Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 11:58 PM EDT

PDB ID	:	4F4C
Title	:	The Crystal Structure of the Multi-Drug Transporter
Authors	:	Jin, M.S.; Oldham, M.L.; Zhang, Q.; Chen, J.
Deposited on	:	2012-05-10
Resolution	:	3.40 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:

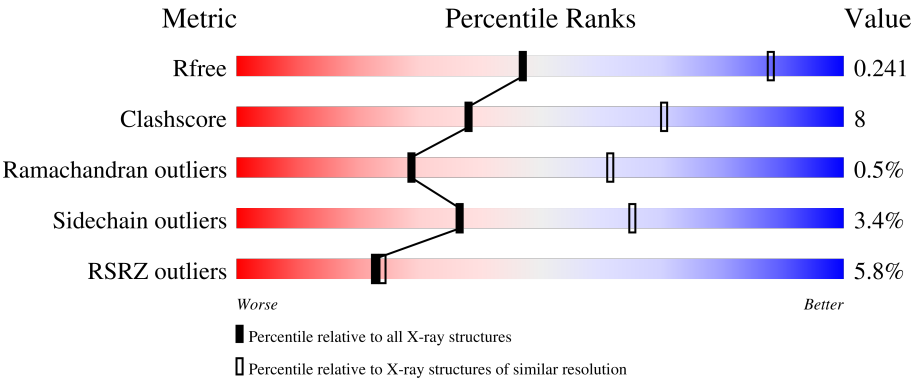
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1321	5%, 77%, 17%, • 5%
2	B	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
2	NAG	B	1	X	-	-	X
2	NAG	B	2	-	-	-	X
2	BMA	B	3	-	-	-	X
2	MAN	B	4	-	-	-	X
3	0SA	A	1405	-	-	-	X
3	0SA	A	1406	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9541 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.

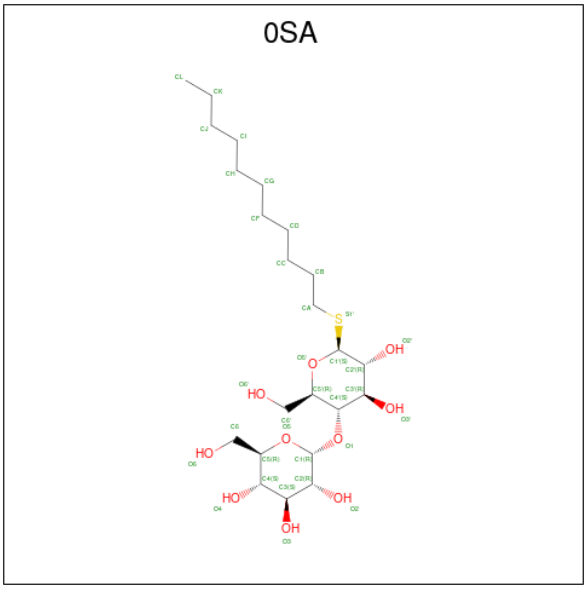
- Molecule 1 is a protein called Multidrug resistance protein pgp-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1250	9423	6011	1593	1772	47	0	0	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0

- Molecule 3 is undecyl 4-O-alpha-D-glucopyranosyl-1-thio-beta-D-glucopyranoside (three-letter code: 0SA) (formula: $C_{23}H_{44}O_{10}S$).



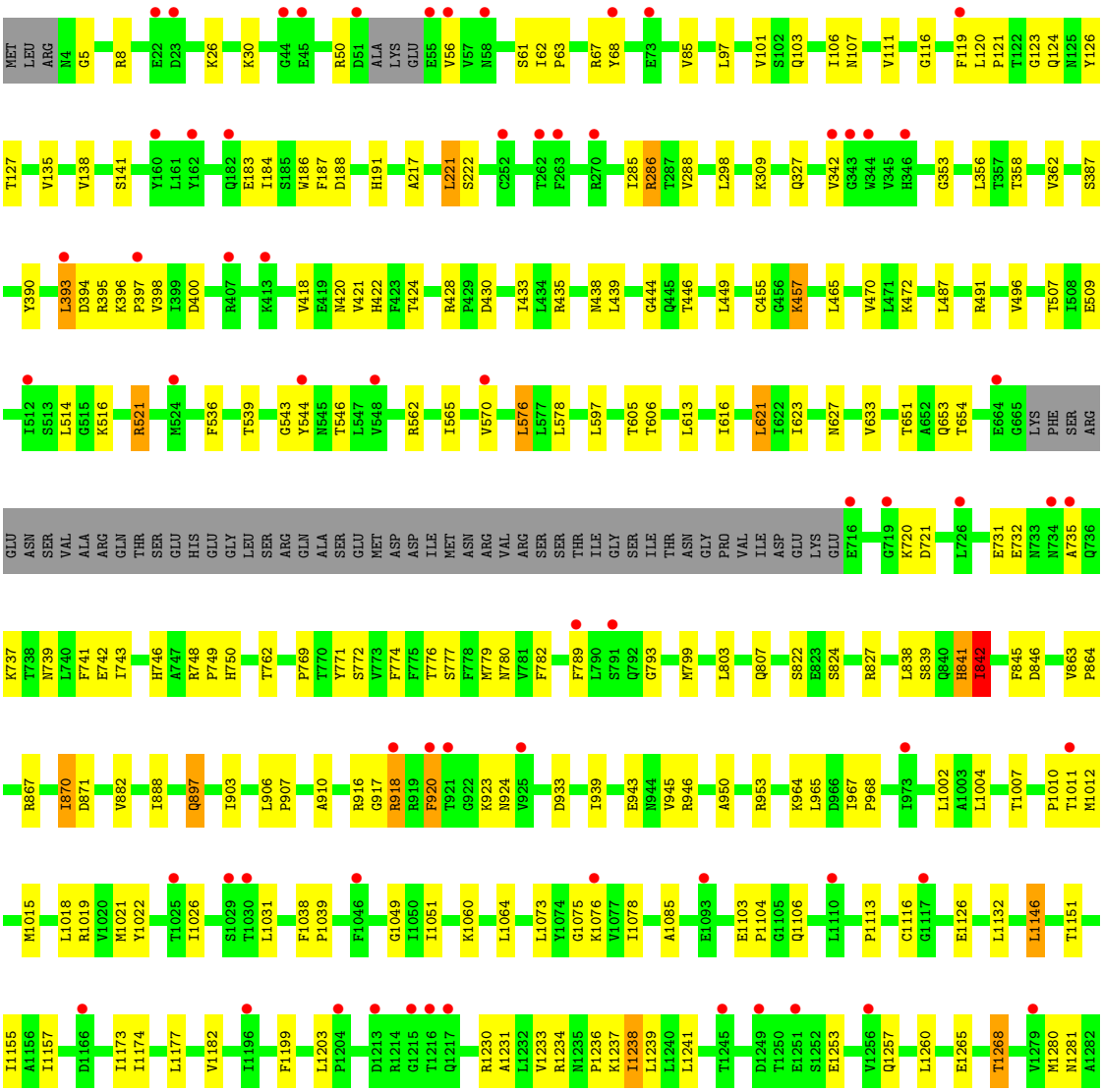
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			34	23	10	1		
3	A	1	Total	C	O	S	0	0
			34	23	10	1		

