Worldwide PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2020 – 10:55 AM BST

PDB ID	:	5KOE
Title	:	The structure of Arabidopsis thaliana FUT1 in complex with XXLG
Authors	:	Alahuhta, P.M.; Lunin, V.V.
Deposited on	:	2016-06-30
Resolution	:	1.79 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 following versions of software and data (see references (i)) were used in the production of this report:

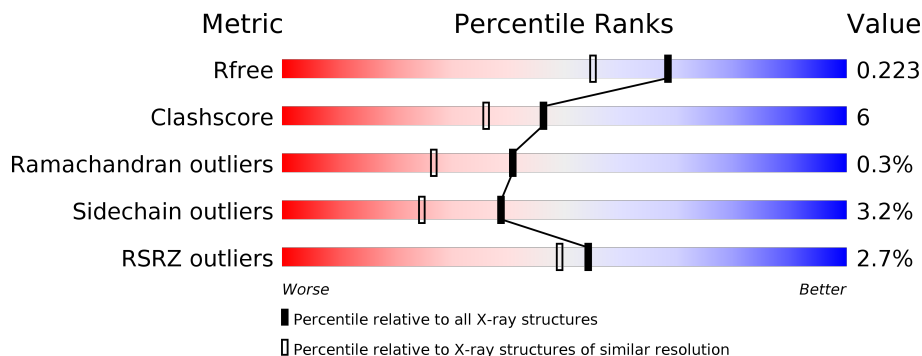|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.79 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	Percentile Ranks	Value
Rfree		0.223
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		3.2%
RSRZ outliers		2.7%

Worse — Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	476	2% / 82% / 9% · 6%
1	B	476	3% / 79% / 14% · 5%
1	C	476	4% / 86% / 10% ·
1	D	476	2% / 83% / 12% · 5%
2	E	8	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	D	607	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 17403 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 Galactoside 2-alpha-L-fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total 3700	C 2379	N 616	O 683	S 22	0	17	0
1	B	452	Total 3772	C 2420	N 625	O 705	S 22	0	19	0
1	C	458	Total 3819	C 2443	N 647	O 707	S 22	0	17	0
1	D	454	Total 3768	C 2416	N 632	O 696	S 24	0	19	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLY	-	expression tag	UNP Q9SWH5
B	83	GLY	-	expression tag	UNP Q9SWH5
C	83	GLY	-	expression tag	UNP Q9SWH5
D	83	GLY	-	expression tag	UNP Q9SWH5

- Molecule 2 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.
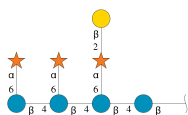
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	8	Total 83	C 45	O 38	0	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

MES

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	S		0	0
			12	6	1	4	1			
3	A	1	Total	C	N	O	S		0	0
			12	6	1	4	1			
3	C	1	Total	C	N	O	S		0	0
			12	6	1	4	1			
3	C	1	Total	C	N	O	S		0	0
			12	6	1	4	1			
3	D	1	Total	C	N	O	S		0	0
			12	6	1	4	1			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Cl	0	0
			4	4		
4	A	8	Total	Cl	0	0
			8	8		
4	D	3	Total	Cl	0	0
			3	3		
4	C	4	Total	Cl	0	0
			4	4		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	K 2	0	0
5	A	2	Total 2	K 2	0	0
5	D	1	Total 1	K 1	0	0
5	C	3	Total 3	K 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
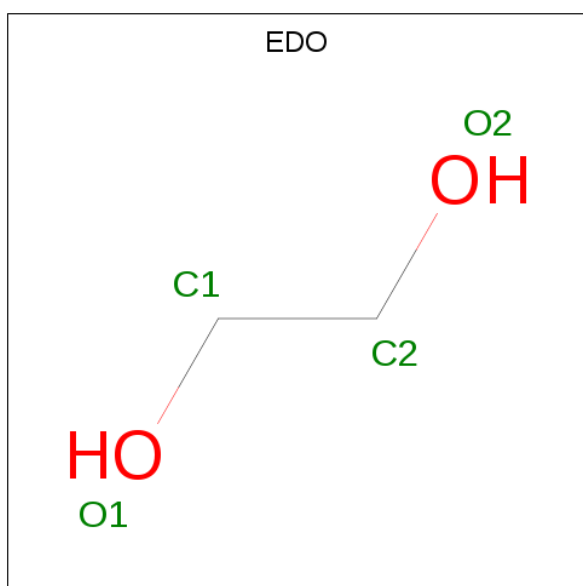
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 8	C 4	O 4	0	1

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0

- Molecule 8 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	544	Total 568	O 568	0	24
8	B	492	Total 506	O 506	0	14
8	C	546	Total 564	O 564	0	18
8	D	495	Total 508	O 508	0	13

