



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:36 PM UTC

PDB ID : 7ORA / pdb_00007ora
Title : Crystal structure of the T478K mutant receptor binding domain of SARS-CoV-2 Spike glycoprotein in complex with COVOX-45 and COVOX-253 Fabs
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2021-06-04
Resolution : 2.60 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

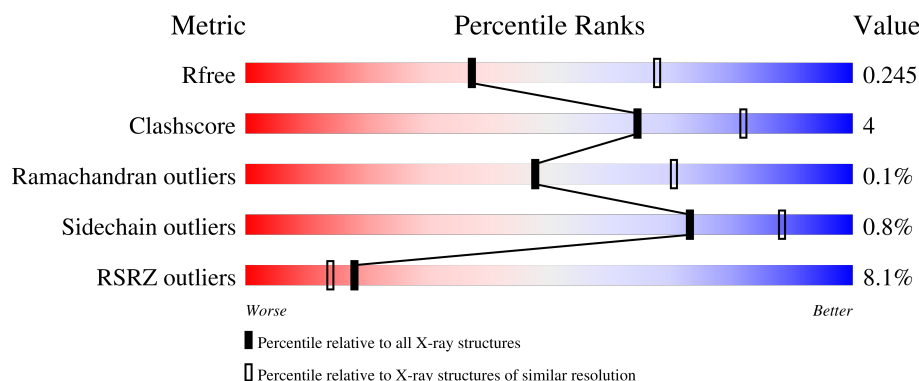
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	C	205	
1	R	205	
2	A	226	
2	D	226	
3	B	214	

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Mol	Chain	Length	Quality of chain
3	E	214	30% 92% 7%
4	F	228	% 86% 13%
4	H	228	88% 10%
5	G	215	3% 89% 10%
5	L	215	2% 88% 10%
6	I	2	50% 50%
7	J	3	100%
7	K	3	67% 33%
7	M	3	100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16719 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	R	197	Total	C	N	O	S	0	0	0
			1563	1001	264	290	8			
1	C	197	Total	C	N	O	S	0	0	0
			1563	1001	264	290	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	324	GLU	-	expression tag	UNP P0DTC2
R	325	THR	-	expression tag	UNP P0DTC2
R	326	GLY	-	expression tag	UNP P0DTC2
R	327	HIS	-	expression tag	UNP P0DTC2
R	328	HIS	-	expression tag	UNP P0DTC2
R	329	HIS	-	expression tag	UNP P0DTC2
R	330	HIS	-	expression tag	UNP P0DTC2
R	331	HIS	-	expression tag	UNP P0DTC2
R	332	HIS	-	expression tag	UNP P0DTC2
R	478	LYS	THR	engineered mutation	UNP P0DTC2
R	527	LYS	PRO	conflict	UNP P0DTC2
C	324	GLU	-	expression tag	UNP P0DTC2
C	325	THR	-	expression tag	UNP P0DTC2
C	326	GLY	-	expression tag	UNP P0DTC2
C	327	HIS	-	expression tag	UNP P0DTC2
C	328	HIS	-	expression tag	UNP P0DTC2
C	329	HIS	-	expression tag	UNP P0DTC2
C	330	HIS	-	expression tag	UNP P0DTC2
C	331	HIS	-	expression tag	UNP P0DTC2
C	332	HIS	-	expression tag	UNP P0DTC2
C	478	LYS	THR	engineered mutation	UNP P0DTC2
C	527	LYS	PRO	conflict	UNP P0DTC2

- Molecule 2 is a protein called COVOX-45 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	216	Total	C	N	O	S	0	0	0
			1631	1037	272	315	7			
2	D	216	Total	C	N	O	S	0	0	0
			1631	1037	272	315	7			

- Molecule 3 is a protein called COVOX-45 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	211	Total	C	N	O	S	0	0	0
			1623	1016	269	334	4			
3	E	211	Total	C	N	O	S	0	0	0
			1623	1016	269	334	4			

- Molecule 4 is a protein called COVOX-253 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	224	Total	C	N	O	S	0	0	0
			1681	1056	284	331	10			
4	H	224	Total	C	N	O	S	0	0	0
			1677	1053	283	331	10			

- Molecule 5 is a protein called COVOX-253 Fab light chain.

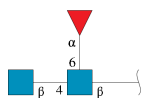
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	214	Total	C	N	O	S	0	0	0
			1628	1016	272	335	5			
5	L	214	Total	C	N	O	S	0	1	0
			1636	1021	275	335	5			

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



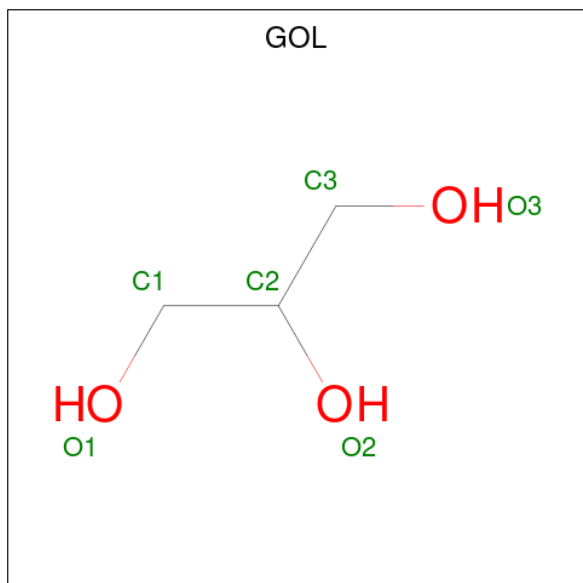
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
7	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
7	M	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	R	1	Total	C	O	0	0
			6	3	3		
8	R	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total 2	Cl 2	0	0
9	B	1	Total 1	Cl 1	0	0
9	F	2	Total 2	Cl 2	0	0
9	H	1	Total 1	Cl 1	0	0

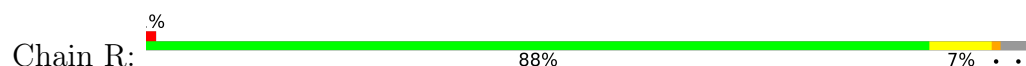
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	R	40	Total 40	O 40	0	0
10	A	31	Total 31	O 31	0	0
10	B	21	Total 21	O 21	0	0
10	F	32	Total 32	O 32	0	0
10	G	20	Total 20	O 20	0	0
10	C	33	Total 33	O 33	0	0
10	D	15	Total 15	O 15	0	0
10	E	19	Total 19	O 19	0	0
10	H	31	Total 31	O 31	0	0
10	L	41	Total 41	O 41	0	0

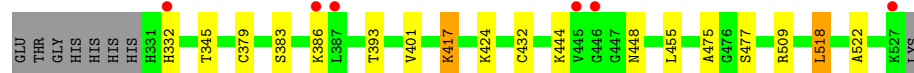
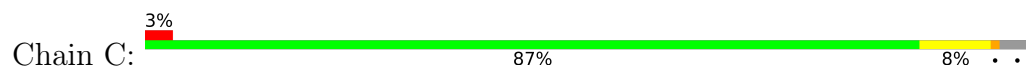
3 Residue-property plots [i](#)

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.

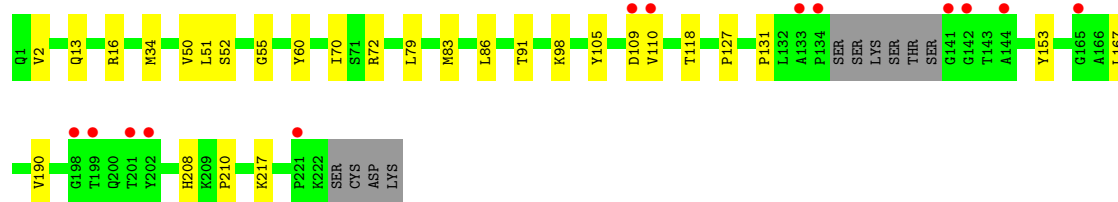
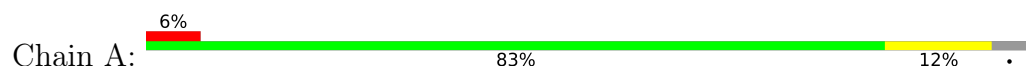
- Molecule 1: Spike protein S1



