



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:26 PM UTC

PDB ID : 9ML8 / pdb_00009ml8
Title : Crystal structure of the SARS-CoV-2 RBD in complex with the rabbit M8b-B1 Fab
Authors : Fan, C.; Bjorkman, P.J.
Deposited on : 2024-12-18
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

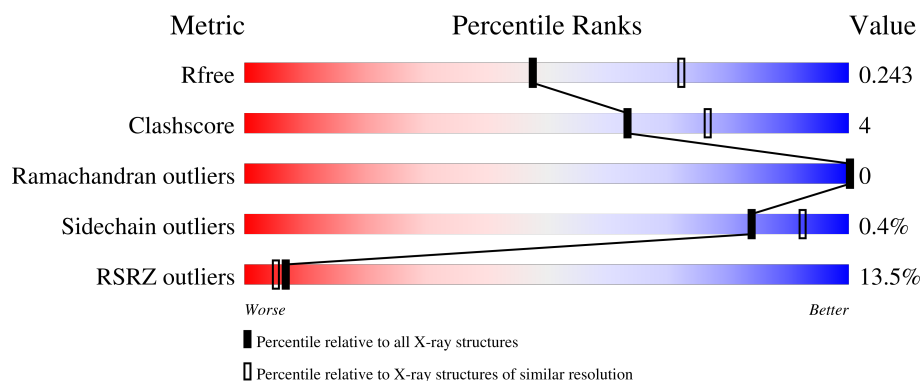
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	212	3% 82% 11% 8%
1	B	212	5% 85% 7% 8%
1	C	212	10% 83% 10% 8%
1	D	212	12% 77% 15% 8%
2	E	235	19% 87% 9% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	235	
2	M	235	
2	P	235	
3	F	217	
3	L	217	
3	N	217	
3	Q	217	
4	G	2	
4	I	2	
4	J	2	
4	K	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20452 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	1	0
			1560	1000	262	290	8			
1	B	196	Total	C	N	O	S	0	1	0
			1560	1000	262	290	8			
1	C	196	Total	C	N	O	S	0	2	0
			1568	1004	264	292	8			
1	D	196	Total	C	N	O	S	0	1	0
			1558	999	260	291	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2
A	538	HIS	-	expression tag	UNP P0DTC2
A	539	HIS	-	expression tag	UNP P0DTC2
B	534	HIS	-	expression tag	UNP P0DTC2
B	535	HIS	-	expression tag	UNP P0DTC2
B	536	HIS	-	expression tag	UNP P0DTC2
B	537	HIS	-	expression tag	UNP P0DTC2
B	538	HIS	-	expression tag	UNP P0DTC2
B	539	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
C	536	HIS	-	expression tag	UNP P0DTC2
C	537	HIS	-	expression tag	UNP P0DTC2
C	538	HIS	-	expression tag	UNP P0DTC2
C	539	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2
D	535	HIS	-	expression tag	UNP P0DTC2
D	536	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	537	HIS	-	expression tag	UNP P0DTC2
D	538	HIS	-	expression tag	UNP P0DTC2
D	539	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called M8b-B1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	224	Total	C	N	O	S	0	0	0
			1683	1078	271	325	9			
2	H	224	Total	C	N	O	S	0	0	0
			1683	1078	271	325	9			
2	M	224	Total	C	N	O	S	0	0	0
			1683	1078	271	325	9			
2	P	224	Total	C	N	O	S	0	0	0
			1683	1078	271	325	9			

- Molecule 3 is a protein called M8b-B1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	216	Total	C	N	O	S	0	1	0
			1643	1030	269	339	5			
3	L	216	Total	C	N	O	S	0	1	0
			1643	1030	269	339	5			
3	N	216	Total	C	N	O	S	0	1	0
			1643	1030	269	339	5			
3	Q	216	Total	C	N	O	S	0	1	0
			1643	1030	269	339	5			

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



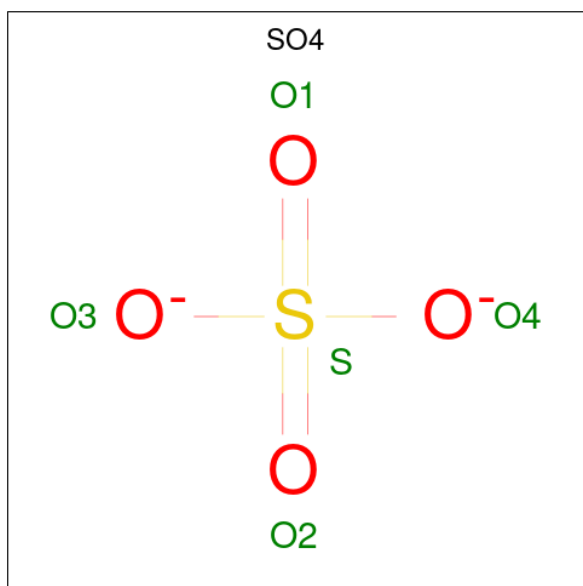
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	N	1	Total	O	S	0	0
			5	4	1		
5	Q	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	58	Total	O	0	0
			58	58		

Continued on next page...

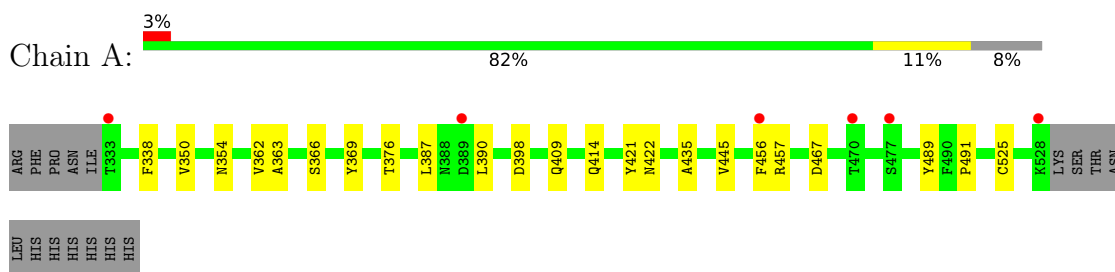
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	63	Total 63	O 63	0	0
6	C	31	Total 31	O 31	0	0
6	D	24	Total 24	O 24	0	0
6	E	102	Total 102	O 102	0	0
6	F	47	Total 47	O 47	0	0
6	H	105	Total 105	O 105	0	0
6	L	51	Total 51	O 51	0	0
6	M	94	Total 94	O 94	0	0
6	N	52	Total 52	O 52	0	0
6	P	81	Total 81	O 81	0	0
6	Q	47	Total 47	O 47	0	0

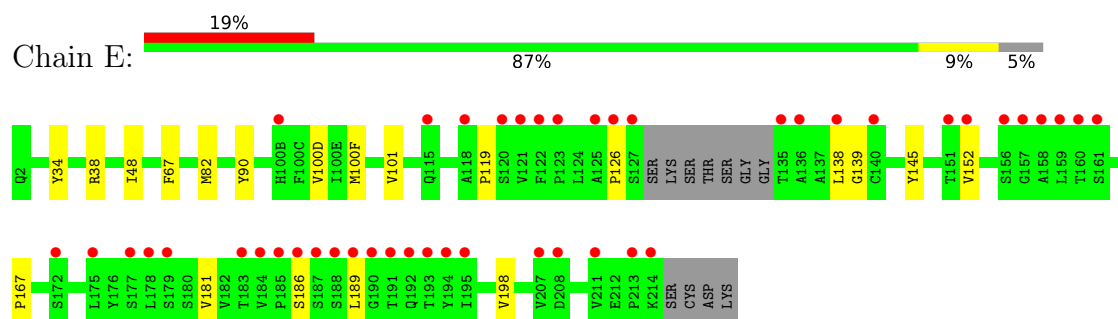
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

