



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 11:36 PM UTC

PDB ID : 7CHH / pdb_00007chh
EMDB ID : EMD-30374
Title : Cryo-EM structure of the SARS-CoV-2 S-6P in complex with BD-368-2 Fabs
Authors : Xiao, J.; Zhu, Q.; Wang, G.
Deposited on : 2020-07-05
Resolution : 3.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

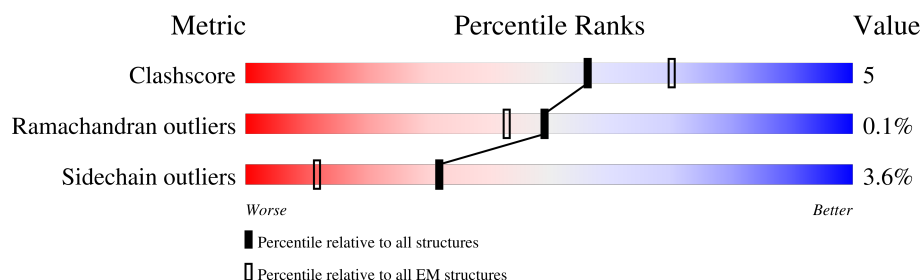
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	A	1208	64% 74% 9% 17%
1	B	1208	67% 73% 9% 18%
1	C	1208	67% 73% 9% 17%
2	D	230	46% 36% 14% • 46%
2	G	230	49% 36% 14% • 46%
2	J	230	50% 36% 14% • 46%
3	E	219	51% 36% 12% • 49%
3	H	219	49% 36% 13% • 49%

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Mol	Chain	Length	Quality of chain
3	K	219	44% 36% 13% 49%
4	F	2	50% 50%
4	I	2	100% 50% 50%
4	L	2	100% 50% 50%
4	M	2	100% 100%
4	N	2	100% 50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29029 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	1003	Total	C	N	O	S	0	0
			7734	4935	1289	1475	35		
1	B	994	Total	C	N	O	S	0	0
			7652	4880	1271	1466	35		
1	C	999	Total	C	N	O	S	0	0
			7672	4897	1270	1470	35		

There are 27 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	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	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	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	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	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called BD-368-2 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	124	Total 947	C 595	N 165	O 183	S 4	0	0
2	G	124	Total 947	C 595	N 165	O 183	S 4	0	0
2	J	124	Total 947	C 595	N 165	O 183	S 4	0	0

- Molecule 3 is a protein called BD-368-2 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	112	Total 852	C 535	N 144	O 169	S 4	0	0
3	H	112	Total 852	C 535	N 144	O 169	S 4	0	0
3	K	112	Total 852	C 535	N 144	O 169	S 4	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

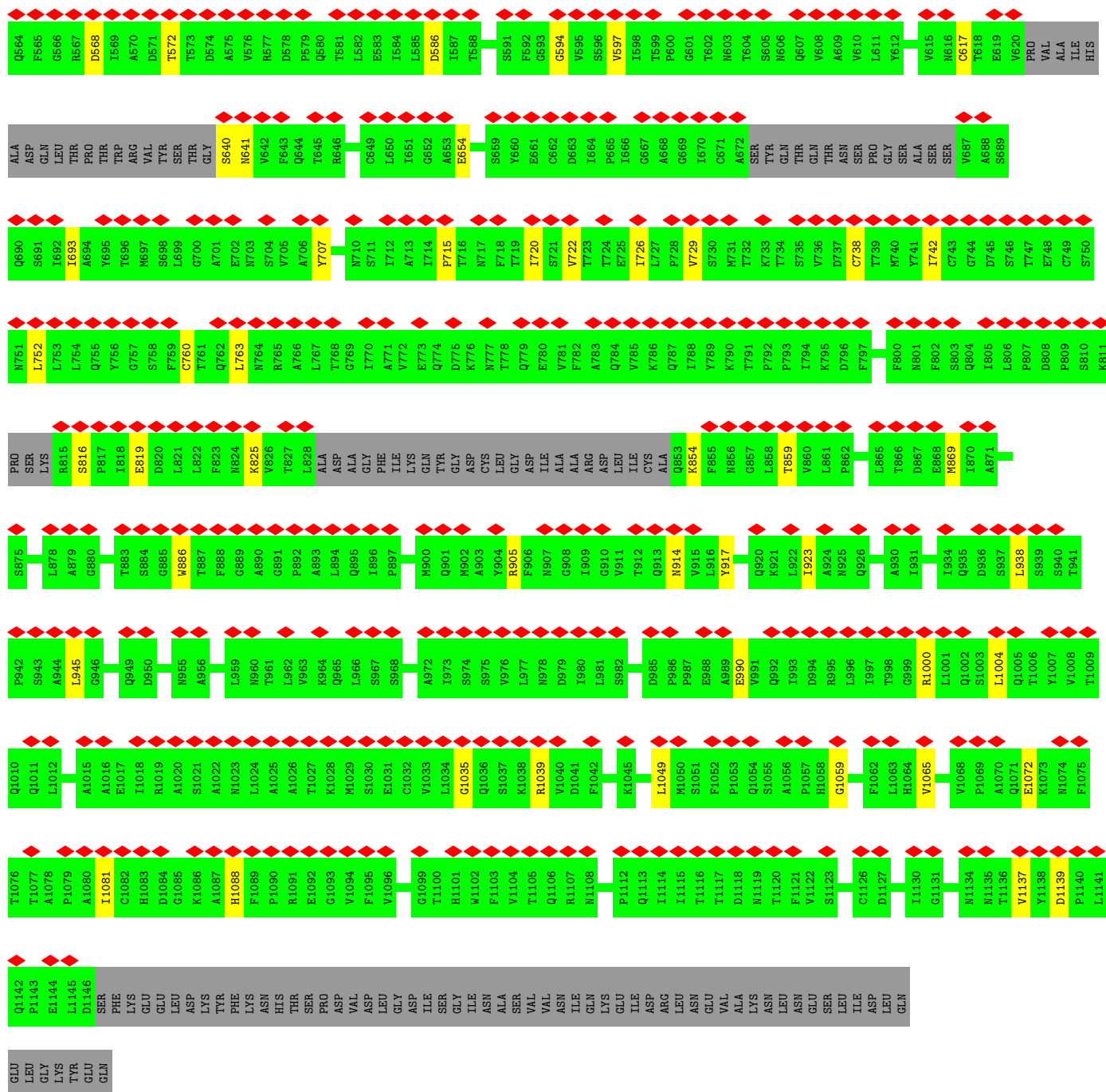


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5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

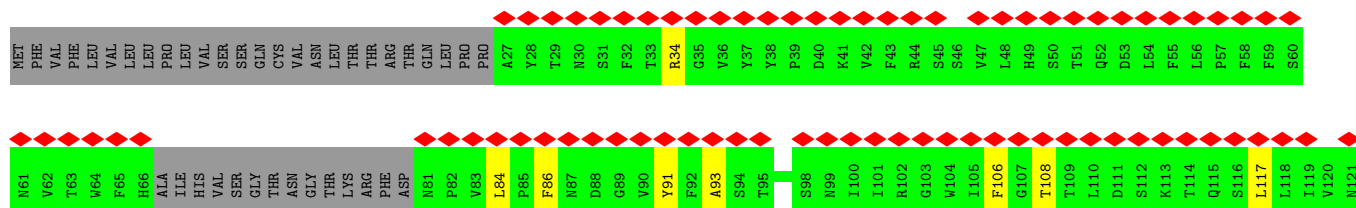
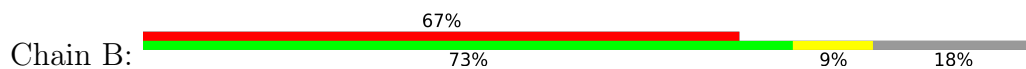
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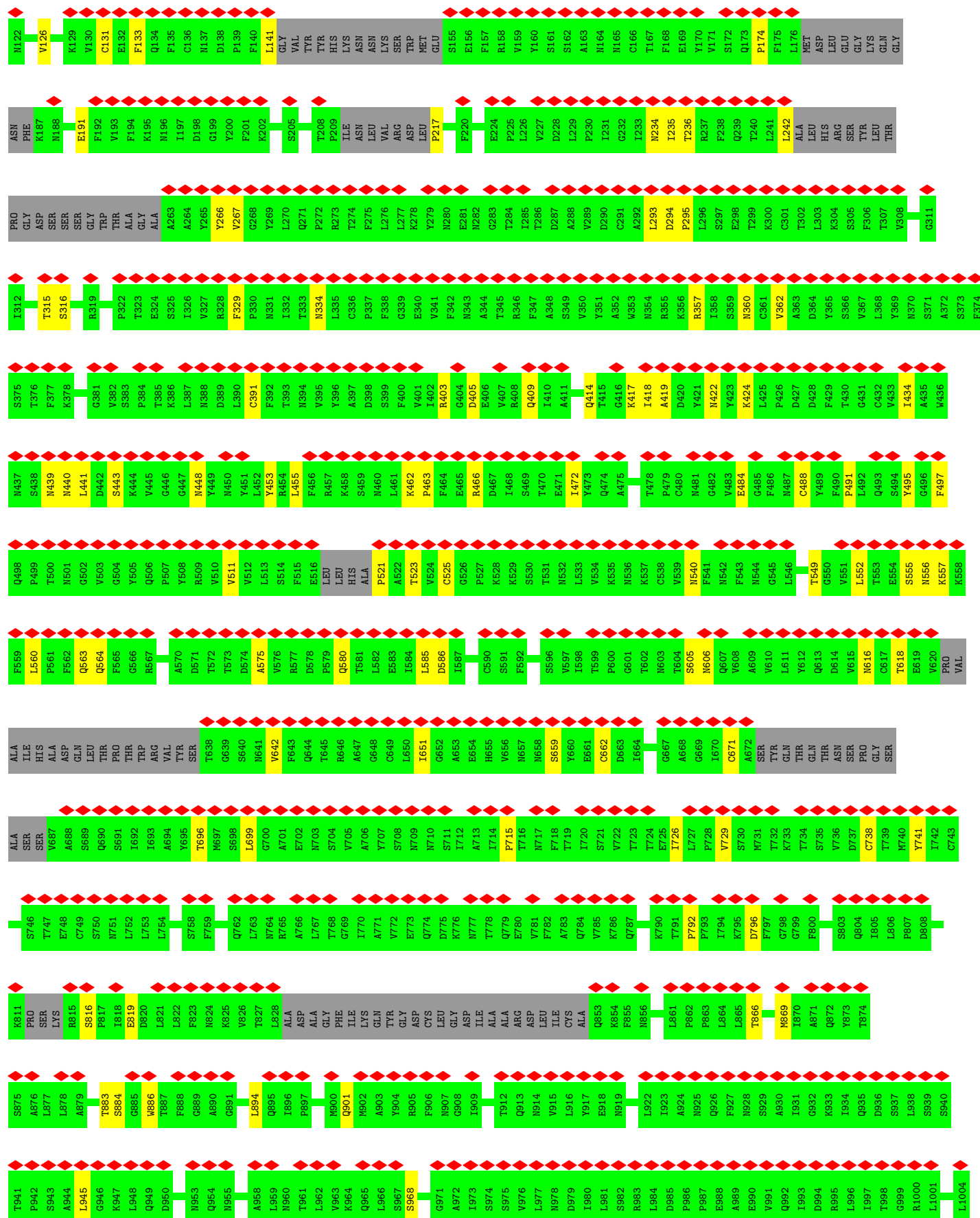
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C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

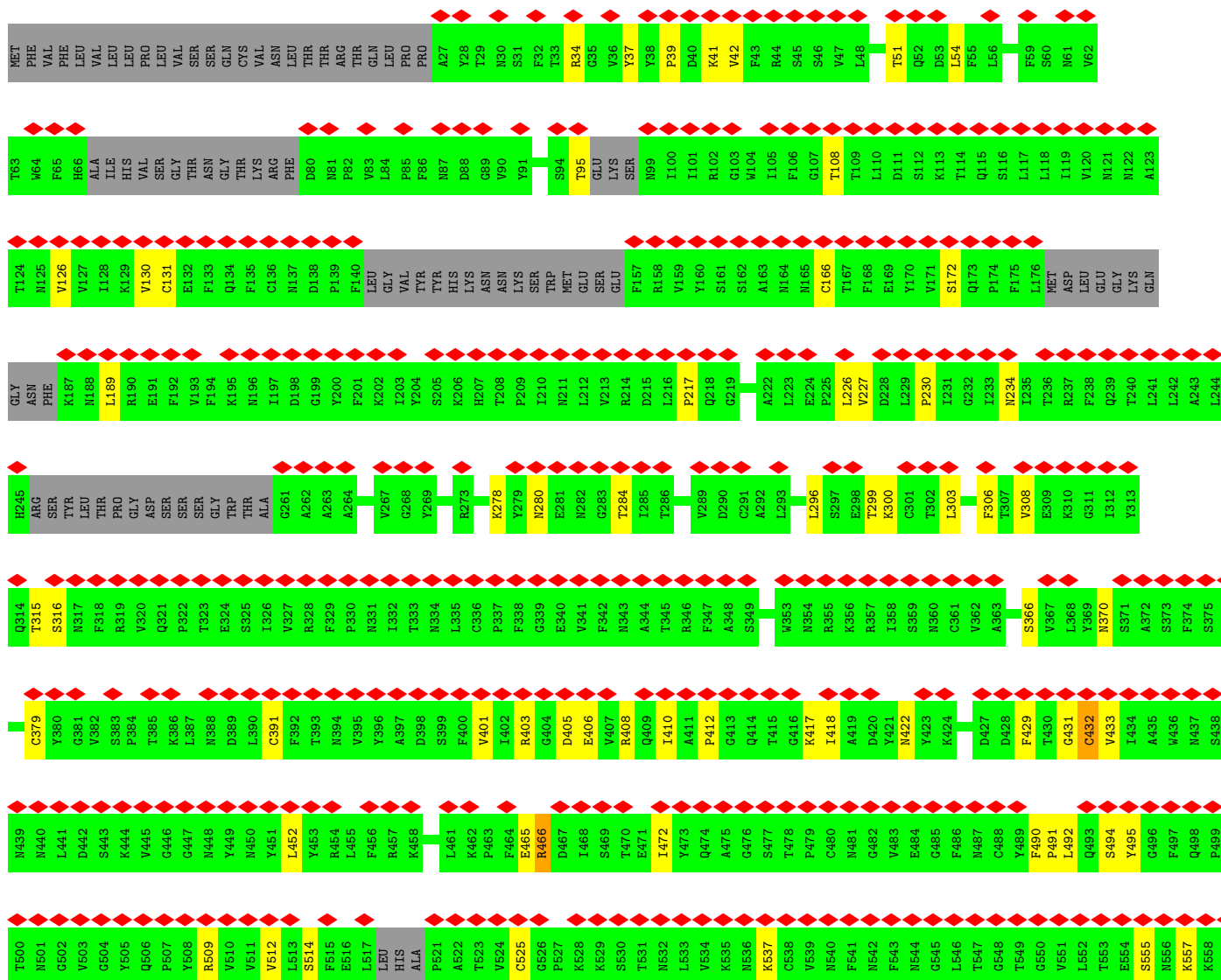
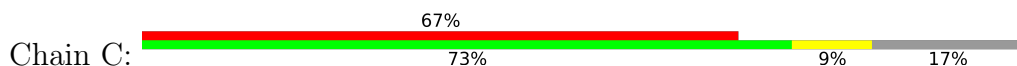


