Full wwPDB X-ray Structure Validation Report ⓘ

Nov 27, 2023 – 12:29 pm GMT

PDB ID	:	8Q1X
Title	:	Structural analysis of PLD3 reveals insights into the mechanism of lysosomal 5' exonuclease-mediated nucleic acid degradation
Authors	:	Roske, Y.; Daumke, O.; Damme, M.
Deposited on	:	2023-08-01
Resolution	:	1.85 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:

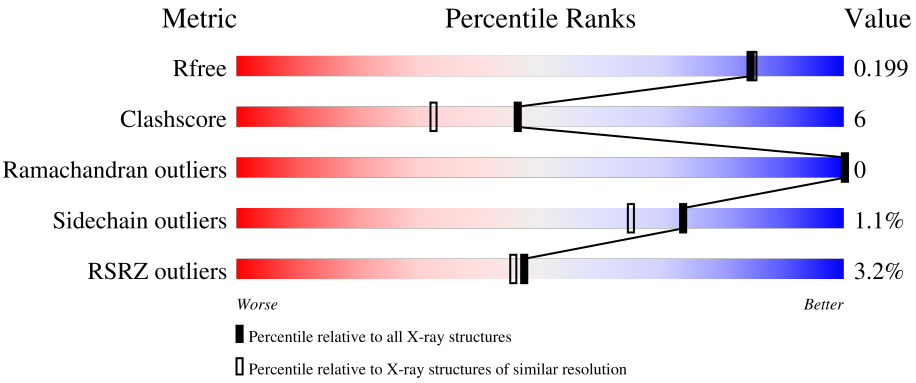
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	433	3% 87% 10%
1	B	433	3% 86% 10%
2	C	6	50% 50%
2	E	6	100%
3	D	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	2	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	MAN	E	6	-	-	-	X
4	PST	A	501	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8057 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.

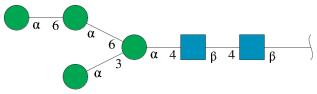
- Molecule 1 is a protein called 5'-3' exonuclease PLD3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	15	0
			3350	2122	582	629	17			
1	B	419	Total	C	N	O	S	0	8	0
			3317	2100	577	623	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	491	ALA	-	expression tag	UNP Q8IV08
A	492	ALA	-	expression tag	UNP Q8IV08
A	493	GLN	-	expression tag	UNP Q8IV08
B	491	ALA	-	expression tag	UNP Q8IV08
B	492	ALA	-	expression tag	UNP Q8IV08
B	493	GLN	-	expression tag	UNP Q8IV08

