:C:619:GLU:O	1:C:619:GLU:HG2	2.14	0.47
1:B:99:ASN:HB2	1:B:177:MET:SD	2.54	0.47
1:A:1073:LYS:HE3	1:A:1073:LYS:HB2	1.72	0.47
1:A:1116:THR:HG22	1:A:1138:TYR:HD1	1.79	0.47
1:B:114:THR:HG22	1:B:115:GLN:H	1.80	0.47
1:C:231:ILE:HG22	1:C:233:ILE:HB	1.97	0.47
2:F:83:MET:HB3	2:F:86:LEU:HD21	1.95	0.47
4:H:18:VAL:HG23	4:H:82(C):LEU:HD11	1.95	0.47
1:A:18:LEU:HD13	1:A:258:TRP:CH2	2.50	0.47
1:B:329:PHE:CG	1:B:330:PRO:HD2	2.49	0.47
1:A:290:ASP:OD1	1:A:291:CYS:N	2.45	0.47
1:B:164:ASN:OD1	1:B:165:ASN:N	2.42	0.47
1:B:417:LYS:NZ	1:B:460:ASN:OD1	2.26	0.47
1:A:96:GLU:O	1:A:188:ASN:HB3	2.14	0.47
1:A:203:ILE:HB	1:A:227:VAL:HG12	1.96	0.47
1:C:325:SER:HB3	1:C:534:VAL:HG21	1.96	0.47
1:B:408:ARG:HH12	1:B:510:VAL:HG11	1.80	0.46
1:A:873:TYR:CE1	1:C:699:LEU:HD13	2.51	0.46
1:B:362:VAL:HG13	1:B:362:VAL:O	2.16	0.46
1:B:362:VAL:HG21	1:B:525:CYS:HB2	1.96	0.46
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.98	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:89:GLN:HG2	5:L:98:PHE:HA	1.96	0.46
1:A:112:SER:HB3	1:A:134:GLN:HA	1.97	0.46
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.97	0.46
1:B:250:THR:HB	1:B:257:GLY:HA2	1.97	0.46
1:A:64:TRP:HH2	1:A:214:ARG:HD3	1.81	0.46
1:B:32:PHE:HD2	1:B:218:GLN:HE22	1.63	0.46
1:B:393:THR:OG1	1:B:518:LEU:N	2.49	0.46
1:B:455:LEU:HB2	1:B:493:GLN:HB2	1.97	0.46
1:A:16:VAL:HG13	1:A:17:ASN:N	2.30	0.46
1:A:334:ASN:ND2	1:A:360:ASN:O	2.47	0.46
1:A:553:THR:OG1	1:A:554:GLU:N	2.48	0.46
1:A:945:LEU:HD12	1:A:948:LEU:HD12	1.98	0.46
1:B:451:TYR:CD2	1:B:495:TYR:HE1	2.33	0.46
1:A:560:LEU:O	1:A:562:PHE:N	2.49	0.46
1:B:634:ARG:HA	1:B:637:SER:HB2	1.98	0.46
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.51	0.46
2:F:38:ARG:NE	2:F:46:GLU:OE1	2.45	0.46
2:F:6:GLU:HG2	2:F:22:CYS:HB3	1.98	0.45
2:F:73:ASP:OD2	2:F:76:LYS:NZ	2.37	0.45
1:A:30:ASN:HB3	1:A:32:PHE:CE1	2.50	0.45
1:A:245:HIS:O	1:A:245:HIS:ND1	2.50	0.45
1:B:105:ILE:HG13	1:B:117:LEU:O	2.17	0.45
1:B:444:LYS:NZ	3:G:28:GLY:O	2.49	0.45
1:B:617:CYS:HB2	1:B:649:CYS:HB3	1.76	0.45
1:C:144:TYR:H	1:C:155:SER:HB2	1.80	0.45
1:A:385:THR:O	1:A:386:LYS:HG3	2.16	0.45
1:A:426:PRO:HG3	1:A:464:PHE:CZ	2.52	0.45
1:B:985:ASP:HB2	1:B:986:PRO:HD2	1.99	0.45
1:C:812:PRO:HB2	1:C:815:ARG:HB2	1.97	0.45
2:D:24:ALA:HB3	2:D:29:PHE:HD1	1.81	0.45
1:A:576:VAL:HG13	1:A:587:ILE:HD11	1.98	0.45
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.49	0.45
1:A:105:ILE:CG2	1:A:239:GLN:HB2	2.47	0.45
1:B:102:ARG:HG3	1:B:102:ARG:HH11	1.82	0.45
1:B:444:LYS:H	1:B:448:ASN:CG	2.19	0.45
4:H:44:ARG:HH12	5:L:103:LYS:HE2	1.82	0.45
1:A:156:GLU:OE1	1:A:156:GLU:N	2.50	0.45
1:B:335:LEU:HG	1:B:364:ASP:OD2	2.16	0.45
1:B:457:ARG:HG2	1:B:458:LYS:H	1.82	0.45
1:A:133:PHE:HB3	1:A:160:TYR:HB3	1.98	0.45
1:C:130:VAL:HG21	1:C:231:ILE:HD12	1.99	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:NH1	1:B:531:THR:O	2.48	0.45
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.99	0.45
1:A:731:MET:HG3	1:A:955:ASN:HD21	1.81	0.45
1:B:1101:HIS:ND1	6:Q:1:NAG:H5	2.31	0.45
1:C:94:SER:OG	1:C:101:ILE:HG13	2.17	0.45
1:C:124:THR:OG1	1:C:125:ASN:N	2.49	0.45
1:A:189:LEU:HB3	1:A:208:THR:O	2.16	0.44
1:B:95:THR:H	1:B:264:ALA:HB3	1.82	0.44
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.99	0.44
1:C:330:PRO:HB3	1:C:530:SER:OG	2.17	0.44
1:B:404:GLY:HA3	1:B:408:ARG:HH22	1.81	0.44
1:C:97:LYS:HE2	1:C:186:PHE:HA	1.99	0.44
2:D:20:LEU:HD12	2:D:81:LEU:HD22	1.99	0.44
4:H:101:ASP:OD1	4:H:101:ASP:N	2.45	0.44
1:A:445:VAL:HA	1:A:499:PRO:HD2	1.99	0.44
1:C:578:ASP:OD1	1:C:583:GLU:N	2.44	0.44
1:A:78:ARG:HD2	1:A:78:ARG:HA	1.73	0.44
1:A:130:VAL:HG12	1:A:130:VAL:O	2.17	0.44
1:A:333:THR:HG22	1:A:334:ASN:N	2.27	0.44
1:C:1088:HIS:CE1	1:C:1122:VAL:HG22	2.52	0.44
2:D:38:ARG:HE	2:D:48:VAL:HG11	1.83	0.44
1:A:1082:CYS:HB2	1:A:1132:ILE:CG2	2.48	0.44
1:B:922:LEU:O	1:B:926:GLN:HG3	2.17	0.44
3:E:48:ILE:HD13	3:E:64:GLY:HA3	2.00	0.44
1:A:699:LEU:HD13	1:B:873:TYR:CE1	2.53	0.44
1:B:79:PHE:HB2	1:B:260:ALA:HB2	1.99	0.44
1:C:207:HIS:O	1:C:207:HIS:ND1	2.51	0.44
1:C:1146:ASP:O	1:C:1149:LYS:NZ	2.46	0.44
3:E:47:LEU:HA	3:E:58:VAL:HG21	1.98	0.44
1:B:117:LEU:HD23	1:B:118:LEU:N	2.33	0.44
1:B:462:LYS:O	1:B:465:GLU:HG3	2.17	0.44
2:F:12:VAL:HG23	2:F:126:SER:H	1.83	0.44
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.53	0.44
5:L:32:TYR:HB3	5:L:91:TYR:HB2	2.00	0.44
1:A:721:SER:OG	1:A:1066:THR:OG1	2.36	0.44
1:B:350:VAL:HG22	1:B:404:GLY:H	1.81	0.44
1:A:433:VAL:HG13	1:A:512:VAL:HG22	1.99	0.44
1:C:14:GLN:HG2	1:C:161:SER:HA	2.00	0.43
1:C:332:ILE:O	1:C:334:ASN:N	2.50	0.43
1:A:546:LEU:H	1:A:546:LEU:HD23	1.83	0.43
1:A:1103:PHE:HZ	6:N:1:NAG:H62	1.82	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:VAL:HG23	1:B:160:TYR:HD1	1.82	0.43
2:D:45:LEU:HD21	2:D:117:TRP:HH2	1.82	0.43
2:F:64:VAL:HG13	2:F:68:PHE:HD2	1.83	0.43
3:K:39:LYS:HB2	3:K:42:LYS:HB2	2.00	0.43
1:A:662:CYS:HB2	1:A:697:MET:HG3	2.00	0.43
1:B:355:ARG:NH2	1:B:400:PHE:HZ	2.16	0.43
1:B:421:TYR:CD2	1:B:456:PHE:HA	2.53	0.43
1:B:456:PHE:O	1:B:491:PRO:HG2	2.17	0.43
3:E:20:ILE:HG13	3:E:72:THR:HG23	2.01	0.43
1:B:403:ARG:NE	1:B:451:TYR:HB3	2.33	0.43
1:B:654:GLU:HG3	1:B:693:ILE:HG22	2.01	0.43
1:A:140:PHE:O	1:A:141:LEU:HD23	2.18	0.43
1:A:402:ILE:HG21	1:A:418:ILE:HD11	2.01	0.43
1:C:524:VAL:O	1:C:524:VAL:HG13	2.19	0.43
1:A:231:ILE:HD12	1:A:233:ILE:HG12	2.00	0.43
1:B:445:VAL:HG22	1:B:499:PRO:HG2	2.00	0.43
1:C:814:LYS:HG3	1:C:872:GLN:HG2	2.00	0.43
2:F:64:VAL:HG13	2:F:68:PHE:CD2	2.54	0.43
4:H:15:GLY:HA2	4:H:82(C):LEU:H	1.83	0.43
2:J:38:ARG:HA	2:J:94:TYR:HA	2.00	0.43
1:C:348:ALA:H	1:C:509:ARG:NH1	2.16	0.43
4:H:52:VAL:HG12	4:H:54:SER:H	1.84	0.43
1:C:97:LYS:HD2	1:C:97:LYS:N	2.34	0.43
1:C:318:PHE:CD2	1:C:623:ALA:HB1	2.54	0.43
1:C:620:VAL:N	1:C:621:PRO:HD2	2.34	0.43
3:K:78:LEU:HD23	3:K:78:LEU:HA	1.91	0.43
1:A:642:VAL:HG22	1:A:651:ILE:HG12	2.01	0.43
1:C:97:LYS:HZ1	1:C:187:LYS:H	1.67	0.43
1:A:34:ARG:O	1:A:56:LEU:HD23	2.19	0.42
1:A:326:ILE:HG21	1:A:534:VAL:HG22	2.01	0.42
1:C:914:ASN:OD1	1:C:914:ASN:N	2.51	0.42
3:E:33:LEU:HD11	3:E:88:CYS:HB3	2.01	0.42
3:E:38:GLN:NE2	3:E:44:PRO:HG3	2.34	0.42
3:K:5:THR:HG23	3:K:100:GLN:NE2	2.34	0.42
3:K:33:LEU:HD11	3:K:88:CYS:HB3	2.00	0.42
1:A:1101:HIS:ND1	6:N:1:NAG:H5	2.34	0.42
1:B:437:ASN:HA	1:B:508:TYR:CD1	2.54	0.42
1:C:462:LYS:HG3	1:C:465:GLU:HB2	2.01	0.42
2:D:114:MET:HB2	3:E:36:TYR:CE2	2.54	0.42
1:A:353:TRP:NE1	1:A:466:ARG:HG3	2.34	0.42
1:B:16:VAL:HG12	1:B:254:SER:HB2	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LEU:O	1:B:632:THR:OG1	2.37	0.42
3:E:90:GLN:HE21	3:E:97:THR:H	1.67	0.42
1:B:65:PHE:CE2	1:B:82:PRO:HG2	2.54	0.42
4:H:6:GLN:H	4:H:105:GLN:HE22	1.67	0.42
1:A:120:VAL:HG12	1:A:122:ASN:N	2.34	0.42
1:A:386:LYS:HD2	1:A:390:LEU:HD23	2.01	0.42
1:A:707:TYR:HB3	1:B:792:PRO:HG3	2.02	0.42
1:B:128:ILE:HD13	1:B:170:TYR:CD2	2.46	0.42
1:A:134:GLN:N	1:A:160:TYR:HB2	2.34	0.42
1:A:391:CYS:HB3	1:A:525:CYS:HA	2.01	0.42
2:J:101:ALA:HA	2:J:109:HIS:O	2.19	0.42
2:J:115:ASP:OD1	2:J:116:VAL:N	2.50	0.42
1:A:634:ARG:HD3	1:A:634:ARG:HA	1.85	0.42
1:B:490:PHE:HA	1:B:491:PRO:HD3	1.90	0.42
2:D:13:GLN:HB3	2:D:86:LEU:HD13	2.01	0.42
3:G:37:GLN:N	3:G:45:LYS:O	2.50	0.42
4:H:4:LEU:HD21	4:H:92:CYS:SG	2.60	0.42
1:C:32:PHE:CD2	1:C:218:GLN:HG3	2.54	0.42
1:C:153:MET:N	1:C:153:MET:SD	2.93	0.42
2:F:5:VAL:O	2:F:22:CYS:HA	2.19	0.42
3:G:38:GLN:NE2	3:G:44:PRO:HG3	2.34	0.42
1:A:457:ARG:HG2	1:A:459:SER:H	1.85	0.42
1:C:361:CYS:O	1:C:524:VAL:HG23	2.19	0.42
3:E:23:CYS:HB2	3:E:35:TRP:CH2	2.55	0.42
3:G:19:VAL:HG21	3:G:78:LEU:HD11	2.01	0.42
1:A:134:GLN:H	1:A:160:TYR:HB2	1.84	0.42
1:C:141:LEU:O	1:C:243:ALA:HA	2.20	0.42
2:F:94:TYR:HE1	2:F:123:VAL:HB	1.84	0.42
1:A:569:ILE:HD11	1:B:47:VAL:HG12	2.02	0.41
1:B:445:VAL:HB	3:G:93:SER:HA	2.01	0.41
3:G:86:TYR:HE2	3:G:104:LEU:HD23	1.85	0.41
1:A:187:LYS:HD3	1:A:210:ILE:O	2.19	0.41
1:B:444:LYS:H	1:B:448:ASN:ND2	2.18	0.41
1:C:325:SER:O	1:C:539:VAL:HG21	2.19	0.41
1:C:410:ILE:HG13	1:C:410:ILE:O	2.19	0.41
2:J:51:ILE:HG12	2:J:72:ARG:HD2	2.02	0.41
1:A:308:VAL:HG22	1:A:602:THR:HB	2.02	0.41
1:B:480:CYS:SG	1:B:486:PHE:HB2	2.59	0.41
2:D:93:VAL:HG22	2:D:122:THR:HG23	2.01	0.41
1:A:118:LEU:O	1:A:120:VAL:HG23	2.20	0.41
1:B:97:LYS:HD2	1:B:182:LYS:HD2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:GLN:HG2	1:B:414:GLN:HB3	2.03	0.41
1:B:1082:CYS:HB2	1:B:1126:CYS:HB2	2.02	0.41
1:A:327:VAL:HG11	1:A:543:PHE:HA	2.03	0.41
1:A:1107:ARG:HG2	1:B:904:TYR:OH	2.20	0.41
1:B:377:PHE:CD1	1:B:434:ILE:HG12	2.50	0.41
3:E:33:LEU:HB3	3:E:51:ALA:HB2	2.02	0.41
3:G:62:PHE:HD2	3:G:75:ILE:HG12	1.85	0.41
5:L:21:LEU:HD12	5:L:73:LEU:HD11	2.01	0.41
1:A:478:THR:HG21	5:L:31:SER:HB3	2.01	0.41
1:B:196:ASN:ND2	1:B:235:ILE:HD12	2.36	0.41
1:B:358:ILE:HD12	1:B:397:ALA:O	2.20	0.41
2:D:104:VAL:HB	2:D:109:HIS:NE2	2.36	0.41
3:G:48:ILE:HG23	3:G:53:SER:O	2.20	0.41
1:A:105:ILE:HB	1:A:241:LEU:HD11	2.02	0.41
1:B:959:LEU:HD12	1:B:959:LEU:HA	1.91	0.41
2:F:13:GLN:HB2	2:F:125:VAL:HG12	2.01	0.41
2:J:64:VAL:HG13	2:J:68:PHE:CD2	2.55	0.41
1:B:449:TYR:HA	1:B:495:TYR:CD2	2.56	0.41
1:C:405:ASP:OD1	1:C:405:ASP:N	2.52	0.41
1:A:58:PHE:CD1	1:A:290:ASP:HB2	2.55	0.41
1:A:347:PHE:CD2	1:A:509:ARG:HD3	2.56	0.41
1:A:453:TYR:HB3	1:A:455:LEU:HG	2.02	0.41
1:A:977:LEU:HD22	1:A:993:ILE:HD12	2.03	0.41
1:B:118:LEU:HD21	1:B:120:VAL:HB	2.01	0.41
1:B:403:ARG:HE	1:B:451:TYR:HB3	1.86	0.41
1:B:603:ASN:OD1	1:B:604:THR:N	2.53	0.41
1:B:705:VAL:HB	1:C:883:THR:HG21	2.02	0.41
1:B:1004:LEU:HD12	1:B:1004:LEU:HA	1.89	0.41
4:H:7:SER:HB3	4:H:21:SER:HB3	2.01	0.41
1:A:417:LYS:HD2	1:A:455:LEU:HD22	2.02	0.41
1:A:433:VAL:HG22	1:A:512:VAL:HG13	2.03	0.41
1:C:438:SER:OG	1:C:442:ASP:OD1	2.24	0.41
2:F:51:ILE:HD12	2:F:58:GLN:HG2	2.03	0.41
1:A:364:ASP:O	1:A:367:VAL:HG12	2.21	0.40
1:A:989:ALA:O	1:A:993:ILE:HG12	2.22	0.40
1:B:131:CYS:SG	1:B:163:ALA:HB1	2.61	0.40
1:C:154:GLU:OE2	1:C:157:PHE:HB2	2.21	0.40
2:D:114:MET:N	3:E:36:TYR:OH	2.50	0.40
1:A:102:ARG:HD3	1:A:102:ARG:HA	1.95	0.40
1:B:65:PHE:HB2	1:B:265:TYR:CD2	2.56	0.40
1:B:449:TYR:HA	1:B:495:TYR:CG	2.56	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:ILE:H	1:C:569:ILE:HD12	1.86	0.40
1:C:938:LEU:HD23	1:C:938:LEU:HA	1.94	0.40
1:C:1056:ALA:HB1	1:C:1057:PRO:HD2	2.03	0.40
2:D:67:ARG:HG3	2:D:68:PHE:CD1	2.57	0.40
2:D:115:ASP:OD1	2:D:116:VAL:N	2.54	0.40
1:A:164:ASN:OD1	1:A:165:ASN:N	2.55	0.40
1:B:518:LEU:HD23	1:B:518:LEU:HA	1.84	0.40
1:C:825:LYS:HG2	1:C:945:LEU:HD23	2.02	0.40
3:G:37:GLN:HB2	3:G:47:LEU:HD11	2.03	0.40
1:A:83:VAL:HG12	1:A:239:GLN:HG2	2.03	0.40
1:A:328:ARG:H	1:A:328:ARG:HG2	1.72	0.40
1:B:354:ASN:O	1:B:355:ARG:HB3	2.22	0.40
1:B:630:THR:N	1:B:633:TRP:HB2	2.36	0.40
1:B:1117:THR:HG22	1:B:1140:PRO:HD2	2.04	0.40
1:C:144:TYR:HA	1:C:246:ARG:HB2	2.03	0.40
1:C:331:ASN:C	1:C:333:THR:H	2.24	0.40
2:F:18:LEU:HB3	2:F:83:MET:HB2	2.04	0.40
1:A:351:TYR:HB3	1:A:454:ARG:HB2	2.04	0.40
1:B:156:GLU:HB3	1:B:158:ARG:HD3	2.04	0.40
1:B:825:LYS:HE2	1:B:825:LYS:HB2	1.96	0.40
1:B:1041:ASP:HB2	1:C:1030:SER:OG	2.21	0.40
4:H:47:TRP:HB2	5:L:98:PHE:CE1	2.57	0.40
2:J:72:ARG:HA	2:J:79:LEU:HA	2.03	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	1071/1195 (90%)	995 (93%)	72 (7%)	4 (0%)	30 49
1	B	1078/1195 (90%)	996 (92%)	79 (7%)	3 (0%)	37 55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1078/1195 (90%)	1005 (93%)	71 (7%)	2 (0%)	44	63
2	D	124/127 (98%)	117 (94%)	7 (6%)	0	100	100
2	F	124/127 (98%)	117 (94%)	7 (6%)	0	100	100
2	J	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
3	E	105/107 (98%)	96 (91%)	8 (8%)	1 (1%)	13	25
3	G	105/107 (98%)	96 (91%)	8 (8%)	1 (1%)	13	25
3	K	105/107 (98%)	99 (94%)	5 (5%)	1 (1%)	13	25
4	H	120/123 (98%)	110 (92%)	10 (8%)	0	100	100
5	L	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
All	All	4139/4518 (92%)	3842 (93%)	285 (7%)	12 (0%)	38	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	327	VAL
3	G	15	VAL
3	K	15	VAL
1	B	399	SER
1	C	530	SER
3	E	15	VAL
1	B	355	ARG
1	A	77	LYS
1	A	331	ASN
1	B	638	THR
1	C	330	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	948/1040 (91%)	945 (100%)	3 (0%)	91	96