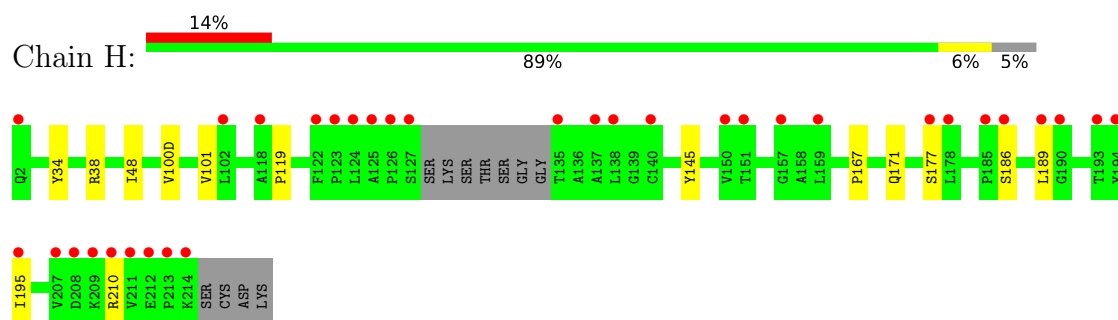
- Molecule 1: Spike protein S1



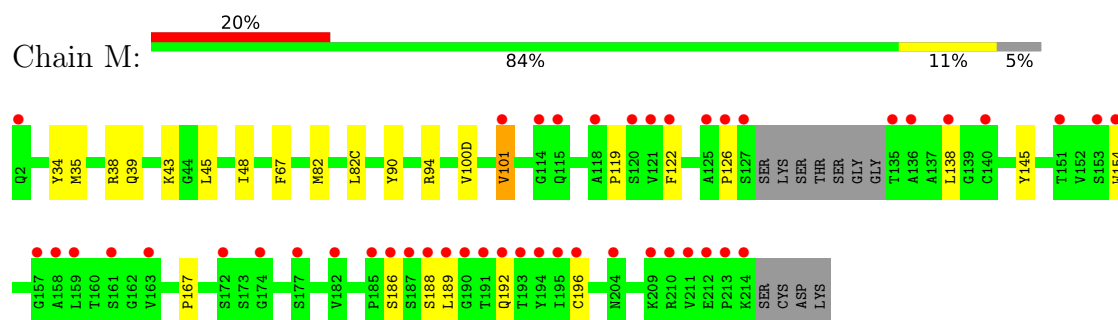
- Molecule 2: M8b-B1 heavy chain



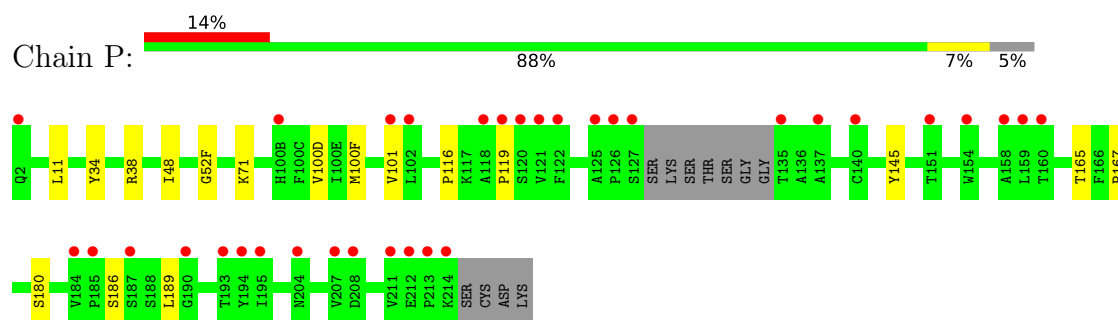
- Molecule 2: M8b-B1 heavy chain



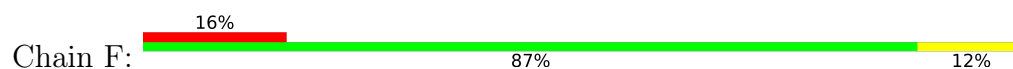
- Molecule 2: M8b-B1 heavy chain

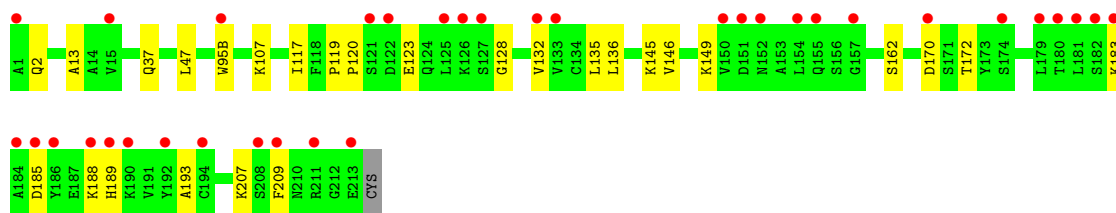


- Molecule 2: M8b-B1 heavy chain



- Molecule 3: M8b-B1 light chain

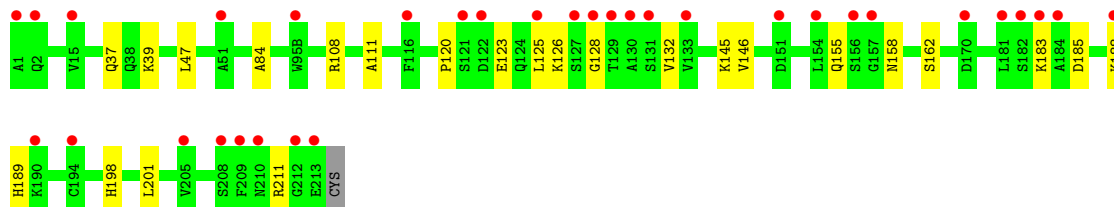
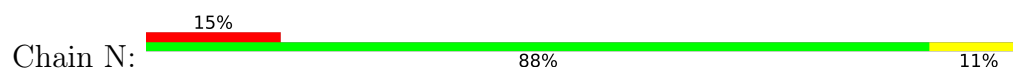




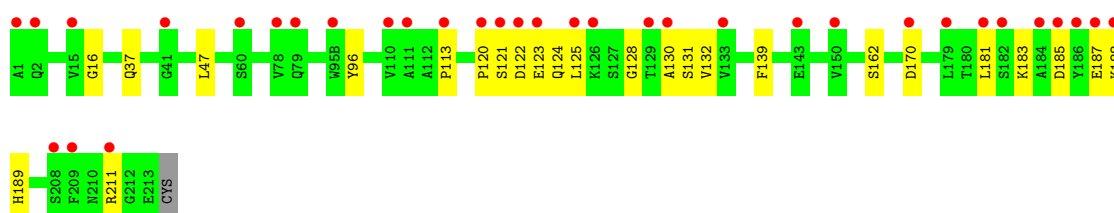
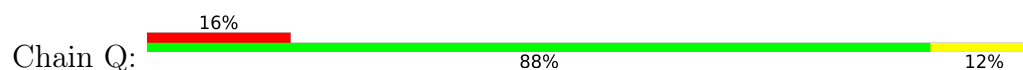
• Molecule 3: M8b-B1 light chain



• Molecule 3: M8b-B1 light chain



• Molecule 3: M8b-B1 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

Chain J:  50% 50%



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

Chain K:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.07Å 173.44Å 129.93Å 90.00° 116.55° 90.00°	Depositor
Resolution (Å)	39.15 – 2.40 39.15 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.15-2.40) 98.4 (39.15-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.223 , 0.247 0.221 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20452	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.10	0/1607	0.31	0/2186
1	B	0.10	0/1607	0.29	0/2186
1	C	0.10	0/1615	0.31	0/2197
1	D	0.12	0/1605	0.33	0/2184
2	E	0.10	0/1730	0.29	0/2362
2	H	0.09	0/1730	0.28	0/2362
2	M	0.10	0/1730	0.28	0/2362
2	P	0.09	0/1730	0.28	0/2362
3	F	0.15	0/1684	0.33	0/2293
3	L	0.09	0/1684	0.30	0/2293
3	N	0.10	0/1684	0.31	0/2293
3	Q	0.10	0/1684	0.30	0/2293
All	All	0.10	0/20090	0.30	0/27373

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1560	0	1485	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1560	0	1485	9	0
1	C	1568	0	1490	12	0
1	D	1558	0	1480	21	0
2	E	1683	0	1630	12	0
2	H	1683	0	1630	7	0
2	M	1683	0	1630	19	0
2	P	1683	0	1630	9	0
3	F	1643	0	1576	16	0
3	L	1643	0	1576	11	0
3	N	1643	0	1576	16	0
3	Q	1643	0	1576	19	0
4	G	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	F	5	0	0	0	0
5	L	5	0	0	0	0
5	N	5	0	0	0	0
5	Q	5	0	0	0	0
6	A	58	0	0	0	0
6	B	63	0	0	1	0
6	C	31	0	0	0	0
6	D	24	0	0	0	0
6	E	102	0	0	0	0
6	F	47	0	0	0	0
6	H	105	0	0	0	0
6	L	51	0	0	0	0
6	M	94	0	0	1	0
6	N	52	0	0	0	0
6	P	81	0	0	0	0
6	Q	47	0	0	0	0
All	All	20452	0	18864	155	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 4.

