wwPDB X-ray Structure Validation Summary Report (i)

May 18, 2023 – 04:08 PM EDT

PDB ID	:	8GB5
Title	:	Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing antibody 25F9
Authors	:	Yuan, M.; Zhu, X.; Wilson, I.A.
Deposited on	:	2023-02-24
Resolution	:	3.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

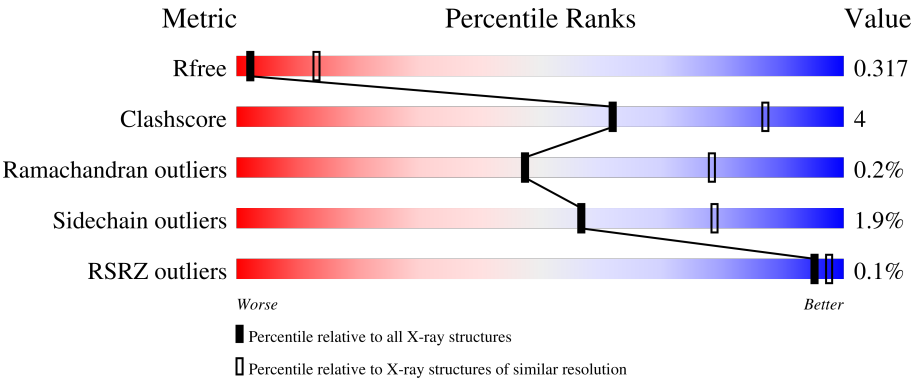
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	205	89% 6% 5%
1	D	205	85% 10% 5%
1	G	205	90% 5% 5%
1	J	205	88% 7% 5%
2	B	231	85% 13% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	231	87% 11%
2	I	231	83% 16%
2	L	231	86% 13%
3	C	216	81% 18%
3	E	216	81% 17%
3	H	216	83% 16%
3	K	216	82% 16%
4	M	3	100%
5	N	5	60% 40%
6	O	4	50% 25% 25%
6	P	4	25% 75%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 19740 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	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			
1	D	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			
1	G	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			
1	J	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	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
D	531	GLY	-	expression tag	UNP P0DTC2
D	532	HIS	-	expression tag	UNP P0DTC2
D	533	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
D	537	HIS	-	expression tag	UNP P0DTC2
G	531	GLY	-	expression tag	UNP P0DTC2
G	532	HIS	-	expression tag	UNP P0DTC2
G	533	HIS	-	expression tag	UNP P0DTC2
G	534	HIS	-	expression tag	UNP P0DTC2
G	535	HIS	-	expression tag	UNP P0DTC2
G	536	HIS	-	expression tag	UNP P0DTC2
G	537	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	531	GLY	-	expression tag	UNP P0DTC2
J	532	HIS	-	expression tag	UNP P0DTC2
J	533	HIS	-	expression tag	UNP P0DTC2
J	534	HIS	-	expression tag	UNP P0DTC2
J	535	HIS	-	expression tag	UNP P0DTC2
J	536	HIS	-	expression tag	UNP P0DTC2
J	537	HIS	-	expression tag	UNP P0DTC2

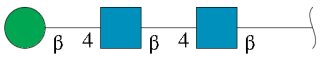
- Molecule 2 is a protein called 25F9 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1725	1100	288	331	6			
2	F	227	Total	C	N	O	S	0	0	0
			1723	1099	288	331	5			
2	I	227	Total	C	N	O	S	0	0	0
			1725	1100	288	331	6			
2	L	228	Total	C	N	O	S	0	0	0
			1729	1102	289	332	6			

- Molecule 3 is a protein called 25F9 Light chain.

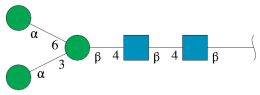
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1585	984	273	323	5			
3	E	213	Total	C	N	O	S	0	0	0
			1579	981	273	321	4			
3	H	214	Total	C	N	O	S	0	0	0
			1585	984	273	323	5			
3	K	213	Total	C	N	O	S	0	0	0
			1579	981	272	322	4			

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



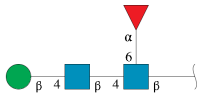
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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.



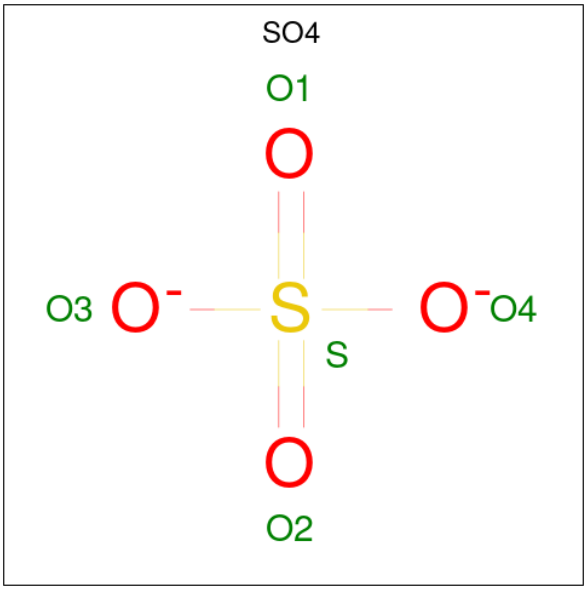
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



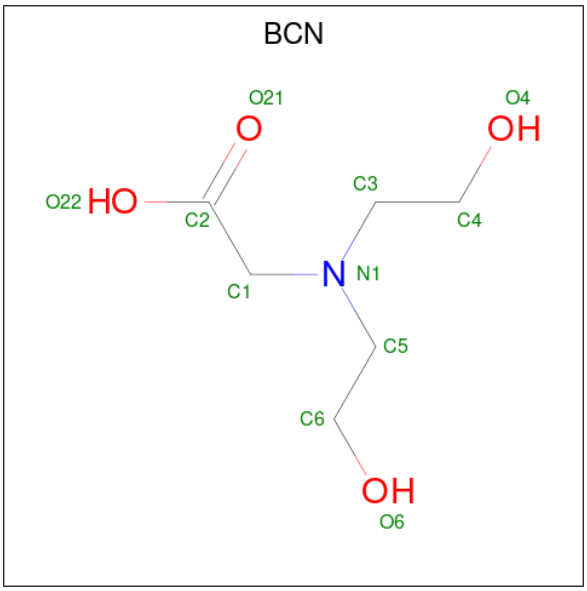
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	4	Total	C	N	O	0	0	0
			49	28	2	19			
6	P	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



