wwPDB X-ray Structure Validation Summary Report (i)

Oct 28, 2024 – 08:10 AM JST

PDB ID	:	5HRT
Title	:	Crystal structure of mouse autotaxin in complex with a DNA aptamer
Authors	:	Kato, K.; Nishimasu, H.; Morita, J.; Ishitani, R.; Nureki, O.
Deposited on	:	2016-01-24
Resolution	:	2.00 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:

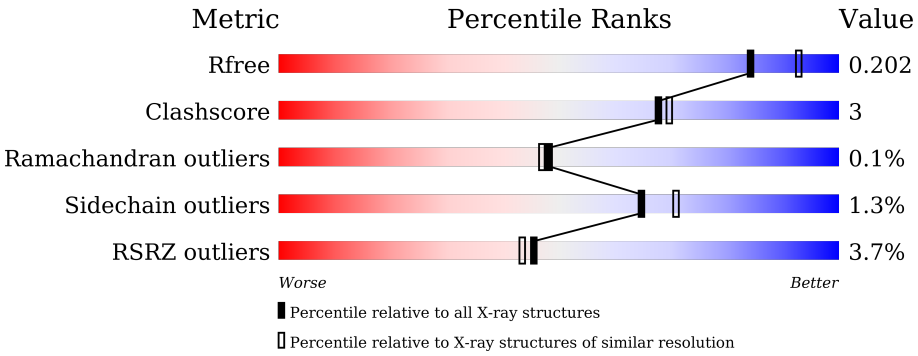
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	831	4%, 88%, 6% • 5%
2	B	34	59%, 26%, 15%
3	C	7	100%
4	D	4	25%, 25%, 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	A	923	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7677 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	786	6306	4005	1090	1163	48	0	5	0

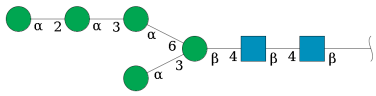
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q9R1E6
A	?	-	VAL	deletion	UNP Q9R1E6
A	?	-	GLU	deletion	UNP Q9R1E6
A	?	-	PRO	deletion	UNP Q9R1E6
A	859	SER	-	expression tag	UNP Q9R1E6
A	860	ARG	-	expression tag	UNP Q9R1E6
A	861	GLU	-	expression tag	UNP Q9R1E6
A	862	ASN	-	expression tag	UNP Q9R1E6
A	863	LEU	-	expression tag	UNP Q9R1E6
A	864	TYR	-	expression tag	UNP Q9R1E6
A	865	PHE	-	expression tag	UNP Q9R1E6
A	866	GLN	-	expression tag	UNP Q9R1E6

- Molecule 2 is a DNA chain called modified DNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	34	712	340	128	211	33	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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
3	C	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 4 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
4	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		

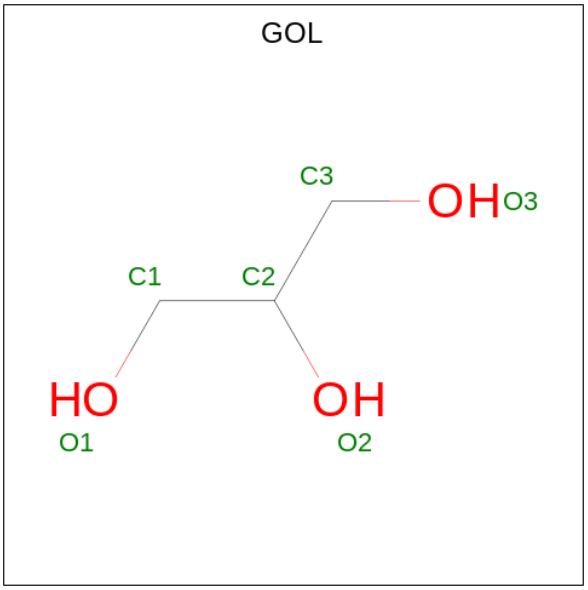
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total K 1 1	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 11 is water.