All (155) 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:D:366:SER:HA	1:D:369:TYR:CE1	2.21	0.76
3:L:16:GLY:HA3	3:Q:16:GLY:HA3	1.70	0.74
1:D:367:VAL:O	1:D:371:SER:HB3	1.88	0.74
3:F:120:PRO:HD3	3:F:132:VAL:HG22	1.70	0.73
3:Q:123:GLU:OE2	3:Q:123:GLU:N	2.17	0.73
2:M:119:PRO:HB3	2:M:145:TYR:HB3	1.71	0.72
3:F:128:GLY:HA2	3:F:183:LYS:HE3	1.69	0.72
2:E:119:PRO:HB3	2:E:145:TYR:HB3	1.72	0.72
3:F:123:GLU:OE2	3:F:123:GLU:N	2.22	0.70
2:P:119:PRO:HB3	2:P:145:TYR:HB3	1.73	0.70
1:D:387:LEU:HA	1:D:390:LEU:HD12	1.75	0.68
3:N:185:ASP:HA	3:N:188:LYS:HE2	1.75	0.68
3:N:108:ARG:HH21	3:N:111:ALA:HB2	1.59	0.66
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.77	0.66
3:Q:120:PRO:HD3	3:Q:132:VAL:HG22	1.75	0.66
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.78	0.65
3:N:128:GLY:HA2	3:N:183:LYS:HE3	1.78	0.64
2:M:167:PRO:HG2	3:N:162:SER:HB2	1.81	0.61
3:F:2:GLN:HB2	3:F:95(B):TRP:CD1	2.38	0.59
2:E:126:PRO:HG3	2:E:138:LEU:HB3	1.84	0.59
1:A:376:THR:HB	1:A:435:ALA:HB3	1.86	0.58
2:M:126:PRO:HB3	2:M:138:LEU:HB3	1.87	0.57
2:H:171:GLN:OE1	2:H:177:SER:OG	2.18	0.56
3:F:185:ASP:HA	3:F:188:LYS:HE2	1.87	0.56
2:M:43:LYS:NZ	6:M:305:HOH:O	2.36	0.56
2:M:82:MET:HE1	2:M:90:TYR:CE2	2.41	0.56
3:N:188:LYS:HG3	3:N:189:HIS:CD2	2.40	0.56
3:N:120:PRO:HD3	3:N:132:VAL:HG22	1.88	0.55
3:N:123:GLU:O	3:N:126:LYS:N	2.28	0.54
1:D:376:THR:HG23	1:D:378:LYS:HG3	1.90	0.54
1:C:457:ARG:NH1	1:C:459:SER:O	2.41	0.53
1:C:358:ILE:HB	1:C:395:VAL:HB	1.90	0.53
2:H:167:PRO:HG2	3:L:162:SER:HB2	1.90	0.53
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.88	0.53
2:M:35:MET:HE1	2:M:94:ARG:HG3	1.91	0.53
3:F:149:LYS:HB2	3:F:193:ALA:HB3	1.91	0.53
1:D:358:ILE:HB	1:D:395:VAL:HB	1.91	0.53
2:P:167:PRO:HG2	3:Q:162:SER:HB2	1.89	0.53
1:B:376:THR:HB	1:B:435:ALA:HB3	1.91	0.53
2:M:188:SER:HB2	2:M:192:GLN:HG2	1.90	0.52
3:Q:187:GLU:C	3:Q:211:ARG:HH22	2.18	0.52
3:Q:37:GLN:HB2	3:Q:47:LEU:HD11	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:PHE:HE2	1:A:363:ALA:HB1	1.74	0.52
1:D:369:TYR:HD1	1:D:370:ASN:N	2.07	0.52
2:P:165:THR:HG23	2:P:180:SER:HB2	1.91	0.52
2:E:34:TYR:HB2	2:E:100(F):MET:HE1	1.92	0.51
2:E:38:ARG:HB3	2:E:48:ILE:HD11	1.92	0.51
2:E:82:MET:HE1	2:E:90:TYR:CE2	2.45	0.51
2:E:67:PHE:HE2	2:E:82:MET:HE2	1.75	0.51
2:M:34:TYR:CZ	2:M:100(D):VAL:HG21	2.45	0.51
3:Q:185:ASP:HA	3:Q:188:LYS:HE2	1.92	0.51
1:D:457:ARG:NH1	1:D:459:SER:O	2.44	0.51
3:N:39:LYS:HD3	3:N:84:ALA:HB2	1.93	0.50
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.42	0.50
1:D:369:TYR:HA	1:D:377:PHE:CE2	2.47	0.50
3:F:117:ILE:HG22	3:F:207:LYS:HD2	1.93	0.50
1:B:456:PHE:CE1	1:B:491:PRO:HA	2.47	0.50
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.94	0.50
1:C:527:PRO:O	1:C:528:LYS:HB2	2.12	0.49
2:E:34:TYR:CZ	2:E:100(D):VAL:HG21	2.47	0.49
3:Q:121:SER:O	3:Q:124:GLN:N	2.46	0.49
2:M:67:PHE:CE2	2:M:82:MET:HE2	2.48	0.49
2:H:34:TYR:CZ	2:H:100(D):VAL:HG21	2.47	0.49
1:D:444:LYS:NZ	1:D:445:VAL:O	2.46	0.49
2:E:67:PHE:CE2	2:E:82:MET:HE2	2.48	0.49
2:H:195:ILE:HG22	2:H:210:ARG:HA	1.95	0.49
3:L:123:GLU:OE1	3:L:123:GLU:N	2.33	0.48
1:D:474[B]:GLN:HG2	1:D:480:CYS:SG	2.54	0.48
1:D:376:THR:HB	1:D:435:ALA:HB3	1.94	0.48
2:M:38:ARG:HB3	2:M:48:ILE:HD11	1.95	0.48
3:N:198:HIS:HB3	3:N:201:LEU:HD13	1.95	0.48
1:C:376:THR:HB	1:C:435:ALA:HB3	1.95	0.48
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.96	0.48
2:P:38:ARG:HB3	2:P:48:ILE:HD11	1.95	0.48
3:Q:189:HIS:H	3:Q:211:ARG:HH21	1.62	0.48
1:A:456:PHE:CZ	1:A:489:TYR:HB2	2.49	0.47
1:B:357[A]:ARG:NH2	6:B:603:HOH:O	2.47	0.47
3:N:145:LYS:HD3	3:N:146:VAL:N	2.29	0.47
1:A:456:PHE:CE1	1:A:491:PRO:HA	2.49	0.47
1:B:334:ASN:OD1	1:B:334:ASN:N	2.44	0.47
1:C:444:LYS:HD2	1:C:445:VAL:H	1.79	0.47
3:L:145:LYS:HD3	3:L:146:VAL:N	2.30	0.47
3:Q:121:SER:C	3:Q:125:LEU:HD23	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:122:ASP:HA	3:Q:125:LEU:HB2	1.96	0.47
3:F:145:LYS:HD3	3:F:146:VAL:N	2.30	0.47
1:D:366:SER:HA	1:D:369:TYR:CZ	2.50	0.46
1:A:409:GLN:HA	1:A:414:GLN:HG2	1.98	0.46
2:P:34:TYR:CZ	2:P:100(D):VAL:HG21	2.50	0.46
2:E:167:PRO:HG2	3:F:162:SER:HB2	1.96	0.46
1:B:354:ASN:O	1:B:398:ASP:HA	2.16	0.45
1:A:362:VAL:HA	1:A:525:CYS:O	2.17	0.45
1:D:455:LEU:HD11	1:D:493:GLN:HB2	1.99	0.45
1:A:366:SER:HA	1:A:369:TYR:CZ	2.51	0.45
1:B:456:PHE:CZ	1:B:489:TYR:HB2	2.52	0.45
1:B:366:SER:HA	1:B:369:TYR:CZ	2.52	0.45
3:Q:120:PRO:HG3	3:Q:130:ALA:HB1	1.98	0.44
3:N:155:GLN:OE1	3:N:158:ASN:ND2	2.47	0.44
3:L:185:ASP:HA	3:L:188:LYS:HE2	2.00	0.44
1:D:392:PHE:HA	1:D:517:LEU:HD23	1.99	0.44
1:B:358:ILE:HB	1:B:395:VAL:HB	1.98	0.43
1:B:360:ASN:H	1:B:523:THR:HB	1.83	0.43
3:F:170:ASP:HB3	3:F:172:THR:HG23	2.00	0.43
3:L:188:LYS:HG3	3:L:189:HIS:CD2	2.52	0.43
2:M:67:PHE:HE2	2:M:82:MET:HE2	1.83	0.43
1:C:382:VAL:HG11	1:C:387:LEU:HD21	1.98	0.43
1:D:454:ARG:HD3	1:D:457:ARG:HG3	2.00	0.43
2:M:82:MET:HB2	2:M:82(C):LEU:HD21	1.99	0.43
3:L:149:LYS:HB2	3:L:193:ALA:HB3	2.00	0.43
2:M:94:ARG:HB3	2:M:101:VAL:HG23	2.00	0.43
2:M:39:GLN:HB2	2:M:45:LEU:HD23	2.00	0.43
1:D:354:ASN:O	1:D:398:ASP:HA	2.18	0.43
2:E:139:GLY:HA3	2:E:181:VAL:HG12	2.01	0.43
2:E:186:SER:HA	2:E:189:LEU:HG	2.00	0.43
2:M:154:TRP:CH2	2:M:196:CYS:HB3	2.53	0.43
3:Q:189:HIS:H	3:Q:211:ARG:NH2	2.17	0.43
1:C:502:GLY:O	1:C:506:GLN:HG3	2.19	0.43
1:D:334:ASN:OD1	1:D:334:ASN:N	2.51	0.43
1:C:388:ASN:HD22	1:C:527:PRO:HD2	1.84	0.42
1:D:425:LEU:HD21	1:D:512:VAL:HG11	2.02	0.42
2:H:186:SER:HA	2:H:189:LEU:HG	2.01	0.42
3:F:188:LYS:HG3	3:F:189:HIS:CE1	2.54	0.42
3:N:189:HIS:O	3:N:211:ARG:NE	2.38	0.42
1:A:421:TYR:CD1	1:A:457:ARG:HB2	2.54	0.42
1:D:379:CYS:SG	1:D:384:PRO:HG3	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HA	1:A:390:LEU:HD23	2.01	0.42
1:A:354:ASN:O	1:A:398:ASP:HA	2.19	0.42
2:P:100(F):MET:HB2	3:Q:96:TYR:CE1	2.54	0.42
3:F:188:LYS:HG3	3:F:189:HIS:ND1	2.35	0.42
2:M:122:PHE:CE1	3:N:123:GLU:HG3	2.54	0.42
3:Q:128:GLY:C	3:Q:183:LYS:HG2	2.45	0.42
2:E:152:VAL:HG22	2:E:198:VAL:HG22	2.02	0.42
3:Q:113:PRO:HB3	3:Q:139:PHE:CD2	2.55	0.42
1:D:377:PHE:CD2	1:D:434:ILE:HG12	2.55	0.41
3:Q:181:LEU:HD13	3:Q:185:ASP:HB3	2.02	0.41
3:F:13:ALA:HA	3:F:107:LYS:HE2	2.02	0.41
1:C:350:VAL:HG22	1:C:422:ASN:HB3	2.02	0.41
3:F:135:LEU:HD12	3:F:136:LEU:N	2.36	0.41
2:M:122:PHE:HE1	3:N:123:GLU:HG3	1.86	0.41
2:M:186:SER:HA	2:M:189:LEU:HG	2.01	0.41
1:D:366:SER:HA	1:D:369:TYR:CD1	2.54	0.41
3:F:119:PRO:HB3	3:F:209:PHE:CE1	2.55	0.41
2:P:52(F):GLY:N	2:P:71:LYS:O	2.49	0.41
3:Q:188:LYS:HG3	3:Q:189:HIS:CD2	2.56	0.41
2:P:11:LEU:HD23	2:P:116:PRO:HG3	2.03	0.41
1:C:461:LEU:HD22	1:C:465:GLU:HB3	2.02	0.40
2:H:38:ARG:HB3	2:H:48:ILE:HD11	2.02	0.40
3:L:163:VAL:HG22	3:L:175:LEU:HD12	2.02	0.40
2:M:154:TRP:CZ3	2:M:196:CYS:HB3	2.56	0.40
1:A:350:VAL:HG22	1:A:422:ASN:HB3	2.03	0.40
1:C:444:LYS:C	1:C:499:PRO:HD3	2.46	0.40
3:N:123:GLU:O	3:N:125:LEU:N	2.54	0.40
3:L:113:PRO:HB3	3:L:139:PHE:CD2	2.57	0.40
2:P:186:SER:HA	2:P:189:LEU:HG	2.02	0.40
3:Q:120:PRO:HB3	3:Q:131:SER:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	195/212 (92%)	190 (97%)	5 (3%)	0	100	100
1	B	195/212 (92%)	191 (98%)	4 (2%)	0	100	100
1	C	196/212 (92%)	190 (97%)	6 (3%)	0	100	100
1	D	195/212 (92%)	192 (98%)	3 (2%)	0	100	100
2	E	220/235 (94%)	217 (99%)	3 (1%)	0	100	100
2	H	220/235 (94%)	218 (99%)	2 (1%)	0	100	100
2	M	220/235 (94%)	217 (99%)	3 (1%)	0	100	100
2	P	220/235 (94%)	218 (99%)	2 (1%)	0	100	100
3	F	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
3	L	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
3	N	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
3	Q	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
All	All	2521/2656 (95%)	2465 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	170/185 (92%)	169 (99%)	1 (1%)	78	89
1	B	170/185 (92%)	169 (99%)	1 (1%)	78	89
1	C	171/185 (92%)	171 (100%)	0	100	100
1	D	170/185 (92%)	168 (99%)	2 (1%)	63	81
2	E	186/195 (95%)	185 (100%)	1 (0%)	81	91
2	H	186/195 (95%)	185 (100%)	1 (0%)	81	91
2	M	186/195 (95%)	185 (100%)	1 (0%)	81	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	186/195 (95%)	185 (100%)	1 (0%)	81	91
3	F	187/187 (100%)	187 (100%)	0	100	100
3	L	187/187 (100%)	187 (100%)	0	100	100
3	N	187/187 (100%)	187 (100%)	0	100	100
3	Q	187/187 (100%)	186 (100%)	1 (0%)	81	91
All	All	2173/2268 (96%)	2164 (100%)	9 (0%)	84	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	VAL
1	B	456	PHE
1	D	369	TYR
1	D	456	PHE
2	E	101	VAL
2	H	101	VAL
2	M	101	VAL
2	P	101	VAL
3	Q	170	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	HIS
1	B	360	ASN
1	C	481	ASN
1	D	388	ASN
1	D	414	GLN
1	D	498	GLN
2	E	171	GLN
2	E	199	ASN
3	F	158	ASN
3	F	160	GLN
2	M	56	ASN
2	P	39	GLN
2	P	115	GLN
3	Q	38	GLN
3	Q	124	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 ⓘ