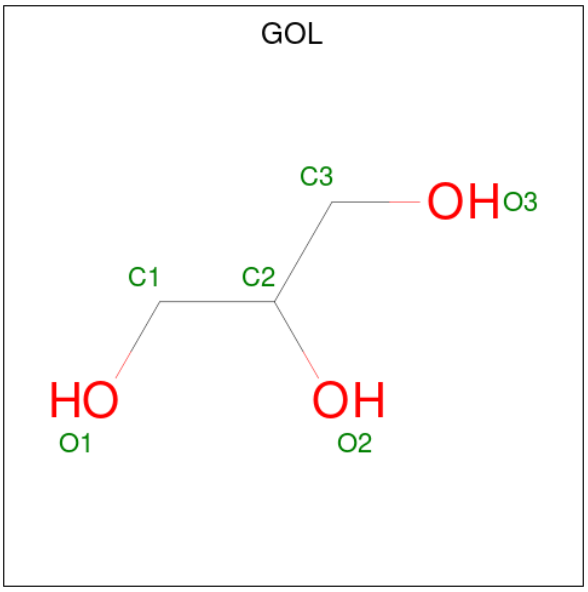
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0

- Molecule 8 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C N O 11 6 1 4	0	0
8	E	1	Total C N O 11 6 1 4	0	0
8	H	1	Total C N O 11 6 1 4	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	K	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total O 3 3	0	0
10	B	3	Total O 3 3	0	0
10	C	6	Total O 6 6	0	0
10	D	2	Total O 2 2	0	0
10	E	5	Total O 5 5	0	0
10	F	4	Total O 4 4	0	0
10	G	3	Total O 3 3	0	0
10	H	6	Total O 6 6	0	0
10	I	7	Total O 7 7	0	0
10	J	2	Total O 2 2	0	0
10	K	14	Total O 14 14	0	0

Continued on next page...

Continued from previous page...

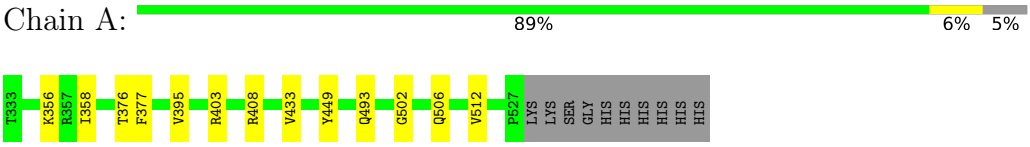
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	6	Total	O	0	0
			6	6		

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.

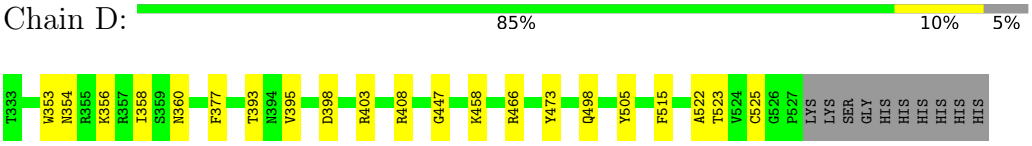
• Molecule 1: Spike protein S1

Chain A:



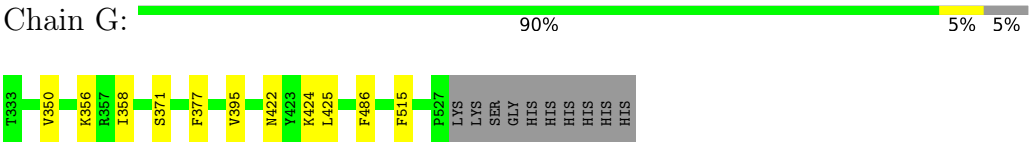
• Molecule 1: Spike protein S1

Chain D:



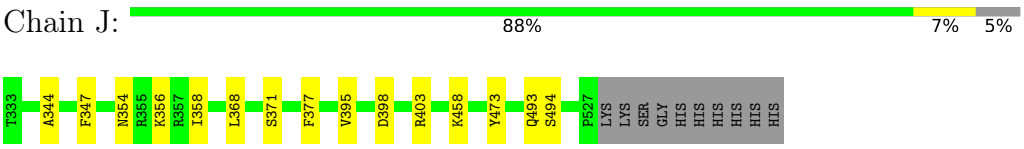
• Molecule 1: Spike protein S1

Chain G:



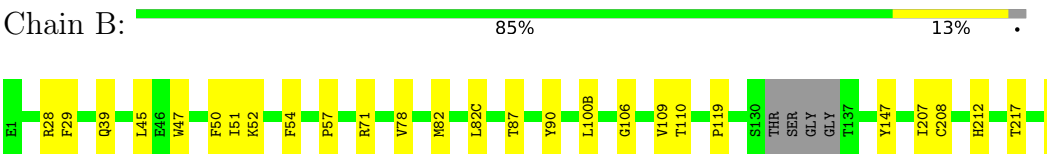
• Molecule 1: Spike protein S1

Chain J:



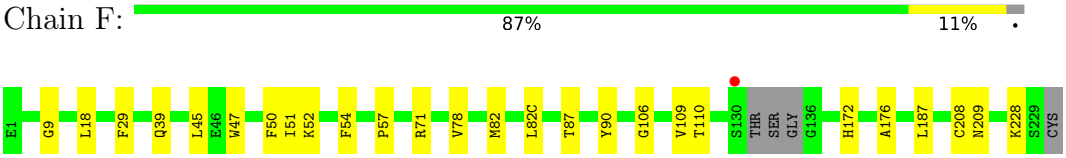
• Molecule 2: 25F9 Heavy chain

Chain B:



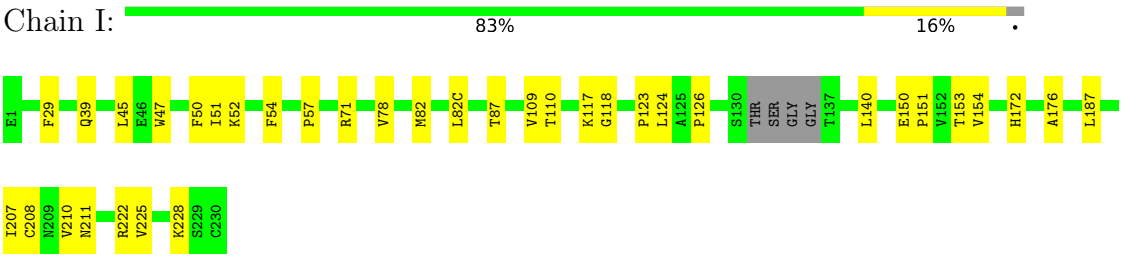
• Molecule 2: 25F9 Heavy chain

Chain F:



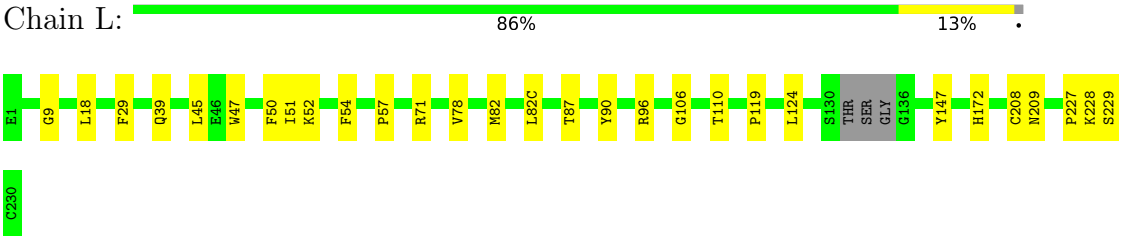
• Molecule 2: 25F9 Heavy chain

Chain I:



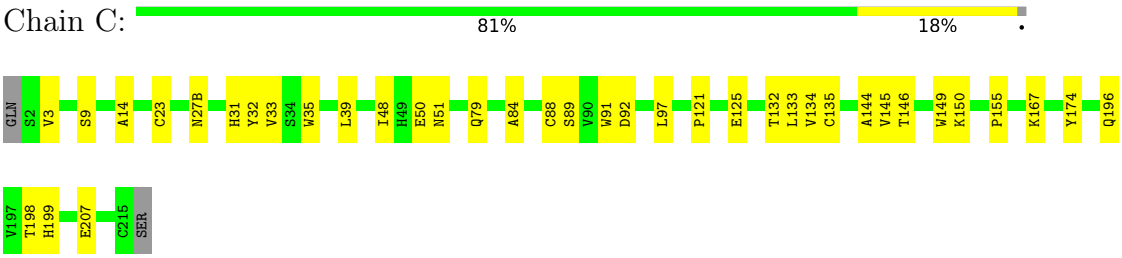
• Molecule 2: 25F9 Heavy chain

Chain L:



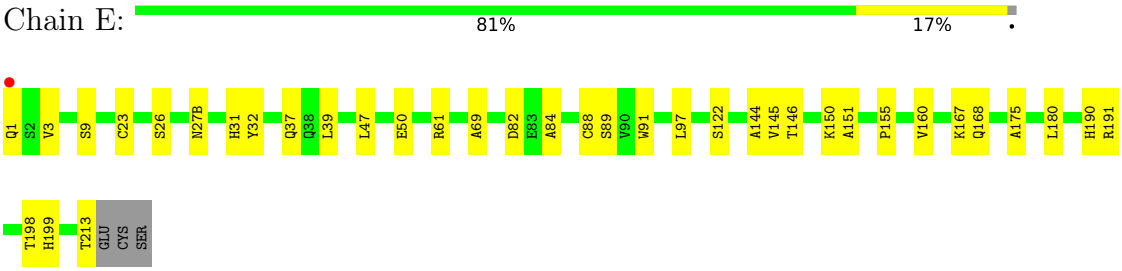
• Molecule 3: 25F9 Light chain

Chain C:



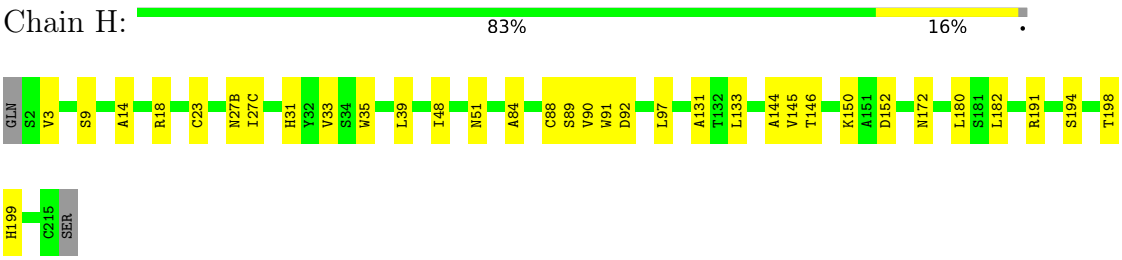
• Molecule 3: 25F9 Light chain

Chain E:



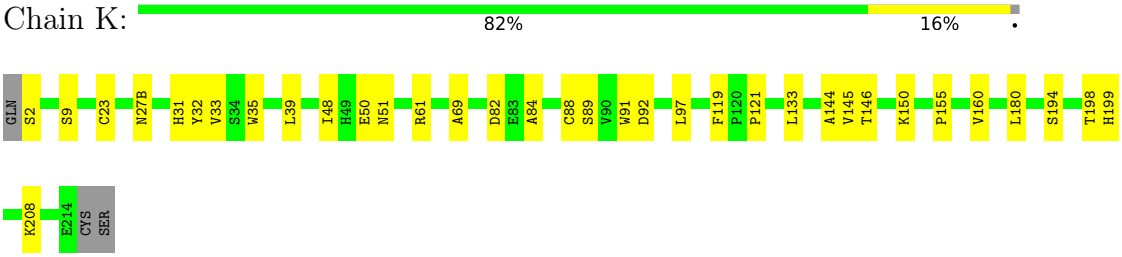
• Molecule 3: 25F9 Light chain

Chain H:



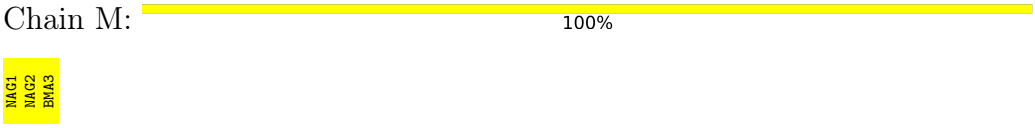
• Molecule 3: 25F9 Light chain

Chain K:



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

Chain M:



• Molecule 5: 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 N:

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

Chain O:

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

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.48Å 105.82Å 118.18Å 83.08° 67.47° 64.04°	Depositor
Resolution (Å)	47.49 – 3.35 47.50 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.49-3.35) 98.5 (47.50-3.35)	Depositor EDS
R_{merge}	0.87	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.275 , 0.320 0.276 , 0.317	Depositor DCC
R_{free} test set	2519 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.000 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	19740	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 85.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3953e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MAN, BMA, BCN, GOL, NAG, SO4, FUC

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	0.25	0/1587	0.48	0/2161
1	D	0.26	0/1587	0.48	0/2161
1	G	0.25	0/1587	0.47	0/2161
1	J	0.26	0/1587	0.48	0/2161
2	B	0.25	0/1769	0.49	0/2409
2	F	0.25	0/1767	0.50	0/2406
2	I	0.25	0/1769	0.50	0/2409
2	L	0.25	0/1773	0.49	0/2414
3	C	0.25	0/1623	0.50	0/2216
3	E	0.25	0/1617	0.49	0/2208
3	H	0.25	0/1623	0.49	0/2216
3	K	0.24	0/1617	0.48	0/2208
All	All	0.25	0/19906	0.49	0/27130

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	A	1543	0	1459	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1543	0	1459	9	0
1	G	1543	0	1459	6	0
1	J	1543	0	1459	8	0
2	B	1725	0	1697	18	0
2	F	1723	0	1696	12	0
2	I	1725	0	1698	19	0
2	L	1729	0	1701	13	0
3	C	1585	0	1532	20	0
3	E	1579	0	1532	21	0
3	H	1585	0	1533	18	0
3	K	1579	0	1528	22	0
4	M	39	0	34	1	0
5	N	61	0	52	1	0
6	O	49	0	43	1	0
6	P	49	0	43	4	0
7	A	5	0	0	1	0
7	D	5	0	0	0	0
7	E	10	0	0	0	0
7	I	5	0	0	0	0
7	J	5	0	0	0	0
7	K	10	0	0	0	0
8	C	11	0	12	1	0
8	E	11	0	11	2	0
8	H	11	0	12	0	0
9	K	6	0	8	1	0
10	A	3	0	0	0	0
10	B	3	0	0	0	0
10	C	6	0	0	1	0
10	D	2	0	0	0	0
10	E	5	0	0	0	0
10	F	4	0	0	0	0
10	G	3	0	0	0	0
10	H	6	0	0	0	0
10	I	7	0	0	0	0
10	J	2	0	0	0	0
10	K	14	0	0	0	0
10	L	6	0	0	0	0
All	All	19740	0	18968	168	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.

