



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:39 PM UTC

PDB ID : 4C9F / pdb_00004c9f
Title : Structure of SIGN-R1 in complex with Sulfodextran
Authors : Silva-Martin, N.; Bartual, S.G.; Rodriguez, A.; Ramirez, E.; Chacon, P.; Anthony, R.M.; Park, C.G.; Hermoso, J.A.
Deposited on : 2013-10-02
Resolution : 2.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

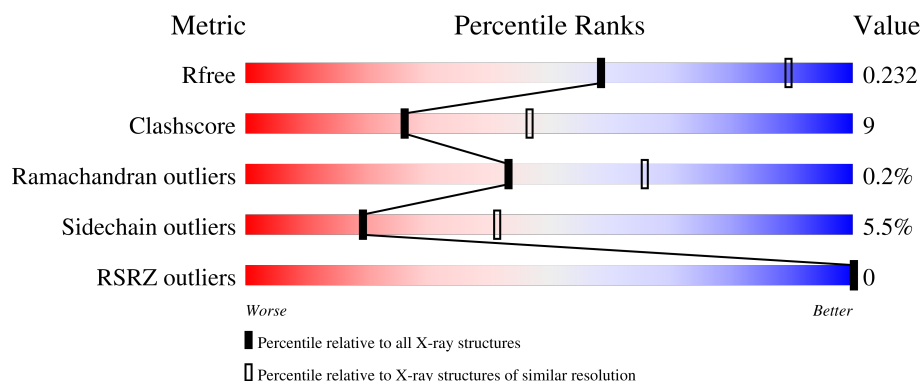
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	134	
1	B	134	
1	C	134	
1	D	134	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
3	G	4	 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GQ1	D	1326	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4680 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.

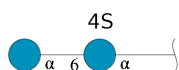
- Molecule 1 is a protein called CD209 ANTIGEN-LIKE PROTEIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			1073	684	180	200	9			
1	B	133	Total	C	N	O	S	0	0	0
			1080	688	181	202	9			
1	C	132	Total	C	N	O	S	0	0	0
			1073	684	180	200	9			
1	D	134	Total	C	N	O	S	0	0	0
			1089	694	183	203	9			

There are 4 discrepancies between the modelled and reference sequences:

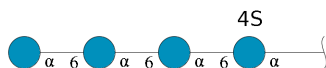
Chain	Residue	Modelled	Actual	Comment	Reference
A	190	LYS	-	expression tag	UNP Q8CJ91
B	190	LYS	-	expression tag	UNP Q8CJ91
C	190	LYS	-	expression tag	UNP Q8CJ91
D	190	LYS	-	expression tag	UNP Q8CJ91

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-4-O-sulfo-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	S	0	0	0
			27	12	14	1			
2	F	2	Total	C	O		0	0	0
			23	12	11				

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-4-O-sulfo-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	4	Total	C	O	S	0	0	0
			49	24	24	1			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



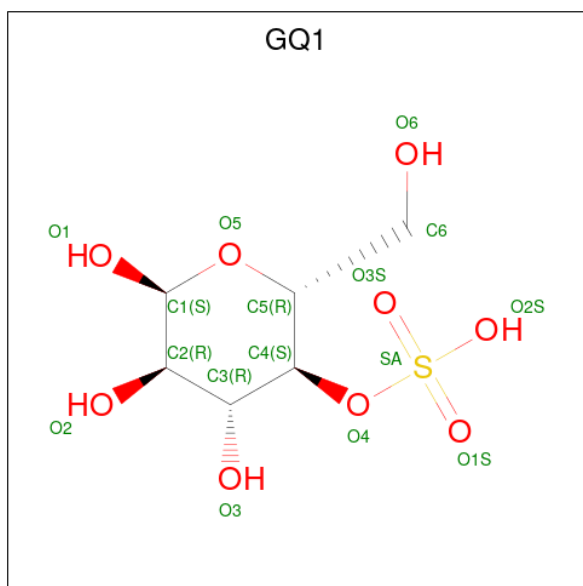
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is 4-O-sulfo-alpha-D-glucopyranose (CCD ID: GQ1) (formula: C₆H₁₂O₉S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	O	S	0	0
			16	6	9	1		
6	D	1	Total	C	O	S	0	0
			16	6	9	1		
6	D	1	Total	C	O	S	0	0
			16	6	9	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	43	Total 43	O 43	0	0
7	B	44	Total 44	O 44	0	0
7	C	40	Total 40	O 40	0	0
7	D	37	Total 37	O 37	0	0

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: CD209 ANTIGEN-LIKE PROTEIN B

Chain A:  84% 10% ..



• Molecule 1: CD209 ANTIGEN-LIKE PROTEIN B

Chain B:  75% 23% ..



• Molecule 1: CD209 ANTIGEN-LIKE PROTEIN B

Chain C:  79% 17% ..



• Molecule 1: CD209 ANTIGEN-LIKE PROTEIN B

Chain D:  78% 19% .



• Molecule 2: alpha-D-glucopyranose-(1-6)-4-O-sulfo-alpha-D-glucopyranose

Chain E:  100%



• Molecule 2: alpha-D-glucopyranose-(1-6)-4-O-sulfo-alpha-D-glucopyranose

Chain F:  100%

GLC2

- Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-4-O-sulfo-alpha-D-glucopyranose

Chain G:

50%

50%

GLC2
GLC3
GLC4

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.03Å 97.96Å 73.85Å 90.00° 120.86° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-2.60) 99.0 (40.00-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.233 0.199 , 0.232	Depositor DCC
R_{free} test set	1345 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 17.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.468 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4680	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 42.07 % 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 2.1526e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GQ1, CA, SO4, GLC

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	1.03	0/1103	1.06	1/1493 (0.1%)
1	B	1.08	0/1110	1.08	0/1503
1	C	1.07	0/1103	1.08	0/1493
1	D	1.06	2/1119 (0.2%)	1.11	2/1514 (0.1%)
All	All	1.06	2/4435 (0.0%)	1.08	3/6003 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	191	LEU	CA-C	5.32	1.59	1.53
1	D	322	CYS	CA-C	5.30	1.59	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	192	CYS	N-CA-C	9.14	122.31	109.15
1	A	262	GLU	N-CA-C	5.32	119.25	112.87
1	D	231	VAL	N-CA-C	5.20	116.11	109.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	290	GLY	Peptide

