



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2020 – 12:12 PM JST

PDB ID : 7BU7
Title : Structure of human beta1 adrenergic receptor bound to BI-167107 and nanobody 6B9
Authors : Xu, X.; Kaindl, J.; Clark, M.; Hubner, H.; Hirata, K.; Sunahara, R.; Gmeiner, P.; Kobilka, B.K.; Liu, X.
Deposited on : 2020-04-04
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 following versions of software and data (see [references ⓘ](#)) 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 : 2.14.6
buster-report : 1.1.7 (2018)
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) : 2.14.6

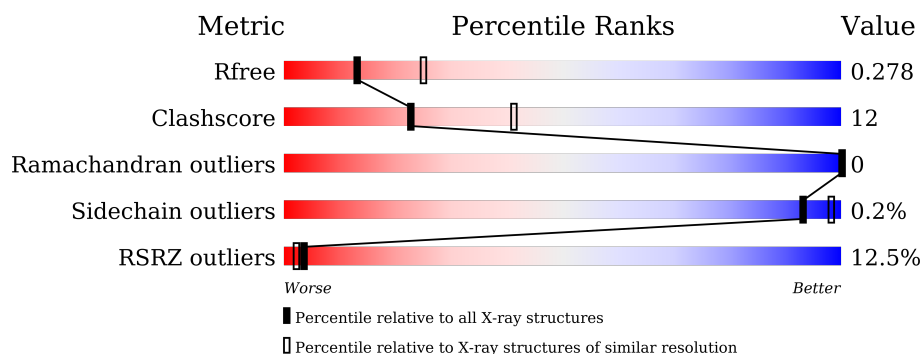
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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 $\leq 5\%$. 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	516	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>13%</div> </div> </div>
2	B	128	<div> <div>34%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>6%</div> </div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
3	D	2	<div> <div>100%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	P6G	A	1414	-	-	X	X
3	GLC	C	1	-	-	-	X
3	GLC	C	2	-	-	X	X
3	GLC	D	2	-	-	-	X
4	SO4	A	1406	-	-	X	-
6	1WV	A	1410	-	-	-	X
8	EPE	A	1412	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 4669 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 Endolysin,Beta-1 adrenergic receptor chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3553	2304	607	620	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	884	ASP	-	expression tag	UNP D9IEF7
A	885	TYR	-	expression tag	UNP D9IEF7
A	886	LYS	-	expression tag	UNP D9IEF7
A	887	ASP	-	expression tag	UNP D9IEF7
A	888	ASP	-	expression tag	UNP D9IEF7
A	889	ASP	-	expression tag	UNP D9IEF7
A	890	ASP	-	expression tag	UNP D9IEF7
A	891	ALA	-	expression tag	UNP D9IEF7
A	944	THR	CYS	engineered mutation	UNP D9IEF7
A	987	ALA	CYS	engineered mutation	UNP D9IEF7
A	1052	ALA	-	linker	UNP D9IEF7
A	1053	ALA	-	linker	UNP D9IEF7

- Molecule 2 is a protein called camelid antibody fragment.

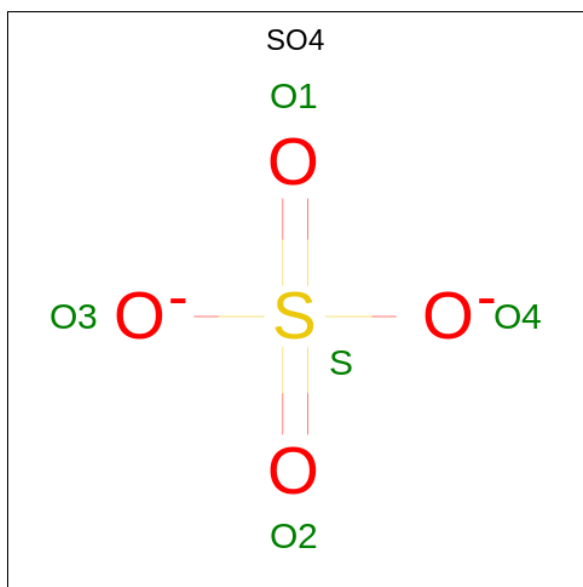
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	0	0	0
			910	569	159	178	4			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			23	12	11			
3	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



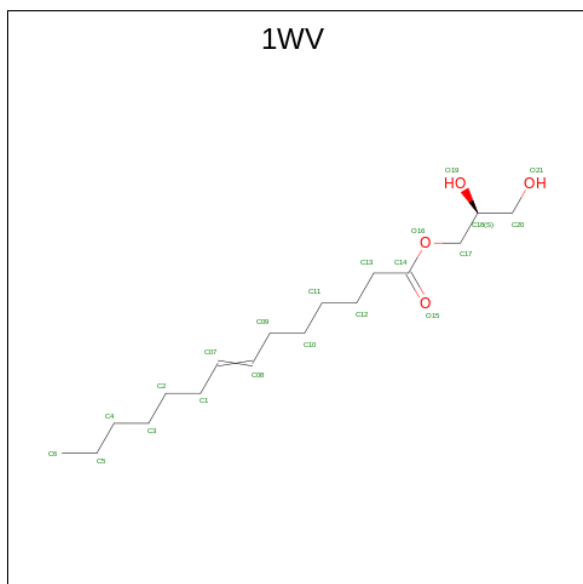
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 6 is (2S)-2,3-dihydroxypropyl (7Z)-tetradec-7-enoate (three-letter code: 1WV) (formula: $C_{17}H_{32}O_4$).

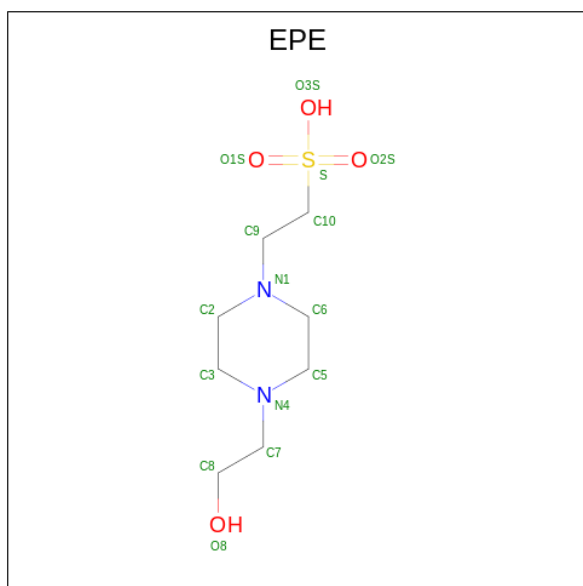


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			15	11	4		

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

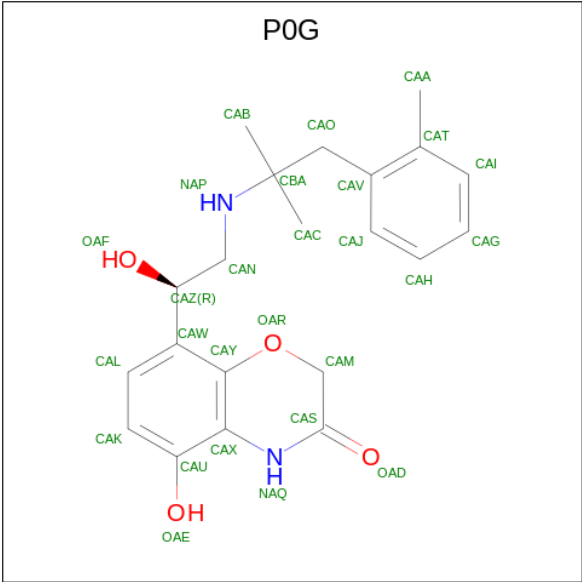
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



