Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 04:20 AM JST

PDB ID	:	7F5G
Title	:	The crystal structure of RBD-Nanobody complex, DL4 (SA4)
Authors	:	Li, T.; Lai, Y.; Zhou, Y.; Tan, J.; Li, D.
Deposited on	:	2021-06-22
Resolution	:	1.75 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 (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:

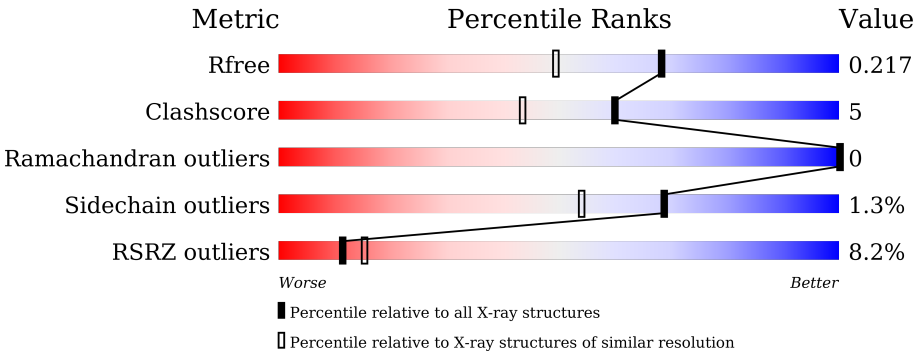
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	213	6% 85% 7% 8%
1	C	213	10% 82% 11% 6%
2	B	146	8% 79% 19%
2	D	146	4% 68% 12% 20%
3	E	4	100%
3	F	4	50% 50%

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
3	NAG	E	3	-	-	-	X
3	FUC	F	4	-	-	-	X
4	GOL	A	602	-	-	-	X
4	GOL	A	605	-	-	-	X
4	GOL	B	201	-	-	-	X
4	GOL	C	601	-	-	-	X
4	GOL	D	203	-	-	-	X
5	ACT	A	608	-	-	-	X
5	ACT	A	612	-	-	-	X
5	ACT	D	206	-	-	X	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5970 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 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	7	0
			1601	1025	270	298	8			
1	C	200	Total	C	N	O	S	0	5	0
			1631	1046	278	299	8			

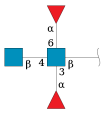
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ALA	-	expression tag	UNP P0DTC2
A	328	GLY	-	expression tag	UNP P0DTC2
A	329	SER	-	expression tag	UNP P0DTC2
A	532	GLY	-	expression tag	UNP P0DTC2
A	533	THR	-	expression tag	UNP P0DTC2
A	534	LEU	-	expression tag	UNP P0DTC2
A	535	GLU	-	expression tag	UNP P0DTC2
A	536	VAL	-	expression tag	UNP P0DTC2
A	537	LEU	-	expression tag	UNP P0DTC2
A	538	PHE	-	expression tag	UNP P0DTC2
A	539	GLN	-	expression tag	UNP P0DTC2
C	327	ALA	-	expression tag	UNP P0DTC2
C	328	GLY	-	expression tag	UNP P0DTC2
C	329	SER	-	expression tag	UNP P0DTC2
C	532	GLY	-	expression tag	UNP P0DTC2
C	533	THR	-	expression tag	UNP P0DTC2
C	534	LEU	-	expression tag	UNP P0DTC2
C	535	GLU	-	expression tag	UNP P0DTC2
C	536	VAL	-	expression tag	UNP P0DTC2
C	537	LEU	-	expression tag	UNP P0DTC2
C	538	PHE	-	expression tag	UNP P0DTC2
C	539	GLN	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Nanobody DL4.

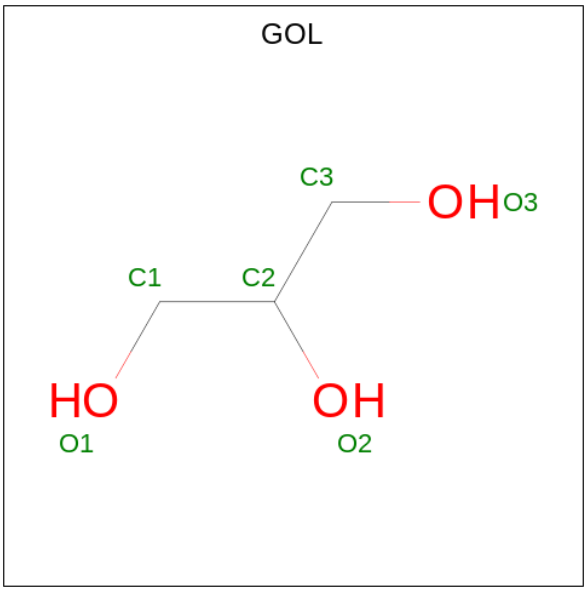
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	118	Total	C	N	O	S	0	4	0
			951	592	171	185	3			
2	D	117	Total	C	N	O	S	0	4	0
			944	585	171	185	3			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[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
3	E	4	Total	C	N	O	0	0	0
			48	28	2	18			
3	F	4	Total	C	N	O	0	0	0
			48	28	2	18			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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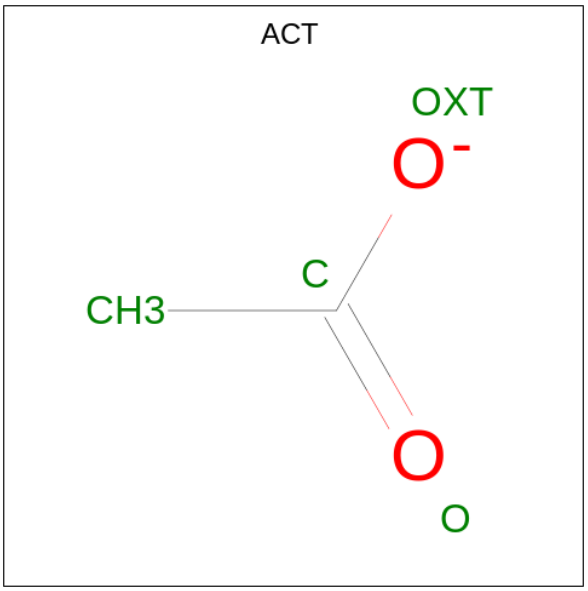
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	204	Total O 204 204	0	0