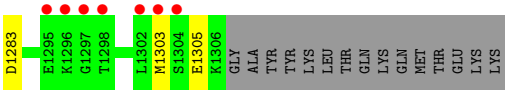
3 Residue-property plots (i)

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: Multidrug resistance protein pgp-1

Chain A:





• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.90Å 155.36Å 162.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.43 – 3.40 46.43 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.43-3.40) 98.7 (46.43-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 3.40Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.250 , 0.283 0.235 , 0.241	Depositor DCC
R_{free} test set	1719 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	140.0	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 88.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9541	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0SA, MAN, NAG, BMA

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	0.43	0/9581	0.59	0/12993

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	9423	0	9395	140	0
2	B	50	0	43	2	0
3	A	68	0	88	7	0
All	All	9541	0	9526	144	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 8.

All (144) 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:444:GLY:H	1:A:605:THR:HG22	1.10	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ARG:HH11	1:A:521:ARG:HG3	1.37	0.89
1:A:920:PHE:O	1:A:920:PHE:HD1	1.54	0.89
1:A:56:VAL:HG11	1:A:387:SER:OG	1.79	0.81
1:A:621:LEU:HD11	1:A:633:VAL:HG13	1.64	0.80
1:A:1126:GLU:HG3	1:A:1157:ILE:HD11	1.67	0.74
1:A:107:ASN:HB3	1:A:119:PHE:CZ	2.24	0.73
1:A:521:ARG:HH11	1:A:521:ARG:CG	2.01	0.73
1:A:1103:GLU:HG3	1:A:1104:PRO:HD2	1.73	0.70
1:A:841:HIS:O	1:A:842:ILE:HB	1.91	0.69
1:A:897:GLN:HE21	1:A:897:GLN:H	1.39	0.69
1:A:917:GLY:O	1:A:918:ARG:HB2	1.91	0.69
1:A:67:ARG:O	1:A:68:TYR:HB2	1.92	0.68
1:A:444:GLY:N	1:A:605:THR:HG22	1.96	0.68
3:A:1406:0SA:C5	3:A:1406:0SA:H30	2.26	0.66
1:A:967:ILE:HB	1:A:968:PRO:HD3	1.77	0.65
1:A:920:PHE:O	1:A:920:PHE:CD1	2.45	0.63
1:A:536:PHE:O	1:A:539:THR:HG22	1.99	0.63
1:A:1280:MET:O	1:A:1281:ASN:HB2	2.01	0.61
1:A:111:VAL:HG13	1:A:116:GLY:HA2	1.81	0.61
1:A:842:ILE:HA	1:A:845:PHE:HD2	1.66	0.60
1:A:939:ILE:O	1:A:943:GLU:HG2	2.02	0.59
1:A:731:GLU:O	1:A:732:GLU:HB2	2.01	0.59
1:A:449:LEU:HD23	1:A:623:ILE:HB	1.84	0.59
1:A:393:LEU:O	1:A:395:ARG:N	2.36	0.59
1:A:769:PRO:O	1:A:772:SER:HB3	2.03	0.59
1:A:106:ILE:HD11	1:A:779:MET:O	2.03	0.58
1:A:1073:LEU:O	1:A:1237:LYS:HG2	2.04	0.58
1:A:286:ARG:NH2	1:A:846:ASP:OD1	2.36	0.57
1:A:298:LEU:HD13	1:A:838:LEU:HD12	1.84	0.57
1:A:422:HIS:HB2	1:A:472:LYS:HB3	1.87	0.57
1:A:920:PHE:HD1	1:A:920:PHE:C	2.09	0.56
1:A:906:LEU:HB3	3:A:1405:0SA:H14	1.88	0.56
1:A:920:PHE:CD1	1:A:920:PHE:C	2.79	0.56
1:A:183:GLU:H	1:A:398:VAL:HG21	1.71	0.56
1:A:487:LEU:HD23	1:A:491:ARG:HH12	1.71	0.55
1:A:1174:ILE:HG22	1:A:1233:VAL:HG11	1.88	0.55
1:A:750:HIS:CE1	1:A:824:SER:HB3	2.41	0.55
1:A:771:TYR:HB2	1:A:803:LEU:HD21	1.89	0.54
1:A:623:ILE:HG12	1:A:633:VAL:HG22	1.90	0.54
1:A:1075:GLY:HA3	1:A:1268:THR:HG21	1.88	0.54
1:A:421:VAL:HG13	1:A:470:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:ILE:HA	1:A:1230:ARG:HG2	1.90	0.53
1:A:103:GLN:NE2	1:A:353:GLY:H	2.06	0.53
1:A:613:LEU:H	1:A:653:GLN:HE22	1.56	0.52
1:A:119:PHE:O	1:A:123:GLY:HA2	2.10	0.52
1:A:418:VAL:HB	1:A:439:LEU:HG	1.92	0.51
1:A:776:THR:HG21	1:A:1019:ARG:HA	1.93	0.51
1:A:1239:LEU:HD22	1:A:1241:LEU:HD12	1.92	0.51
1:A:393:LEU:C	1:A:395:ARG:H	2.14	0.51
1:A:184:ILE:CG2	1:A:946:ARG:CZ	2.89	0.51
1:A:863:VAL:HB	1:A:864:PRO:HD3	1.93	0.50
1:A:1257:GLN:HA	1:A:1260:LEU:HD12	1.92	0.50
1:A:26:LYS:HG2	1:A:30:LYS:HE2	1.92	0.50
1:A:748:ARG:N	1:A:749:PRO:HD2	2.27	0.50
1:A:217:ALA:O	1:A:221:LEU:HB2	2.12	0.50
1:A:521:ARG:HG3	1:A:521:ARG:NH1	2.17	0.50
1:A:578:LEU:HD22	1:A:597:LEU:HD22	1.92	0.50
3:A:1406:0SA:H30	3:A:1406:0SA:H35	1.92	0.50
1:A:1199:PHE:O	1:A:1203:LEU:HB2	2.11	0.50