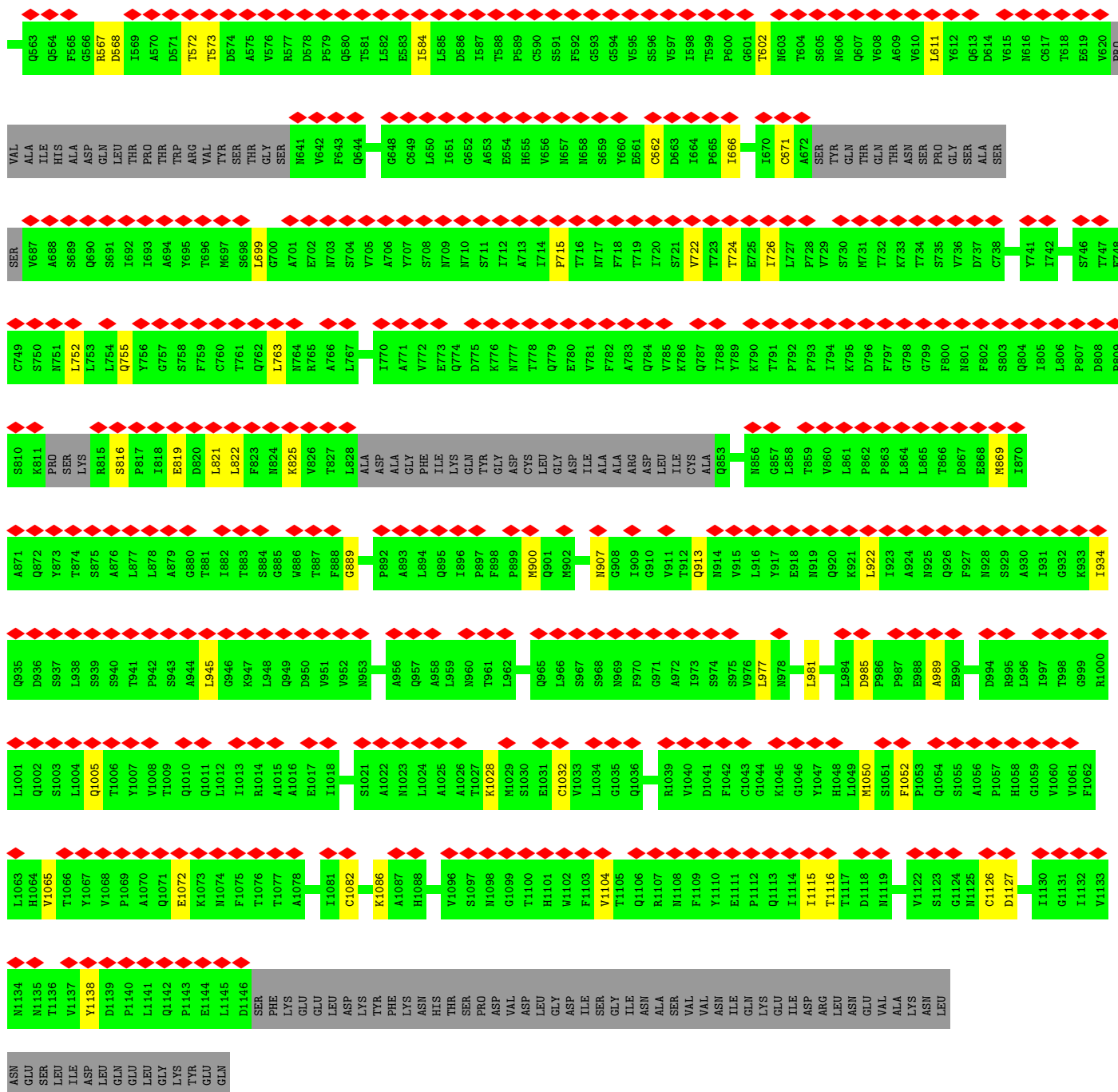
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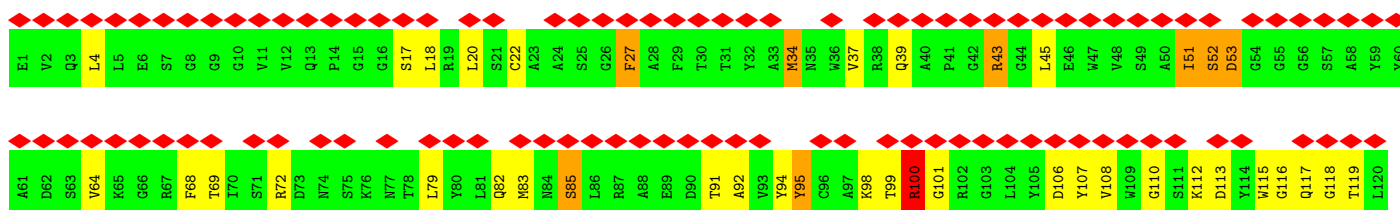
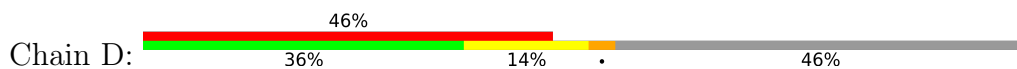


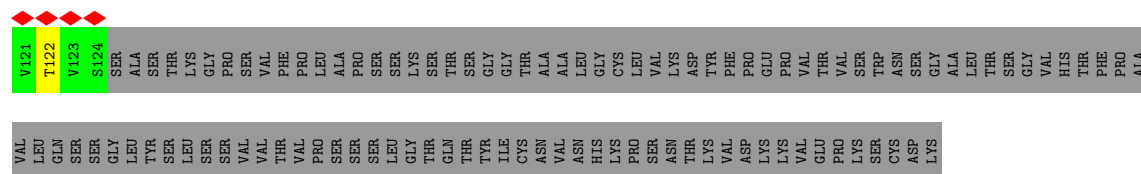
- Molecule 1: Spike glycoprotein



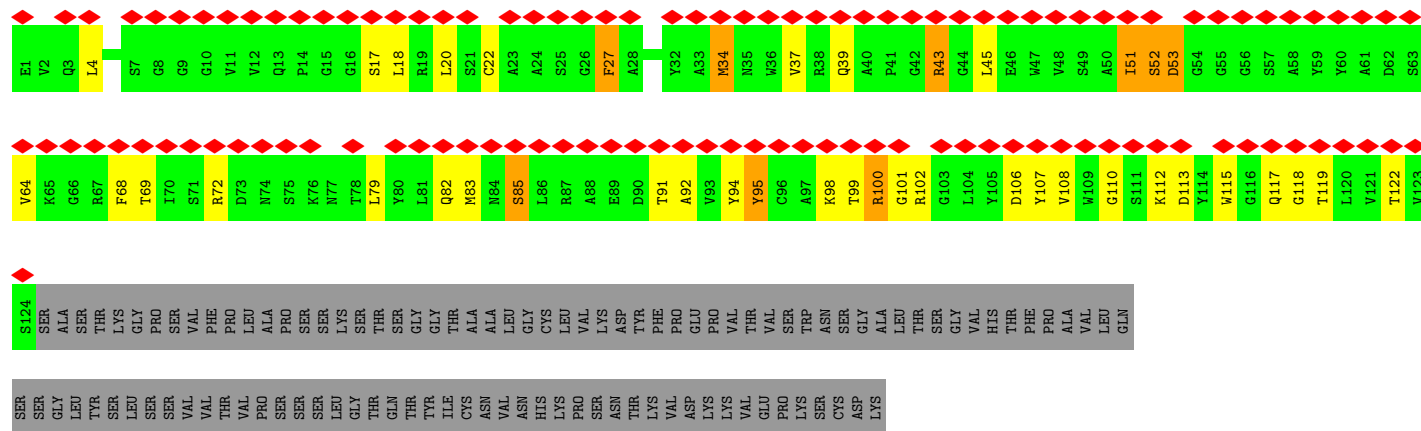
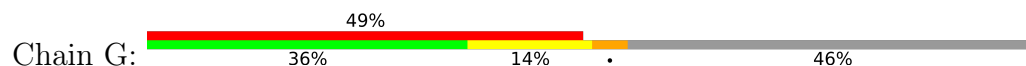


• Molecule 2: BD-368-2 Fab heavy chain

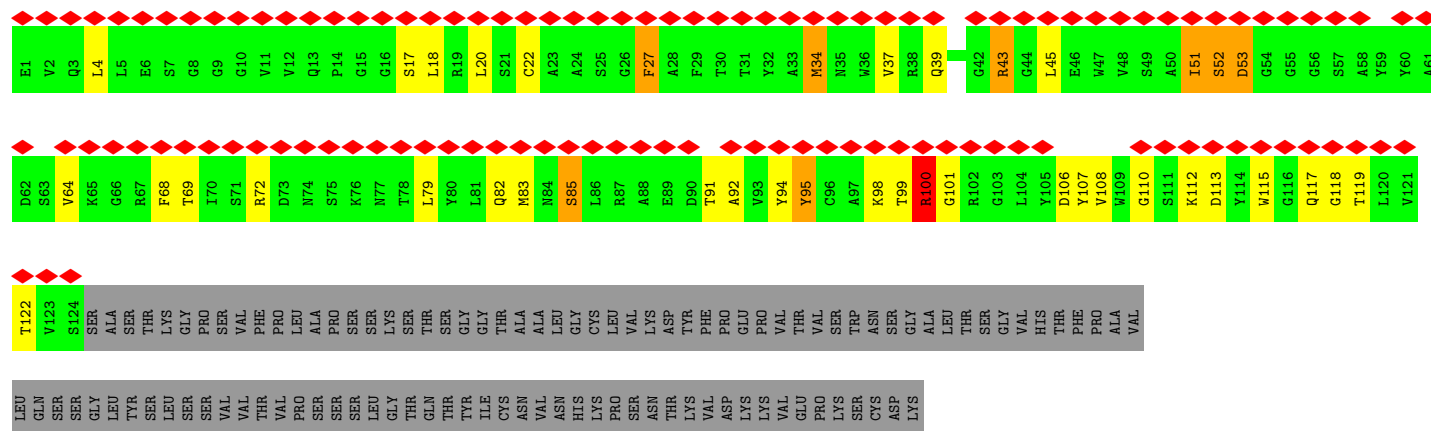
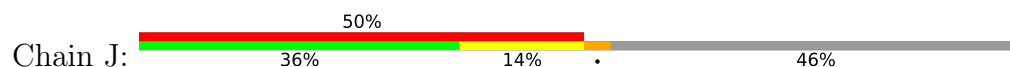




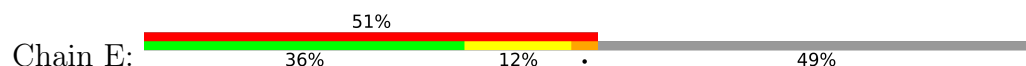
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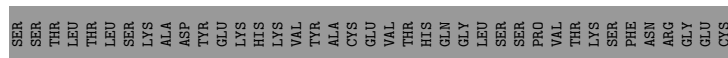
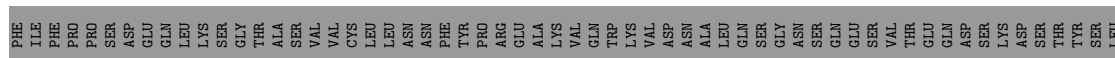
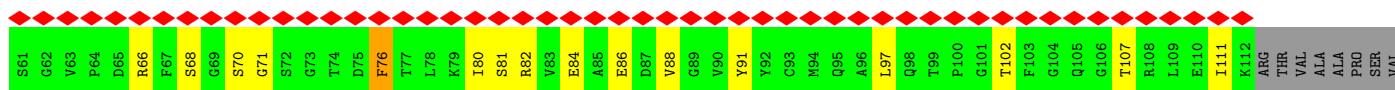


• Molecule 2: BD-368-2 Fab heavy chain

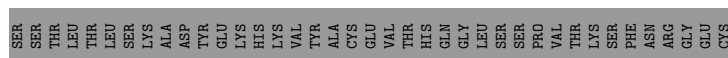
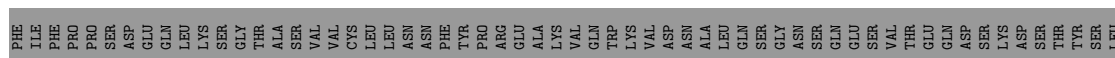
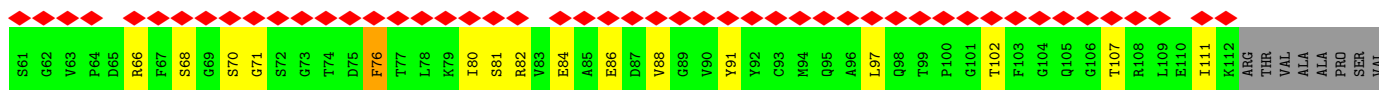
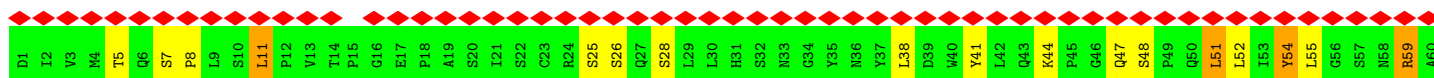
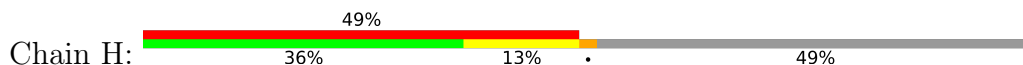


• Molecule 3: BD-368-2 Fab light chain

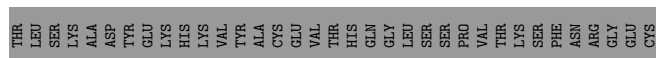
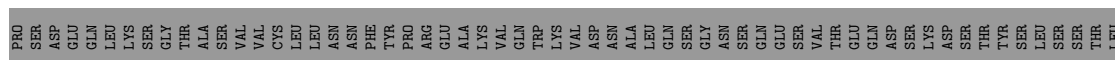
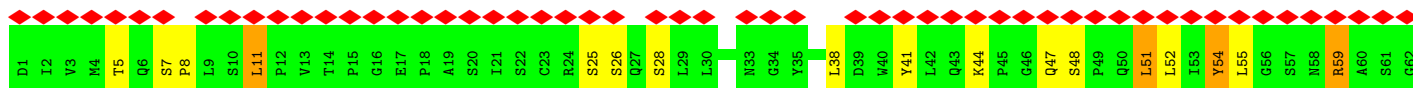
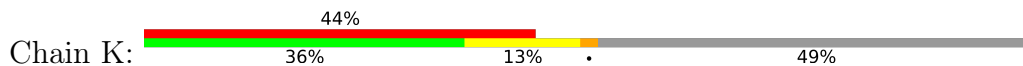




