Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 09:33 PM EDT

PDB ID	:	7UZC
Title	:	Structure of the SARS-CoV-2 RBD in complex with the mouse antibody Fab fragment, M8a-34
Authors	:	Fan, C.; Bjorkman, P.J.
Deposited on	:	2022-05-08
Resolution	:	2.20 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:

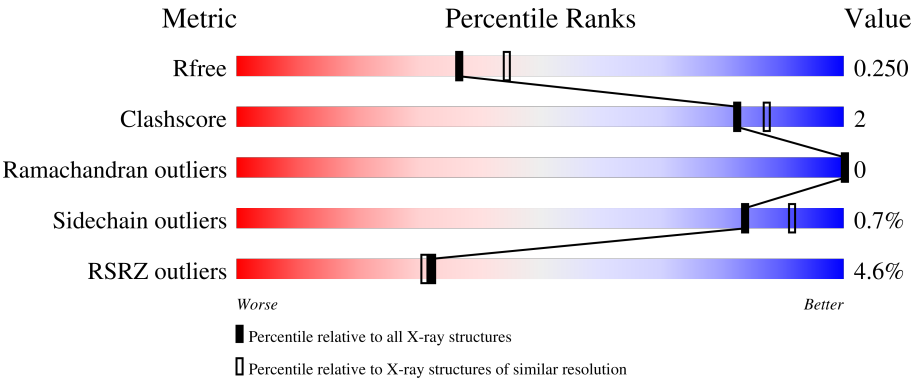
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	231	7% 75% 10% 15%
1	B	231	3% 77% 8% 15%
2	E	235	9% 90% 6% .
2	H	235	4% 89% 6% .
3	F	218	2% 95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	218	94% 6%
4	C	5	40% 60%
5	D	4	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BMA	D	3	-	-	-	X
5	MAN	D	4	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10482 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	0	0
			1552	995	259	290	8			
1	B	196	Total	C	N	O	S	0	0	0
			1552	995	259	290	8			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	MET	-	initiating methionine	UNP P0DTC2
A	310	GLY	-	expression tag	UNP P0DTC2
A	311	TRP	-	expression tag	UNP P0DTC2
A	312	SER	-	expression tag	UNP P0DTC2
A	313	CYS	-	expression tag	UNP P0DTC2
A	314	ILE	-	expression tag	UNP P0DTC2
A	315	ILE	-	expression tag	UNP P0DTC2
A	316	LEU	-	expression tag	UNP P0DTC2
A	317	PHE	-	expression tag	UNP P0DTC2
A	318	LEU	-	expression tag	UNP P0DTC2
A	319	VAL	-	expression tag	UNP P0DTC2
A	320	ALA	-	expression tag	UNP P0DTC2
A	321	THR	-	expression tag	UNP P0DTC2
A	322	ALA	-	expression tag	UNP P0DTC2
A	323	THR	-	expression tag	UNP P0DTC2
A	324	GLY	-	expression tag	UNP P0DTC2
A	325	VAL	-	expression tag	UNP P0DTC2
A	326	HIS	-	expression tag	UNP P0DTC2
A	327	SER	-	expression tag	UNP P0DTC2
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	309	MET	-	initiating methionine	UNP P0DTC2
B	310	GLY	-	expression tag	UNP P0DTC2
B	311	TRP	-	expression tag	UNP P0DTC2
B	312	SER	-	expression tag	UNP P0DTC2
B	313	CYS	-	expression tag	UNP P0DTC2
B	314	ILE	-	expression tag	UNP P0DTC2
B	315	ILE	-	expression tag	UNP P0DTC2
B	316	LEU	-	expression tag	UNP P0DTC2
B	317	PHE	-	expression tag	UNP P0DTC2
B	318	LEU	-	expression tag	UNP P0DTC2
B	319	VAL	-	expression tag	UNP P0DTC2
B	320	ALA	-	expression tag	UNP P0DTC2
B	321	THR	-	expression tag	UNP P0DTC2
B	322	ALA	-	expression tag	UNP P0DTC2
B	323	THR	-	expression tag	UNP P0DTC2
B	324	GLY	-	expression tag	UNP P0DTC2
B	325	VAL	-	expression tag	UNP P0DTC2
B	326	HIS	-	expression tag	UNP P0DTC2
B	327	SER	-	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