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	951/1040 (91%)	951 (100%)	0	100	100
1	C	951/1040 (91%)	948 (100%)	3 (0%)	91	96
2	D	101/102 (99%)	101 (100%)	0	100	100
2	F	101/102 (99%)	101 (100%)	0	100	100
2	J	101/102 (99%)	101 (100%)	0	100	100
3	E	91/91 (100%)	91 (100%)	0	100	100
3	G	91/91 (100%)	91 (100%)	0	100	100
3	K	91/91 (100%)	91 (100%)	0	100	100
4	H	101/103 (98%)	100 (99%)	1 (1%)	73	87
5	L	89/90 (99%)	89 (100%)	0	100	100
All	All	3616/3892 (93%)	3609 (100%)	7 (0%)	91	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	386	LYS
1	A	646	ARG
1	A	978	ASN
1	C	121	ASN
1	C	462	LYS
1	C	493	GLN
4	H	41	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	GLN
1	A	493	GLN
1	A	955	ASN
1	B	122	ASN
1	B	239	GLN
1	B	501	ASN
1	B	935	GLN
4	H	64	GLN
5	L	37	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	$\# Z  > 2$
6	NAG	I	1	6,1	14,14,15	0.31	0	17,19,21	0.67	1 (5%)
6	NAG	I	2	6	14,14,15	0.34	0	17,19,21	0.48	0
7	NAG	M	1	7,1	14,14,15	0.23	0	17,19,21	0.47	0
7	NAG	M	2	7	14,14,15	0.27	0	17,19,21	0.38	0
6	NAG	N	1	6,1	14,14,15	0.20	0	17,19,21	0.47	0
6	NAG	N	2	6	14,14,15	0.23	0	17,19,21	0.39	0
6	NAG	O	1	6,1	14,14,15	0.19	0	17,19,21	0.66	0
6	NAG	O	2	6	14,14,15	0.37	0	17,19,21	0.38	0
6	NAG	P	1	6,1	14,14,15	0.28	0	17,19,21	0.62	0
6	NAG	P	2	6	14,14,15	0.29	0	17,19,21	0.51	0
6	NAG	Q	1	6,1	14,14,15	0.24	0	17,19,21	0.45	0
6	NAG	Q	2	6	14,14,15	0.22	0	17,19,21	0.47	0
6	NAG	R	1	6,1	14,14,15	0.21	0	17,19,21	0.56	0
6	NAG	R	2	6	14,14,15	0.29	0	17,19,21	0.43	0
6	NAG	S	1	6,1	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	S	2	6	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	T	1	6,1	14,14,15	0.24	0	17,19,21	0.48	0
6	NAG	T	2	6	14,14,15	0.25	0	17,19,21	0.45	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
6	NAG	I	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
7	NAG	M	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	2/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	NAG	O	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	NAG	P	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	NAG	R	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1	NAG	C1-O5-C5	2.27	115.22	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	1	NAG	O5-C5-C6-O6
7	M	2	NAG	O5-C5-C6-O6
7	M	1	NAG	C4-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
7	M	2	NAG	C4-C5-C6-O6
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	Q	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