1:A:424:THR:HA	1:A:433:ILE:HD12	1.95	0.49
1:A:521:ARG:CG	1:A:521:ARG:NH1	2.68	0.49
2:B:2:NAG:H3	2:B:3:BMA:O5	2.12	0.49
2:B:2:NAG:H5	2:B:3:BMA:O2	2.13	0.49
1:A:516:LYS:HB2	1:A:570:VAL:HG12	1.95	0.48
1:A:186:TRP:CD1	1:A:396:LYS:HE2	2.48	0.48
1:A:910:ALA:HB2	3:A:1405:0SA:H19	1.95	0.48
1:A:651:THR:HA	1:A:654:THR:HG22	1.96	0.48
1:A:61:SER:HB3	1:A:63:PRO:HD2	1.96	0.48
1:A:720:LYS:HG2	1:A:721:ASP:H	1.78	0.48
1:A:1076:LYS:HE2	1:A:1078:ILE:HD11	1.95	0.48
1:A:1155:ILE:HG12	1:A:1238:ILE:HG12	1.95	0.48
1:A:491:ARG:HG2	1:A:950:ALA:HA	1.95	0.47
1:A:309:LYS:HD2	1:A:827:ARG:HE	1.80	0.47
1:A:327:GLN:HB3	1:A:807:GLN:HE21	1.79	0.47
1:A:358:THR:O	1:A:362:VAL:HG23	2.14	0.47
1:A:135:VAL:HG11	1:A:1002:LEU:HB2	1.96	0.47
1:A:188:ASP:OD1	1:A:946:ARG:NH2	2.47	0.47
1:A:487:LEU:HD12	1:A:487:LEU:H	1.80	0.47
1:A:762:THR:HG23	1:A:882:VAL:HG21	1.97	0.47
1:A:1004:LEU:HB3	1:A:1012:MET:HB2	1.95	0.47
1:A:1007:THR:O	1:A:1010:PRO:HB3	2.14	0.47
1:A:1106:GLN:HE21	1:A:1283:ASP:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ASN:HD21	1:A:741:PHE:HB2	1.79	0.47
1:A:1075:GLY:CA	1:A:1268:THR:HG21	2.44	0.46
1:A:107:ASN:HB3	1:A:119:PHE:CE2	2.51	0.46
1:A:916:ARG:HH22	3:A:1406:0SA:H36	1.80	0.46
1:A:1146:LEU:HB3	1:A:1151:THR:HG21	1.97	0.46
1:A:1113:PRO:HG2	1:A:1116:CYS:HB3	1.98	0.46
1:A:446:THR:HG23	1:A:606:THR:HB	1.99	0.45
1:A:455:CYS:SG	1:A:457:LYS:HD2	2.55	0.45
1:A:782:PHE:HA	1:A:789:PHE:CE1	2.52	0.45
1:A:1177:LEU:H	1:A:1177:LEU:HD12	1.82	0.45
1:A:743:ILE:HG22	1:A:870:ILE:HD12	1.98	0.45
1:A:390:TYR:HA	1:A:393:LEU:HB3	1.98	0.44
1:A:777:SER:OG	1:A:1019:ARG:NH2	2.50	0.44
1:A:119:PHE:HB3	1:A:121:PRO:HD2	1.98	0.44
1:A:1085:ALA:H	1:A:1132:LEU:HD13	1.81	0.44
1:A:187:PHE:CZ	1:A:945:VAL:HG21	2.52	0.44
1:A:342:VAL:HG11	1:A:793:GLY:HA3	2.00	0.44
1:A:435:ARG:HH21	1:A:627:ASN:HB3	1.83	0.44
1:A:1031:LEU:CD2	3:A:1405:0SA:H16	2.47	0.44
1:A:933:ASP:HB3	1:A:964:LYS:NZ	2.33	0.43
1:A:1015:MET:O	1:A:1019:ARG:HG3	2.17	0.43
1:A:1253:GLU:O	1:A:1257:GLN:HB2	2.18	0.43
1:A:774:PHE:CE1	1:A:799:MET:HB3	2.54	0.43
1:A:62:ILE:N	1:A:63:PRO:CD	2.82	0.43
1:A:507:THR:HA	1:A:546:THR:O	2.19	0.43
1:A:839:SER:HB3	1:A:1064:LEU:HD12	2.00	0.43
1:A:822:SER:HB2	1:A:867:ARG:HG3	2.00	0.43
1:A:101:VAL:HB	1:A:138:VAL:HG11	2.01	0.43
1:A:576:LEU:HD23	1:A:606:THR:HG23	2.01	0.43
1:A:1018:LEU:HD23	1:A:1021:MET:HE1	2.00	0.43
1:A:285:ILE:HA	1:A:288:VAL:HG12	2.00	0.43
1:A:782:PHE:HA	1:A:789:PHE:HE1	1.84	0.43
1:A:1022:TYR:O	1:A:1026:ILE:HB	2.19	0.43
1:A:97:LEU:HD21	1:A:141:SER:HB3	2.01	0.42
1:A:906:LEU:N	1:A:907:PRO:HD2	2.34	0.42
1:A:742:GLU:O	1:A:746:HIS:HD2	2.02	0.42
1:A:910:ALA:HB1	3:A:1406:0SA:H12	2.01	0.42
1:A:863:VAL:HG22	1:A:1051:ILE:HD13	2.01	0.42
1:A:119:PHE:CE2	1:A:126:TYR:CG	3.07	0.42
1:A:514:LEU:HD22	1:A:953:ARG:HG2	2.01	0.42
1:A:562:ARG:HA	1:A:565:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:O	1:A:546:THR:HG22	2.19	0.42
1:A:1177:LEU:HD12	1:A:1234:ARG:NH1	2.35	0.41
1:A:85:VAL:HG13	1:A:222:SER:CB	2.51	0.41
1:A:111:VAL:HG23	1:A:119:PHE:CE1	2.56	0.41
1:A:184:ILE:HG21	1:A:946:ARG:NH1	2.36	0.41
1:A:1231:ALA:O	1:A:1236:PRO:HD3	2.20	0.41
1:A:420:ASN:H	1:A:438:ASN:ND2	2.18	0.41
1:A:613:LEU:O	1:A:616:ILE:HG22	2.21	0.41
1:A:396:LYS:HA	1:A:397:PRO:HD3	1.86	0.41
1:A:509:GLU:HB3	1:A:544:TYR:HB3	2.02	0.41
1:A:864:PRO:O	1:A:867:ARG:HB3	2.22	0.40
1:A:1182:VAL:HG21	1:A:1233:VAL:HG13	2.02	0.40
1:A:85:VAL:HG13	1:A:222:SER:HB3	2.03	0.40
1:A:737:LYS:HA	1:A:1049:GLY:HA3	2.02	0.40
1:A:841:HIS:ND1	1:A:1060:LYS:HB2	2.36	0.40
1:A:1038:PHE:N	1:A:1039:PRO:HD2	2.36	0.40
1:A:731:GLU:O	1:A:732:GLU:CB	2.69	0.40
1:A:888:ILE:HG23	1:A:903:ILE:HD11	2.04	0.40
1:A:1280:MET:O	1:A:1281:ASN:CB	2.69	0.40
1:A:5:GLY:HA2	1:A:8:ARG:HG2	2.02	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	1244/1321 (94%)	1175 (94%)	63 (5%)	6 (0%)	29 61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ASP