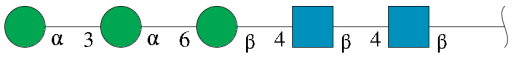
- Molecule 2 is a protein called M8a-34 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	225	Total	C	N	O	S	0	0	0
			1705	1081	280	337	7			
2	H	225	Total	C	N	O	S	0	0	0
			1705	1081	280	337	7			

- Molecule 3 is a protein called M8a-34 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	218	Total	C	N	O	S	0	0	0
			1685	1056	285	339	5			
3	L	218	Total	C	N	O	S	0	0	0
			1685	1056	285	339	5			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

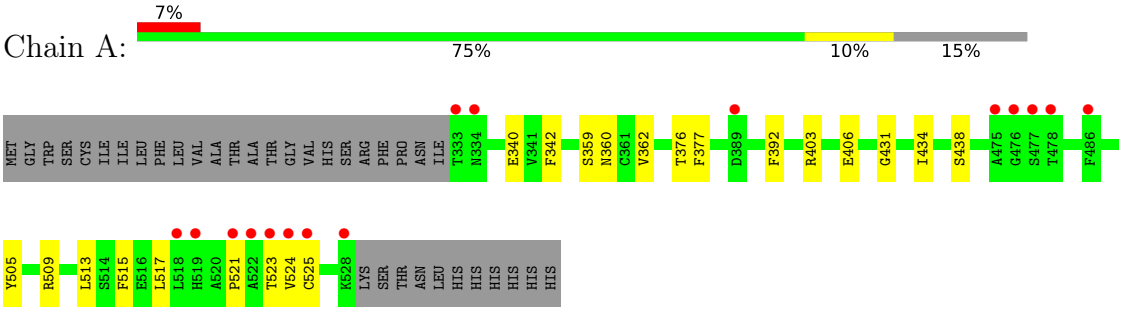
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total	O	0	0
			80	80		
6	B	83	Total	O	0	0
			83	83		
6	E	44	Total	O	0	0
			44	44		
6	F	69	Total	O	0	0
			69	69		
6	H	98	Total	O	0	0
			98	98		
6	L	113	Total	O	0	0
			113	113		

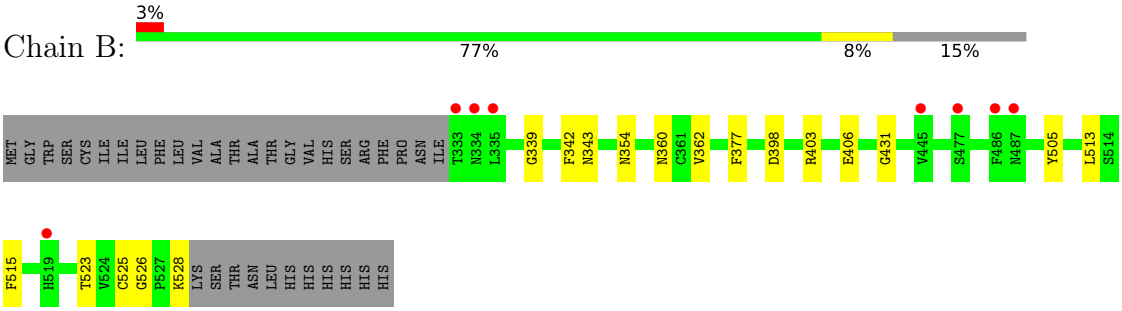
3 Residue-property plots (i)

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.