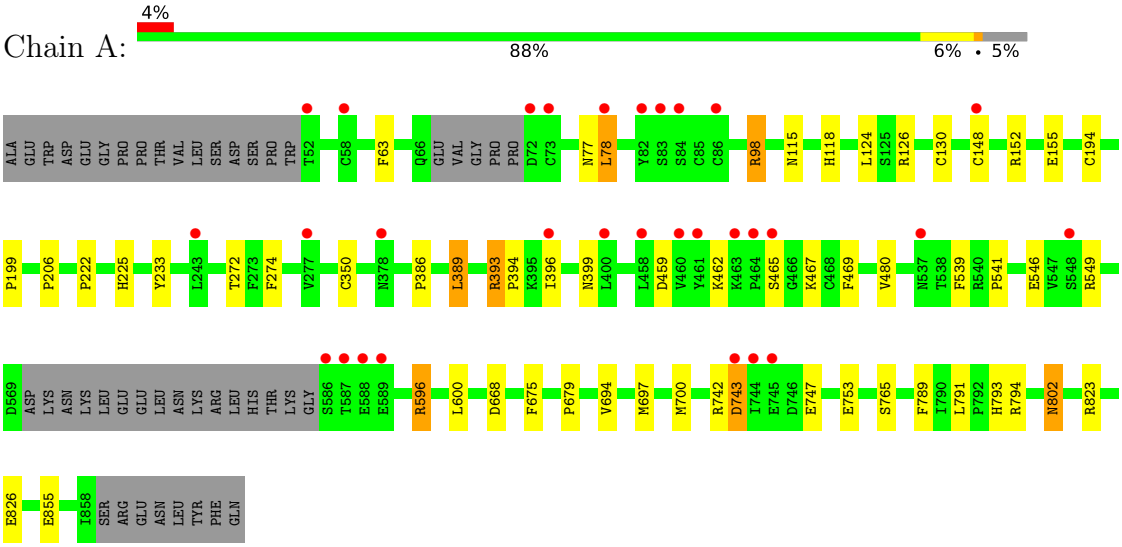
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	441	Total O 441 441	0	0
11	B	18	Total O 18 18	0	0

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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2

Chain A:

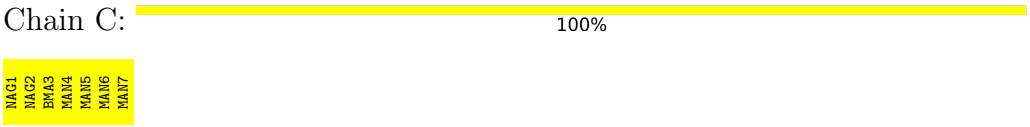


• Molecule 2: modified DNA (34-MER)

Chain B:

• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 C:



• Molecule 4: 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:


NAG1
NAG2
BMA3
MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	120.06Å 208.76Å 90.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.15 – 2.00 45.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.15-2.00) 93.2 (45.15-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.44 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.164 , 0.202 0.164 , 0.202	Depositor DCC
R_{free} test set	1981 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7677	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: CL, BMA, NA, NAG, CA, ZN, MAN, OMG, A2M, GOL, OMC, K

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	0.86	2/6492 (0.0%)	0.82	8/8825 (0.1%)
2	B	1.25	2/564 (0.4%)	1.09	0/868
All	All	0.90	4/7056 (0.1%)	0.85	8/9693 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	480	VAL	CB-CG2	6.96	1.67	1.52
2	B	2012	DC	C3'-O3'	-6.06	1.36	1.44
1	A	130	CYS	CB-SG	5.93	1.92	1.82
2	B	2027	DT	C1'-N1	5.36	1.56	1.49

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	743	ASP	CB-CG-OD2	-10.80	108.58	118.30
1	A	194	CYS	CA-CB-SG	-8.89	98.00	114.00
1	A	148	CYS	CA-CB-SG	-7.42	100.64	114.00
1	A	596	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	A	549	ARG	NE-CZ-NH2	-6.83	116.88	120.30

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	6306	0	5989	38	0
2	B	712	0	402	8	0
3	C	83	0	70	0	0
4	D	50	0	42	1	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	A	60	0	79	11	0
11	A	441	0	0	7	0
11	B	18	0	0	0	0
All	All	7677	0	6582	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 3.