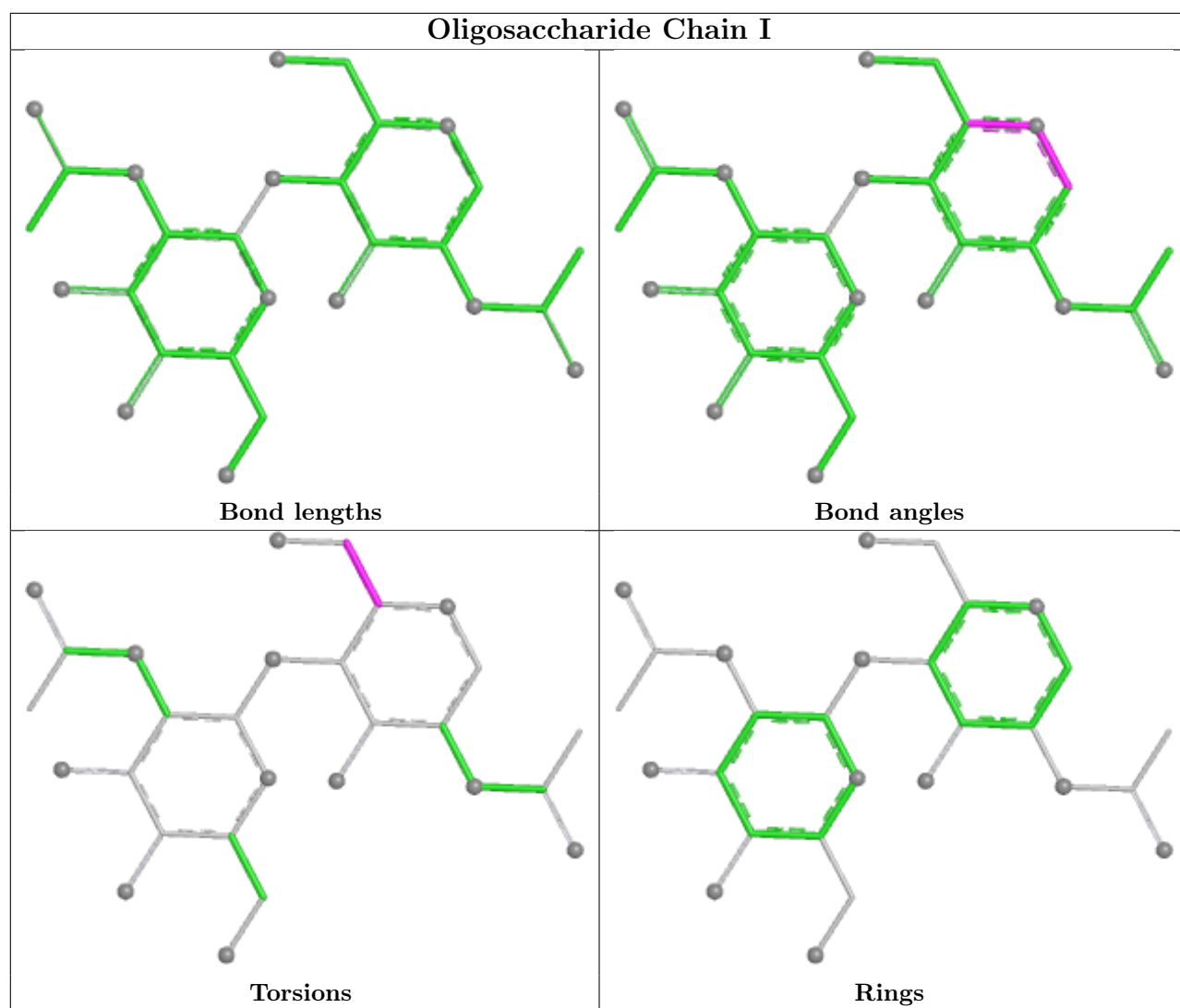
Mol	Chain	Res	Type	Atoms
6	Q	2	NAG	C8-C7-N2-C2
6	Q	2	NAG	O7-C7-N2-C2
6	T	1	NAG	C8-C7-N2-C2
6	T	1	NAG	O7-C7-N2-C2
6	O	1	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
6	P	2	NAG	C1-C2-N2-C7
6	R	1	NAG	C4-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	O	1	NAG	C3-C2-N2-C7
6	P	1	NAG	C3-C2-N2-C7
6	P	2	NAG	C3-C2-N2-C7
6	O	1	NAG	C1-C2-N2-C7
6	P	1	NAG	C1-C2-N2-C7
6	R	1	NAG	O5-C5-C6-O6

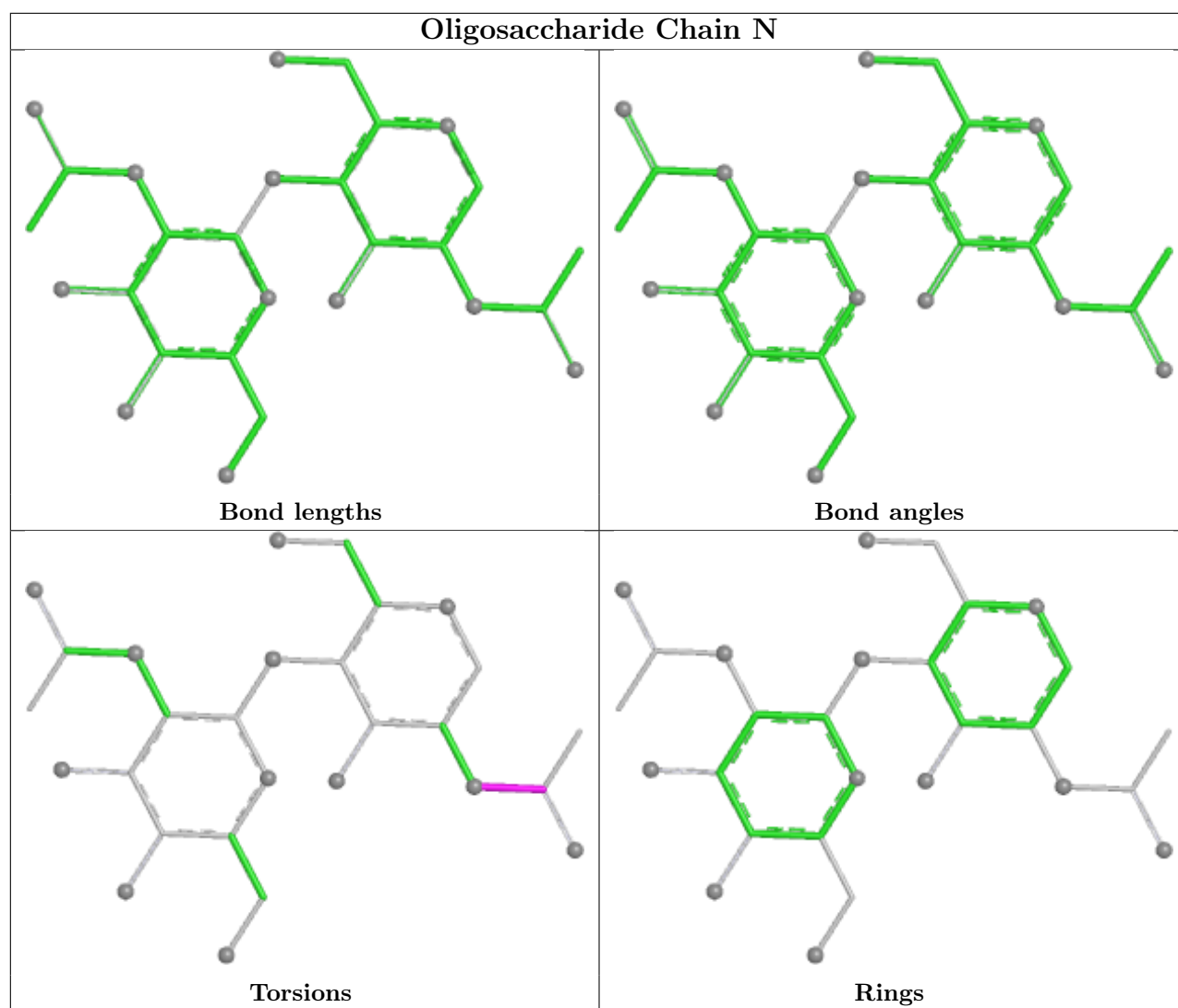
There are no ring outliers.

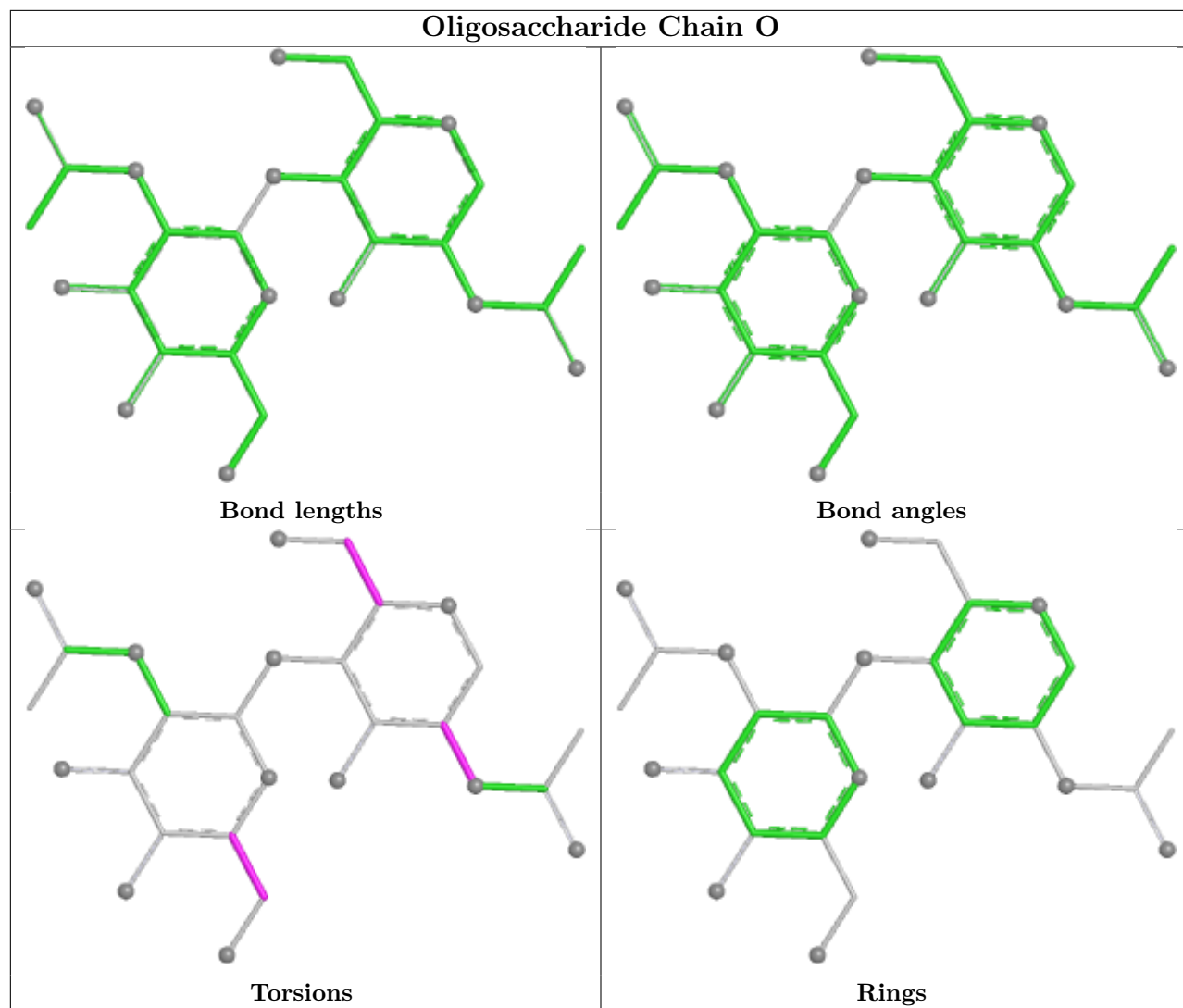
2 monomers are involved in 3 short contacts:

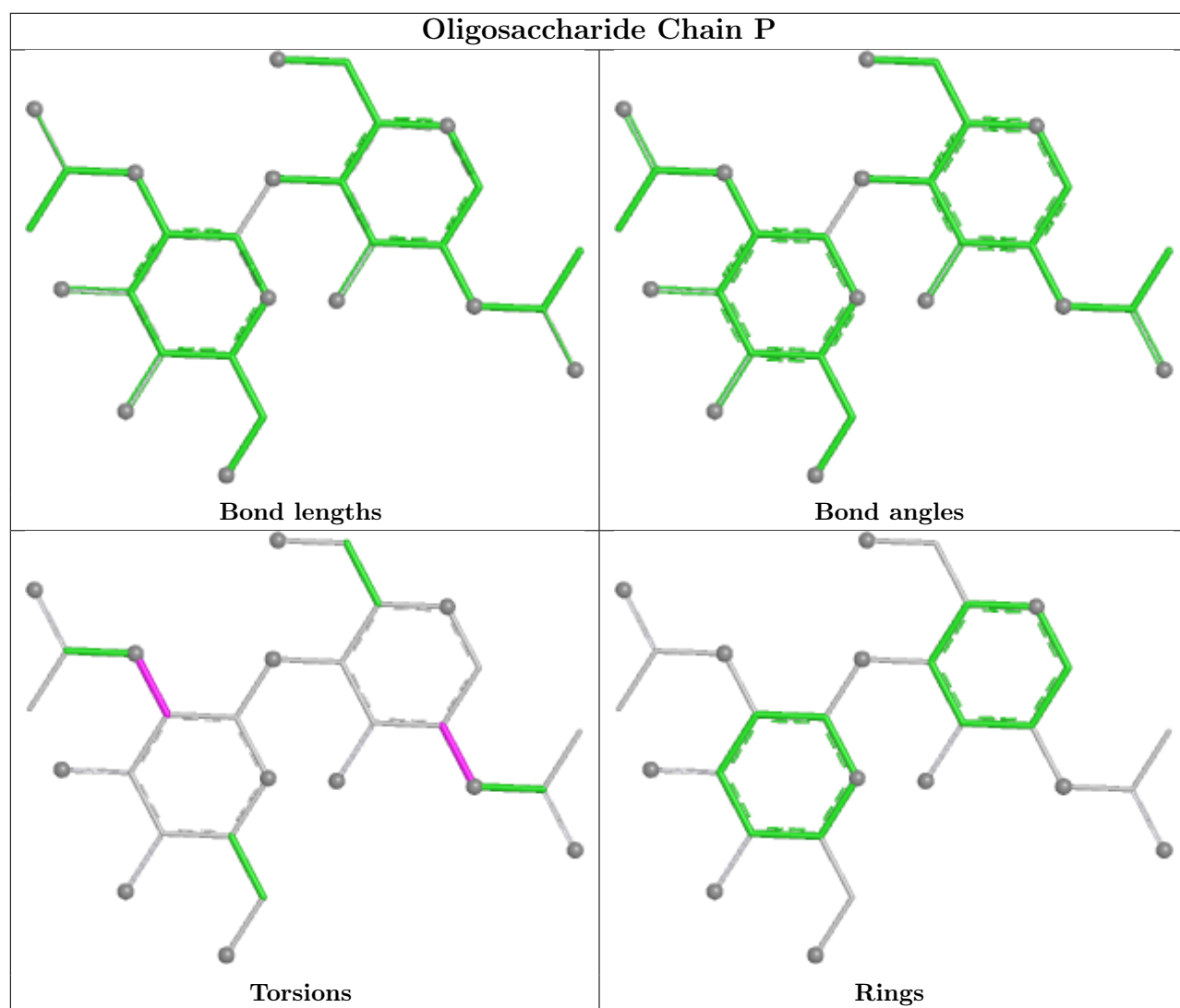
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	1	NAG	2	0
6	Q	1	NAG	1	0

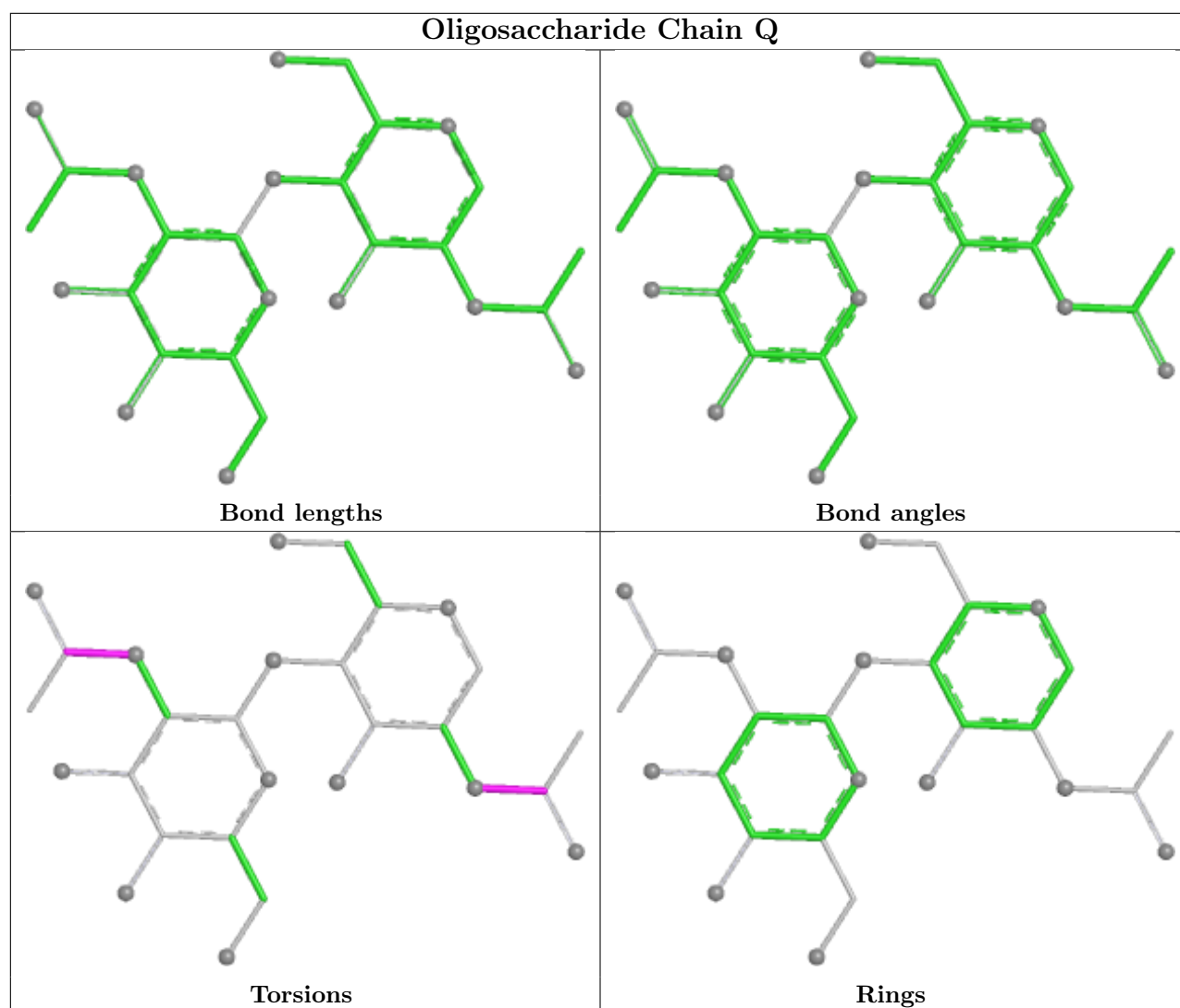
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