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	1073	0	1017	17	0
1	B	1080	0	1024	25	0
1	C	1073	0	1017	23	0
1	D	1089	0	1037	18	0
2	E	27	0	21	2	0
2	F	23	0	20	2	0
3	G	49	0	39	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	0	0	0
5	B	25	0	0	1	0
5	C	15	0	0	0	0
5	D	5	0	0	0	0
6	D	48	0	35	7	0
7	A	43	0	0	5	0
7	B	44	0	0	3	0
7	C	40	0	0	4	0
7	D	37	0	0	0	0
All	All	4680	0	4210	82	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 (82) 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:191:LEU:HD11	1:D:213:GLN:HE21	1.29	0.94
6:D:1326:GQ1:HS2	6:D:1326:GQ1:H2HA	0.95	0.88
6:D:1326:GQ1:O2S	6:D:1326:GQ1:O2	1.90	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1326:GQ1:O2S	6:D:1326:GQ1:H3A	1.77	0.85
1:B:296:GLU:OE2	2:F:2:GLC:O2	2.01	0.76
6:D:1326:GQ1:O2S	6:D:1326:GQ1:C3	2.39	0.70
1:A:320:THR:HG22	1:A:320:THR:O	1.93	0.68
1:A:234:ASN:ND2	7:A:2016:HOH:O	2.26	0.68
1:C:234:ASN:OD1	7:C:2015:HOH:O	2.12	0.67
1:C:202:LEU:HD12	1:D:244:GLN:OE1	1.94	0.67
1:D:207:TYR:CE2	1:D:316:LYS:HD3	2.31	0.64
1:B:227:LYS:O	1:B:227:LYS:HD3	2.03	0.59
1:B:262:GLU:CG	1:B:289:ILE:HG22	2.32	0.59
1:A:287:ASN:OD1	1:A:287:ASN:C	2.46	0.58
1:C:311:LYS:NZ	3:G:2:GLC:H2	2.17	0.58
1:C:217:ASN:ND2	7:C:2011:HOH:O	2.11	0.57
1:D:260:LYS:HD2	1:D:266:LEU:HD12	1.87	0.57
1:D:232:ILE:HG23	1:D:267:TRP:CD2	2.40	0.56
1:D:234:ASN:HB2	6:D:1327:GQ1:O1S	2.06	0.55
2:E:1:GQ1:H6AA	2:E:2:GLC:O2	2.06	0.55
1:B:221:THR:O	1:B:225:GLU:HG2	2.07	0.54
1:B:323:THR:HG22	1:B:323:THR:O	2.07	0.54
1:C:211:LYS:HG2	1:D:193:ARG:HG3	1.89	0.54
1:A:256:LEU:HD23	1:A:295:VAL:HG21	1.90	0.53
1:A:234:ASN:C	1:A:234:ASN:HD22	2.15	0.53
1:B:191:LEU:C	1:B:191:LEU:HD23	2.34	0.52
2:F:1:GQ1:H6AA	2:F:2:GLC:O2	2.09	0.52
1:B:254:MET:HE3	1:B:295:VAL:HG12	1.92	0.52
1:A:253:TRP:CE2	1:A:311:LYS:HG3	2.45	0.51
1:C:203:LEU:N	1:D:244:GLN:OE1	2.40	0.51
1:A:214:ARG:NE	7:A:2011:HOH:O	2.44	0.51
1:C:203:LEU:HD23	1:D:244:GLN:HG3	1.94	0.49
1:C:234:ASN:ND2	7:C:2017:HOH:O	2.45	0.49
1:A:214:ARG:CD	7:A:2011:HOH:O	2.61	0.48
1:C:254:MET:HE1	1:C:302:TRP:CD1	2.47	0.48
1:C:311:LYS:HZ2	3:G:2:GLC:H2	1.77	0.48
1:A:203:LEU:HD11	1:A:237:GLU:OE1	2.14	0.47
1:A:244:GLN:NE2	1:B:203:LEU:H	2.12	0.47
1:D:296:GLU:OE1	1:D:311:LYS:HE3	2.15	0.47
2:E:1:GQ1:C6	2:E:2:GLC:O2	2.64	0.46
1:C:306:LYS:NZ	7:C:2035:HOH:O	2.46	0.46
1:A:192:CYS:O	1:B:249:LYS:NZ	2.49	0.46
1:A:191:LEU:N	7:A:2001:HOH:O	2.48	0.46
1:C:233:ILE:N	1:C:233:ILE:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:GLU:OE2	1:B:289:ILE:HG22	2.16	0.46
1:B:323:THR:N	7:B:2042:HOH:O	2.40	0.45
6:D:1326:GQ1:O2S	6:D:1326:GQ1:C2	2.64	0.45
1:C:243:GLN:NE2	1:C:299:GLY:O	2.50	0.45
1:B:211:LYS:HD2	5:B:1328:SO4:O2	2.17	0.45
1:A:249:LYS:HD3	1:B:192:CYS:SG	2.57	0.44
1:B:199:TRP:CE2	1:B:208:PHE:HB2	2.53	0.44
1:B:322:CYS:O	1:B:323:THR:C	2.60	0.44
1:D:229:GLN:HE21	1:D:229:GLN:HB2	1.57	0.44
1:B:231:VAL:HG21	1:B:242:LEU:HD11	2.00	0.44
1:D:276:ARG:HB2	6:D:1326:GQ1:H2A	2.00	0.44
1:A:214:ARG:HD2	7:A:2011:HOH:O	2.17	0.44
1:D:231:VAL:HG21	1:D:242:LEU:CD1	2.48	0.44
1:D:287:ASN:O	1:D:288:ASN:C	2.60	0.44
3:G:1:GQ1:H6AA	3:G:2:GLC:O2	2.18	0.43
1:B:322:CYS:HA	7:B:2042:HOH:O	2.18	0.43
1:C:253:TRP:CE2	1:C:311:LYS:HG3	2.53	0.43
1:A:194:LEU:HD13	1:A:201:PHE:CD1	2.53	0.43
1:B:238:GLU:O	1:B:242:LEU:HG	2.19	0.43
1:A:241:PHE:O	1:A:244:GLN:HG3	2.19	0.42
1:C:287:ASN:O	1:C:288:ASN:C	2.62	0.42
1:B:287:ASN:OD1	1:B:287:ASN:C	2.61	0.42
1:B:311:LYS:NZ	7:B:2037:HOH:O	2.51	0.42
1:D:199:TRP:CD2	1:D:208:PHE:HB2	2.54	0.42
1:B:213:GLN:HA	1:B:311:LYS:O	2.19	0.42
1:B:195:CYS:O	1:B:196:PRO:C	2.61	0.42
1:D:231:VAL:HG21	1:D:242:LEU:HD11	2.00	0.42
1:C:199:TRP:CE2	1:C:208:PHE:HB2	2.55	0.42
1:C:256:LEU:HD23	1:C:295:VAL:HG21	2.01	0.42
1:A:191:LEU:HA	1:B:211:LYS:O	2.20	0.41
1:C:244:GLN:NE2	1:D:203:LEU:H	2.18	0.41
1:B:232:ILE:HG23	1:B:267:TRP:CD2	2.55	0.41
1:C:199:TRP:CD2	1:C:208:PHE:HB2	2.56	0.41
1:C:254:MET:HE3	1:C:295:VAL:HG12	2.02	0.41
1:B:207:TYR:HA	1:B:315:CYS:O	2.21	0.40
1:C:191:LEU:N	1:C:191:LEU:HD13	2.36	0.40
1:C:241:PHE:O	1:C:244:GLN:HG3	2.22	0.40
1:D:323:THR:O	1:D:323:THR:HG22	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	130/134 (97%)	121 (93%)	9 (7%)	0	100	100
1	B	131/134 (98%)	128 (98%)	3 (2%)	0	100	100
1	C	130/134 (97%)	126 (97%)	3 (2%)	1 (1%)	16	34
1	D	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
All	All	523/536 (98%)	499 (95%)	23 (4%)	1 (0%)	43	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	288	ASN

5.3.2 Protein sidechains

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	117/119 (98%)	109 (93%)	8 (7%)	14	32
1	B	118/119 (99%)	113 (96%)	5 (4%)	26	52
1	C	117/119 (98%)	111 (95%)	6 (5%)	21	45
1	D	119/119 (100%)	112 (94%)	7 (6%)	18	38
All	All	471/476 (99%)	445 (94%)	26 (6%)	19	41

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	A	214	ARG
1	A	229	GLN
1	A	234	ASN
1	A	244	GLN
1	A	262	GLU
1	A	274	SER
1	A	320	THR
1	B	194	LEU
1	B	211	LYS
1	B	225	GLU
1	B	244	GLN
1	B	272	THR
1	C	191	LEU
1	C	193	ARG
1	C	194	LEU
1	C	229	GLN
1	C	244	GLN
1	C	320	THR
1	D	191	LEU
1	D	211	LYS
1	D	229	GLN
1	D	244	GLN
1	D	272	THR
1	D	274	SER
1	D	317	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	A	217	ASN
1	A	229	GLN
1	A	244	GLN
1	B	213	GLN
1	B	244	GLN
1	C	234	ASN
1	C	244	GLN
1	C	282	ASN
1	D	213	GLN
1	D	229	GLN
1	D	234	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	GQ1	E	1	2,4	16,16,16	0.76	0	21,24,24	1.40	4 (19%)
2	GLC	E	2	2	11,11,12	0.94	1 (9%)	15,15,17	1.66	3 (20%)
2	GQ1	F	1	2,4	12,12,16	0.89	0	17,17,24	2.38	5 (29%)
2	GLC	F	2	2	11,11,12	0.89	0	15,15,17	1.50	2 (13%)
3	GQ1	G	1	3	16,16,16	0.69	0	21,24,24	1.43	4 (19%)
3	GLC	G	2	3	11,11,12	0.54	0	15,15,17	1.25	2 (13%)
3	GLC	G	3	3	11,11,12	0.88	0	15,15,17	2.25	1 (6%)
3	GLC	G	4	3	11,11,12	1.16	2 (18%)	15,15,17	2.27	5 (33%)