3 Residue-property plots ⓘ

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: Galactoside 2-alpha-L-fucosyltransferase
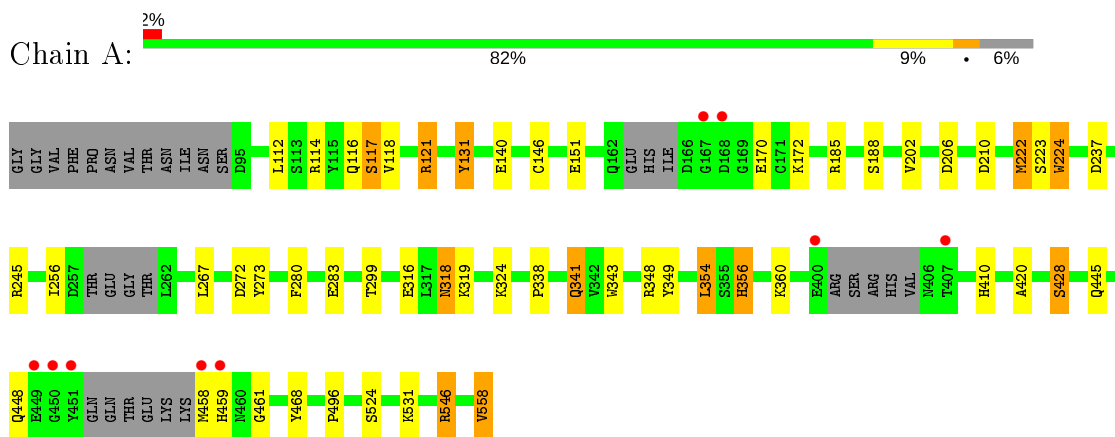
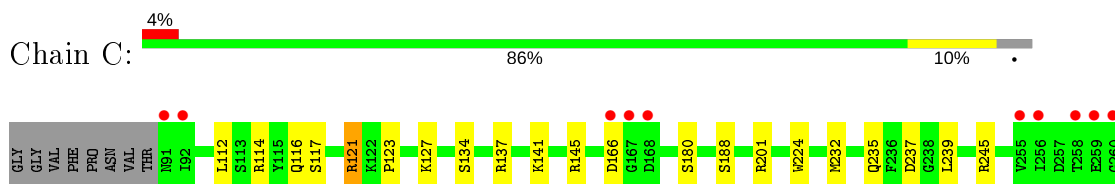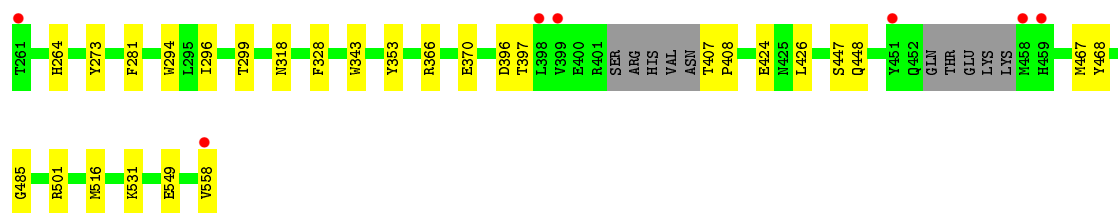- Molecule 1: Galactoside 2-alpha-L-fucosyltransferase
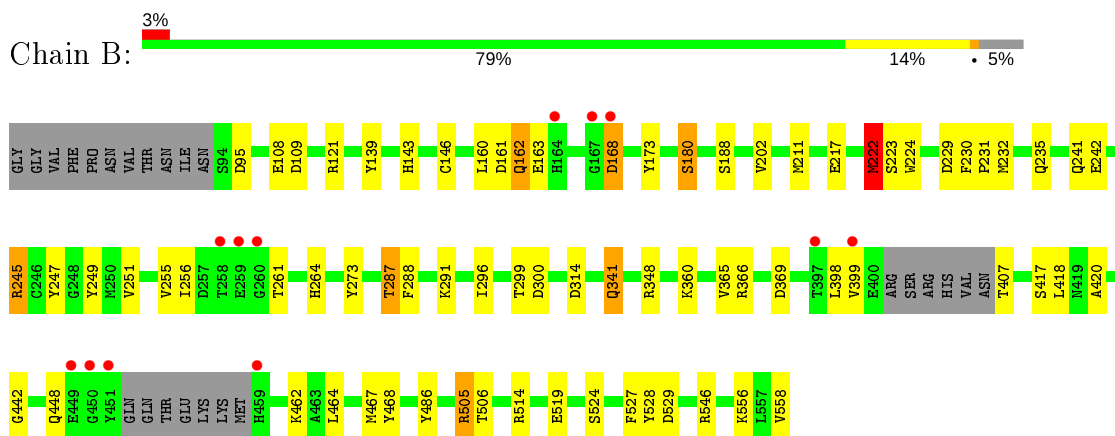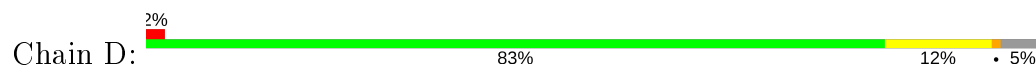

- Molecule 1: Galactoside 2-alpha-L-fucosyltransferase

• Molecule 1: Galactoside 2-alpha-L-fucosyltransferase
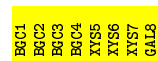

• Molecule 2: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.75Å 80.15Å 157.62Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	157.53 – 1.79 73.54 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.5 (157.53-1.79) 99.6 (73.54-1.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.166 , 0.217 0.174 , 0.223	Depositor DCC
R_{free} test set	9305 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l 0.010 for -k,-h,-l 0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17403	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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 33.32 % 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 8.1476e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BGC, CL, K, EDO, XYS, MES, GAL

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	1.23	12/3801 (0.3%)	1.10	12/5147 (0.2%)
1	B	1.19	9/3876 (0.2%)	1.14	23/5253 (0.4%)
1	C	1.20	8/3925 (0.2%)	1.11	16/5321 (0.3%)
1	D	1.14	0/3876	1.10	18/5258 (0.3%)
All	All	1.19	29/15478 (0.2%)	1.11	69/20979 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	TYR	CE2-CZ	-6.46	1.30	1.38
1	A	428	SER	CB-OG	-6.41	1.33	1.42
1	A	117	SER	CB-OG	5.86	1.49	1.42
1	B	249	TYR	CB-CG	-5.79	1.43	1.51
1	A	343	TRP	CB-CG	-5.78	1.39	1.50
1	C	201	ARG	CZ-NH1	5.77	1.40	1.33
1	A	316	GLU	CD-OE1	5.66	1.31	1.25
1	C	468	TYR	CB-CG	-5.61	1.43	1.51
1	A	349	TYR	CE1-CZ	-5.59	1.31	1.38
1	B	528	TYR	CG-CD2	-5.57	1.31	1.39
1	C	424	GLU	CG-CD	5.51	1.60	1.51
1	C	396	ASP	CB-CG	-5.51	1.40	1.51
1	A	151	GLU	CD-OE1	5.46	1.31	1.25
1	A	283	GLU	CD-OE1	5.46	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	328	PHE	CG-CD1	-5.40	1.30	1.38
1	B	180	SER	CA-CB	5.38	1.61	1.52
1	B	486	TYR	CE1-CZ	5.33	1.45	1.38
1	C	353	TYR	CE1-CZ	-5.29	1.31	1.38
1	B	173	TYR	CE1-CZ	-5.23	1.31	1.38
1	C	485	GLY	N-CA	-5.19	1.38	1.46
1	C	137	ARG	CZ-NH1	-5.16	1.26	1.33
1	A	131	TYR	CE2-CZ	5.16	1.45	1.38
1	A	224	TRP	CG-CD1	-5.15	1.29	1.36
1	B	95	ASP	CB-CG	5.09	1.62	1.51
1	B	247	TYR	CZ-OH	5.08	1.46	1.37
1	A	524	SER	CB-OG	5.07	1.48	1.42
1	A	140	GLU	CD-OE2	5.04	1.31	1.25
1	B	442	GLY	C-O	5.04	1.31	1.23
1	A	459	HIS	C-O	5.00	1.32	1.23