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Mol	Chain	Res	Type
1	A	842	ILE
1	A	735	ALA
1	A	393	LEU
1	A	871	ASP
1	A	1265	GLU

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	984/1099 (90%)	951 (97%)	33 (3%)	37 65

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	120	LEU
1	A	124	GLN
1	A	127	THR
1	A	191	HIS
1	A	221	LEU
1	A	286	ARG
1	A	356	LEU
1	A	400	ASP
1	A	428	ARG
1	A	430	ASP
1	A	457	LYS
1	A	465	LEU
1	A	496	VAL
1	A	521	ARG
1	A	576	LEU
1	A	621	LEU
1	A	780	ASN
1	A	841	HIS
1	A	842	ILE
1	A	870	ILE

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Mol	Chain	Res	Type
1	A	897	GLN
1	A	918	ARG
1	A	920	PHE
1	A	923	LYS
1	A	924	ASN
1	A	965	LEU
1	A	1011	THR
1	A	1146	LEU
1	A	1238	ILE
1	A	1268	THR
1	A	1303	MET
1	A	1305	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	191	HIS
1	A	249	GLN
1	A	330	ASN
1	A	383	GLN
1	A	438	ASN
1	A	486	ASN
1	A	554	GLN
1	A	739	ASN
1	A	746	HIS
1	A	750	HIS
1	A	780	ASN
1	A	807	GLN
1	A	831	ASN
1	A	840	GLN
1	A	897	GLN
1	A	949	GLN
1	A	1106	GLN
1	A	1172	ASN
1	A	1186	GLN
1	A	1301	GLN

5.3.3 RNA

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)

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	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	1.43	3 (21%)	17,19,21	1.41	1 (5%)
2	NAG	B	2	2	14,14,15	1.69	2 (14%)	17,19,21	1.24	2 (11%)
2	BMA	B	3	2	11,11,12	1.17	1 (9%)	15,15,17	0.66	0
2	MAN	B	4	2	11,11,12	1.11	1 (9%)	15,15,17	0.83	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C1-C2	4.96	1.59	1.52
2	B	1	NAG	O5-C5	3.04	1.49	1.43
2	B	2	NAG	C3-C2	2.80	1.58	1.52
2	B	1	NAG	O5-C1	2.76	1.48	1.43
2	B	4	MAN	C2-C3	2.51	1.56	1.52
2	B	3	BMA	C2-C3	2.11	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	2.10	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C1-O5-C5	4.78	118.67	112.19
2	B	2	NAG	C4-C3-C2	2.69	114.96	111.02
2	B	4	MAN	C1-O5-C5	2.21	115.18	112.19
2	B	2	NAG	C1-C2-N2	-2.08	106.94	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1