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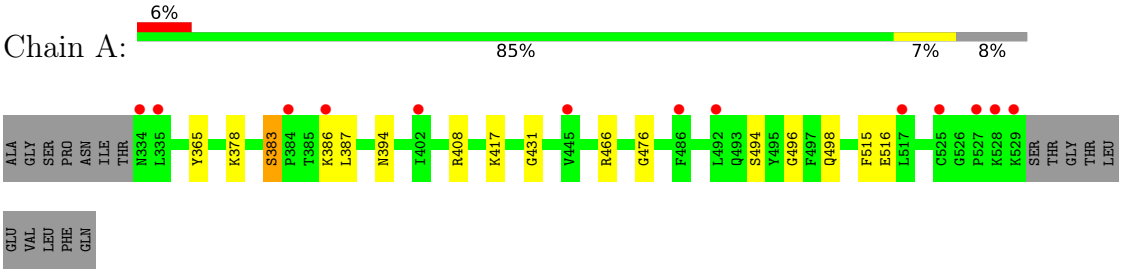
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	118	Total O 118 118	0	0
6	C	171	Total O 171 171	0	0
6	D	120	Total O 120 120	0	0

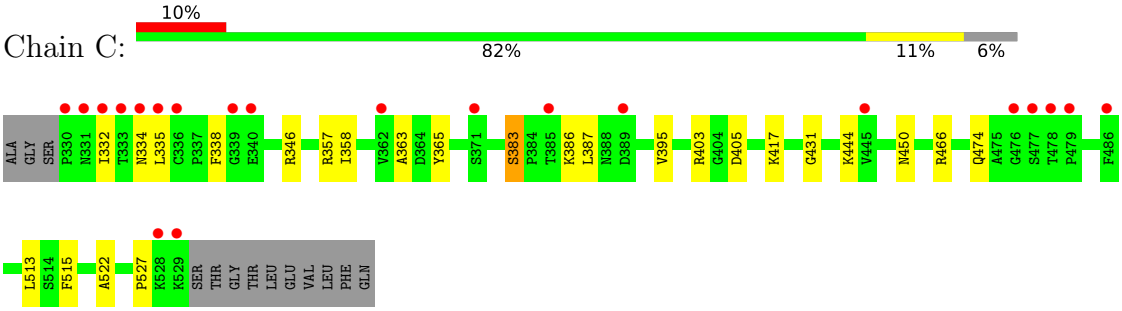
3 Residue-property plots (i)

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.

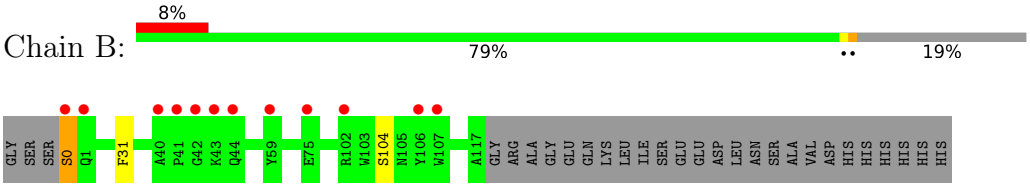
• Molecule 1: Spike glycoprotein



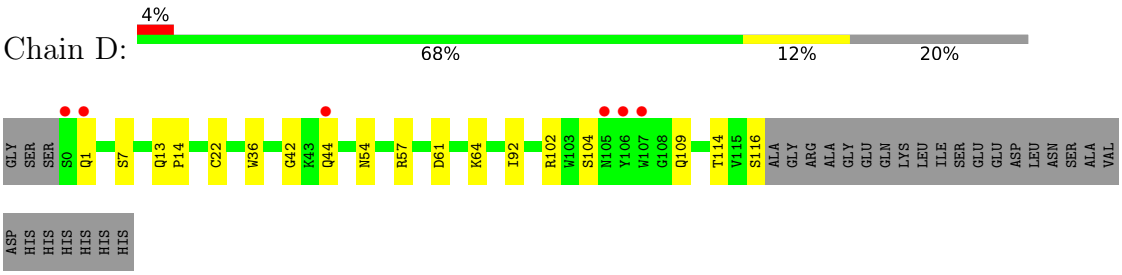
• Molecule 1: Spike glycoprotein



• Molecule 2: Nanobody DL4

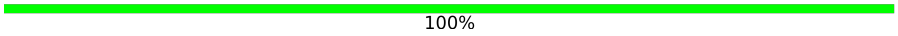


• Molecule 2: Nanobody DL4



• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.82Å 95.04Å 118.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.58 – 1.75 36.58 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.58-1.75) 100.0 (36.58-1.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.188 , 0.217 0.188 , 0.217	Depositor DCC
R_{free} test set	4590 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	1.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5970	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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 46.29 % 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 1.1691e-04. 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: GOL, ACT, FUC, 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	0.39	0/1655	0.57	0/2252
1	C	0.37	0/1683	0.58	0/2287
2	B	0.40	0/981	0.59	0/1326
2	D	0.38	0/970	0.59	0/1310
All	All	0.38	0/5289	0.58	0/7175

