Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2020 – 08:23 AM BST

PDB ID	:	3QYQ
Title	:	1.8 Angstrom resolution crystal structure of a putative deoxyribose-phosphate aldolase from Toxoplasma gondii ME49
Authors	:	Halavaty, A.S.; Ruan, J.; Minasov, G.; Shuvalova, L.; Ueno, A.; Igarashi, M.; Ngo, H.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2011-03-03
Resolution	:	1.80 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

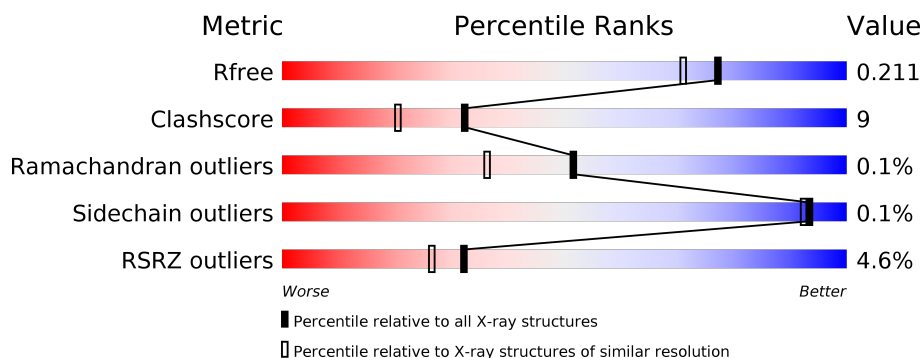|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.80 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		0.211
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		0.1%
RSRZ outliers		4.6%

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	293	4% / 81% / 12% / 7%
1	B	293	2% / 76% / 15% / 9%
1	C	293	5% / 79% / 14% / 7%
1	D	293	5% / 78% / 14% / 8%
2	E	2	50% / 50%
2	F	2	50% / 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9940 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 Deoxyribose-phosphate aldolase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total 2215	C 1391	N 389	O 421	S 14	0	16	0
1	B	268	Total 2155	C 1355	N 374	O 413	S 13	0	14	0
1	C	273	Total 2234	C 1401	N 384	O 434	S 15	0	20	0
1	D	270	Total 2229	C 1397	N 386	O 431	S 15	0	23	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP B6KPX4
A	-15	GLY	-	expression tag	UNP B6KPX4
A	-14	SER	-	expression tag	UNP B6KPX4
A	-13	SER	-	expression tag	UNP B6KPX4
A	-12	HIS	-	expression tag	UNP B6KPX4
A	-11	HIS	-	expression tag	UNP B6KPX4
A	-10	HIS	-	expression tag	UNP B6KPX4
A	-9	HIS	-	expression tag	UNP B6KPX4
A	-8	HIS	-	expression tag	UNP B6KPX4
A	-7	HIS	-	expression tag	UNP B6KPX4
A	-6	GLU	-	expression tag	UNP B6KPX4
A	-5	ASN	-	expression tag	UNP B6KPX4
A	-4	LEU	-	expression tag	UNP B6KPX4
A	-3	TYR	-	expression tag	UNP B6KPX4
A	-2	PHE	-	expression tag	UNP B6KPX4
A	-1	GLN	-	expression tag	UNP B6KPX4
A	0	GLY	-	expression tag	UNP B6KPX4
B	-16	MET	-	expression tag	UNP B6KPX4
B	-15	GLY	-	expression tag	UNP B6KPX4
B	-14	SER	-	expression tag	UNP B6KPX4
B	-13	SER	-	expression tag	UNP B6KPX4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP B6KPX4
B	-11	HIS	-	expression tag	UNP B6KPX4
B	-10	HIS	-	expression tag	UNP B6KPX4
B	-9	HIS	-	expression tag	UNP B6KPX4
B	-8	HIS	-	expression tag	UNP B6KPX4
B	-7	HIS	-	expression tag	UNP B6KPX4
B	-6	GLU	-	expression tag	UNP B6KPX4
B	-5	ASN	-	expression tag	UNP B6KPX4
B	-4	LEU	-	expression tag	UNP B6KPX4
B	-3	TYR	-	expression tag	UNP B6KPX4
B	-2	PHE	-	expression tag	UNP B6KPX4
B	-1	GLN	-	expression tag	UNP B6KPX4
B	0	GLY	-	expression tag	UNP B6KPX4
C	-16	MET	-	expression tag	UNP B6KPX4
C	-15	GLY	-	expression tag	UNP B6KPX4
C	-14	SER	-	expression tag	UNP B6KPX4
C	-13	SER	-	expression tag	UNP B6KPX4
C	-12	HIS	-	expression tag	UNP B6KPX4
C	-11	HIS	-	expression tag	UNP B6KPX4
C	-10	HIS	-	expression tag	UNP B6KPX4
C	-9	HIS	-	expression tag	UNP B6KPX4
C	-8	HIS	-	expression tag	UNP B6KPX4
C	-7	HIS	-	expression tag	UNP B6KPX4
C	-6	GLU	-	expression tag	UNP B6KPX4
C	-5	ASN	-	expression tag	UNP B6KPX4
C	-4	LEU	-	expression tag	UNP B6KPX4
C	-3	TYR	-	expression tag	UNP B6KPX4
C	-2	PHE	-	expression tag	UNP B6KPX4
C	-1	GLN	-	expression tag	UNP B6KPX4
C	0	GLY	-	expression tag	UNP B6KPX4
D	-16	MET	-	expression tag	UNP B6KPX4
D	-15	GLY	-	expression tag	UNP B6KPX4
D	-14	SER	-	expression tag	UNP B6KPX4
D	-13	SER	-	expression tag	UNP B6KPX4
D	-12	HIS	-	expression tag	UNP B6KPX4
D	-11	HIS	-	expression tag	UNP B6KPX4
D	-10	HIS	-	expression tag	UNP B6KPX4
D	-9	HIS	-	expression tag	UNP B6KPX4
D	-8	HIS	-	expression tag	UNP B6KPX4
D	-7	HIS	-	expression tag	UNP B6KPX4
D	-6	GLU	-	expression tag	UNP B6KPX4
D	-5	ASN	-	expression tag	UNP B6KPX4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	LEU	-	expression tag	UNP B6KPX4
D	-3	TYR	-	expression tag	UNP B6KPX4
D	-2	PHE	-	expression tag	UNP B6KPX4
D	-1	GLN	-	expression tag	UNP B6KPX4
D	0	GLY	-	expression tag	UNP B6KPX4

• Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.
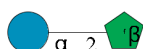
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total 23	C 12	O 11	0	0	0
2	F	2	Total 23	C 12	O 11	0	0	0
2	G	2	Total 23	C 12	O 11	0	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	240	Total 250	O 250	0	13
4	B	259	Total 267	O 267	0	11
4	C	206	Total 215	O 215	0	14
4	D	222	Total 226	O 226	0	7

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: Deoxyribose-phosphate aldolase, putative
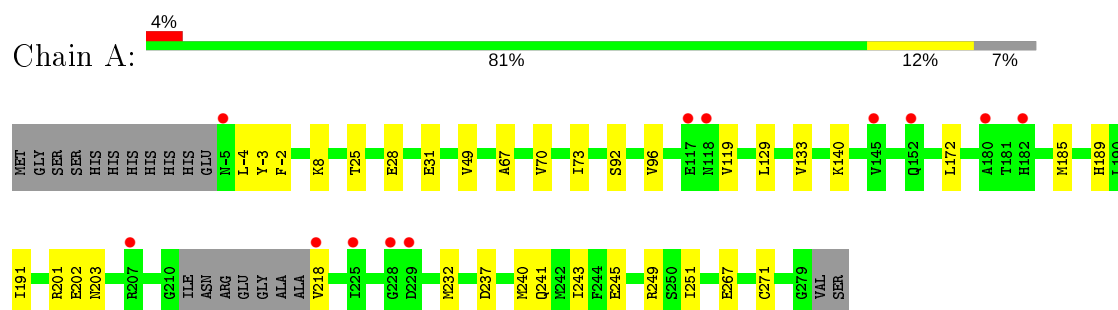
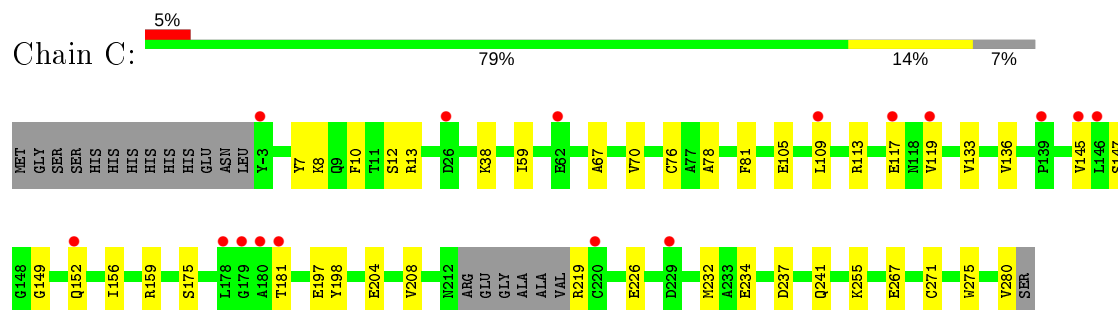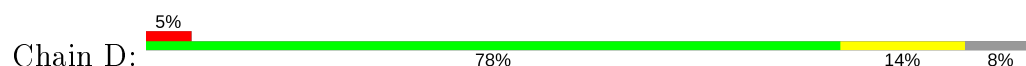

- Molecule 1: Deoxyribose-phosphate aldolase, putative
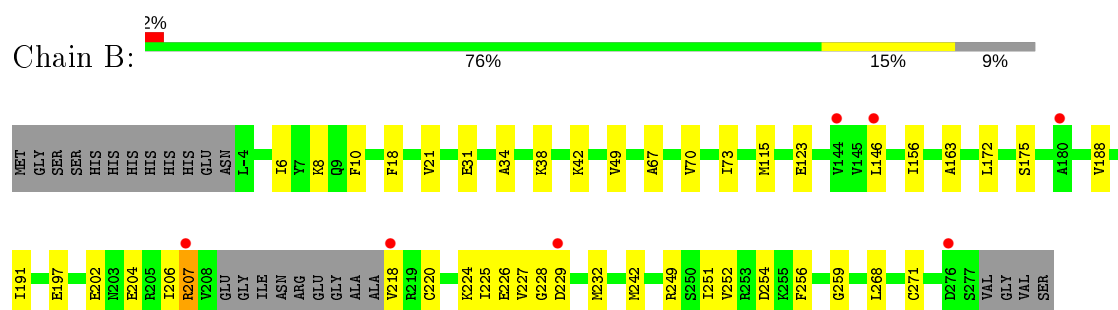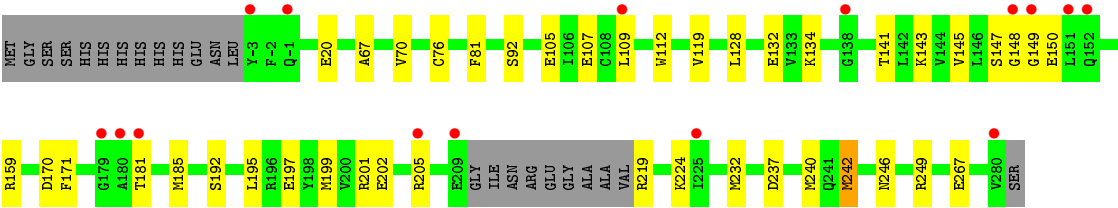

- Molecule 1: Deoxyribose-phosphate aldolase, putative

- Molecule 1: Deoxyribose-phosphate aldolase, putative
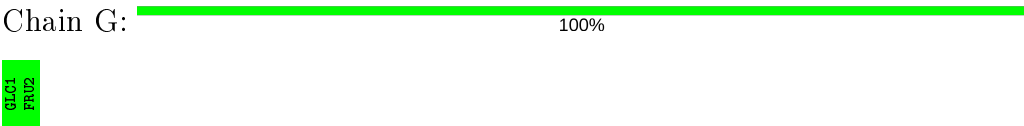
• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E:

• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain F:

• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.92Å 72.19Å 73.05Å 62.90° 89.80° 88.85°	Depositor
Resolution (Å)	29.49 – 1.80 29.49 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.49-1.80) 97.3 (29.49-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.166 , 0.201 0.176 , 0.211	Depositor DCC
R_{free} test set	5879 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.9	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l 0.005 for -h,l,k 0.008 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9940	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, SO4, FRU

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	0.38	0/2245	0.64	0/3025
1	B	0.39	0/2184	0.67	0/2945
1	C	0.39	0/2263	0.66	0/3052
1	D	0.37	0/2258	0.67	0/3043
All	All	0.38	0/8950	0.66	0/12065

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207[A]	ARG	Sidechain

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	2215	0	2220	36	0
1	B	2155	0	2161	42	0
1	C	2234	0	2220	50	0
1	D	2229	0	2221	46	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
2	G	23	0	21	0	0
3	A	30	0	0	1	0
3	B	15	0	0	0	0
3	C	10	0	0	1	0
3	D	25	0	0	1	0
4	A	250	0	0	5	0
4	B	267	0	0	7	0
4	C	215	0	0	8	0
4	D	226	0	0	10	0
All	All	9940	0	8885	158	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 9.