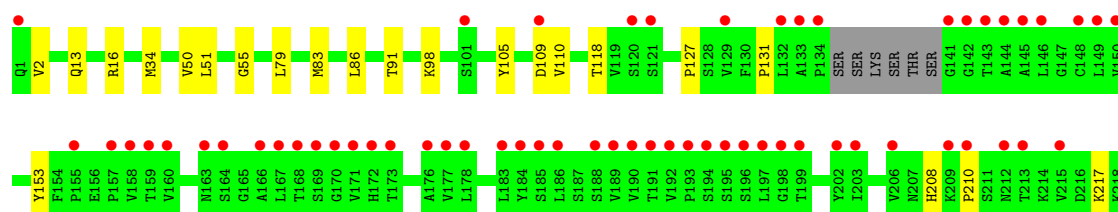
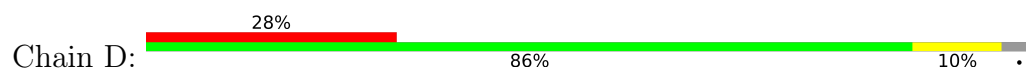
- Molecule 1: Spike protein S1

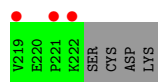


- Molecule 2: COVOX-45 Fab heavy chain

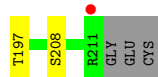
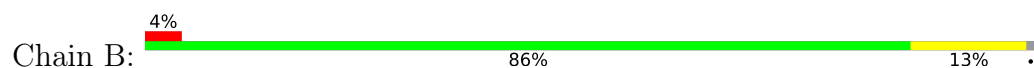


- Molecule 2: COVOX-45 Fab heavy chain

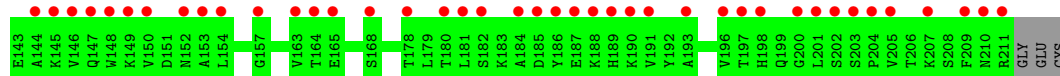
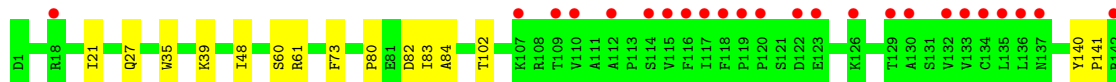
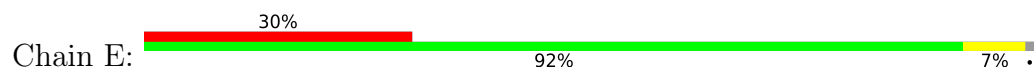




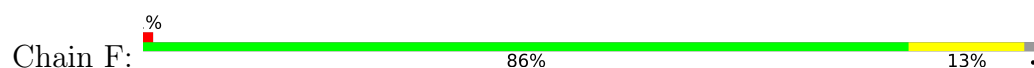
• Molecule 3: COVOX-45 Fab light chain



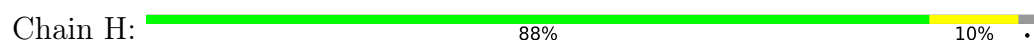
• Molecule 3: COVOX-45 Fab light chain



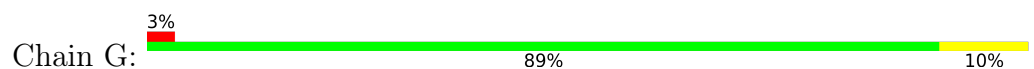
• Molecule 4: COVOX-253 Fab heavy chain



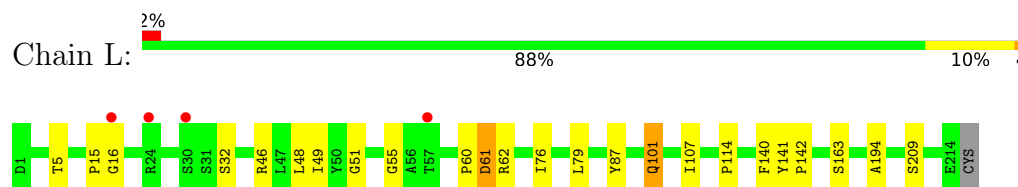
• Molecule 4: COVOX-253 Fab heavy chain



• Molecule 5: COVOX-253 Fab light chain



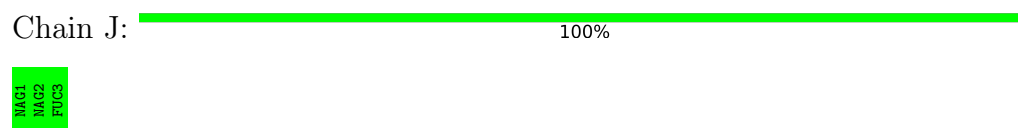
- Molecule 5: COVOX-253 Fab light chain



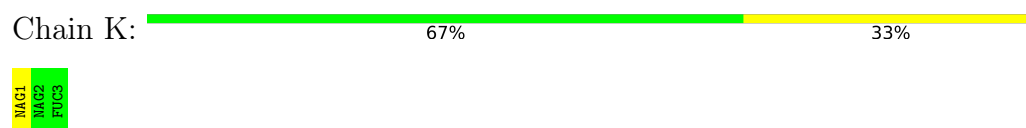
- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



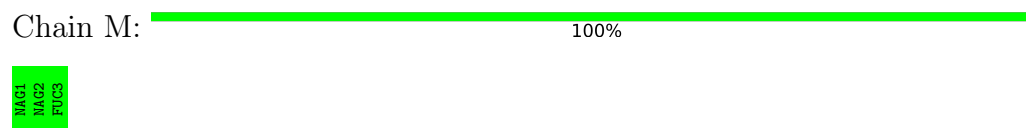
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.57Å 182.38Å 142.41Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	51.50 – 2.60 51.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.2 (51.50-2.60) 90.2 (51.50-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.204 , 0.245 0.205 , 0.245	Depositor DCC
R_{free} test set	3647 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16719	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

5.1 Standard geometry

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

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	C	0.09	0/1608	0.28	0/2187
1	R	0.09	0/1608	0.28	0/2187
2	A	0.09	0/1672	0.27	0/2276
2	D	0.09	0/1672	0.27	0/2276
3	B	0.09	0/1657	0.27	0/2254
3	E	0.08	0/1657	0.27	0/2254
4	F	0.11	0/1719	0.30	0/2342
4	H	0.11	0/1715	0.31	0/2338
5	G	0.09	0/1664	0.28	0/2259
5	L	0.11	0/1675	0.30	0/2273
All	All	0.10	0/16647	0.29	0/22646