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	1601	0	1511	11	0
1	C	1631	0	1564	23	0
2	B	951	0	905	3	0
2	D	944	0	897	15	0
3	E	48	0	43	0	0
3	F	48	0	43	0	0
4	A	42	0	55	2	0
4	B	6	0	8	0	0
4	C	18	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	24	0	32	4	0
5	A	28	0	21	1	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	8	0	6	2	0
6	A	204	0	0	2	0
6	B	118	0	0	0	0
6	C	171	0	0	3	0
6	D	120	0	0	0	0
All	All	5970	0	5115	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (48) 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:B:0:SER:HB2	1:C:522:ALA:H	1.42	0.84
2:D:64:LYS:O	5:D:206:ACT:H1	1.86	0.74
1:C:332:ILE:HG22	1:C:334:ASN:H	1.57	0.67
1:C:450:ASN:OD1	2:D:54:ASN:ND2	2.28	0.67
1:C:417:LYS:H	4:C:602:GOL:H2	1.60	0.67
2:B:0:SER:HB2	1:C:522:ALA:N	2.11	0.66
1:C:383:SER:HB3	1:C:386:LYS:HG2	1.77	0.65
1:C:444:LYS:NZ	6:C:704:HOH:O	2.30	0.65
1:C:403[A]:ARG:NH1	6:C:702:HOH:O	2.28	0.58
2:D:44:GLN:OE1	2:D:44:GLN:N	2.38	0.56
2:B:0:SER:CB	1:C:522:ALA:H	2.18	0.56
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.42	0.55
1:A:466[A]:ARG:NH2	6:A:702:HOH:O	2.39	0.54
1:A:378:LYS:NZ	6:A:704:HOH:O	2.40	0.54
1:C:346[A]:ARG:HG2	1:C:346[A]:ARG:HH11	1.74	0.52
1:A:408:ARG:HD2	5:A:612:ACT:H1	1.91	0.50
1:A:476:GLY:HA3	4:A:605:GOL:H2	1.94	0.49
1:C:338:PHE:HE2	1:C:363:ALA:HB1	1.77	0.49
2:D:61:ASP:O	5:D:206:ACT:H3	2.13	0.48
2:D:114:THR:HG21	4:D:202:GOL:H12	1.96	0.48
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.49	0.47
2:D:102:ARG:HG2	2:D:102:ARG:HH11	1.79	0.47
1:C:417:LYS:HG2	4:C:602:GOL:H31	1.97	0.47
1:C:466[B]:ARG:NH2	6:C:703:HOH:O	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLY:O	1:A:498[B]:GLN:HG2	2.15	0.46
1:C:474:GLN:HB3	4:C:601:GOL:H32	1.98	0.46
1:C:332:ILE:HB	1:C:335:LEU:HG	1.97	0.46
2:D:13:GLN:HA	2:D:116:SER:HB3	1.97	0.46
2:D:7:SER:HA	4:D:201:GOL:H2	1.98	0.46
1:A:431:GLY:HA2	1:A:515:PHE:HD2	1.81	0.45
1:C:357:ARG:HG2	1:C:357:ARG:HH11	1.82	0.45
1:A:383:SER:HB3	1:A:386:LYS:HG2	1.99	0.45
2:D:57:ARG:HB2	4:D:205:GOL:H11	1.98	0.44
1:C:363:ALA:O	1:C:527:PRO:HD3	2.17	0.44
2:D:1[B]:GLN:HE21	2:D:1[B]:GLN:HB3	1.71	0.43
2:D:42:GLY:O	4:D:203:GOL:H2	2.19	0.43
1:C:357:ARG:HG2	1:C:357:ARG:NH1	2.34	0.42
2:D:22:CYS:HB2	2:D:36:TRP:CZ2	2.54	0.42
1:A:365:TYR:CD2	1:A:387:LEU:HB3	2.53	0.42
1:C:403[B]:ARG:NH1	1:C:405:ASP:HB2	2.35	0.42
2:D:92:ILE:HD11	2:D:109:GLN:O	2.20	0.42
1:A:394:ASN:HB2	1:A:516:GLU:OE2	2.21	0.41
2:D:14:PRO:HD3	2:D:116:SER:HB3	2.02	0.41
1:A:417:LYS:HG2	4:A:606:GOL:O2	2.20	0.41
1:C:358:ILE:HB	1:C:395:VAL:HB	2.02	0.40
1:C:365:TYR:CD2	1:C:387:LEU:HB3	2.56	0.40
2:D:102:ARG:HH11	2:D:102:ARG:CG	2.34	0.40
1:C:431:GLY:HA3	1:C:513:LEU: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	201/213 (94%)	192 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	203/213 (95%)	198 (98%)	5 (2%)	0	100	100
2	B	120/146 (82%)	117 (98%)	3 (2%)	0	100	100
2	D	119/146 (82%)	113 (95%)	6 (5%)	0	100	100
All	All	643/718 (90%)	620 (96%)	23 (4%)	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	174/183 (95%)	172 (99%)	2 (1%)	73	60
1	C	178/183 (97%)	177 (99%)	1 (1%)	86	79
2	B	102/121 (84%)	99 (97%)	3 (3%)	42	19
2	D	102/121 (84%)	101 (99%)	1 (1%)	76	63
All	All	556/608 (91%)	549 (99%)	7 (1%)	69	54

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	383	SER
1	A	494	SER
2	B	0	SER
2	B	31	PHE
2	B	104	SER
1	C	383	SER
2	D	104	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	13	GLN