8 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	G	1	4,1	14,14,15	0.79	0	17,19,21	1.21	2 (11%)
4	NAG	G	2	4	14,14,15	0.71	0	17,19,21	0.99	0
4	NAG	I	1	4,1	14,14,15	0.73	0	17,19,21	0.99	1 (5%)
4	NAG	I	2	4	14,14,15	0.70	0	17,19,21	0.87	0
4	NAG	J	1	4,1	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
4	NAG	J	2	4	14,14,15	0.70	0	17,19,21	0.80	0
4	NAG	K	1	4,1	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
4	NAG	K	2	4	14,14,15	0.70	0	17,19,21	0.95	1 (5%)

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	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C1-O5-C5	3.02	116.24	112.19
4	K	1	NAG	C1-O5-C5	2.45	115.46	112.19
4	G	1	NAG	C2-N2-C7	2.20	125.84	122.90
4	I	1	NAG	C1-O5-C5	2.18	115.11	112.19
4	J	1	NAG	C1-O5-C5	2.10	115.00	112.19
4	K	2	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

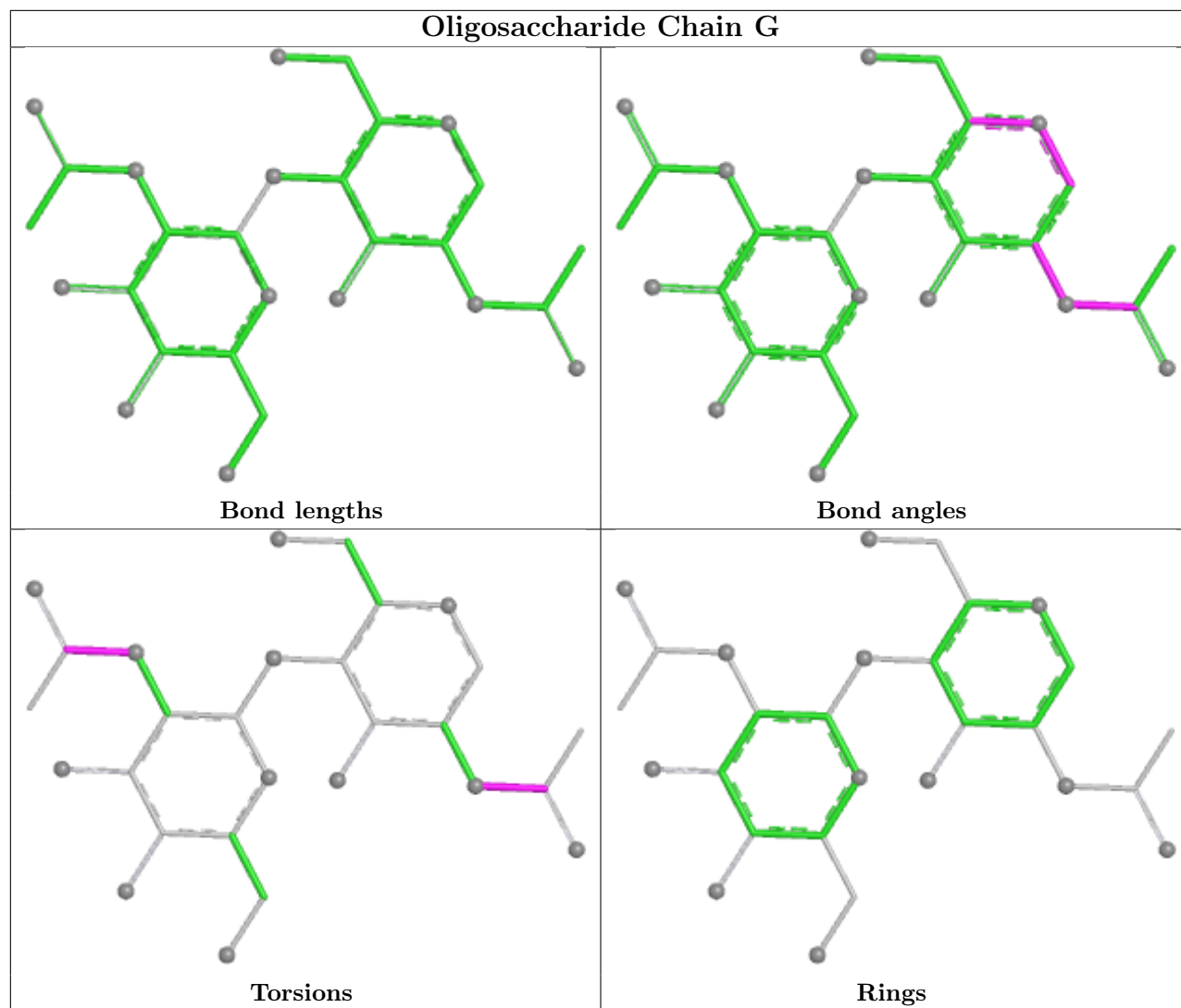
All (8) torsion outliers are listed below:

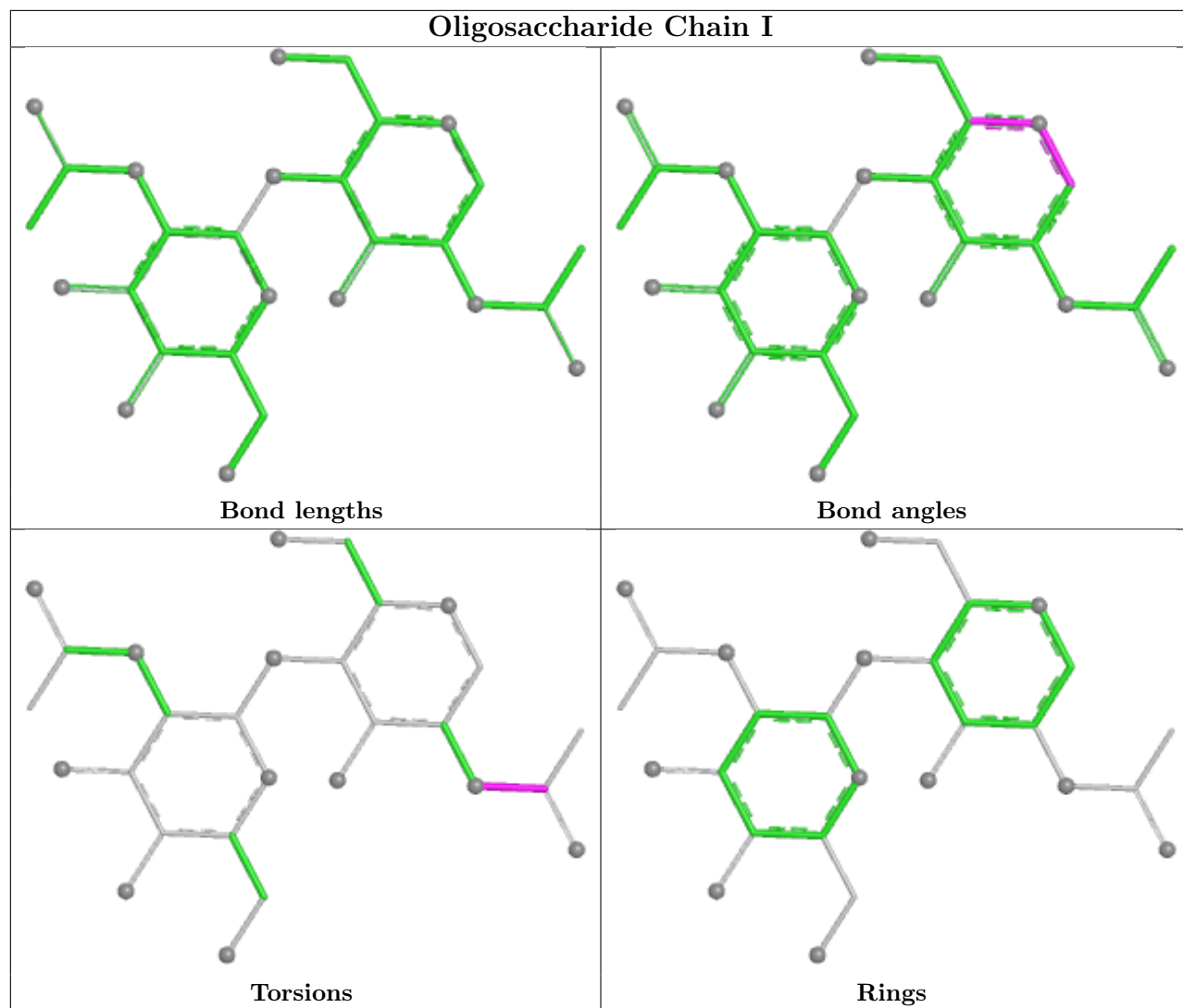
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2

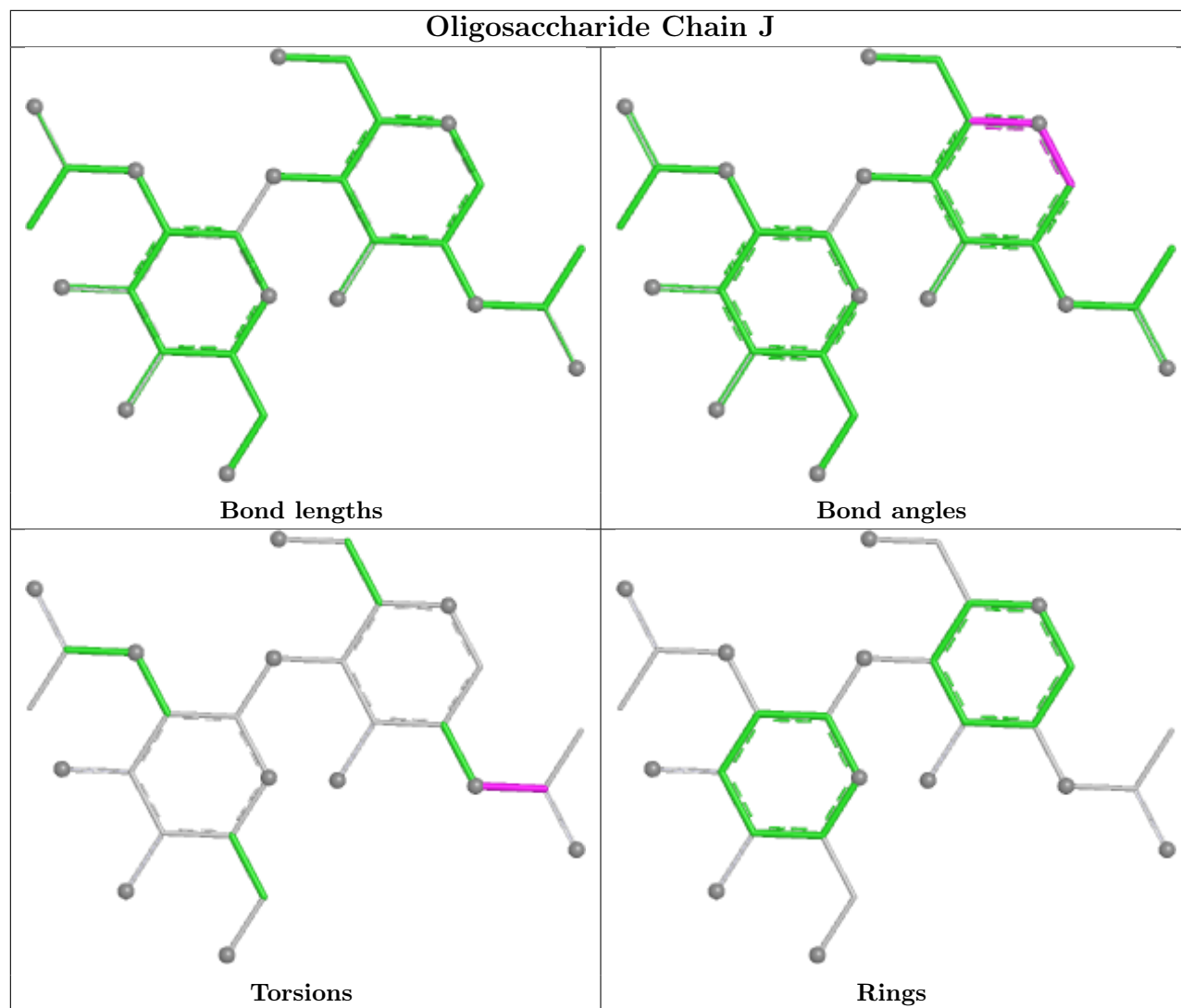
There are no ring outliers.