The worst 5 of 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:2019:A2M:C1'	2:B:2019:A2M:O4'	1.64	1.22
2:B:2032:A2M:C1'	2:B:2032:A2M:O4'	1.65	1.19
1:A:826:GLU:HB3	10:A:923:GOL:H12	1.50	0.91
1:A:546:GLU:OE2	1:A:596:ARG:NH1	2.05	0.90
2:B:2033:OMG:HM22	2:B:2034:OMG:H5'	1.61	0.81

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	786/831 (95%)	764 (97%)	21 (3%)	1 (0%)	48 47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	PRO

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	695/756 (92%)	686 (99%)	9 (1%)	65 71

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	467	LYS
1	A	802	ASN
1	A	152	ARG
1	A	199	PRO
1	A	389	LEU

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

Mol	Chain	Res	Type
1	A	77	ASN
1	A	115	ASN
1	A	797	ASN
1	A	802	ASN
1	A	852	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	OMC	B	2020	2	19,22,23	3.11	7 (36%)	26,31,34	0.77	1 (3%)
2	A2M	B	2019	2	18,25,26	4.89	9 (50%)	18,36,39	2.69	4 (22%)
2	OMC	B	2007	2	19,22,23	2.87	7 (36%)	26,31,34	0.97	2 (7%)
2	A2M	B	2032	2	18,25,26	5.00	9 (50%)	18,36,39	2.57	3 (16%)
2	OMG	B	2033	2	18,26,27	2.51	6 (33%)	19,38,41	1.28	2 (10%)
2	A2M	B	2014	2	18,25,26	4.59	9 (50%)	18,36,39	3.11	5 (27%)
2	OMG	B	2034	2	18,26,27	2.61	7 (38%)	19,38,41	1.64	6 (31%)
2	OMG	B	2015	2	18,26,27	2.55	7 (38%)	19,38,41	1.27	3 (15%)
2	OMG	B	2009	2,6	18,26,27	2.34	7 (38%)	19,38,41	1.60	4 (21%)

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
2	OMC	B	2020	2	-	2/9/27/28	0/2/2/2
2	A2M	B	2019	2	-	0/5/27/28	0/3/3/3
2	OMC	B	2007	2	-	7/9/27/28	0/2/2/2
2	A2M	B	2032	2	-	0/5/27/28	0/3/3/3
2	OMG	B	2033	2	-	0/5/27/28	0/3/3/3
2	A2M	B	2014	2	-	0/5/27/28	0/3/3/3
2	OMG	B	2034	2	-	2/5/27/28	0/3/3/3
2	OMG	B	2015	2	-	2/5/27/28	0/3/3/3
2	OMG	B	2009	2,6	-	0/5/27/28	0/3/3/3

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2032	A2M	O4'-C1'	17.31	1.65	1.41
2	B	2019	A2M	O4'-C1'	16.93	1.64	1.41
2	B	2014	A2M	O4'-C1'	15.62	1.62	1.41
2	B	2032	A2M	O4'-C4'	-7.10	1.29	1.45
2	B	2014	A2M	O4'-C4'	-6.99	1.29	1.45

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2014	A2M	C5-C6-N6	8.30	132.96	120.35
2	B	2019	A2M	C5-C6-N6	7.86	132.29	120.35
2	B	2032	A2M	C5-C6-N6	7.04	131.05	120.35
2	B	2014	A2M	N6-C6-N1	-6.38	105.32	118.57
2	B	2014	A2M	N3-C2-N1	-6.34	118.77	128.68

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2007	OMC	C1'-C2'-O2'-CM2
2	B	2015	OMG	C1'-C2'-O2'-CM2
2	B	2020	OMC	C3'-C4'-C5'-O5'
2	B	2020	OMC	O4'-C4'-C5'-O5'
2	B	2007	OMC	C2'-C1'-N1-C6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2019	A2M	1	0
2	B	2007	OMC	1	0
2	B	2032	A2M	4	0
2	B	2033	OMG	2	0
2	B	2034	OMG	1	0