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	GQ1	E	1	2,4	-	7/7/27/27	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GQ1	F	1	2,4	-	2/2/22/27	0/1/1/1
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GQ1	G	1	3	-	4/7/27/27	0/1/1/1
3	GLC	G	2	3	-	2/2/19/22	0/1/1/1
3	GLC	G	3	3	-	2/2/19/22	0/1/1/1
3	GLC	G	4	3	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	4	GLC	C2-C3	2.25	1.55	1.52
3	G	4	GLC	C1-C2	2.22	1.57	1.52
2	E	2	GLC	C2-C3	2.21	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	GLC	C1-O5-C5	7.93	122.82	112.19
3	G	4	GLC	C1-C2-C3	5.98	118.35	109.64
2	F	1	GQ1	O4-C4-C5	-5.57	95.59	109.32
3	G	4	GLC	C1-O5-C5	4.57	118.31	112.19
2	F	1	GQ1	C3-C4-C5	4.27	117.97	110.23
3	G	1	GQ1	C4-O4-SA	3.82	128.19	119.04
2	F	1	GQ1	O5-C5-C6	3.67	115.55	106.44
2	F	2	GLC	O5-C5-C6	3.66	114.79	107.66
2	E	2	GLC	C1-O5-C5	3.27	116.58	112.19
2	E	1	GQ1	C4-O4-SA	3.25	126.84	119.04
2	E	2	GLC	C1-C2-C3	3.25	114.37	109.64
3	G	1	GQ1	C2-C3-C4	3.17	116.88	109.68
2	E	1	GQ1	C2-C3-C4	2.96	116.39	109.68
3	G	2	GLC	C1-O5-C5	2.92	116.10	112.19
3	G	1	GQ1	C1-C2-C3	2.83	116.13	110.36
2	F	2	GLC	C1-C2-C3	2.81	113.73	109.64
2	E	1	GQ1	O5-C1-C2	-2.61	105.72	110.30
2	F	1	GQ1	O5-C5-C4	2.45	114.12	109.70
3	G	4	GLC	O3-C3-C2	2.31	114.76	110.05
3	G	4	GLC	O4-C4-C5	2.29	114.97	109.32
3	G	2	GLC	O5-C5-C6	2.18	111.91	107.66
2	F	1	GQ1	C1-C2-C3	-2.13	106.01	110.36
3	G	4	GLC	C3-C4-C5	-2.12	106.39	110.23
2	E	1	GQ1	O5-C5-C6	2.07	111.57	106.44
2	E	2	GLC	O3-C3-C4	-2.02	105.60	110.38
3	G	1	GQ1	C6-C5-C4	2.01	119.04	113.38

There are no chirality outliers.

All (22) torsion outliers are listed below:

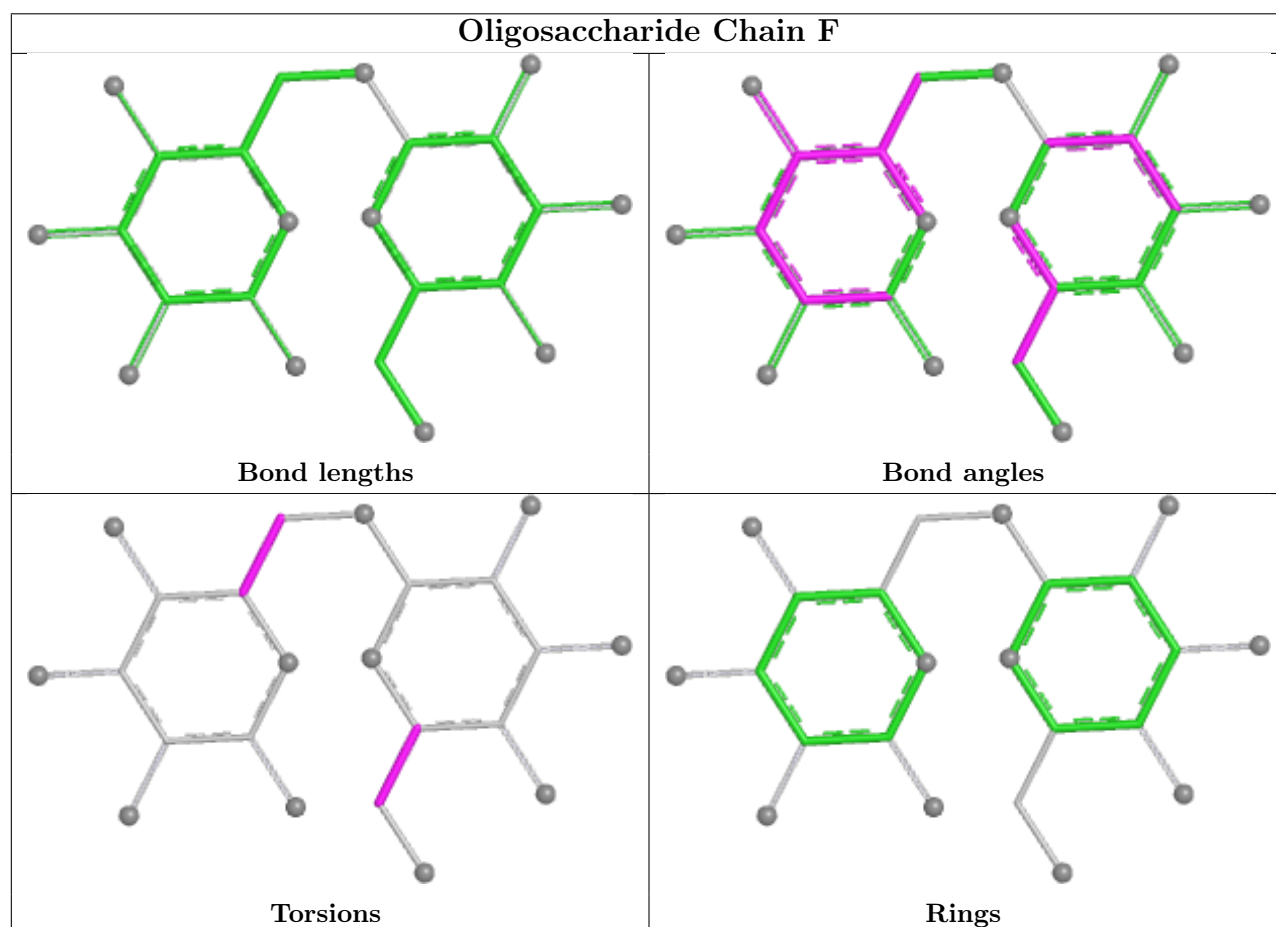
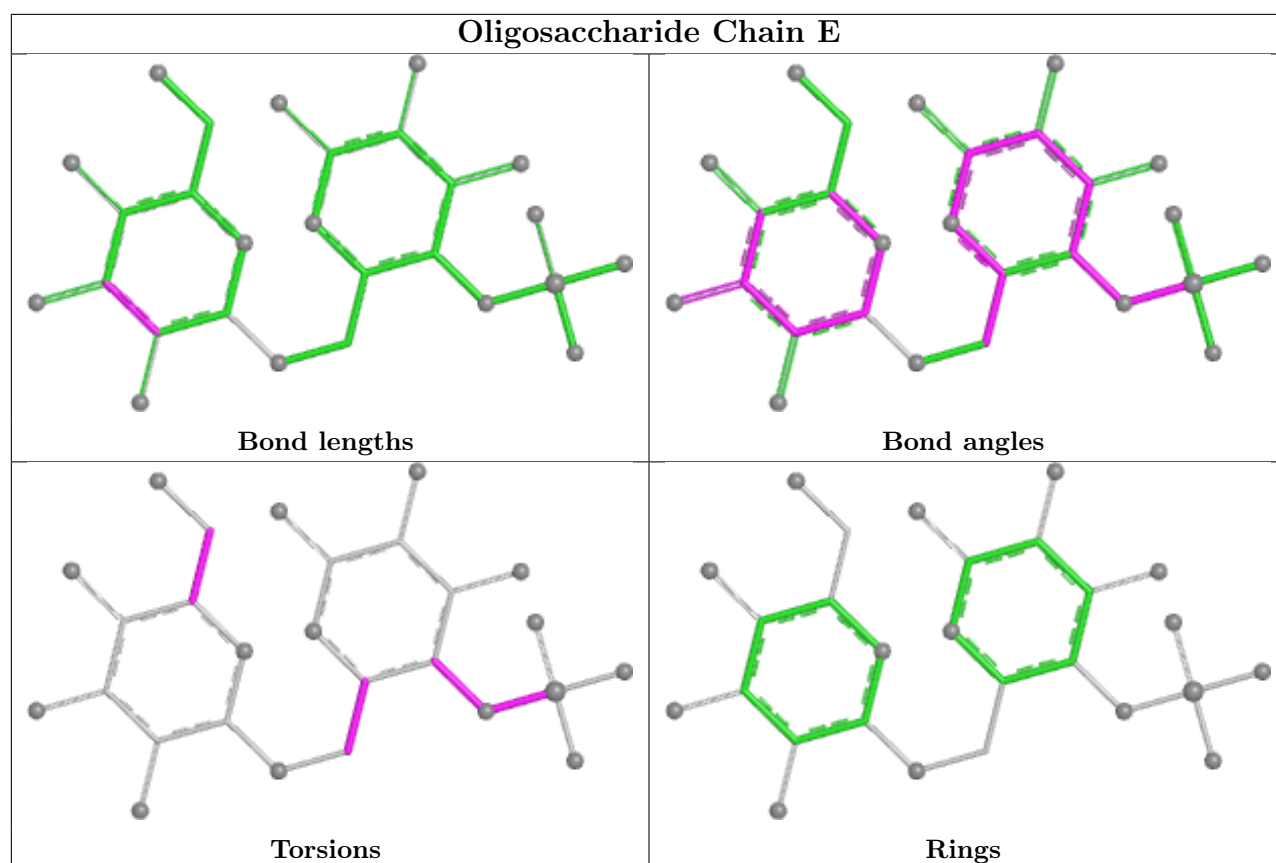
Mol	Chain	Res	Type	Atoms
2	E	1	GQ1	C4-O4-SA-O1S
2	E	1	GQ1	C4-O4-SA-O2S
2	E	1	GQ1	C4-O4-SA-O3S
2	E	1	GQ1	C3-C4-O4-SA
2	E	1	GQ1	C5-C4-O4-SA
3	G	1	GQ1	C3-C4-O4-SA
3	G	1	GQ1	C5-C4-O4-SA
3	G	2	GLC	C4-C5-C6-O6
3	G	2	GLC	O5-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	F	1	GQ1	O5-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	F	1	GQ1	C4-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
3	G	3	GLC	O5-C5-C6-O6
3	G	1	GQ1	O5-C5-C6-O6
2	E	1	GQ1	O5-C5-C6-O6
3	G	3	GLC	C4-C5-C6-O6
3	G	4	GLC	O5-C5-C6-O6
3	G	1	GQ1	C4-C5-C6-O6
2	E	1	GQ1	C4-C5-C6-O6