All (158) 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:B:225:ILE:HD11	1:B:242[B]:MET:SD	1.73	1.29
1:A:240[B]:MET:SD	1:A:243[B]:ILE:HD11	2.02	0.99
1:B:146:LEU:HB2	4:B:321:HOH:O	1.65	0.97
1:C:271[B]:CYS:SG	4:C:504:HOH:O	2.28	0.91
1:B:225:ILE:CD1	1:B:242[B]:MET:SD	2.60	0.88
1:D:150[B]:GLU:HG3	1:D:181:THR:HG21	1.60	0.84
1:D:76[B]:CYS:SG	4:D:334:HOH:O	2.35	0.82
1:C:149:GLY:HA3	1:C:181:THR:OG1	1.81	0.81
1:D:195[B]:LEU:HD22	4:D:561:HOH:O	1.80	0.80
1:C:76[B]:CYS:SG	4:C:334:HOH:O	2.40	0.79
1:D:195[B]:LEU:HD23	1:D:195[B]:LEU:O	1.82	0.79
1:A:203:ASN:OD1	1:A:218:VAL:HG23	1.83	0.78
1:D:81:PHE:CE2	1:D:109[B]:LEU:HG	2.20	0.77
1:D:128[A]:LEU:HD12	4:D:841:HOH:O	1.86	0.76
1:C:109[A]:LEU:HD11	1:C:147[A]:SER:OG	1.90	0.72
1:D:242[A]:MET:HE2	1:D:242[A]:MET:HA	1.71	0.72
1:D:195[B]:LEU:HD23	1:D:195[B]:LEU:C	2.10	0.71
1:D:150[B]:GLU:CG	1:D:181:THR:HG21	2.22	0.69
1:A:202:GLU:HG3	1:A:218:VAL:HG22	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76[B]:CYS:SG	4:C:342:HOH:O	2.53	0.67
1:D:249:ARG:NH2	3:D:284:SO4:O3	2.25	0.64
1:A:243[B]:ILE:HG22	1:A:251:ILE:HG13	1.79	0.64
1:C:67:ALA:O	1:C:70[A]:VAL:HG22	1.97	0.64
1:C:271[A]:CYS:SG	4:C:603:HOH:O	2.55	0.63
1:A:8[A]:LYS:HG2	1:C:7:TYR:CD2	2.35	0.62
1:C:109[B]:LEU:HD23	1:C:145:VAL:HB	1.82	0.62
1:A:232:MET:CE	1:A:267:GLU:HG2	2.31	0.61
1:A:249:ARG:NH2	3:A:287:SO4:O1	2.32	0.61
1:B:249:ARG:NH1	4:B:674:HOH:O	2.32	0.61
1:B:175:SER:O	1:B:226[A]:GLU:HG3	2.00	0.61
1:B:115[B]:MET:HG3	1:B:156:ILE:HG23	1.82	0.61
1:A:240[B]:MET:HE1	1:C:10:PHE:HA	1.83	0.60
1:A:49[A]:VAL:HG13	1:A:73:ILE:HD12	1.83	0.60
1:B:197[A]:GLU:HG3	4:B:405:HOH:O	2.00	0.60
1:B:252:VAL:HG23	1:B:254[B]:ASP:OD2	2.01	0.60
1:C:271[B]:CYS:SG	4:C:845:HOH:O	2.56	0.60
1:D:81:PHE:CD2	1:D:109[B]:LEU:HG	2.37	0.60
1:C:119:VAL:HG11	1:C:159:ARG:HD3	1.84	0.59
1:A:201[B]:ARG:NH2	4:A:364:HOH:O	2.35	0.59
1:B:204:GLU:HG2	1:C:234:GLU:HG3	1.84	0.59
1:C:12[B]:SER:HB3	1:C:232[B]:MET:CE	2.32	0.59
1:B:6:ILE:HD11	1:D:240[B]:MET:HG3	1.85	0.59
1:A:140:LYS:NZ	4:A:501:HOH:O	2.35	0.59
1:D:242[A]:MET:CE	1:D:242[A]:MET:HA	2.33	0.59
1:B:49[A]:VAL:HG13	1:B:73:ILE:HD12	1.84	0.58
1:C:197[B]:GLU:HA	1:C:197[B]:GLU:OE2	2.03	0.57
1:B:228[A]:GLY:O	1:B:229[A]:ASP:C	2.42	0.57
1:C:255:LYS:HE3	4:C:332:HOH:O	2.04	0.57
1:A:189[B]:HIS:CE1	1:C:280:VAL:HG13	2.40	0.56
1:B:172:LEU:HD12	1:B:191:ILE:HG23	1.87	0.56
1:D:224:LYS:NZ	4:D:786:HOH:O	2.35	0.56
1:D:185:MET:HE1	1:D:237[A]:ASP:OD1	2.06	0.56
1:A:240[B]:MET:CE	1:C:10:PHE:HA	2.36	0.56
1:C:181:THR:O	3:C:282:SO4:O3	2.23	0.56
1:C:152:GLN:O	1:C:156:ILE:HD12	2.06	0.55
1:B:232:MET:HE2	1:B:268:LEU:HD23	1.89	0.55
1:D:195[B]:LEU:CD2	1:D:195[B]:LEU:C	2.75	0.55
1:B:31[A]:GLU:HG2	4:B:332:HOH:O	2.07	0.54
1:B:229[B]:ASP:OD2	1:B:229[B]:ASP:N	2.39	0.53
1:D:134[A]:LYS:NZ	1:D:170:ASP:OD2	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HD13	1:B:218:VAL:HG13	1.91	0.53
1:C:67:ALA:O	1:C:70[B]:VAL:HG12	2.08	0.53
1:D:76[B]:CYS:SG	1:D:105:GLU:OE1	2.66	0.53
1:A:243[B]:ILE:HG22	1:A:251:ILE:CG1	2.39	0.53
1:D:109[B]:LEU:HD23	1:D:145:VAL:HB	1.91	0.52
1:D:195[B]:LEU:CD2	4:D:561:HOH:O	2.49	0.52
1:A:67:ALA:O	1:A:70:VAL:HG22	2.10	0.52
1:C:119:VAL:CG1	1:C:159:ARG:HD3	2.38	0.52
1:C:81:PHE:CE2	1:C:109[B]:LEU:HG	2.45	0.52
1:D:67:ALA:O	1:D:70:VAL:HG22	2.10	0.52
1:D:128[A]:LEU:CD1	4:D:841:HOH:O	2.51	0.52
1:A:245[B]:GLU:HG2	1:C:280:VAL:HG11	1.91	0.52
1:D:92:SER:OG	1:D:132:GLU:HG2	2.09	0.52
1:A:240[B]:MET:O	1:A:243[B]:ILE:HG12	2.10	0.51
1:A:245[A]:GLU:HG2	1:C:280:VAL:HG11	1.92	0.51
1:C:8:LYS:HG2	1:C:271[A]:CYS:SG	2.51	0.51
1:B:232:MET:HE1	1:B:268:LEU:HA	1.93	0.51
1:C:12[B]:SER:HB3	1:C:232[B]:MET:HE3	1.92	0.51
1:A:240[B]:MET:HA	1:A:243[B]:ILE:HG12	1.94	0.50
1:D:119:VAL:HG11	1:D:159:ARG:HH11	1.77	0.49
1:B:42:LYS:HD3	4:B:365:HOH:O	2.12	0.49