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	222[A]	MET	CG-SD-CE	9.57	115.51	100.20
1	B	222[B]	MET	CG-SD-CE	9.57	115.51	100.20
1	C	145	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	B	245	ARG	NE-CZ-NH1	-8.93	115.83	120.30
1	B	95	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	467	MET	CG-SD-CE	7.98	112.97	100.20
1	C	145	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	A	206	ASP	CB-CG-OD1	7.35	124.91	118.30
1	C	468	TYR	CB-CG-CD1	-7.19	116.69	121.00
1	D	234	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	C	467	MET	CG-SD-CE	7.06	111.49	100.20
1	B	229	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	B	486	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	B	486	TYR	CB-CG-CD1	7.01	125.21	121.00
1	C	366	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	426	LEU	CA-CB-CG	6.85	131.06	115.30
1	B	505	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	121	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	B	109	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	229	ASP	CB-CG-OD1	6.76	124.39	118.30
1	C	549	GLU	OE1-CD-OE2	-6.62	115.36	123.30
1	D	333	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	114	ARG	NE-CZ-NH1	-6.49	117.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	396	ASP	N-CA-CB	-6.31	99.24	110.60
1	D	371	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	272	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	348	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	211	MET	CG-SD-CE	-6.25	90.20	100.20
1	B	529	ASP	CB-CG-OD1	6.23	123.91	118.30
1	C	137	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	B	514	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	C	328	PHE	CB-CG-CD2	-6.05	116.56	120.80
1	B	528	TYR	CB-CG-CD1	6.05	124.63	121.00
1	C	137	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	B	109	ASP	CB-CG-OD1	5.91	123.61	118.30
1	D	145	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	C	121[A]	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	C	121[B]	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	D	275	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	D	314	ASP	CB-CG-OD1	5.68	123.42	118.30
1	D	348	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	D	522	PHE	CB-CG-CD1	5.63	124.75	120.80
1	A	114	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	316	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	D	187	LEU	CB-CG-CD2	5.54	120.42	111.00
1	A	546	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	B	314	ASP	CB-CG-OD1	5.46	123.22	118.30
1	D	371	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	D	275	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	300	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	514	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	354	LEU	CB-CG-CD1	5.32	120.04	111.00
1	D	121[A]	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	D	121[B]	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	245[A]	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	245[B]	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	558[A]	VAL	CB-CA-C	-5.28	101.37	111.40
1	A	558[B]	VAL	CB-CA-C	-5.28	101.37	111.40
1	B	348	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	D	285	ASP	CB-CG-OD1	5.26	123.03	118.30
1	D	265	LEU	CA-CB-CG	5.23	127.32	115.30
1	D	201	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	304	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	B	95	ASP	N-CA-CB	5.17	119.91	110.60
1	B	348	ARG	NE-CZ-NH1	5.15	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	366	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	501[A]	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	C	501[B]	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	D	468	TYR	CB-CG-CD1	-5.00	118.00	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	161	ASP	Peptide

5.2 Too-close contacts (i)

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	3700	0	3573	44	0
1	B	3772	0	3622	51	0
1	C	3819	0	3663	36	0
1	D	3768	0	3608	46	0
2	E	83	0	69	0	0
3	A	24	0	26	1	0
3	C	24	0	26	1	0
3	D	12	0	13	0	0
4	A	8	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	1	0
4	D	3	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
6	A	4	0	6	0	0
6	C	4	0	6	2	0
6	D	8	0	12	0	0
7	C	6	0	8	2	0
7	D	6	0	8	5	0
8	A	568	0	0	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	506	0	0	17	1
8	C	564	0	0	18	1
8	D	508	0	0	24	0
All	All	17403	0	14640	186	1

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 6.