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

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	C	1563	0	1474	15	0
1	R	1563	0	1474	13	0
2	A	1631	0	1596	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1631	0	1596	13	0
3	B	1623	0	1572	16	0
3	E	1623	0	1572	11	0
4	F	1681	0	1652	15	0
4	H	1677	0	1641	12	0
5	G	1628	0	1566	13	0
5	L	1636	0	1579	14	0
6	I	24	0	22	1	0
7	J	38	0	34	0	0
7	K	38	0	34	0	0
7	M	38	0	34	0	0
8	C	12	0	16	0	0
8	F	6	0	8	0	0
8	L	6	0	8	1	0
8	R	12	0	16	0	0
9	A	2	0	0	0	0
9	B	1	0	0	0	0
9	F	2	0	0	1	0
9	H	1	0	0	0	0
10	A	31	0	0	0	0
10	B	21	0	0	1	0
10	C	33	0	0	3	0
10	D	15	0	0	0	0
10	E	19	0	0	2	0
10	F	32	0	0	0	0
10	G	20	0	0	1	0
10	H	31	0	0	1	0
10	L	41	0	0	1	0
10	R	40	0	0	0	0
All	All	16719	0	15894	126	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 (126) 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:D:13:GLN:HB2	2:D:16:ARG:HD3	1.66	0.78
5:L:46:ARG:NH2	10:L:401:HOH:O	2.20	0.74
3:E:39:LYS:NZ	10:E:301:HOH:O	2.28	0.66
5:G:1:ASP:N	10:G:301:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:VAL:HG21	2:D:105:TYR:HB3	1.80	0.63
1:R:478:LYS:HG2	5:G:32:SER:HB3	1.80	0.62
4:F:100:HIS:HB3	4:F:112:ILE:HD11	1.82	0.61
2:A:13:GLN:HB2	2:A:16:ARG:HG3	1.82	0.60
2:A:127:PRO:HB3	2:A:153:TYR:HB3	1.83	0.60
3:E:61:ARG:NH1	3:E:82:ASP:OD2	2.35	0.60
3:B:103:LYS:NZ	10:B:406:HOH:O	2.34	0.60
4:F:203:THR:OG1	4:F:220:LYS:NZ	2.27	0.59
5:G:61:ASP:OD1	5:G:61:ASP:N	2.34	0.59
1:C:444:LYS:HD2	1:C:448:ASN:HA	1.85	0.59
2:A:50:VAL:HG21	2:A:105:TYR:HB3	1.85	0.59
4:H:100:HIS:HB3	4:H:112:ILE:HD11	1.83	0.58
5:L:61:ASP:OD1	5:L:61:ASP:N	2.33	0.58
2:A:34:MET:HB3	2:A:79:LEU:HD22	1.86	0.57
1:C:509:ARG:NH1	10:C:803:HOH:O	2.32	0.57
4:H:38:ARG:HB3	4:H:48:ILE:HD11	1.85	0.57
2:A:131:PRO:HD3	2:A:217:LYS:HE2	1.87	0.56
2:D:131:PRO:HD3	2:D:217:LYS:HE2	1.86	0.56
1:C:383:SER:HB3	1:C:386:LYS:HG2	1.88	0.56
2:A:51:LEU:HD11	2:A:55:GLY:HA2	1.88	0.56
2:A:83:MET:HB3	2:A:86:LEU:HD21	1.87	0.55
2:D:127:PRO:HB3	2:D:153:TYR:HB3	1.89	0.54
5:G:40:LYS:NZ	5:G:82:GLU:O	2.34	0.54
1:R:383:SER:HB3	1:R:386:LYS:HG2	1.89	0.54
2:D:2:VAL:HB	2:D:110:VAL:HG21	1.90	0.53
4:H:210:HIS:ND1	4:H:213:SER:OG	2.38	0.53
5:L:49:ILE:HD13	5:L:55:GLY:HA2	1.89	0.53
5:G:38:GLN:HB2	5:G:48:LEU:HD11	1.91	0.53
3:B:39:LYS:HG3	3:B:84:ALA:HB2	1.89	0.53
4:F:174:HIS:ND1	9:F:403:CL:CL	2.75	0.52
3:E:21:ILE:HG21	3:E:102:THR:HG21	1.91	0.52
4:H:41:ARG:NH2	10:H:402:HOH:O	2.41	0.52
4:F:210:HIS:ND1	4:F:213:SER:OG	2.41	0.52
2:A:167:LEU:HD21	2:A:190:VAL:HG21	1.92	0.52
3:B:35:TRP:CE2	3:B:73:PHE:HB2	2.45	0.52
1:R:393:THR:HA	1:R:522:ALA:HA	1.92	0.51
1:R:383:SER:HB3	1:R:386:LYS:HE2	1.92	0.51
1:R:342:PHE:HB2	6:I:1:NAG:H82	1.92	0.50
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.94	0.50
3:E:39:LYS:HG3	3:E:84:ALA:HB2	1.93	0.50
5:L:16:GLY:N	5:L:79:LEU:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:MET:HB3	2:D:79:LEU:HD22	1.93	0.49
5:G:6:GLN:O	5:G:101:GLN:NE2	2.45	0.49
1:C:518:LEU:HD21	2:D:98:LYS:NZ	2.26	0.49
4:H:129:PRO:HB3	4:H:155:TYR:HB3	1.93	0.49
1:R:518:LEU:HD21	2:A:98:LYS:NZ	2.28	0.49
1:C:383:SER:HB3	1:C:386:LYS:HE2	1.94	0.49
5:L:163:SER:HB3	8:L:301:GOL:H31	1.95	0.49
4:F:129:PRO:HB3	4:F:155:TYR:HB3	1.96	0.48
5:G:2:ILE:HD13	5:G:29:VAL:HG12	1.96	0.48
3:E:35:TRP:CE2	3:E:73:PHE:HB2	2.49	0.47
3:B:46:LEU:HD21	3:B:49:TYR:HB3	1.95	0.47
5:G:19:ALA:HB3	5:G:76:ILE:HB	1.97	0.47
3:E:27:GLN:NE2	10:E:303:HOH:O	2.47	0.47
1:C:455:LEU:HD21	4:H:54:GLY:C	2.40	0.47
4:H:11:VAL:HG21	4:H:157:PRO:HG3	1.97	0.46
1:C:417:LYS:HE3	1:C:455:LEU:HD12	1.96	0.46
5:G:49:ILE:HD13	5:G:55:GLY:HA2	1.98	0.46
4:H:73:ASP:HB3	4:H:76:THR:HG22	1.97	0.46
4:F:161:THR:HG23	4:F:209:ASN:HB3	1.98	0.45
1:R:478:LYS:N	1:R:478:LYS:HD2	2.31	0.45
2:D:51:LEU:HD11	2:D:55:GLY:HA2	1.98	0.45
3:B:15:VAL:HG11	3:E:60:SER:HB2	1.98	0.45
4:F:91:THR:HG23	4:F:120:THR:HA	1.98	0.45
5:G:8:PRO:HG3	5:G:11:LEU:HD13	1.98	0.45
1:C:379:CYS:HA	1:C:432:CYS:HA	1.99	0.45
5:L:60:PRO:HB2	5:L:62:ARG:HG2	1.99	0.45
3:B:54:LEU:HD21	3:B:60:SER:HA	1.99	0.45
5:L:5:THR:HA	5:L:101:GLN:OE1	2.17	0.45
1:R:331:HIS:O	1:R:332:HIS:ND1	2.49	0.44
2:A:208:HIS:CD2	2:A:210:PRO:HD2	2.51	0.44
1:R:475:ALA:O	4:F:106:CYS:N	2.48	0.44
4:F:60:TYR:HE1	4:F:70:ILE:HG13	1.83	0.44
1:R:401:VAL:HG22	1:R:509:ARG:HG2	2.00	0.44
1:C:345:THR:O	10:C:801:HOH:O	2.21	0.43
4:H:161:THR:HG23	4:H:209:ASN:HB3	2.00	0.43
1:R:334:ASN:N	1:R:334:ASN:OD1	2.51	0.43
4:F:73:ASP:HB3	4:F:76:THR:HG22	1.99	0.43
2:D:208:HIS:CD2	2:D:210:PRO:HD2	2.53	0.43
5:L:114:PRO:HB3	5:L:140:PHE:CD2	2.53	0.43
1:C:475:ALA:O	4:H:106:CYS:N	2.50	0.43
5:L:101:GLN:H	5:L:101:GLN:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:194:ALA:HB2	5:L:209:SER:HB3	2.01	0.43
3:B:115:VAL:HA	3:B:135:LEU:O	2.19	0.43
2:D:91:THR:HG23	2:D:118:THR:HA	1.99	0.43
3:B:37:GLN:HB2	3:B:47:LEU:HD11	2.00	0.43
3:B:21:ILE:HG21	3:B:102:THR:HG21	2.01	0.43
5:L:48:LEU:HD11	5:L:87:TYR:HE2	1.83	0.43
3:E:80:PRO:O	3:E:83:ILE:HD12	2.19	0.42
1:C:393:THR:HA	1:C:522:ALA:HA	2.01	0.42
3:E:140:TYR:CG	3:E:141:PRO:HA	2.55	0.42
1:R:417:LYS:HD3	1:R:417:LYS:HA	1.64	0.42
2:A:52:SER:O	2:A:72:ARG:NH1	2.51	0.42
3:E:35:TRP:HB2	3:E:48:ILE:HB	2.00	0.42
4:H:194:VAL:HG11	4:H:204:TYR:CE1	2.54	0.42
1:C:424:LYS:HD3	10:C:819:HOH:O	2.19	0.41
4:F:50:TRP:CD1	4:F:59:ASN:HB2	2.55	0.41
1:C:477:SER:OG	4:H:108:ASP:OD2	2.37	0.41
2:D:34:MET:HE1	2:D:98:LYS:HG3	2.01	0.41
1:C:401:VAL:HG22	1:C:509:ARG:HG2	2.01	0.41
5:L:15:PRO:HD3	5:L:107:ILE:HG23	2.02	0.41
2:A:2:VAL:HB	2:A:110:VAL:HG21	2.03	0.41
3:B:47:LEU:HA	3:B:58:VAL:HG21	2.01	0.41
5:L:32:SER:HA	5:L:51:GLY:HA2	2.02	0.41
3:B:145:LYS:HB3	3:B:197:THR:OG1	2.21	0.41
3:E:140:TYR:CD1	3:E:141:PRO:HA	2.56	0.41
4:F:64:PHE:HB3	4:F:68:VAL:CG2	2.51	0.41
5:L:141:TYR:CG	5:L:142:PRO:HA	2.56	0.41
1:R:379:CYS:SG	1:R:384:PRO:HB3	2.60	0.41
4:F:193:THR:HG21	5:G:138:ASN:ND2	2.36	0.41
2:A:60:TYR:CZ	2:A:70:ILE:HG22	2.56	0.41
3:B:80:PRO:O	3:B:83:ILE:HD12	2.20	0.40
3:B:183:LYS:O	3:B:187:GLU:HG2	2.21	0.40
4:F:38:ARG:HB3	4:F:48:ILE:HD11	2.02	0.40
5:G:36:TRP:CE2	5:G:74:LEU:HB2	2.56	0.40
5:G:121:PRO:HD3	5:G:133:VAL:HG22	2.02	0.40
2:A:91:THR:HG23	2:A:118:THR:HA	2.02	0.40
1:C:518:LEU:HD21	2:D:98:LYS:HZ2	1.86	0.40
3:B:35:TRP:HB2	3:B:48:ILE:HB	2.02	0.40
3:B:45:LYS:HD3	3:B:45:LYS:HA	1.86	0.40
3:B:193:ALA:HB2	3:B:208:SER:HB3	2.04	0.40
4:F:164:TRP:CH2	4:F:206:CYS:HB3	2.56	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	C	195/205 (95%)	186 (95%)	9 (5%)	0	100	100
1	R	195/205 (95%)	186 (95%)	9 (5%)	0	100	100
2	A	212/226 (94%)	204 (96%)	7 (3%)	1 (0%)	24	46
2	D	212/226 (94%)	203 (96%)	8 (4%)	1 (0%)	24	46
3	B	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
3	E	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
4	F	220/228 (96%)	212 (96%)	8 (4%)	0	100	100
4	H	220/228 (96%)	211 (96%)	9 (4%)	0	100	100
5	G	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
5	L	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
All	All	2097/2176 (96%)	2013 (96%)	82 (4%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	109	ASP
2	D	109	ASP