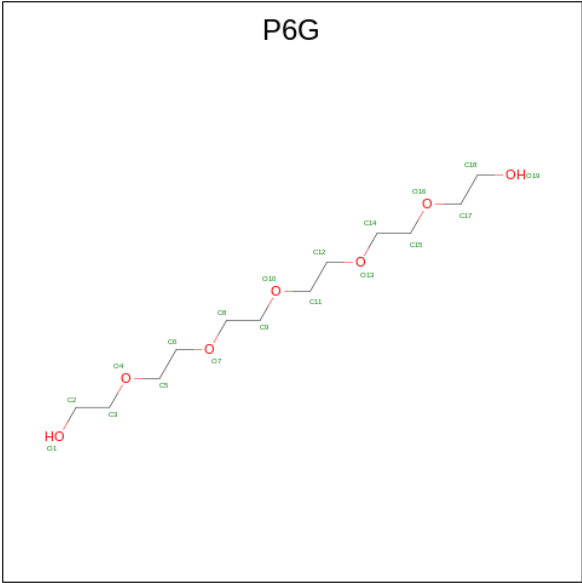
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is 8-[(1R)-2-{[1,1-dimethyl-2-(2-methylphenyl)ethyl]amino}-1-hydroxyethyl]-5-hydroxy-2H-1,4-benzoxazin-3(4H)-one (three-letter code: P0G) (formula: C₂₁H₂₆N₂O₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			27	21	2	4		

- Molecule 10 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			19	12	7		

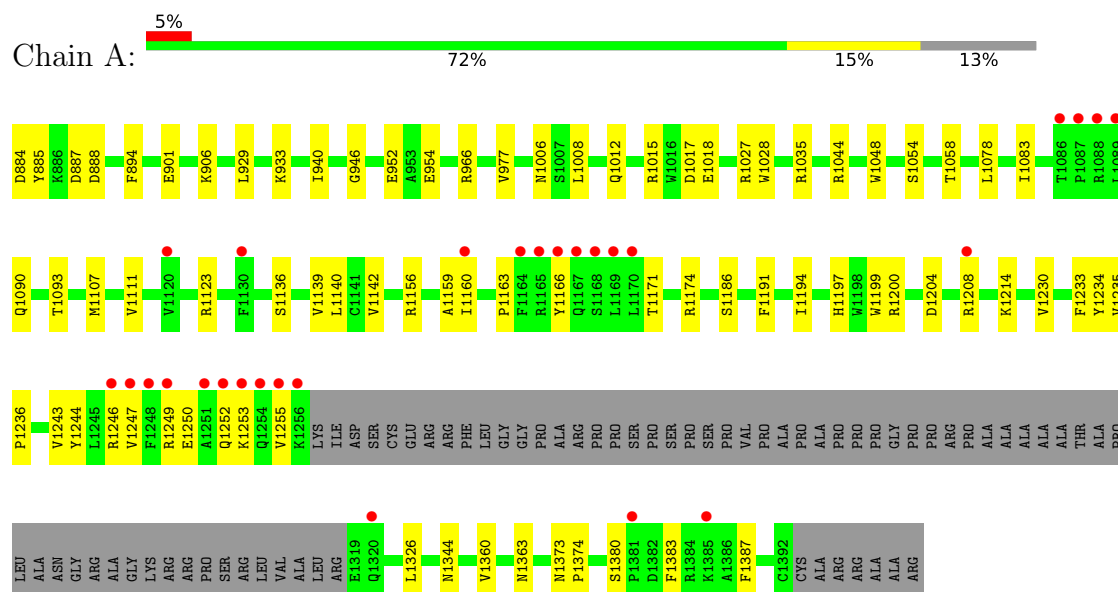
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	25	Total 25	O 25	0	0

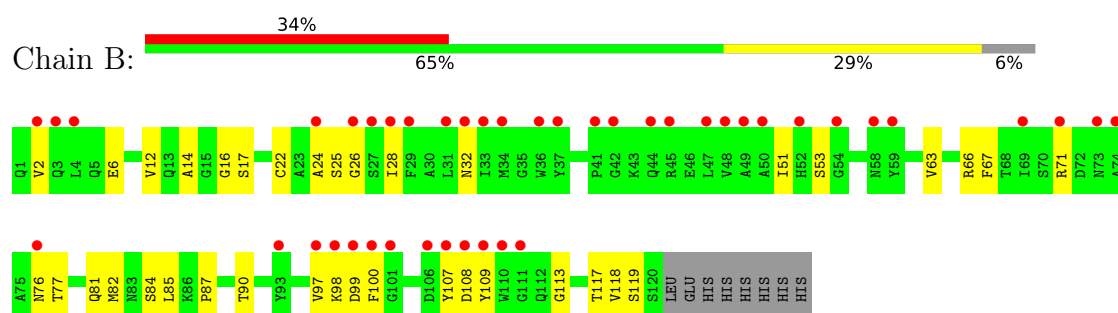
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Endolysin,Endolysin,Beta-1 adrenergic receptor chimera



- Molecule 2: camelid antibody fragment



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  100%

GLU1
GLU2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	377.98Å 66.22Å 47.86Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	19.98 – 2.60 49.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.98-2.60) 96.4 (49.76-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.243 , 0.270 0.249 , 0.278	Depositor DCC
R_{free} test set	2000 reflections (5.66%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4669	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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: P0G, NA, GLC, SO4, P6G, 1WV, EPE, CLR

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	0.40	0/3632	0.48	0/4931
2	B	0.33	0/927	0.50	0/1256
All	All	0.39	0/4559	0.48	0/6187

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3553	0	3608	68	0
2	B	910	0	878	28	0
3	C	23	0	20	6	0
3	D	23	0	20	2	0
4	A	30	0	0	3	0
5	A	28	0	46	1	0
6	A	15	0	18	0	0
7	A	1	0	0	0	0
8	A	15	0	17	1	0
9	A	27	0	25	5	0
10	A	19	0	26	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	25	0	0	0	0
All	All	4669	0	4658	107	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 12.