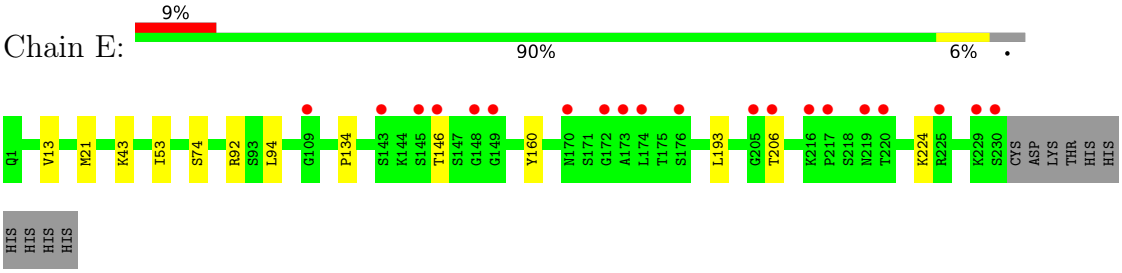
• Molecule 1: Spike protein S1



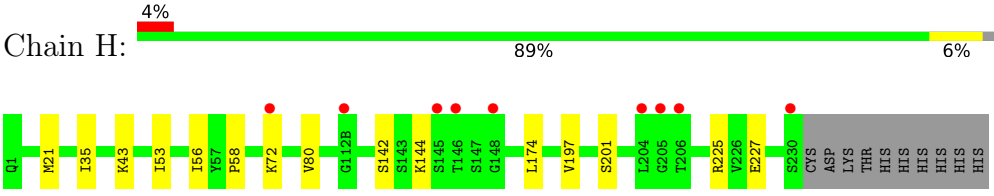
• Molecule 1: Spike protein S1



• Molecule 2: M8a-34 Fab heavy chain

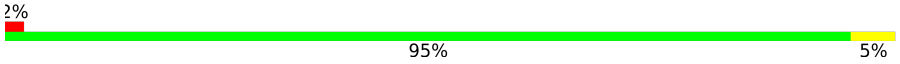


• Molecule 2: M8a-34 Fab heavy chain



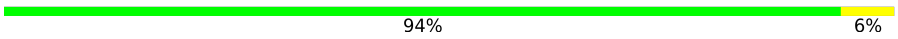
• Molecule 3: M8a-34 Fab light chain

Chain F:



• Molecule 3: M8a-34 Fab light chain

Chain L:

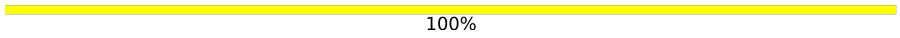


• Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.47Å 165.16Å 93.72Å 90.00° 106.63° 90.00°	Depositor
Resolution (Å)	39.23 – 2.20 39.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.23-2.20) 98.5 (39.23-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.172 , 0.243 0.197 , 0.250	Depositor DCC
R_{free} test set	1999 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10482	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, MAN, 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	0.43	0/1596	0.62	0/2172
1	B	0.43	0/1596	0.62	0/2172
2	E	0.39	0/1750	0.65	1/2386 (0.0%)
2	H	0.41	0/1750	0.65	0/2386
3	F	0.42	0/1721	0.62	0/2337
3	L	0.45	0/1721	0.63	0/2337
All	All	0.42	0/10134	0.63	1/13790 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	193	LEU	CA-CB-CG	5.23	127.32	115.30

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	A	1552	0	1472	12	0
1	B	1552	0	1472	9	0
2	E	1705	0	1660	7	0
2	H	1705	0	1660	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1685	0	1637	6	0
3	L	1685	0	1637	8	0
4	C	61	0	52	2	0
5	D	50	0	43	1	0
6	A	80	0	0	0	0
6	B	83	0	0	0	0
6	E	44	0	0	1	0
6	F	69	0	0	0	0
6	H	98	0	0	0	0
6	L	113	0	0	1	0
All	All	10482	0	9633	49	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 2.