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	C	169/177 (96%)	166 (98%)	3 (2%)	51	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	169/177 (96%)	167 (99%)	2 (1%)	63	83
2	A	179/189 (95%)	179 (100%)	0	100	100
2	D	179/189 (95%)	179 (100%)	0	100	100
3	B	186/188 (99%)	185 (100%)	1 (0%)	81	92
3	E	186/188 (99%)	186 (100%)	0	100	100
4	F	193/196 (98%)	191 (99%)	2 (1%)	68	86
4	H	192/196 (98%)	189 (98%)	3 (2%)	55	79
5	G	183/184 (100%)	182 (100%)	1 (0%)	81	92
5	L	184/184 (100%)	181 (98%)	3 (2%)	55	79
All	All	1820/1868 (97%)	1805 (99%)	15 (1%)	73	88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	417	LYS
1	R	518	LEU
3	B	11	LEU
4	F	4	LEU
4	F	89	GLU
5	G	61	ASP
1	C	332	HIS
1	C	417	LYS
1	C	518	LEU
4	H	89	GLU
4	H	203	THR
4	H	214	ASN
5	L	61	ASP
5	L	76	ILE
5	L	101	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	39	GLN
2	A	172	HIS
3	B	38	GLN
3	B	53	ASN
3	B	160	GLN

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Mol	Chain	Res	Type
4	F	1	GLN
4	F	3	GLN
4	F	62	GLN
4	F	202	GLN
1	C	354	ASN
2	D	13	GLN
3	E	27	GLN
3	E	53	ASN
3	E	79	GLN
4	H	43	GLN
4	H	202	GLN
5	L	148	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

11 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	I	1	1,6	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
6	FUC	I	2	6	10,10,11	0.73	0	14,14,16	0.69	0
7	NAG	J	1	7,4	14,14,15	0.21	0	17,19,21	0.48	0
7	NAG	J	2	7	14,14,15	0.32	0	17,19,21	0.37	0
7	FUC	J	3	7	10,10,11	0.79	0	14,14,16	0.83	0
7	NAG	K	1	1,7	14,14,15	0.30	0	17,19,21	0.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	K	2	7	14,14,15	0.32	0	17,19,21	0.41	0
7	FUC	K	3	7	10,10,11	0.76	0	14,14,16	0.67	0
7	NAG	M	1	7,4	14,14,15	0.33	0	17,19,21	0.60	0
7	NAG	M	2	7	14,14,15	0.30	0	17,19,21	0.38	0
7	FUC	M	3	7	10,10,11	0.74	0	14,14,16	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	FUC	I	2	6	-	-	0/1/1/1
7	NAG	J	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	FUC	J	3	7	-	-	0/1/1/1
7	NAG	K	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	FUC	K	3	7	-	-	0/1/1/1
7	NAG	M	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	2/6/23/26	0/1/1/1
7	FUC	M	3	7	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	1	NAG	C1-O5-C5	2.45	115.47	112.19
6	I	1	NAG	C1-O5-C5	2.43	115.45	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	2	NAG	O5-C5-C6-O6
7	M	2	NAG	O5-C5-C6-O6
7	M	2	NAG	C4-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6

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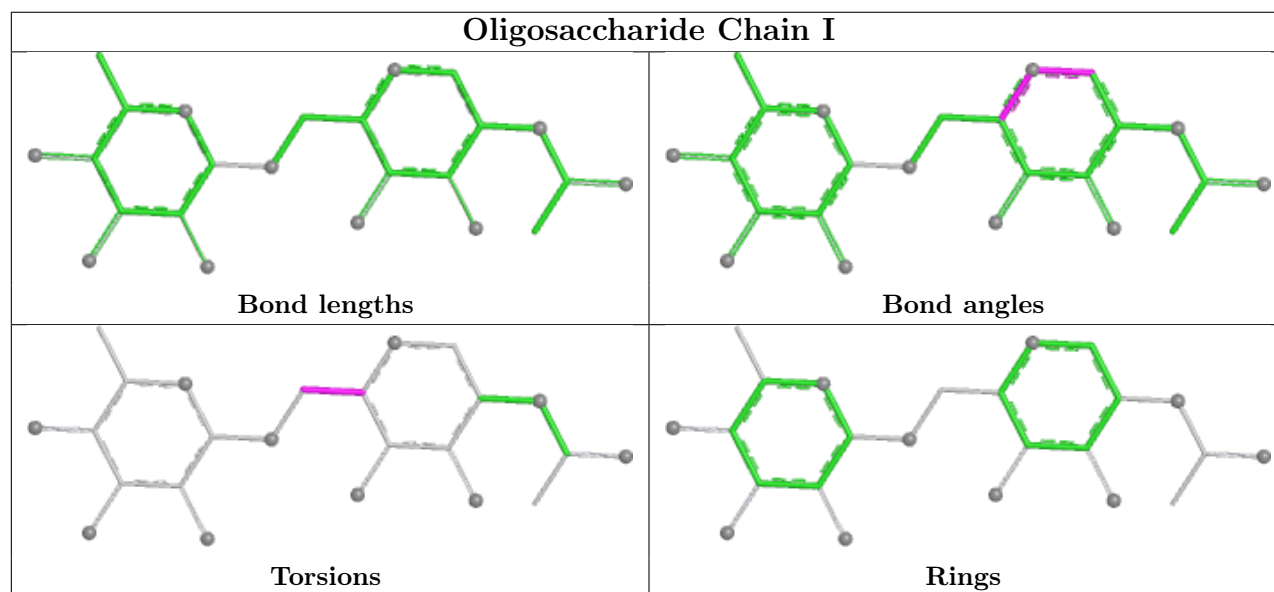
Mol	Chain	Res	Type	Atoms
6	I	1	NAG	C4-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6
7	K	1	NAG	O5-C5-C6-O6