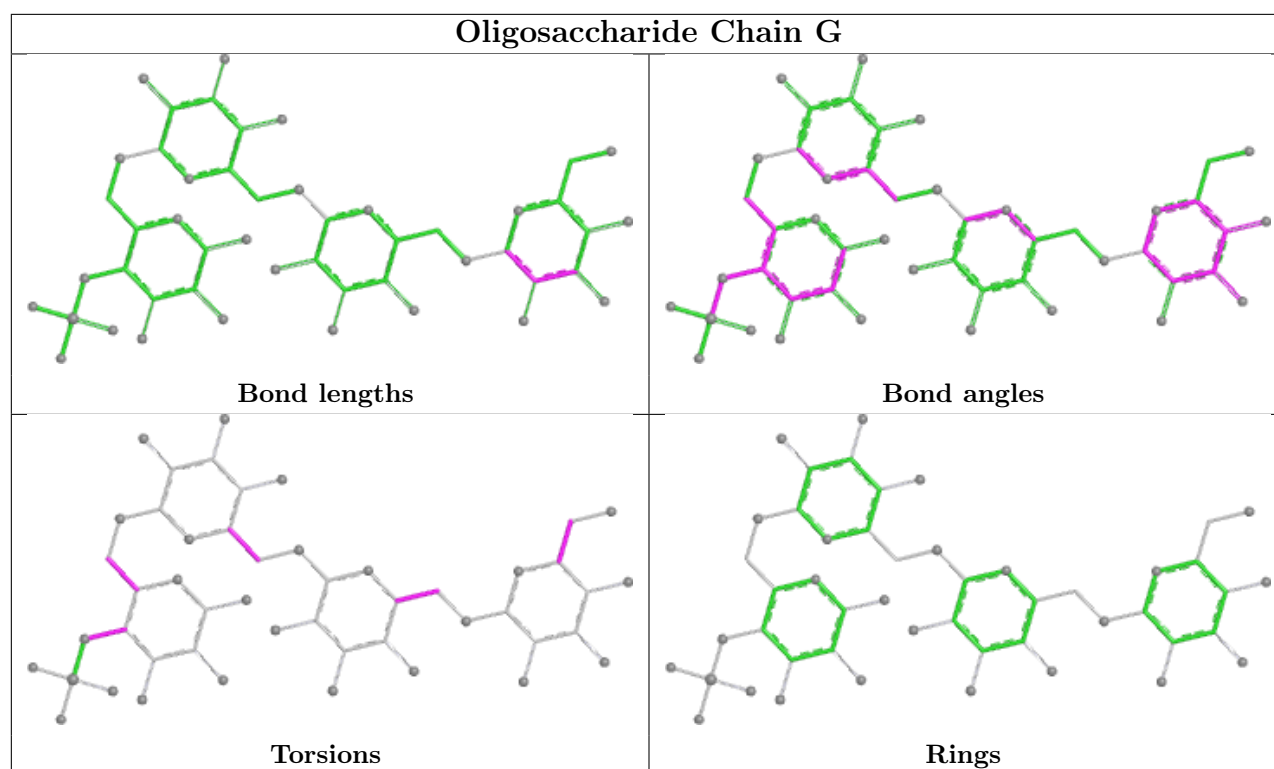
There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	GQ1	2	0
2	F	2	GLC	2	0
2	E	2	GLC	2	0
3	G	2	GLC	3	0
3	G	1	GQ1	1	0
2	F	1	GQ1	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, 4 are monoatomic - leaving 13 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	GQ1	D	1327	-	16,16,16	0.93	0	21,24,24	2.34	11 (52%)
6	GQ1	D	1325	-	16,16,16	1.33	3 (18%)	21,24,24	2.80	5 (23%)
5	SO4	C	1324	-	4,4,4	0.63	0	6,6,6	0.29	0
5	SO4	D	1324	-	4,4,4	0.35	0	6,6,6	0.80	0
5	SO4	B	1326	-	4,4,4	0.50	0	6,6,6	0.42	0
6	GQ1	D	1326	-	16,16,16	1.13	3 (18%)	21,24,24	1.74	3 (14%)
5	SO4	B	1325	-	4,4,4	0.48	0	6,6,6	0.58	0
5	SO4	B	1327	-	4,4,4	0.48	0	6,6,6	0.36	0
5	SO4	B	1328	-	4,4,4	0.59	0	6,6,6	1.18	0
5	SO4	B	1324	-	4,4,4	0.19	0	6,6,6	0.53	0
5	SO4	A	1323	-	4,4,4	0.43	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	C	1323	-	4,4,4	0.55	0	6,6,6	0.51	0
5	SO4	C	1326	-	4,4,4	0.50	0	6,6,6	0.15	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	GQ1	D	1327	-	-	6/7/27/27	0/1/1/1
6	GQ1	D	1325	-	-	4/7/27/27	0/1/1/1
6	GQ1	D	1326	-	-	3/7/27/27	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1325	GQ1	C3-C2	-2.52	1.45	1.52
6	D	1326	GQ1	C1-C2	2.18	1.57	1.52
6	D	1326	GQ1	O5-C1	2.17	1.48	1.42
6	D	1325	GQ1	C1-C2	2.15	1.57	1.52
6	D	1326	GQ1	O1-C1	2.09	1.46	1.39
6	D	1325	GQ1	C4-C5	2.04	1.58	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1325	GQ1	O2-C2-C3	-7.18	93.45	110.38
6	D	1325	GQ1	O2-C2-C1	6.06	123.23	109.25
6	D	1325	GQ1	O3-C3-C2	-5.98	96.28	110.38
6	D	1327	GQ1	C1-O5-C5	4.43	122.22	113.65
6	D	1326	GQ1	C1-O5-C5	4.35	122.06	113.65
6	D	1327	GQ1	C2-C3-C4	4.00	118.75	109.68
6	D	1327	GQ1	O3-C3-C2	-3.83	101.35	110.38
6	D	1327	GQ1	O5-C5-C4	3.62	117.20	109.72
6	D	1326	GQ1	O2-C2-C1	3.47	117.25	109.25
6	D	1325	GQ1	O3-C3-C4	3.41	118.67	109.94
6	D	1327	GQ1	O1-C1-C2	-3.25	99.56	108.98
6	D	1325	GQ1	O5-C5-C4	3.23	116.41	109.72
6	D	1327	GQ1	O2-C2-C3	-3.21	102.81	110.38
6	D	1326	GQ1	O5-C5-C6	2.63	112.96	106.44
6	D	1327	GQ1	O2-C2-C1	-2.42	103.67	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1327	GQ1	O5-C1-C2	2.35	114.43	110.30
6	D	1327	GQ1	C4-O4-SA	2.29	124.54	119.04
6	D	1327	GQ1	C3-C4-C5	2.13	115.65	110.93
6	D	1327	GQ1	O2S-SA-O3S	-2.01	101.54	108.56