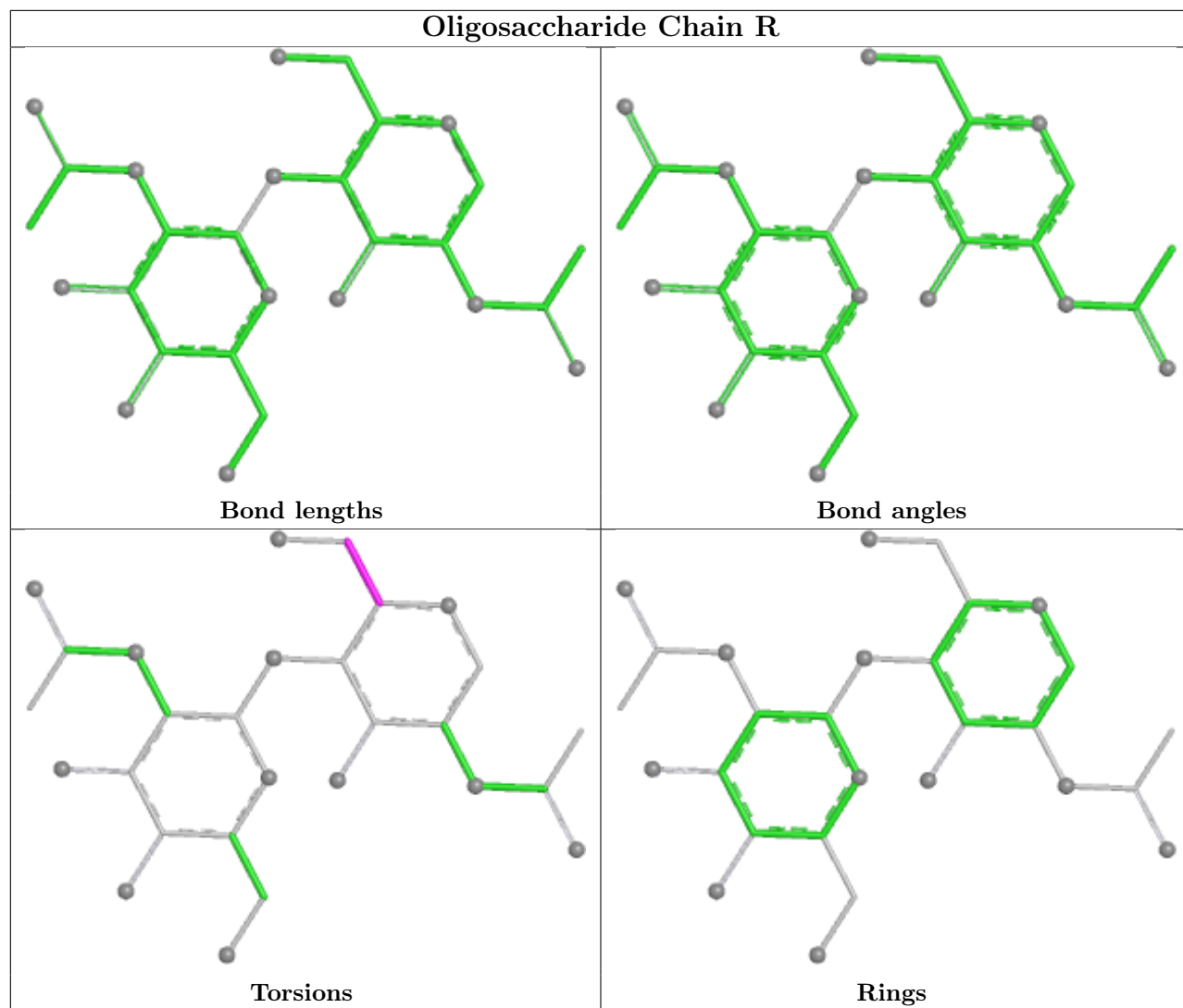




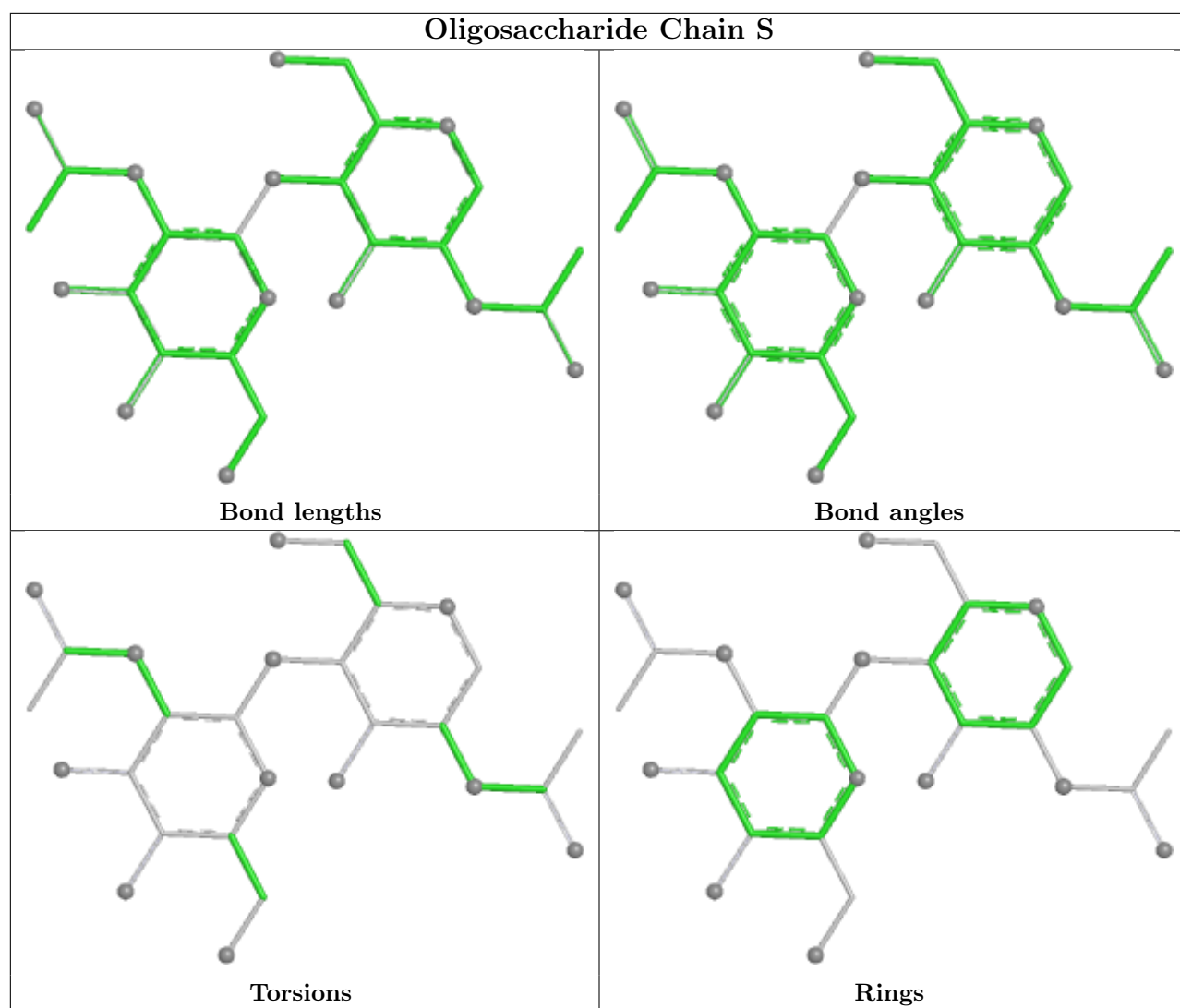


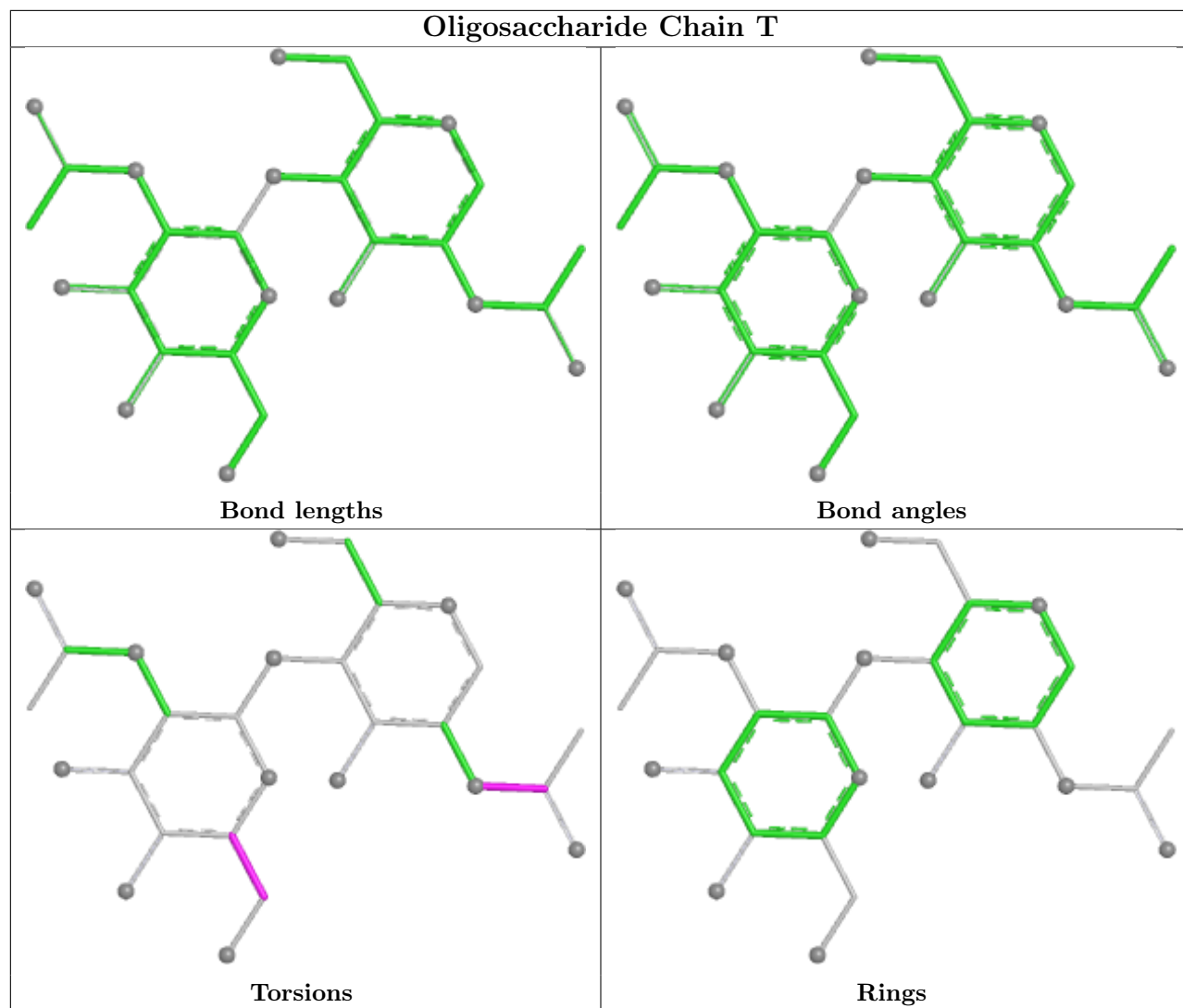


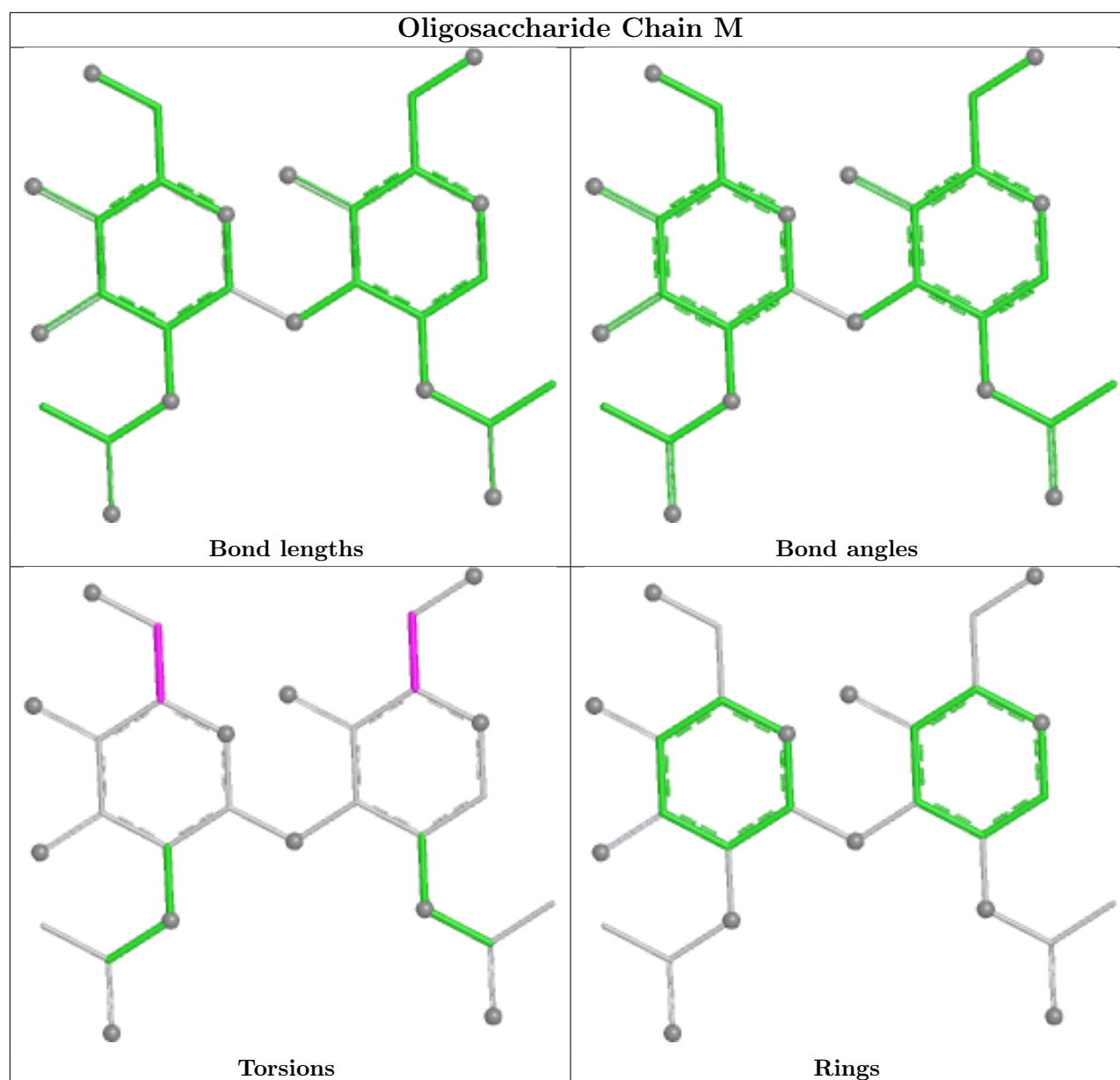












## 5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.48	0
8	NAG	B	1304	1	14,14,15	0.40	0	17,19,21	0.54	0
8	NAG	C	1311	1	14,14,15	0.22	0	17,19,21	0.38	0
8	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.43	0
8	NAG	C	1305	1	14,14,15	0.32	0	17,19,21	0.53	0
8	NAG	C	1303	1	14,14,15	0.25	0	17,19,21	0.55	0
8	NAG	A	1303	1	14,14,15	0.30	0	17,19,21	0.64	0
8	NAG	C	1301	1	14,14,15	0.47	0	17,19,21	0.46	0
8	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.43	0
8	NAG	A	1307	1	14,14,15	0.21	0	17,19,21	0.39	0
8	NAG	A	1306	1	14,14,15	0.29	0	17,19,21	0.49	0
8	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.47	0
8	NAG	C	1309	1	14,14,15	0.23	0	17,19,21	0.61	0
8	NAG	C	1312	1	14,14,15	0.25	0	17,19,21	0.53	0
8	NAG	B	1301	1	14,14,15	0.21	0	17,19,21	0.45	0
8	NAG	C	1313	1	14,14,15	0.27	0	17,19,21	0.53	0
8	NAG	A	1304	1	14,14,15	0.28	0	17,19,21	0.51	0
8	NAG	C	1302	-	14,14,15	0.21	0	17,19,21	0.42	0
8	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.53	0
8	NAG	C	1307	1	14,14,15	0.21	0	17,19,21	0.47	0
8	NAG	A	1305	1	14,14,15	0.24	0	17,19,21	0.44	0
8	NAG	B	1303	1	14,14,15	0.26	0	17,19,21	0.39	0
8	NAG	C	1310	1	14,14,15	0.32	0	17,19,21	0.54	0
8	NAG	B	1302	1	14,14,15	0.27	0	17,19,21	0.49	0
8	NAG	C	1306	1	14,14,15	0.23	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
8	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
8	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1302	1	-	0/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1313	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1302	-	-	2/6/23/26	0/1/1/1
8	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
8	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
8	NAG	C	1306	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1312	NAG	C4-C5-C6-O6
8	C	1302	NAG	C4-C5-C6-O6
8	C	1301	NAG	O5-C5-C6-O6
8	A	1306	NAG	C4-C5-C6-O6
8	C	1303	NAG	C4-C5-C6-O6
8	C	1302	NAG	O5-C5-C6-O6
8	C	1312	NAG	O5-C5-C6-O6
8	B	1305	NAG	C4-C5-C6-O6
8	A	1307	NAG	O5-C5-C6-O6
8	C	1305	NAG	O5-C5-C6-O6
8	C	1301	NAG	C4-C5-C6-O6
8	C	1310	NAG	O5-C5-C6-O6
8	A	1306	NAG	O5-C5-C6-O6
8	A	1307	NAG	C4-C5-C6-O6
8	C	1303	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	B	1305	NAG	O5-C5-C6-O6
8	C	1311	NAG	C4-C5-C6-O6
8	B	1301	NAG	C4-C5-C6-O6
8	C	1305	NAG	C4-C5-C6-O6
8	C	1311	NAG	O5-C5-C6-O6
8	C	1310	NAG	C4-C5-C6-O6
8	B	1304	NAG	C8-C7-N2-C2
8	B	1304	NAG	O7-C7-N2-C2
8	C	1301	NAG	C8-C7-N2-C2
8	C	1301	NAG	O7-C7-N2-C2
8	C	1304	NAG	C8-C7-N2-C2
8	C	1304	NAG	O7-C7-N2-C2
8	B	1301	NAG	O5-C5-C6-O6
8	B	1303	NAG	C4-C5-C6-O6
8	C	1313	NAG	C4-C5-C6-O6
8	B	1302	NAG	C4-C5-C6-O6
8	B	1302	NAG	O5-C5-C6-O6
8	B	1303	NAG	O5-C5-C6-O6
8	C	1307	NAG	O5-C5-C6-O6
8	C	1313	NAG	O5-C5-C6-O6
8	B	1304	NAG	C4-C5-C6-O6
8	C	1304	NAG	C4-C5-C6-O6
8	C	1304	NAG	O5-C5-C6-O6
8	A	1303	NAG	C1-C2-N2-C7
8	C	1303	NAG	C1-C2-N2-C7
8	C	1306	NAG	C4-C5-C6-O6
8	C	1308	NAG	C4-C5-C6-O6
8	C	1306	NAG	O5-C5-C6-O6
8	C	1308	NAG	O5-C5-C6-O6
8	B	1304	NAG	O5-C5-C6-O6
8	A	1303	NAG	C3-C2-N2-C7
8	C	1303	NAG	C3-C2-N2-C7
8	C	1309	NAG	C3-C2-N2-C7
8	C	1313	NAG	C3-C2-N2-C7
8	B	1302	NAG	C1-C2-N2-C7
8	B	1303	NAG	C1-C2-N2-C7
8	C	1309	NAG	C1-C2-N2-C7
8	C	1313	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	338:PHE	C	339:GLY	N	4.28
1	A	526:GLY	C	527:PRO	N	4.25

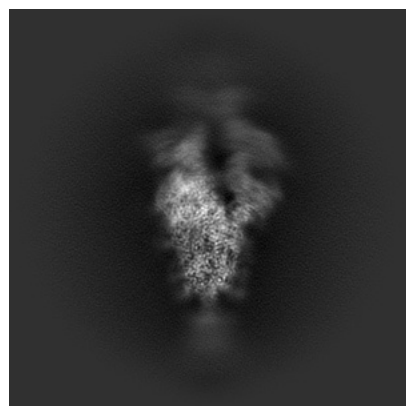
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25794. These allow visual inspection of the internal detail of the map and identification of artifacts.