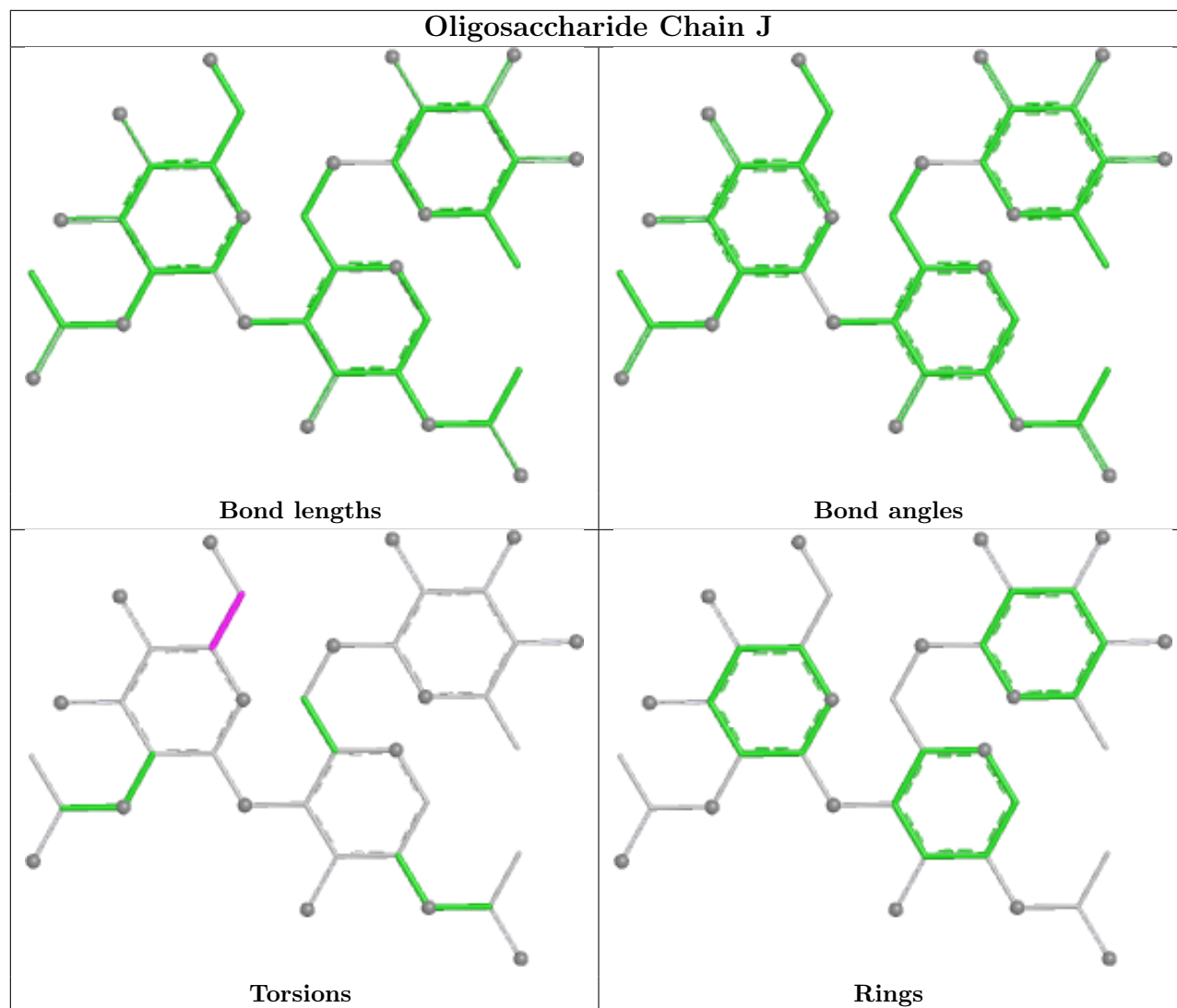
There are no ring outliers.

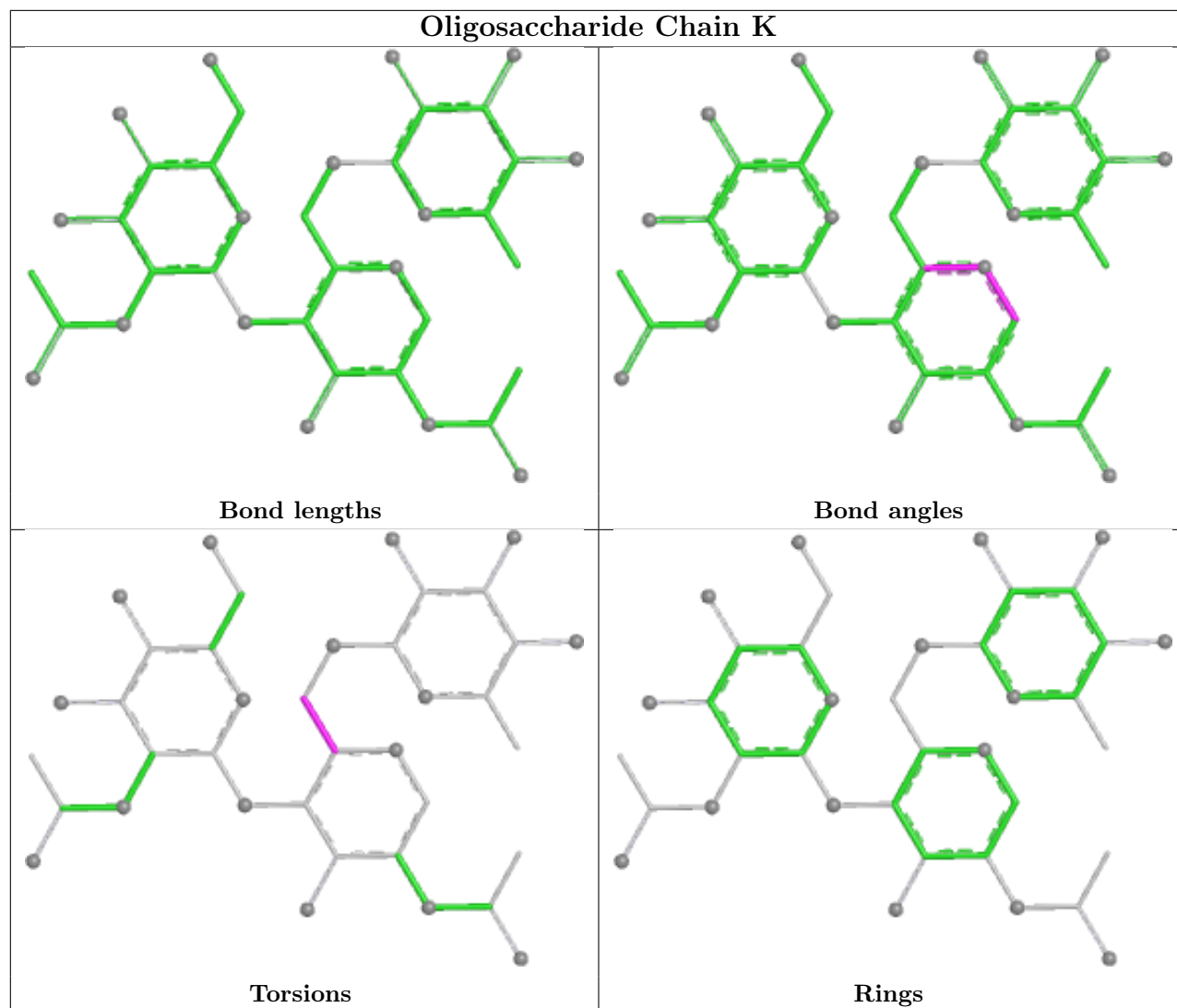
1 monomer is involved in 1 short contact:

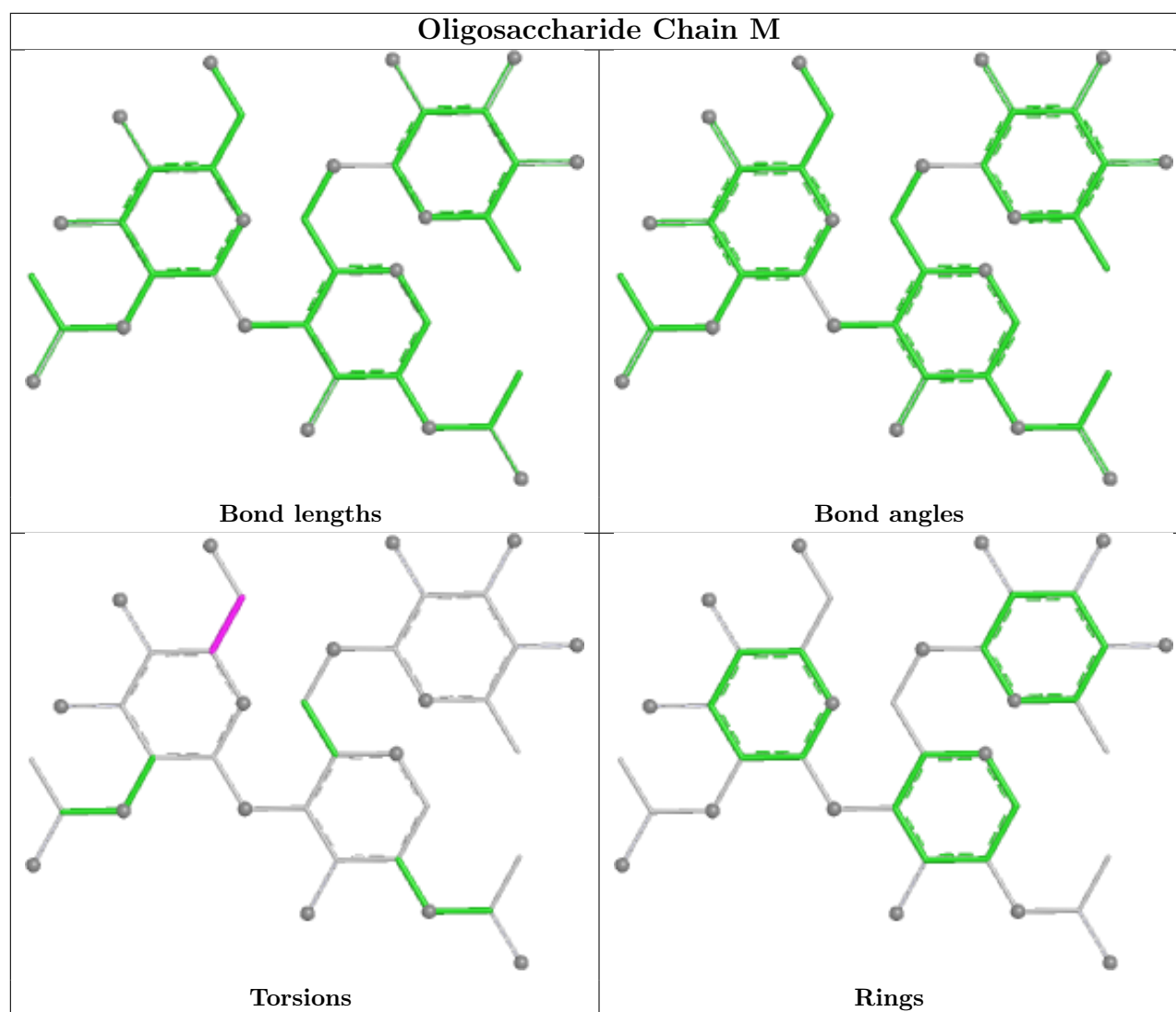
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	1	0

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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	GOL	R	702	-	5,5,5	0.90	0	5,5,5	1.10	0
8	GOL	C	701	-	5,5,5	0.71	0	5,5,5	1.22	0
8	GOL	R	701	-	5,5,5	0.72	0	5,5,5	1.21	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	C	702	-	5,5,5	0.92	0	5,5,5	1.08	0
8	GOL	L	301	-	5,5,5	0.73	0	5,5,5	1.19	1 (20%)
8	GOL	F	401	-	5,5,5	0.74	0	5,5,5	1.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	R	702	-	-	0/4/4/4	-
8	GOL	C	701	-	-	4/4/4/4	-
8	GOL	R	701	-	-	0/4/4/4	-
8	GOL	C	702	-	-	0/4/4/4	-
8	GOL	L	301	-	-	2/4/4/4	-
8	GOL	F	401	-	-	1/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	301	GOL	C3-C2-C1	-2.14	103.93	111.80
8	R	701	GOL	C3-C2-C1	-2.13	103.99	111.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	701	GOL	C1-C2-C3-O3
8	C	701	GOL	O1-C1-C2-C3
8	L	301	GOL	O1-C1-C2-C3
8	F	401	GOL	O2-C2-C3-O3
8	C	701	GOL	O1-C1-C2-O2
8	C	701	GOL	O2-C2-C3-O3
8	L	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	301	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	C	197/205 (96%)	0.07	6 (3%) 52 47	28, 47, 81, 106	0
1	R	197/205 (96%)	-0.11	3 (1%) 72 68	26, 43, 73, 126	0
2	A	216/226 (95%)	0.41	13 (6%) 27 22	29, 55, 149, 201	0
2	D	216/226 (95%)	0.96	63 (29%) 1 1	30, 68, 178, 231	0
3	B	211/214 (98%)	0.34	8 (3%) 44 38	30, 62, 141, 183	0
3	E	211/214 (98%)	1.09	65 (30%) 1 1	33, 102, 226, 250	0
4	F	224/228 (98%)	0.01	3 (1%) 75 71	31, 51, 75, 121	0
4	H	224/228 (98%)	-0.22	0 100 100	29, 40, 70, 103	0
5	G	214/215 (99%)	0.11	6 (2%) 55 49	33, 59, 95, 128	0
5	L	214/215 (99%)	-0.12	4 (1%) 66 61	27, 43, 66, 90	1 (0%)
All	All	2124/2176 (97%)	0.25	171 (8%) 18 14	26, 50, 167, 250	1 (0%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	192	VAL	4.7
3	E	191	VAL	4.7
3	E	190	LYS	4.4
3	E	134	CYS	4.2
2	A	134	PRO	3.9
3	E	186	TYR	3.9
3	B	184	ALA	3.8
2	D	160	VAL	3.8
3	E	133	VAL	3.8
1	R	331	HIS	3.7
3	E	203	SER	3.7
3	E	116	PHE	3.6
2	D	134	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
3	E	180	THR	3.6
2	D	206	VAL	3.5
3	E	135	LEU	3.5
2	D	222	LYS	3.5
2	A	141	GLY	3.5
3	E	144	ALA	3.4
2	D	194	SER	3.3
1	C	527	LYS	3.3
3	E	146	VAL	3.3
2	D	145	ALA	3.3
3	B	191	VAL	3.3
2	D	141	GLY	3.2
2	D	129	VAL	3.2
2	A	142	GLY	3.2
2	D	133	ALA	3.2
2	A	110	VAL	3.2
3	E	142	ARG	3.1
3	E	197	THR	3.1
3	E	184	ALA	3.1
2	D	177	VAL	3.1
3	E	152	ASN	3.0
3	E	119	PRO	3.0
2	D	173	THR	3.0
3	E	178	THR	3.0
5	G	31	SER	2.9
2	A	199	THR	2.9
2	D	149	LEU	2.9
3	E	149	LYS	2.9
2	D	101	SER	2.9
1	C	446	GLY	2.9
2	D	120	SER	2.9
3	E	132	VAL	2.9
3	E	210	ASN	2.8
2	D	142	GLY	2.8
3	E	145	LYS	2.8
4	F	201	THR	2.8
2	D	183	LEU	2.8
2	D	203	ILE	2.8
2	D	109	ASP	2.8
1	R	332	HIS	2.8
3	E	181	LEU	2.8
2	D	209	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	190	VAL	2.7
2	D	199	THR	2.7
2	D	166	ALA	2.7
2	D	189	VAL	2.7
3	E	118	PHE	2.7
2	D	176	ALA	2.7
2	A	133	ALA	2.6
2	D	215	VAL	2.6
3	E	130	ALA	2.6
2	A	201	THR	2.6
2	D	132	LEU	2.6
2	D	167	LEU	2.6
3	B	152	ASN	2.6
2	D	195	SER	2.6
2	D	213	THR	2.6
2	A	202	TYR	2.6
2	D	184	TYR	2.6
1	C	445	VAL	2.6
2	D	163	ASN	2.6
5	L	57	THR	2.6
2	D	202	TYR	2.6
3	E	165	GLU	2.6
2	D	185	SER	2.5
2	D	188	SER	2.5
3	E	187	GLU	2.5
3	E	157	GLY	2.5
2	D	191	THR	2.5
2	D	121	SER	2.5
2	D	193	PRO	2.5
3	E	107	LYS	2.5
3	E	198	HIS	2.5
3	E	196	VAL	2.5
3	E	148	TRP	2.5
5	G	155	LEU	2.4
3	E	163	VAL	2.4
3	E	129	THR	2.4
2	D	146	LEU	2.4
3	E	136	LEU	2.4
3	E	201	LEU	2.4
2	D	171	VAL	2.4
3	E	154	LEU	2.4
2	A	109	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	198	GLY	2.4
2	D	221	PRO	2.4
3	E	153	ALA	2.4
2	D	197	LEU	2.4
3	B	181	LEU	2.4
2	D	210	PRO	2.4
5	G	15	PRO	2.4
2	A	144	ALA	2.4
5	G	32	SER	2.3
3	E	147	GLN	2.3
3	E	200	GLY	2.3
4	F	1	GLN	2.3
2	D	158	VAL	2.3
3	E	205	VAL	2.3
3	E	188	LYS	2.3
3	E	168	SER	2.3
3	E	120	PRO	2.3
3	B	150	VAL	2.3
2	D	178	LEU	2.3
2	D	144	ALA	2.3
3	E	207	LYS	2.3
3	E	114	SER	2.3
2	D	186	LEU	2.3
1	C	332	HIS	2.2
3	E	150	VAL	2.2
5	G	214	GLU	2.2
1	R	334	ASN	2.2
2	D	155	PRO	2.2
2	D	157	PRO	2.2
2	A	198	GLY	2.2
2	D	164	SER	2.2
5	L	16	GLY	2.2
5	G	79	LEU	2.2
4	F	141	THR	2.2
1	C	386	LYS	2.2
2	D	148	CYS	2.2
3	E	112	ALA	2.1
3	E	193	ALA	2.1
3	E	18	ARG	2.1
3	E	211	ARG	2.1
2	D	1	GLN	2.1
3	E	137	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	196	SER	2.1
3	E	109	THR	2.1
3	B	188	LYS	2.1
3	E	115	VAL	2.1
3	E	117	ILE	2.1
2	D	169	SER	2.1
3	E	209	PHE	2.1
3	E	126	LYS	2.1
1	C	387	LEU	2.1
3	B	154	LEU	2.1
3	E	202	SER	2.1
3	E	123	GLU	2.1
2	D	143	THR	2.1
2	D	159	THR	2.1
3	E	164	THR	2.1
2	D	170	GLY	2.1
3	E	110	VAL	2.1
3	B	211	ARG	2.0
5	L	24[A]	ARG	2.0
5	L	30	SER	2.0
2	A	221	PRO	2.0
2	D	212	ASN	2.0
2	D	219	VAL	2.0
3	E	122	ASP	2.0
3	E	185	ASP	2.0
3	E	182	SER	2.0
2	D	168	THR	2.0
3	E	204	PRO	2.0
2	D	172	HIS	2.0
3	E	189	HIS	2.0
2	A	165	GLY	2.0
2	D	150	VAL	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.