1:B:67:ALA:O	1:B:70:VAL:HG22	2.13	0.48
1:D:185:MET:HE2	1:D:237[A]:ASP:CG	2.33	0.48
1:C:133:VAL:O	1:C:136:VAL:HG22	2.14	0.48
1:C:38:LYS:NZ	1:C:67:ALA:HB2	2.29	0.48
1:D:267:GLU:OE2	4:D:838:HOH:O	2.20	0.48
1:C:219:ARG:HB2	4:C:947:HOH:O	2.13	0.48
1:B:227[A]:VAL:HG22	1:B:259:GLY:O	2.13	0.48
1:A:-4:LEU:N	1:A:-4:LEU:HD12	2.29	0.48
1:B:18:PHE:CZ	1:B:251:ILE:HG22	2.49	0.48
1:C:70[B]:VAL:HG22	1:C:70[B]:VAL:O	2.13	0.48
1:D:232:MET:SD	1:D:267:GLU:HG2	2.53	0.48
1:B:123:GLU:HG3	1:B:163:ALA:HB2	1.95	0.47
1:A:119:VAL:HG11	4:A:844:HOH:O	2.15	0.47
1:B:206:ILE:HD12	1:B:207[A]:ARG:N	2.30	0.47
1:B:232:MET:CE	1:B:268:LEU:HD23	2.44	0.47
1:C:175[B]:SER:HB2	1:C:226[B]:GLU:OE2	2.15	0.47
1:D:205:ARG:NH1	4:D:456:HOH:O	2.44	0.47
1:C:119:VAL:HG11	1:C:159:ARG:CD	2.44	0.47
1:A:232:MET:HE3	1:A:267:GLU:HG2	1.96	0.46
1:B:204:GLU:HG2	1:C:234:GLU:CG	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ILE:CD1	1:B:242[B]:MET:CG	2.93	0.46
1:C:12[B]:SER:HB3	1:C:232[B]:MET:HE1	1.98	0.46
1:D:109[A]:LEU:HD11	1:D:147[A]:SER:OG	2.15	0.46
1:D:149[A]:GLY:HA3	1:D:181:THR:HB	1.97	0.46
1:D:143:LYS:HG2	1:D:171:PHE:HB2	1.97	0.46
1:B:224:LYS:HE2	1:B:226[B]:GLU:OE2	2.16	0.46
1:B:10:PHE:HA	1:D:240[B]:MET:SD	2.55	0.46
1:C:113:ARG:O	1:C:117[B]:GLU:HG3	2.16	0.46
1:D:20:GLU:OE1	1:D:143:LYS:NZ	2.48	0.46
1:D:192:SER:HB3	1:D:246:ASN:HD21	1.80	0.46
1:A:271:CYS:SG	4:A:355:HOH:O	2.53	0.45
1:A:8[B]:LYS:HG2	1:A:271:CYS:SG	2.56	0.45
1:D:128[B]:LEU:HG	4:D:394:HOH:O	2.15	0.45
1:A:243[B]:ILE:HD12	1:C:13:ARG:HG2	1.98	0.45
1:B:220:CYS:HA	4:B:341:HOH:O	2.16	0.45
1:A:241[B]:GLN:O	1:A:245[B]:GLU:HG3	2.17	0.45
1:A:129:LEU:O	1:A:133:VAL:HG23	2.17	0.45
1:B:34:ALA:O	1:B:38:LYS:HG3	2.17	0.44
1:D:185:MET:HE2	1:D:237[B]:ASP:HB3	1.98	0.44
1:C:59:ILE:HG23	1:C:70[B]:VAL:HG21	1.99	0.44
1:A:172:LEU:HD12	1:A:191:ILE:HG23	2.00	0.44
1:B:207[A]:ARG:HH22	1:C:181:THR:HB	1.82	0.44
1:B:252:VAL:CG2	1:B:254[B]:ASP:OD2	2.66	0.44
1:A:31:GLU:HG2	4:A:343:HOH:O	2.18	0.43
1:C:198:TYR:OH	1:C:219:ARG:NH1	2.51	0.43
1:C:237:ASP:O	1:C:241[A]:GLN:HG3	2.18	0.43
1:A:-3:TYR:OH	1:B:197[A]:GLU:HB2	2.18	0.43
1:B:21:VAL:CG1	1:B:49[A]:VAL:HG12	2.49	0.43
1:A:240[B]:MET:HG2	1:C:275:TRP:CE2	2.53	0.43
1:B:242[B]:MET:HG3	1:B:256:PHE:CE1	2.54	0.43
1:D:195[B]:LEU:HD23	1:D:199:MET:HG2	2.00	0.42
1:D:185:MET:CE	1:D:237[A]:ASP:CG	2.88	0.42
1:C:109[A]:LEU:CD1	1:C:147[A]:SER:OG	2.63	0.42
1:B:204:GLU:CG	1:C:234:GLU:HG3	2.50	0.42
1:D:197:GLU:O	1:D:201[A]:ARG:HG2	2.19	0.42
1:D:232:MET:HB3	1:D:232:MET:HE2	1.87	0.42
1:C:204:GLU:O	1:C:208:VAL:HG22	2.19	0.42
1:C:78:ALA:HB1	1:C:81:PHE:CD2	2.55	0.42
1:C:76[B]:CYS:SG	1:C:105:GLU:OE1	2.76	0.42
1:A:237:ASP:O	1:A:241[B]:GLN:HG3	2.20	0.42
1:B:206:ILE:HD12	1:B:207[B]:ARG:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LYS:HG2	1:B:271:CYS:SG	2.59	0.42
1:D:105:GLU:HG2	1:D:141:THR:HB	2.02	0.42
1:D:119:VAL:HG11	1:D:159:ARG:CD	2.49	0.41
1:D:202:GLU:OE1	1:D:219:ARG:HG2	2.20	0.41
1:D:112:TRP:CZ2	1:D:149[B]:GLY:HA3	2.55	0.41
1:C:175[A]:SER:OG	1:C:226[A]:GLU:HB3	2.20	0.41
1:C:267:GLU:HG3	4:C:845:HOH:O	2.20	0.41
1:B:188:VAL:HG11	1:B:242[B]:MET:SD	2.61	0.41
1:B:229[A]:ASP:HA	4:B:933[A]:HOH:O	2.20	0.41
1:A:25:THR:O	1:A:28:GLU:HG2	2.21	0.41
1:A:92:SER:O	1:A:96:VAL:HG23	2.21	0.41
1:A:185:MET:HG3	1:A:241[B]:GLN:OE1	2.21	0.41
1:D:242[A]:MET:CA	1:D:242[A]:MET:CE	2.98	0.40
1:A:-2:PHE:CE2	1:B:202:GLU:HG2	2.56	0.40
1:C:81:PHE:CD2	1:C:109[B]:LEU:HG	2.57	0.40
1:D:107:GLU:OE2	4:D:384:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/293 (97%)	279 (98%)	6 (2%)	0	100	100
1	B	278/293 (95%)	270 (97%)	8 (3%)	0	100	100
1	C	289/293 (99%)	282 (98%)	7 (2%)	0	100	100
1	D	289/293 (99%)	279 (96%)	8 (3%)	2 (1%)	22	10
All	All	1141/1172 (97%)	1110 (97%)	29 (2%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	148[A]	GLY
1	D	148[B]	GLY