All (186) 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)
1:C:516[A]:MET:CE	1:C:558[A]:VAL:HG11	1.49	1.41
7:D:607:GOL:O3	8:D:702:HOH:O	1.54	1.24
1:B:527[A]:PHE:CE1	8:B:730:HOH:O	1.76	1.22
1:C:121[B]:ARG:CG	8:C:1095:HOH:O	1.84	1.22
1:B:527[A]:PHE:CD1	8:B:730:HOH:O	1.74	1.19
1:A:410[B]:HIS:HE1	8:A:730:HOH:O	1.17	1.19
1:D:356[A]:HIS:CE1	8:D:709:HOH:O	1.91	1.18
1:A:410[A]:HIS:CE1	8:A:726:HOH:O	1.93	1.18
1:A:410[B]:HIS:CE1	8:A:730:HOH:O	1.88	1.16
7:D:607:GOL:O1	8:D:703:HOH:O	1.67	1.13
1:C:121[B]:ARG:HG3	8:C:1095:HOH:O	1.45	1.10
1:D:356[B]:HIS:ND1	8:D:706:HOH:O	1.80	1.09
1:B:546[B]:ARG:HD3	1:B:558[B]:VAL:HG11	1.34	1.08
4:C:604:CL:CL	8:C:813[B]:HOH:O	2.09	1.07
1:C:516[A]:MET:CE	1:C:558[A]:VAL:CG1	2.32	1.07
1:C:516[A]:MET:HE3	1:C:558[A]:VAL:HG11	1.25	1.06
1:D:121[A]:ARG:NH2	8:D:707[A]:HOH:O	1.89	1.05
1:A:356[A]:HIS:CD2	8:A:716:HOH:O	2.08	1.04
1:B:341[A]:GLN:HG2	8:B:705:HOH:O	1.61	0.99
1:D:356[B]:HIS:CD2	8:D:710:HOH:O	2.14	0.98
1:D:534[A]:THR:OG1	8:D:705:HOH:O	1.78	0.98
1:C:516[A]:MET:HE1	1:C:558[A]:VAL:HG11	1.42	0.98
1:D:182:LEU:HD22	1:D:460[B]:ASN:OD1	1.67	0.94
1:B:341[A]:GLN:CG	8:B:705:HOH:O	2.14	0.92
1:B:222[A]:MET:CE	1:B:223[A]:SER:H	1.84	0.90
1:C:318[A]:ASN:ND2	8:C:705:HOH:O	2.03	0.90
1:B:222[A]:MET:HE2	1:B:223[A]:SER:H	1.35	0.89
1:A:121:ARG:HD2	8:A:853:HOH:O	1.72	0.88
1:A:172[A]:LYS:NZ	8:A:705[A]:HOH:O	2.09	0.86
1:C:318[A]:ASN:CG	8:C:705:HOH:O	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356[B]:HIS:CE1	8:D:706:HOH:O	2.22	0.83
1:D:279[B]:MET:CE	8:D:745:HOH:O	2.27	0.82
1:D:356[B]:HIS:NE2	8:D:710:HOH:O	2.11	0.82
1:C:318[A]:ASN:OD1	8:C:705:HOH:O	1.97	0.82
1:B:558[B]:VAL:OXT	8:B:704:HOH:O	1.99	0.80
1:C:121[A]:ARG:HD2	8:C:912:HOH:O	1.79	0.80
1:B:546[B]:ARG:HD3	1:B:558[B]:VAL:CG1	2.12	0.80
7:D:607:GOL:H12	8:D:1119:HOH:O	1.83	0.79
1:D:410[A]:HIS:CE1	8:D:720:HOH:O	2.38	0.75
1:D:341[A]:GLN:OE1	1:D:458[A]:MET:SD	2.45	0.75
1:A:172[A]:LYS:CE	8:A:705[A]:HOH:O	2.35	0.75
1:C:318[B]:ASN:OD1	8:C:706:HOH:O	2.04	0.75
1:D:341[B]:GLN:NE2	8:D:711:HOH:O	2.18	0.74
1:A:222[A]:MET:HA	1:A:222[A]:MET:HE3	1.70	0.74
1:D:448[B]:GLN:HA	1:D:448[B]:GLN:OE1	1.86	0.74
1:A:172[A]:LYS:HE2	8:A:705[A]:HOH:O	1.87	0.74
1:D:458[A]:MET:SD	8:D:936:HOH:O	2.46	0.73
8:A:1151[B]:HOH:O	1:C:516[B]:MET:HE3	1.88	0.73
1:B:341[A]:GLN:OE1	8:B:705:HOH:O	2.06	0.73
1:B:261:THR:HG23	1:B:291[A]:LYS:HG3	1.70	0.73
1:B:546[B]:ARG:CD	1:B:558[B]:VAL:HG11	2.16	0.73
1:B:121[A]:ARG:NH1	1:B:121[A]:ARG:HG3	2.04	0.72
1:B:121[A]:ARG:HH11	1:B:121[A]:ARG:HG3	1.56	0.71
1:B:369:ASP:OD2	1:B:505:ARG:NH1	2.22	0.71
1:B:222[A]:MET:HE2	1:B:223[A]:SER:N	2.05	0.71
7:C:611:GOL:O1	8:C:708:HOH:O	2.09	0.71
1:B:288:PHE:CE1	1:B:291[A]:LYS:HE2	2.26	0.71
1:C:516[A]:MET:HE3	1:C:558[A]:VAL:CG1	2.09	0.71
1:B:139:TYR:OH	1:B:143:HIS:HD2	1.74	0.70
1:A:356[A]:HIS:ND1	8:A:708:HOH:O	2.25	0.68
1:D:121[A]:ARG:CZ	8:D:707[A]:HOH:O	2.35	0.67
1:A:222[A]:MET:CE	1:A:223[A]:SER:H	2.08	0.67
3:C:602:MES:O1	8:C:1004[B]:HOH:O	2.14	0.66
1:B:188:SER:HB2	1:B:299:THR:HG23	1.76	0.66
1:C:447:SER:HB2	8:C:917:HOH:O	1.96	0.65
1:A:131:TYR:CD1	1:A:319[B]:LYS:HE2	2.32	0.65
1:D:420:ALA:HB2	1:D:448[A]:GLN:HE22	1.61	0.65
1:A:546:ARG:NH1	8:A:710:HOH:O	2.29	0.64
1:D:188:SER:HB2	1:D:299:THR:HG23	1.80	0.64
1:B:287:THR:HG21	8:B:1125:HOH:O	1.98	0.64
1:B:160[A]:LEU:O	1:B:162:GLN:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356[A]:HIS:ND1	8:D:709:HOH:O	2.10	0.62
1:D:458[B]:MET:O	1:D:459[B]:HIS:C	2.36	0.62
1:B:222[A]:MET:HA	1:B:222[A]:MET:HE3	1.81	0.62
1:B:241:GLN:HG2	8:B:795:HOH:O	1.97	0.62
1:A:558[A]:VAL:OXT	1:A:558[A]:VAL:HG12	2.00	0.62
1:A:318:ASN:HD21	1:A:324:LYS:HE3	1.64	0.61
1:A:222[A]:MET:CE	1:A:223[A]:SER:N	2.65	0.60
1:A:118:VAL:HG12	8:A:1198:HOH:O	2.02	0.60
1:C:188:SER:HB2	1:C:299:THR:HG23	1.83	0.59
1:C:516[A]:MET:HE2	1:C:558[A]:VAL:CG1	2.29	0.58
1:B:222[A]:MET:HE3	1:B:223[A]:SER:H	1.66	0.58
1:B:222[A]:MET:CE	1:B:223[A]:SER:N	2.61	0.57
1:B:505:ARG:CG	1:B:505:ARG:HH11	2.18	0.57
1:D:245:ARG:HG2	1:D:264[B]:HIS:NE2	2.19	0.57
1:D:279[B]:MET:HE1	8:D:745:HOH:O	2.00	0.56
7:D:607:GOL:C1	8:D:708:HOH:O	2.52	0.56
1:A:222[A]:MET:HE3	1:A:223[A]:SER:H	1.70	0.56
1:A:222[A]:MET:HE2	1:A:223[A]:SER:N	2.21	0.55
1:B:251:VAL:HG22	1:B:256:ILE:HD11	1.88	0.55
1:A:172[A]:LYS:NZ	8:A:707:HOH:O	2.23	0.55
1:B:365:VAL:HB	1:B:417[B]:SER:HB2	1.90	0.54
1:A:112:LEU:HD22	1:A:116[A]:GLN:NE2	2.23	0.53
1:A:222[A]:MET:CA	1:A:222[A]:MET:HE3	2.37	0.53
1:D:112:LEU:O	1:D:116[A]:GLN:HB3	2.07	0.53
1:B:287:THR:HG22	8:B:933:HOH:O	2.08	0.53
1:A:188:SER:HB2	1:A:299:THR:HG23	1.90	0.52
1:A:356[A]:HIS:CE1	8:A:708:HOH:O	2.62	0.52
1:D:96:LYS:HG2	1:D:115:TYR:HB3	1.91	0.52
1:B:217:GLU:OE1	1:B:223[B]:SER:HA	2.10	0.52
1:B:360:LYS:HE2	8:B:816:HOH:O	2.10	0.51
1:A:356[A]:HIS:NE2	8:A:716:HOH:O	2.33	0.51
1:B:288:PHE:CD1	1:B:291[A]:LYS:HE2	2.46	0.51
1:B:464:LEU:HD11	1:B:468[B]:TYR:HE2	1.77	0.50
1:C:121[B]:ARG:HG2	8:C:1095:HOH:O	1.77	0.50
1:A:222[B]:MET:HA	1:A:222[B]:MET:CE	2.41	0.50
1:B:341[A]:GLN:CD	8:B:705:HOH:O	2.34	0.50
1:B:287:THR:CG2	8:B:1125:HOH:O	2.58	0.50
1:C:232:MET:HE1	1:C:296:ILE:HD13	1.94	0.50
1:D:121[A]:ARG:HG2	1:D:472:LEU:CD2	2.42	0.50
1:A:185:ARG:NH1	8:A:706:HOH:O	2.45	0.50
1:D:116[A]:GLN:NE2	1:D:343:TRP:HE1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121[B]:ARG:CD	8:C:1095:HOH:O	2.36	0.49
1:B:139:TYR:OH	1:B:143:HIS:CD2	2.62	0.49
1:B:232:MET:HE1	1:B:296:ILE:HG13	1.94	0.49
8:A:1163:HOH:O	1:D:458[A]:MET:HB3	2.13	0.49
1:B:121[B]:ARG:HD2	8:B:1098:HOH:O	2.12	0.49
1:C:516[A]:MET:HE1	1:C:558[A]:VAL:CG1	2.22	0.49
1:A:338:PRO:HD3	1:A:468:TYR:CZ	2.48	0.48
1:B:462:LYS:NZ	8:B:732:HOH:O	2.46	0.48
1:C:116[A]:GLN:NE2	8:C:707:HOH:O	2.05	0.48
7:C:611:GOL:C1	8:C:708:HOH:O	2.60	0.48
1:A:360:LYS:HE2	8:A:953:HOH:O	2.13	0.48
1:D:426[B]:LEU:HA	1:D:426[B]:LEU:HD23	1.63	0.48
1:D:264[B]:HIS:CE1	8:D:903:HOH:O	2.66	0.48
1:A:356[A]:HIS:CG	8:A:708:HOH:O	2.65	0.48
1:A:267[A]:LEU:HD13	1:A:280:PHE:CE1	2.50	0.47
1:B:230:PHE:CD1	1:B:231:PRO:HD2	2.49	0.47
1:B:235:GLN:NE2	8:B:716:HOH:O	2.37	0.47
1:C:112:LEU:O	1:C:116[A]:GLN:HB3	2.14	0.47
1:A:210:ASP:OD1	8:A:706:HOH:O	2.21	0.47
1:C:235:GLN:OE1	1:C:245[C]:ARG:NH2	2.48	0.47
1:B:242:GLU:HB3	8:B:765:HOH:O	2.15	0.47
1:D:245:ARG:HG2	1:D:264[B]:HIS:CE1	2.49	0.47
1:D:480:ALA:HB1	1:D:550:ASP:HB2	1.96	0.47
1:B:143:HIS:CD2	1:B:202:VAL:HG13	2.50	0.46
1:C:281:PHE:HB2	6:C:610:EDO:C2	2.46	0.46
1:D:177:ILE:HD11	1:D:296:ILE:HG22	1.97	0.46
1:D:229:ASP:OD2	8:D:712[A]:HOH:O	2.21	0.46
1:B:121[A]:ARG:NH1	8:B:731:HOH:O	2.46	0.46
1:D:447:SER:HB2	8:D:736:HOH:O	2.16	0.45
1:B:505:ARG:HG2	1:B:505:ARG:HH11	1.80	0.45
1:A:420:ALA:HA	1:A:445:GLN:HE22	1.82	0.45
1:B:341[B]:GLN:HB2	8:C:702:HOH:O	2.17	0.45
1:D:279[B]:MET:HE3	8:D:745:HOH:O	2.06	0.45
1:A:256:ILE:HA	8:A:788:HOH:O	2.16	0.45
1:A:445:GLN:NE2	8:A:746:HOH:O	2.48	0.45
1:A:356[A]:HIS:CE1	8:A:936:HOH:O	2.70	0.44
1:C:407:THR:N	1:C:408:PRO:HD3	2.32	0.44
1:D:150:THR:HA	7:D:607:GOL:H2	1.99	0.44
1:A:222[A]:MET:HE3	1:A:223[A]:SER:N	2.31	0.44
1:B:121[A]:ARG:CG	1:B:121[A]:ARG:HH11	2.26	0.44
1:C:239:LEU:HD21	1:C:245[C]:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:GLU:O	1:B:556:LYS:HE2	2.17	0.44
1:A:558[A]:VAL:OXT	1:A:558[A]:VAL:CG1	2.64	0.43
3:A:602:MES:C2	8:A:725:HOH:O	2.65	0.43
1:C:235:GLN:OE1	1:C:245[C]:ARG:CZ	2.66	0.43
1:D:341[A]:GLN:HE22	1:D:458[A]:MET:N	2.16	0.43
1:C:127:LYS:HD2	8:C:1186:HOH:O	2.18	0.43
1:A:458:MET:HA	1:A:461:GLY:H	1.83	0.43
1:D:108:GLU:OE2	1:D:116[B]:GLN:NE2	2.48	0.43
1:D:166:ASP:OD1	1:D:166:ASP:N	2.51	0.43
1:D:420:ALA:HB2	1:D:448[A]:GLN:NE2	2.31	0.43
1:B:420:ALA:HB2	1:B:448[B]:GLN:NE2	2.33	0.43
1:D:146:CYS:HB2	1:D:202:VAL:HG21	2.00	0.43
1:C:516[A]:MET:HE2	1:C:516[A]:MET:HB2	1.59	0.43
1:A:222[A]:MET:CA	1:A:222[A]:MET:CE	2.96	0.43
1:C:281:PHE:HB2	6:C:610:EDO:H22	2.00	0.43
1:D:531[B]:LYS:HG2	8:D:733:HOH:O	2.18	0.42
8:A:1163:HOH:O	1:D:458[A]:MET:CB	2.67	0.42
1:C:232:MET:HE3	1:C:232:MET:HB3	1.93	0.42
1:D:279[B]:MET:HE1	8:D:1040:HOH:O	2.19	0.42
1:C:116[A]:GLN:NE2	1:C:343:TRP:HE1	2.18	0.42
1:C:232:MET:HE1	1:C:296:ILE:CD1	2.50	0.42
1:B:146:CYS:HB2	1:B:202:VAL:HG21	2.01	0.41
1:C:123:PRO:HA	8:C:1089[B]:HOH:O	2.20	0.41
1:A:341[A]:GLN:NE2	8:A:759:HOH:O	2.53	0.41
1:D:531[A]:LYS:HG2	1:D:531[A]:LYS:HZ2	1.75	0.41
1:B:160[B]:LEU:HD21	1:B:264:HIS:HB3	2.03	0.41
1:A:356[A]:HIS:HD2	8:A:716:HOH:O	1.71	0.41
1:A:267[B]:LEU:HD13	1:A:267[B]:LEU:HA	1.78	0.41
1:C:264:HIS:HA	1:C:294:TRP:O	2.21	0.41
1:C:141:LYS:HB2	1:C:141:LYS:HE2	1.78	0.40
1:D:329:HIS:O	1:D:333:ARG:HG3	2.21	0.40
1:D:445[B]:GLN:HA	1:D:446:PRO:HD3	1.90	0.40
1:A:146:CYS:HB2	1:A:202:VAL:HG21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:918:HOH:O	8:C:1143:HOH:O[1_655]	2.15	0.05