• Molecule 3: BD-368-2 Fab light chain



• Molecule 3: BD-368-2 Fab light chain



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



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



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



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- Molecule 4: 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, C1	Depositor
Number of particles used	85053	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0122	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.005, 1.005, 1.005	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	0.31	0/7904	0.61	4/10764 (0.0%)
1	B	0.31	0/7822	0.58	0/10653
1	C	0.30	0/7843	0.58	3/10689 (0.0%)
2	D	0.32	0/968	0.78	4/1311 (0.3%)
2	G	0.31	0/968	0.78	4/1311 (0.3%)
2	J	0.32	0/968	0.78	4/1311 (0.3%)
3	E	0.26	0/871	0.67	2/1183 (0.2%)
3	H	0.26	0/871	0.67	2/1183 (0.2%)
3	K	0.26	0/871	0.67	2/1183 (0.2%)
All	All	0.30	0/29086	0.62	25/39588 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
2	D	0	1
2	G	0	1
2	J	0	1
All	All	0	7

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	100	ARG	CB-CG-CD	-6.80	95.66	111.30
2	J	100	ARG	CB-CG-CD	-6.79	95.67	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	100	ARG	CB-CG-CD	-6.77	95.72	111.30
1	C	432	CYS	CA-CB-SG	6.30	128.88	114.40
1	A	165	ASN	CA-C-N	-6.28	111.32	122.74
1	A	165	ASN	C-N-CA	-6.28	111.32	122.74
2	D	43	ARG	CA-CB-CG	6.21	126.51	114.10
2	G	43	ARG	CA-CB-CG	6.21	126.51	114.10
3	H	59	ARG	CB-CG-CD	6.17	125.49	111.30
2	J	43	ARG	CA-CB-CG	6.17	126.43	114.10
3	E	59	ARG	CB-CG-CD	6.16	125.48	111.30
3	K	59	ARG	CB-CG-CD	6.16	125.46	111.30
1	C	466	ARG	CG-CD-NE	5.56	124.23	112.00
1	A	379	CYS	CA-CB-SG	5.49	127.02	114.40
1	A	166	CYS	CA-CB-SG	5.38	126.78	114.40
2	D	100	ARG	CA-CB-CG	5.17	124.44	114.10
2	J	100	ARG	CA-CB-CG	5.15	124.40	114.10
2	G	100	ARG	CA-CB-CG	5.14	124.39	114.10
3	K	59	ARG	CA-CB-CG	5.14	124.38	114.10
3	E	59	ARG	CA-CB-CG	5.12	124.33	114.10
3	H	59	ARG	CA-CB-CG	5.11	124.33	114.10
2	J	43	ARG	CB-CG-CD	5.06	122.94	111.30
1	C	130	VAL	N-CA-C	-5.04	106.52	111.77
2	G	43	ARG	CB-CG-CD	5.04	122.89	111.30
2	D	43	ARG	CB-CG-CD	5.03	122.86	111.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ASN	Peptide
1	A	517	LEU	Peptide
1	A	617	CYS	Peptide
1	B	293	LEU	Peptide
2	D	100	ARG	Peptide
2	G	100	ARG	Peptide
2	J	100	ARG	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	7734	0	7469	71	0
1	B	7652	0	7364	64	0
1	C	7672	0	7368	72	0
2	D	947	0	907	20	0
2	G	947	0	907	19	0
2	J	947	0	907	19	0
3	E	852	0	833	11	0
3	H	852	0	833	10	0
3	K	852	0	833	11	0
4	F	28	0	25	0	0
4	I	28	0	25	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	1	0
5	A	168	0	156	0	0
5	B	140	0	130	0	0
5	C	126	0	117	0	0
All	All	29029	0	27949	281	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 5.