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	237/237 (100%)	237 (100%)	0	100	100
1	B	231/237 (98%)	231 (100%)	0	100	100
1	C	241/237 (102%)	241 (100%)	0	100	100
1	D	240/237 (101%)	238 (99%)	2 (1%)	81	78
All	All	949/948 (100%)	947 (100%)	2 (0%)	93	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	242[A]	MET
1	D	242[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	182	HIS
1	D	-1	GLN
1	D	246	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)

6 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	GLC	E	1	2	11,11,12	0.59	0	15,15,17	1.46	3 (20%)
2	FRU	E	2	2	11,12,12	0.77	0	10,18,18	0.82	0
2	GLC	F	1	2	11,11,12	0.74	0	15,15,17	1.64	3 (20%)
2	FRU	F	2	2	11,12,12	0.74	0	10,18,18	0.70	0
2	GLC	G	1	2	11,11,12	0.56	0	15,15,17	0.90	0
2	FRU	G	2	2	11,12,12	0.81	0	10,18,18	0.64	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
2	GLC	E	1	2	-	2/2/19/22	0/1/1/1
2	FRU	E	2	2	-	3/5/24/24	0/1/1/1
2	GLC	F	1	2	-	0/2/19/22	0/1/1/1
2	FRU	F	2	2	-	3/5/24/24	0/1/1/1
2	GLC	G	1	2	-	0/2/19/22	0/1/1/1
2	FRU	G	2	2	-	0/5/24/24	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	GLC	O5-C5-C6	3.38	112.50	107.20
2	E	1	GLC	O6-C6-C5	-3.15	100.47	111.29
2	E	1	GLC	C1-O5-C5	3.05	116.33	112.19
2	F	1	GLC	O5-C1-C2	-3.05	106.07	110.77
2	F	1	GLC	C6-C5-C4	-2.60	106.91	113.00
2	E	1	GLC	C6-C5-C4	-2.15	107.96	113.00

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	FRU	O1-C1-C2-O2
2	E	2	FRU	O1-C1-C2-C3
2	E	2	FRU	O1-C1-C2-O2
2	E	1	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	E	2	FRU	O1-C1-C2-O5
2	F	2	FRU	C4-C5-C6-O6
2	F	2	FRU	O5-C5-C6-O6