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Mol	Chain	Res	Type
2	B	54	ASN
1	C	519	HIS
2	D	3	GLN
2	D	5	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)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.58	0	17,19,21	0.69	0
3	FUC	E	2	3	10,10,11	0.78	0	14,14,16	0.87	0
3	NAG	E	3	3	14,14,15	0.53	0	17,19,21	0.42	0
3	FUC	E	4	3	10,10,11	0.84	0	14,14,16	0.89	0
3	NAG	F	1	1,3	14,14,15	0.55	0	17,19,21	0.75	1 (5%)
3	FUC	F	2	3	10,10,11	0.59	0	14,14,16	0.82	0
3	NAG	F	3	3	14,14,15	0.41	0	17,19,21	0.49	0
3	FUC	F	4	3	10,10,11	1.12	1 (10%)	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
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
3	NAG	E	3	3	-	0/6/23/26	0/1/1/1
3	FUC	E	4	3	-	-	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
3	NAG	F	3	3	-	0/6/23/26	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	FUC	O5-C1	-2.31	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	NAG	C1-O5-C5	2.18	115.14	112.19

There are no chirality outliers.

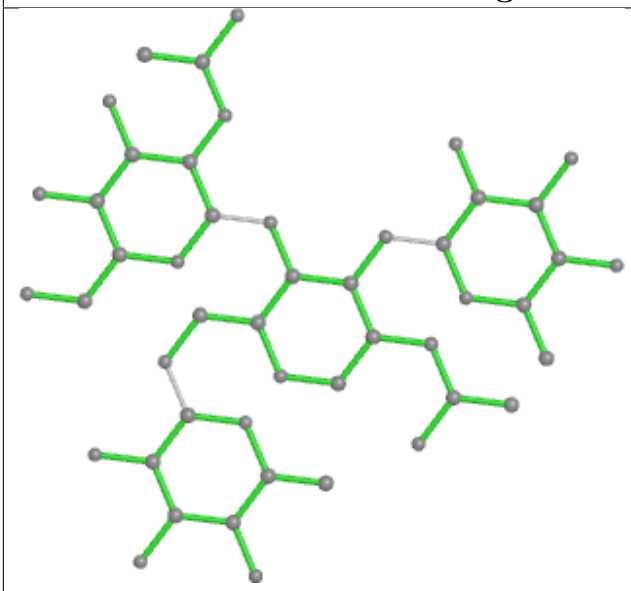
There are no torsion outliers.

There are no ring outliers.

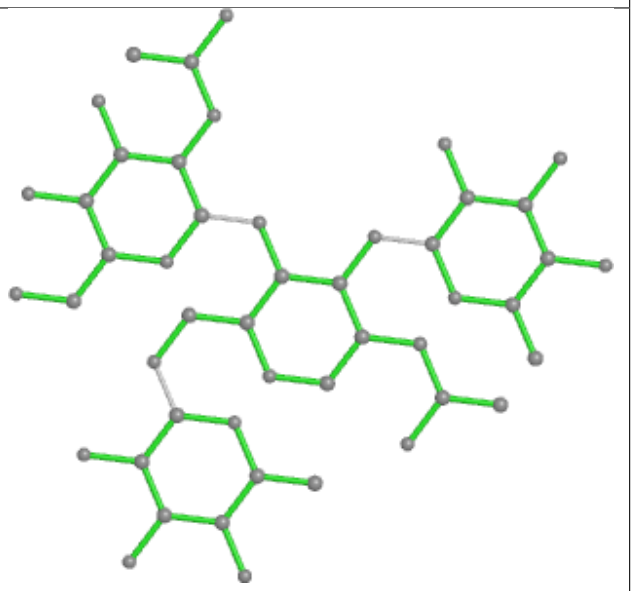
No monomer is involved in short contacts.