All (107) 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:A:1028:TRP:HA	3:C:2:GLC:O3	1.57	1.03
1:A:1360:VAL:HG22	9:A:1413:P0G:HAH	1.51	0.91
1:A:1028:TRP:CA	3:C:2:GLC:O3	2.20	0.89
1:A:1107:MET:HE2	1:A:1142:VAL:HG23	1.56	0.88
1:A:1107:MET:CE	1:A:1142:VAL:HG23	2.12	0.79
1:A:1107:MET:HE2	1:A:1142:VAL:CG2	2.18	0.74
1:A:901:GLU:OE2	1:A:1035:ARG:NH1	2.24	0.70
1:A:1107:MET:CE	1:A:1142:VAL:CG2	2.69	0.70
10:A:1414:P6G:H181	10:A:1414:P6G:H82	1.76	0.68
1:A:1028:TRP:N	3:C:2:GLC:O3	2.26	0.68
2:B:24:ALA:HB3	2:B:76:ASN:HB3	1.75	0.68
1:A:1160:ILE:HG23	2:B:100:PHE:CD2	2.29	0.67
1:A:1093:THR:HG21	1:A:1156:ARG:HH11	1.61	0.66
1:A:1246:ARG:HH12	1:A:1249:ARG:HD3	1.61	0.66
2:B:82:MET:HB3	2:B:85:LEU:HD21	1.76	0.66
1:A:1027:ARG:HB3	3:C:2:GLC:O4	1.95	0.65
2:B:87:PRO:HA	2:B:118:VAL:HG13	1.80	0.62
1:A:1194:ILE:HA	1:A:1199:TRP:CD1	2.34	0.62
1:A:1197:HIS:CG	1:A:1200:ARG:HE	2.17	0.62
3:D:1:GLC:H62	3:D:2:GLC:C2	2.31	0.61
1:A:1027:ARG:CB	3:C:2:GLC:O4	2.49	0.60
2:B:90:THR:HG22	2:B:118:VAL:H	1.66	0.60
1:A:1230:VAL:HA	1:A:1234:TYR:HB2	1.85	0.59
3:D:1:GLC:H62	3:D:2:GLC:C1	2.34	0.58
1:A:977:VAL:HG21	1:A:1008:LEU:HB3	1.86	0.57
10:A:1414:P6G:H122	10:A:1414:P6G:O19	2.04	0.57
1:A:1171:THR:HG23	1:A:1174:ARG:H	1.70	0.57
2:B:6:GLU:OE2	2:B:113:GLY:N	2.37	0.57
1:A:1344:ASN:HD21	9:A:1413:P0G:CAS	2.17	0.57
5:A:1409:CLR:H212	5:A:1409:CLR:H183	1.86	0.57
2:B:14:ALA:N	2:B:119:SER:O	2.39	0.56
1:A:1123:ARG:HD2	1:A:1214:LYS:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1380:SER:HG	1:A:1383:PHE:HD2	1.52	0.55
1:A:1246:ARG:NH1	1:A:1249:ARG:HD3	2.22	0.54
1:A:966:ARG:HD2	4:A:1406:SO4:O2	2.07	0.54
1:A:1107:MET:HE1	1:A:1142:VAL:CG2	2.38	0.54
2:B:2:VAL:HG13	2:B:25:SER:O	2.08	0.53
1:A:1250:GLU:HA	1:A:1253:LYS:HD3	1.91	0.53
1:A:1360:VAL:HG22	9:A:1413:P0G:CAH	2.33	0.52
2:B:99:ASP:HB3	2:B:107:TYR:HB3	1.90	0.52
1:A:1246:ARG:HH22	1:A:1249:ARG:HH11	1.56	0.52
1:A:1252:GLN:HA	1:A:1255:VAL:HG12	1.90	0.52
1:A:887:ASP:OD1	1:A:888:ASP:N	2.44	0.49
2:B:63:VAL:HG11	2:B:67:PHE:HB2	1.95	0.49
2:B:67:PHE:CE1	2:B:82:MET:HG2	2.47	0.49
1:A:1054:SER:O	1:A:1058:THR:HG23	2.12	0.49
2:B:17:SER:HA	2:B:82:MET:O	2.14	0.48
1:A:966:ARG:NH1	4:A:1406:SO4:O4	2.47	0.48
2:B:63:VAL:HG22	2:B:67:PHE:CD2	2.49	0.47
1:A:1107:MET:HG3	1:A:1111:VAL:HB	1.97	0.47
8:A:1412:EPE:O8	8:A:1412:EPE:H51	2.14	0.47
1:A:1233:PHE:C	1:A:1236:PRO:HD2	2.34	0.47
1:A:1235:VAL:CG2	1:A:1236:PRO:HD3	2.44	0.47
10:A:1414:P6G:H81	10:A:1414:P6G:O19	2.15	0.47
1:A:1017:ASP:OD1	1:A:1044:ARG:NE	2.38	0.47
2:B:67:PHE:HA	2:B:81:GLN:O	2.14	0.47
1:A:1139:VAL:HG22	9:A:1413:P0G:CAL	2.45	0.46
2:B:2:VAL:HG21	2:B:28:ILE:HG23	1.96	0.46
2:B:98:LYS:HD3	2:B:108:ASP:OD1	2.15	0.46
2:B:32:ASN:OD1	2:B:53:SER:HB3	2.16	0.46
1:A:929:LEU:HG	1:A:933:LYS:HE3	1.98	0.45
2:B:63:VAL:HG13	2:B:67:PHE:H	1.81	0.45
2:B:67:PHE:CD1	2:B:82:MET:HG2	2.52	0.45
10:A:1414:P6G:H122	10:A:1414:P6G:C18	2.46	0.45
2:B:12:VAL:HG11	2:B:16:GLY:HA3	1.98	0.45
1:A:1163:PRO:O	1:A:1166:TYR:HB3	2.17	0.45
1:A:1244:TYR:HB3	1:A:1326:LEU:HD22	1.99	0.45
1:A:885:TYR:CD1	1:A:885:TYR:C	2.90	0.45
1:A:1136:SER:HB2	1:A:1191:PHE:CD1	2.52	0.45
1:A:940:ILE:HD12	1:A:952:GLU:HB3	1.99	0.45
1:A:1204:ASP:HB3	1:A:1208:ARG:NH1	2.32	0.45
1:A:1139:VAL:HG22	9:A:1413:P0G:CAK	2.46	0.45
10:A:1414:P6G:C18	10:A:1414:P6G:H82	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:VAL:CG1	2:B:109:TYR:HB2	2.47	0.45
1:A:894:PHE:CE1	1:A:954:GLU:HG2	2.52	0.44
1:A:1048:TRP:HB3	10:A:1414:P6G:H92	1.99	0.44
1:A:1136:SER:HB2	1:A:1191:PHE:HD1	1.83	0.44
1:A:1107:MET:CE	1:A:1142:VAL:HG22	2.44	0.44
2:B:22:CYS:O	2:B:77:THR:HA	2.17	0.44
2:B:51:ILE:HD13	2:B:71:ARG:HG3	1.99	0.44
2:B:2:VAL:HG22	2:B:26:GLY:HA3	1.98	0.44
1:A:1140:LEU:HD12	1:A:1186:SER:HB3	1.99	0.44
10:A:1414:P6G:H181	10:A:1414:P6G:C8	2.46	0.44
1:A:1006:ASN:HB2	4:A:1404:SO4:O1	2.18	0.43
1:A:1107:MET:HE1	1:A:1142:VAL:HG22	2.01	0.43
1:A:977:VAL:HG22	1:A:1012:GLN:HB2	2.00	0.43
1:A:1093:THR:HG21	1:A:1156:ARG:NH1	2.32	0.43
1:A:1083:ILE:O	1:A:1090:GLN:NE2	2.52	0.43
1:A:1246:ARG:HH22	1:A:1249:ARG:NH1	2.17	0.43
1:A:884:ASP:N	1:A:884:ASP:OD1	2.52	0.42
1:A:1048:TRP:CD2	10:A:1414:P6G:H91	2.54	0.42
1:A:1027:ARG:HB2	3:C:2:GLC:O4	2.19	0.42
1:A:1015:ARG:NH2	1:A:1018:GLU:OE1	2.53	0.42
2:B:66:ARG:HD2	2:B:84:SER:HB2	2.01	0.42
2:B:97:VAL:HG12	2:B:109:TYR:HB2	2.02	0.41
1:A:1156:ARG:O	1:A:1160:ILE:HG12	2.20	0.41
1:A:1160:ILE:HD12	2:B:100:PHE:CG	2.55	0.41
1:A:1078:LEU:HG	1:A:1387:PHE:CD1	2.55	0.41
1:A:1243:VAL:O	1:A:1247:VAL:HG23	2.21	0.41
1:A:1235:VAL:HG22	1:A:1236:PRO:HD3	2.02	0.41
10:A:1414:P6G:C18	10:A:1414:P6G:C8	2.99	0.41
2:B:90:THR:HG22	2:B:117:THR:HA	2.03	0.41
1:A:1159:ALA:HB2	1:A:1166:TYR:CZ	2.55	0.41
10:A:1414:P6G:C8	10:A:1414:P6G:O19	2.69	0.41
1:A:906:LYS:HA	1:A:946:GLY:O	2.22	0.40
1:A:1373:ASN:N	1:A:1374:PRO:HD2	2.36	0.40
10:A:1414:P6G:C12	10:A:1414:P6G:O16	2.69	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	443/516 (86%)	437 (99%)	6 (1%)	0	100	100
2	B	118/128 (92%)	117 (99%)	1 (1%)	0	100	100
All	All	561/644 (87%)	554 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	376/426 (88%)	375 (100%)	1 (0%)	92	98
2	B	94/102 (92%)	94 (100%)	0	100	100
All	All	470/528 (89%)	469 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1363	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GLC	C	1	3	12,12,12	1.21	1 (8%)	17,17,17	2.54	9 (52%)
3	GLC	C	2	3	11,11,12	2.04	5 (45%)	15,15,17	5.01	10 (66%)
3	GLC	D	1	3	12,12,12	1.53	3 (25%)	17,17,17	2.70	9 (52%)
3	GLC	D	2	3	11,11,12	1.71	2 (18%)	15,15,17	2.53	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
3	GLC	C	1	3	-	2/2/22/22	0/1/1/1
3	GLC	C	2	3	-	2/2/19/22	0/1/1/1
3	GLC	D	1	3	-	1/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	GLC	O3-C3	4.49	1.53	1.43
3	D	2	GLC	O5-C1	3.88	1.49	1.43
3	D	2	GLC	C2-C3	-2.89	1.48	1.52
3	D	1	GLC	O5-C1	2.76	1.49	1.42
3	C	2	GLC	C2-C3	2.60	1.56	1.52
3	C	2	GLC	C4-C5	2.50	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	GLC	O4-C4	2.39	1.48	1.43
3	C	2	GLC	O5-C5	2.38	1.48	1.43
3	D	1	GLC	C3-C2	-2.36	1.46	1.52
3	C	1	GLC	O5-C1	2.18	1.48	1.42
3	C	2	GLC	O5-C1	2.06	1.47	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	GLC	O2-C2-C1	-10.94	86.76	109.15
3	C	2	GLC	O5-C5-C6	-9.87	91.73	107.20
3	D	2	GLC	C1-C2-C3	7.03	118.31	109.67
3	C	2	GLC	C1-C2-C3	6.90	118.15	109.67
3	C	2	GLC	O3-C3-C2	6.16	121.79	109.99
3	D	1	GLC	C3-C4-C5	-5.73	100.02	110.24
3	D	1	GLC	O4-C4-C5	5.50	122.96	109.30
3	C	1	GLC	O5-C5-C6	-4.91	94.23	106.44
3	C	1	GLC	O4-C4-C5	4.05	119.36	109.30
3	C	2	GLC	O6-C6-C5	-3.94	97.77	111.29
3	C	2	GLC	O2-C2-C3	3.87	117.88	110.14
3	D	2	GLC	O3-C3-C2	-3.69	102.92	109.99
3	C	2	GLC	O4-C4-C5	3.69	118.45	109.30
3	C	1	GLC	O2-C2-C3	-3.60	102.04	110.35
3	D	2	GLC	C2-C3-C4	3.42	116.82	110.89
3	D	1	GLC	O5-C1-C2	3.37	116.30	110.28
3	C	1	GLC	O1-C1-C2	3.29	118.29	109.03
3	C	1	GLC	O5-C5-C4	3.21	115.52	109.69
3	D	1	GLC	O4-C4-C3	3.01	117.31	110.35
3	C	2	GLC	O5-C1-C2	-2.81	106.43	110.77
3	D	1	GLC	O3-C3-C4	2.80	116.83	110.35
3	C	1	GLC	O3-C3-C2	2.76	116.73	110.35
3	D	1	GLC	O2-C2-C1	2.64	115.27	109.16
3	C	2	GLC	C3-C4-C5	-2.47	105.84	110.24
3	D	1	GLC	C4-C3-C2	-2.46	106.53	110.82
3	C	2	GLC	O5-C5-C4	2.43	116.74	110.83
3	C	1	GLC	O3-C3-C4	-2.41	104.77	110.35
3	D	1	GLC	O2-C2-C3	-2.34	104.94	110.35
3	C	1	GLC	C3-C4-C5	-2.30	106.14	110.24
3	D	2	GLC	O2-C2-C3	-2.27	105.59	110.14
3	D	2	GLC	O4-C4-C3	2.13	115.27	110.35
3	D	1	GLC	C1-C2-C3	2.13	114.73	110.31
3	C	1	GLC	C1-C2-C3	2.03	114.52	110.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