All (281) 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)
2:G:99:THR:HG22	2:G:101:GLY:H	1.56	0.71
2:D:99:THR:HG22	2:D:101:GLY:H	1.56	0.71
2:J:99:THR:HG22	2:J:101:GLY:H	1.56	0.70
1:A:346:ARG:NH1	1:A:347:PHE:O	2.25	0.69
1:B:106:PHE:HB2	1:B:117:LEU:HB2	1.77	0.67
1:C:452:LEU:HD21	1:C:492:LEU:HB3	1.78	0.66
1:B:360:ASN:H	1:B:523:THR:HB	1.61	0.65
2:D:22:CYS:HB3	2:D:79:LEU:HB3	1.80	0.64
2:G:22:CYS:HB3	2:G:79:LEU:HB3	1.79	0.63
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.64	0.62
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.81	0.62
1:A:108:THR:HB	1:A:114:THR:HG21	1.82	0.62
1:C:308:VAL:HG22	1:C:602:THR:HG23	1.81	0.62
2:J:22:CYS:HB3	2:J:79:LEU:HB3	1.79	0.61
1:C:366:SER:O	1:C:370:ASN:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ILE:HA	1:C:491:PRO:HD3	1.82	0.61
3:K:84:GLU:HG3	3:K:86:GLU:H	1.65	0.61
3:E:84:GLU:HG3	3:E:86:GLU:H	1.65	0.61
1:B:424:LYS:O	1:B:466:ARG:NH2	2.32	0.60
1:B:560:LEU:HB2	1:C:41:LYS:HD2	1.83	0.60
1:B:448:ASN:HB3	1:B:497:PHE:HD1	1.67	0.60
1:A:130:VAL:HB	1:A:168:PHE:HB2	1.82	0.60
3:H:84:GLU:HG3	3:H:86:GLU:H	1.65	0.60
1:A:358:ILE:HB	1:A:395:VAL:HB	1.84	0.59
1:B:106:PHE:HB3	1:B:235:ILE:HD11	1.84	0.59
1:A:327:VAL:HG22	1:A:542:ASN:HB3	1.83	0.59
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.85	0.59
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.85	0.58
1:A:472:ILE:HA	1:A:491:PRO:HD3	1.84	0.58
1:B:642:VAL:HG22	1:B:651:ILE:HG12	1.86	0.57
1:A:379:CYS:HB3	1:A:432:CYS:HA	1.86	0.57
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.85	0.57
1:C:226:LEU:HG	1:C:227:VAL:HG13	1.85	0.57
1:A:654:GLU:HB3	1:A:693:ILE:HG22	1.87	0.56
1:C:922:LEU:HD11	4:N:1:NAG:H3	1.87	0.56
1:A:640:SER:OG	1:A:641:ASN:N	2.38	0.56
2:D:116:GLY:O	3:E:48:SER:OG	2.18	0.56
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.71	0.55
1:B:484:GLU:OE2	2:G:102:ARG:NH2	2.33	0.55
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.88	0.55
1:A:432:CYS:HB2	1:A:513:LEU:HD12	1.89	0.55
1:C:95:THR:HA	1:C:189:LEU:HA	1.89	0.54
2:J:85:SER:O	2:J:85:SER:OG	2.26	0.54
3:H:44:LYS:HB2	3:H:47:GLN:HB3	1.90	0.54
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.90	0.54
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.72	0.54
3:E:44:LYS:HB2	3:E:47:GLN:HB3	1.90	0.54
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.89	0.54
1:A:65:PHE:HE2	1:A:84:LEU:HD13	1.72	0.54
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.90	0.54
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.88	0.54
1:A:763:LEU:HD13	1:A:1004:LEU:HD22	1.90	0.54
1:C:763:LEU:HD21	1:C:1005:GLN:HG3	1.91	0.54
1:B:866:THR:HG22	1:B:869:MET:HE3	1.90	0.53
2:D:85:SER:O	2:D:85:SER:OG	2.26	0.53
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:44:LYS:HB2	3:K:47:GLN:HB3	1.90	0.53
1:A:42:VAL:HG11	1:C:567:ARG:HE	1.73	0.53
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.40	0.53
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.91	0.53
1:A:117:LEU:HD13	1:A:130:VAL:HG22	1.90	0.53
2:J:39:GLN:HB2	2:J:45:LEU:HD23	1.91	0.53
1:A:516:GLU:HG3	1:A:517:LEU:H	1.74	0.52
3:K:44:LYS:NZ	3:K:88:VAL:O	2.40	0.52
1:B:472:ILE:HA	1:B:491:PRO:HD3	1.90	0.52
2:J:37:VAL:HG11	2:J:115:TRP:HZ3	1.75	0.52
1:C:1028:LYS:O	1:C:1032:CYS:HB2	2.10	0.52
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.91	0.52
1:C:611:LEU:HD11	1:C:666:ILE:HG23	1.91	0.52
1:C:568:ASP:OD1	1:C:572:THR:OG1	2.27	0.52
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.91	0.51
1:A:729:VAL:HG22	1:A:1059:GLY:HA2	1.92	0.51
1:A:869:MET:HG2	1:C:699:LEU:HD11	1.91	0.51
1:B:424:LYS:H	1:B:466:ARG:HE	1.58	0.51
1:B:440:ASN:OD1	1:B:441:LEU:N	2.43	0.51
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.93	0.51
1:A:444:LYS:HE2	1:A:448:ASN:HA	1.93	0.51
1:B:575:ALA:HA	1:B:586:ASP:HA	1.92	0.51
2:G:39:GLN:HB2	2:G:45:LEU:HD23	1.91	0.51
1:A:344:ALA:HB3	1:A:347:PHE:HE2	1.76	0.51
1:B:126:VAL:HG23	1:B:174:PRO:HA	1.92	0.51
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.38	0.51
3:H:44:LYS:NZ	3:H:88:VAL:O	2.40	0.51
3:K:71:GLY:HA3	3:K:76:PHE:HA	1.93	0.51
1:A:105:ILE:HG22	1:A:239:GLN:HB2	1.92	0.51
1:B:357:ARG:NH2	1:C:230:PRO:O	2.43	0.51
2:D:53:ASP:OD1	2:D:53:ASP:N	2.43	0.51
1:B:329:PHE:O	1:B:580:GLN:NE2	2.42	0.51
1:C:821:LEU:O	1:C:825:LYS:HB2	2.11	0.51
1:A:361:CYS:H	1:A:524:VAL:HG12	1.75	0.51
1:C:126:VAL:HB	1:C:172:SER:HB3	1.93	0.51
2:G:37:VAL:HG11	2:G:115:TRP:HZ3	1.75	0.51
2:D:37:VAL:HG11	2:D:115:TRP:HZ3	1.75	0.50
2:G:53:ASP:OD1	2:G:53:ASP:N	2.43	0.50
2:J:18:LEU:H	2:J:83:MET:HB2	1.77	0.50
1:A:130:VAL:HG21	1:A:231:ILE:HD12	1.94	0.50
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:71:GLY:HA3	3:E:76:PHE:HA	1.93	0.50
1:A:461:LEU:HD21	1:A:466:ARG:HG3	1.93	0.50
1:C:403:ARG:HD2	1:C:405:ASP:HB2	1.94	0.50
1:C:278:LYS:HB2	1:C:306:PHE:HE2	1.77	0.50
3:H:71:GLY:HA3	3:H:76:PHE:HA	1.93	0.50
1:B:552:LEU:HD23	1:B:585:LEU:HD13	1.93	0.50
1:B:1116:THR:OG1	1:B:1118:ASP:OD1	2.27	0.50
2:D:18:LEU:H	2:D:83:MET:HB2	1.76	0.50
2:G:18:LEU:H	2:G:83:MET:HB2	1.76	0.50
1:A:720:ILE:HD12	1:A:923:ILE:HG23	1.93	0.49
2:J:53:ASP:OD1	2:J:53:ASP:N	2.43	0.49
1:B:968:SER:OG	1:C:755:GLN:O	2.30	0.49
1:B:34:ARG:NH1	1:B:217:PRO:O	2.45	0.49
2:D:107:TYR:O	2:D:110:GLY:N	2.45	0.49
1:B:659:SER:OG	1:B:696:THR:O	2.28	0.49
1:C:724:THR:HG23	1:C:934:ILE:HD11	1.93	0.49
2:J:107:TYR:O	2:J:110:GLY:N	2.45	0.49
3:E:44:LYS:NZ	3:E:88:VAL:O	2.40	0.49
1:B:334:ASN:O	1:B:362:VAL:N	2.44	0.49
1:C:907:ASN:ND2	1:C:913:GLN:OE1	2.46	0.49
3:H:81:SER:OG	3:H:82:ARG:NH1	2.46	0.49
2:G:85:SER:O	2:G:85:SER:OG	2.26	0.49
1:B:605:SER:OG	1:B:606:ASN:N	2.45	0.49
2:G:107:TYR:O	2:G:110:GLY:N	2.45	0.49
3:K:54:TYR:HD1	3:K:54:TYR:H	1.61	0.48
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.30	0.48
1:B:729:VAL:HG22	1:B:1059:GLY:HA2	1.95	0.48
3:E:81:SER:OG	3:E:82:ARG:NH1	2.46	0.48
3:H:54:TYR:HD1	3:H:54:TYR:H	1.61	0.48
3:K:81:SER:OG	3:K:82:ARG:NH1	2.46	0.48
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.94	0.48
1:B:108:THR:OG1	1:B:234:ASN:O	2.30	0.48
1:B:1045:LYS:NZ	1:C:889:GLY:O	2.44	0.48
1:C:406:GLU:OE1	1:C:408:ARG:NH2	2.45	0.48
3:H:66:ARG:NH2	3:H:84:GLU:OE2	2.46	0.48
2:J:34:MET:HG3	2:J:79:LEU:HD22	1.96	0.48
1:C:39:PRO:HG2	1:C:51:THR:HG21	1.95	0.48
1:C:1116:THR:HG22	1:C:1138:TYR:HD2	1.78	0.48
1:A:453:TYR:HE1	1:A:455:LEU:HD13	1.79	0.48
3:H:8:PRO:HG2	3:H:11:LEU:HD21	1.96	0.48
1:A:816:SER:HB2	1:A:819:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.95	0.48
3:K:8:PRO:HG2	3:K:11:LEU:HD21	1.96	0.48
1:B:417:LYS:HE2	1:B:455:LEU:HD12	1.95	0.48
1:C:819:GLU:HA	1:C:822:LEU:HD12	1.96	0.48
1:A:752:LEU:HD21	1:A:990:GLU:HG2	1.96	0.47
3:E:54:TYR:H	3:E:54:TYR:HD1	1.61	0.47
1:B:886:TRP:HZ3	1:B:901:GLN:HG3	1.79	0.47
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.49	0.47
1:B:555:SER:OG	1:B:556:ASN:N	2.45	0.47
1:B:403:ARG:NE	1:B:405:ASP:OD1	2.39	0.47
3:E:66:ARG:NH2	3:E:84:GLU:OE2	2.46	0.47
2:G:34:MET:HG3	2:G:79:LEU:HD22	1.96	0.47
1:B:738:CYS:O	1:B:741:TYR:N	2.47	0.47
1:C:280:ASN:HD21	1:C:284:THR:HB	1.79	0.47
2:D:34:MET:HG3	2:D:79:LEU:HD22	1.96	0.47
2:J:51:ILE:HD12	2:J:72:ARG:HD2	1.96	0.47
2:D:51:ILE:HD12	2:D:72:ARG:HD2	1.96	0.46
1:C:412:PRO:HG3	1:C:429:PHE:HB3	1.96	0.46
2:G:99:THR:HA	2:G:112:LYS:HA	1.97	0.46
2:D:99:THR:HA	2:D:112:LYS:HA	1.97	0.46
3:E:8:PRO:HG2	3:E:11:LEU:HD21	1.96	0.46
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.47	0.46
1:A:1081:ILE:HG13	1:A:1088:HIS:HB2	1.96	0.46
3:K:66:ARG:NH2	3:K:84:GLU:OE2	2.46	0.46
1:C:1127:ASP:OD1	1:C:1127:ASP:N	2.45	0.46
2:D:69:THR:HB	2:D:82:GLN:HB3	1.98	0.46
1:C:985:ASP:O	1:C:989:ALA:N	2.42	0.46
1:A:305:SER:OG	1:A:306:PHE:N	2.49	0.46
2:G:51:ILE:HD12	2:G:72:ARG:HD2	1.96	0.46
1:C:1050:MET:HE2	1:C:1052:PHE:HE2	1.80	0.46
2:D:52:SER:O	2:D:72:ARG:NH1	2.49	0.46
1:B:439:ASN:O	1:B:443:SER:OG	2.34	0.46
2:G:64:VAL:HB	2:G:68:PHE:HD1	1.81	0.46
1:A:299:THR:HG21	1:A:597:VAL:HG21	1.98	0.45
1:A:886:TRP:HB3	1:A:1035:GLY:HA2	1.97	0.45
2:J:52:SER:O	2:J:72:ARG:NH1	2.49	0.45
2:G:52:SER:O	2:G:72:ARG:NH1	2.49	0.45
1:B:131:CYS:HB2	1:B:133:PHE:CE1	2.52	0.45
1:C:34:ARG:HH21	1:C:217:PRO:HG2	1.82	0.45
2:D:91:THR:HG23	2:D:122:THR:HA	1.99	0.45
2:J:69:THR:HB	2:J:82:GLN:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ASP:OD1	1:A:572:THR:OG1	2.30	0.45
2:J:91:THR:HG23	2:J:122:THR:HA	1.99	0.45
1:A:299:THR:O	1:A:303:LEU:HB2	2.17	0.45
2:G:69:THR:HB	2:G:82:GLN:HB3	1.98	0.45
1:A:281:GLU:O	1:C:557:LYS:NZ	2.50	0.45
2:J:99:THR:HA	2:J:112:LYS:HA	1.98	0.45
1:B:141:LEU:N	1:B:242:LEU:O	2.50	0.45
2:J:64:VAL:HB	2:J:68:PHE:HD1	1.81	0.45
1:A:85:PRO:HA	1:A:237:ARG:HA	1.99	0.44
1:A:1088:HIS:CD2	1:A:1137:VAL:HG21	2.53	0.44
1:B:409:GLN:HA	1:B:414:GLN:HG2	1.99	0.44
2:D:64:VAL:HB	2:D:68:PHE:HD1	1.81	0.44
1:B:616:ASN:HB3	1:B:618:THR:H	1.82	0.44
1:C:431:GLY:HA3	1:C:514:SER:HA	1.98	0.44
1:C:1082:CYS:HB2	1:C:1126:CYS:HB2	1.80	0.44
1:A:50:SER:HA	1:A:276:LEU:HA	2.00	0.44
1:B:409:GLN:HB3	1:B:419:ALA:HB2	2.00	0.44
1:B:662:CYS:HB2	1:B:671:CYS:HB3	1.77	0.44
1:C:465:GLU:C	1:C:466:ARG:HD3	2.42	0.44
2:G:91:THR:HG23	2:G:122:THR:HA	1.99	0.44
1:B:521:PRO:HA	1:B:564:GLN:HB2	1.99	0.44
1:C:131:CYS:HA	1:C:166:CYS:HA	1.99	0.44
1:C:662:CYS:HB2	1:C:671:CYS:HB3	1.73	0.44
1:A:715:PRO:HA	1:A:1072:GLU:HA	2.00	0.43
1:C:410:ILE:HG22	1:C:433:VAL:HG11	2.00	0.43
3:H:51:LEU:HD21	3:H:54:TYR:HB3	2.00	0.43
3:K:91:TYR:HB2	3:K:107:THR:HB	2.00	0.43
1:B:699:LEU:HD11	1:C:869:MET:HB3	2.01	0.43
1:B:883:THR:OG1	1:B:884:SER:N	2.51	0.43
1:C:977:LEU:O	1:C:981:LEU:HB2	2.18	0.43
1:C:900:MET:HE2	1:C:900:MET:HB3	1.69	0.43
1:B:540:ASN:HA	1:B:549:THR:HA	2.01	0.43
1:B:816:SER:HB3	1:B:819:GLU:OE1	2.19	0.43
1:A:715:PRO:HD3	1:B:894:LEU:HD13	2.00	0.43
1:C:299:THR:O	1:C:303:LEU:HB2	2.18	0.43
1:C:433:VAL:HG12	1:C:512:VAL:HG22	1.99	0.43
3:H:91:TYR:HB2	3:H:107:THR:HB	2.00	0.43
1:A:825:LYS:HD3	1:A:825:LYS:HA	1.82	0.43
1:C:108:THR:OG1	1:C:234:ASN:O	2.33	0.43
3:E:91:TYR:HB2	3:E:107:THR:HB	2.00	0.43
1:A:125:ASN:HA	1:A:174:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1050:MET:HE2	1:C:1052:PHE:CE2	2.54	0.43
1:A:738:CYS:HB3	1:A:760:CYS:HB2	1.66	0.43
1:A:914:ASN:O	1:A:917:TYR:N	2.52	0.43
1:B:453:TYR:HB3	1:B:495:TYR:HE2	1.84	0.43
1:C:278:LYS:HB2	1:C:306:PHE:CE2	2.54	0.43
1:C:726:ILE:HD13	1:C:945:LEU:HD13	2.01	0.43
1:C:573:THR:O	1:C:573:THR:OG1	2.36	0.42
1:C:715:PRO:HA	1:C:1072:GLU:HA	2.00	0.42
2:J:100:ARG:NH1	3:K:54:TYR:HE2	2.17	0.42
1:A:726:ILE:HG12	1:A:945:LEU:HD23	2.01	0.42
3:E:51:LEU:HD21	3:E:54:TYR:HB3	2.00	0.42
1:A:484:GLU:O	2:D:100:ARG:NH2	2.52	0.42
1:A:121:ASN:HA	1:A:126:VAL:HG12	2.02	0.42
2:G:95:TYR:HB3	2:G:118:GLY:HA2	2.01	0.42
1:C:417:LYS:HA	1:C:417:LYS:HD3	1.82	0.42
3:K:51:LEU:HD21	3:K:54:TYR:HB3	2.00	0.42
1:C:300:LYS:HE2	1:C:602:THR:HG21	2.01	0.42
1:A:395:VAL:HG23	1:A:524:VAL:HG21	2.02	0.42
2:D:95:TYR:HB3	2:D:118:GLY:HA2	2.01	0.42
2:G:27:PHE:CE1	2:G:98:LYS:HD3	2.55	0.42
1:A:84:LEU:HA	1:A:85:PRO:HD3	1.85	0.42
1:B:315:THR:OG1	1:B:316:SER:N	2.52	0.42
1:B:563:GLN:HE22	1:C:42:VAL:HA	1.84	0.42
1:B:796:ASP:OD1	1:B:796:ASP:N	2.53	0.42
1:B:434:ILE:HB	1:B:511:VAL:HG23	2.02	0.42
1:B:557:LYS:HA	1:B:557:LYS:HD3	1.90	0.42
1:C:494:SER:OG	1:C:495:TYR:N	2.53	0.42
2:G:92:ALA:HB3	2:G:94:TYR:HE1	1.85	0.42
2:D:27:PHE:CE1	2:D:98:LYS:HD3	2.55	0.42
1:A:289:VAL:HG11	1:A:300:LYS:HD3	2.01	0.41
1:A:395:VAL:HG22	1:A:515:PHE:CE1	2.54	0.41
1:C:296:LEU:O	1:C:299:THR:OG1	2.28	0.41
2:J:92:ALA:HB3	2:J:94:TYR:HE1	1.85	0.41
1:B:84:LEU:HD13	1:B:267:VAL:HG11	2.02	0.41
1:A:409:GLN:HB3	1:A:419:ALA:HB2	2.02	0.41
1:C:537:LYS:HB3	1:C:537:LYS:HE3	1.76	0.41
1:B:726:ILE:HD13	1:B:945:LEU:HD23	2.01	0.41
1:C:37:TYR:OH	1:C:54:LEU:O	2.28	0.41
1:A:108:THR:OG1	1:A:234:ASN:O	2.35	0.41
1:A:317:ASN:HA	1:A:594:GLY:HA2	2.03	0.41
2:D:92:ALA:HB3	2:D:94:TYR:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:27:PHE:CE1	2:J:98:LYS:HD3	2.55	0.41
1:C:752:LEU:HD23	1:C:752:LEU:HA	1.91	0.41
1:C:816:SER:HB3	1:C:819:GLU:OE2	2.21	0.41
1:A:167:THR:HG22	1:A:168:PHE:CD1	2.56	0.41
1:A:328:ARG:HE	1:A:328:ARG:HB3	1.70	0.41
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.88	0.41
1:A:1139:ASP:OD1	1:A:1139:ASP:N	2.43	0.41
2:J:95:TYR:HB3	2:J:118:GLY:HA2	2.01	0.41
1:B:86:PHE:N	1:B:236:THR:O	2.53	0.41
1:C:472:ILE:HG22	1:C:490:PHE:HD1	1.85	0.41
1:A:428:ASP:OD1	1:A:428:ASP:N	2.53	0.40
1:B:462:LYS:NZ	1:B:463:PRO:O	2.54	0.40
1:B:472:ILE:HD12	1:B:488:CYS:HB3	2.02	0.40
1:C:555:SER:HB3	1:C:584:ILE:HG13	2.02	0.40
1:A:1039:ARG:H	1:A:1039:ARG:HG2	1.60	0.40
1:B:93:ALA:HB3	1:B:266:TYR:HB2	2.04	0.40
1:B:1094:VAL:HG23	1:C:900:MET:HE1	2.03	0.40
1:C:315:THR:OG1	1:C:316:SER:N	2.54	0.40
1:A:854:LYS:HG2	1:A:859:THR:HA	2.03	0.40
1:C:1086:LYS:HE3	1:C:1086:LYS:HB2	1.84	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	981/1208 (81%)	924 (94%)	57 (6%)	0	100	100
1	B	972/1208 (80%)	917 (94%)	53 (6%)	2 (0%)	43	74
1	C	977/1208 (81%)	936 (96%)	41 (4%)	0	100	100
2	D	122/230 (53%)	114 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	122/230 (53%)	114 (93%)	8 (7%)	0	100	100
2	J	122/230 (53%)	114 (93%)	8 (7%)	0	100	100
3	E	110/219 (50%)	105 (96%)	5 (4%)	0	100	100
3	H	110/219 (50%)	105 (96%)	5 (4%)	0	100	100
3	K	110/219 (50%)	105 (96%)	5 (4%)	0	100	100
All	All	3626/4971 (73%)	3434 (95%)	190 (5%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	ASP
1	B	295	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	852/1056 (81%)	852 (100%)	0	100	100
1	B	844/1056 (80%)	844 (100%)	0	100	100
1	C	843/1056 (80%)	843 (100%)	0	100	100
2	D	96/188 (51%)	80 (83%)	16 (17%)	2	13
2	G	96/188 (51%)	80 (83%)	16 (17%)	2	13
2	J	96/188 (51%)	80 (83%)	16 (17%)	2	13
3	E	96/192 (50%)	75 (78%)	21 (22%)	1	5
3	H	96/192 (50%)	75 (78%)	21 (22%)	1	5
3	K	96/192 (50%)	75 (78%)	21 (22%)	1	5
All	All	3115/4308 (72%)	3004 (96%)	111 (4%)	32	57

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	4	LEU
2	D	17	SER
2	D	20	LEU
2	D	27	PHE
2	D	34	MET
2	D	43	ARG
2	D	51	ILE
2	D	52	SER
2	D	53	ASP
2	D	85	SER
2	D	95	TYR
2	D	106	ASP
2	D	108	VAL
2	D	113	ASP
2	D	117	GLN
2	D	119	THR
3	E	5	THR
3	E	7	SER
3	E	11	LEU
3	E	25	SER
3	E	26	SER
3	E	28	SER
3	E	38	LEU
3	E	41	TYR
3	E	48	SER
3	E	51	LEU
3	E	52	LEU
3	E	54	TYR
3	E	55	LEU
3	E	59	ARG
3	E	68	SER
3	E	70	SER
3	E	76	PHE
3	E	80	ILE
3	E	97	LEU
3	E	102	THR
3	E	111	ILE
2	G	4	LEU
2	G	17	SER
2	G	20	LEU
2	G	27	PHE
2	G	34	MET
2	G	43	ARG

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Mol	Chain	Res	Type
2	G	51	ILE
2	G	52	SER
2	G	53	ASP
2	G	85	SER
2	G	95	TYR
2	G	106	ASP
2	G	108	VAL
2	G	113	ASP
2	G	117	GLN
2	G	119	THR
3	H	5	THR
3	H	7	SER
3	H	11	LEU
3	H	25	SER
3	H	26	SER
3	H	28	SER
3	H	38	LEU
3	H	41	TYR
3	H	48	SER
3	H	51	LEU
3	H	52	LEU
3	H	54	TYR
3	H	55	LEU
3	H	59	ARG
3	H	68	SER
3	H	70	SER
3	H	76	PHE
3	H	80	ILE
3	H	97	LEU
3	H	102	THR
3	H	111	ILE
2	J	4	LEU
2	J	17	SER
2	J	20	LEU
2	J	27	PHE
2	J	34	MET
2	J	43	ARG
2	J	51	ILE
2	J	52	SER
2	J	53	ASP
2	J	85	SER
2	J	95	TYR