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

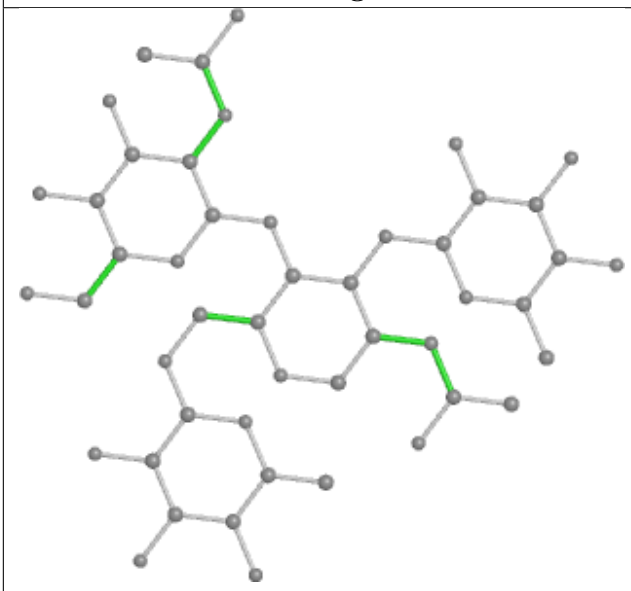
Oligosaccharide Chain E



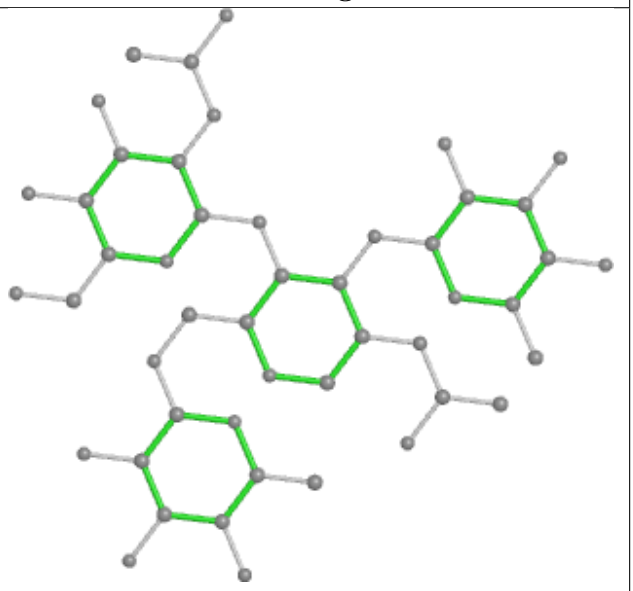
Bond lengths



Bond angles

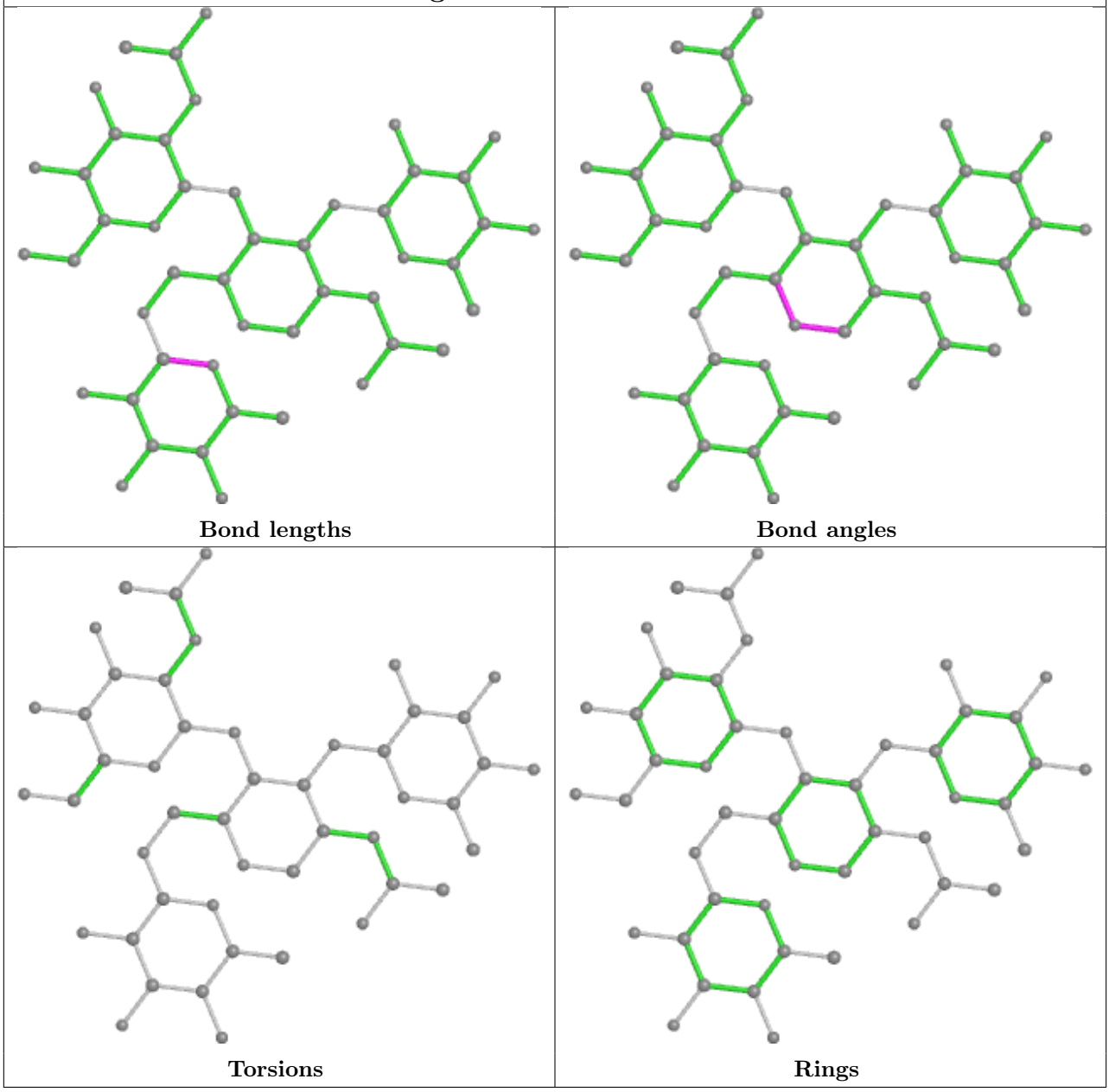


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

26 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	$\#\|Z\|>2$
4	GOL	A	604	-	5,5,5	0.63	0	5,5,5	1.01	0
4	GOL	A	603	-	5,5,5	0.86	0	5,5,5	1.04	1 (20%)
5	ACT	A	612	-	3,3,3	1.29	0	3,3,3	1.44	0
4	GOL	C	601	-	5,5,5	0.97	0	5,5,5	0.94	0
5	ACT	A	611	-	3,3,3	1.37	1 (33%)	3,3,3	1.36	0
5	ACT	A	609	-	3,3,3	1.36	1 (33%)	3,3,3	1.41	0
4	GOL	A	606	-	5,5,5	0.93	0	5,5,5	0.92	0
5	ACT	D	206	-	3,3,3	0.87	0	3,3,3	1.84	2 (66%)
4	GOL	A	601	-	5,5,5	0.81	0	5,5,5	1.04	0
4	GOL	A	602	-	5,5,5	0.84	0	5,5,5	1.01	0
4	GOL	A	605	-	5,5,5	0.86	0	5,5,5	0.98	0
4	GOL	D	202	-	5,5,5	0.94	0	5,5,5	1.02	0
5	ACT	A	608	-	3,3,3	1.30	0	3,3,3	1.39	0
5	ACT	D	204	-	3,3,3	1.26	0	3,3,3	1.50	0
4	GOL	D	201	-	5,5,5	0.77	0	5,5,5	1.10	0
4	GOL	D	205	-	5,5,5	0.81	0	5,5,5	1.06	0
5	ACT	A	607	-	3,3,3	1.34	0	3,3,3	1.34	0
4	GOL	A	614	-	5,5,5	1.73	1 (20%)	5,5,5	0.92	0
5	ACT	A	613	-	3,3,3	1.46	1 (33%)	3,3,3	1.34	0
4	GOL	C	602	-	5,5,5	0.81	0	5,5,5	0.92	0
4	GOL	C	603	-	5,5,5	0.83	0	5,5,5	1.03	0
4	GOL	D	203	-	5,5,5	1.08	1 (20%)	5,5,5	0.99	0
5	ACT	B	202	-	3,3,3	1.48	1 (33%)	3,3,3	1.32	0
5	ACT	A	610	-	3,3,3	1.41	1 (33%)	3,3,3	1.34	0
5	ACT	C	604	-	3,3,3	1.33	0	3,3,3	1.54	0
4	GOL	B	201	-	5,5,5	0.83	0	5,5,5	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	604	-	-	2/4/4/4	-
4	GOL	D	201	-	-	0/4/4/4	-
4	GOL	D	205	-	-	0/4/4/4	-
4	GOL	A	601	-	-	2/4/4/4	-
4	GOL	A	603	-	-	0/4/4/4	-
4	GOL	A	602	-	-	2/4/4/4	-
4	GOL	A	605	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	601	-	-	2/4/4/4	-
4	GOL	A	614	-	-	2/4/4/4	-
4	GOL	D	202	-	-	2/4/4/4	-
4	GOL	D	203	-	-	0/4/4/4	-
4	GOL	C	602	-	-	2/4/4/4	-
4	GOL	C	603	-	-	0/4/4/4	-
4	GOL	B	201	-	-	2/4/4/4	-
4	GOL	A	606	-	-	4/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	614	GOL	O2-C2	-3.43	1.33	1.43
5	B	202	ACT	CH3-C	2.31	1.58	1.49
5	A	613	ACT	CH3-C	2.15	1.58	1.49
4	D	203	GOL	O2-C2	-2.07	1.37	1.43
5	A	611	ACT	CH3-C	2.06	1.57	1.49
5	A	610	ACT	CH3-C	2.04	1.57	1.49