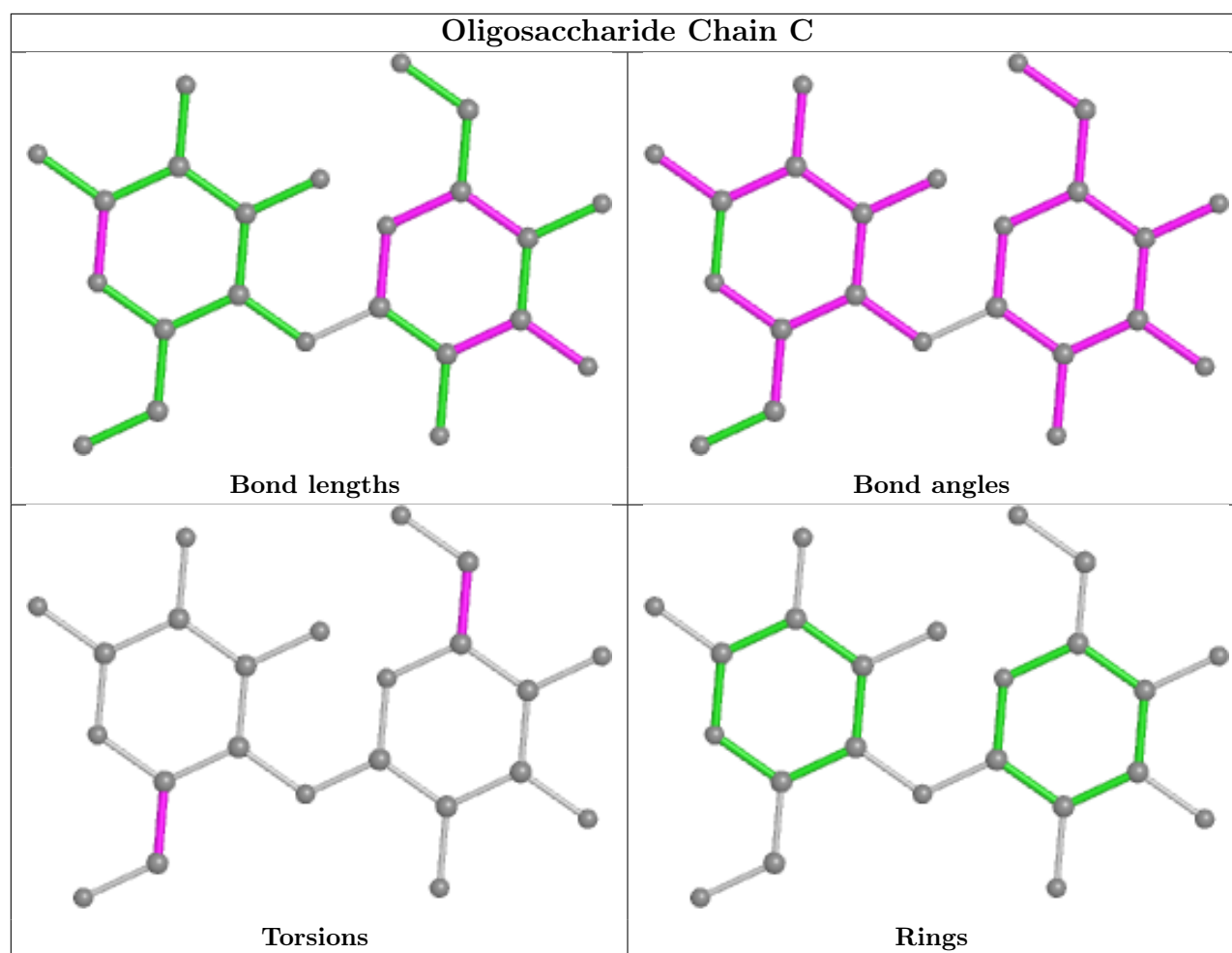
Mol	Chain	Res	Type	Atoms
3	C	1	GLC	O5-C5-C6-O6
3	C	1	GLC	C4-C5-C6-O6
3	C	2	GLC	O5-C5-C6-O6
3	C	2	GLC	C4-C5-C6-O6
3	D	1	GLC	C4-C5-C6-O6