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	452/476 (95%)	441 (98%)	11 (2%)	0	100	100
1	B	464/476 (98%)	444 (96%)	17 (4%)	3 (1%)	25	12
1	C	469/476 (98%)	457 (97%)	11 (2%)	1 (0%)	47	33
1	D	466/476 (98%)	449 (96%)	14 (3%)	3 (1%)	25	12
All	All	1851/1904 (97%)	1791 (97%)	53 (3%)	7 (0%)	41	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	459[A]	HIS
1	D	459[B]	HIS
1	C	180	SER
1	D	94	SER
1	B	168[A]	ASP
1	B	168[B]	ASP
1	B	180	SER

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	407/423 (96%)	390 (96%)	17 (4%)	30	15
1	B	416/423 (98%)	396 (95%)	20 (5%)	25	11
1	C	419/423 (99%)	409 (98%)	10 (2%)	49	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	411/423 (97%)	400 (97%)	11 (3%)	44	31
All	All	1653/1692 (98%)	1595 (96%)	58 (4%)	39	21

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	SER
1	A	170	GLU
1	A	222[A]	MET
1	A	222[B]	MET
1	A	224	TRP
1	A	237	ASP
1	A	273	TYR
1	A	318	ASN
1	A	341[A]	GLN
1	A	341[B]	GLN
1	A	354	LEU
1	A	356[A]	HIS
1	A	356[B]	HIS
1	A	428	SER
1	A	448	GLN
1	A	496	PRO
1	A	531	LYS
1	B	108	GLU
1	B	162	GLN
1	B	163	GLU
1	B	168[A]	ASP
1	B	168[B]	ASP
1	B	222[A]	MET
1	B	222[B]	MET
1	B	224	TRP
1	B	245	ARG
1	B	255	VAL
1	B	273	TYR
1	B	287	THR
1	B	341[A]	GLN
1	B	341[B]	GLN
1	B	398	LEU
1	B	399	VAL
1	B	407	THR
1	B	418	LEU
1	B	506	THR