5	A	609	ACT	CH3-C	2.04	1.57	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	206	ACT	O-C-CH3	-2.37	113.12	122.33
5	D	206	ACT	OXT-C-O	2.07	129.69	122.05
4	A	603	GOL	C3-C2-C1	-2.01	103.90	111.70

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	GOL	O1-C1-C2-C3
4	A	604	GOL	O1-C1-C2-C3
4	A	606	GOL	O1-C1-C2-O2
4	A	606	GOL	O1-C1-C2-C3
4	A	606	GOL	C1-C2-C3-O3
4	A	614	GOL	C1-C2-C3-O3
4	B	201	GOL	C1-C2-C3-O3
4	C	601	GOL	C1-C2-C3-O3
4	C	602	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	602	GOL	O1-C1-C2-C3
4	D	202	GOL	C1-C2-C3-O3
4	A	606	GOL	O2-C2-C3-O3
4	A	602	GOL	O1-C1-C2-C3
4	A	601	GOL	O1-C1-C2-O2
4	A	604	GOL	O1-C1-C2-O2
4	A	614	GOL	O2-C2-C3-O3
4	B	201	GOL	O2-C2-C3-O3
4	C	601	GOL	O2-C2-C3-O3
4	D	202	GOL	O2-C2-C3-O3
4	A	602	GOL	O1-C1-C2-O2
4	A	605	GOL	C1-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	612	ACT	1	0
4	C	601	GOL	1	0
4	A	606	GOL	1	0
5	D	206	ACT	2	0
4	A	605	GOL	1	0
4	D	202	GOL	1	0
4	D	201	GOL	1	0
4	D	205	GOL	1	0
4	C	602	GOL	2	0
4	D	203	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	196/213 (92%)	0.56	13 (6%) 18 24	14, 25, 40, 65	0
1	C	200/213 (93%)	0.71	21 (10%) 6 8	16, 27, 48, 73	0
2	B	118/146 (80%)	0.77	12 (10%) 6 9	15, 22, 47, 65	0
2	D	117/146 (80%)	0.37	6 (5%) 28 34	15, 22, 45, 56	0
All	All	631/718 (87%)	0.61	52 (8%) 11 15	14, 25, 46, 73	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	THR	12.7
1	C	332	ILE	11.7
2	D	106	TYR	10.1
1	C	331	ASN	8.5
1	C	330	PRO	7.8
2	D	107	TRP	7.4
2	B	41	PRO	7.3
2	B	42	GLY	6.7
2	B	0	SER	6.6
1	C	529	LYS	5.2
1	C	335	LEU	4.5
1	C	334	ASN	4.5
2	D	0	SER	4.3
1	A	335	LEU	4.0
2	B	107	TRP	3.9
2	B	106[A]	TYR	3.8
1	A	445	VAL	3.6
2	B	1	GLN	3.4
1	A	528	LYS	3.4
1	A	486[A]	PHE	3.4
1	C	528	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	385	THR	3.1
1	C	486[A]	PHE	3.0
1	C	477	SER	3.0
1	C	336	CYS	2.9
2	D	1[A]	GLN	2.8
2	D	105	ASN	2.8
1	C	445	VAL	2.8
1	A	529	LYS	2.5
2	D	44	GLN	2.5
1	A	517	LEU	2.5
1	A	384	PRO	2.5
2	B	44	GLN	2.5
1	C	479	PRO	2.4
1	C	371	SER	2.4
1	C	389	ASP	2.4
1	C	476	GLY	2.4
1	A	402	ILE	2.3
2	B	43	LYS	2.3
1	A	527	PRO	2.2
1	A	492	LEU	2.2
1	A	334	ASN	2.2
1	C	478	THR	2.2
1	C	362	VAL	2.1
2	B	40	ALA	2.1
2	B	59	TYR	2.1
1	C	340	GLU	2.1
1	A	525	CYS	2.1
2	B	102	ARG	2.0
1	A	386	LYS	2.0
2	B	75	GLU	2.0
1	C	339	GLY	2.0