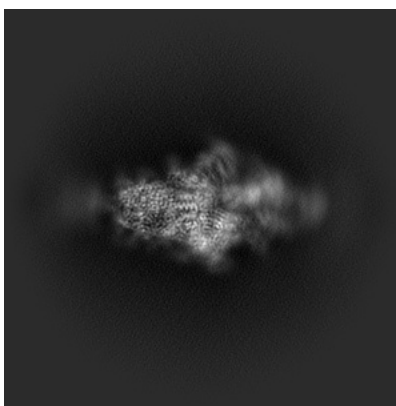
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

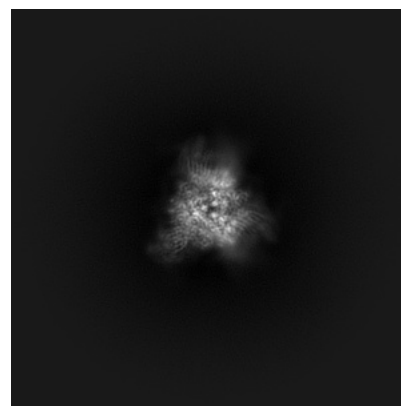
#### 6.1.1 Primary map



X

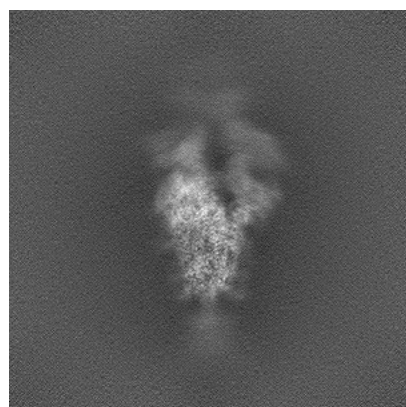


Y

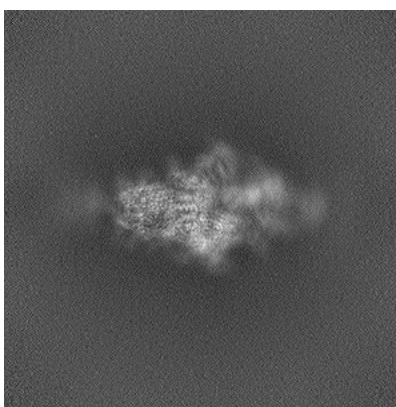


Z

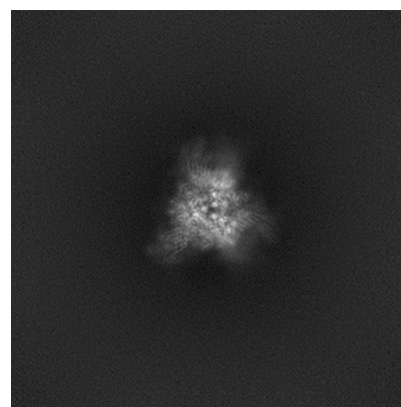
#### 6.1.2 Raw map



X



Y



Z

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

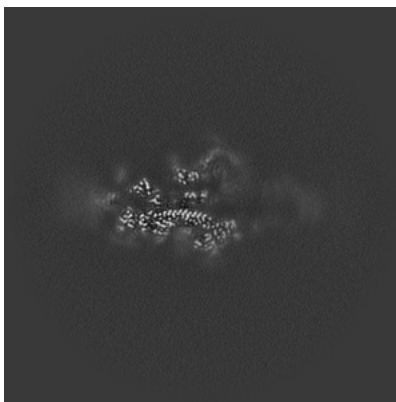


## 6.2 Central slices [i](#)

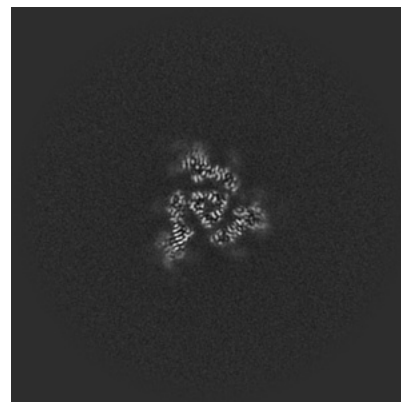
### 6.2.1 Primary map



X Index: 260

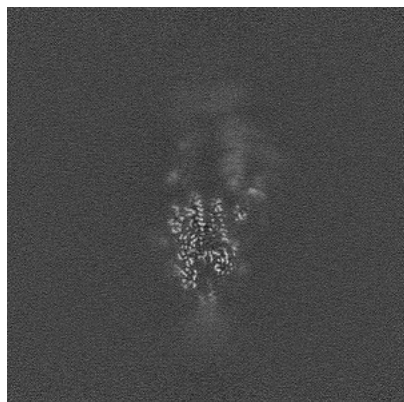


Y Index: 260

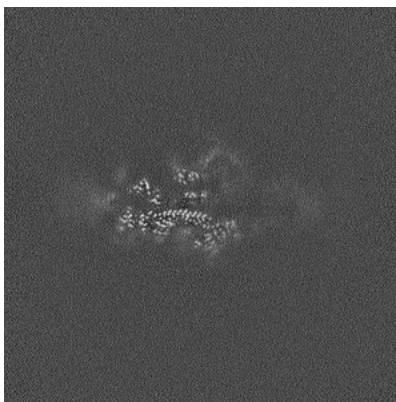


Z Index: 260

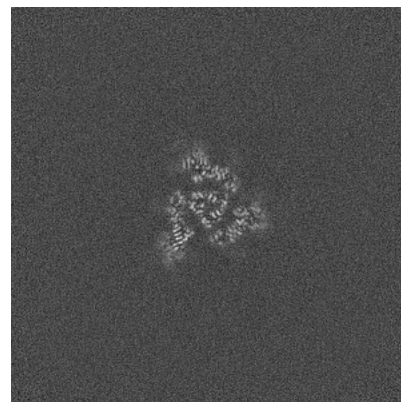
### 6.2.2 Raw map



X Index: 260



Y Index: 260

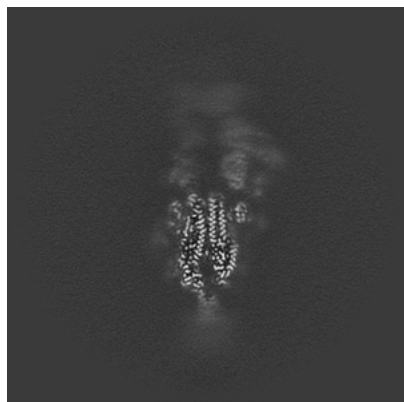


Z Index: 260

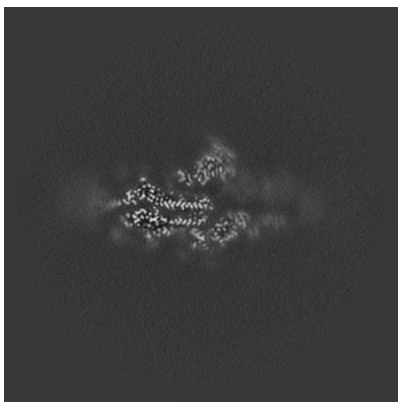
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

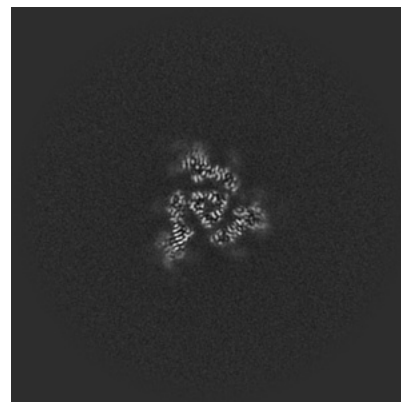
### 6.3.1 Primary map



X Index: 264

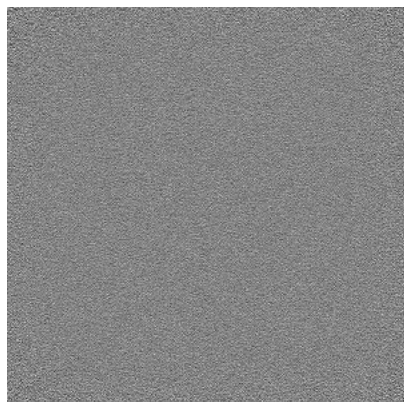


Y Index: 252

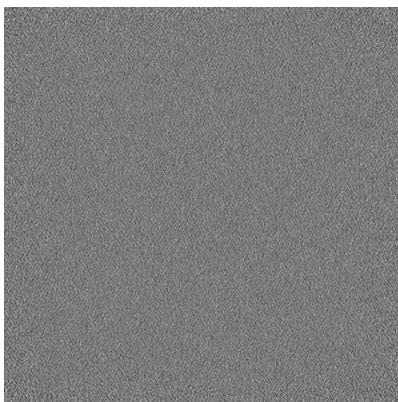


Z Index: 260

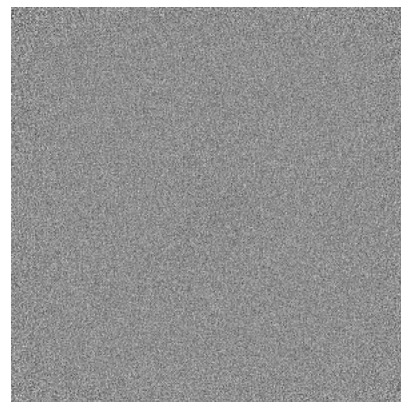
### 6.3.2 Raw map



X Index: 0



Y Index: 0

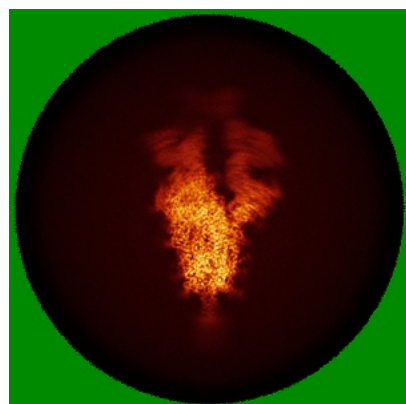


Z Index: 519

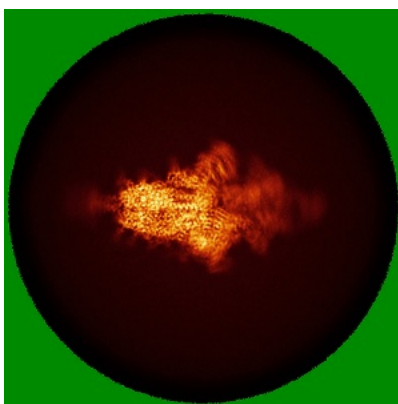
The images above show the largest variance slices of the map in three orthogonal directions.