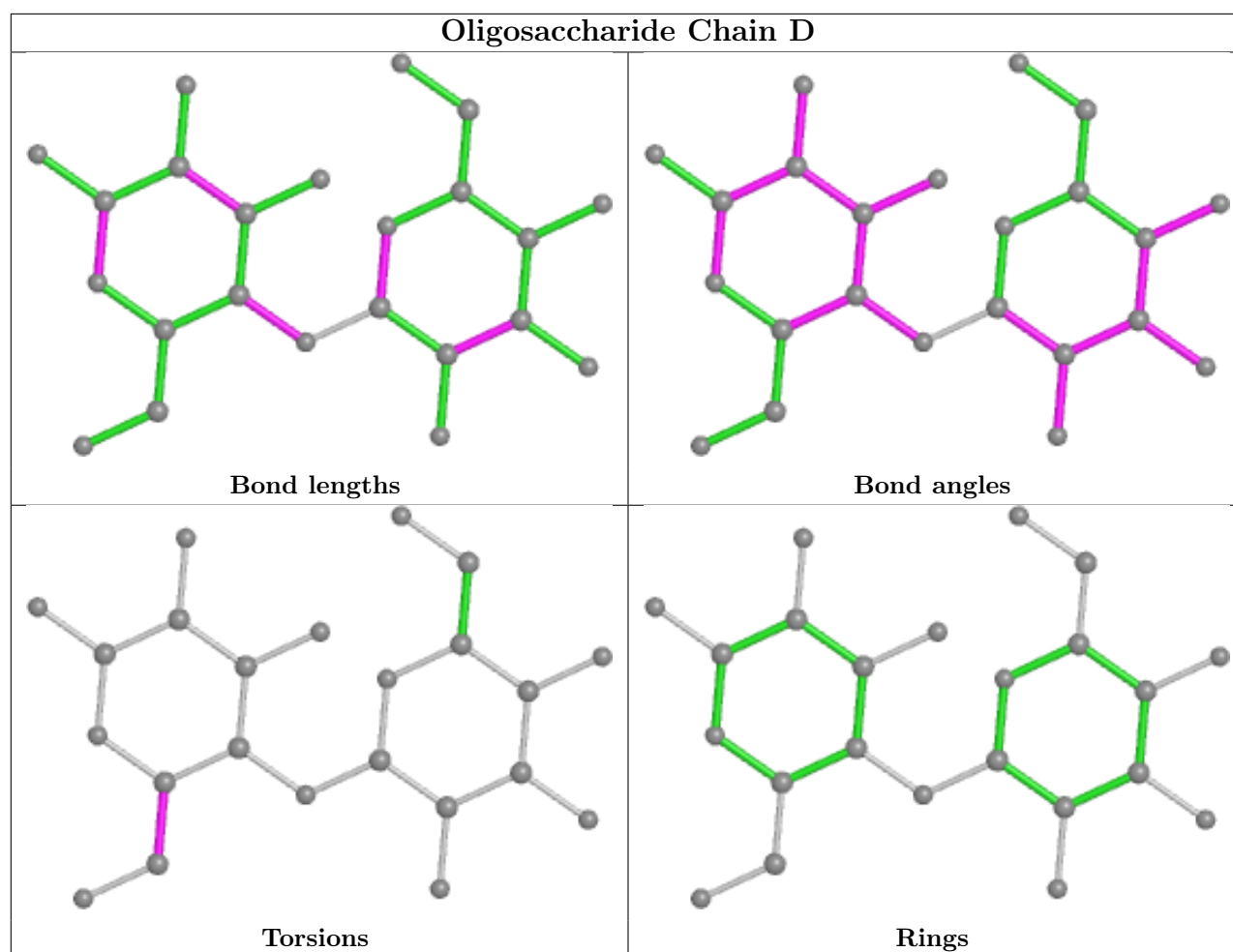
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	GLC	2	0
3	C	2	GLC	6	0
3	D	1	GLC	2	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 12 ligands modelled in this entry, 1 is 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	$\# Z > 2$
4	SO4	A	1403	-	4,4,4	0.11	0	6,6,6	0.09	0
4	SO4	A	1408	-	4,4,4	0.14	0	6,6,6	0.07	0
9	P0G	A	1413	-	27,29,29	1.25	2 (7%)	32,42,42	1.37	3 (9%)
4	SO4	A	1407	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	1406	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CLR	A	1409	-	31,31,31	0.69	0	48,48,48	1.14	5 (10%)
6	1WV	A	1410	-	14,14,20	1.91	3 (21%)	15,15,21	2.37	4 (26%)
4	SO4	A	1405	-	4,4,4	0.14	0	6,6,6	0.06	0
10	P6G	A	1414	-	18,18,18	0.72	0	17,17,17	0.73	0
8	EPE	A	1412	-	15,15,15	2.20	1 (6%)	18,20,20	2.14	6 (33%)
4	SO4	A	1404	-	4,4,4	0.16	0	6,6,6	0.12	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
9	P0G	A	1413	-	-	4/15/24/24	0/3/3/3
5	CLR	A	1409	-	-	3/10/68/68	0/4/4/4
10	P6G	A	1414	-	-	13/16/16/16	-
8	EPE	A	1412	-	-	5/9/19/19	0/1/1/1
6	1WV	A	1410	-	-	8/14/14/20	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1412	EPE	C10-S	-8.43	1.65	1.77
6	A	1410	1WV	O15-C14	5.18	1.37	1.22
9	A	1413	P0G	CBA-NAP	-4.18	1.45	1.49
9	A	1413	P0G	CAW-CAZ	-3.71	1.49	1.52
6	A	1410	1WV	C07-C08	3.45	1.51	1.28
6	A	1410	1WV	O16-C17	-2.43	1.39	1.45

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1410	1WV	O16-C14-O15	-7.36	105.01	123.59
8	A	1412	EPE	O2S-S-C10	5.01	112.95	106.92
9	A	1413	P0G	OAR-CAY-CAW	4.53	123.12	116.75
6	A	1410	1WV	O15-C14-C13	-4.17	107.45	123.73
9	A	1413	P0G	OAR-CAY-CAX	-3.94	116.18	121.22
5	A	1409	CLR	C3-C4-C5	-3.89	105.42	112.03
8	A	1412	EPE	C5-C6-N1	-3.64	103.17	110.64
8	A	1412	EPE	C3-C2-N1	-3.30	103.87	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1412	EPE	O1S-S-C10	2.86	110.36	106.92
9	A	1413	P0G	CAC-CBA-CAO	2.62	113.40	109.95
5	A	1409	CLR	O1-C3-C2	2.60	116.78	110.16
8	A	1412	EPE	O3S-S-C10	2.45	109.73	105.77
8	A	1412	EPE	O2S-S-O1S	-2.36	105.78	113.95
6	A	1410	1WV	C09-C08-C07	-2.24	111.62	126.84
5	A	1409	CLR	C21-C20-C17	2.15	116.22	112.92
5	A	1409	CLR	C19-C10-C5	-2.15	104.87	108.34
6	A	1410	1WV	O21-C20-C18	-2.14	99.92	110.20
5	A	1409	CLR	C7-C8-C9	2.11	112.27	109.71

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1413	P0G	CAV-CAO-CBA-CAB
9	A	1413	P0G	CAV-CAO-CBA-CAC
9	A	1413	P0G	CAV-CAO-CBA-NAP
8	A	1412	EPE	C9-C10-S-O2S
10	A	1414	P6G	O10-C11-C12-O13
10	A	1414	P6G	O7-C8-C9-O10
6	A	1410	1WV	O15-C14-O16-C17
10	A	1414	P6G	O16-C17-C18-O19
5	A	1409	CLR	C22-C23-C24-C25
8	A	1412	EPE	C9-C10-S-O3S
6	A	1410	1WV	C08-C09-C10-C11
5	A	1409	CLR	C17-C20-C22-C23
10	A	1414	P6G	O4-C5-C6-O7
6	A	1410	1WV	C09-C10-C11-C12
8	A	1412	EPE	C10-C9-N1-C6
6	A	1410	1WV	C11-C12-C13-C14
6	A	1410	1WV	O19-C18-C20-O21
10	A	1414	P6G	O1-C2-C3-O4
10	A	1414	P6G	C8-C9-O10-C11
5	A	1409	CLR	C21-C20-C22-C23
10	A	1414	P6G	C5-C6-O7-C8
9	A	1413	P0G	CAZ-CAN-NAP-CBA
8	A	1412	EPE	C9-C10-S-O1S
10	A	1414	P6G	C6-C5-O4-C3
6	A	1410	1WV	C07-C08-C09-C10
8	A	1412	EPE	C10-C9-N1-C2
10	A	1414	P6G	C11-C12-O13-C14

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Mol	Chain	Res	Type	Atoms
10	A	1414	P6G	C18-C17-O16-C15
10	A	1414	P6G	C2-C3-O4-C5
10	A	1414	P6G	C15-C14-O13-C12
10	A	1414	P6G	C9-C8-O7-C6
6	A	1410	1WV	C17-C18-C20-O21
6	A	1410	1WV	C12-C13-C14-O15