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

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

6.3 Carbohydrates (i)

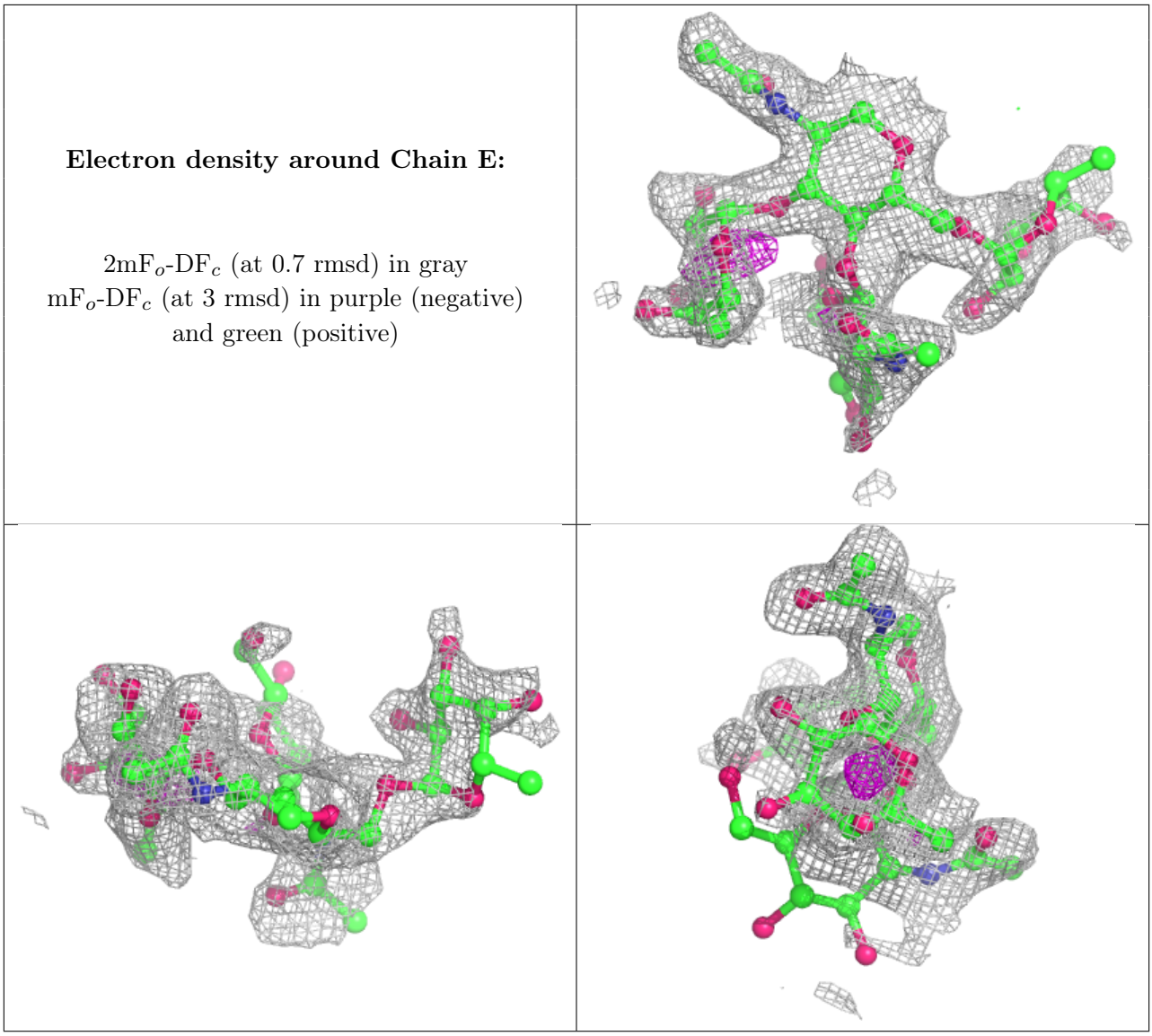
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	FUC	E	2	10/11	0.52	0.39	57,65,69,72	0
3	NAG	E	3	14/15	0.61	0.47	76,81,93,102	0
3	FUC	E	4	10/11	0.68	0.40	84,89,92,92	0
3	FUC	F	2	10/11	0.70	0.35	49,56,58,60	0
3	NAG	F	3	14/15	0.74	0.34	64,73,81,86	0
3	NAG	E	1	14/15	0.75	0.20	42,55,75,78	0
3	FUC	F	4	10/11	0.79	0.60	88,92,100,101	0
3	NAG	F	1	14/15	0.80	0.27	37,50,66,79	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.