5.5 Carbohydrates (i)

11 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1	3,1	14,14,15	0.79	1 (7%)	17,19,21	1.03	1 (5%)
3	NAG	C	2	3	14,14,15	0.85	1 (7%)	17,19,21	0.78	0
3	BMA	C	3	3	11,11,12	1.46	1 (9%)	15,15,17	1.11	1 (6%)
3	MAN	C	4	3	11,11,12	0.92	0	15,15,17	1.35	2 (13%)
3	MAN	C	5	3	11,11,12	1.96	3 (27%)	15,15,17	1.08	1 (6%)
3	MAN	C	6	3	11,11,12	1.60	3 (27%)	15,15,17	1.56	3 (20%)
3	MAN	C	7	3	11,11,12	1.54	2 (18%)	15,15,17	1.11	2 (13%)
4	NAG	D	1	4,1	14,14,15	0.58	0	17,19,21	0.69	0
4	NAG	D	2	4	14,14,15	0.44	0	17,19,21	1.31	2 (11%)
4	BMA	D	3	4	11,11,12	3.84	6 (54%)	15,15,17	3.46	7 (46%)
4	MAN	D	4	4	11,11,12	1.96	4 (36%)	15,15,17	1.40	3 (20%)

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	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	1/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	BMA	O5-C5	8.63	1.60	1.43
4	D	3	BMA	O2-C2	-5.33	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	BMA	C2-C3	-5.28	1.44	1.52
3	C	5	MAN	C2-C3	4.66	1.59	1.52
4	D	4	MAN	C1-C2	4.39	1.62	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3	BMA	O5-C5-C6	7.36	118.74	107.20
4	D	3	BMA	O2-C2-C3	-6.37	97.38	110.14
4	D	3	BMA	C1-C2-C3	5.84	116.85	109.67
4	D	3	BMA	C1-O5-C5	4.86	118.77	112.19
3	C	6	MAN	C1-O5-C5	3.70	117.20	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

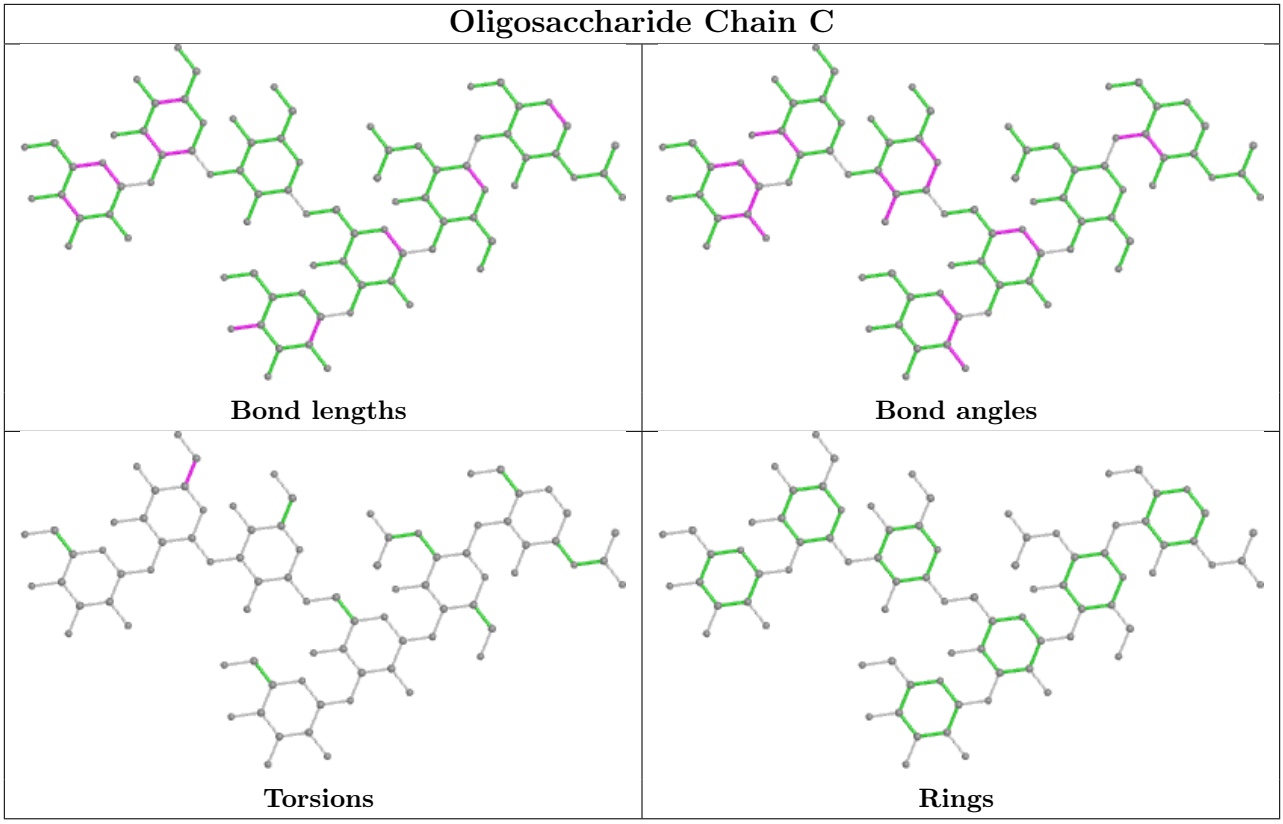
All (1) ring outliers are listed below:

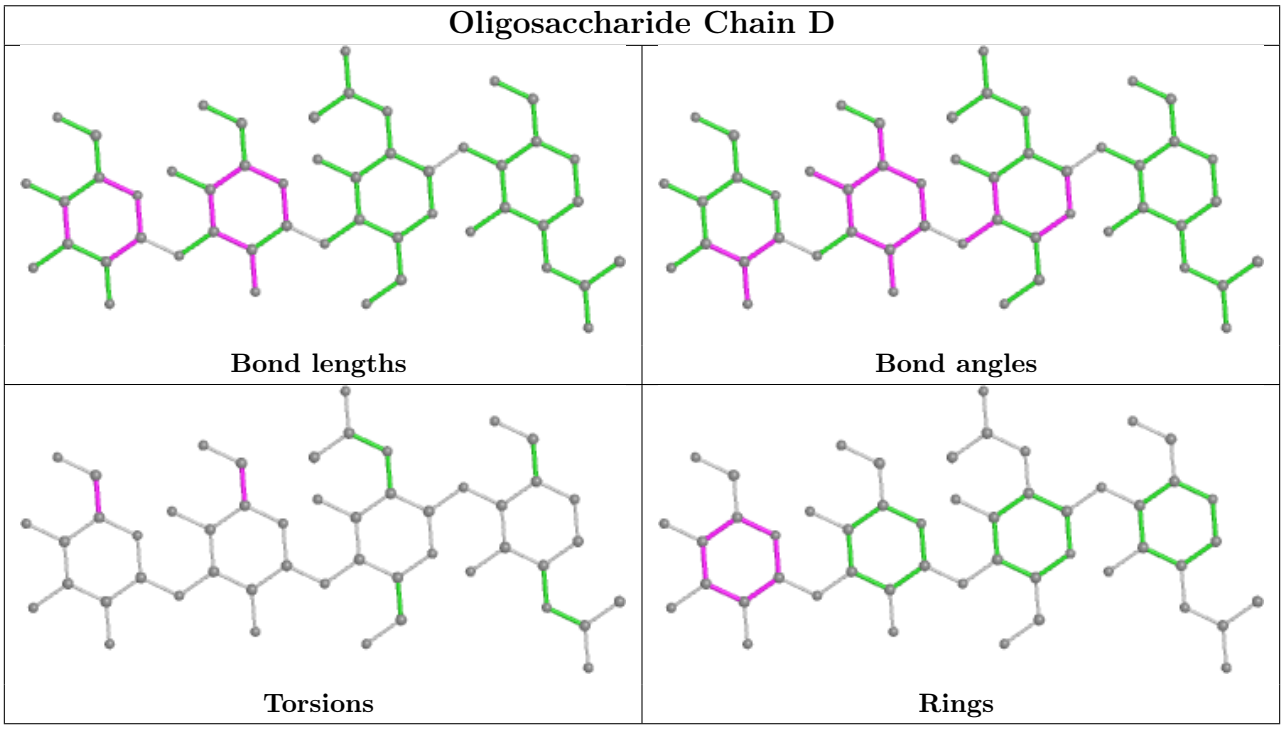
Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	BMA	1	0
4	D	2	NAG	1	0