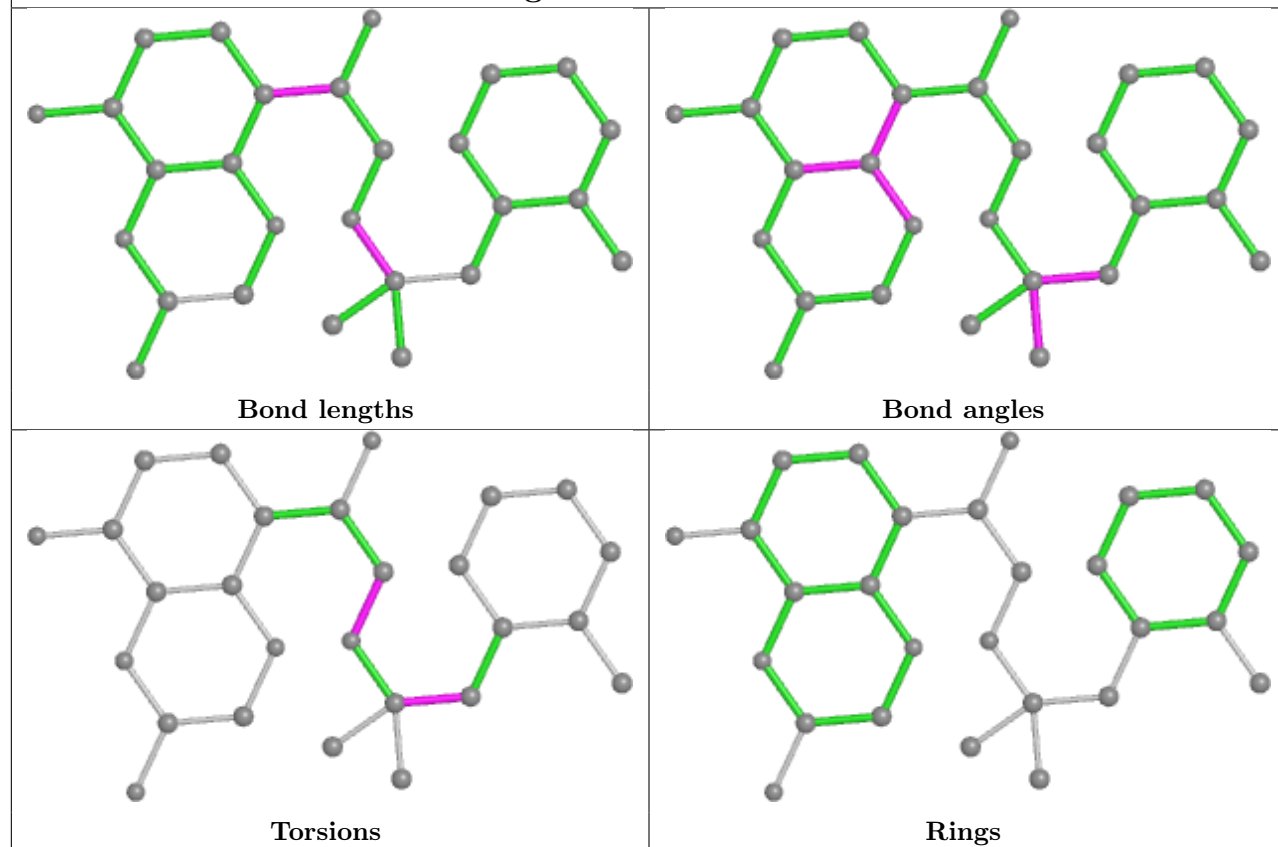
There are no ring outliers.

6 monomers are involved in 21 short contacts:

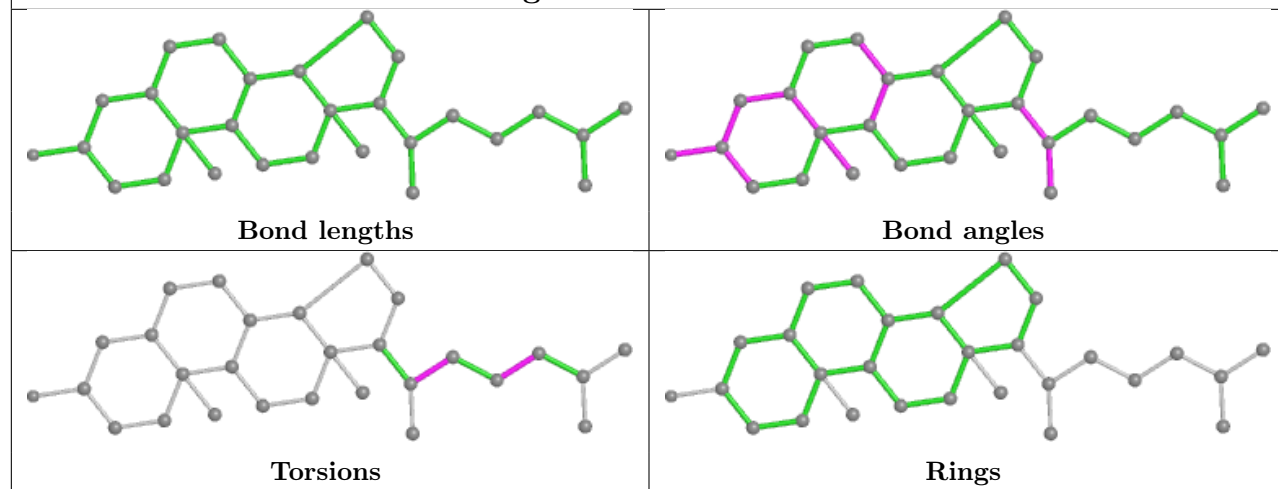
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1413	P0G	5	0
4	A	1406	SO4	2	0
5	A	1409	CLR	1	0
10	A	1414	P6G	11	0
8	A	1412	EPE	1	0
4	A	1404	SO4	1	0

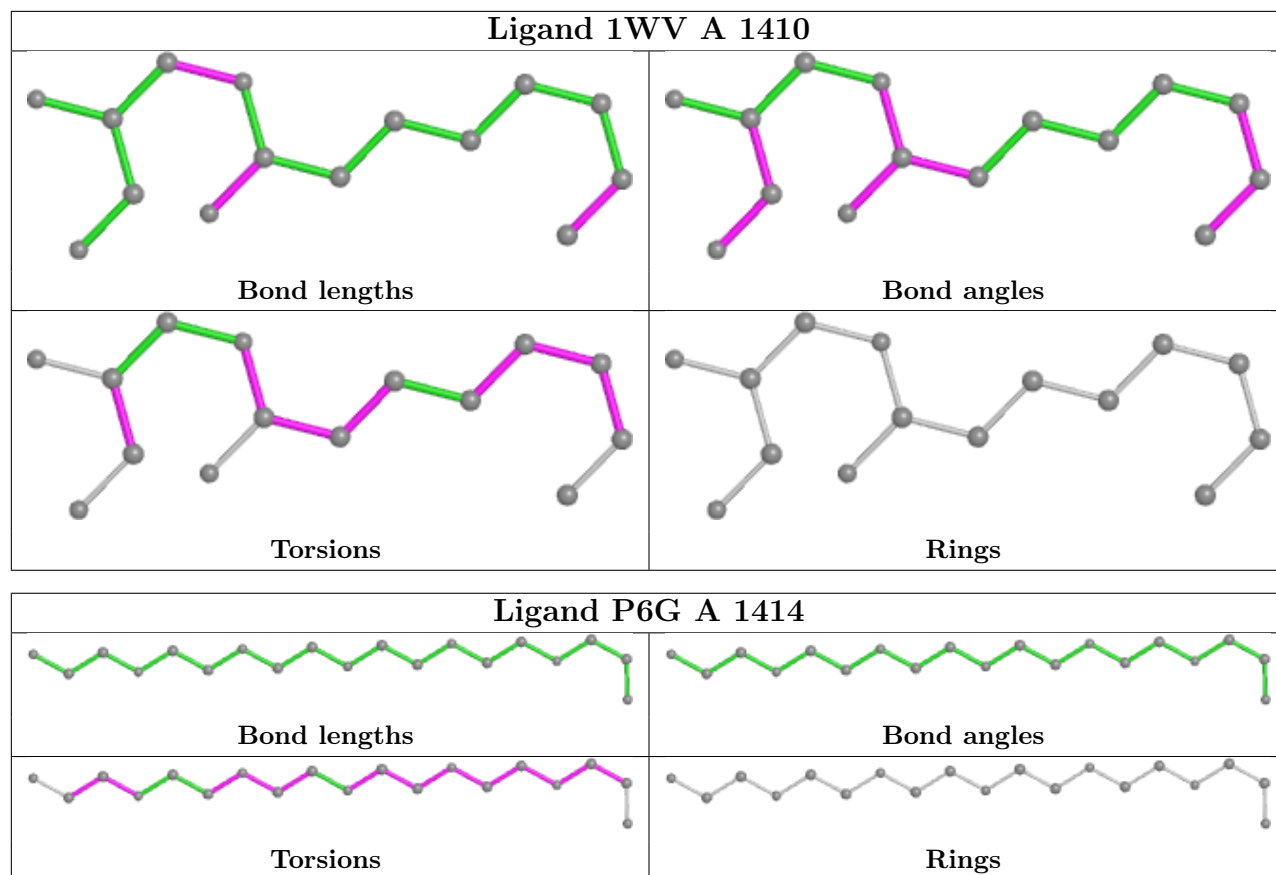
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand P0G A 1413