All (6) torsion outliers are listed below:

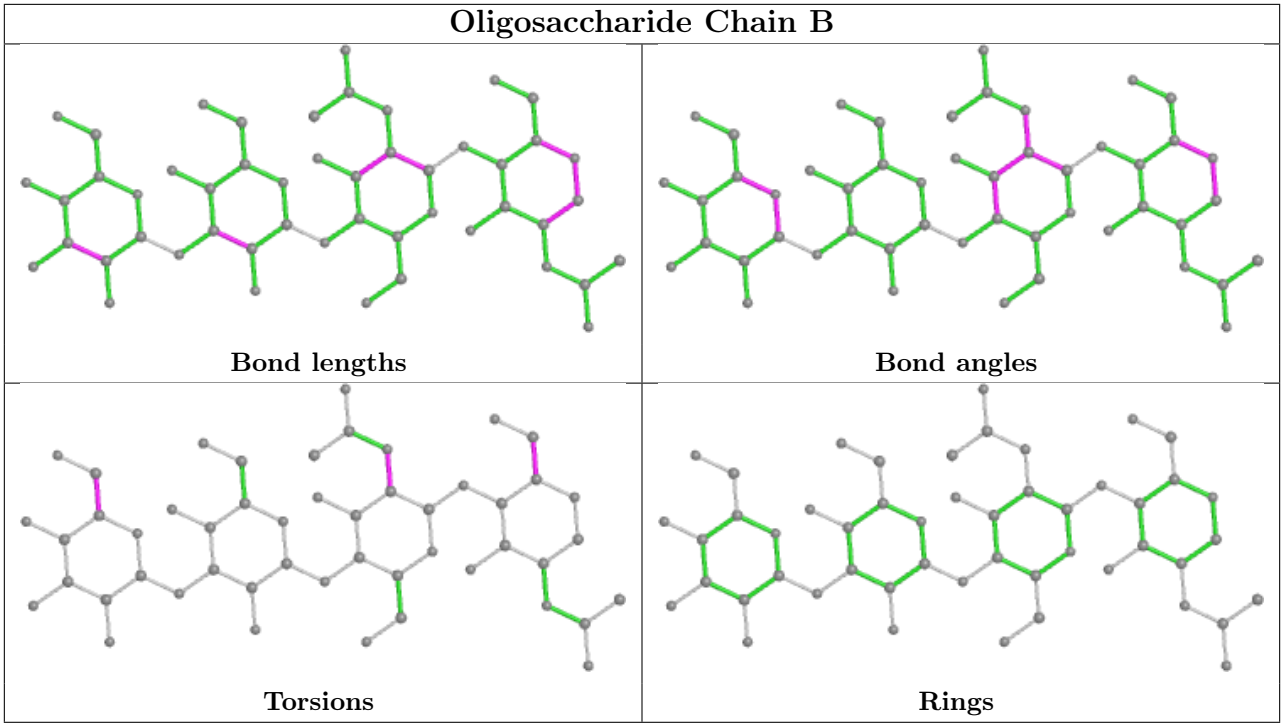
Mol	Chain	Res	Type	Atoms
2	B	4	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	2	0
2	B	3	BMA	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)

2 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	0SA	A	1406	-	35,35,35	0.48	0	45,46,46	1.06	2 (4%)
3	0SA	A	1405	-	35,35,35	0.49	0	45,46,46	0.90	1 (2%)

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	0SA	A	1406	-	-	8/20/60/60	0/2/2/2
3	0SA	A	1405	-	-	2/20/60/60	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1406	0SA	O5'-C1'-S1'	-3.43	101.63	109.82
3	A	1406	0SA	CA-S1'-C1'	2.77	105.27	100.09
3	A	1405	0SA	O5'-C1'-C2'	-2.24	107.50	110.31

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1406	0SA	CB-CA-S1'-C1'
3	A	1406	0SA	O5'-C1'-S1'-CA
3	A	1406	0SA	O5-C5-C6-O6
3	A	1406	0SA	C4-C5-C6-O6
3	A	1406	0SA	CG-CH-CI-CJ
3	A	1406	0SA	CC-CD-CF-CG
3	A	1405	0SA	C3'-C4'-O1-C1
3	A	1405	0SA	C5'-C4'-O1-C1
3	A	1406	0SA	CH-CI-CJ-CK
3	A	1406	0SA	O5'-C5'-C6'-O6'