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





5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	GOL	A	924	-	5,5,5	0.48	0	5,5,5	1.00	0
10	GOL	A	922	-	5,5,5	0.40	0	5,5,5	0.34	0
10	GOL	A	920	-	5,5,5	0.77	0	5,5,5	1.22	1 (20%)
10	GOL	A	926	-	5,5,5	0.52	0	5,5,5	0.66	0
10	GOL	A	918	-	5,5,5	0.49	0	5,5,5	0.50	0
10	GOL	A	925	-	5,5,5	0.35	0	5,5,5	0.44	0
10	GOL	A	923	-	5,5,5	0.51	0	5,5,5	1.09	0
10	GOL	A	919	-	5,5,5	0.32	0	5,5,5	0.46	0
10	GOL	A	927	-	5,5,5	0.70	0	5,5,5	0.90	0
10	GOL	A	921	-	5,5,5	0.32	0	5,5,5	1.01	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
10	GOL	A	924	-	-	2/4/4/4	-
10	GOL	A	922	-	-	2/4/4/4	-
10	GOL	A	920	-	-	4/4/4/4	-
10	GOL	A	926	-	-	4/4/4/4	-
10	GOL	A	918	-	-	3/4/4/4	-
10	GOL	A	925	-	-	2/4/4/4	-
10	GOL	A	923	-	-	2/4/4/4	-
10	GOL	A	919	-	-	4/4/4/4	-
10	GOL	A	927	-	-	4/4/4/4	-
10	GOL	A	921	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	920	GOL	C3-C2-C1	-2.26	102.92	111.70

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	918	GOL	O1-C1-C2-C3
10	A	919	GOL	O1-C1-C2-C3
10	A	920	GOL	C1-C2-C3-O3
10	A	921	GOL	C1-C2-C3-O3
10	A	921	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	924	GOL	1	0
10	A	920	GOL	3	0
10	A	923	GOL	7	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	786/831 (94%)	-0.13	30 (3%) 44 42	10, 30, 67, 96	5 (0%)
2	B	25/34 (73%)	0.08	0 100 100	33, 60, 105, 108	0
All	All	811/865 (93%)	-0.12	30 (3%) 45 43	10, 31, 72, 108	5 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	744	ILE	6.1
1	A	587	THR	4.4
1	A	461	TYR	4.0
1	A	458	LEU	3.7
1	A	464	PRO	3.6

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

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
2	OMG	B	2034	24/25	0.43	0.20	88,99,102,103	0
2	OMG	B	2033	24/25	0.70	0.17	77,91,96,98	0
2	A2M	B	2019	23/24	0.72	0.16	112,124,129,133	0
2	OMC	B	2020	21/22	0.72	0.19	106,124,132,137	0
2	A2M	B	2032	23/24	0.74	0.16	73,76,86,92	0
2	OMG	B	2015	24/25	0.91	0.10	58,65,75,80	0
2	OMC	B	2007	21/22	0.94	0.10	51,57,70,76	0
2	A2M	B	2014	23/24	0.94	0.11	47,59,68,71	0
2	OMG	B	2009	24/25	0.97	0.08	39,45,50,54	0