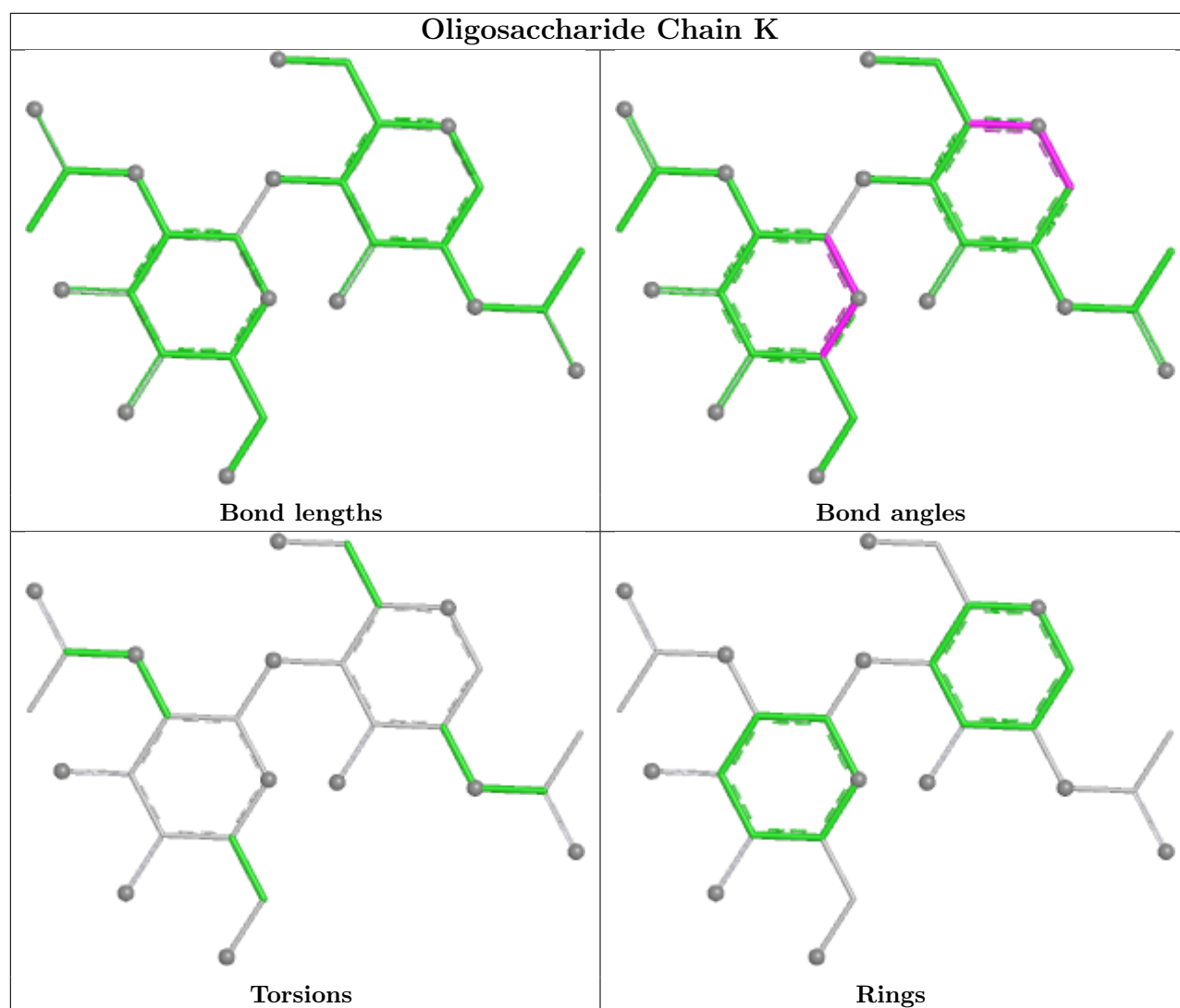
No monomer is involved in short contacts.

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](#)

7 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	SO4	A	601	-	4,4,4	0.68	0	6,6,6	0.08	0
5	SO4	L	301	-	4,4,4	0.68	0	6,6,6	0.08	0
5	SO4	F	301	-	4,4,4	0.67	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	Q	301	-	4,4,4	0.68	0	6,6,6	0.09	0
5	SO4	N	301	-	4,4,4	0.67	0	6,6,6	0.10	0
5	SO4	C	601	-	4,4,4	0.68	0	6,6,6	0.10	0
5	SO4	D	601	-	4,4,4	0.68	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	196/212 (92%)	0.37	6 (3%) 51 47	24, 45, 65, 92	1 (0%)
1	B	196/212 (92%)	0.49	11 (5%) 30 26	26, 46, 81, 95	1 (0%)
1	C	196/212 (92%)	0.73	21 (10%) 11 8	23, 53, 84, 100	2 (1%)
1	D	196/212 (92%)	0.88	25 (12%) 7 6	37, 57, 101, 124	1 (0%)
2	E	224/235 (95%)	0.76	45 (20%) 3 2	24, 41, 102, 124	0
2	H	224/235 (95%)	0.68	34 (15%) 5 4	23, 40, 97, 124	0
2	M	224/235 (95%)	0.84	46 (20%) 2 2	26, 43, 108, 129	0
2	P	224/235 (95%)	0.76	34 (15%) 5 4	27, 44, 101, 132	0
3	F	216/217 (99%)	1.05	35 (16%) 4 4	30, 56, 108, 129	1 (0%)
3	L	216/217 (99%)	0.87	20 (9%) 14 11	29, 54, 105, 122	1 (0%)
3	N	216/217 (99%)	1.05	33 (15%) 5 4	29, 56, 109, 136	1 (0%)
3	Q	216/217 (99%)	1.12	34 (15%) 5 4	33, 59, 107, 127	1 (0%)
All	All	2544/2656 (95%)	0.81	344 (13%) 7 5	23, 51, 101, 136	9 (0%)