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Mol	Chain	Res	Type
1	B	524	SER
1	C	117	SER
1	C	134	SER
1	C	166	ASP
1	C	224	TRP
1	C	237	ASP
1	C	273	TYR
1	C	370	GLU
1	C	397	THR
1	C	448	GLN
1	C	531	LYS
1	D	122	LYS
1	D	123	PRO
1	D	162[A]	GLN
1	D	162[B]	GLN
1	D	166	ASP
1	D	224	TRP
1	D	245	ARG
1	D	256	ILE
1	D	273	TYR
1	D	318	ASN
1	D	541	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	444	HIS
1	A	445	GLN
1	B	143	HIS
1	B	425	ASN
1	C	93	ASN
1	C	276	HIS
1	C	448	GLN
1	D	301	ASN

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
2	BGC	E	1	2	12,12,12	0.82	0	17,17,17	1.28	1 (5%)
2	BGC	E	2	2	11,11,12	0.91	0	15,15,17	1.34	1 (6%)
2	BGC	E	3	2	11,11,12	1.10	1 (9%)	15,15,17	1.36	1 (6%)
2	BGC	E	4	2	11,11,12	1.07	1 (9%)	15,15,17	0.99	1 (6%)
2	XYS	E	5	2	9,9,10	1.04	1 (11%)	10,12,14	1.17	1 (10%)
2	XYS	E	6	2	9,9,10	1.63	2 (22%)	10,12,14	2.06	4 (40%)
2	XYS	E	7	2	9,9,10	1.68	2 (22%)	10,12,14	1.30	2 (20%)
2	GAL	E	8	2	11,11,12	1.99	2 (18%)	15,15,17	1.10	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	E	4	2	-	0/2/19/22	0/1/1/1
2	XYS	E	5	2	-	-	0/1/1/1
2	XYS	E	6	2	-	-	1/1/1/1
2	XYS	E	7	2	-	-	0/1/1/1
2	GAL	E	8	2	-	2/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	8	GAL	O5-C1	5.48	1.52	1.43
2	E	6	XYS	O5-C1	3.64	1.50	1.42
2	E	7	XYS	O5-C5	3.49	1.49	1.42
2	E	8	GAL	C2-C3	2.96	1.56	1.52
2	E	6	XYS	C5-C4	2.69	1.58	1.52
2	E	4	BGC	C2-C3	2.68	1.56	1.52
2	E	3	BGC	C2-C3	-2.39	1.49	1.52
2	E	7	XYS	C4-C3	-2.32	1.49	1.52
2	E	5	XYS	O4-C4	2.09	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	XYS	C5-O5-C1	3.82	117.40	111.52
2	E	6	XYS	C4-C3-C2	-3.10	107.25	110.92
2	E	6	XYS	C1-C2-C3	-3.07	105.89	109.67
2	E	2	BGC	O5-C5-C6	3.06	112.00	107.20
2	E	3	BGC	C6-C5-C4	-3.02	105.92	113.00
2	E	7	XYS	O4-C4-C3	-2.94	104.26	110.14
2	E	5	XYS	C5-O5-C1	2.90	115.98	111.52
2	E	1	BGC	C1-O5-C5	-2.63	108.69	113.66
2	E	8	GAL	O6-C6-C5	-2.52	102.66	111.29
2	E	4	BGC	C1-O5-C5	-2.50	108.80	112.19
2	E	6	XYS	C5-C4-C3	2.12	112.28	109.67
2	E	7	XYS	O2-C2-C3	-2.07	105.99	110.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	8	GAL	O5-C5-C6-O6
2	E	8	GAL	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	6	XYS	C1-C2-C3-C4-C5-O5

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
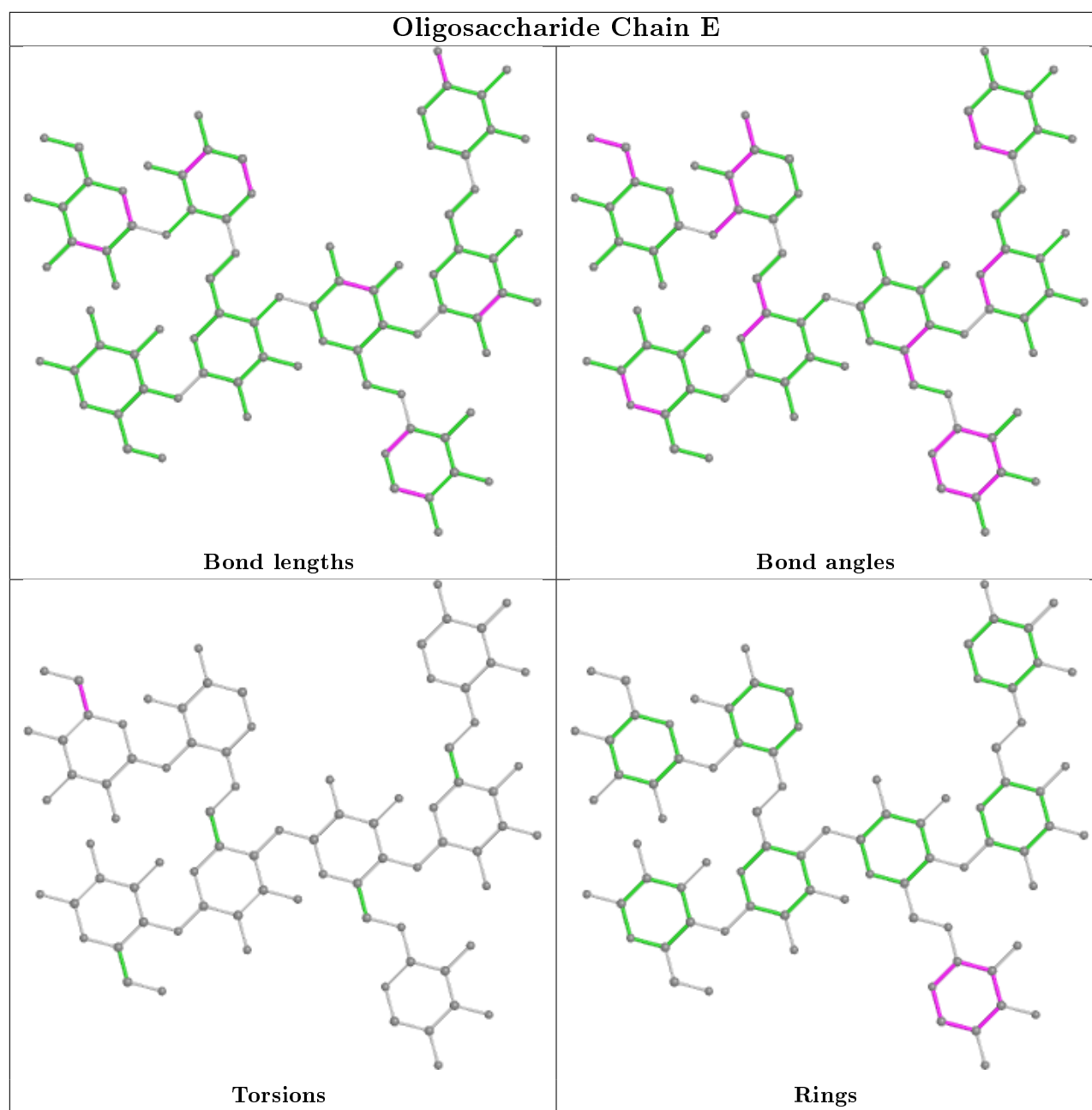
5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 27 are monoatomic - leaving 11 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
6	EDO	A	613	-	3,3,3	0.40	0	2,2,2	0.67	0
6	EDO	D	606[A]	-	3,3,3	0.61	0	2,2,2	0.16	0
3	MES	C	601	-	12,12,12	1.78	1 (8%)	14,16,16	1.94	3 (21%)
3	MES	D	601	-	12,12,12	2.18	1 (8%)	14,16,16	1.32	2 (14%)
7	GOL	C	611	-	5,5,5	0.36	0	5,5,5	0.57	0
3	MES	A	602	-	12,12,12	1.83	1 (8%)	14,16,16	1.62	2 (14%)
3	MES	C	602	-	12,12,12	2.12	1 (8%)	14,16,16	1.89	4 (28%)
7	GOL	D	607	-	5,5,5	0.26	0	5,5,5	0.55	0
6	EDO	C	610	-	3,3,3	0.49	0	2,2,2	0.75	0
3	MES	A	601	-	12,12,12	1.60	1 (8%)	14,16,16	1.36	3 (21%)
6	EDO	D	606[B]	-	3,3,3	0.49	0	2,2,2	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	613	-	-	1/1/1/1	-
6	EDO	D	606[A]	-	-	0/1/1/1	-
3	MES	C	601	-	-	3/6/14/14	0/1/1/1
3	MES	D	601	-	-	0/6/14/14	0/1/1/1
7	GOL	C	611	-	-	3/4/4/4	-
3	MES	A	602	-	-	5/6/14/14	0/1/1/1
3	MES	C	602	-	-	3/6/14/14	0/1/1/1
7	GOL	D	607	-	-	0/4/4/4	-
6	EDO	C	610	-	-	1/1/1/1	-
3	MES	A	601	-	-	0/6/14/14	0/1/1/1
6	EDO	D	606[B]	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	MES	C8-S	-7.13	1.67	1.77
3	C	602	MES	C8-S	-6.95	1.67	1.77
3	A	602	MES	C8-S	-5.77	1.69	1.77
3	C	601	MES	C8-S	-5.42	1.69	1.77
3	A	601	MES	C8-S	-5.01	1.70	1.77