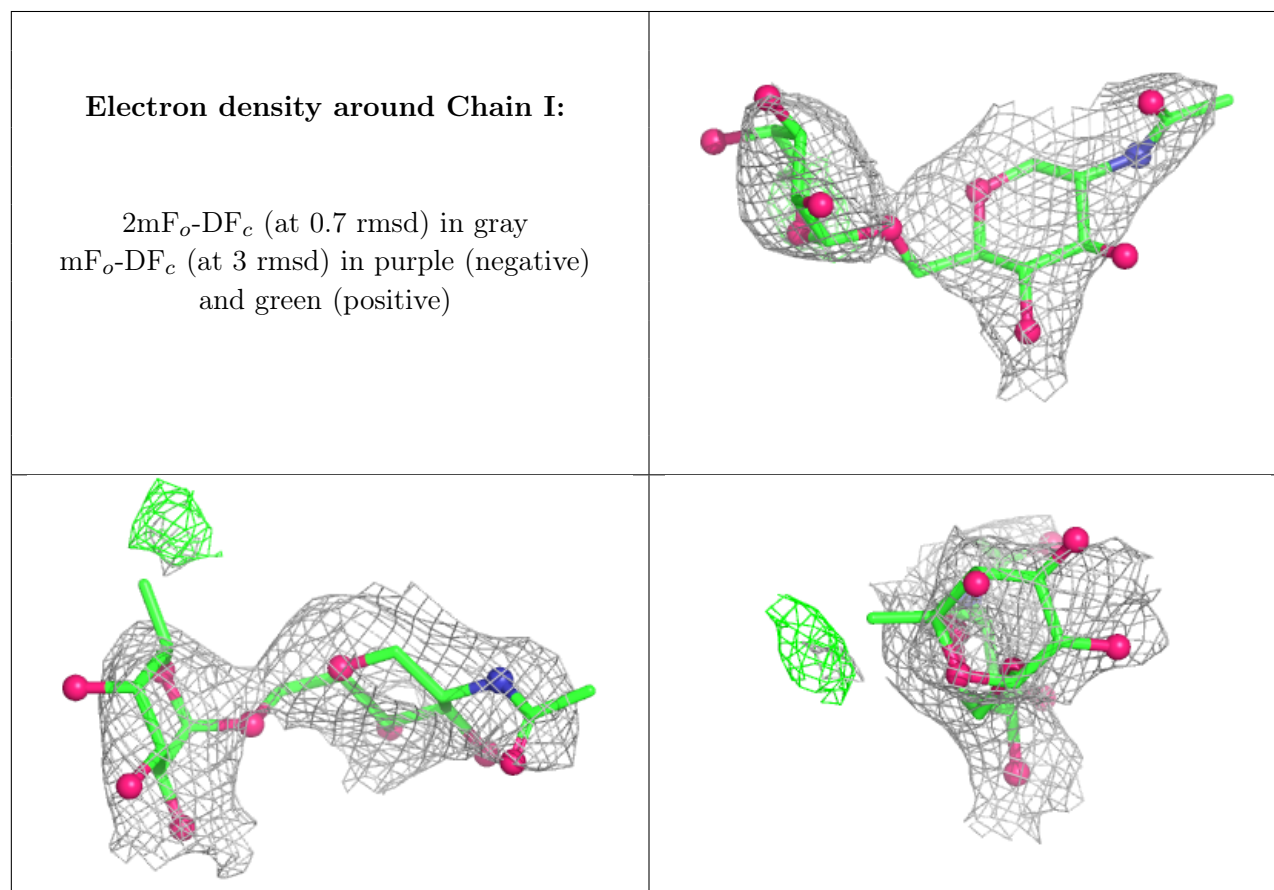
6.3 Carbohydrates [i](#)

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.

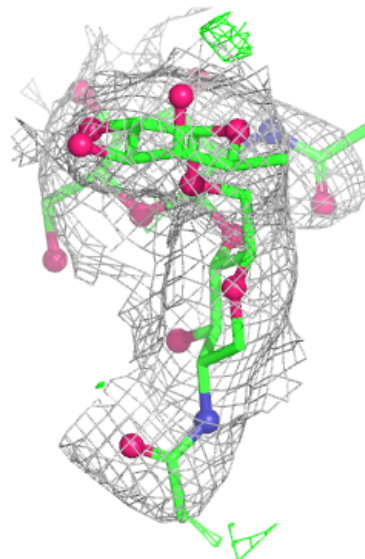
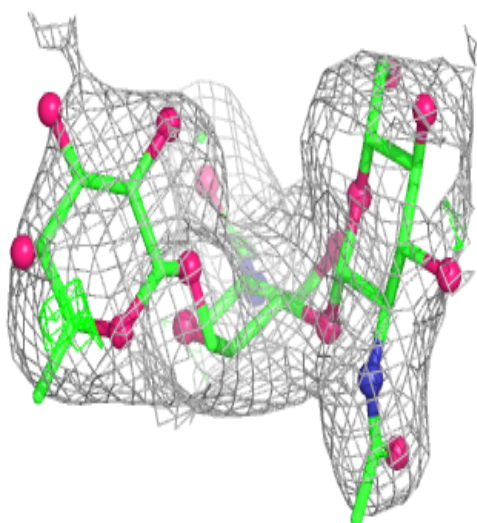
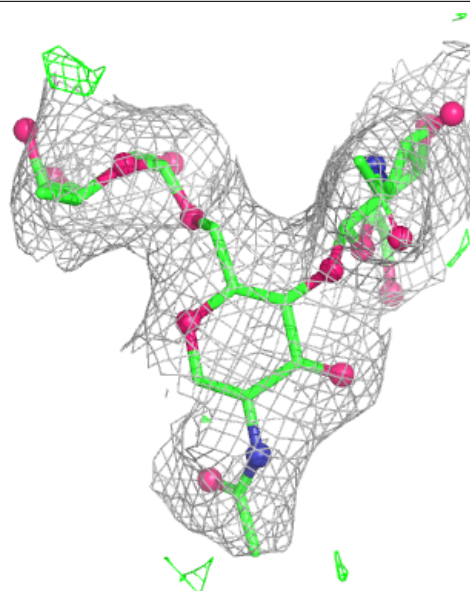
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	I	1	14/15	-	-	61,81,100,105	0
6	FUC	I	2	10/11	-	-	97,111,114,116	0
7	NAG	J	1	14/15	-	-	67,75,84,87	0
7	NAG	J	2	14/15	-	-	83,93,101,106	0
7	FUC	J	3	10/11	-	-	67,81,85,88	0
7	FUC	M	3	10/11	0.46	0.17	64,69,87,94	0
7	NAG	K	2	14/15	-	-	88,98,111,117	0
7	FUC	K	3	10/11	-	-	87,97,109,121	0
7	NAG	M	2	14/15	0.62	0.17	85,99,110,111	0
7	NAG	K	1	14/15	0.78	0.14	46,75,92,96	0
7	NAG	M	1	14/15	0.81	0.11	69,81,88,97	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.