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	1325	GQ1	C3-C4-O4-SA
6	D	1326	GQ1	C3-C4-O4-SA
6	D	1326	GQ1	C5-C4-O4-SA
6	D	1327	GQ1	C3-C4-O4-SA
6	D	1327	GQ1	C5-C4-O4-SA
6	D	1327	GQ1	O5-C5-C6-O6
6	D	1325	GQ1	O5-C5-C6-O6
6	D	1325	GQ1	C4-C5-C6-O6
6	D	1327	GQ1	C4-C5-C6-O6
6	D	1326	GQ1	O5-C5-C6-O6
6	D	1327	GQ1	C4-O4-SA-O1S
6	D	1325	GQ1	C5-C4-O4-SA
6	D	1327	GQ1	C4-O4-SA-O2S

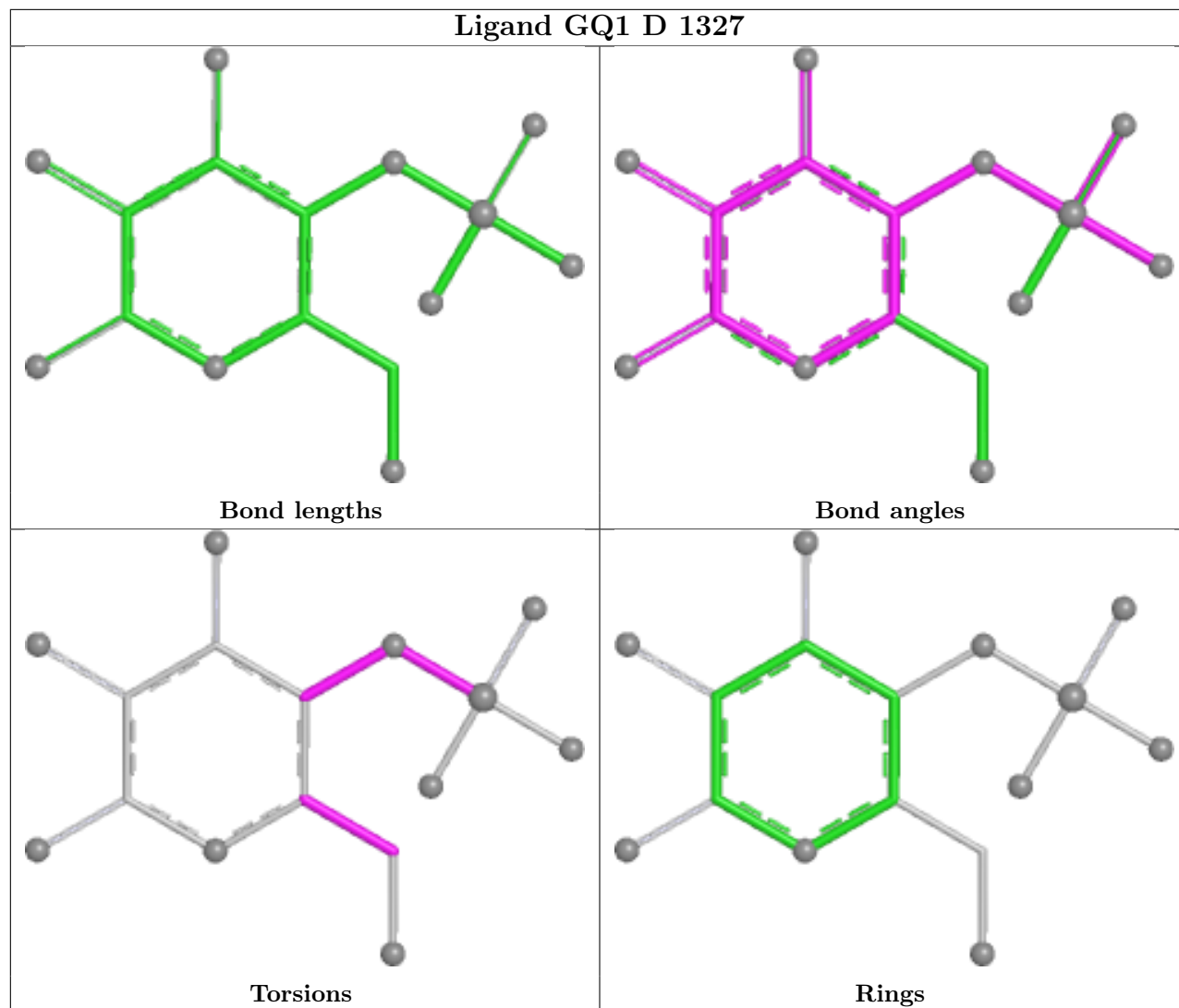
There are no ring outliers.