The worst 5 of 168 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:H:131:ALA:HB3	3:H:182:LEU:O	1.73	0.89
3:K:92:ASP:HB2	3:K:97:LEU:HD11	1.63	0.79
3:H:92:ASP:HB2	3:H:97:LEU:HD11	1.66	0.77
1:J:371:SER:HB2	6:P:1:NAG:H3	1.67	0.76
1:G:358:ILE:HB	1:G:395:VAL:HG23	1.69	0.73

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	193/205 (94%)	189 (98%)	4 (2%)	0	100	100
1	D	193/205 (94%)	185 (96%)	8 (4%)	0	100	100
1	G	193/205 (94%)	187 (97%)	6 (3%)	0	100	100
1	J	193/205 (94%)	187 (97%)	6 (3%)	0	100	100
2	B	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
2	F	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
2	I	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
2	L	224/231 (97%)	218 (97%)	6 (3%)	0	100	100
3	C	212/216 (98%)	201 (95%)	9 (4%)	2 (1%)	17	51
3	E	211/216 (98%)	202 (96%)	8 (4%)	1 (0%)	29	63
3	H	212/216 (98%)	204 (96%)	7 (3%)	1 (0%)	29	63
3	K	211/216 (98%)	202 (96%)	9 (4%)	0	100	100
All	All	2511/2608 (96%)	2423 (96%)	84 (3%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	3	VAL
3	E	3	VAL
3	H	3	VAL
3	C	134	VAL

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	168/177 (95%)	163 (97%)	5 (3%)	41	69
1	D	168/177 (95%)	164 (98%)	4 (2%)	49	74
1	G	168/177 (95%)	166 (99%)	2 (1%)	71	85
1	J	168/177 (95%)	163 (97%)	5 (3%)	41	69
2	B	193/195 (99%)	191 (99%)	2 (1%)	76	87
2	F	192/195 (98%)	188 (98%)	4 (2%)	53	77
2	I	193/195 (99%)	190 (98%)	3 (2%)	62	81
2	L	193/195 (99%)	188 (97%)	5 (3%)	46	73
3	C	178/180 (99%)	175 (98%)	3 (2%)	60	80
3	E	177/180 (98%)	175 (99%)	2 (1%)	73	86
3	H	178/180 (99%)	175 (98%)	3 (2%)	60	80
3	K	177/180 (98%)	175 (99%)	2 (1%)	73	86
All	All	2153/2208 (98%)	2113 (98%)	40 (2%)	57	79

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	356	LYS
2	L	54	PHE
1	J	377	PHE
1	J	494	SER
2	L	172	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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)

16 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	M	1	4,1	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	M	2	4	14,14,15	0.32	0	17,19,21	0.39	0
4	BMA	M	3	4	11,11,12	0.53	0	15,15,17	0.96	1 (6%)
5	NAG	N	1	5,1	14,14,15	0.73	1 (7%)	17,19,21	0.69	0
5	NAG	N	2	5	14,14,15	0.54	0	17,19,21	1.30	3 (17%)
5	BMA	N	3	5	11,11,12	0.98	1 (9%)	15,15,17	1.73	5 (33%)
5	MAN	N	4	5	11,11,12	0.95	0	15,15,17	1.03	1 (6%)
5	MAN	N	5	5	11,11,12	0.68	0	15,15,17	1.06	2 (13%)
6	NAG	O	1	6,1	14,14,15	0.74	1 (7%)	17,19,21	0.69	0
6	NAG	O	2	6	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
6	BMA	O	3	6	11,11,12	0.77	0	15,15,17	0.72	0
6	FUC	O	4	6	10,10,11	0.69	0	14,14,16	0.84	0
6	NAG	P	1	6,1	14,14,15	0.46	0	17,19,21	1.06	1 (5%)
6	NAG	P	2	6	14,14,15	0.81	1 (7%)	17,19,21	1.03	1 (5%)
6	BMA	P	3	6	11,11,12	0.70	0	15,15,17	0.71	0
6	FUC	P	4	6	10,10,11	0.81	0	14,14,16	1.07	1 (7%)

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	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
5	NAG	N	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	N	2	5	-	3/6/23/26	0/1/1/1
5	BMA	N	3	5	-	2/2/19/22	0/1/1/1
5	MAN	N	4	5	-	1/2/19/22	0/1/1/1
5	MAN	N	5	5	-	1/2/19/22	0/1/1/1
6	NAG	O	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	FUC	O	4	6	-	-	0/1/1/1
6	NAG	P	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	BMA	P	3	6	-	1/2/19/22	0/1/1/1
6	FUC	P	4	6	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	2	NAG	C1-C2	2.74	1.56	1.52
5	N	1	NAG	C1-C2	2.49	1.56	1.52
6	O	1	NAG	O5-C1	-2.32	1.40	1.43
5	N	3	BMA	C2-C3	2.13	1.55	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	1	NAG	C1-O5-C5	3.64	117.12	112.19
5	N	2	NAG	C2-N2-C7	3.62	128.05	122.90
6	P	2	NAG	C2-N2-C7	3.31	127.62	122.90
5	N	3	BMA	C3-C4-C5	3.02	115.63	110.24
5	N	3	BMA	C2-C3-C4	2.94	115.98	110.89

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	2	NAG	C1-C2-N2-C7
6	P	2	NAG	C1-C2-N2-C7
5	N	2	NAG	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
6	O	2	NAG	C1-C2-N2-C7

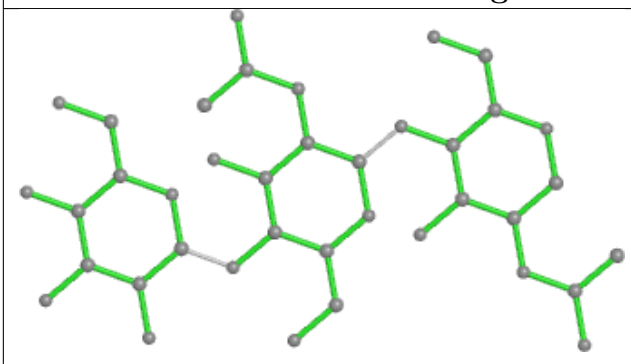
There are no ring outliers.