6.3 Carbohydrates (i)

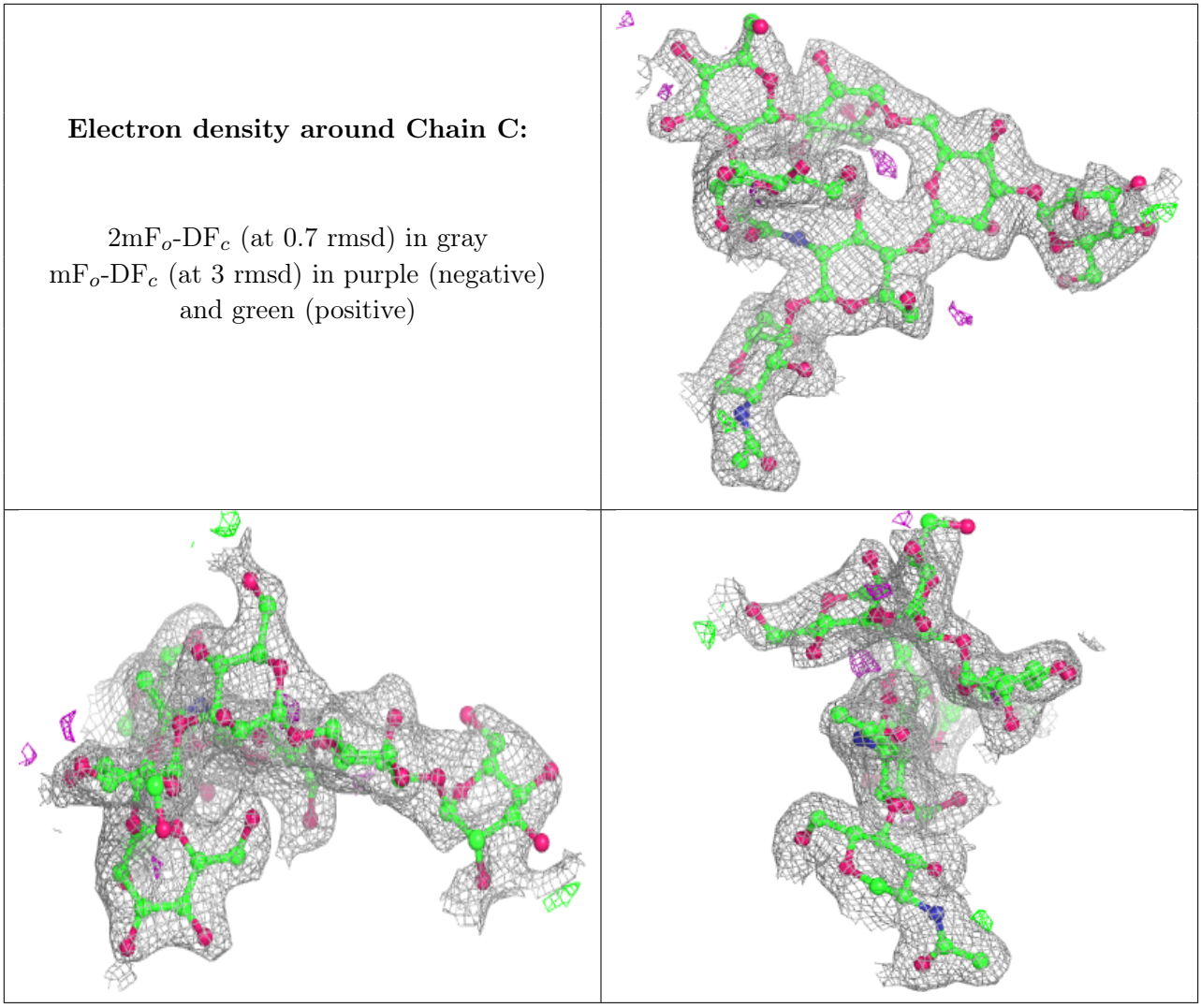
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MAN	C	7	11/12	0.60	0.15	78,84,85,87	0
4	MAN	D	4	11/12	0.68	0.13	71,73,75,76	0
4	BMA	D	3	11/12	0.82	0.15	45,54,62,68	0
3	MAN	C	5	11/12	0.87	0.16	56,63,67,69	0
3	MAN	C	4	11/12	0.87	0.11	62,63,67,69	0
3	BMA	C	3	11/12	0.88	0.10	52,59,63,70	0
3	MAN	C	6	11/12	0.90	0.12	41,51,54,54	0
4	NAG	D	1	14/15	0.93	0.08	28,34,40,45	0
4	NAG	D	2	14/15	0.93	0.10	39,44,51,52	0
3	NAG	C	2	14/15	0.94	0.08	32,35,39,46	0
3	NAG	C	1	14/15	0.97	0.06	20,23,26,29	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.