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

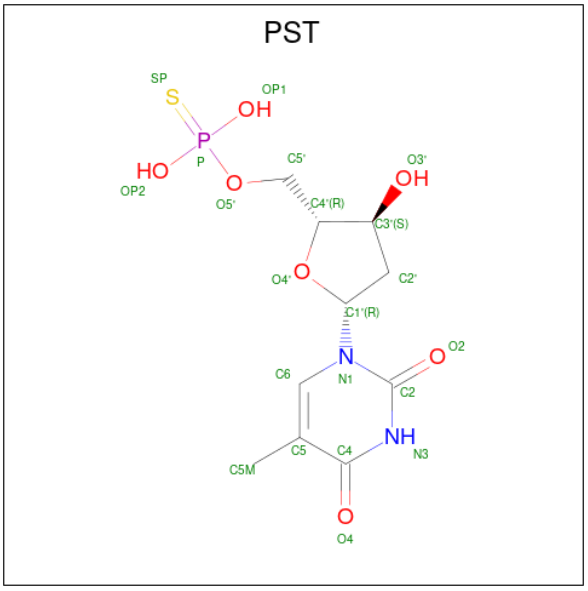


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

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

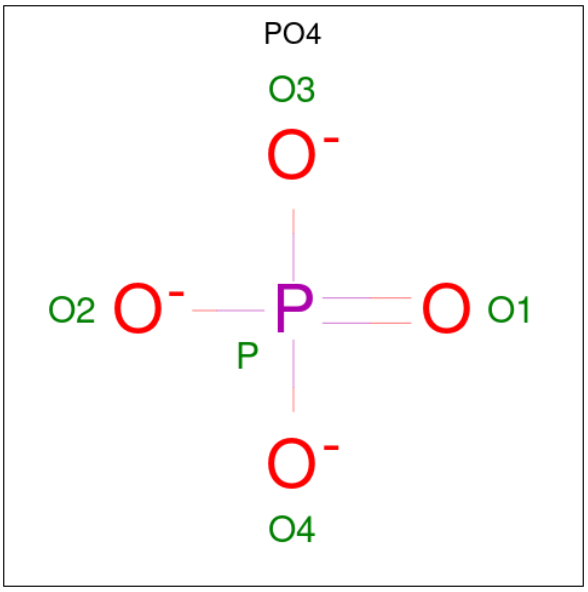
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C N O 42 24 3 15	0	1	0
3	F	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 is THYMIDINE-5'-THIOPHOSPHATE (three-letter code: PST) (formula: $C_{10}H_{15}N_2O_7PS$).



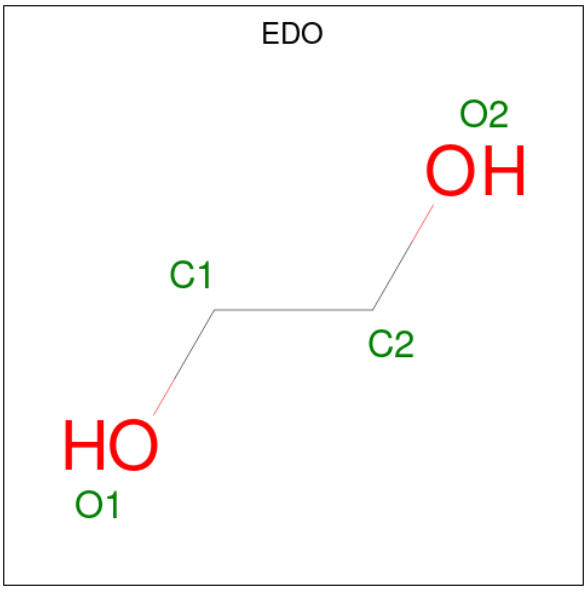
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 17 10 2 5	0	0
4	A	1	Total O P S 4 2 1 1	0	0
4	B	1	Total C N O 17 10 2 5	0	0
4	B	1	Total O P S 4 2 1 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0

Continued on next page...

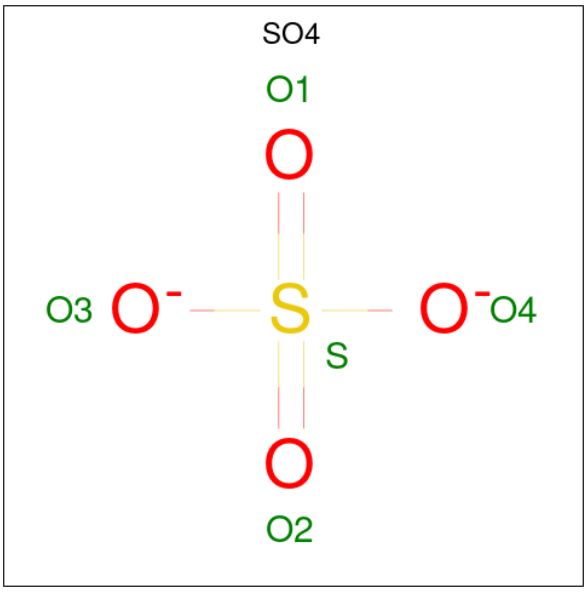
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mn 1 1	0	0
7	B	1	Total Mn 1 1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Mg 1 1	0	0
9	B	1	Total Mg 1 1	0	0

- Molecule 10 is water.

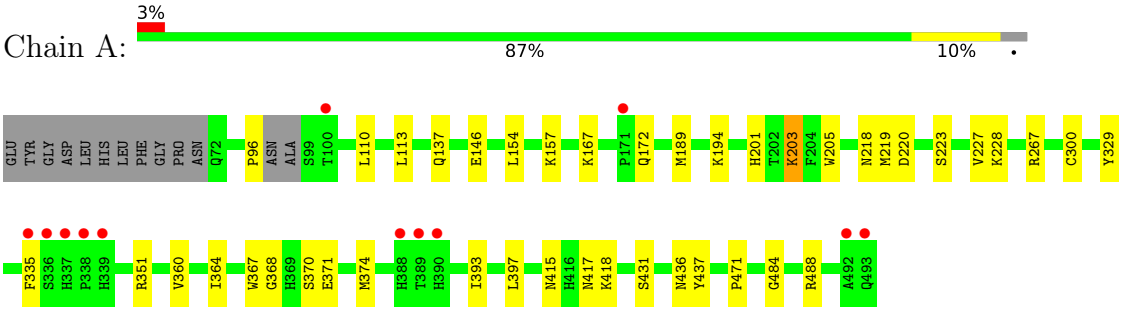
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	525	Total O 526 526	0	1
10	B	509	Total O 509 509	0	0