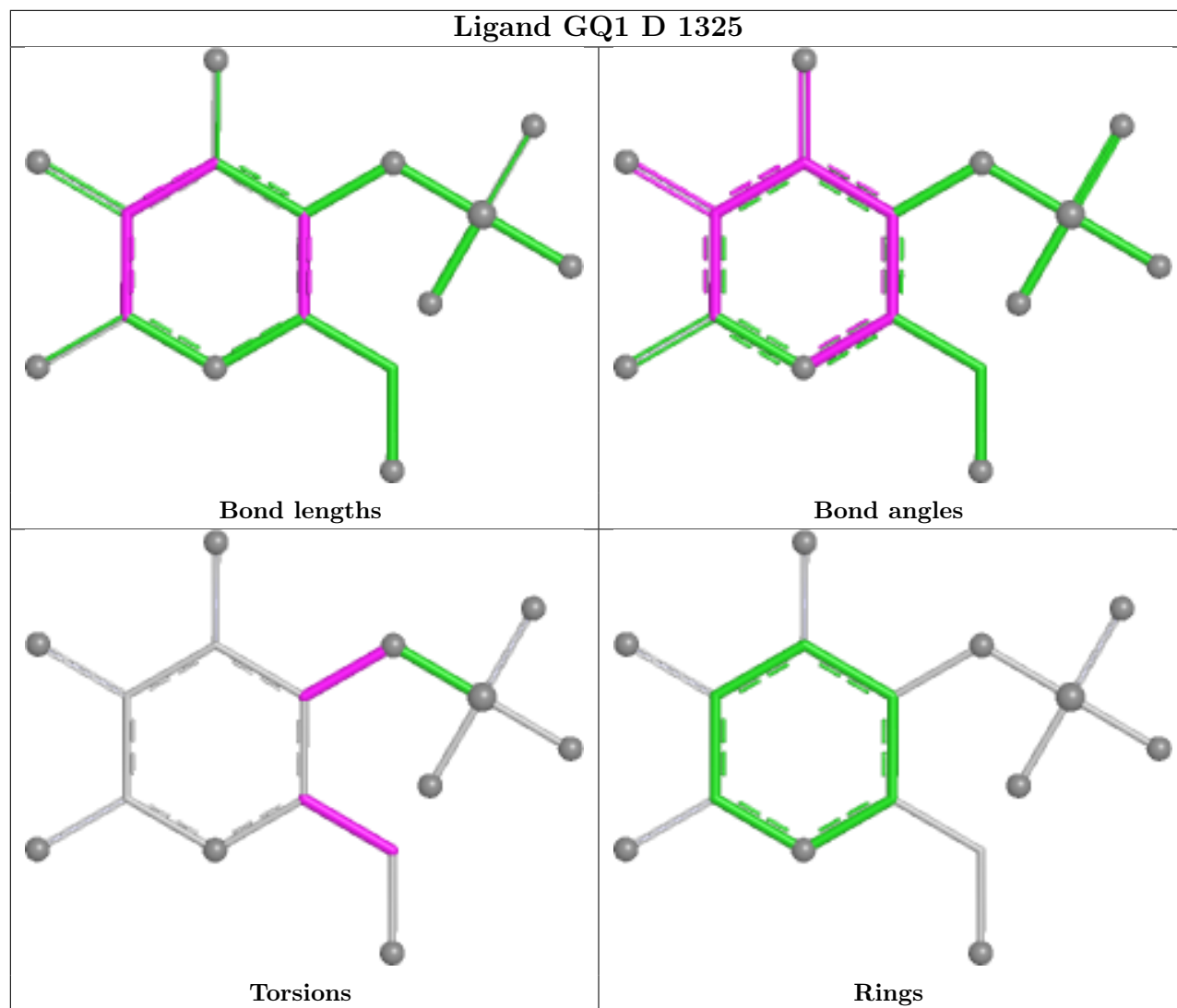
3 monomers are involved in 8 short contacts:

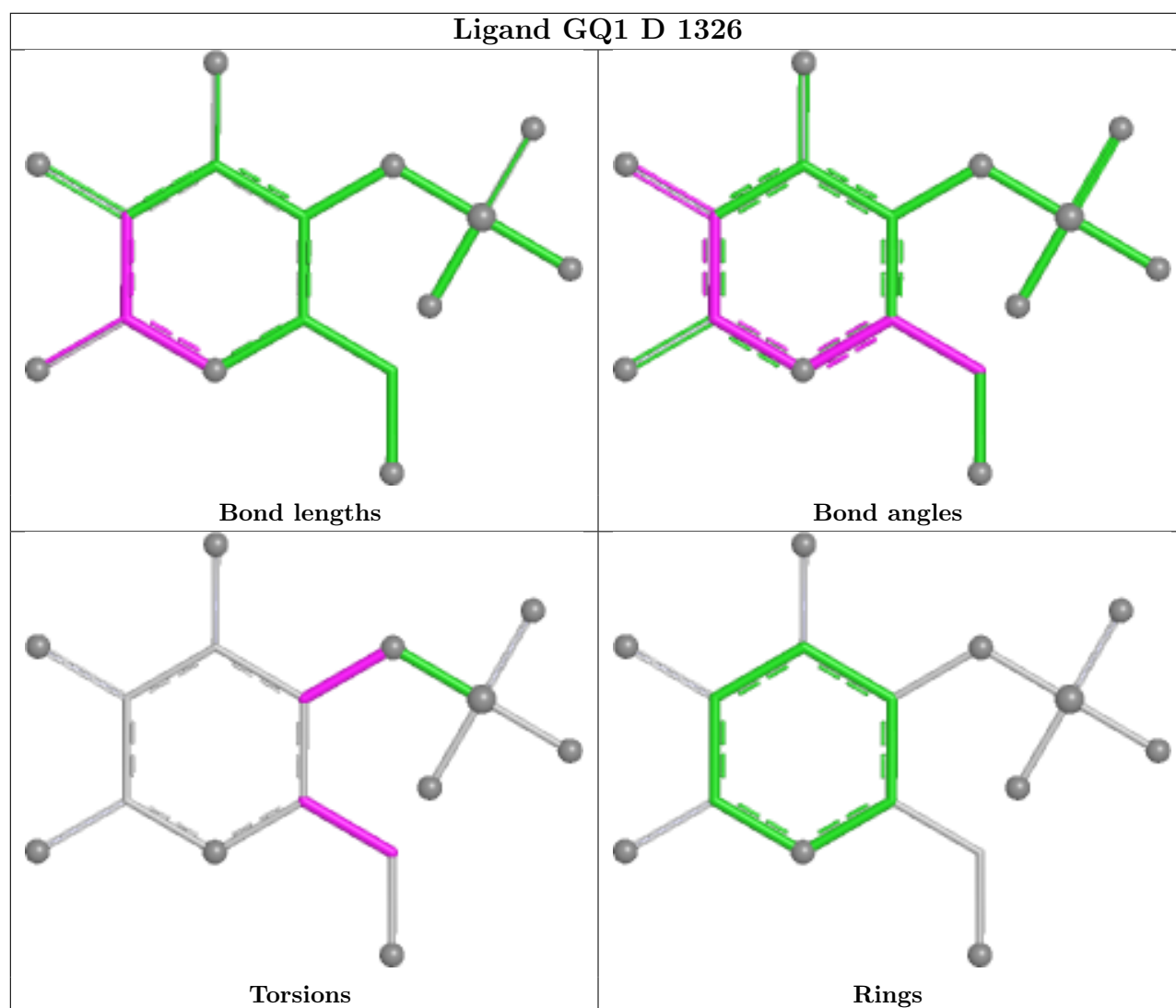
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1327	GQ1	1	0
6	D	1326	GQ1	6	0
5	B	1328	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.







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	132/134 (98%)	-1.49	0 100 100	20, 33, 54, 77	0
1	B	133/134 (99%)	-1.51	0 100 100	20, 30, 52, 69	0
1	C	132/134 (98%)	-1.47	0 100 100	20, 31, 54, 69	0
1	D	134/134 (100%)	-1.46	0 100 100	22, 30, 52, 78	0
All	All	531/536 (99%)	-1.48	0 100 100	20, 31, 54, 78	0

There are no RSRZ outliers to report.