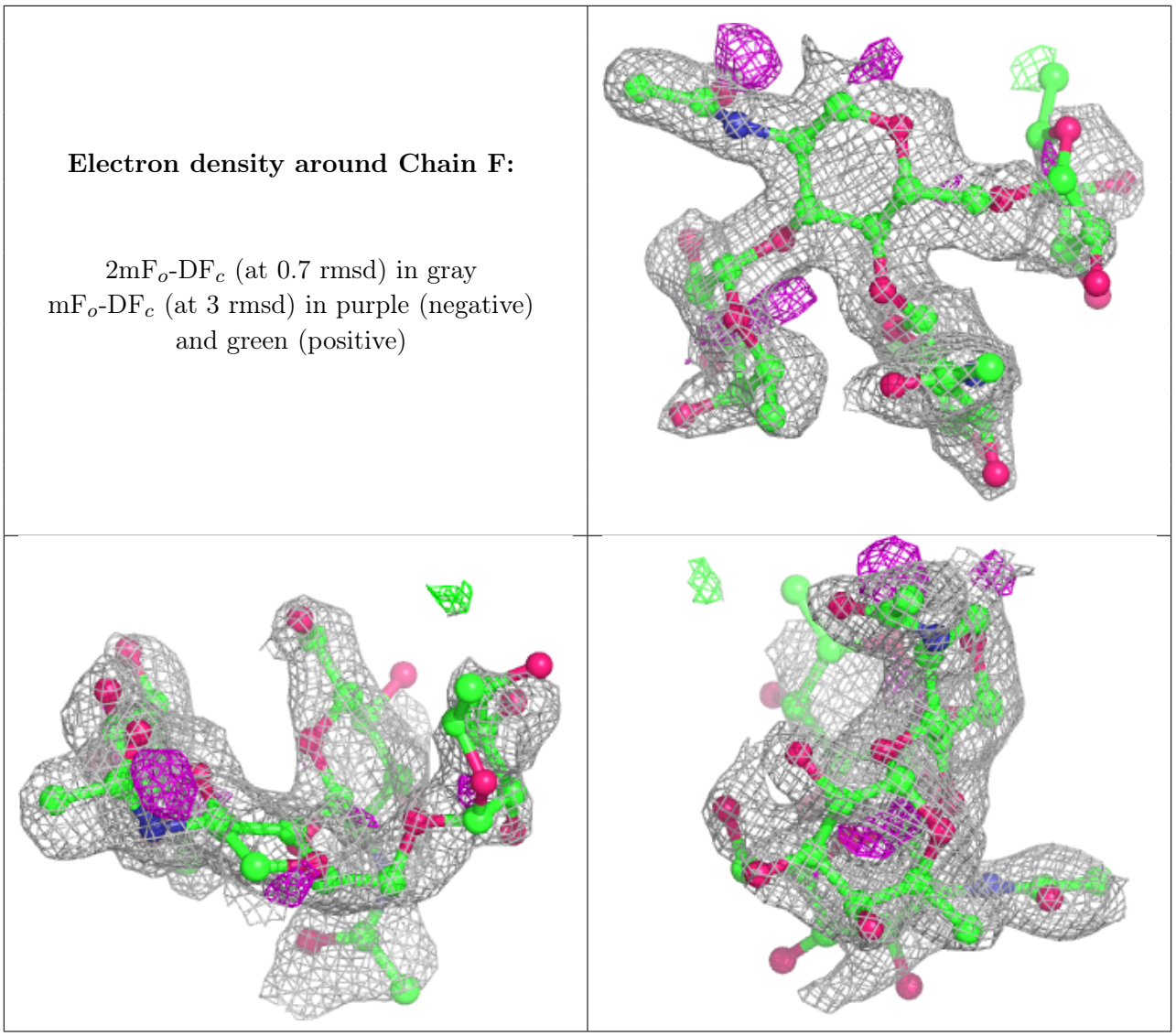
Electron density around Chain E:

$2mF_o$-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 F:

$2mF_o$-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
4	GOL	A	605	6/6	0.55	0.46	51,54,59,71	0
5	ACT	A	608	4/4	0.57	0.41	29,41,44,46	0
5	ACT	A	611	4/4	0.63	0.35	48,51,52,54	0
5	ACT	A	613	4/4	0.64	0.27	41,47,48,53	0
4	GOL	A	602	6/6	0.65	0.42	41,46,52,56	0
4	GOL	B	201	6/6	0.65	0.53	38,46,51,56	0
4	GOL	C	602	6/6	0.65	0.32	37,51,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	D	203	6/6	0.68	0.52	39,49,55,55	0
4	GOL	C	601	6/6	0.69	0.48	43,54,61,62	0
5	ACT	C	604	4/4	0.70	0.23	44,44,50,58	0
5	ACT	B	202	4/4	0.71	0.22	37,42,43,48	0
5	ACT	A	612	4/4	0.74	0.51	49,52,53,58	0
4	GOL	A	603	6/6	0.74	0.28	40,47,51,55	0
4	GOL	D	205	6/6	0.75	0.23	40,44,46,58	0
5	ACT	A	610	4/4	0.76	0.24	42,47,50,54	0
4	GOL	A	606	6/6	0.77	0.24	39,42,46,48	0
5	ACT	D	206	4/4	0.77	0.43	27,30,32,38	0
5	ACT	D	204	4/4	0.80	0.19	32,38,38,42	0
4	GOL	C	603	6/6	0.80	0.30	37,44,52,56	0
4	GOL	A	604	6/6	0.81	0.18	33,37,43,45	0
4	GOL	D	201	6/6	0.84	0.16	38,44,51,53	0
4	GOL	A	614	6/6	0.85	0.35	28,35,37,45	0
5	ACT	A	607	4/4	0.89	0.15	48,50,52,54	0
4	GOL	D	202	6/6	0.92	0.55	37,42,46,47	0
5	ACT	A	609	4/4	0.92	0.24	40,42,46,50	0
4	GOL	A	601	6/6	0.94	0.14	36,41,48,51	0

6.5 Other polymers (i)

There are no such residues in this entry.