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.

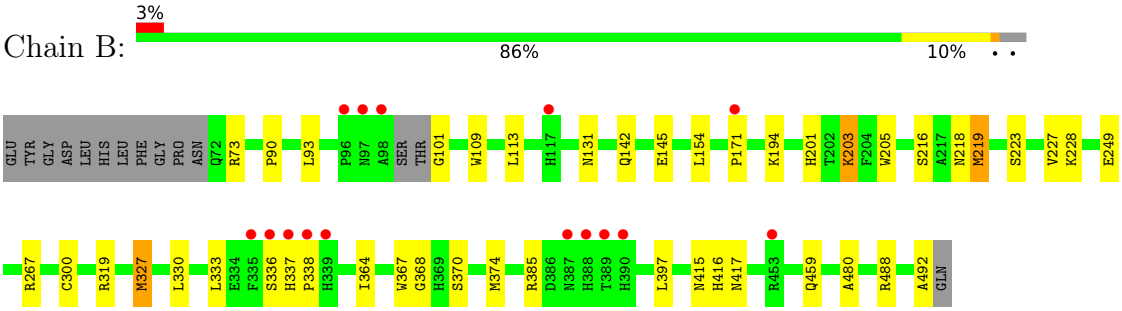
• Molecule 1: 5'-3' exonuclease PLD3

Chain A:



• Molecule 1: 5'-3' exonuclease PLD3

Chain B:

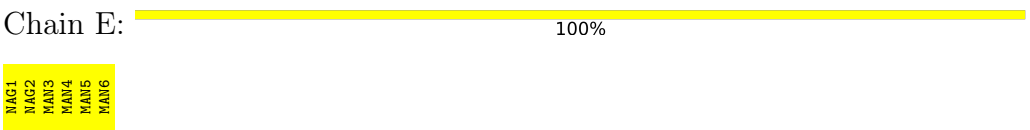


• Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain D:

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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.53Å 115.45Å 101.33Å 90.00° 106.62° 90.00°	Depositor
Resolution (Å)	35.78 – 1.85 48.55 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.5 (35.78-1.85) 98.5 (48.55-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.174 , 0.199 0.175 , 0.199	Depositor DCC
R_{free} test set	2101 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8057	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: MN, MG, MAN, NAG, EDO, OCS, PO4, SO4, PST

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	0.42	0/3471	0.63	0/4735
1	B	0.43	0/3419	0.65	2/4664 (0.0%)
All	All	0.43	0/6890	0.64	2/9399 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	219	MET	CG-SD-CE	8.96	114.53	100.20
1	B	327	MET	CG-SD-CE	-5.89	90.77	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	319	ARG	Sidechain