All (344) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	1	ALA	6.6
3	N	125	LEU	6.3
3	F	1	ALA	6.3
3	Q	1	ALA	5.7
3	N	1	ALA	5.4
2	E	127	SER	5.2
3	F	209	PHE	5.0
2	M	127	SER	4.5
1	D	372	ALA	4.5
2	E	195	ILE	4.4
2	H	127	SER	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	195	ILE	4.3
1	C	333	THR	4.2
1	D	528	LYS	4.2
1	B	333	THR	4.0
1	D	333	THR	3.9
2	M	213	PRO	3.9
2	M	125	ALA	3.9
2	M	190	GLY	3.9
3	Q	182	SER	3.9
1	C	369	TYR	3.9
2	P	2	GLN	3.8
2	E	213	PRO	3.8
1	D	371	SER	3.8
2	H	190	GLY	3.8
2	M	186	SER	3.8
3	N	212	GLY	3.8
3	L	125	LEU	3.8
2	P	127	SER	3.7
3	F	182	SER	3.7
2	E	161	SER	3.7
2	M	159	LEU	3.7
2	H	125	ALA	3.7
2	M	214	LYS	3.7
2	P	125	ALA	3.6
3	N	182	SER	3.6
1	D	368	LEU	3.6
2	E	159	LEU	3.6
3	N	209	PHE	3.6
1	A	333	THR	3.6
2	P	214	LYS	3.6
3	N	190	LYS	3.6
2	E	118	ALA	3.6
2	E	214	LYS	3.5
3	F	126	LYS	3.5
2	E	194	TYR	3.5
2	P	151	THR	3.5
3	Q	170	ASP	3.5
3	Q	187	GLU	3.5
2	M	194	TYR	3.5
2	E	186	SER	3.5
1	B	369	TYR	3.4
3	L	170	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	125	ALA	3.4
1	D	369	TYR	3.4
2	H	208	ASP	3.4
2	H	2	GLN	3.4
2	M	193	THR	3.4
1	B	528	LYS	3.4
2	M	151	THR	3.4
3	F	95(B)	TRP	3.3
2	E	135	THR	3.3
3	F	122	ASP	3.3
3	N	188	LYS	3.3
2	M	211	VAL	3.3
3	N	128	GLY	3.3
3	N	15	VAL	3.3
2	H	151	THR	3.3
3	N	194	CYS	3.3
3	F	170	ASP	3.2
2	P	118	ALA	3.2
2	E	177	SER	3.2
2	M	188	SER	3.2
2	H	213	PRO	3.2
3	L	154	LEU	3.2
3	F	184	ALA	3.2
1	D	527	PRO	3.2
3	F	188	LYS	3.2
2	M	118	ALA	3.2
2	P	126	PRO	3.2
3	F	125	LEU	3.2
2	P	158	ALA	3.1
3	F	194	CYS	3.1
3	N	130	ALA	3.1
3	Q	209	PHE	3.1
2	M	121	VAL	3.1
2	H	138	LEU	3.1
2	H	207	VAL	3.1
2	M	135	THR	3.1
2	P	193	THR	3.1
1	B	367	VAL	3.1
1	D	367	VAL	3.1
2	P	195	ILE	3.1
3	L	129	THR	3.0
1	D	382	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	129	THR	3.0
3	N	213	GLU	3.0
1	C	381	GLY	3.0
2	E	192	GLN	3.0
2	E	185	PRO	3.0
1	A	389	ASP	3.0
1	D	370	ASN	3.0
1	D	385	THR	2.9
1	C	528	LYS	2.9
1	D	365	TYR	2.9
2	H	214	LYS	2.9
2	M	172	SER	2.9
2	E	115	GLN	2.9
2	M	140	CYS	2.9
2	E	193	THR	2.9
2	M	189	LEU	2.9
2	M	187	SER	2.9
3	N	154	LEU	2.9
3	L	209	PHE	2.9
3	F	127	SER	2.8
2	H	135	THR	2.8
3	L	188	LYS	2.8
2	P	100(B)	HIS	2.8
3	N	208	SER	2.8
1	A	456	PHE	2.8
3	F	189	HIS	2.8
2	M	177	SER	2.8
3	Q	2	GLN	2.8
3	Q	185	ASP	2.8
3	Q	186	TYR	2.8
2	M	161	SER	2.8
3	N	127	SER	2.8
1	D	387	LEU	2.8
3	F	179	LEU	2.7
2	E	188	SER	2.7
2	P	101	VAL	2.7
3	N	156	SER	2.7
2	M	191	THR	2.7
2	P	119	PRO	2.7
3	Q	113	PRO	2.7
1	D	390	LEU	2.7
1	B	372	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	385	THR	2.7
2	P	135	THR	2.7
3	L	95(B)	TRP	2.7
3	N	95(B)	TRP	2.7
3	Q	123	GLU	2.7
3	Q	129	THR	2.7
3	L	2	GLN	2.7
2	P	208	ASP	2.6
2	E	190	GLY	2.6
2	E	140	CYS	2.6
2	M	196	CYS	2.6
2	E	158	ALA	2.6
2	M	158	ALA	2.6
2	H	195	ILE	2.6
2	M	185	PRO	2.6
2	E	138	LEU	2.6
3	Q	79	GLN	2.6
3	Q	95(B)	TRP	2.6
2	P	190	GLY	2.6
3	F	185	ASP	2.6
1	C	456	PHE	2.6
2	E	211	VAL	2.6
2	E	183	THR	2.6
2	M	154	TRP	2.6
2	H	126	PRO	2.6
3	N	170	ASP	2.6
2	M	138	LEU	2.6
3	N	181	LEU	2.6
2	M	115	GLN	2.6
2	P	211	VAL	2.6
2	E	191	THR	2.6
3	F	181	LEU	2.5
1	C	367	VAL	2.5
3	F	133	VAL	2.5
3	N	2	GLN	2.5
2	E	120	SER	2.5
3	Q	121	SER	2.5
3	N	133	VAL	2.5
1	D	373	SER	2.5
2	P	160	THR	2.5
2	E	123	PRO	2.5
2	E	189	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	181	LEU	2.5
3	Q	126	LYS	2.5
2	P	184	VAL	2.5
2	H	118	ALA	2.5
3	F	208	SER	2.5
2	E	157	GLY	2.5
2	H	189	LEU	2.5
3	Q	133	VAL	2.5
3	Q	60	SER	2.5
2	M	126	PRO	2.4
1	A	528	LYS	2.4
3	F	151	ASP	2.4
2	M	2	GLN	2.4
2	E	122	PHE	2.4
1	C	445	VAL	2.4
3	Q	208	SER	2.4
2	H	123	PRO	2.4
3	L	122	ASP	2.4
3	N	122	ASP	2.4
3	Q	122	ASP	2.4
3	Q	179	LEU	2.4
1	B	382	VAL	2.4
3	Q	111	ALA	2.4
3	Q	130	ALA	2.4
2	H	193	THR	2.4
3	N	121	SER	2.4
3	Q	143	GLU	2.4
3	F	192	TYR	2.4
2	H	211	VAL	2.4
2	M	163	VAL	2.4
3	L	150	VAL	2.4
2	E	136	ALA	2.4
2	P	194	TYR	2.4
3	F	186	TYR	2.4
3	Q	150	VAL	2.4
2	P	120	SER	2.3
3	F	121	SER	2.3
2	H	209	LYS	2.3
2	P	207	VAL	2.3
3	L	191	VAL	2.3
3	N	183	LYS	2.3
3	Q	78	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	481	ASN	2.3
2	P	137	ALA	2.3
3	Q	184	ALA	2.3
1	C	470	THR	2.3
1	D	381	GLY	2.3
2	P	159	LEU	2.3
3	F	154	LEU	2.3
2	H	122	PHE	2.3
2	H	150	VAL	2.3
2	P	121	VAL	2.3
3	N	205	VAL	2.3
2	E	126	PRO	2.3
3	Q	120	PRO	2.3
2	E	151	THR	2.3
3	Q	211	ARG	2.3
2	M	120	SER	2.3
2	E	100(B)	HIS	2.3
2	M	192	GLN	2.3
2	M	122	PHE	2.3
2	E	184	VAL	2.3
2	M	157	GLY	2.3
3	Q	41	GLY	2.3
1	A	477	SER	2.3
1	C	373	SER	2.3
1	D	477	SER	2.3
2	M	101	VAL	2.3
3	L	133	VAL	2.3
1	B	365	TYR	2.3
3	Q	188	LYS	2.2
2	P	122	PHE	2.2
2	H	185	PRO	2.2
2	H	210	ARG	2.2
1	D	480	CYS	2.2
2	H	140	CYS	2.2
1	C	387	LEU	2.2
2	E	178	LEU	2.2
1	B	373	SER	2.2
1	C	371	SER	2.2
2	H	177	SER	2.2
2	P	154	TRP	2.2
2	P	212	GLU	2.2
3	F	213	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	210	ARG	2.2
1	D	374	PHE	2.2
2	M	182	VAL	2.2
3	F	190	LYS	2.2
3	L	126	LYS	2.2
3	F	180	THR	2.2
2	H	159	LEU	2.2
2	P	102	LEU	2.2
3	Q	125	LEU	2.2
2	E	172	SER	2.2
2	E	208	ASP	2.2
1	C	357[A]	ARG	2.2
1	C	408	ARG	2.2
2	P	213	PRO	2.2
1	D	362	VAL	2.2
2	E	121	VAL	2.2
3	F	150	VAL	2.2
1	D	435	ALA	2.2
2	M	209	LYS	2.2
2	M	204	ASN	2.2
1	D	526	GLY	2.2
2	E	175	LEU	2.2
3	L	128	GLY	2.2
2	M	153	SER	2.2
2	P	187	SER	2.2
3	F	211	ARG	2.2
1	C	444	LYS	2.2
3	N	116	PHE	2.2
3	F	15	VAL	2.1
3	F	132	VAL	2.1
3	L	15	VAL	2.1
3	Q	15	VAL	2.1
2	P	204	ASN	2.1
3	N	184	ALA	2.1
3	N	210	ASN	2.1
1	A	470	THR	2.1
1	D	431	GLY	2.1
2	H	102	LEU	2.1
2	M	174	GLY	2.1
3	N	157	GLY	2.1
2	H	194	TYR	2.1
2	E	156	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	174	SER	2.1
3	N	151	ASP	2.1
2	P	185	PRO	2.1
2	H	137	ALA	2.1
3	F	152	ASN	2.1
1	C	365	TYR	2.1
1	C	505	TYR	2.1
2	P	140	CYS	2.1
2	E	179	SER	2.1
2	E	187	SER	2.1
3	L	185	ASP	2.1
2	E	152	VAL	2.1
2	E	207	VAL	2.1
3	F	155	GLN	2.1
1	B	381	GLY	2.1
2	H	178	LEU	2.1
2	M	114	GLY	2.1
3	L	212	GLY	2.1
2	M	212	GLU	2.1
3	F	183	LYS	2.1
1	B	527	PRO	2.1
2	H	124	LEU	2.1
1	D	476	GLY	2.1
2	E	160	THR	2.1
3	L	123	GLU	2.1
1	D	380	TYR	2.1
1	B	477	SER	2.1
2	H	186	SER	2.1
1	C	382	VAL	2.0
3	Q	110	VAL	2.0
2	M	136	ALA	2.0
1	C	368	LEU	2.0
2	H	212	GLU	2.0
3	L	190	LYS	2.0
1	C	383	SER	2.0
3	N	131	SER	2.0
3	N	51	ALA	2.0
2	H	157	GLY	2.0
3	F	157	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