Ligand CLR A 1409





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	447/516 (86%)	0.53	28 (6%) 20 15	39, 72, 115, 145	0
2	B	120/128 (93%)	1.60	43 (35%) 0 0	89, 118, 132, 139	0
All	All	567/644 (88%)	0.76	71 (12%) 3 2	39, 78, 125, 145	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1255	VAL	9.9
2	B	74	ALA	9.2
2	B	107	TYR	7.1
1	A	1252	GLN	7.0
1	A	1169	LEU	6.9
2	B	37	TYR	6.8
1	A	1256	LYS	6.7
1	A	1253	LYS	6.1
2	B	33	ILE	6.0
1	A	1168	SER	5.8
2	B	97	VAL	5.6
1	A	1166	TYR	5.4
2	B	48	VAL	5.4
1	A	1087	PRO	5.4
1	A	1164	PHE	5.4
1	A	1249	ARG	5.3
2	B	29	PHE	5.2
1	A	1088	ARG	5.2
2	B	109	TYR	5.1
2	B	26	GLY	5.1
1	A	1320	GLN	5.1
1	A	1385	LYS	5.0
2	B	73	ASN	5.0
1	A	1165	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	1248	PHE	4.2
2	B	69	ILE	4.0
2	B	28	ILE	3.8
1	A	1381	PRO	3.8
2	B	76	ASN	3.7
1	A	1251	ALA	3.6
2	B	71	ARG	3.5
2	B	99	ASP	3.4
2	B	45	ARG	3.4
2	B	49	ALA	3.4
2	B	44	GLN	3.4
1	A	1254	GLN	3.3
2	B	98	LYS	3.3
1	A	1130	PHE	3.1
2	B	4	LEU	3.1
2	B	58	ASN	3.1
1	A	1246	ARG	3.0
2	B	54	GLY	3.0
2	B	110	TRP	3.0
1	A	1160	ILE	2.9
2	B	2	VAL	2.9
1	A	1170	LEU	2.9
2	B	24	ALA	2.9
2	B	101	GLY	2.8
2	B	111	GLY	2.8
2	B	31	LEU	2.7
2	B	3	GLN	2.7
2	B	52	HIS	2.6
2	B	32	ASN	2.5
2	B	36	TRP	2.5
1	A	1086	THR	2.5
2	B	93	TYR	2.5
2	B	42	GLY	2.5
2	B	50	ALA	2.5
1	A	1089	LEU	2.4
2	B	108	ASP	2.3
1	A	1247	VAL	2.3
2	B	27	SER	2.2
2	B	59	TYR	2.2
2	B	100	PHE	2.2
1	A	1167	GLN	2.2
2	B	41	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1120	VAL	2.2
1	A	1208	ARG	2.1
2	B	106	ASP	2.1
2	B	34	MET	2.0
2	B	47	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](#)

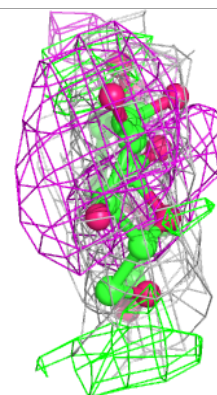
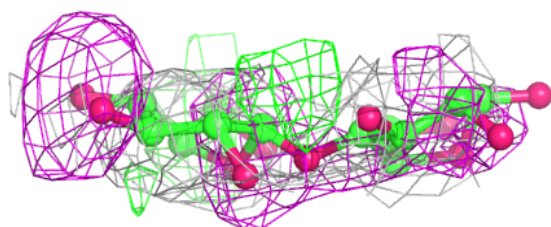
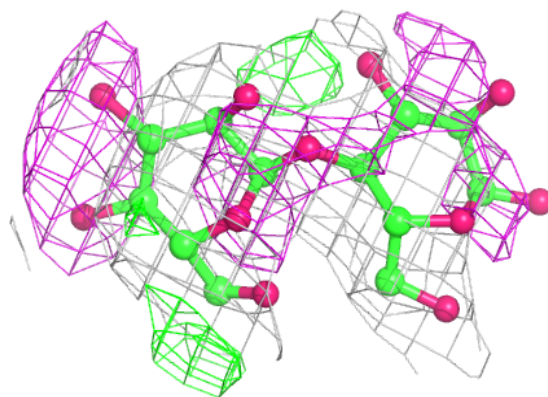
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	C	1	12/12	0.53	0.41	87,112,122,124	0
3	GLC	C	2	11/12	0.56	0.54	75,84,103,110	0
3	GLC	D	2	11/12	0.57	0.42	71,84,94,101	0
3	GLC	D	1	12/12	0.61	0.39	59,69,80,82	0

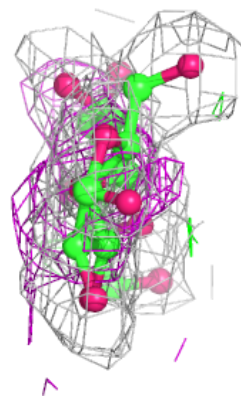
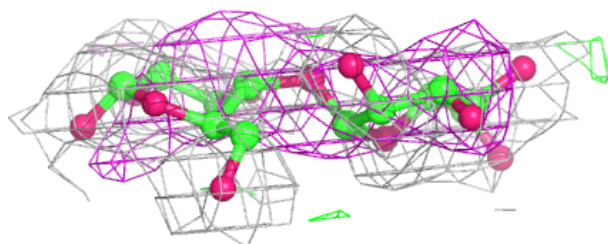
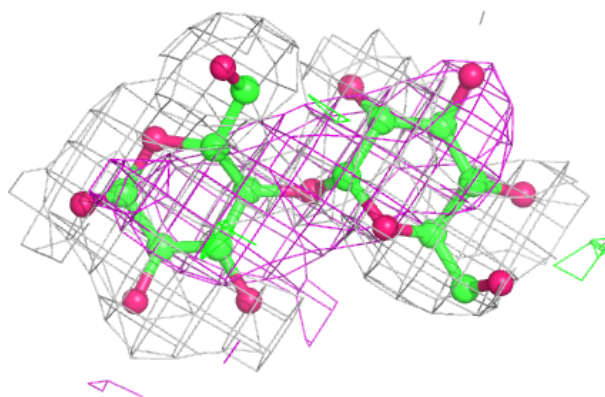
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