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	3350	0	3268	35	0
1	B	3317	0	3226	48	0
2	C	72	0	61	0	0
2	E	72	0	61	1	0
3	D	42	0	38	1	0
3	F	28	0	25	0	0
4	A	21	0	12	3	0
4	B	21	0	10	9	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	32	0	48	3	0
6	B	28	0	42	3	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	10	0	0	1	0
8	B	10	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	526	0	0	12	1
10	B	509	0	0	9	1
All	All	8057	0	6791	87	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:TRP:HE1	1:B:219:MET:HE3	1.48	0.79
1:A:218:ASN:ND2	4:A:502:PST:SP	2.53	0.78
1:B:480:ALA:HB3	1:B:492:ALA:HB2	1.67	0.76
1:B:203:LYS:NZ	4:B:503:PST:SP	2.63	0.70
1:B:416[A]:HIS:CE1	4:B:502:PST:H4'	2.25	0.70
1:B:416[B]:HIS:HE2	4:B:503:PST:P	2.14	0.70
1:A:371:GLU:OE2	10:A:601:HOH:O	2.08	0.70
1:B:249[B]:GLU:OE2	10:B:601:HOH:O	2.11	0.67
1:A:194:LYS:NZ	10:A:608:HOH:O	2.26	0.67
1:A:201:HIS:HE2	4:A:502:PST:P	2.17	0.66
1:A:205:TRP:HE1	1:A:219:MET:CE	2.10	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:GLY:O	1:B:488:ARG:HD2	1.96	0.65
3:D:1[B]:NAG:H4	3:D:2:NAG:C1	2.27	0.65
1:B:364:ILE:HG21	1:B:374:MET:HE1	1.79	0.64
1:B:171:PRO:O	10:B:602:HOH:O	2.14	0.64
1:A:96:PRO:HD2	6:A:509:EDO:H21	1.80	0.64
1:A:205:TRP:HE1	1:A:219:MET:HE3	1.65	0.62
1:B:216:SER:HB2	1:B:416[B]:HIS:ND1	2.14	0.61
1:A:335:PHE:H	1:A:436:ASN:HD21	1.46	0.61
8:A:514:SO4:O3	10:A:603:HOH:O	2.16	0.61
1:B:218:ASN:ND2	4:B:503:PST:SP	2.61	0.61
1:B:73:ARG:NH2	10:B:608:HOH:O	2.33	0.60
4:B:502:PST:H5"	10:B:742:HOH:O	2.01	0.60
1:B:131:ASN:HD22	6:B:509:EDO:H22	1.67	0.59
1:A:146:GLU:O	10:A:604:HOH:O	2.18	0.56
1:B:415:ASN:HD21	1:B:417:ASN:HD21	1.54	0.56
1:B:416[A]:HIS:CE1	4:B:502:PST:C4'	2.88	0.55
1:A:335:PHE:H	1:A:436:ASN:ND2	2.04	0.55
1:B:370:SER:O	1:B:488:ARG:HD3	2.07	0.55
1:B:90:PRO:HD2	1:B:93:LEU:HD22	1.88	0.55
1:B:327:MET:CE	1:B:416[B]:HIS:HA	2.37	0.54
1:A:219:MET:HE2	10:A:703:HOH:O	2.07	0.54
1:B:327:MET:CE	1:B:416[A]:HIS:HA	2.39	0.52
1:A:351:ARG:NH2	10:A:614:HOH:O	2.41	0.52
1:B:416[A]:HIS:HE1	4:B:502:PST:H4'	1.70	0.52
1:B:327:MET:HE3	1:B:416[B]:HIS:CD2	2.44	0.52
1:A:471:PRO:HD3	6:A:509:EDO:H22	1.93	0.51
1:A:172[B]:GLN:NE2	10:A:616:HOH:O	2.43	0.51
1:A:203:LYS:NZ	4:A:502:PST:SP	2.83	0.51
6:A:511:EDO:H21	10:A:891:HOH:O	2.10	0.51
1:B:205:TRP:HE1	1:B:219:MET:CE	2.20	0.51
1:B:267:ARG:HH21	6:B:510:EDO:H21	1.75	0.50
1:B:219:MET:HE3	10:B:688:HOH:O	2.10	0.50
1:B:228:LYS:HB3	1:B:415:ASN:HA	1.94	0.50
1:B:415:ASN:HD21	1:B:417:ASN:ND2	2.09	0.50
1:B:416[A]:HIS:HE1	4:B:502:PST:C4'	2.23	0.50
1:B:194:LYS:NZ	10:B:620:HOH:O	2.46	0.49
1:B:228:LYS:O	1:B:416[A]:HIS:HB2	2.12	0.49
1:A:228:LYS:HG2	10:A:756:HOH:O	2.13	0.49
1:A:113:LEU:HD22	1:A:154:LEU:HD11	1.94	0.49
1:B:113:LEU:HD22	1:B:154:LEU:HD11	1.95	0.48
1:A:228:LYS:HB3	1:A:415:ASN:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLU:OE2	6:B:509:EDO:H21	2.13	0.48
1:A:154:LEU:O	1:A:157:LYS:HG2	2.14	0.48
1:A:146:GLU:HG3	10:A:604:HOH:O	2.13	0.47
1:A:167:LYS:HA	1:A:189:MET:HE3	1.96	0.47
1:B:201:HIS:NE2	4:B:503:PST:O5'	2.37	0.47
1:A:360:VAL:HB	1:A:393:ILE:HG12	1.97	0.47
1:A:484:GLY:N	10:A:602:HOH:O	2.10	0.46
1:B:364:ILE:CG2	1:B:374:MET:HE1	2.45	0.46
1:B:101:GLY:N	10:B:614:HOH:O	2.48	0.46
1:B:327:MET:HE3	1:B:416[B]:HIS:HA	1.97	0.46
1:A:220:ASP:OD2	1:A:220:ASP:OD1	2.33	0.45
1:B:109:TRP:CH2	1:B:219:MET:CE	3.00	0.45
1:B:330:LEU:HD13	1:B:374:MET:HG2	1.98	0.45
1:A:189:MET:HE3	1:A:189:MET:HB3	1.78	0.45
1:B:327:MET:HE3	1:B:416[A]:HIS:HA	1.98	0.45
1:A:351:ARG:HD3	10:A:913:HOH:O	2.17	0.45
1:B:142:GLN:NE2	10:B:623:HOH:O	2.49	0.44
1:A:364:ILE:O	1:A:397:LEU:HA	2.18	0.43
1:B:216:SER:O	1:B:416[B]:HIS:CE1	2.71	0.43
1:A:223:SER:HA	1:A:227[A]:VAL:HG22	1.99	0.43
1:B:459:GLN:NE2	2:E:1:NAG:H83	2.34	0.43
1:A:329:TYR:O	1:A:374:MET:HG2	2.19	0.42
1:B:333:LEU:O	1:B:336:SER:HB2	2.20	0.42
1:B:223:SER:HA	1:B:227[A]:VAL:HG22	2.01	0.42
1:B:223:SER:HA	1:B:227[A]:VAL:CG2	2.49	0.42
1:A:368:GLY:O	1:A:488:ARG:HD2	2.18	0.42
1:A:223:SER:HA	1:A:227[A]:VAL:CG2	2.50	0.42
1:A:370:SER:O	1:A:488:ARG:HD3	2.19	0.41
1:B:337:HIS:HA	1:B:338:PRO:C	2.39	0.41
1:A:220:ASP:OD2	1:A:220:ASP:CB	2.69	0.41
1:B:385:ARG:NH1	10:B:603:HOH:O	2.27	0.41
1:B:364:ILE:O	1:B:397:LEU:HA	2.21	0.41
1:A:431:SER:HB3	1:A:437:TYR:HB3	2.03	0.40
1:B:327:MET:CE	1:B:416[B]:HIS:HD2	2.34	0.40
1:A:110:LEU:HA	1:A:110:LEU:HD23	1.80	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:686:HOH:O	10:B:775:HOH:O[2_555]	2.17	0.03