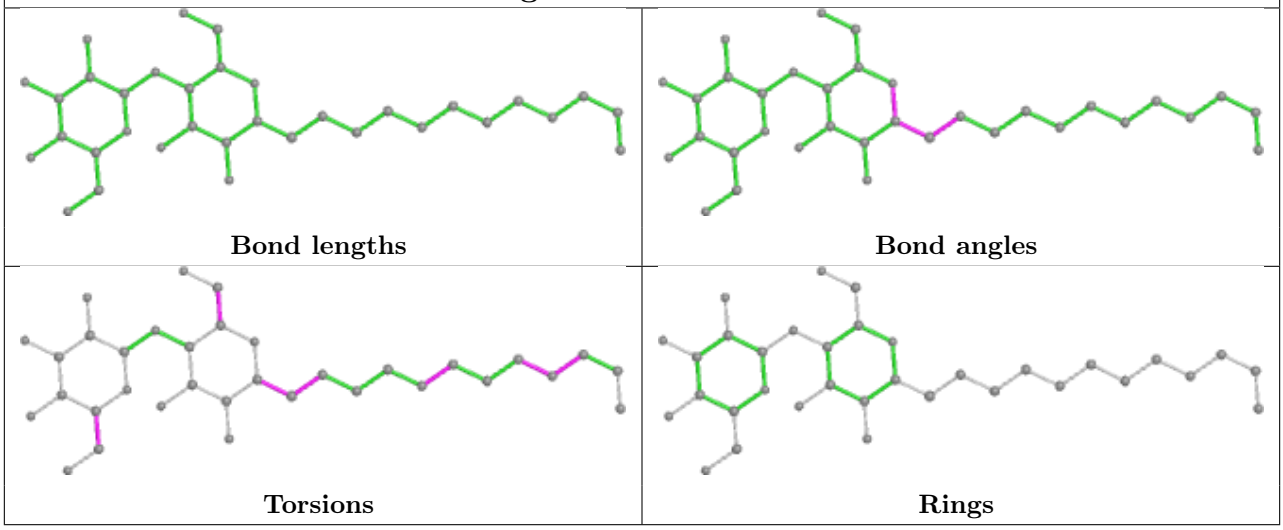
There are no ring outliers.

2 monomers are involved in 7 short contacts:

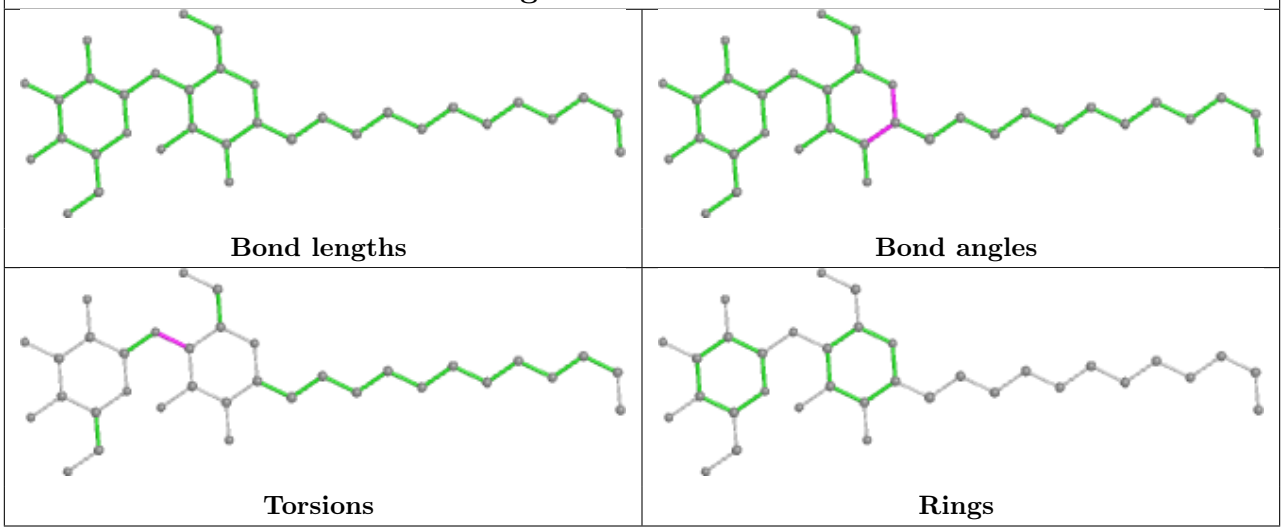
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1406	0SA	4	0
3	A	1405	0SA	3	0

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 then 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 0SA A 1406



Ligand 0SA A 1405



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1250/1321 (94%)	0.54	72 (5%)	23	24	105, 140, 192, 200	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	GLU	4.6
1	A	56	VAL	4.5
1	A	1256	VAL	4.5
1	A	119	PHE	4.5
1	A	1279	VAL	4.2
1	A	1296	LYS	3.9
1	A	920	PHE	3.7
1	A	1245	THR	3.6
1	A	1204	PRO	3.6
1	A	58	ASN	3.5
1	A	1298	THR	3.5
1	A	263	PHE	3.4
1	A	51	ASP	3.3
1	A	343	GLY	3.3
1	A	397	PRO	3.3
1	A	1295	GLU	3.3
1	A	68	TYR	3.2
1	A	921	THR	3.2
1	A	918	ARG	3.1
1	A	23	ASP	3.1
1	A	512	ILE	3.0
1	A	45	GLU	3.0
1	A	1025	THR	3.0
1	A	1251	GLU	2.9
1	A	413	LYS	2.9
1	A	524	MET	2.9
1	A	1029	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	789	PHE	2.8
1	A	1110	LEU	2.8
1	A	1166	ASP	2.8
1	A	791	SER	2.8
1	A	44	GLY	2.8
1	A	726	LEU	2.7
1	A	162	TYR	2.7
1	A	664	GLU	2.7
1	A	342	VAL	2.7
1	A	1117	GLY	2.6
1	A	1249	ASP	2.6
1	A	1213	ASP	2.6
1	A	1196	ILE	2.6
1	A	734	ASN	2.6
1	A	22	GLU	2.5
1	A	270	ARG	2.5
1	A	1030	THR	2.5
1	A	1046	PHE	2.5
1	A	719	GLY	2.5
1	A	1303	MET	2.5
1	A	1216	THR	2.5
1	A	973	ILE	2.4
1	A	544	TYR	2.4
1	A	1297	GLY	2.4
1	A	735	ALA	2.4
1	A	1302	LEU	2.4
1	A	393	LEU	2.3
1	A	262	THR	2.3
1	A	182	GLN	2.3
1	A	570	VAL	2.3
1	A	1011	THR	2.3
1	A	73	GLU	2.2
1	A	160	TYR	2.2
1	A	925	VAL	2.1
1	A	1304	SER	2.1
1	A	344	TRP	2.1
1	A	1217	GLN	2.1
1	A	55	GLU	2.1
1	A	346	HIS	2.1
1	A	548	VAL	2.1
1	A	252	CYS	2.0
1	A	407	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1093	GLU	2.0
1	A	1076	LYS	2.0
1	A	1215	GLY	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)