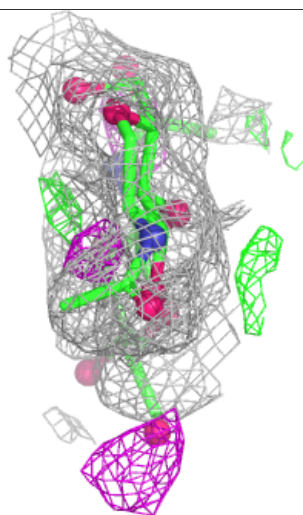
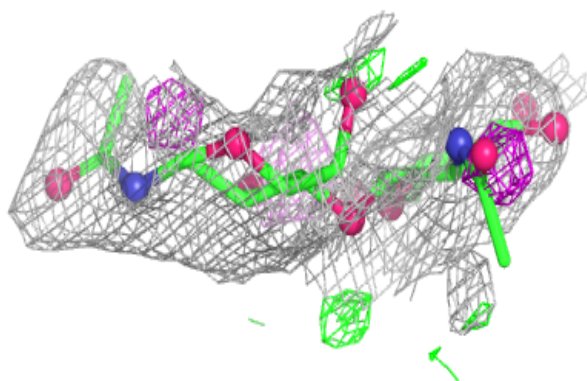
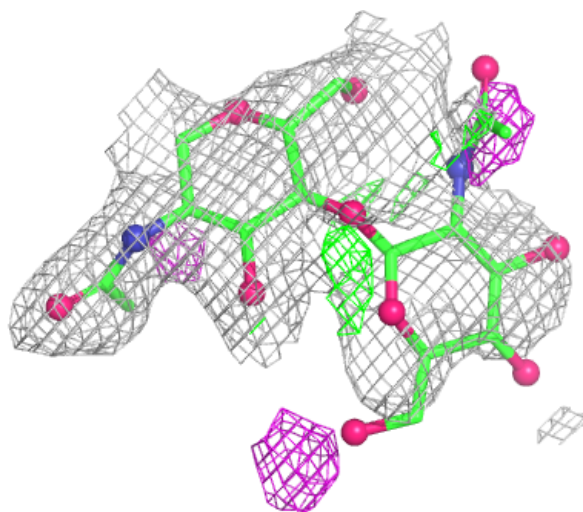
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	G	1	14/15	-	-	53,79,92,102	0
4	NAG	G	2	14/15	-	-	104,109,115,115	0
4	NAG	I	1	14/15	-	-	59,79,83,87	0
4	NAG	I	2	14/15	-	-	90,100,109,113	0
4	NAG	J	1	14/15	-	-	68,86,96,102	0
4	NAG	J	2	14/15	-	-	107,111,115,117	0
4	NAG	K	1	14/15	-	-	78,99,105,109	0
4	NAG	K	2	14/15	-	-	110,117,124,125	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

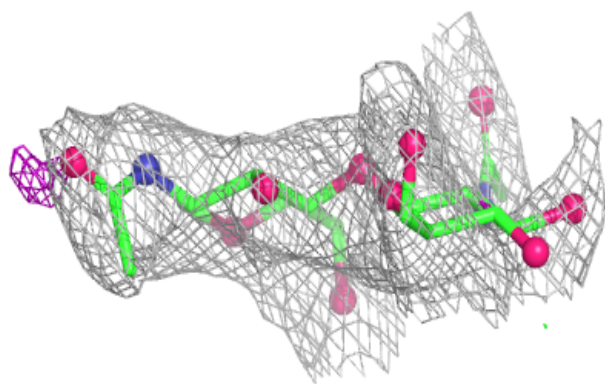
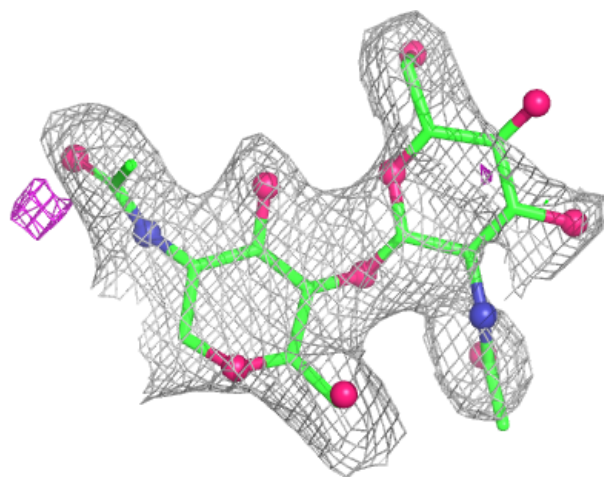
Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



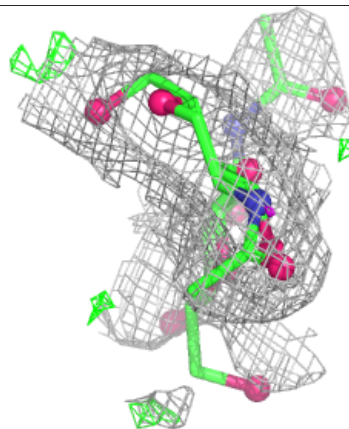
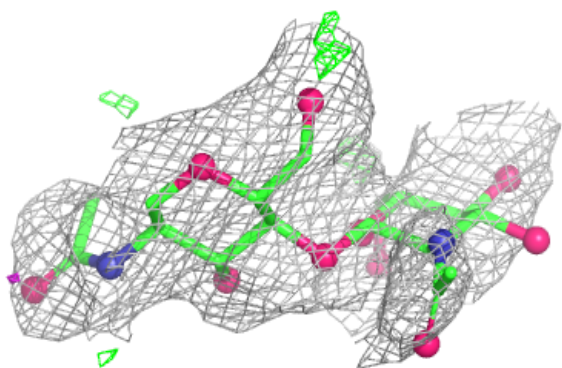
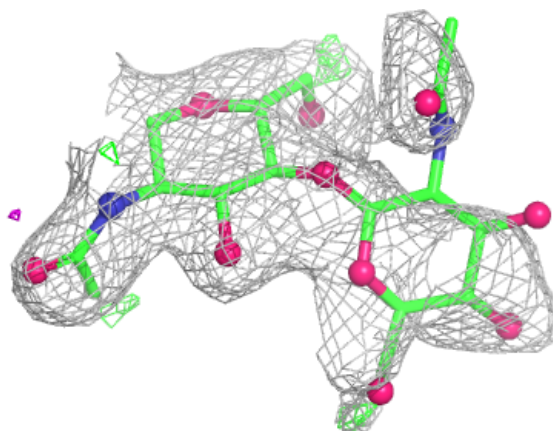
Electron density around Chain I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

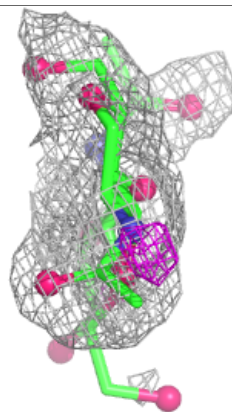
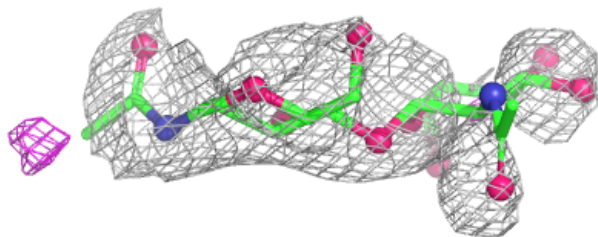
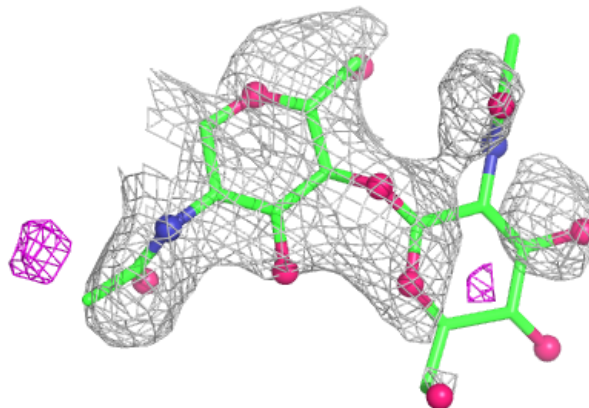


Electron density around Chain J:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain K:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	Q	301	5/5	0.61	0.15	91,91,97,102	0
5	SO4	F	301	5/5	0.62	0.13	81,86,92,100	0
5	SO4	N	301	5/5	0.64	0.16	80,84,96,98	0
5	SO4	L	301	5/5	0.72	0.12	77,79,90,93	0
5	SO4	C	601	5/5	0.80	0.21	62,62,80,80	0
5	SO4	D	601	5/5	0.86	0.16	66,69,82,82	0
5	SO4	A	601	5/5	0.89	0.13	48,53,69,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.