8 monomers are involved in 7 short contacts:

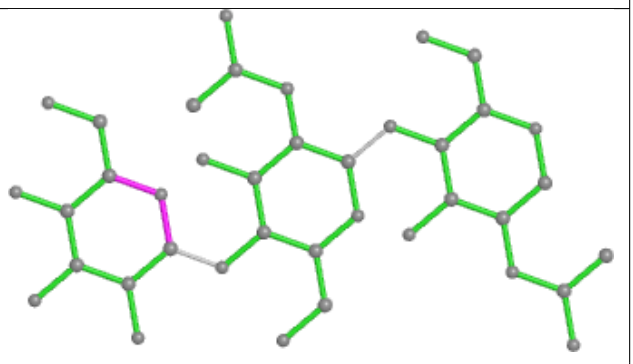
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	1	NAG	2	0
4	M	2	NAG	1	0
5	N	3	BMA	1	0
4	M	1	NAG	1	0
6	O	2	NAG	1	0
6	P	2	NAG	2	0
5	N	2	NAG	1	0
6	P	4	FUC	1	0

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

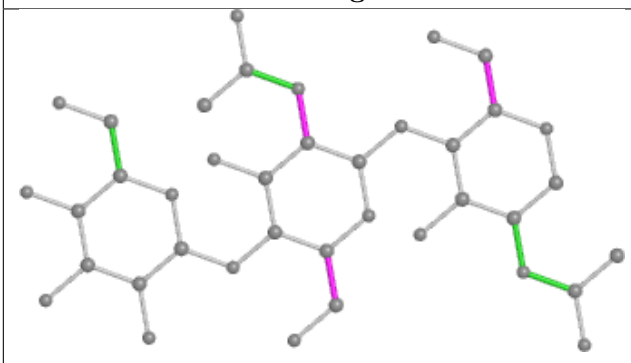
Oligosaccharide Chain M



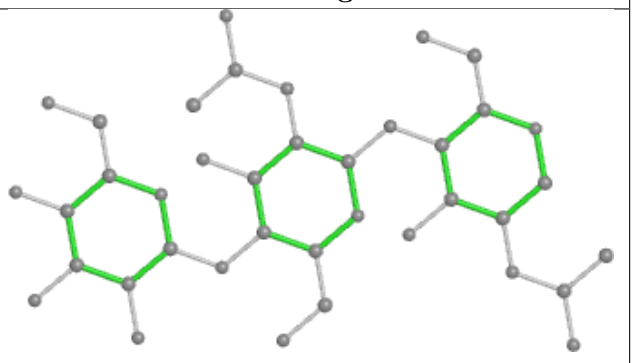
Bond lengths



Bond angles

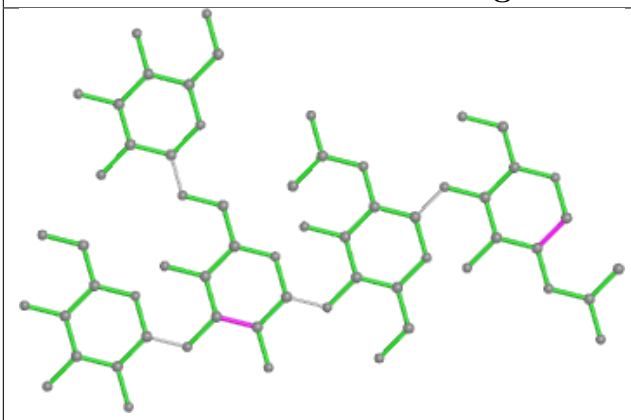


Torsions

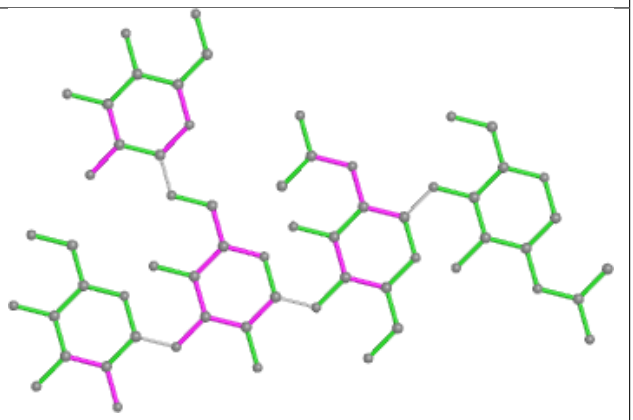


Rings

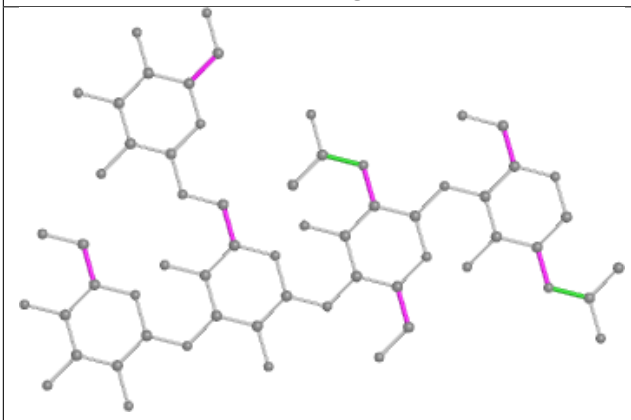
Oligosaccharide Chain N



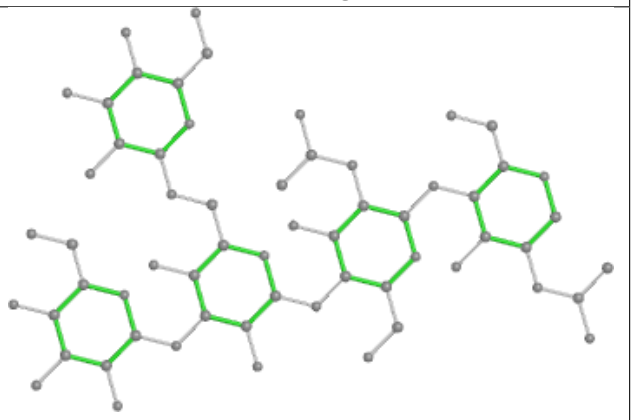
Bond lengths



Bond angles

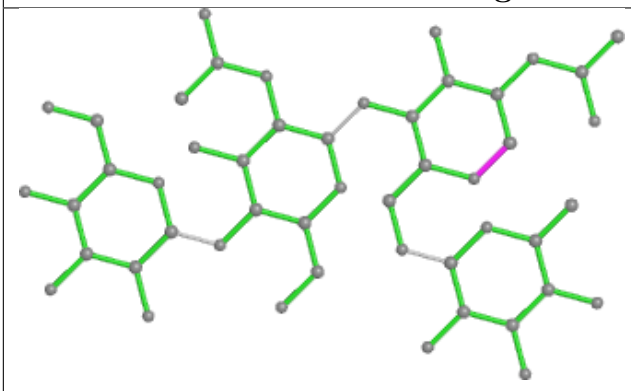


Torsions

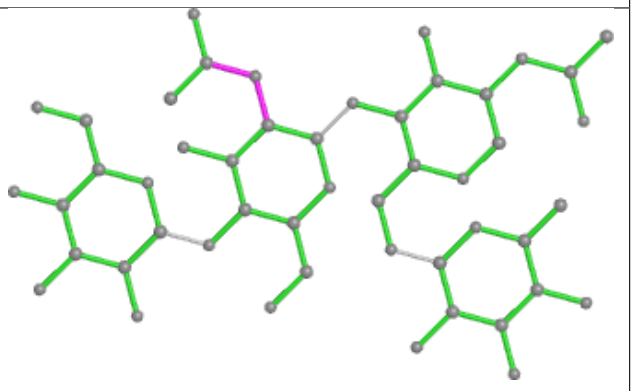


Rings

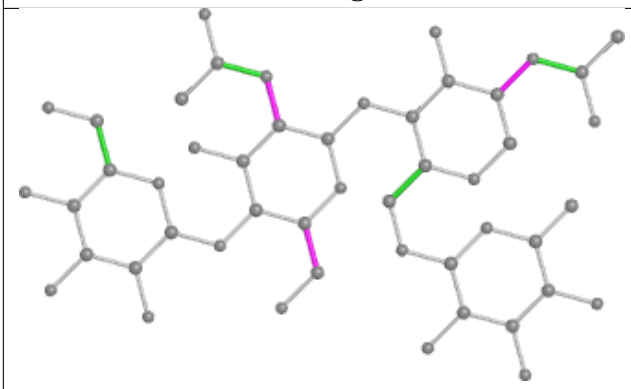
Oligosaccharide Chain O



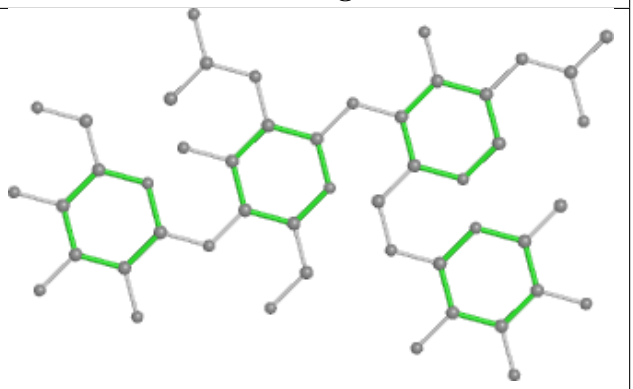
Bond lengths



Bond angles

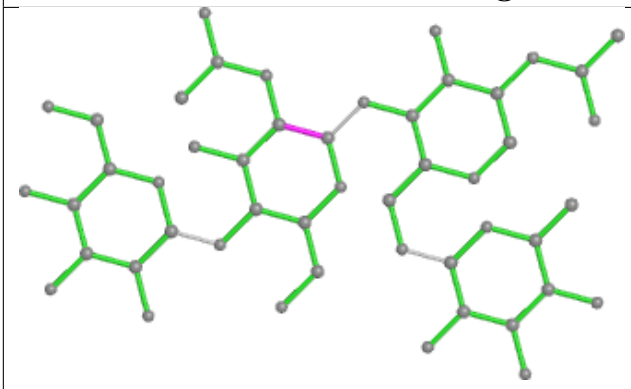


Torsions

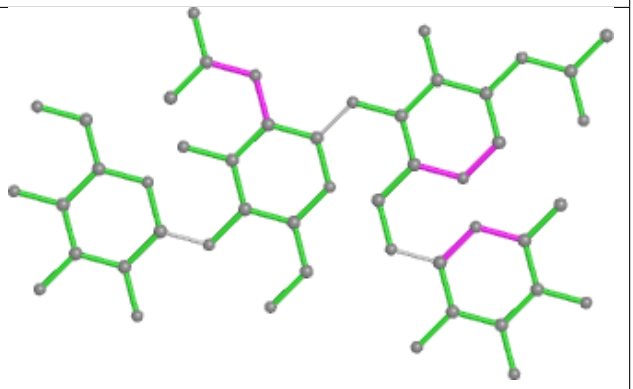


Rings

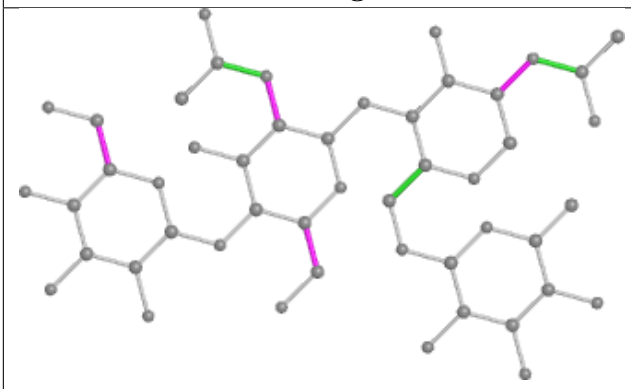
Oligosaccharide Chain P



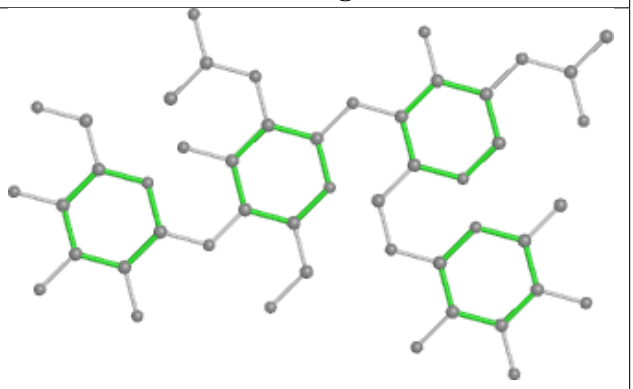
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
7	SO4	D	601	-	4,4,4	0.13	0	6,6,6	0.10	0
7	SO4	K	303	-	4,4,4	0.14	0	6,6,6	0.08	0
7	SO4	I	301	-	4,4,4	0.13	0	6,6,6	0.10	0
7	SO4	E	302	-	4,4,4	0.15	0	6,6,6	0.06	0
7	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.09	0
8	BCN	C	301	-	10,10,10	0.96	0	11,11,11	0.99	0
8	BCN	E	303	3	10,10,10	0.99	0	11,11,11	1.06	0
7	SO4	K	302	-	4,4,4	0.15	0	6,6,6	0.10	0