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

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings
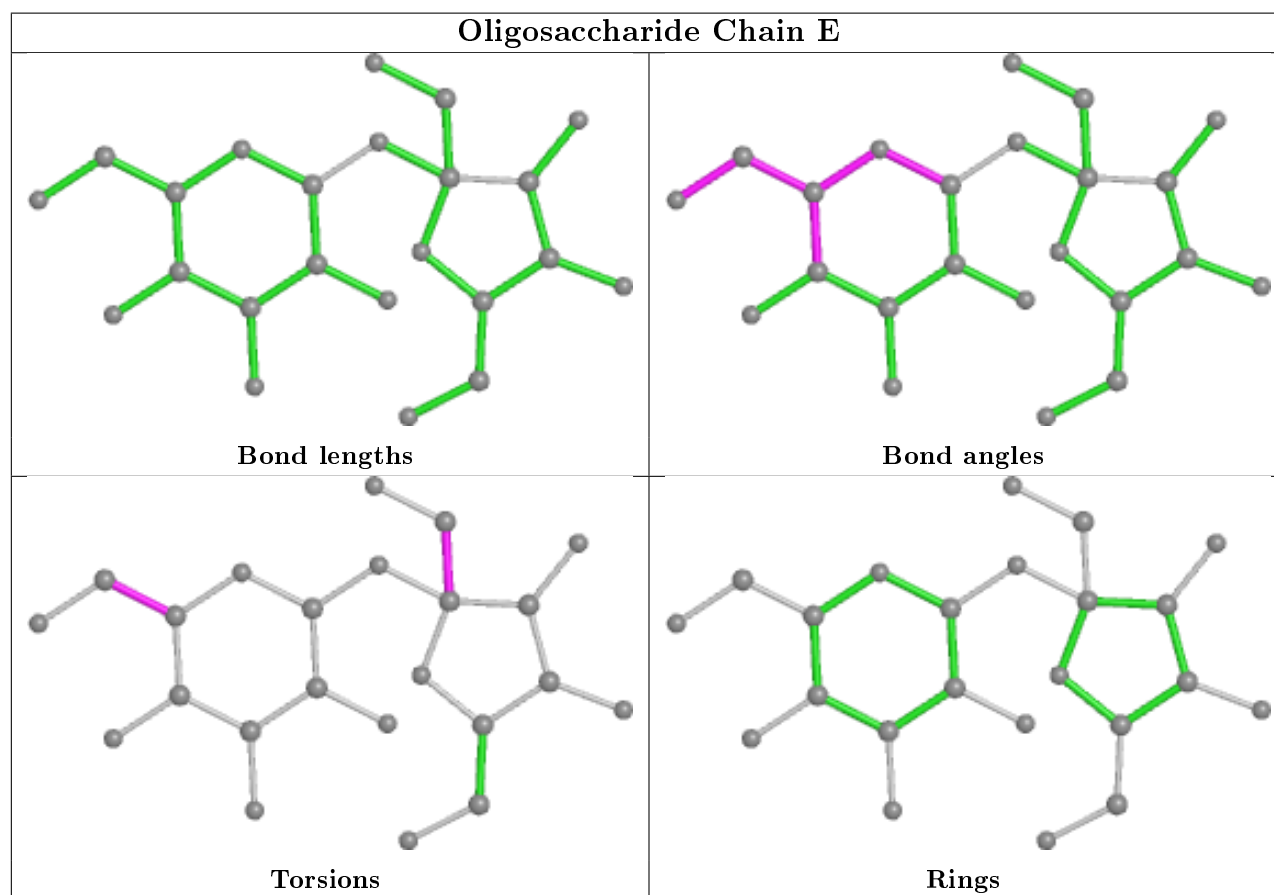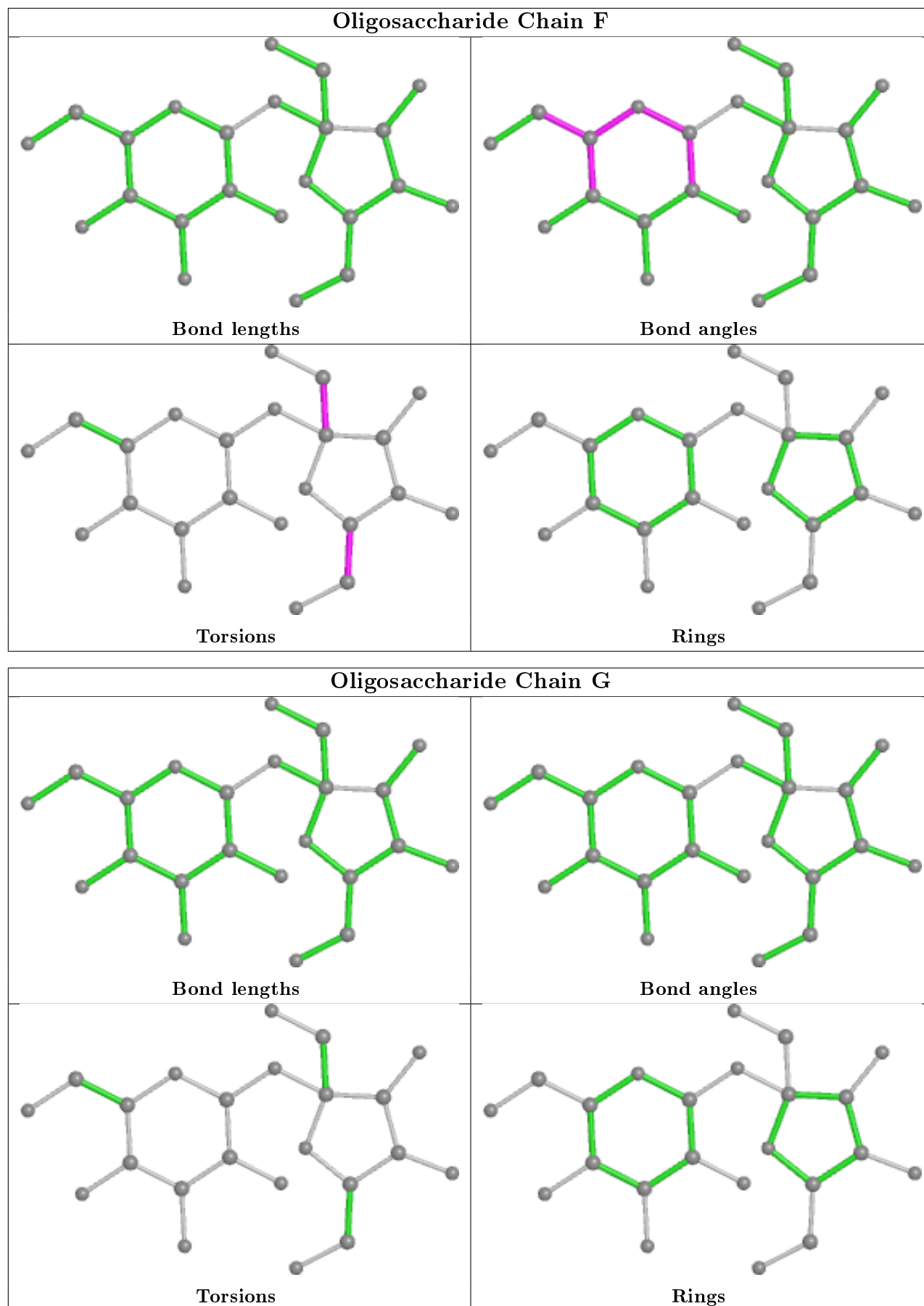
5.6 Ligand geometry (i)

16 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	$\#|Z| > 2$
3	SO4	D	285	-	4,4,4	0.16	0	6,6,6	0.09	0
3	SO4	A	283	-	4,4,4	0.14	0	6,6,6	0.18	0
3	SO4	B	282	-	4,4,4	0.13	0	6,6,6	0.29	0
3	SO4	A	287	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	B	5	-	4,4,4	0.18	0	6,6,6	0.20	0
3	SO4	C	283	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	A	284	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	A	286[A]	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	283	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	D	283	-	4,4,4	0.12	0	6,6,6	0.08	0
3	SO4	D	284	-	4,4,4	0.18	0	6,6,6	0.10	0
3	SO4	A	282	-	4,4,4	0.18	0	6,6,6	0.20	0
3	SO4	C	282	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	D	4	-	4,4,4	0.24	0	6,6,6	0.38	0
3	SO4	A	285	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	D	282	-	4,4,4	0.15	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	287	SO4	1	0
3	D	284	SO4	1	0
3	C	282	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	273/293 (93%)	0.19	12 (4%)	34	28	17, 31, 47, 58	0
1	B	268/293 (91%)	0.16	7 (2%)	56	51	18, 28, 44, 53	0
1	C	273/293 (93%)	0.22	16 (5%)	22	17	19, 30, 46, 59	0
1	D	270/293 (92%)	0.17	15 (5%)	24	19	20, 30, 48, 61	0
All	All	1084/1172 (92%)	0.19	50 (4%)	32	26	17, 30, 46, 61	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	180	ALA	7.7
1	D	180	ALA	6.9
1	A	229	ASP	4.4
1	D	209	GLU	4.2
1	D	152	GLN	3.9
1	D	179	GLY	3.9
1	D	280	VAL	3.8
1	D	-3	TYR	3.7
1	B	229[A]	ASP	3.6
1	B	207[A]	ARG	3.5
1	D	181	THR	3.5
1	C	119	VAL	3.5
1	C	179	GLY	3.5
1	C	152	GLN	3.4
1	A	207	ARG	3.4
1	B	218	VAL	3.3
1	A	117	GLU	3.3
1	A	218	VAL	3.2
1	A	180	ALA	3.2
1	C	220	CYS	3.1
1	A	228	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	117[A]	GLU	2.8
1	C	-3	TYR	2.8
1	A	-5	ASN	2.8
1	B	146	LEU	2.7
1	C	181	THR	2.7
1	D	151	LEU	2.7
1	B	180	ALA	2.7
1	D	205	ARG	2.6
1	C	145	VAL	2.5
1	C	139	PRO	2.4
1	A	145	VAL	2.4
1	A	152	GLN	2.3
1	D	225	ILE	2.3
1	D	-1	GLN	2.3
1	A	118	ASN	2.3
1	B	144	VAL	2.2
1	D	148[A]	GLY	2.2
1	C	26	ASP	2.2
1	D	138	GLY	2.2
1	C	229	ASP	2.2
1	A	225	ILE	2.1
1	B	276	ASP	2.1
1	C	109[A]	LEU	2.1
1	C	146	LEU	2.1
1	A	182	HIS	2.1
1	C	178[A]	LEU	2.1
1	D	149[A]	GLY	2.1
1	C	62[A]	GLU	2.0
1	D	109[A]	LEU	2.0