All (49) 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)
3:F:99:VAL:HG13	3:F:126:ILE:HG12	1.74	0.69
3:F:210:LYS:HE3	3:F:234:CYS:SG	2.37	0.65
1:A:362:VAL:HA	1:A:525:CYS:O	2.03	0.59
3:L:204:ALA:O	3:L:208:LYS:HG2	2.02	0.59
2:E:134:PRO:HB3	2:E:160:TYR:HB3	1.84	0.58
3:F:15:LEU:H	3:F:15:LEU:HD12	1.69	0.57
1:B:362:VAL:HA	1:B:525:CYS:O	2.05	0.57
3:L:183:VAL:HG22	3:L:195:LEU:HD12	1.88	0.56
1:B:360:ASN:H	1:B:523:THR:HB	1.73	0.53
1:A:340:GLU:N	1:A:340:GLU:OE1	2.41	0.52
2:E:43:LYS:HB2	2:E:53:ILE:HD11	1.93	0.50
1:A:359:SER:HA	1:A:524:VAL:CG2	2.42	0.50
4:C:3:BMA:O4	4:C:4:MAN:H5	2.12	0.50
1:A:360:ASN:H	1:A:523:THR:HB	1.78	0.49
3:L:140:PRO:HD3	3:L:152:VAL:HG22	1.95	0.48
3:L:43:GLN:HB2	3:L:53:LEU:HD11	1.95	0.48
3:L:8:PRO:HG2	3:L:11:LEU:HD13	1.96	0.48
2:E:146:THR:HB	3:F:136:PHE:HE2	1.79	0.47
1:A:392:PHE:CD1	1:A:515:PHE:HB3	2.48	0.47
2:H:35:ILE:HA	2:H:58:PRO:HB2	1.97	0.46
2:E:13:VAL:HG11	2:E:94:LEU:HD13	1.97	0.46
1:B:403:ARG:HG2	1:B:406:GLU:OE1	2.16	0.46
2:H:56:ILE:HD13	2:H:80:VAL:HG13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:21:MET:HE2	2:H:21:MET:HB2	1.83	0.45
1:A:521:PRO:HG2	2:E:206:THR:OG1	2.17	0.45
1:B:526:GLY:O	1:B:528:LYS:HE2	2.17	0.45
1:A:403:ARG:HG2	1:A:406:GLU:OE1	2.17	0.44
1:B:339:GLY:O	1:B:343:ASN:HB2	2.17	0.44
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.52	0.44
3:L:167:GLN:OE1	3:L:174:LEU:HD23	2.17	0.44
2:H:72:LYS:HB3	2:H:72:LYS:HE2	1.64	0.44
1:B:354:ASN:O	1:B:398:ASP:HA	2.18	0.44
3:L:15:LEU:HD22	3:L:15:LEU:H	1.83	0.44
1:B:342:PHE:HB2	5:D:1:NAG:H82	1.99	0.43
2:H:174:LEU:HD21	2:H:197:VAL:HG21	2.01	0.43
2:H:225:ARG:NH1	2:H:227:GLU:OE2	2.51	0.43
1:A:342:PHE:HB2	4:C:1:NAG:H82	2.02	0.42
3:F:43:GLN:HB2	3:F:53:LEU:HD11	2.01	0.42
1:B:431:GLY:HA3	1:B:513:LEU:O	2.19	0.42
1:A:431:GLY:HA3	1:A:513:LEU:O	2.20	0.42
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.55	0.42
3:F:140:PRO:HD3	3:F:152:VAL:HG22	2.01	0.41
2:H:43:LYS:HB2	2:H:53:ILE:HD11	2.02	0.41
1:A:438:SER:CB	1:A:509:ARG:HG3	2.51	0.41
2:E:74:SER:O	2:E:92:ARG:HD2	2.20	0.41
3:L:86:ASP:HB3	6:L:352:HOH:O	2.21	0.41
2:H:142:SER:OG	2:H:144:LYS:HE2	2.21	0.40
1:A:376:THR:O	1:A:434:ILE:HA	2.22	0.40
2:E:21:MET:HB3	6:E:322:HOH:O	2.22	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 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	194/231 (84%)	189 (97%)	5 (3%)	0	100	100
1	B	194/231 (84%)	189 (97%)	5 (3%)	0	100	100
2	E	223/235 (95%)	217 (97%)	6 (3%)	0	100	100
2	H	223/235 (95%)	218 (98%)	5 (2%)	0	100	100
3	F	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
3	L	216/218 (99%)	210 (97%)	6 (3%)	0	100	100
All	All	1266/1368 (92%)	1235 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 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	169/200 (84%)	166 (98%)	3 (2%)	59	72
1	B	169/200 (84%)	167 (99%)	2 (1%)	71	83
2	E	190/200 (95%)	189 (100%)	1 (0%)	88	94
2	H	190/200 (95%)	189 (100%)	1 (0%)	88	94
3	F	190/190 (100%)	189 (100%)	1 (0%)	88	94
3	L	190/190 (100%)	190 (100%)	0	100	100
All	All	1098/1180 (93%)	1090 (99%)	8 (1%)	84	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	PHE
1	A	505	TYR
1	A	517	LEU
1	B	377	PHE
1	B	505	TYR
2	E	224	LYS
3	F	207	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	201	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

9 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	C	1	1,4	14,14,15	0.22	0	17,19,21	0.70	1 (5%)
4	NAG	C	2	4	14,14,15	0.28	0	17,19,21	1.49	2 (11%)
4	BMA	C	3	4	11,11,12	2.37	4 (36%)	15,15,17	2.85	4 (26%)
4	MAN	C	4	4	11,11,12	1.52	3 (27%)	15,15,17	1.46	2 (13%)
4	MAN	C	5	4	11,11,12	1.22	1 (9%)	15,15,17	1.21	2 (13%)
5	NAG	D	1	5,1	14,14,15	0.21	0	17,19,21	0.64	0
5	NAG	D	2	5	14,14,15	0.24	0	17,19,21	1.05	2 (11%)
5	BMA	D	3	5	11,11,12	1.43	2 (18%)	15,15,17	1.46	1 (6%)
5	MAN	D	4	5	11,11,12	1.41	2 (18%)	15,15,17	1.35	1 (6%)