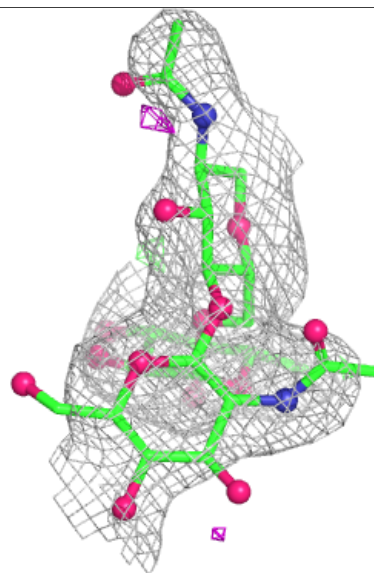
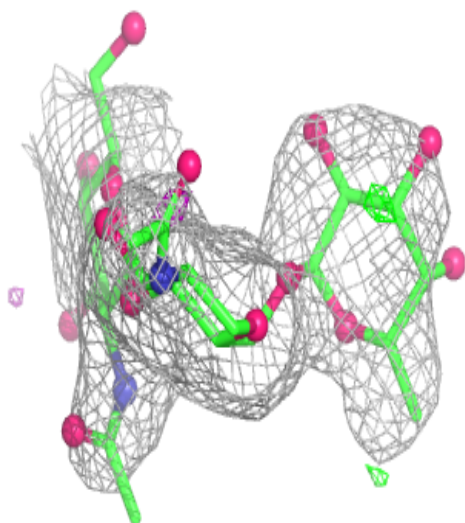
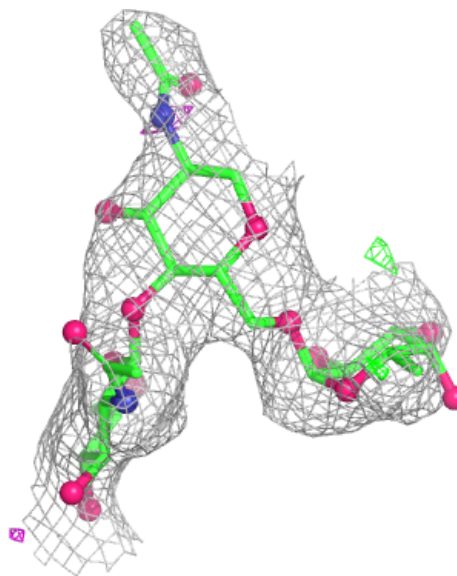
Electron density around Chain J:

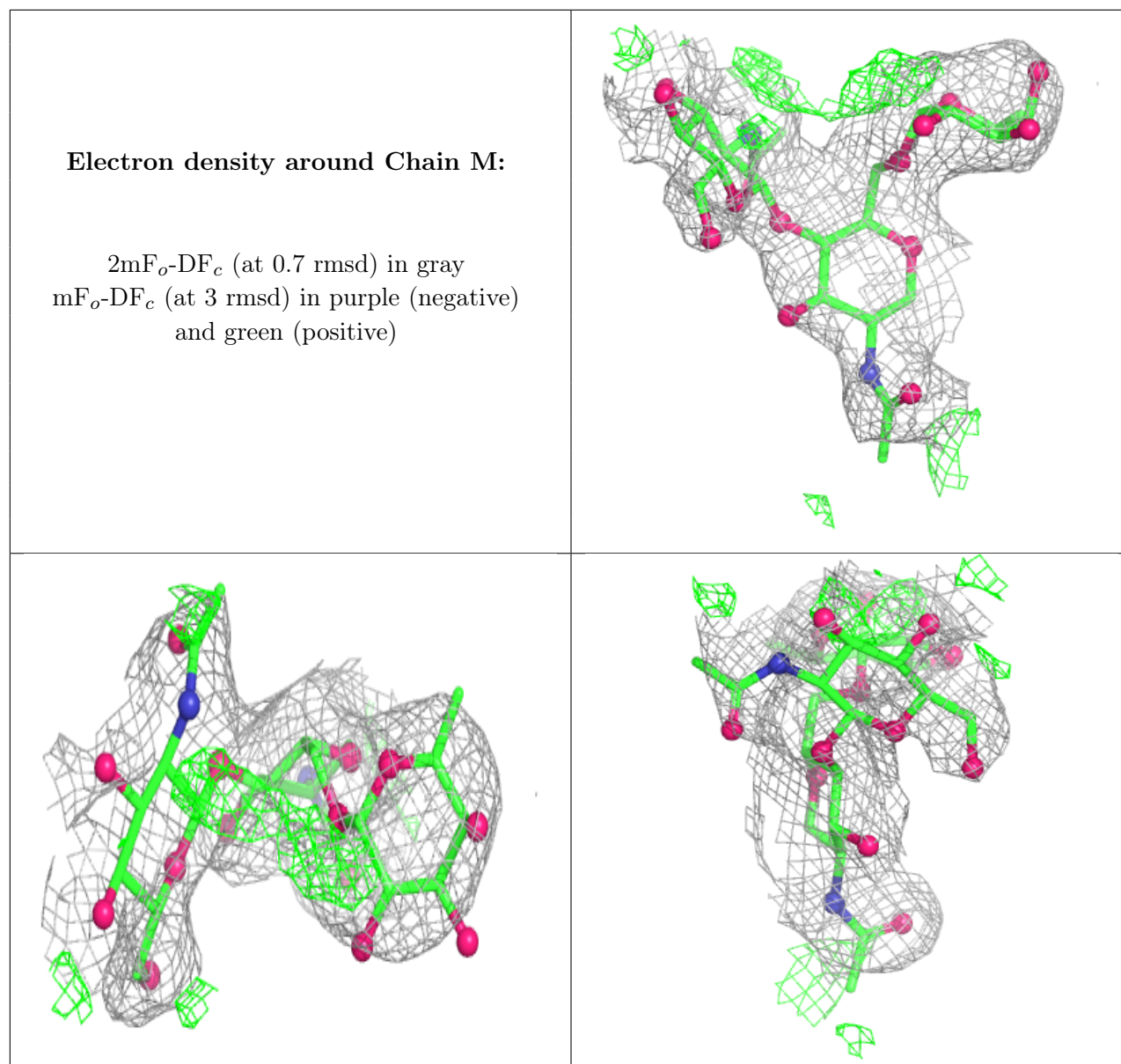
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(Å ²)	Q<0.9
8	GOL	F	401	6/6	0.84	0.17	53,57,62,65	0
8	GOL	R	701	6/6	0.85	0.15	53,64,68,74	0
8	GOL	C	701	6/6	0.88	0.14	60,66,70,70	0
8	GOL	C	702	6/6	0.91	0.10	43,46,55,58	0
8	GOL	L	301	6/6	0.91	0.13	44,46,50,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CL	A	301	1/1	0.91	0.07	62,62,62,62	0
9	CL	A	302	1/1	0.91	0.14	72,72,72,72	0
8	GOL	R	702	6/6	0.93	0.09	42,44,52,55	0
9	CL	F	403	1/1	0.93	0.07	68,68,68,68	0
9	CL	B	301	1/1	0.96	0.08	61,61,61,61	0
9	CL	H	301	1/1	0.98	0.07	41,41,41,41	0
9	CL	F	402	1/1	0.99	0.04	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.