7	SO4	E	301	-	4,4,4	0.13	0	6,6,6	0.07	0
9	GOL	K	301	-	5,5,5	0.90	0	5,5,5	0.98	0
8	BCN	H	301	-	10,10,10	0.95	0	11,11,11	1.06	0
7	SO4	J	601	-	4,4,4	0.15	0	6,6,6	0.12	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
9	GOL	K	301	-	-	0/4/4/4	-
8	BCN	C	301	-	-	4/10/10/10	-
8	BCN	H	301	-	-	6/10/10/10	-
8	BCN	E	303	3	-	3/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	301	BCN	N1-C1-C2-O21
8	H	301	BCN	N1-C1-C2-O22
8	C	301	BCN	N1-C1-C2-O21
8	C	301	BCN	N1-C1-C2-O22
8	E	303	BCN	N1-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	SO4	1	0
8	C	301	BCN	1	0
8	E	303	BCN	2	0
9	K	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, 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	195/205 (95%)	-0.45	0 100 100	42, 73, 90, 105	0
1	D	195/205 (95%)	-0.48	0 100 100	40, 61, 85, 103	0
1	G	195/205 (95%)	-0.38	0 100 100	44, 79, 112, 117	0
1	J	195/205 (95%)	-0.13	0 100 100	59, 99, 125, 138	0
2	B	227/231 (98%)	-0.33	0 100 100	66, 85, 108, 124	0
2	F	227/231 (98%)	-0.60	1 (0%) 92 94	31, 54, 88, 112	0
2	I	227/231 (98%)	-0.50	0 100 100	36, 66, 89, 106	0
2	L	228/231 (98%)	-0.19	0 100 100	70, 99, 118, 140	0
3	C	214/216 (99%)	-0.27	0 100 100	35, 84, 105, 124	0
3	E	213/216 (98%)	-0.51	1 (0%) 91 93	25, 51, 76, 105	0
3	H	214/216 (99%)	-0.40	0 100 100	33, 63, 91, 106	0
3	K	213/216 (98%)	-0.07	0 100 100	56, 93, 118, 142	0
All	All	2543/2608 (97%)	-0.36	2 (0%) 95 97	25, 75, 112, 142	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	1	GLN	2.1
2	F	130	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