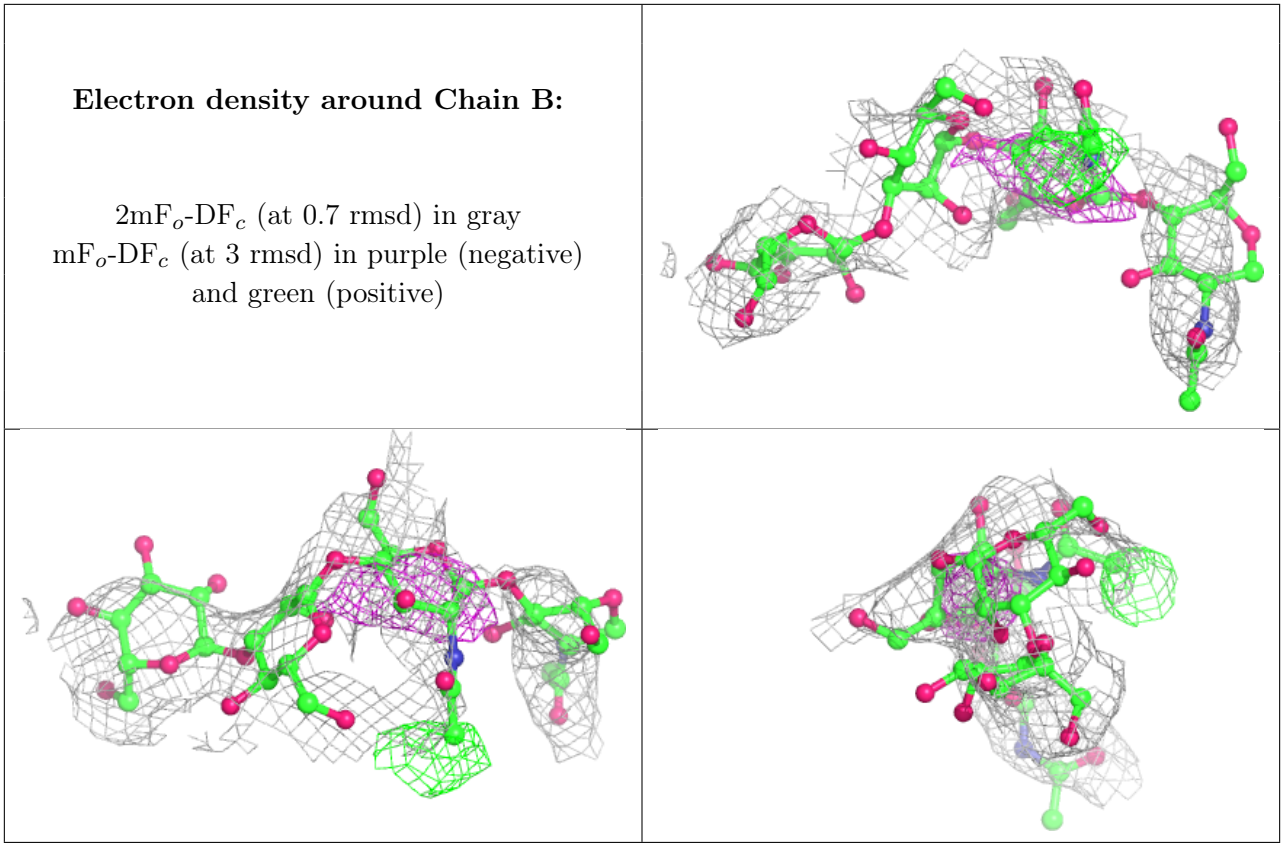
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	2	14/15	0.55	0.53	196,200,200,200	0
2	MAN	B	4	11/12	0.58	0.51	191,200,200,200	0
2	NAG	B	1	14/15	0.59	0.57	195,199,200,200	0
2	BMA	B	3	11/12	0.60	0.44	200,200,200,200	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 B:

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



6.4 Ligands

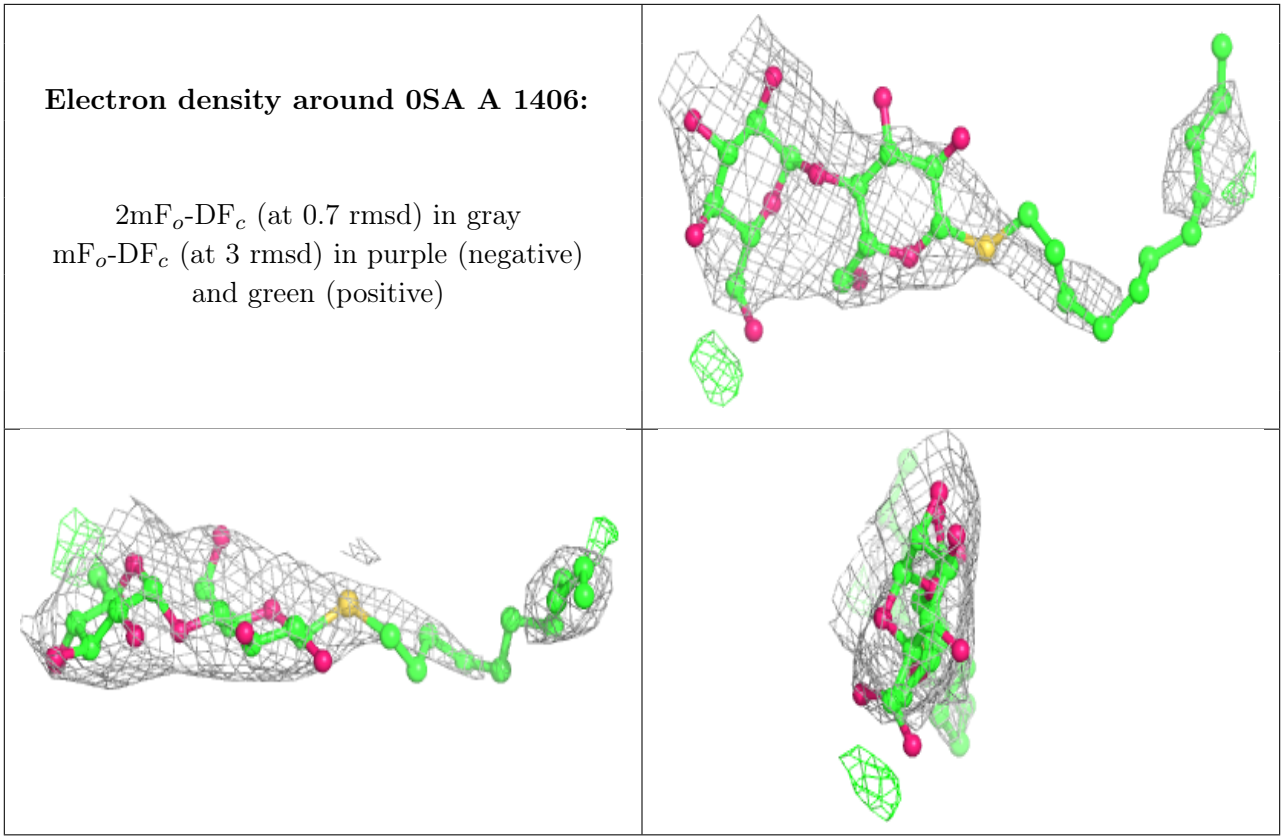
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	0SA	A	1406	34/34	0.56	0.52	134,190,198,198	0
3	0SA	A	1405	34/34	0.63	0.58	147,171,178,179	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.

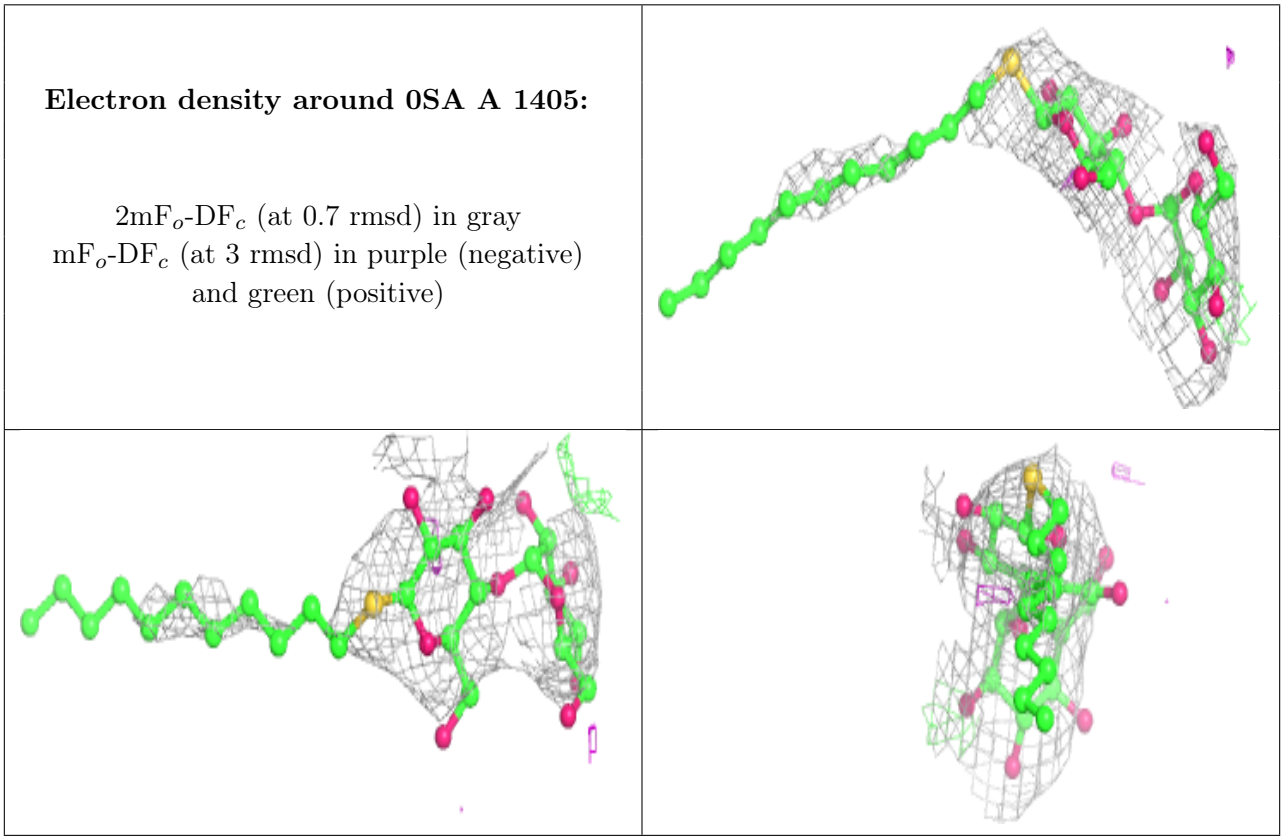
Electron density around 0SA A 1406:

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



Electron density around 0SA A 1405:

$2mF_o$-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.