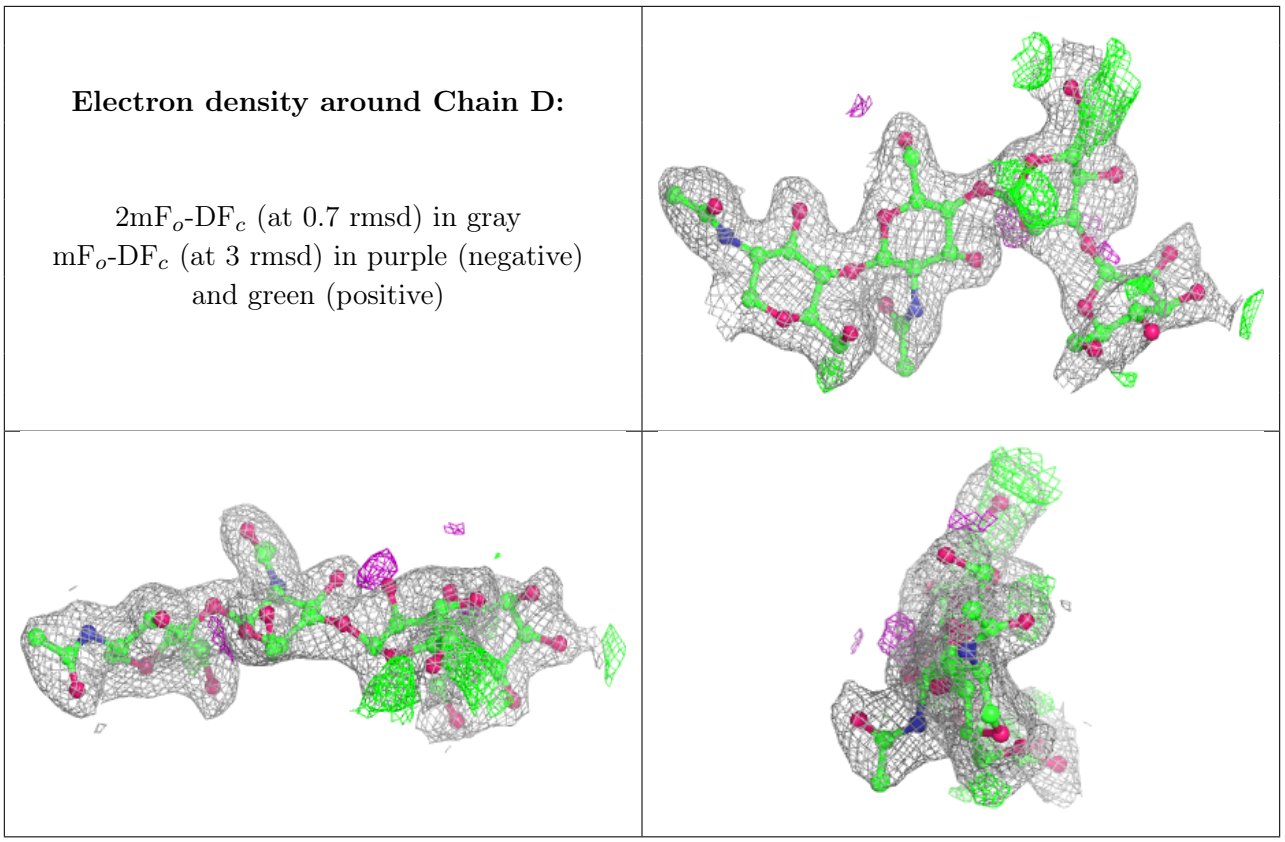
Electron density around Chain C:

$2mF_o$-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

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
10	GOL	A	922	6/6	0.73	0.13	68,69,70,71	0
10	GOL	A	926	6/6	0.81	0.17	44,56,57,60	0
10	GOL	A	927	6/6	0.85	0.21	52,58,65,67	0
10	GOL	A	918	6/6	0.86	0.16	57,62,63,65	0
10	GOL	A	925	6/6	0.86	0.15	57,61,61,62	0
10	GOL	A	921	6/6	0.87	0.16	60,62,63,64	0
10	GOL	A	919	6/6	0.88	0.14	53,57,59,60	0
10	GOL	A	923	6/6	0.88	0.16	63,66,67,68	0
10	GOL	A	924	6/6	0.88	0.18	56,64,65,65	0
10	GOL	A	920	6/6	0.89	0.15	47,59,62,64	0
6	CA	B	2101	1/1	0.97	0.05	49,49,49,49	0
8	CL	A	916	1/1	0.97	0.07	42,42,42,42	0
6	CA	A	914	1/1	0.99	0.03	22,22,22,22	0
9	K	A	917	1/1	0.99	0.02	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NA	A	915	1/1	0.99	0.05	30,30,30,30	0
5	ZN	A	913	1/1	1.00	0.01	25,25,25,25	0
5	ZN	A	912	1/1	1.00	0.01	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.