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	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	MAN	C	4	4	-	2/2/19/22	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
5	NAG	D	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	2/6/23/26	0/1/1/1
5	BMA	D	3	5	-	0/2/19/22	0/1/1/1
5	MAN	D	4	5	-	2/2/19/22	1/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3	BMA	C4-C5	5.99	1.65	1.53
4	C	3	BMA	C4-C3	3.53	1.61	1.52
4	C	4	MAN	C4-C5	3.07	1.59	1.53
5	D	4	MAN	O5-C5	2.78	1.49	1.43
5	D	4	MAN	C1-C2	2.58	1.58	1.52
4	C	5	MAN	C4-C5	2.58	1.58	1.53
5	D	3	BMA	O5-C5	2.58	1.48	1.43
5	D	3	BMA	C4-C5	2.51	1.58	1.53
4	C	3	BMA	C1-C2	2.20	1.57	1.52
4	C	4	MAN	C4-C3	2.14	1.57	1.52
4	C	3	BMA	O5-C1	2.09	1.47	1.43
4	C	4	MAN	O5-C5	2.04	1.47	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3	BMA	C1-O5-C5	-6.70	103.12	112.19
4	C	3	BMA	C1-C2-C3	-6.24	102.00	109.67
4	C	2	NAG	O4-C4-C3	-4.84	99.17	110.35
5	D	4	MAN	C1-O5-C5	4.01	117.63	112.19
5	D	3	BMA	C1-C2-C3	-3.79	105.01	109.67
4	C	3	BMA	C3-C4-C5	3.54	116.55	110.24
4	C	4	MAN	C1-O5-C5	3.50	116.94	112.19
4	C	3	BMA	O5-C1-C2	-3.35	105.60	110.77
4	C	2	NAG	C1-O5-C5	3.14	116.45	112.19
5	D	2	NAG	C1-O5-C5	3.06	116.34	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	5	MAN	C1-O5-C5	2.94	116.17	112.19
4	C	4	MAN	C3-C4-C5	2.71	115.08	110.24
4	C	1	NAG	C1-O5-C5	2.19	115.16	112.19
5	D	2	NAG	O4-C4-C3	2.04	115.07	110.35
4	C	5	MAN	O2-C2-C3	-2.04	106.06	110.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3	BMA	C4-C5-C6-O6
5	D	4	MAN	C4-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
5	D	4	MAN	O5-C5-C6-O6
4	C	4	MAN	C4-C5-C6-O6
5	D	2	NAG	C4-C5-C6-O6
4	C	4	MAN	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6