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

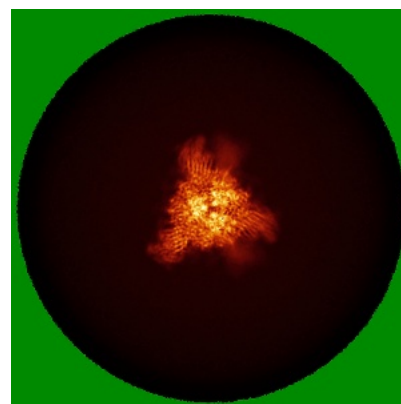
### 6.4.1 Primary map



X

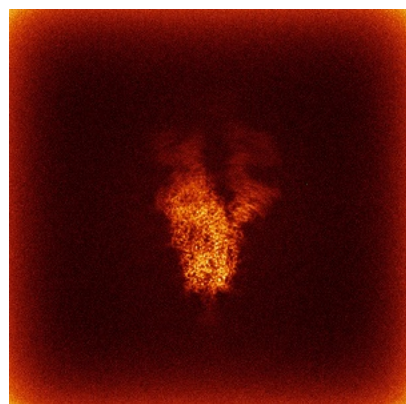


Y

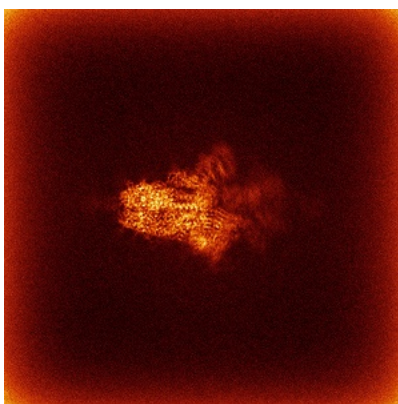


Z

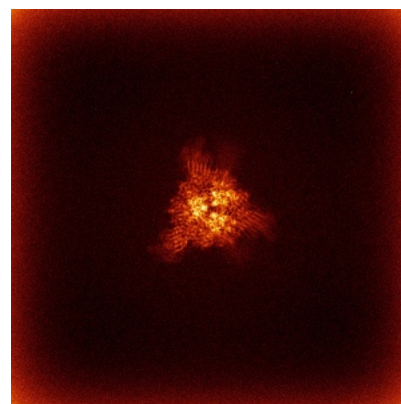
### 6.4.2 Raw map



X



Y

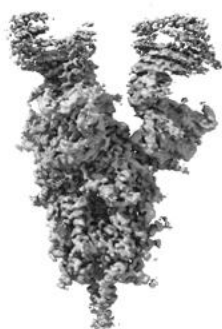


Z

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



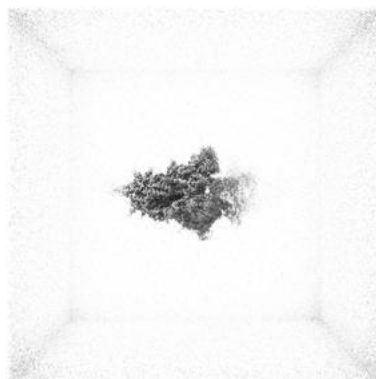
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0838. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

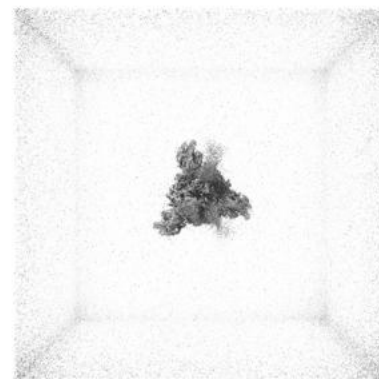
### 6.5.2 Raw map



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.



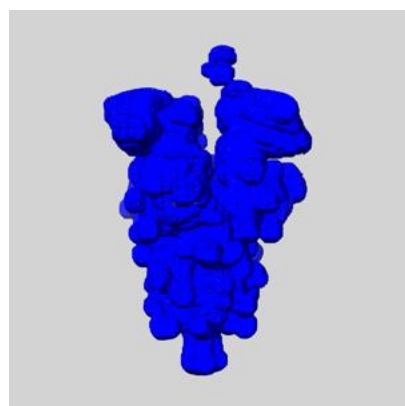
## 6.6 Mask visualisation [i](#)

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

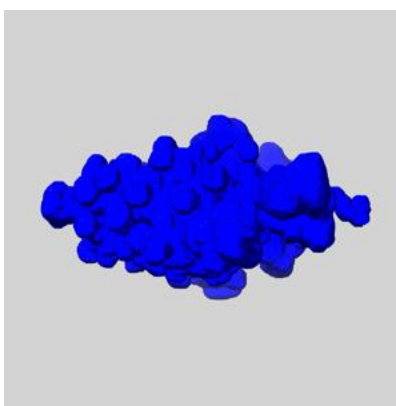
A mask typically either:

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

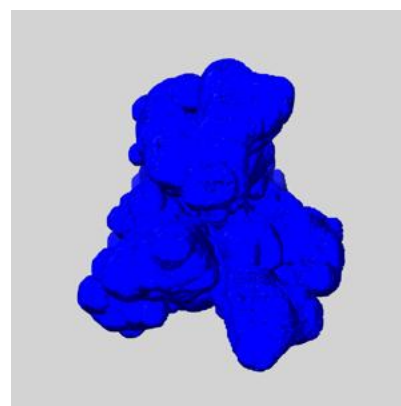
### 6.6.1 emd\_25794\_msk\_1.map [i](#)



X



Y

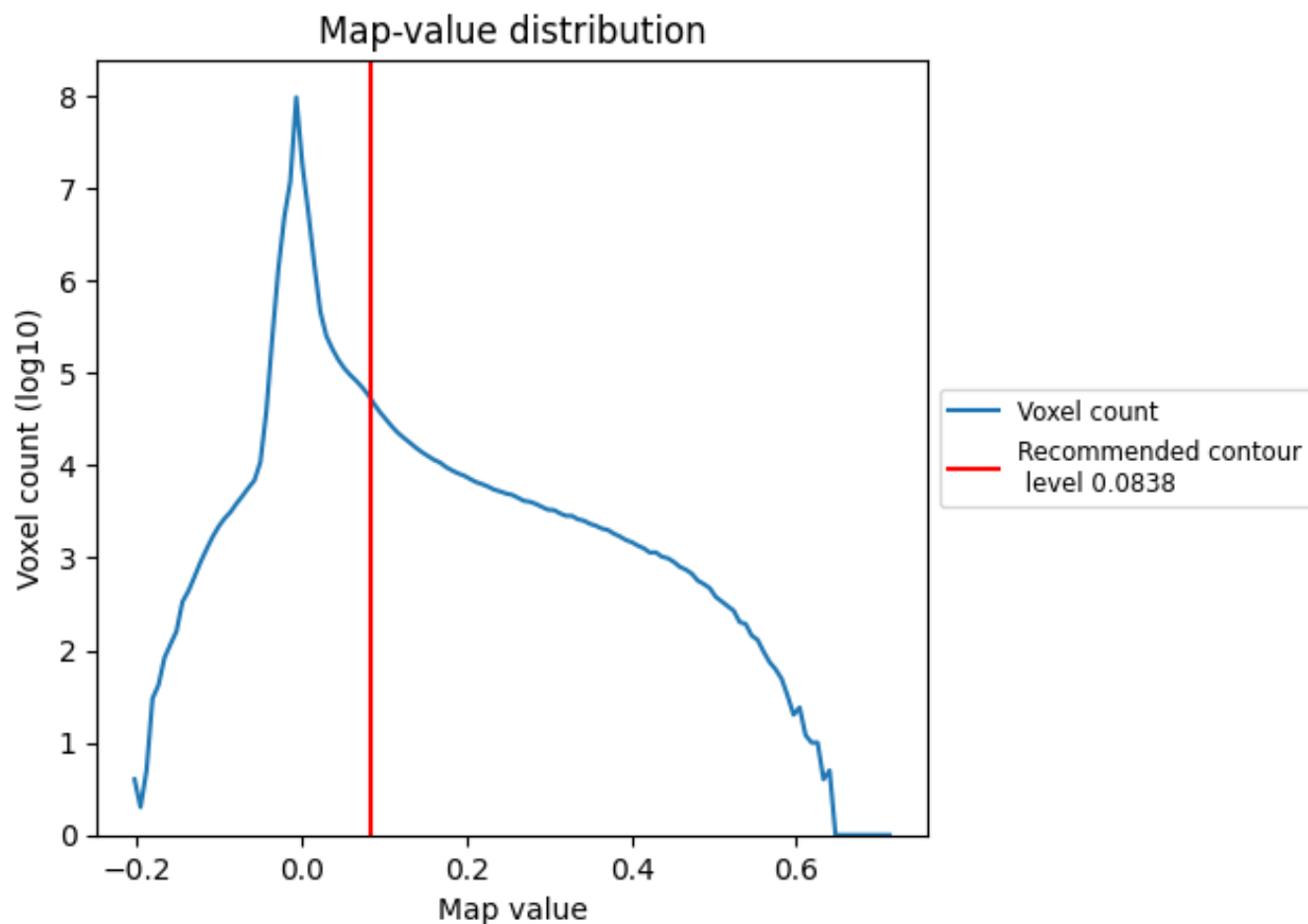


Z

## 7 Map analysis [i](#)

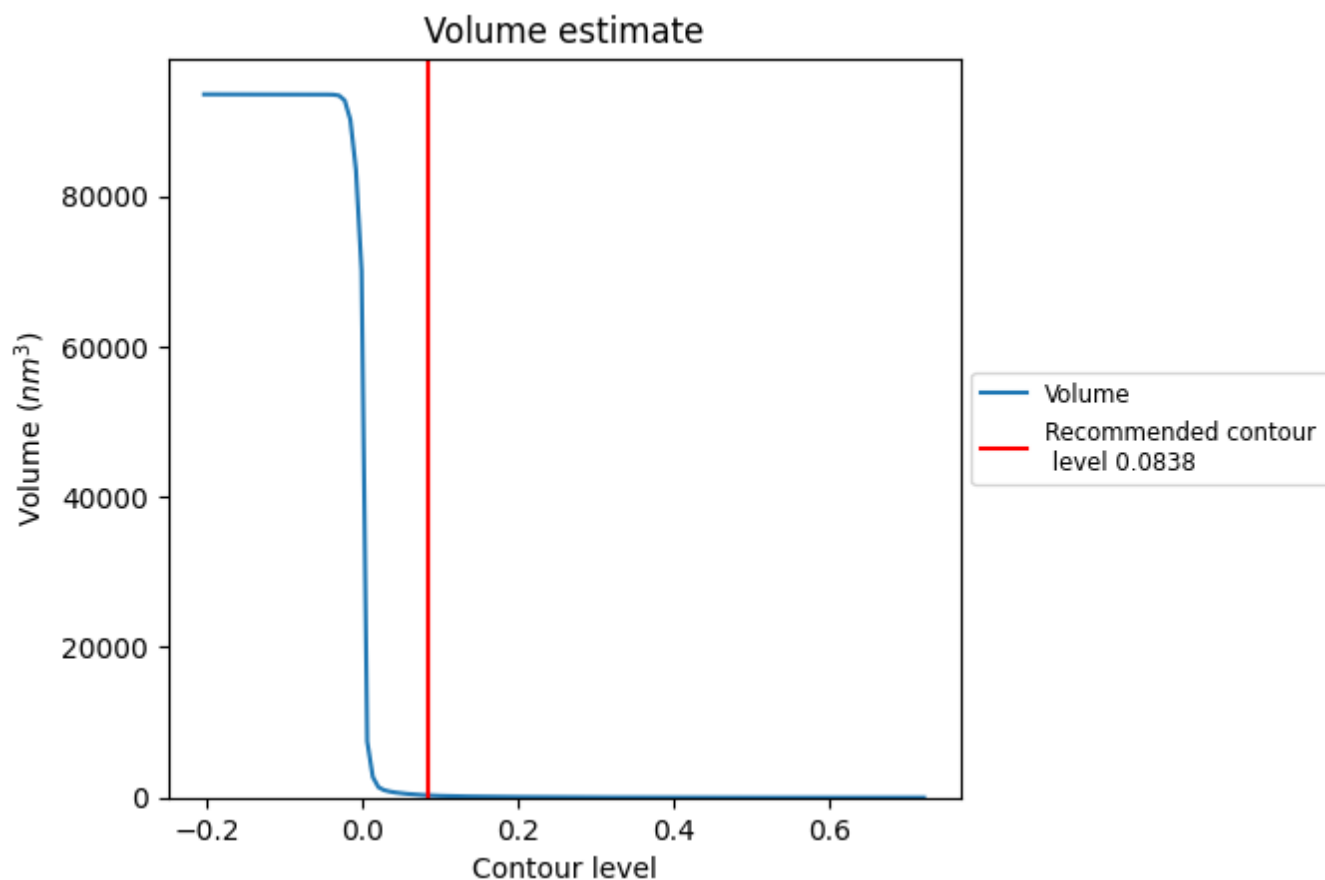
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