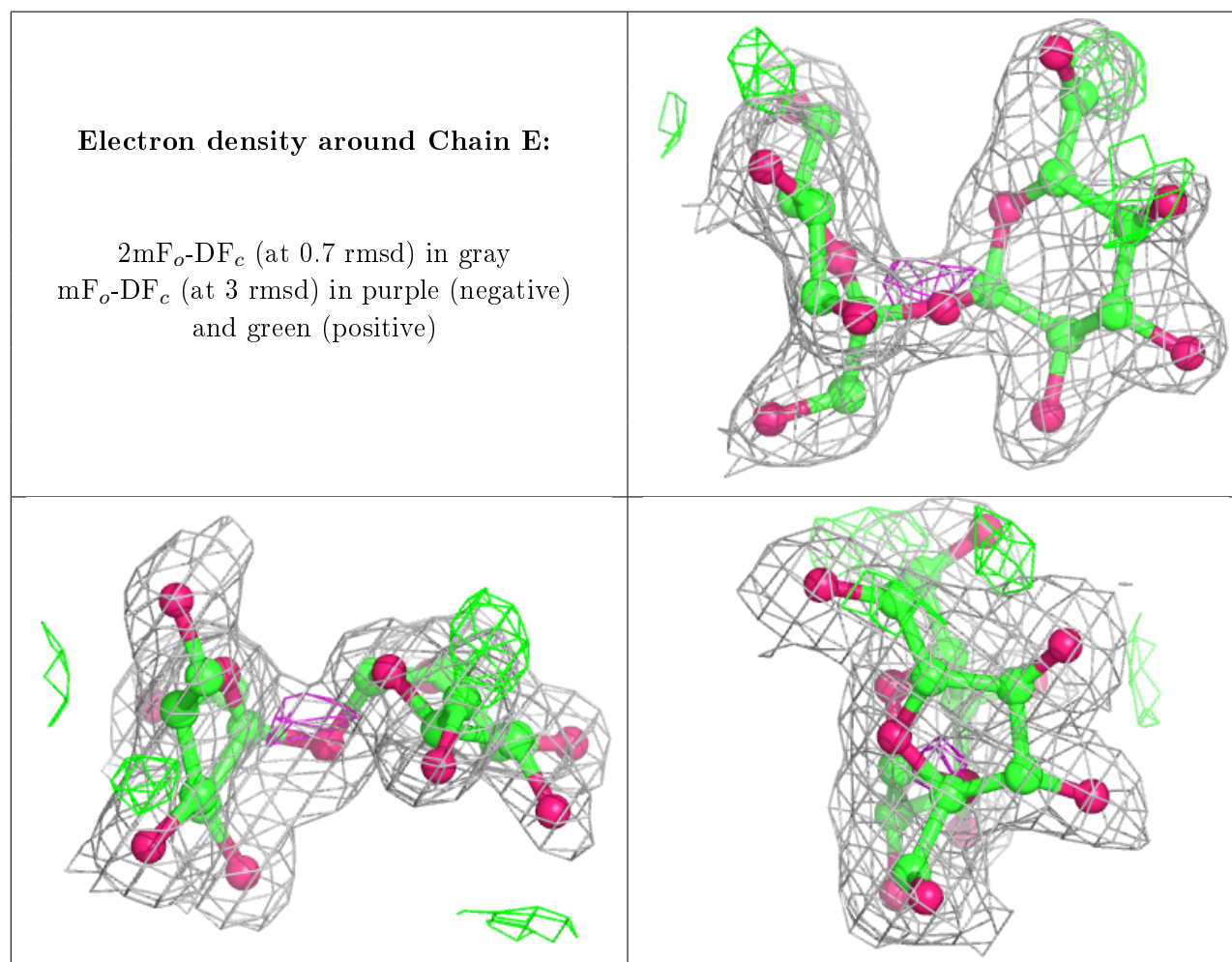## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