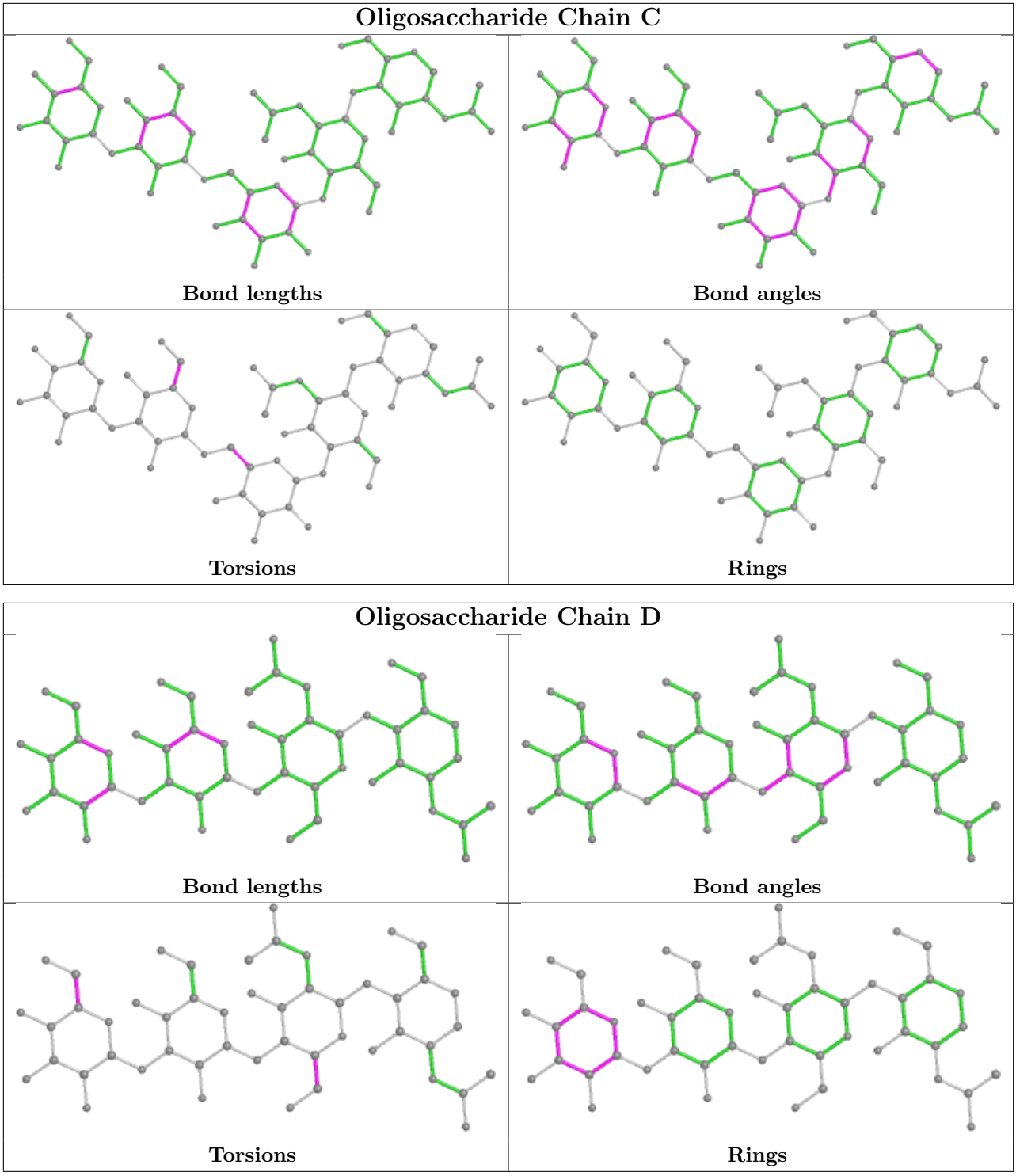
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	4	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1	NAG	1	0
4	C	1	NAG	1	0
4	C	3	BMA	1	0
4	C	4	MAN	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)

There are no ligands in this entry.

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, 95^{th} 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	196/231 (84%)	0.44	16 (8%) 11 10	28, 43, 77, 97	0
1	B	196/231 (84%)	0.34	8 (4%) 37 35	29, 43, 68, 86	0
2	E	225/235 (95%)	0.40	20 (8%) 9 8	34, 51, 84, 96	0
2	H	225/235 (95%)	0.10	9 (4%) 38 36	30, 42, 68, 86	0
3	F	218/218 (100%)	0.05	5 (2%) 60 58	29, 47, 67, 82	0
3	L	218/218 (100%)	-0.11	1 (0%) 91 90	27, 39, 54, 80	0
All	All	1278/1368 (93%)	0.20	59 (4%) 32 31	27, 44, 75, 97	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	521	PRO	7.0
2	E	148	GLY	6.6
1	B	333	THR	6.5
3	F	234	CYS	6.4
2	E	206	THR	5.4
2	H	148	GLY	5.3
2	E	173	ALA	4.9
1	A	519	HIS	4.8
1	A	486	PHE	4.7
1	B	334	ASN	4.4
1	B	486	PHE	4.3
2	E	230	SER	4.3
1	B	335	LEU	3.8
1	A	524	VAL	3.7
1	A	476	GLY	3.6
2	E	216	LYS	3.6
2	H	145	SER	3.3
2	E	176	SER	3.3
2	E	149	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	232	GLY	3.1
2	H	146	THR	3.1
3	F	233	GLU	3.1
1	A	518	LEU	3.0
2	E	172	GLY	3.0
2	H	205	GLY	2.9
2	H	206	THR	2.9
2	E	145	SER	2.9
3	F	84	ARG	2.9
2	E	174	LEU	2.9
1	B	477	SER	2.8
2	E	146	THR	2.8
2	E	205	GLY	2.7
1	A	523	THR	2.7
2	E	170	ASN	2.7
2	E	220	THR	2.7
1	A	522	ALA	2.7
3	L	234	CYS	2.6
2	H	230	SER	2.5
2	E	229	LYS	2.5
1	A	477	SER	2.5
1	B	445	VAL	2.4
2	H	72	LYS	2.3
1	A	528	LYS	2.3
1	A	333	THR	2.3
2	H	204	LEU	2.3
2	E	143	SER	2.3
1	B	519	HIS	2.2
1	A	334	ASN	2.2
1	B	487	ASN	2.2
1	A	525	CYS	2.2
2	E	225	ARG	2.2
3	F	146	LYS	2.2
2	E	217	PRO	2.2
2	E	109	GLY	2.2
1	A	475	ALA	2.1
1	A	389	ASP	2.1
2	E	219	ASN	2.1
2	H	112(B)	GLY	2.0
1	A	478	THR	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)