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Mol	Chain	Res	Type
2	J	106	ASP
2	J	108	VAL
2	J	113	ASP
2	J	117	GLN
2	J	119	THR
3	K	5	THR
3	K	7	SER
3	K	11	LEU
3	K	25	SER
3	K	26	SER
3	K	28	SER
3	K	38	LEU
3	K	41	TYR
3	K	48	SER
3	K	51	LEU
3	K	52	LEU
3	K	54	TYR
3	K	55	LEU
3	K	59	ARG
3	K	68	SER
3	K	70	SER
3	K	76	PHE
3	K	80	ILE
3	K	97	LEU
3	K	102	THR
3	K	111	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	137	ASN
1	A	245	HIS
1	A	314	GLN
1	A	439	ASN
1	A	762	GLN
1	A	764	ASN
1	A	787	GLN
1	A	913	GLN
1	A	969	ASN
1	A	1054	GLN
1	B	30	ASN

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Mol	Chain	Res	Type
1	B	165	ASN
1	B	321	GLN
1	B	354	ASN
1	B	481	ASN
1	B	540	ASN
1	B	641	ASN
1	B	955	ASN
1	B	960	ASN
1	B	992	GLN
1	B	1048	HIS
1	B	1058	HIS
1	B	1101	HIS
1	C	314	GLN
1	C	414	GLN
1	C	498	GLN
1	C	506	GLN
1	C	907	ASN
1	C	949	GLN
1	C	953	ASN
1	C	1010	GLN
2	D	35	ASN
2	G	35	ASN
2	J	35	ASN
2	J	84	ASN

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 ⓘ

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	F	1	1,4	14,14,15	0.28	0	17,19,21	0.74	1 (5%)
4	NAG	F	2	4	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	I	1	1,4	14,14,15	0.31	0	17,19,21	1.09	1 (5%)
4	NAG	I	2	4	14,14,15	0.24	0	17,19,21	0.48	0
4	NAG	L	1	1,4	14,14,15	0.33	0	17,19,21	0.85	0
4	NAG	L	2	4	14,14,15	1.39	1 (7%)	17,19,21	1.46	1 (5%)
4	NAG	M	1	1,4	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	M	2	4	14,14,15	0.35	0	17,19,21	0.54	0
4	NAG	N	1	1,4	14,14,15	0.31	0	17,19,21	0.57	0
4	NAG	N	2	4	14,14,15	0.36	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	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	2	NAG	O5-C1	4.94	1.52	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2	NAG	C1-O5-C5	5.83	119.99	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C2-N2-C7	3.23	127.23	122.90
4	F	1	NAG	C1-O5-C5	2.43	115.44	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

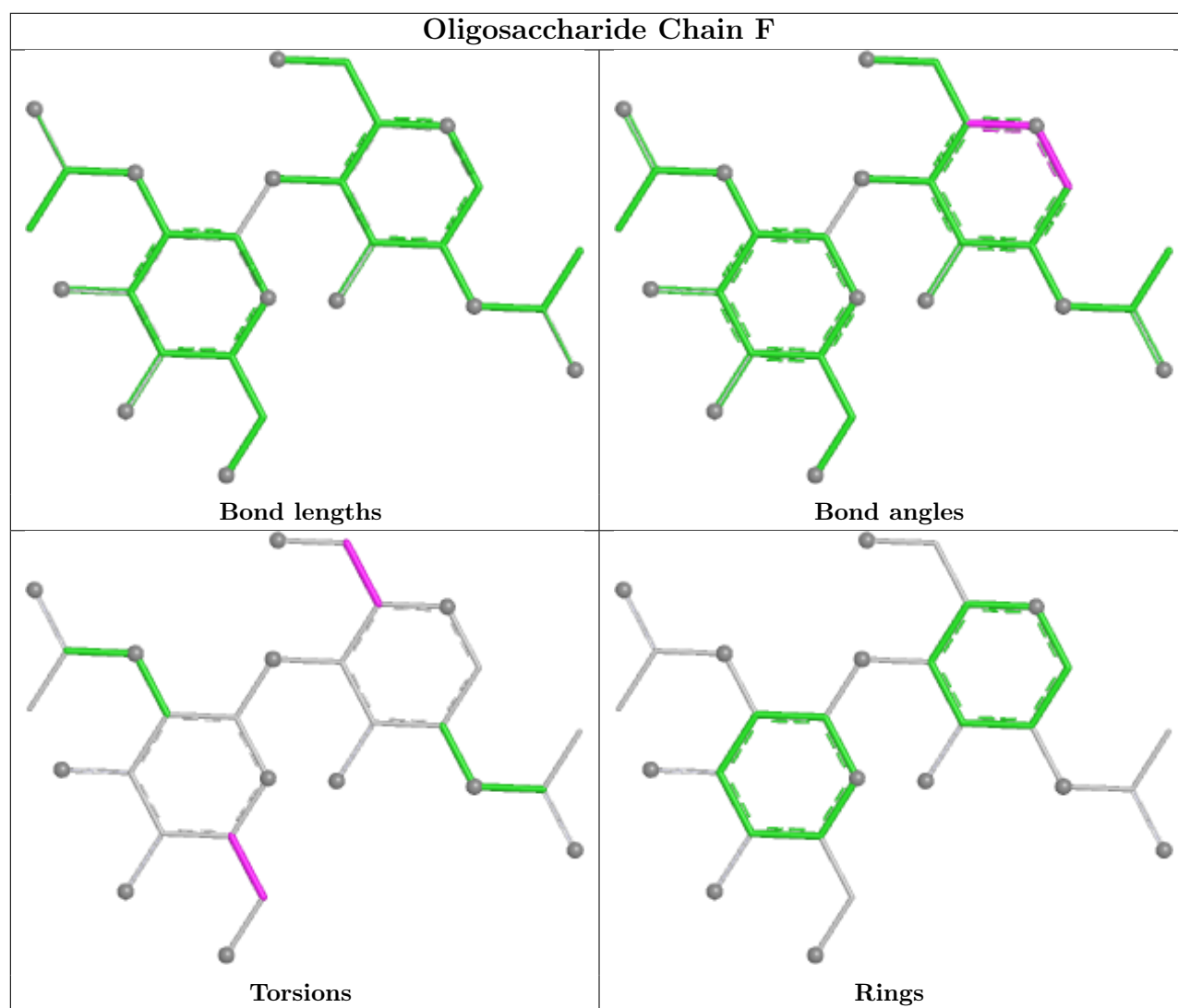
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C1-C2-N2-C7
4	I	1	NAG	C3-C2-N2-C7

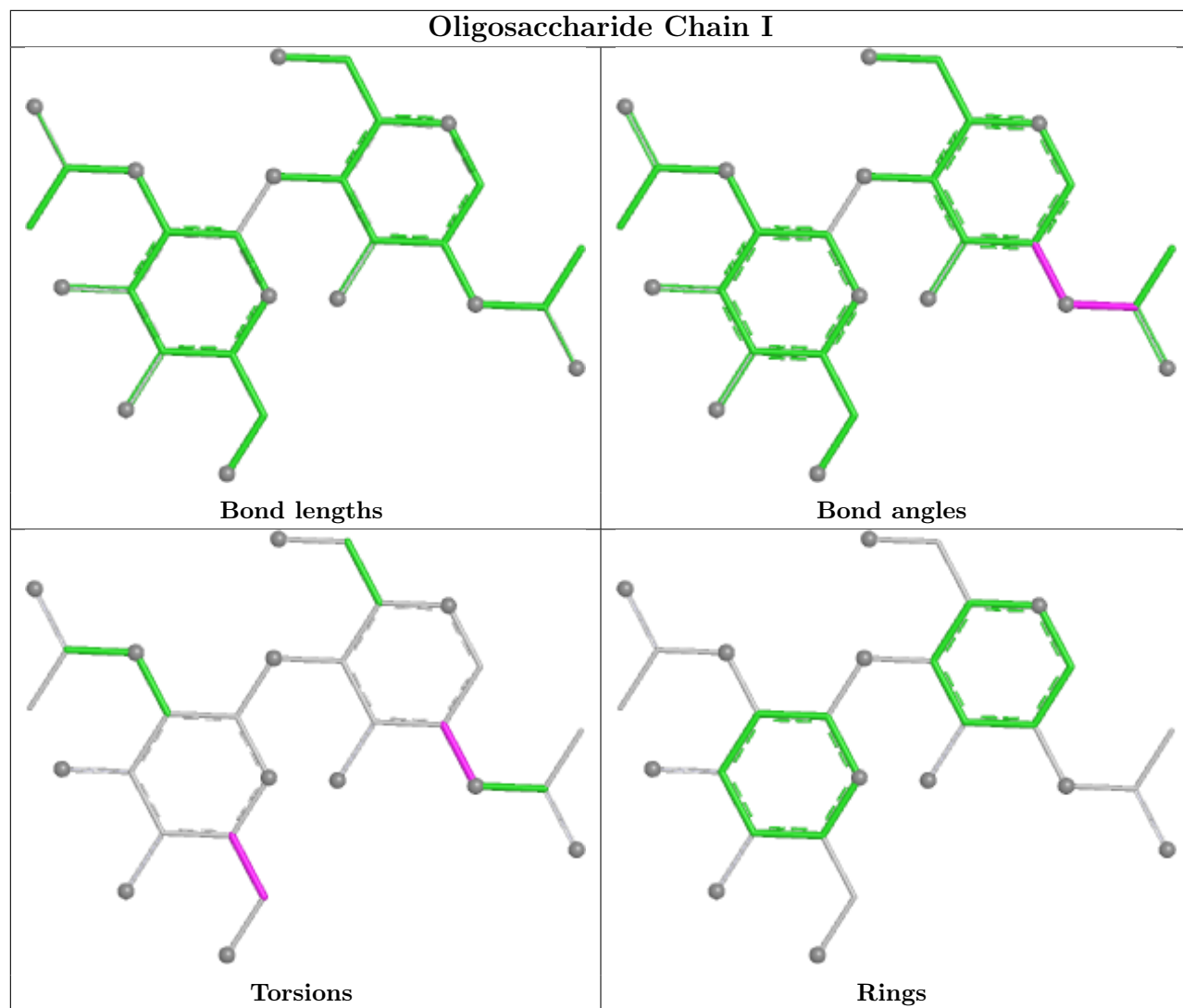
There are no ring outliers.

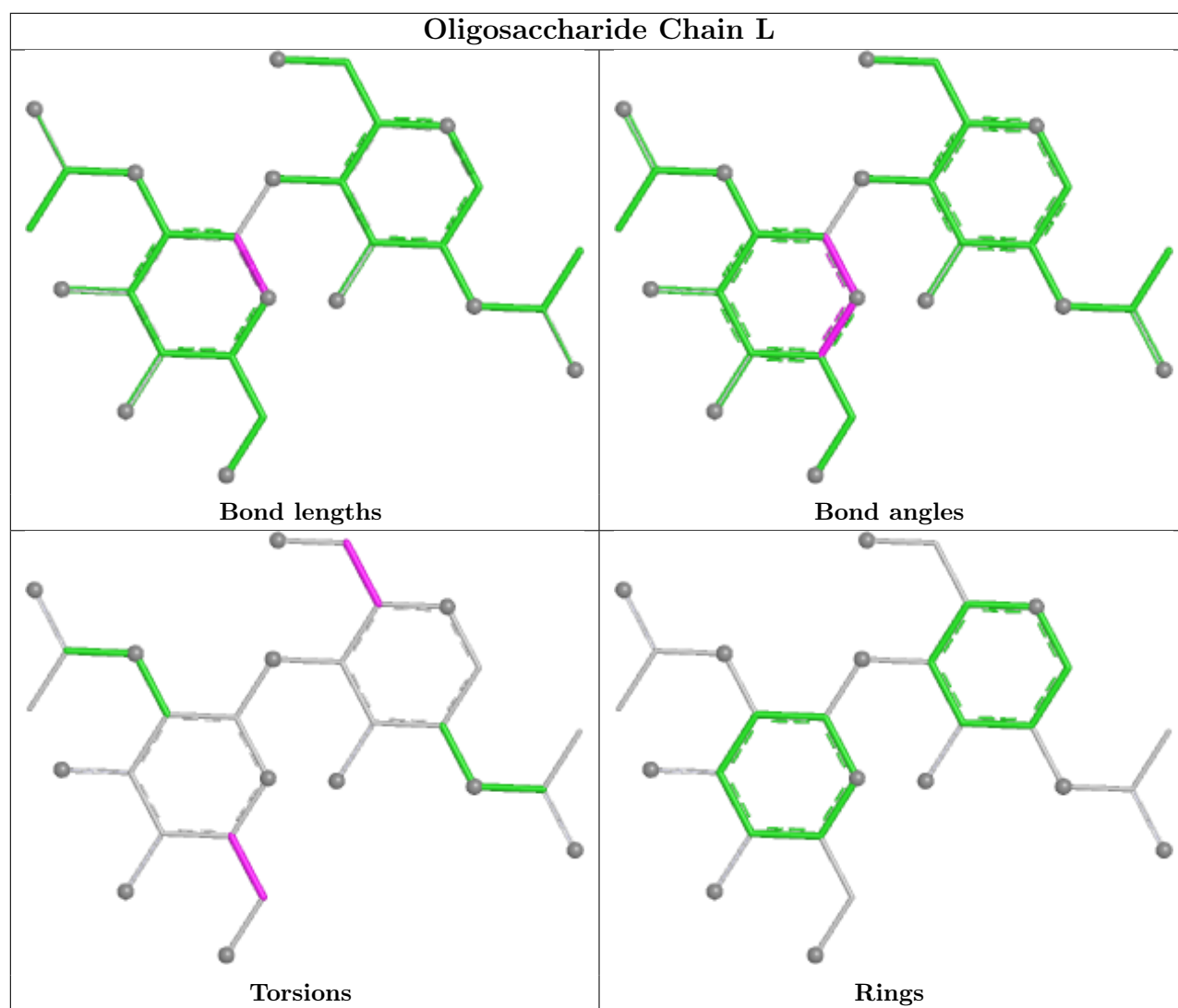
1 monomer is involved in 1 short contact:

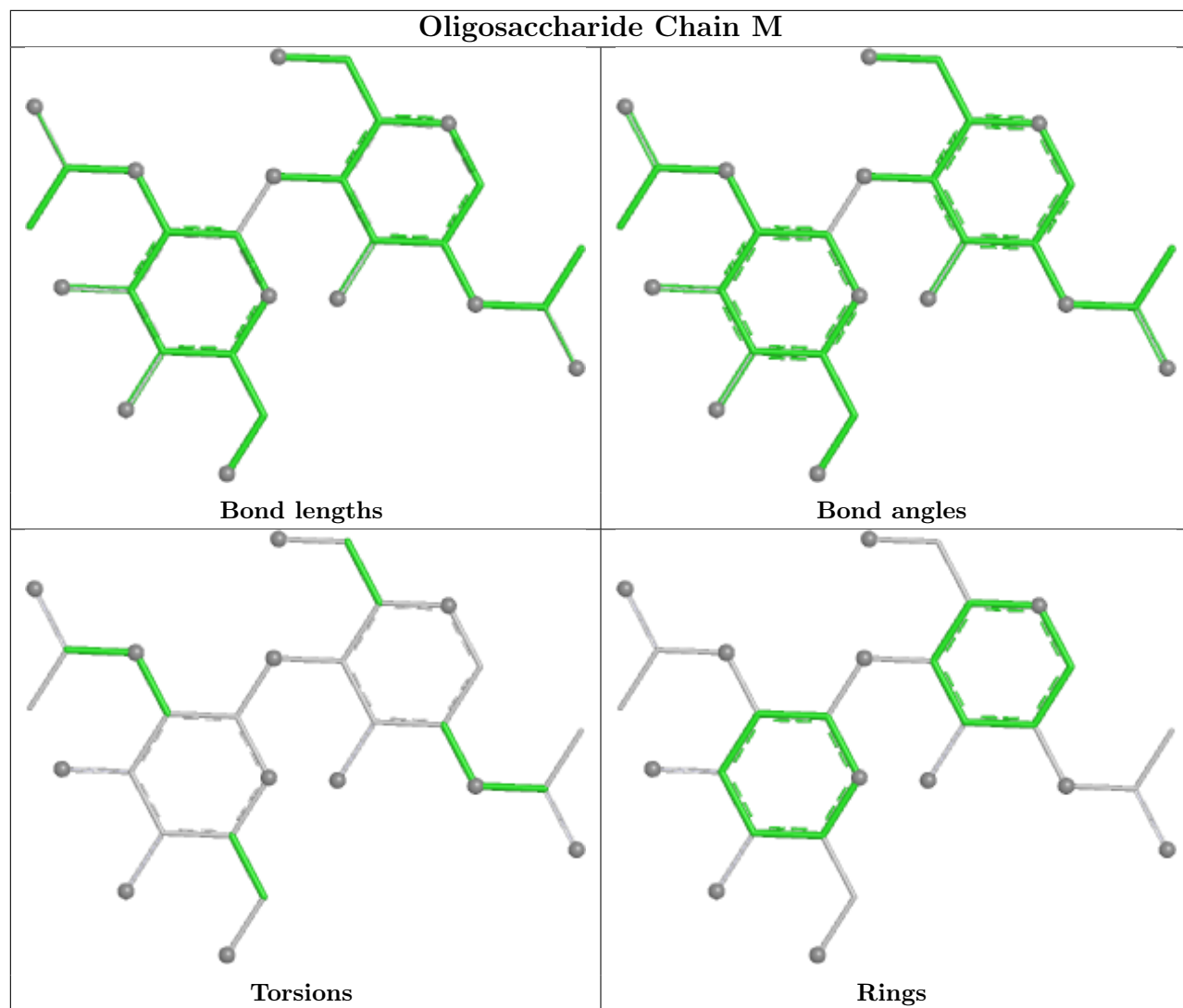
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1	NAG	1	0

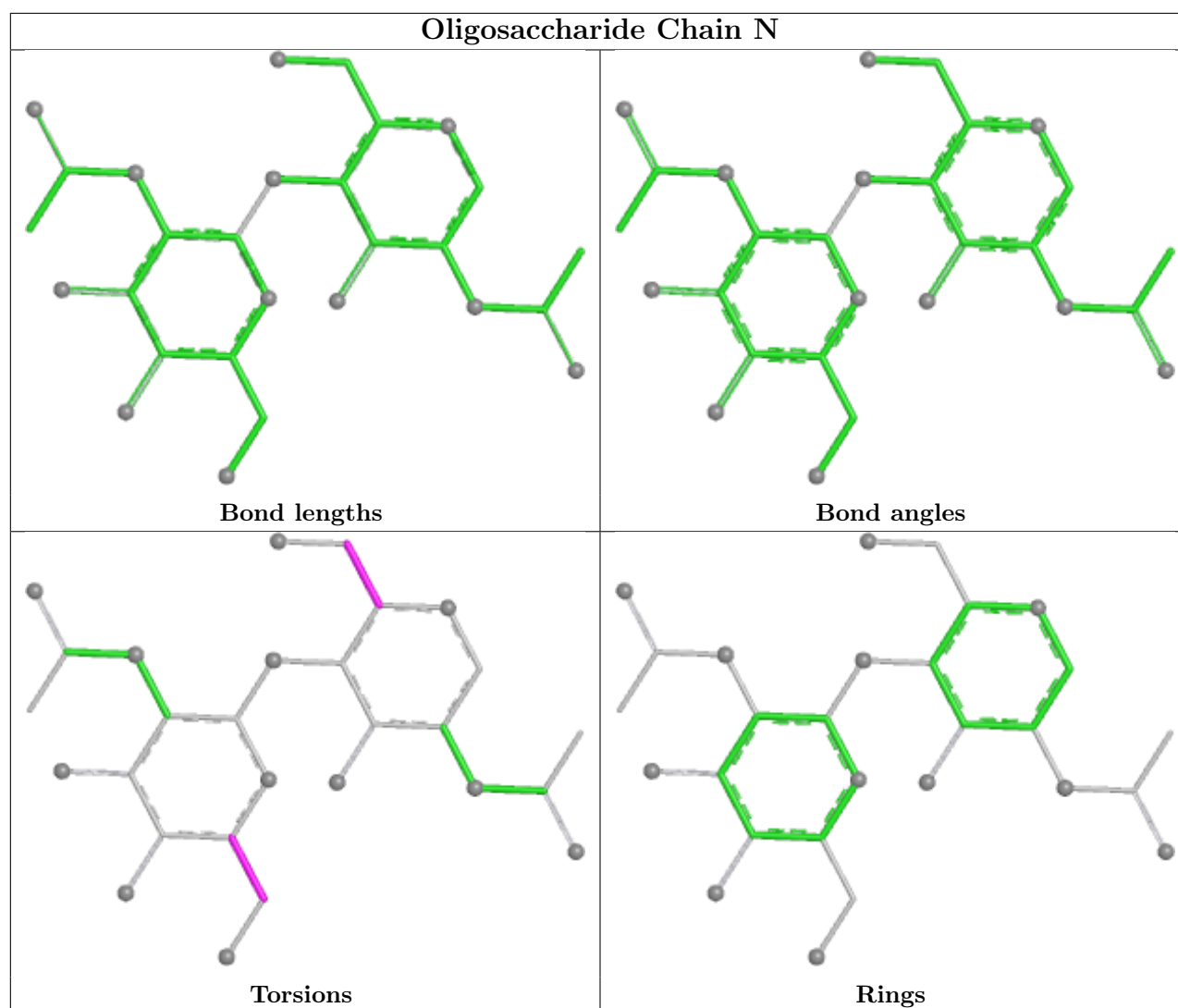
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

31 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	$\# Z > 2$
5	NAG	A	1307	1	14,14,15	0.54	0	17,19,21	0.65	1 (5%)
5	NAG	A	1303	1	14,14,15	0.28	0	17,19,21	0.62	1 (5%)
5	NAG	A	1313	1	14,14,15	0.91	1 (7%)	17,19,21	2.37	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1303	1	14,14,15	0.82	1 (7%)	17,19,21	2.36	3 (17%)
5	NAG	A	1306	1	14,14,15	0.27	0	17,19,21	0.59	0
5	NAG	C	1309	1	14,14,15	0.38	0	17,19,21	0.65	1 (5%)
5	NAG	A	1311	1	14,14,15	0.43	0	17,19,21	0.52	0
5	NAG	C	1313	1	14,14,15	0.43	0	17,19,21	0.57	0
5	NAG	A	1309	1	14,14,15	0.33	0	17,19,21	0.57	0
5	NAG	B	1312	1	14,14,15	1.11	1 (7%)	17,19,21	2.39	4 (23%)
5	NAG	A	1312	1	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	A	1301	1	14,14,15	0.31	0	17,19,21	0.62	1 (5%)
5	NAG	B	1311	-	14,14,15	0.39	0	17,19,21	1.03	1 (5%)
5	NAG	B	1301	1	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
5	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.54	0
5	NAG	C	1304	1	14,14,15	0.46	0	17,19,21	0.65	1 (5%)
5	NAG	C	1301	1	14,14,15	0.32	0	17,19,21	0.52	0
5	NAG	C	1312	-	14,14,15	0.28	0	17,19,21	0.53	0
5	NAG	C	1305	1	14,14,15	0.37	0	17,19,21	0.42	0
5	NAG	A	1314	-	14,14,15	0.27	0	17,19,21	0.57	0
5	NAG	A	1310	1	14,14,15	0.48	0	17,19,21	0.59	0
5	NAG	B	1313	1	14,14,15	0.38	0	17,19,21	0.64	1 (5%)
5	NAG	B	1310	1	14,14,15	0.42	0	17,19,21	0.63	1 (5%)
5	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.55	0
5	NAG	B	1314	-	14,14,15	0.32	0	17,19,21	0.52	0
5	NAG	C	1310	1	14,14,15	0.59	0	17,19,21	1.00	1 (5%)
5	NAG	C	1311	1	14,14,15	0.78	1 (7%)	17,19,21	2.35	3 (17%)
5	NAG	C	1308	1	14,14,15	0.74	1 (7%)	17,19,21	2.35	3 (17%)
5	NAG	B	1304	1	14,14,15	0.45	0	17,19,21	0.61	1 (5%)
5	NAG	A	1302	1	14,14,15	0.27	0	17,19,21	0.52	0
5	NAG	B	1307	1	14,14,15	0.24	0	17,19,21	0.50	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
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1313	1	-	6/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1312	1	-	6/6/23/26	0/1/1/1
5	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1311	-	-	4/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1312	-	-	1/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1314	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1313	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1314	-	-	2/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1311	1	-	6/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	6/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1312	NAG	C1-C2	3.18	1.56	1.52
5	A	1313	NAG	C1-C2	2.87	1.56	1.52
5	B	1303	NAG	C1-C2	2.38	1.55	1.52
5	C	1311	NAG	C1-C2	2.22	1.55	1.52
5	C	1308	NAG	C1-C2	2.11	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1303	NAG	C2-N2-C7	8.33	134.06	122.90
5	C	1311	NAG	C2-N2-C7	8.32	134.06	122.90
5	C	1308	NAG	C2-N2-C7	8.28	134.00	122.90
5	A	1313	NAG	C2-N2-C7	8.27	133.99	122.90
5	B	1312	NAG	C2-N2-C7	8.26	133.96	122.90
5	A	1313	NAG	C1-C2-N2	4.07	116.85	110.43
5	C	1311	NAG	C1-C2-N2	3.98	116.71	110.43
5	B	1303	NAG	C1-C2-N2	3.92	116.62	110.43
5	C	1308	NAG	C1-C2-N2	3.88	116.55	110.43
5	B	1312	NAG	C1-C2-N2	3.81	116.44	110.43
5	B	1301	NAG	C2-N2-C7	3.27	127.28	122.90
5	B	1311	NAG	C2-N2-C7	3.21	127.21	122.90
5	C	1310	NAG	C2-N2-C7	3.11	127.06	122.90
5	B	1312	NAG	C1-O5-C5	2.34	115.33	112.19
5	C	1304	NAG	C1-O5-C5	2.27	115.23	112.19
5	C	1309	NAG	C1-O5-C5	2.26	115.22	112.19
5	B	1310	NAG	C1-O5-C5	2.19	115.12	112.19
5	B	1312	NAG	C8-C7-N2	2.19	119.75	116.12
5	A	1307	NAG	C1-O5-C5	2.19	115.12	112.19
5	C	1311	NAG	C8-C7-N2	2.18	119.73	116.12
5	B	1303	NAG	C8-C7-N2	2.16	119.70	116.12
5	A	1301	NAG	C1-O5-C5	2.15	115.07	112.19
5	C	1308	NAG	C8-C7-N2	2.15	119.68	116.12
5	A	1313	NAG	C8-C7-N2	2.15	119.68	116.12
5	B	1313	NAG	C1-O5-C5	2.14	115.05	112.19
5	A	1303	NAG	C1-O5-C5	2.12	115.03	112.19
5	B	1304	NAG	C1-O5-C5	2.04	114.91	112.19

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1303	NAG	O5-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	A	1301	NAG	C4-C5-C6-O6
5	B	1312	NAG	O5-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	A	1312	NAG	O5-C5-C6-O6
5	A	1313	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1307	NAG	O5-C5-C6-O6
5	B	1314	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	C	1311	NAG	O5-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	B	1311	NAG	O5-C5-C6-O6
5	C	1313	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	A	1310	NAG	C4-C5-C6-O6
5	A	1311	NAG	C4-C5-C6-O6
5	A	1313	NAG	C4-C5-C6-O6
5	A	1314	NAG	C4-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	B	1312	NAG	C4-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	A	1310	NAG	O5-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	A	1312	NAG	C4-C5-C6-O6
5	B	1311	NAG	C4-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	A	1314	NAG	O5-C5-C6-O6
5	A	1309	NAG	C4-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	A	1307	NAG	C4-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	B	1314	NAG	C4-C5-C6-O6
5	C	1313	NAG	C4-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	A	1313	NAG	C8-C7-N2-C2
5	A	1313	NAG	O7-C7-N2-C2
5	B	1303	NAG	C8-C7-N2-C2
5	B	1303	NAG	O7-C7-N2-C2
5	B	1312	NAG	C8-C7-N2-C2
5	B	1312	NAG	O7-C7-N2-C2
5	C	1308	NAG	C8-C7-N2-C2
5	C	1308	NAG	O7-C7-N2-C2
5	C	1311	NAG	C8-C7-N2-C2
5	C	1311	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	A	1311	NAG	O5-C5-C6-O6
5	C	1311	NAG	C4-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	C	1312	NAG	O5-C5-C6-O6
5	B	1301	NAG	C1-C2-N2-C7
5	B	1302	NAG	C4-C5-C6-O6
5	B	1313	NAG	O5-C5-C6-O6
5	A	1313	NAG	C1-C2-N2-C7
5	B	1303	NAG	C1-C2-N2-C7
5	B	1311	NAG	C1-C2-N2-C7
5	B	1312	NAG	C1-C2-N2-C7
5	C	1308	NAG	C1-C2-N2-C7
5	C	1310	NAG	C1-C2-N2-C7
5	C	1311	NAG	C1-C2-N2-C7
5	A	1313	NAG	C3-C2-N2-C7
5	B	1301	NAG	C3-C2-N2-C7
5	B	1303	NAG	C3-C2-N2-C7
5	B	1311	NAG	C3-C2-N2-C7
5	B	1312	NAG	C3-C2-N2-C7
5	C	1308	NAG	C3-C2-N2-C7
5	C	1310	NAG	C3-C2-N2-C7
5	C	1311	NAG	C3-C2-N2-C7
5	B	1301	NAG	C4-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	C	1310	NAG	C4-C5-C6-O6

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](#)

There are no chain breaks in this entry.