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.
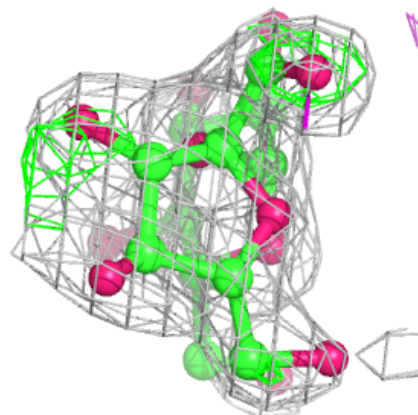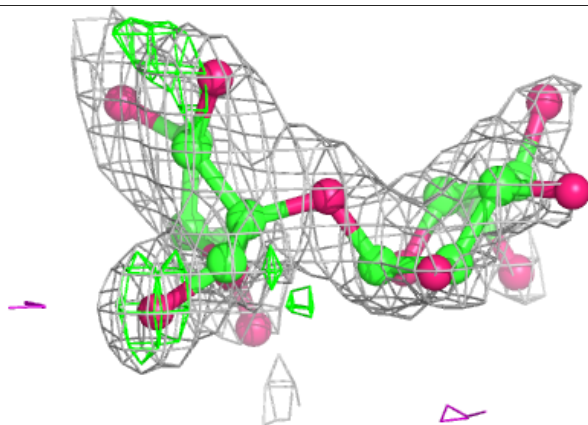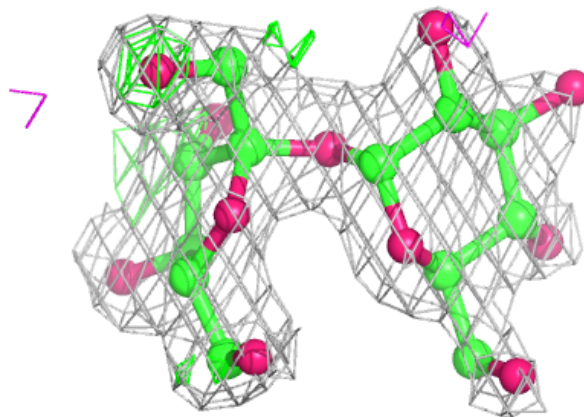
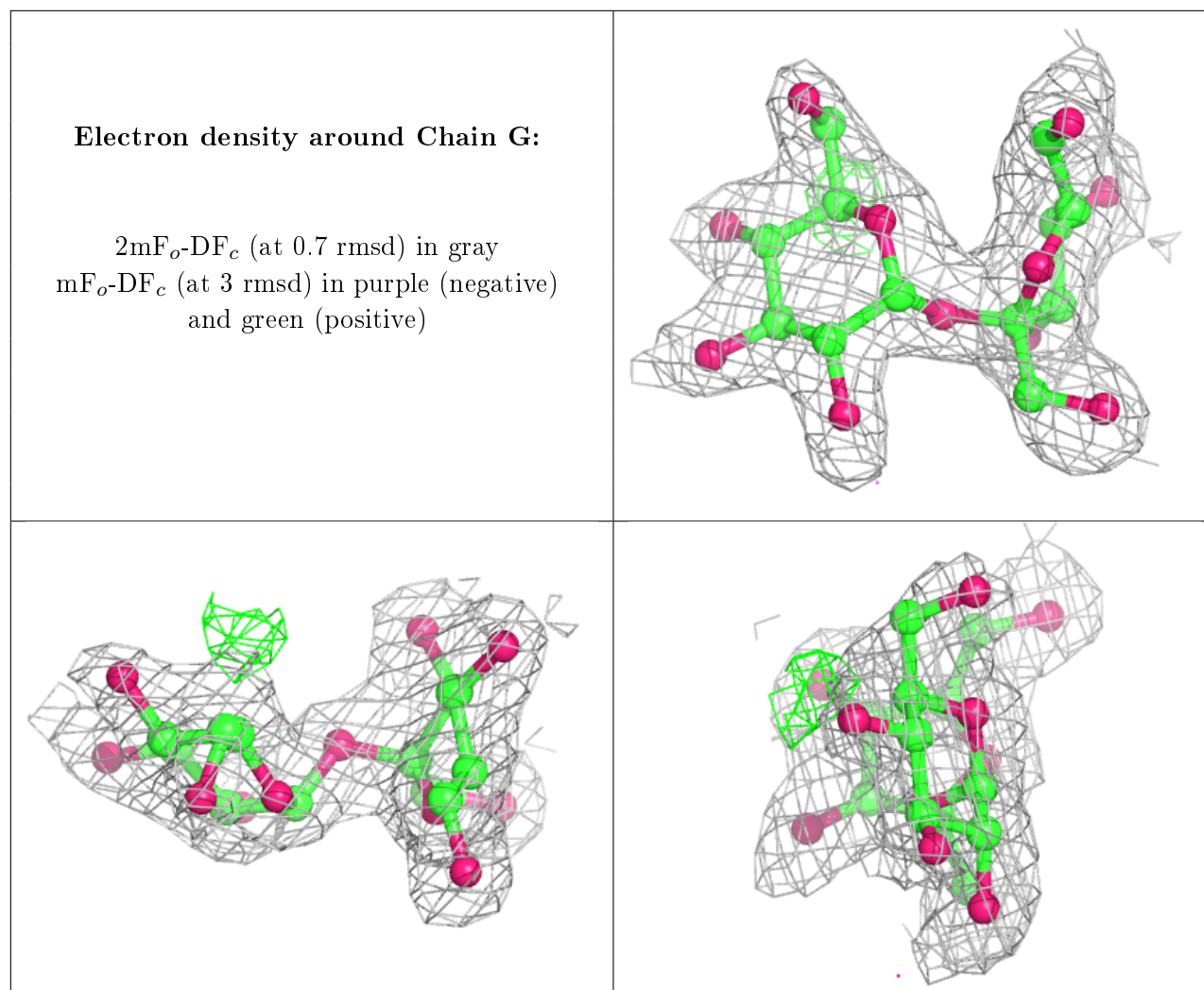| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRU	F	2	12/12	0.65	0.22	46,53,61,66	12
2	FRU	E	2	12/12	0.77	0.20	33,39,41,42	12
2	GLC	E	1	11/12	0.83	0.30	46,47,48,49	11
2	FRU	G	2	12/12	0.88	0.14	33,37,40,42	12
2	GLC	G	1	11/12	0.89	0.22	43,45,48,48	11
2	GLC	F	1	11/12	0.89	0.21	46,52,61,64	11

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)

Electron density around Chain G:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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
3	SO4	A	287	5/5	0.57	0.37	34,41,43,48	5
3	SO4	C	282	5/5	0.80	0.23	53,55,55,55	5
3	SO4	B	283	5/5	0.83	0.18	56,57,57,58	5
3	SO4	D	284	5/5	0.84	0.28	44,51,52,53	5
3	SO4	C	283	5/5	0.90	0.19	53,53,54,55	5
3	SO4	D	285	5/5	0.90	0.24	27,35,38,41	5
3	SO4	A	285	5/5	0.92	0.22	87,88,88,88	0
3	SO4	D	283	5/5	0.93	0.17	30,38,43,43	5
3	SO4	A	284	5/5	0.94	0.26	82,82,83,84	0

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	286[A]	5/5	0.95	0.20	45,46,47,48	5
3	SO4	A	282	5/5	0.97	0.14	33,35,37,38	5
3	SO4	D	282	5/5	0.97	0.12	39,40,42,43	5
3	SO4	B	5	5/5	0.98	0.11	37,42,43,43	0
3	SO4	D	4	5/5	0.99	0.07	28,30,34,38	0
3	SO4	A	283	5/5	0.99	0.06	38,39,42,44	0
3	SO4	B	282	5/5	0.99	0.06	40,41,43,45	0

6.5 Other polymers (i)

There are no such residues in this entry.