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

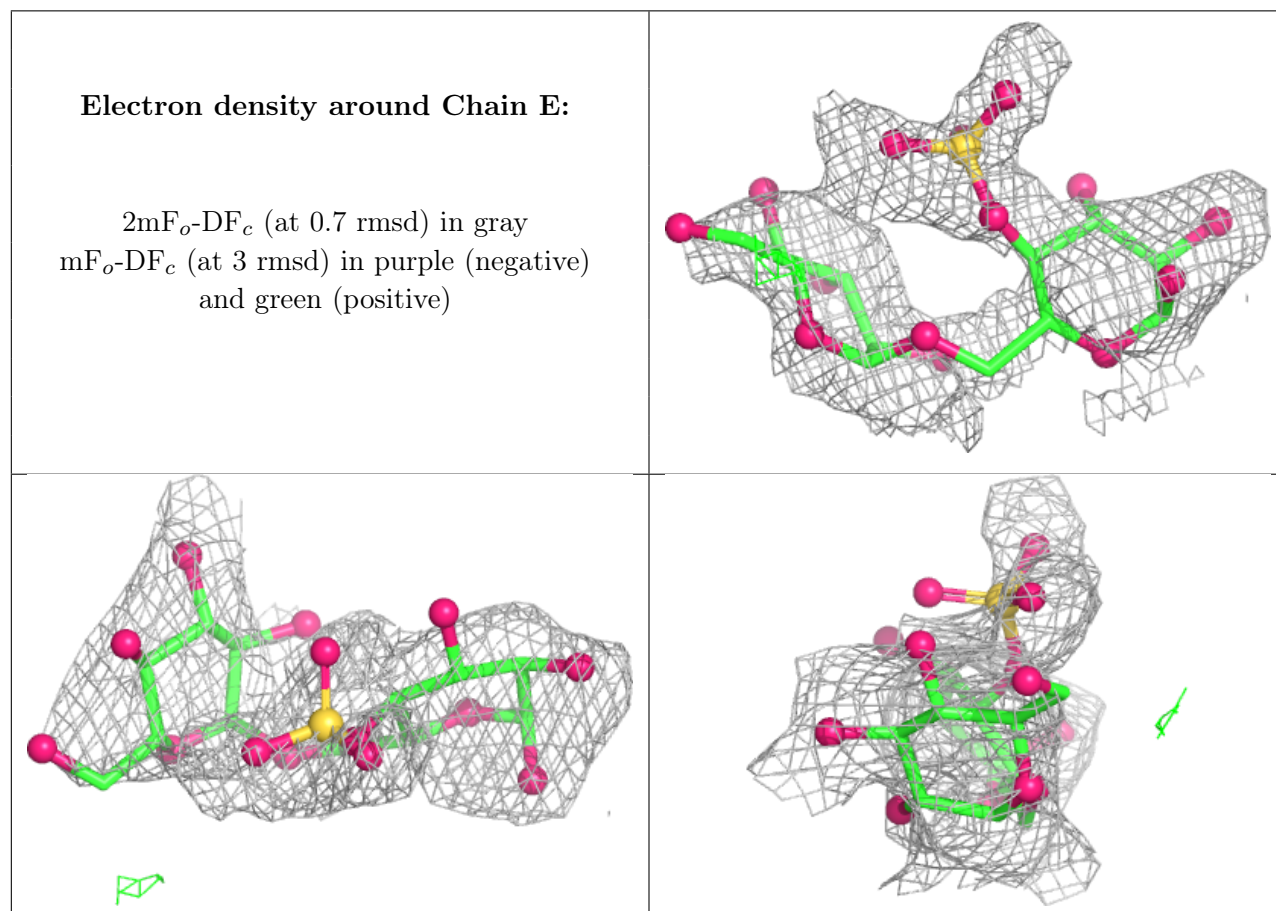
There are no non-standard protein/DNA/RNA residues in this entry.

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.

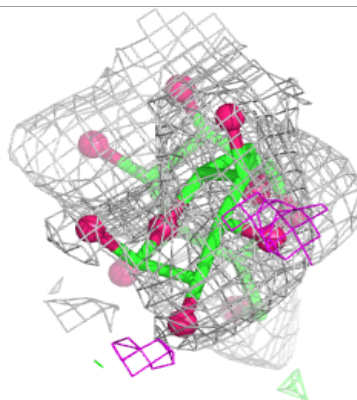
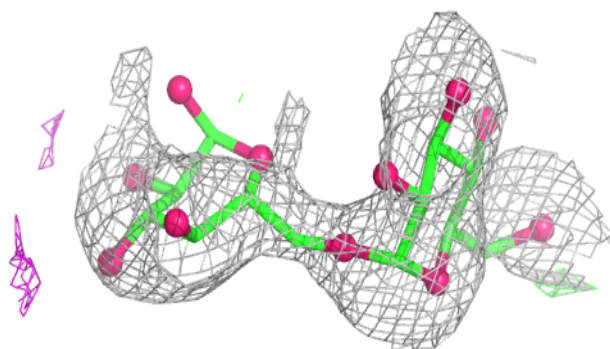
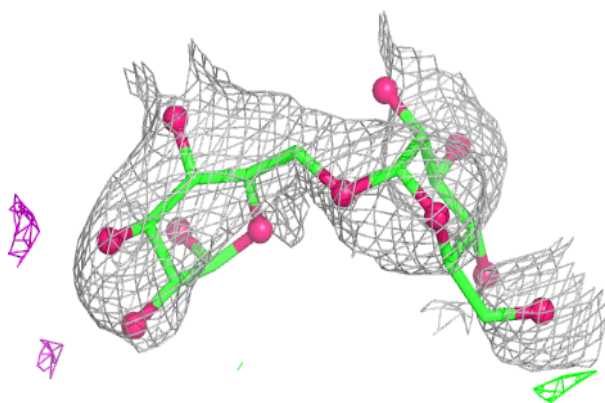
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GQ1	G	1	16/16	0.96	0.07	74,106,135,145	0
3	GLC	G	3	11/12	0.97	0.07	92,104,112,112	0
2	GQ1	F	1	12/16	0.98	0.08	56,72,89,89	0
2	GQ1	E	1	16/16	0.98	0.06	70,105,140,142	0
2	GLC	E	2	11/12	0.98	0.06	68,83,85,86	0
3	GLC	G	4	11/12	0.98	0.08	76,96,104,105	0
2	GLC	F	2	11/12	0.99	0.06	56,74,81,86	0
3	GLC	G	2	11/12	0.99	0.05	73,95,102,106	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.

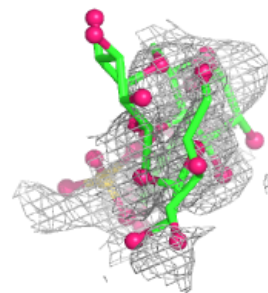
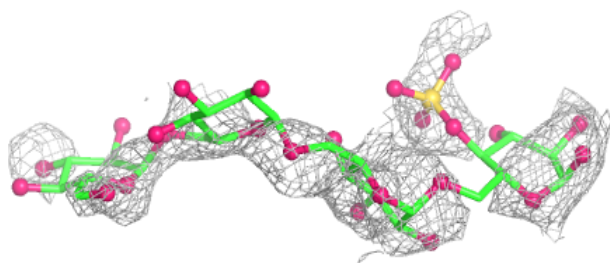
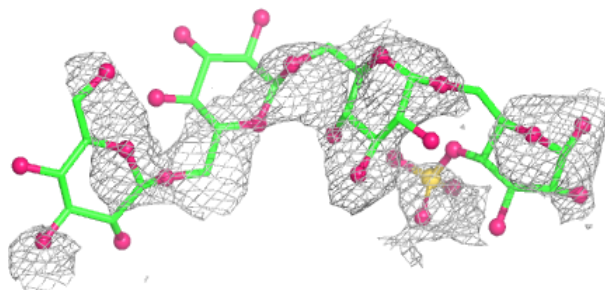


Electron density around Chain F:

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

**Electron density around Chain G:**

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



6.4 Ligands

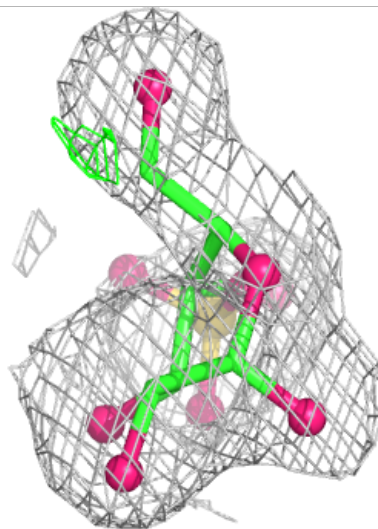
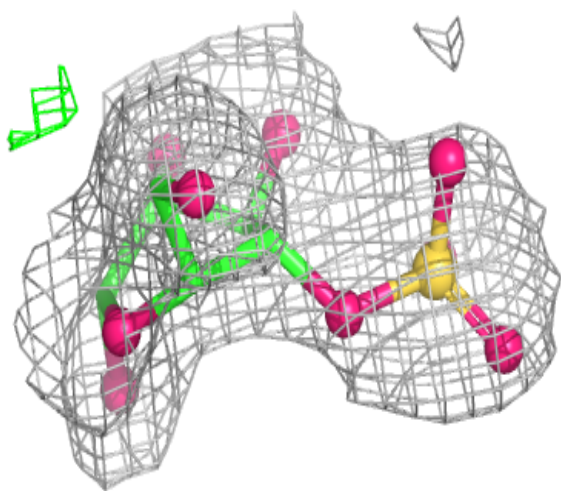
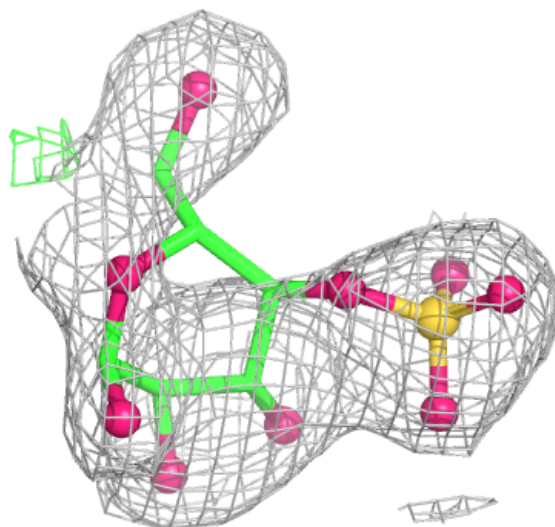
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	C	1326	5/5	0.98	0.06	117,120,127,128	0
4	CA	D	401	1/1	0.99	0.05	53,53,53,53	0
5	SO4	B	1325	5/5	0.99	0.05	63,67,76,77	0
5	SO4	B	1326	5/5	0.99	0.08	66,74,78,80	0
5	SO4	B	1327	5/5	0.99	0.06	45,45,48,49	0
5	SO4	B	1328	5/5	0.99	0.05	43,46,50,50	0
5	SO4	C	1323	5/5	0.99	0.05	53,61,65,68	0
5	SO4	C	1324	5/5	0.99	0.04	61,62,70,74	0
4	CA	C	401	1/1	0.99	0.05	54,54,54,54	0
6	GQ1	D	1325	16/16	0.99	0.04	38,61,69,73	0
6	GQ1	D	1326	16/16	0.99	0.06	51,72,104,110	0
6	GQ1	D	1327	16/16	0.99	0.04	54,71,87,100	0
5	SO4	A	1323	5/5	1.00	0.02	42,44,50,51	0
5	SO4	D	1324	5/5	1.00	0.01	32,33,35,39	0
5	SO4	B	1324	5/5	1.00	0.03	32,34,37,42	0
4	CA	A	401	1/1	1.00	0.05	56,56,56,56	0
4	CA	B	401	1/1	1.00	0.05	50,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

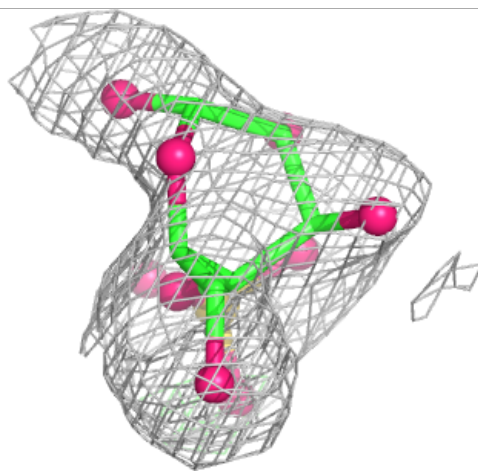
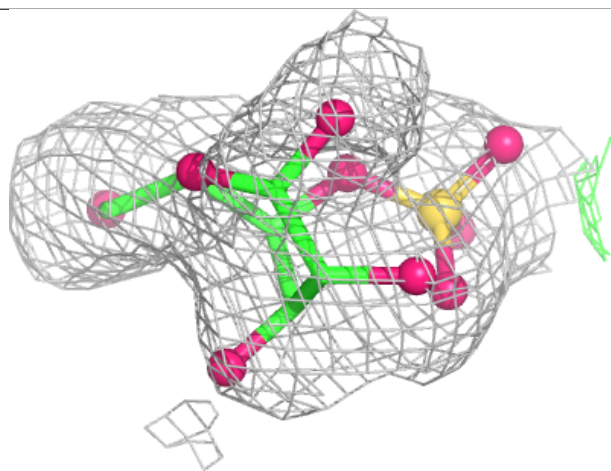
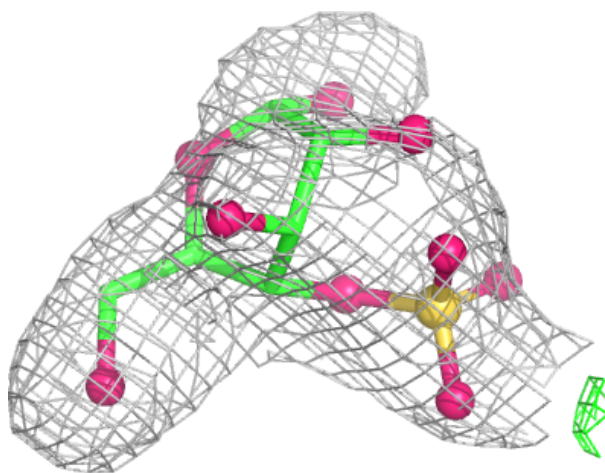
Electron density around GQ1 D 1325:

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



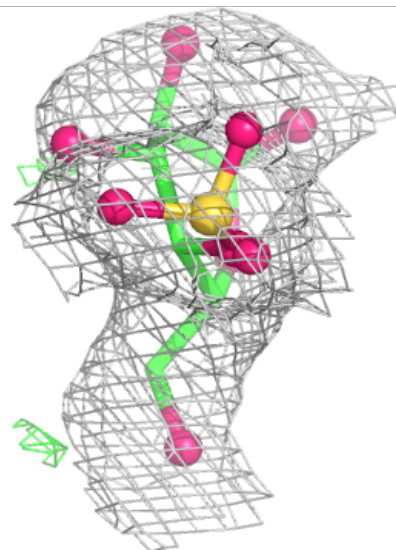
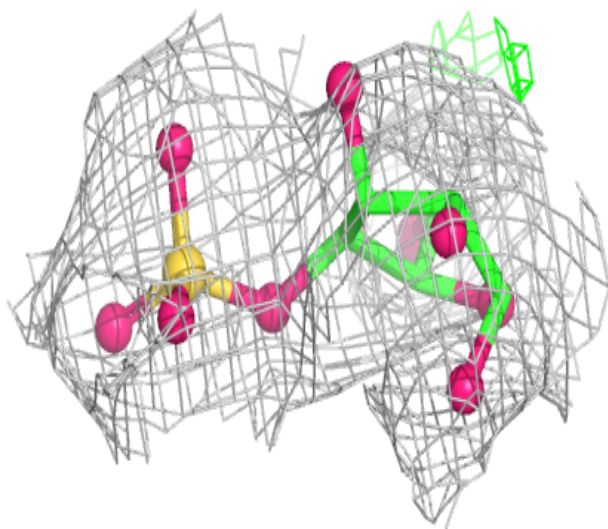
Electron density around GQ1 D 1326:

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



Electron density around GQ1 D 1327:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.