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



6.4 Ligands ⓘ

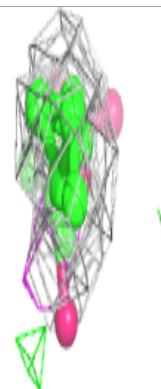
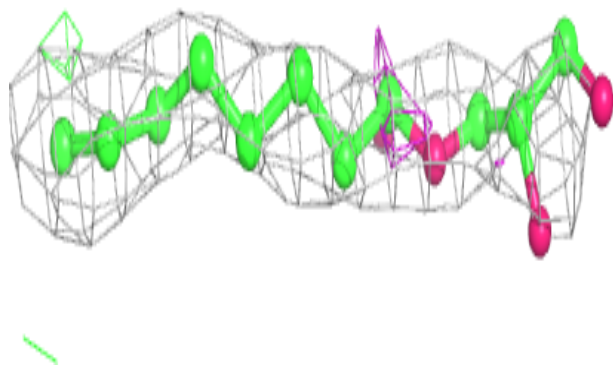
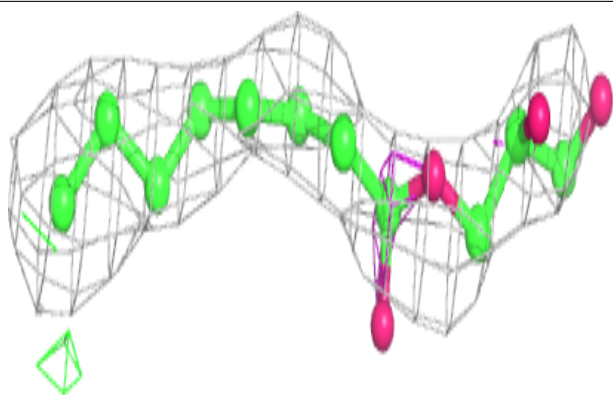
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	1WV	A	1410	15/21	0.70	0.45	69,85,104,106	0
8	EPE	A	1412	15/15	0.73	0.53	63,87,116,125	0
4	SO4	A	1407	5/5	0.76	0.27	81,89,125,128	0
10	P6G	A	1414	19/19	0.80	0.44	67,83,97,99	0
5	CLR	A	1409	28/28	0.86	0.41	72,88,92,94	0
4	SO4	A	1408	5/5	0.89	0.21	90,92,104,104	0
9	P0G	A	1413	27/27	0.90	0.22	62,78,83,88	0
7	NA	A	1411	1/1	0.92	0.10	70,70,70,70	0
4	SO4	A	1405	5/5	0.96	0.13	62,70,79,85	0
4	SO4	A	1404	5/5	0.97	0.23	52,54,57,65	0
4	SO4	A	1406	5/5	0.98	0.12	74,75,81,87	0
4	SO4	A	1403	5/5	0.98	0.21	57,59,60,66	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.

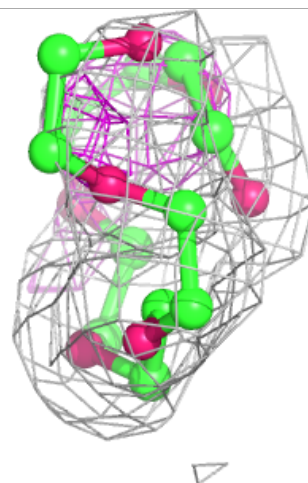
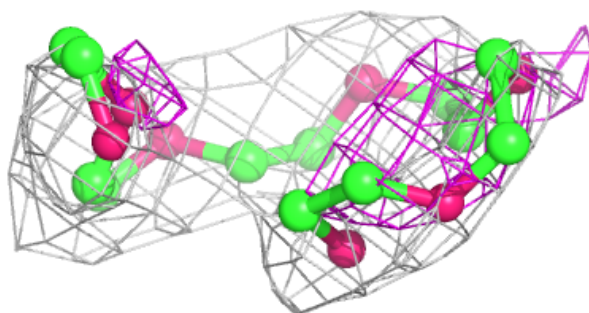
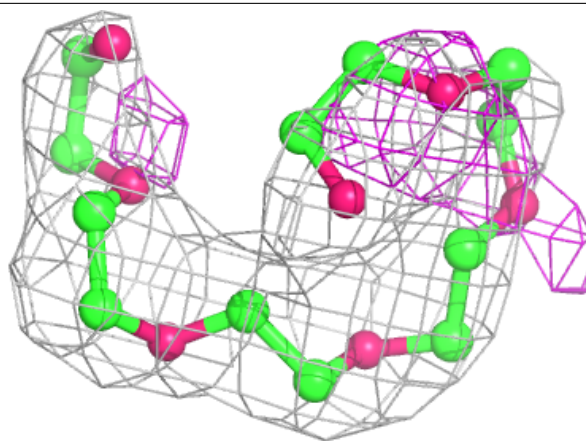
Electron density around 1WV A 1410:

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



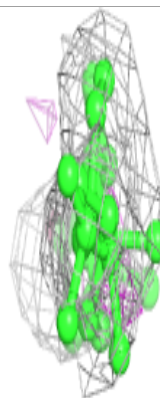
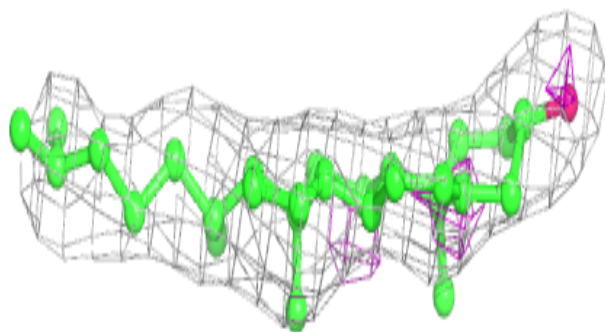
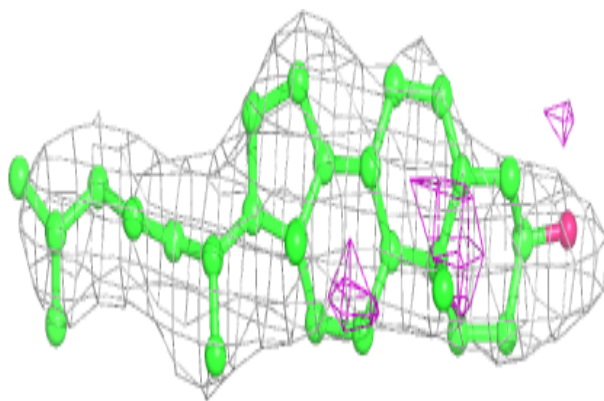
Electron density around P6G A 1414:

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

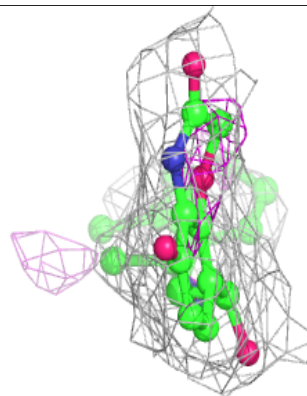
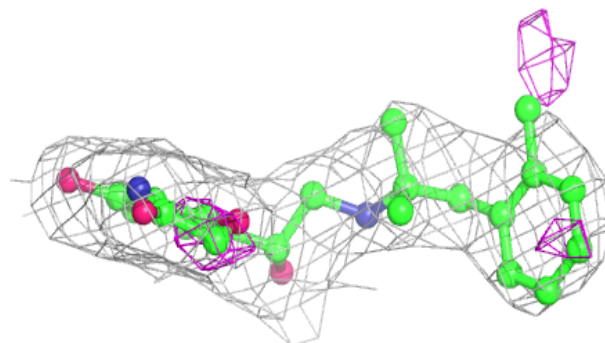
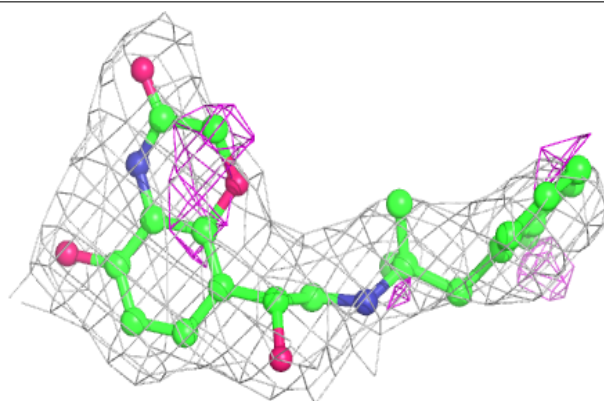


Electron density around CLR A 1409:

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

**Electron density around P0G A 1413:**

$2mF_o-DF_c$ (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.