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	MES	O3S-S-C8	4.76	113.47	105.77
3	C	601	MES	C2-C3-N4	3.99	116.16	110.10
3	C	601	MES	O2S-S-C8	3.18	110.74	106.92
3	A	601	MES	O3S-S-O1S	-3.16	103.56	111.27
3	C	601	MES	O3S-S-C8	3.13	110.83	105.77
3	C	602	MES	O1S-S-C8	3.04	110.58	106.92
3	C	602	MES	O3S-S-C8	2.98	110.58	105.77
3	D	601	MES	O1S-S-C8	2.95	110.47	106.92
3	C	602	MES	O2S-S-C8	2.65	110.10	106.92
3	D	601	MES	O3S-S-C8	2.59	109.95	105.77
3	C	602	MES	C2-C3-N4	2.52	113.93	110.10
3	A	601	MES	O3S-S-C8	2.50	109.81	105.77
3	A	602	MES	O2S-S-O1S	-2.21	106.31	113.95
3	A	601	MES	O2S-S-C8	2.09	109.43	106.92

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	MES	C7-C8-S-O1S
3	C	602	MES	C7-C8-S-O3S
7	C	611	GOL	O1-C1-C2-C3
3	A	602	MES	C8-C7-N4-C3
3	A	602	MES	C8-C7-N4-C5
3	A	602	MES	C7-C8-S-O1S
3	A	602	MES	C7-C8-S-O2S
3	A	602	MES	C7-C8-S-O3S
7	C	611	GOL	O1-C1-C2-O2
3	C	601	MES	C7-C8-S-O3S
3	C	602	MES	C7-C8-S-O2S
3	C	601	MES	C7-C8-S-O1S
6	C	610	EDO	O1-C1-C2-O2
3	C	601	MES	C8-C7-N4-C5
6	A	613	EDO	O1-C1-C2-O2
6	D	606[B]	EDO	O1-C1-C2-O2
7	C	611	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	611	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	MES	1	0
3	C	602	MES	1	0
7	D	607	GOL	5	0
6	C	610	EDO	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB($Å^2$)	Q<0.9
1	A	446/476 (93%)	-0.36	9 (2%)	65	61	9, 19, 45, 82	3 (0%)
1	B	452/476 (94%)	-0.32	12 (2%)	54	49	9, 20, 57, 94	0
1	C	458/476 (96%)	-0.20	17 (3%)	41	36	11, 22, 54, 87	1 (0%)
1	D	454/476 (95%)	-0.22	10 (2%)	62	57	11, 22, 52, 90	1 (0%)
All	All	1810/1904 (95%)	-0.27	48 (2%)	54	49	9, 21, 53, 94	5 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	258	THR	11.3
1	A	451	TYR	7.1
1	D	256	ILE	6.2
1	C	459	HIS	5.4
1	D	258	THR	5.1
1	C	260	GLY	4.7
1	B	258	THR	4.6
1	B	168[A]	ASP	3.9
1	A	450	GLY	3.7
1	A	168	ASP	3.7
1	A	459	HIS	3.7
1	B	449	GLU	3.6
1	C	458	MET	3.6
1	C	168	ASP	3.4
1	B	451	TYR	3.4
1	D	407	THR	3.3
1	A	458	MET	3.2
1	C	92	ILE	3.2
1	B	397	THR	3.1
1	A	407	THR	3.0
1	A	449	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	399	VAL	2.9
1	B	259	GLU	2.9
1	C	166	ASP	2.9
1	B	450	GLY	2.8
1	C	91	ASN	2.7
1	D	167	GLY	2.7
1	B	260	GLY	2.6
1	A	167	GLY	2.6
1	A	400	GLU	2.6
1	D	458[A]	MET	2.6
1	B	167	GLY	2.6
1	B	164	HIS	2.5
1	C	558[A]	VAL	2.4
1	C	256	ILE	2.3
1	D	451	TYR	2.3
1	C	398	LEU	2.2
1	D	94	SER	2.2
1	C	261	THR	2.1
1	B	459	HIS	2.1
1	D	259	GLU	2.1
1	C	451	TYR	2.1
1	D	398	LEU	2.1
1	C	259	GLU	2.1
1	C	167	GLY	2.0
1	D	260	GLY	2.0
1	C	399	VAL	2.0
1	C	255	VAL	2.0