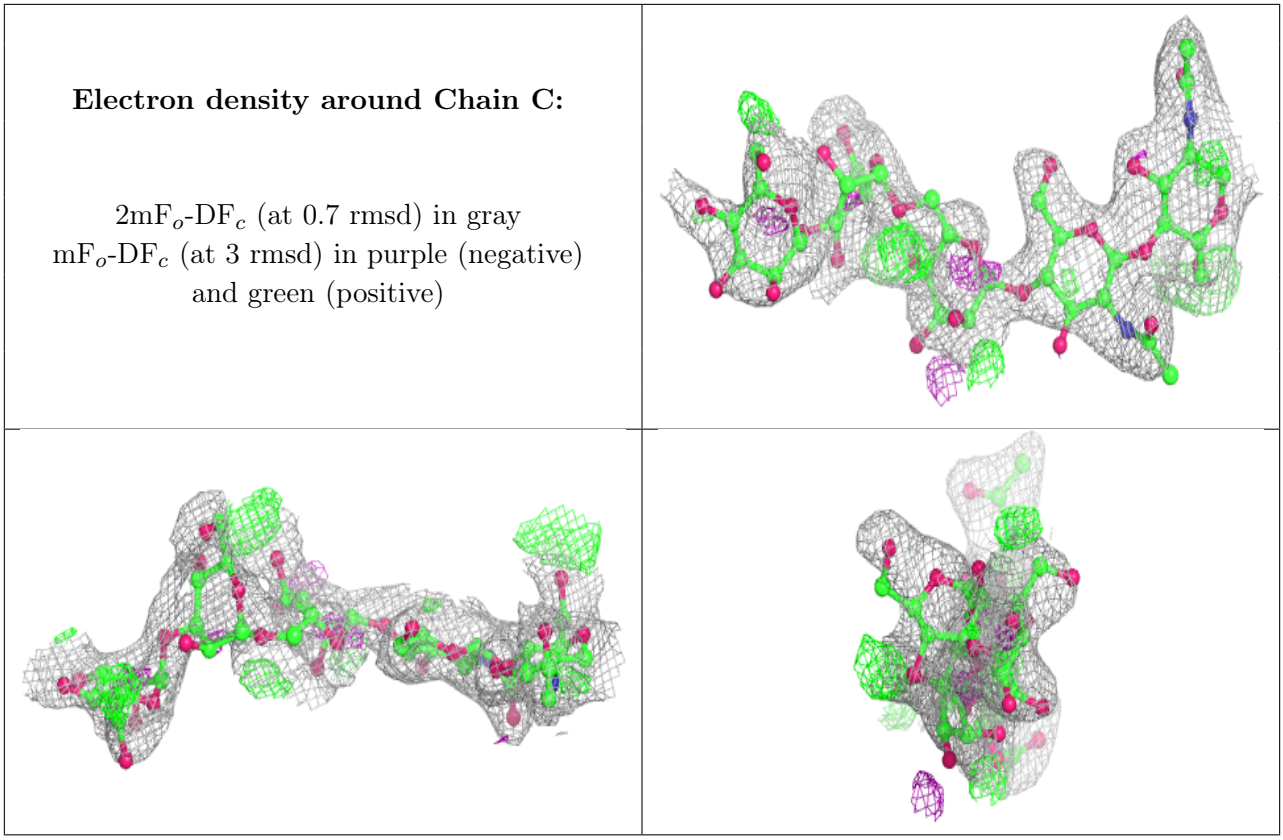
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	BMA	C	3	11/12	0.42	0.32	84,89,95,97	0
4	MAN	C	4	11/12	0.55	0.32	82,94,98,100	0
5	MAN	D	4	11/12	0.57	0.50	95,106,110,110	0
4	MAN	C	5	11/12	0.64	0.24	84,89,97,97	0
5	BMA	D	3	11/12	0.74	0.49	95,105,107,110	0
5	NAG	D	2	14/15	0.75	0.34	75,81,95,99	0
4	NAG	C	2	14/15	0.81	0.26	68,78,84,90	0
4	NAG	C	1	14/15	0.84	0.13	51,60,78,79	0
5	NAG	D	1	14/15	0.87	0.15	52,60,70,77	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.