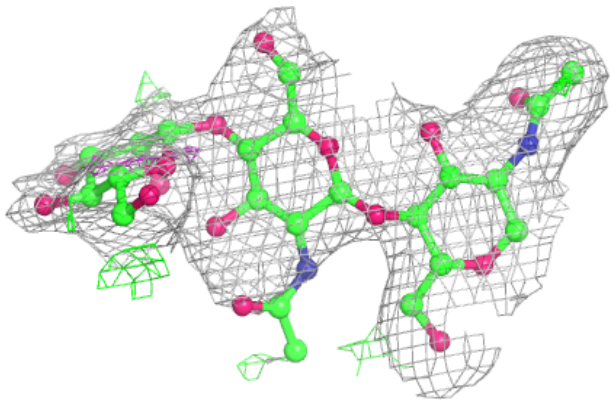
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

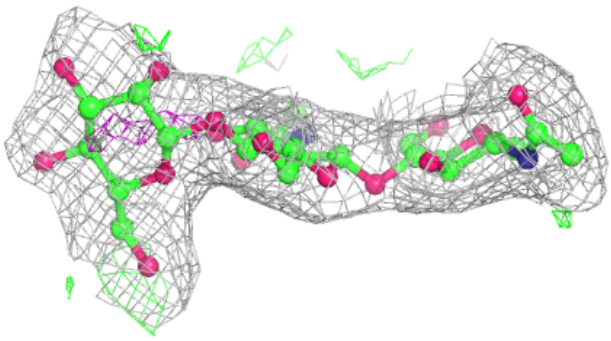
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	M	3	11/12	0.76	0.24	62,90,107,116	0
6	BMA	O	3	11/12	0.78	0.23	67,74,107,116	0
6	BMA	P	3	11/12	0.80	0.17	73,82,100,100	0
6	FUC	O	4	10/11	0.84	0.24	57,89,102,108	0
6	FUC	P	4	10/11	0.84	0.31	47,98,115,115	0
5	NAG	N	2	14/15	0.85	0.25	68,86,98,115	0
5	MAN	N	4	11/12	0.85	0.34	60,100,116,132	0
6	NAG	O	2	14/15	0.88	0.22	89,101,107,109	0
6	NAG	P	1	14/15	0.89	0.28	56,82,112,112	0
4	NAG	M	2	14/15	0.89	0.24	75,93,115,117	0
5	BMA	N	3	11/12	0.89	0.19	72,86,101,106	0
5	MAN	N	5	11/12	0.91	0.26	65,81,100,101	0
6	NAG	O	1	14/15	0.91	0.22	51,84,96,105	0
5	NAG	N	1	14/15	0.92	0.22	61,71,102,105	0
4	NAG	M	1	14/15	0.92	0.15	32,57,83,96	0
6	NAG	P	2	14/15	0.93	0.24	73,91,116,118	0

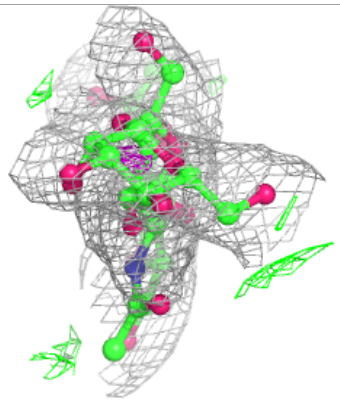
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

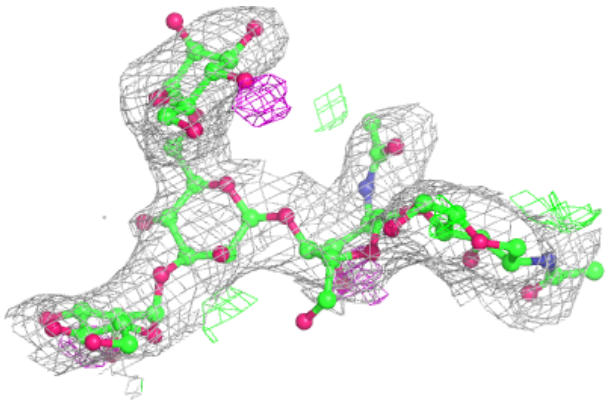


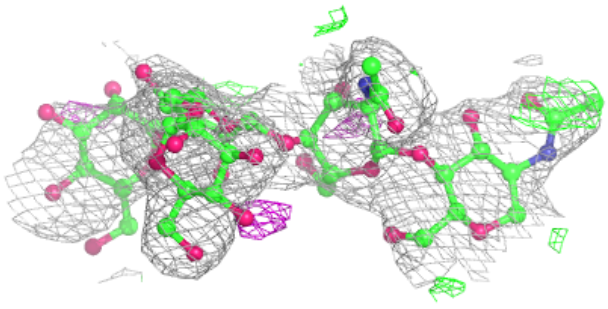


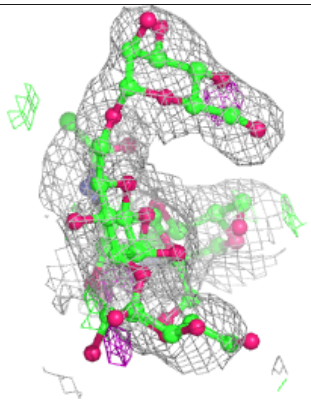


Electron density around Chain N:

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

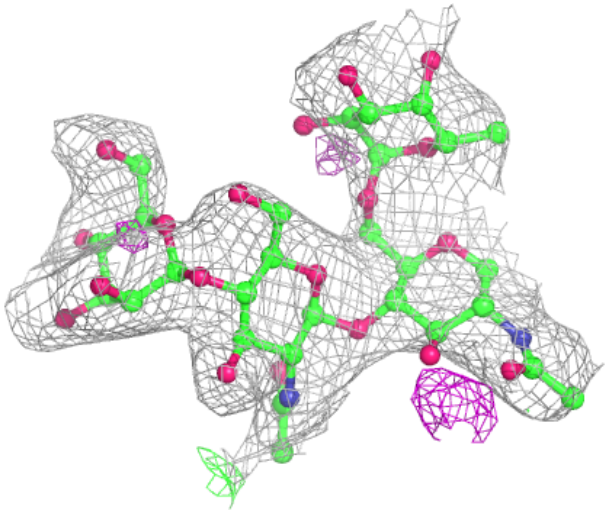


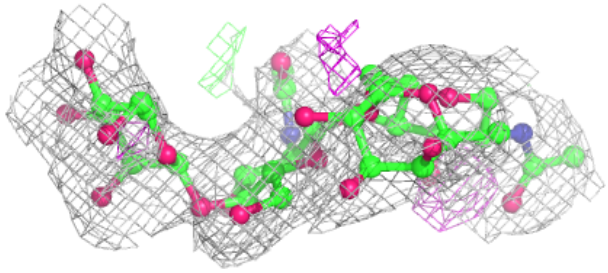


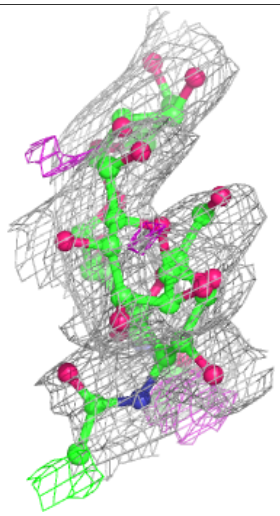


Electron density around Chain O:

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

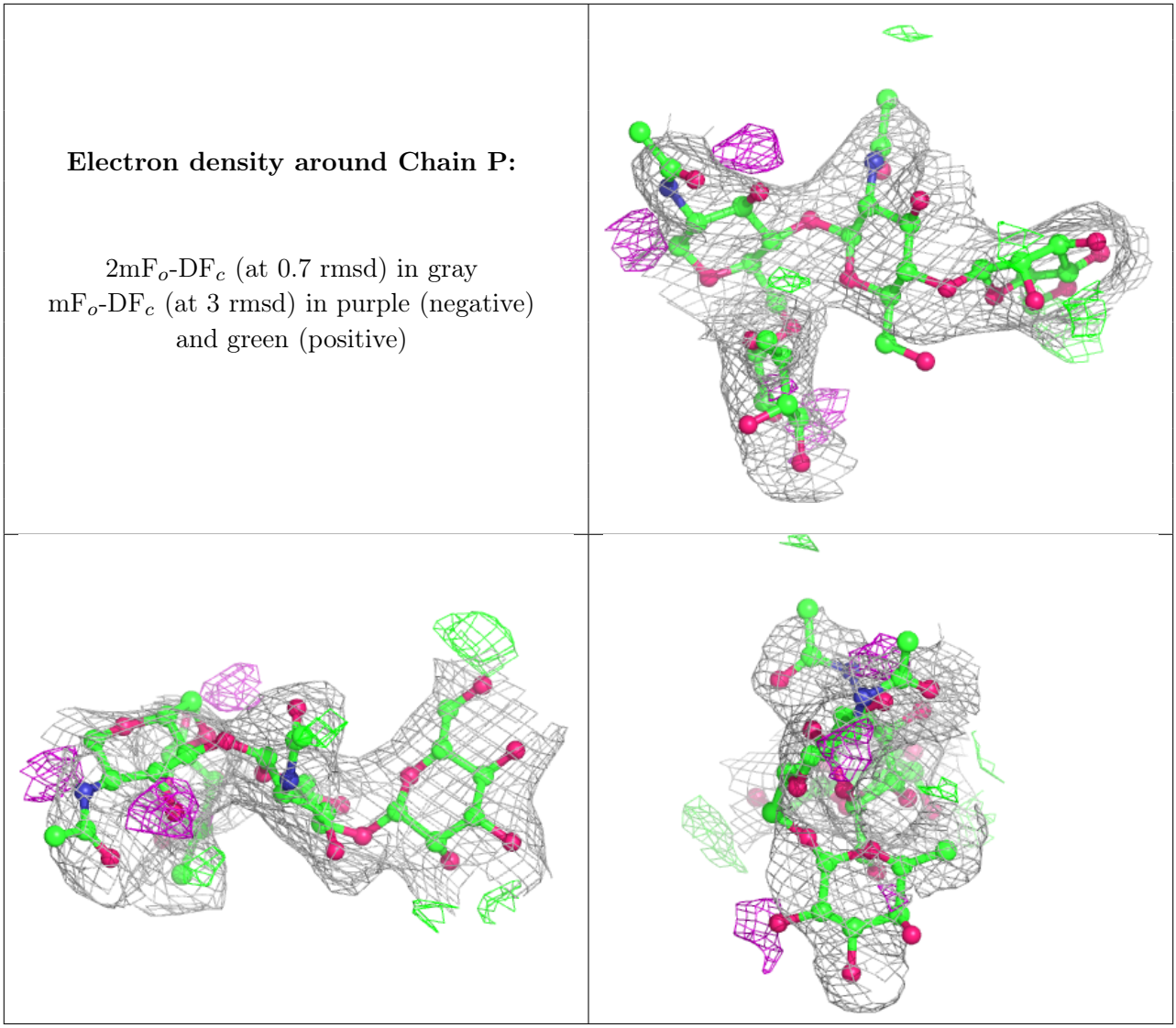






Electron density around Chain P:

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



6.4 Ligands

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
7	SO4	J	601	5/5	0.94	0.15	57,76,99,99	0
8	BCN	E	303	11/11	0.94	0.15	47,68,75,79	0
8	BCN	C	301	11/11	0.95	0.12	38,49,66,79	0
7	SO4	I	301	5/5	0.95	0.21	70,90,120,123	0
8	BCN	H	301	11/11	0.95	0.11	39,51,67,68	0
7	SO4	D	601	5/5	0.96	0.21	57,72,93,102	0
7	SO4	E	302	5/5	0.96	0.10	48,52,87,114	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	K	302	5/5	0.96	0.17	57,65,85,104	0
7	SO4	K	303	5/5	0.97	0.10	68,71,93,99	0
9	GOL	K	301	6/6	0.97	0.13	29,40,56,56	0
7	SO4	E	301	5/5	0.98	0.34	81,84,104,125	0
7	SO4	A	601	5/5	0.99	0.13	53,57,75,80	0

6.5 Other polymers (i)

There are no such residues in this entry.