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

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

6.3 Carbohydrates (i)

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

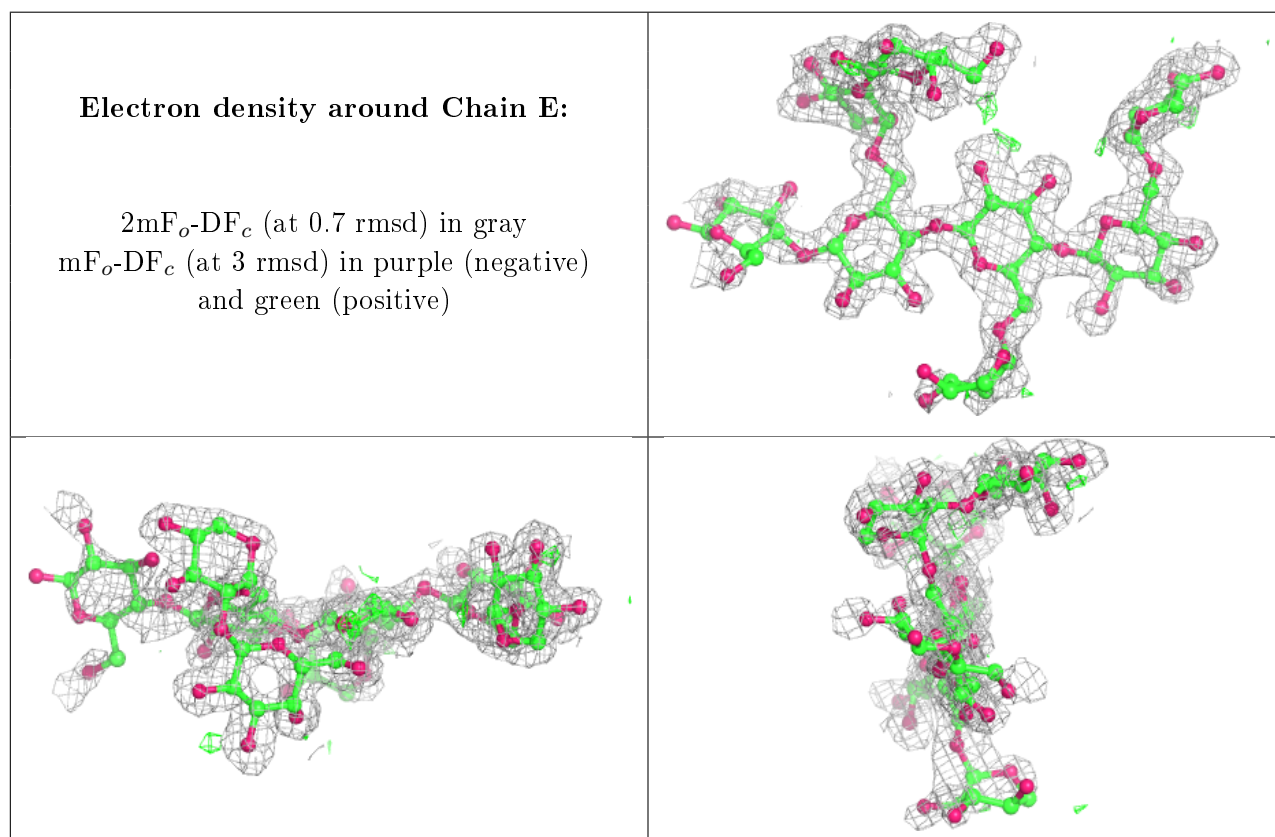| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	E	1	12/12	0.61	0.26	46,57,61,63	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XYS	E	6	9/10	0.68	0.30	48,51,55,56	9
2	BGC	E	4	11/12	0.88	0.14	24,27,31,32	11
2	BGC	E	3	11/12	0.88	0.09	23,27,34,39	11
2	XYS	E	5	9/10	0.89	0.13	22,24,26,29	9
2	BGC	E	2	11/12	0.89	0.15	25,31,37,39	11
2	GAL	E	8	11/12	0.91	0.11	15,17,19,19	11
2	XYS	E	7	9/10	0.93	0.12	19,24,25,25	9

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:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	C	611	6/6	0.66	0.27	35,36,37,39	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	D	607	6/6	0.87	0.24	24,28,28,29	6
3	MES	C	602	12/12	0.88	0.16	38,44,48,50	12
6	EDO	C	610	4/4	0.90	0.18	7,7,7,7	4
5	K	C	609	1/1	0.92	0.09	40,40,40,40	1
3	MES	A	602	12/12	0.92	0.17	26,33,39,41	12
6	EDO	A	613	4/4	0.92	0.15	33,34,34,36	4
4	CL	D	604	1/1	0.93	0.08	40,40,40,40	0
5	K	C	608	1/1	0.94	0.09	43,43,43,43	0
4	CL	A	610	1/1	0.94	0.11	41,41,41,41	1
6	EDO	D	606[A]	4/4	0.94	0.11	37,41,45,46	4
3	MES	A	601	12/12	0.94	0.12	25,32,35,36	12
6	EDO	D	606[B]	4/4	0.94	0.11	15,16,16,16	4
3	MES	D	601	12/12	0.95	0.13	49,50,52,53	0
4	CL	C	606	1/1	0.95	0.08	39,39,39,39	0
3	MES	C	601	12/12	0.96	0.12	39,43,50,50	0
4	CL	B	603	1/1	0.96	0.09	48,48,48,48	0
4	CL	B	601	1/1	0.97	0.05	28,28,28,28	0
5	K	A	612	1/1	0.97	0.12	38,38,38,38	0
4	CL	A	609	1/1	0.97	0.07	42,42,42,42	0
4	CL	A	606	1/1	0.97	0.08	37,37,37,37	0
4	CL	C	603	1/1	0.98	0.04	32,32,32,32	0
4	CL	C	605	1/1	0.98	0.07	36,36,36,36	0
5	K	A	611	1/1	0.98	0.05	20,20,20,20	0
5	K	B	606	1/1	0.98	0.13	40,40,40,40	0
4	CL	A	604	1/1	0.98	0.04	32,32,32,32	0
4	CL	D	602	1/1	0.99	0.06	33,33,33,33	0
4	CL	C	604	1/1	0.99	0.12	21,21,21,21	1
5	K	C	607	1/1	0.99	0.05	26,26,26,26	0
4	CL	A	607	1/1	0.99	0.07	44,44,44,44	0
5	K	B	605	1/1	0.99	0.06	23,23,23,23	0
4	CL	A	603	1/1	0.99	0.05	18,18,18,18	0
5	K	D	605	1/1	0.99	0.04	25,25,25,25	0
4	CL	B	602	1/1	0.99	0.05	29,29,29,29	0
4	CL	A	608	1/1	0.99	0.04	27,27,27,27	0
4	CL	A	605	1/1	0.99	0.04	29,29,29,29	0
4	CL	B	604	1/1	0.99	0.05	28,28,28,28	0
4	CL	D	603	1/1	1.00	0.04	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.