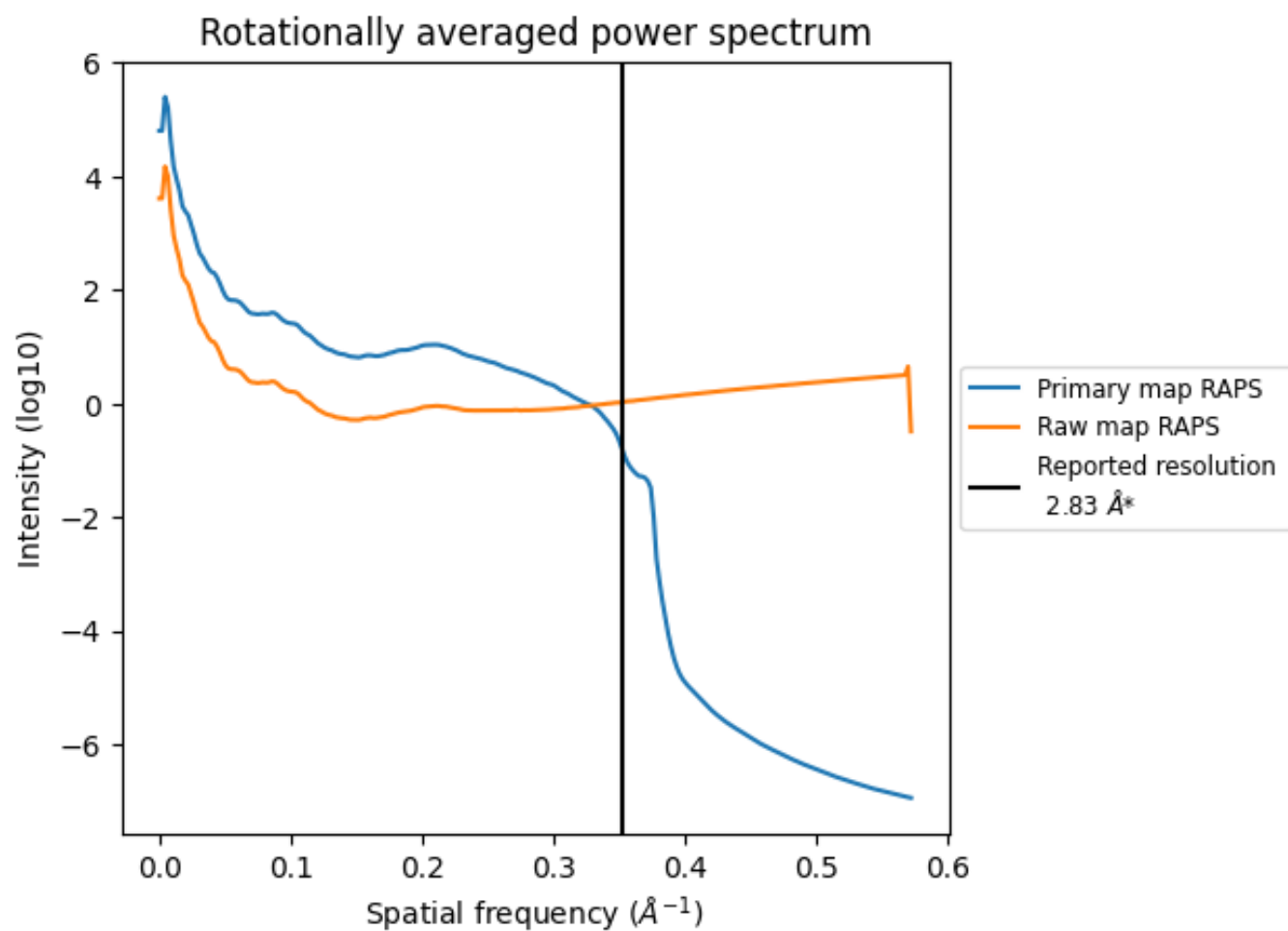
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm<sup>3</sup>; this corresponds to an approximate mass of 267 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 ⓘ



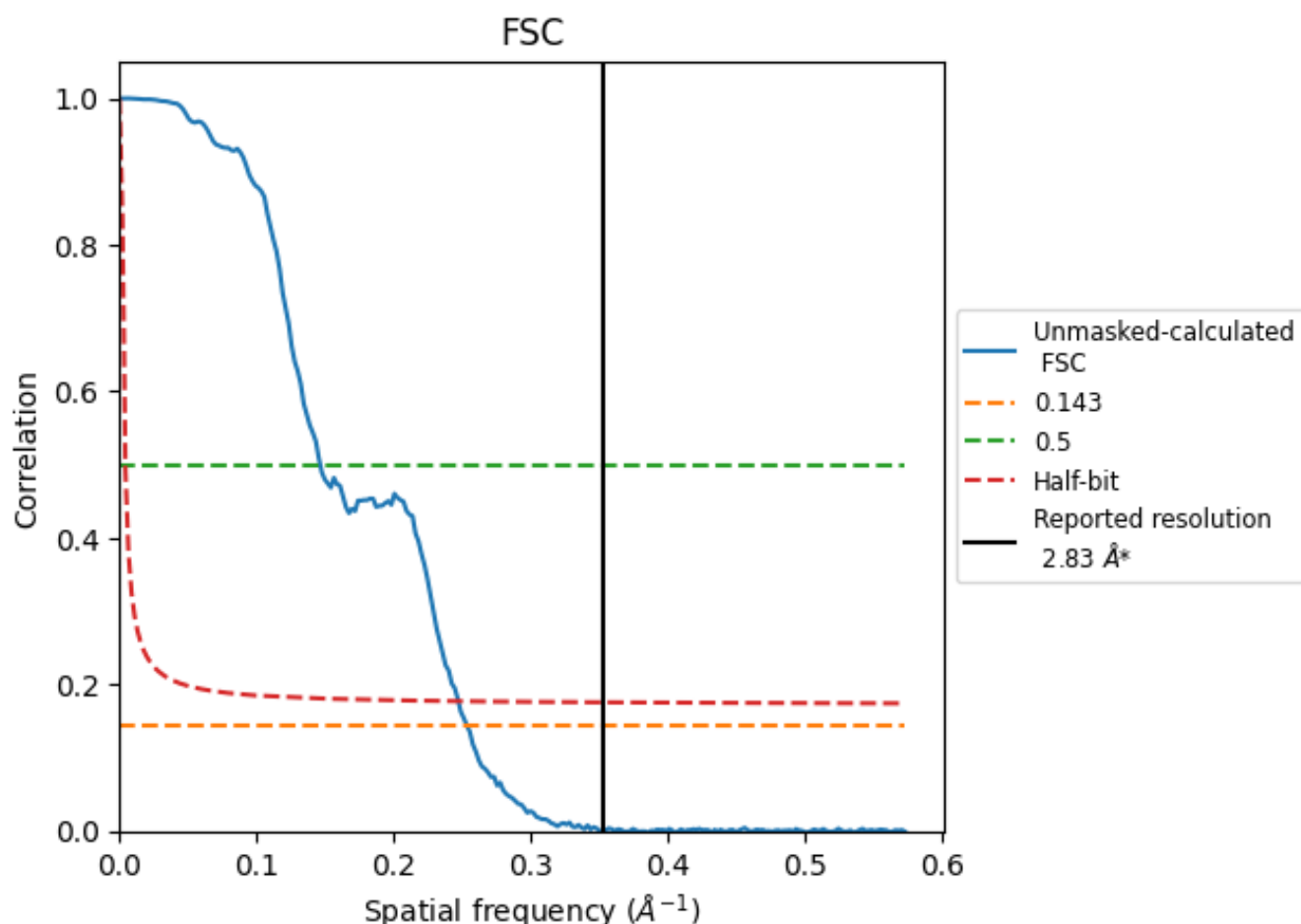
\*Reported resolution corresponds to spatial frequency of 0.353 Å<sup>-1</sup>



## 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 0.353  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

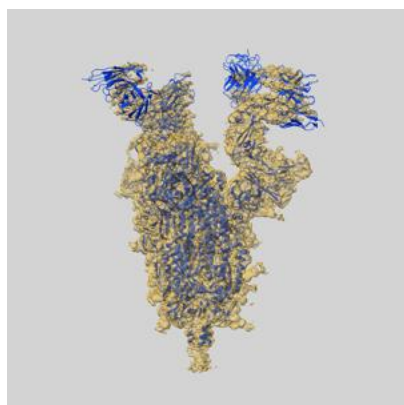
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	2.83	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	6.84	4.05

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 6.84 differs from the reported value 2.83 by more than 10 %

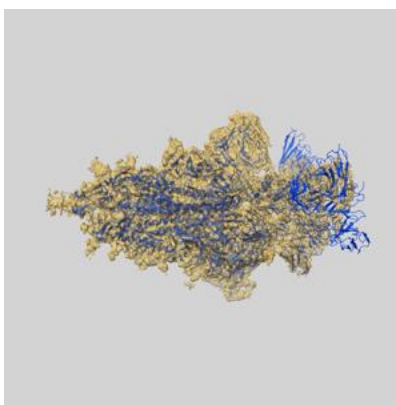
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25794 and PDB model 7TB8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

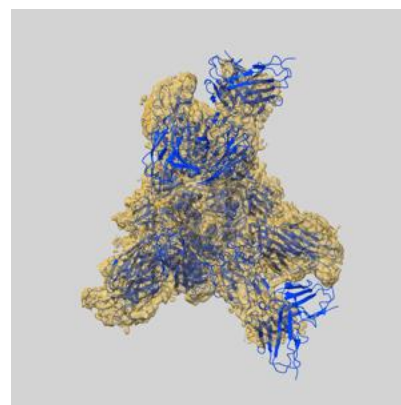
### 9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0838 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](#)



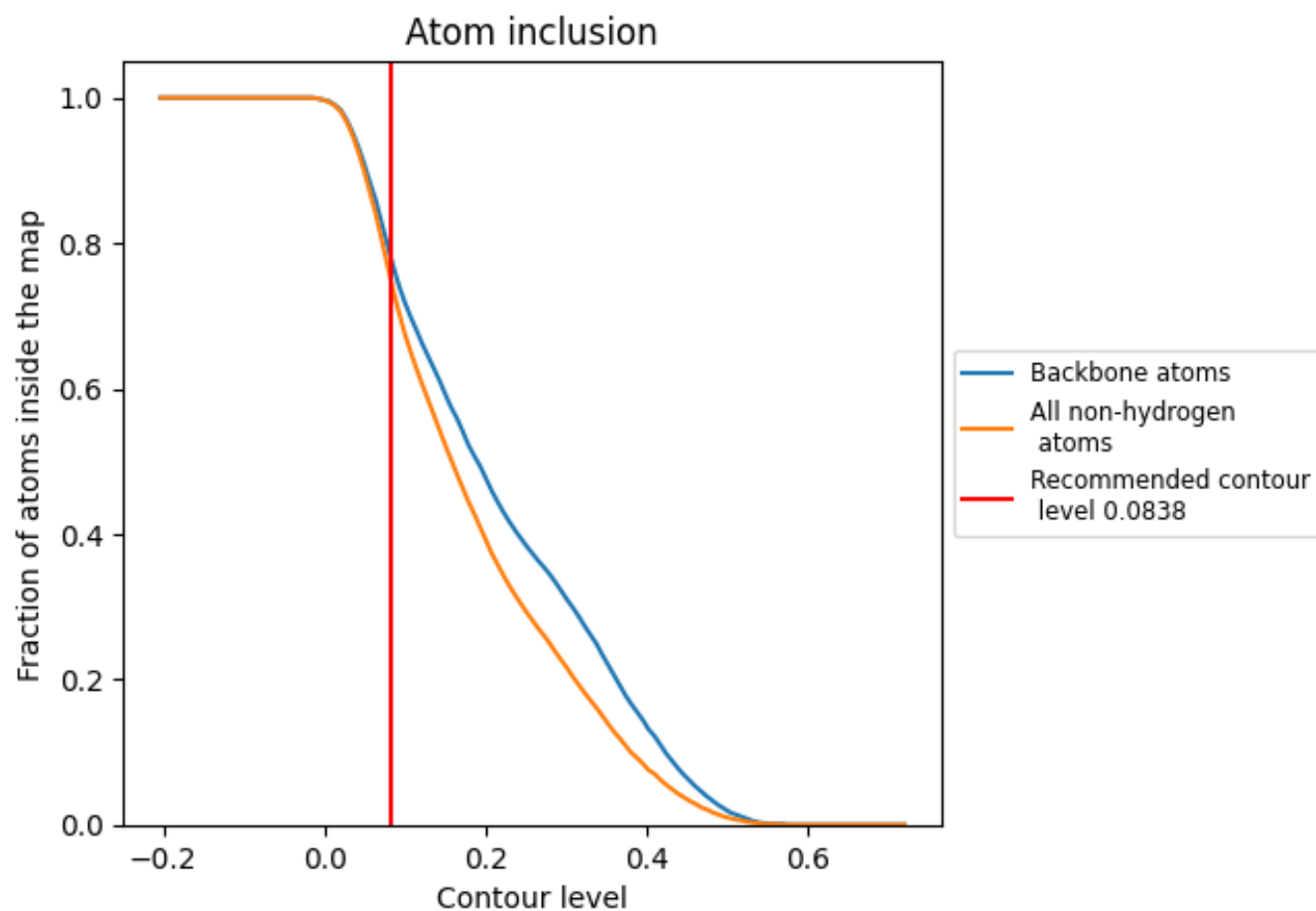
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0838).











































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 74% 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 (0.0838) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7440	 0.4100
A	 0.8790	 0.4610
B	 0.9310	 0.5050
C	 0.8570	 0.4700
D	 0.1930	 0.1340
E	 0.1320	 0.1170
F	 0.4960	 0.2790
G	 0.5530	 0.3280
H	 0.0720	 0.1190
I	 0.9290	 0.4000
J	 0.1240	 0.0940
K	 0.0500	 0.0860
L	 0.0040	 0.0990
M	 0.7500	 0.3500
N	 0.9290	 0.5130
O	 0.9640	 0.5090
P	 0.8930	 0.4460
Q	 0.9640	 0.5200
R	 0.9640	 0.5420
S	 0.9290	 0.4560
T	 1.0000	 0.5430