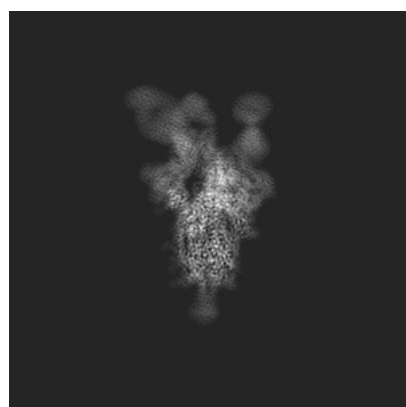
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30374. These allow visual inspection of the internal detail of the map and identification of artifacts.

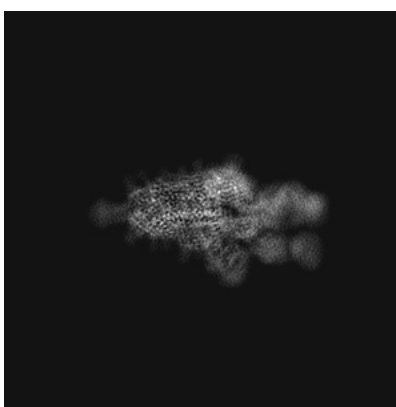
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

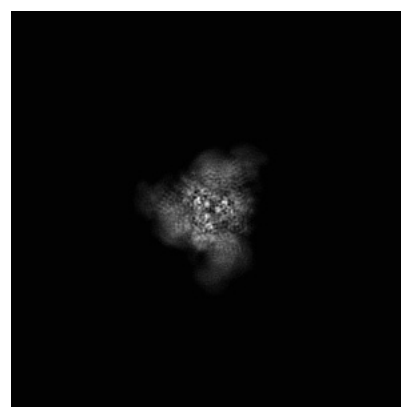
6.1.1 Primary map



X



Y

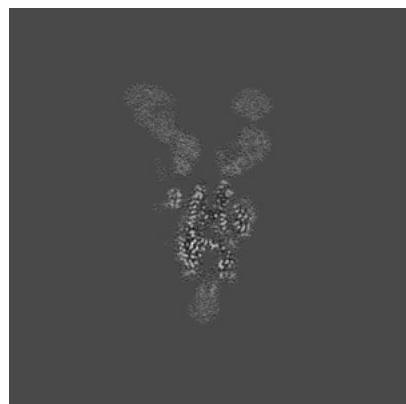


Z

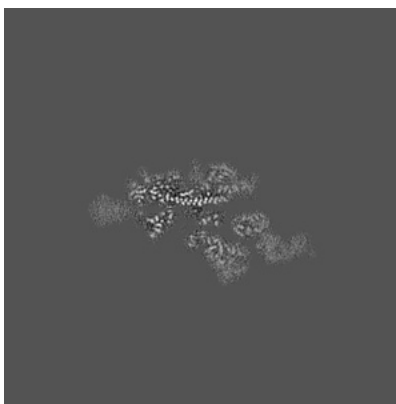
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

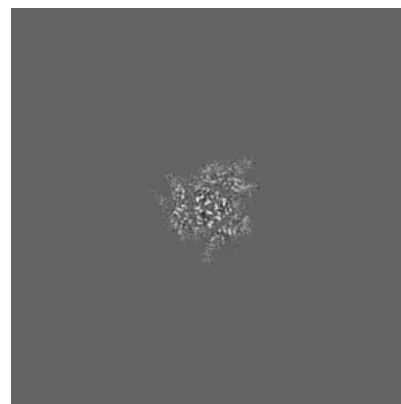
6.2.1 Primary map



X Index: 200



Y Index: 200

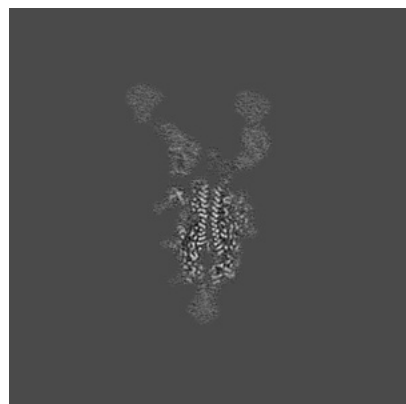


Z Index: 200

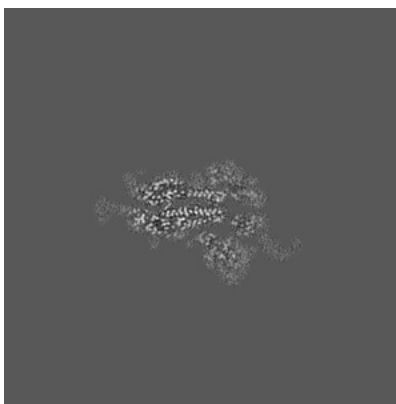
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

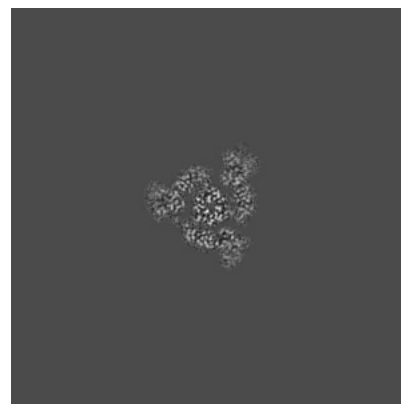
6.3.1 Primary map



X Index: 195



Y Index: 207

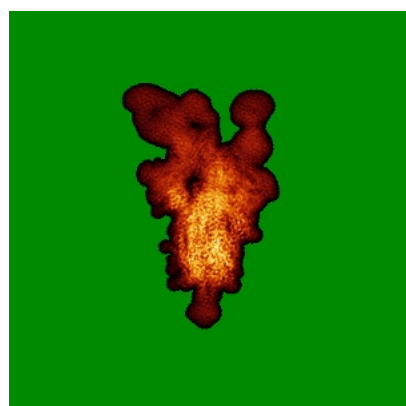


Z Index: 211

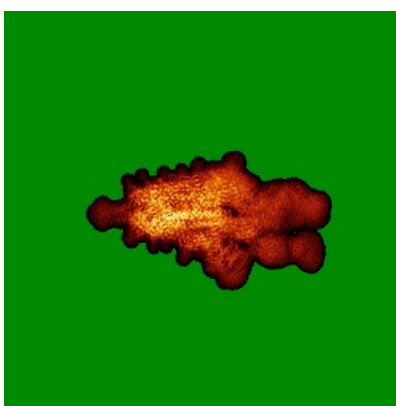
The images above show the largest variance slices of the map in three orthogonal directions.

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

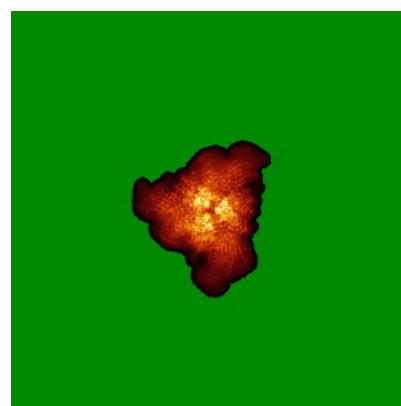
6.4.1 Primary map



X



Y

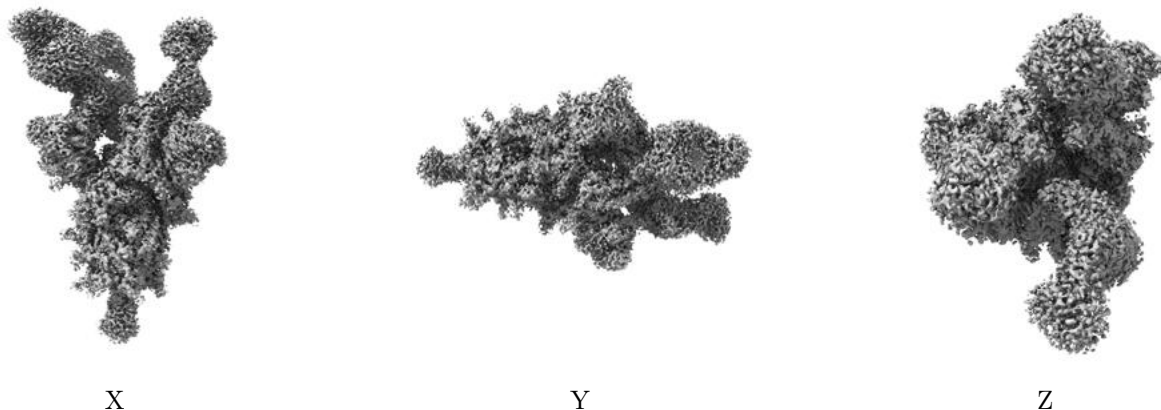


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0122. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

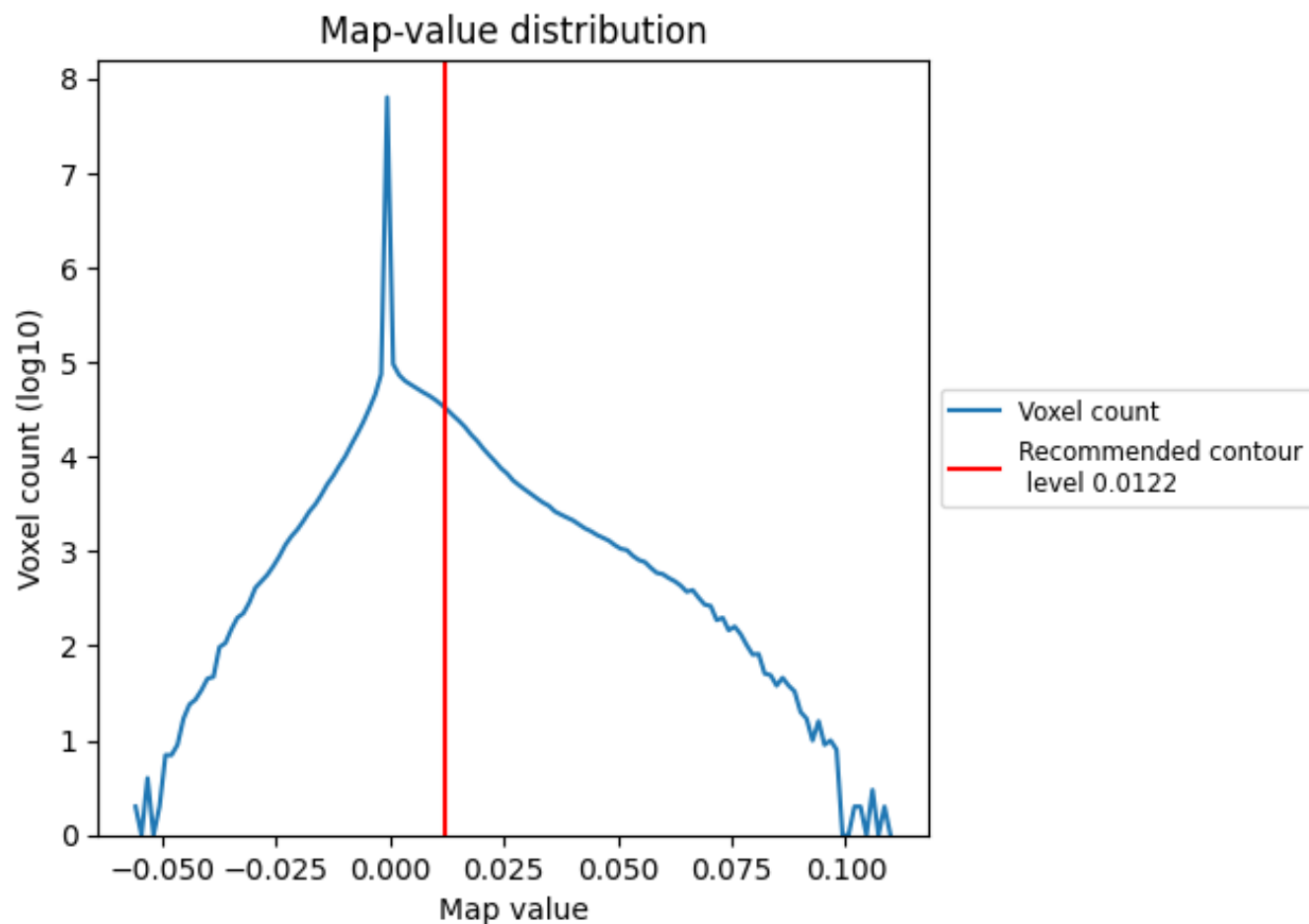
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

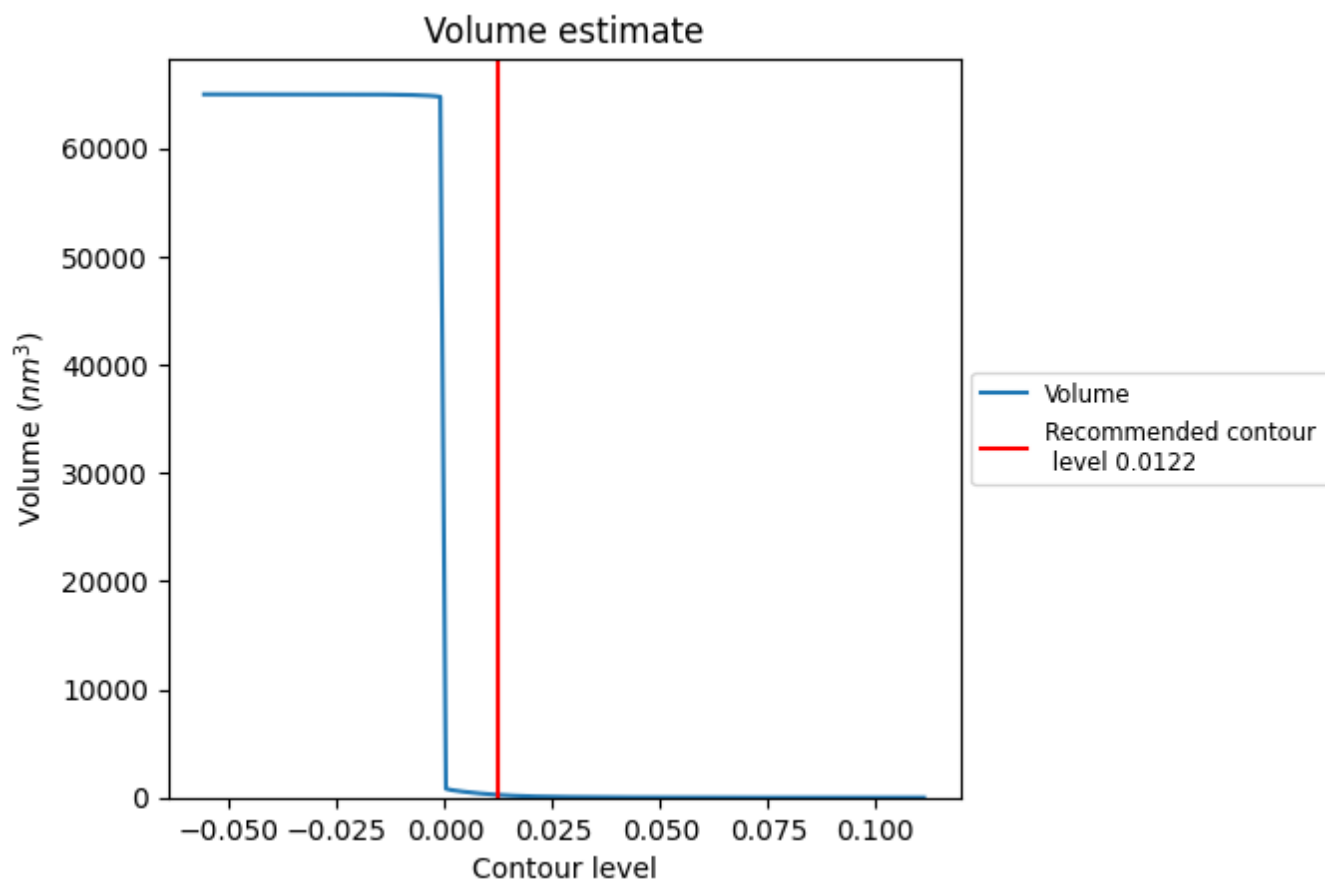
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