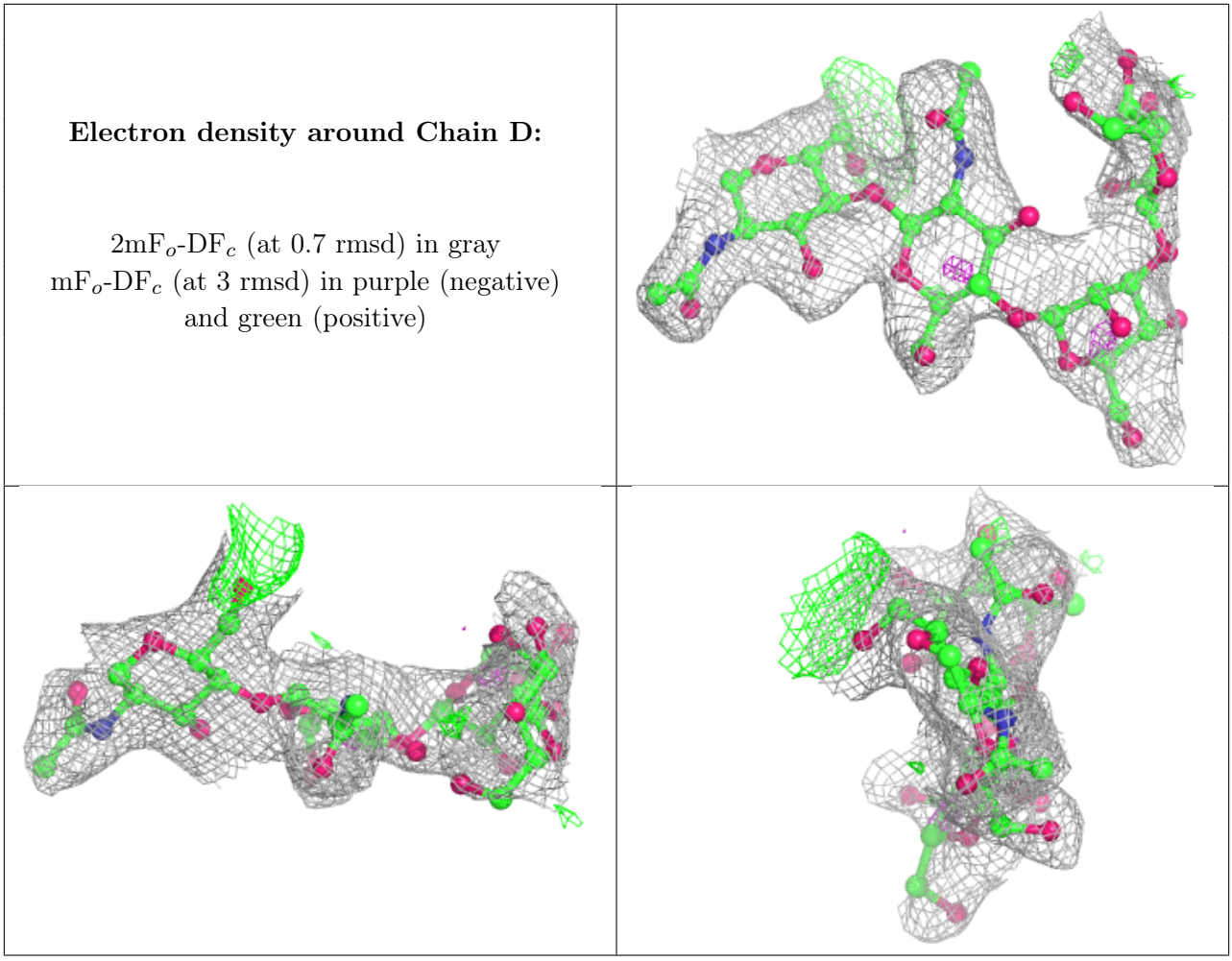
Electron density around Chain C:

$2mF_o$-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 D:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.