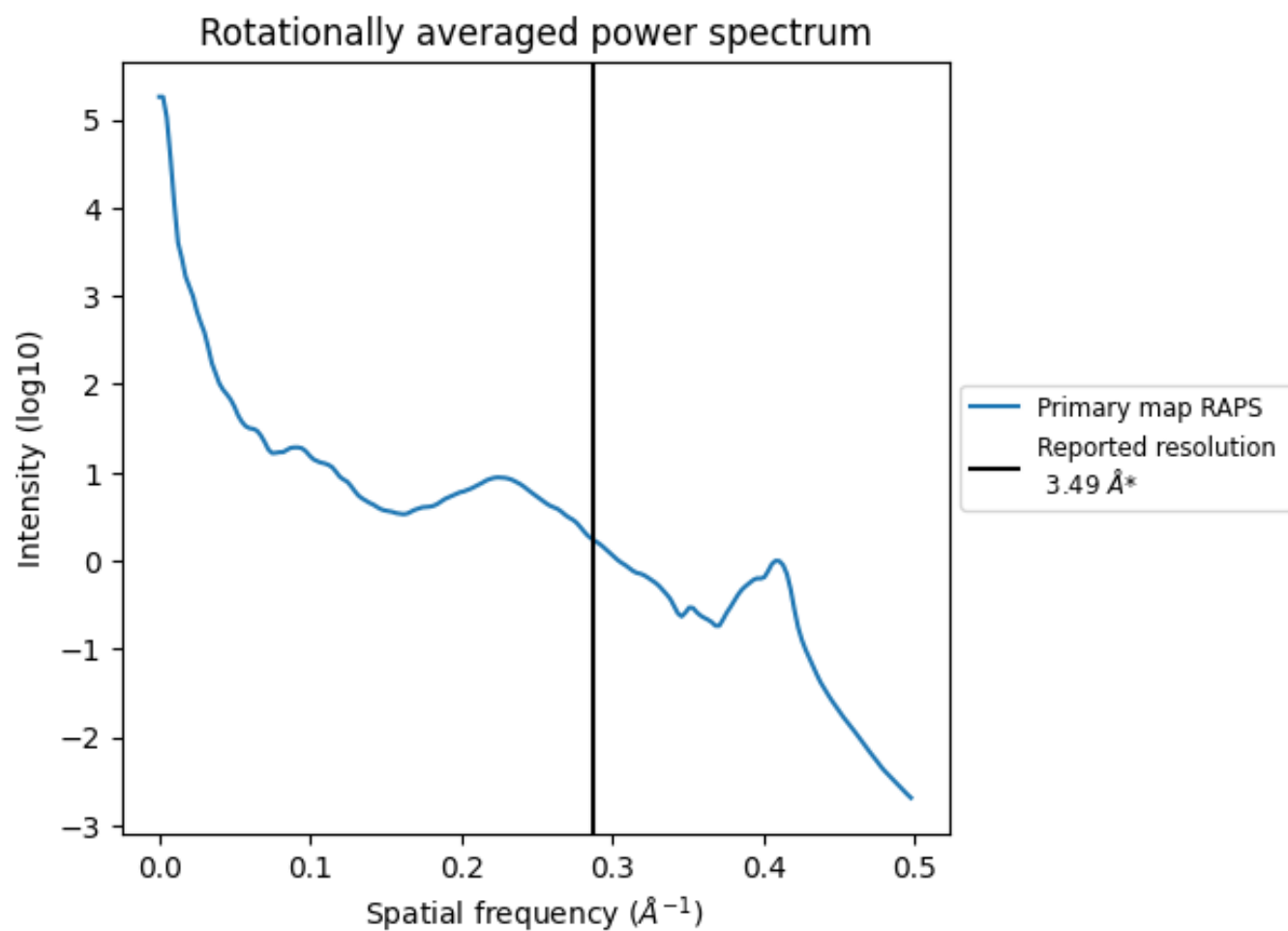
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 254 nm³; this corresponds to an approximate mass of 230 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 0.287 Å⁻¹

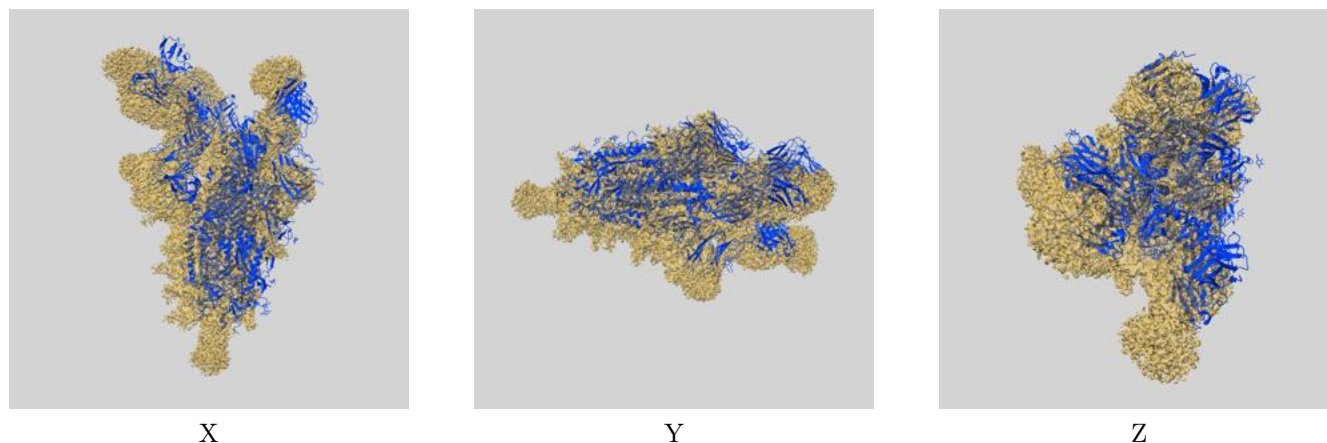
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

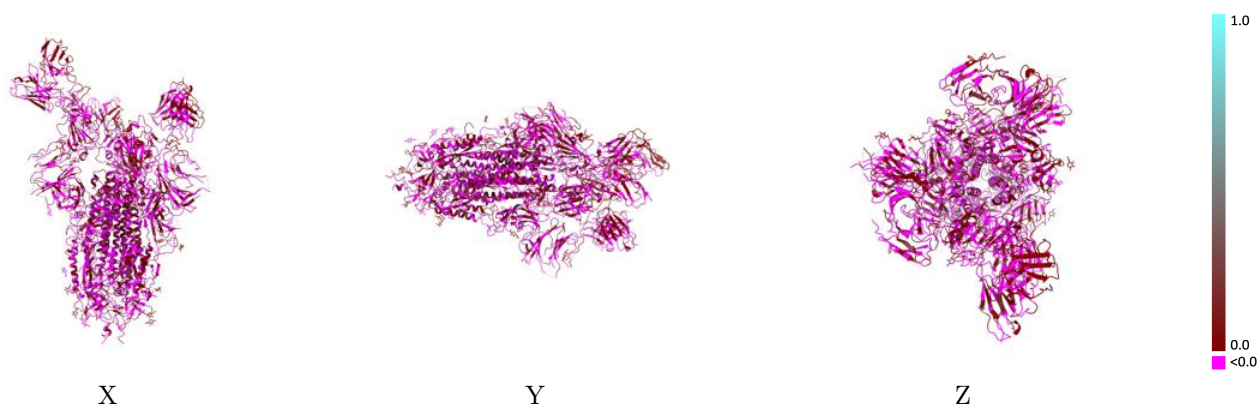
This section contains information regarding the fit between EMDB map EMD-30374 and PDB model 7CHH. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



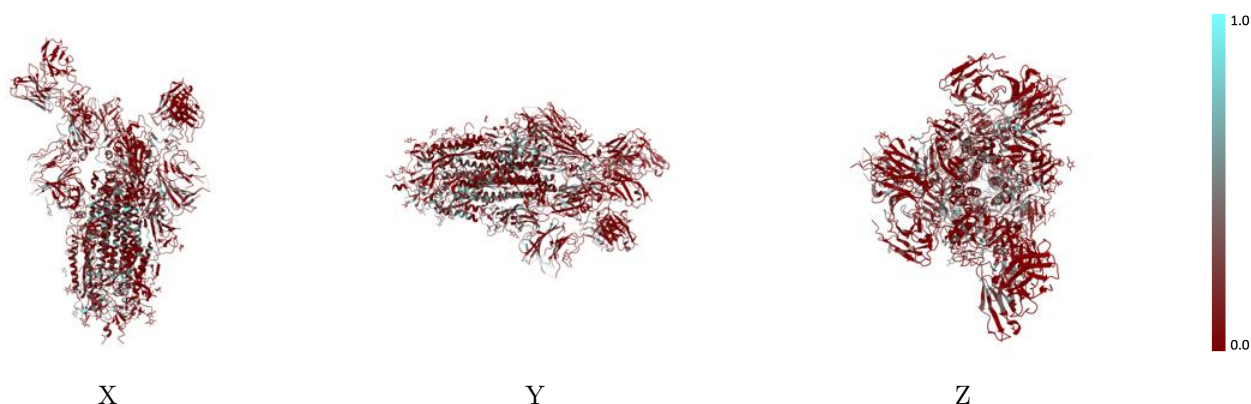
The images above show the 3D surface view of the map at the recommended contour level 0.0122 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



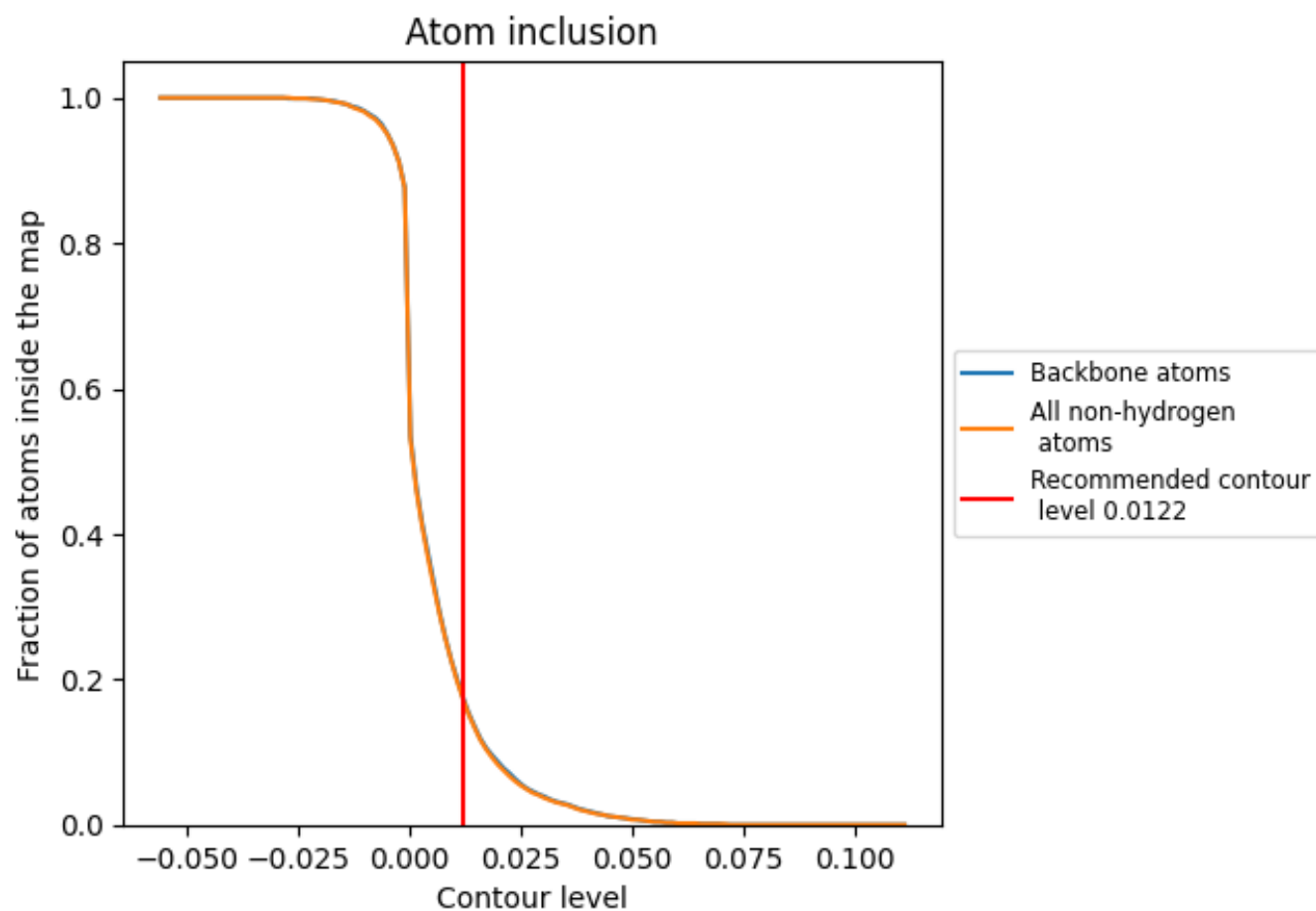
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0122).

9.4 Atom inclusion [i](#)



At the recommended contour level, 17% of all backbone atoms, 17% 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 (0.0122) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1710	 -0.0090
A	 0.2080	 -0.0060
B	 0.1830	 -0.0160
C	 0.1750	 -0.0050
D	 0.1700	 -0.0180
E	 0.0130	 -0.0150
F	 0.4290	 0.0720
G	 0.0970	 0.0170
H	 0.0530	 -0.0030
I	 0.0000	 0.0530
J	 0.0850	 -0.0270
K	 0.1330	 -0.0160
L	 0.0000	 -0.0280
M	 0.0000	 0.0010
N	 0.0000	 -0.0280