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	430/433 (99%)	419 (97%)	11 (3%)	0	100	100
1	B	422/433 (98%)	408 (97%)	14 (3%)	0	100	100
All	All	852/866 (98%)	827 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	366/365 (100%)	359 (98%)	7 (2%)	57	43
1	B	361/365 (99%)	359 (99%)	2 (1%)	86	83
All	All	727/730 (100%)	718 (99%)	9 (1%)	73	62

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137[A]	GLN
1	A	137[B]	GLN
1	A	203	LYS
1	A	267	ARG
1	A	367	TRP
1	A	417	ASN
1	A	418	LYS
1	B	203	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	367	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	436	ASN
1	B	178	GLN
1	B	182	GLN
1	B	417	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	OCS	B	300	1	7,8,9	0.93	0	6,11,13	1.57	1 (16%)
1	OCS	A	300	1	7,8,9	0.88	0	6,11,13	1.71	2 (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
1	OCS	B	300	1	-	3/4/7/9	-
1	OCS	A	300	1	-	3/4/7/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	300	OCS	OD2-SG-CB	3.16	110.78	105.74
1	B	300	OCS	OD2-SG-CB	2.73	110.09	105.74
1	A	300	OCS	OD3-SG-CB	2.18	109.52	106.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	300	OCS	CA-CB-SG-OD1
1	A	300	OCS	CA-CB-SG-OD2
1	B	300	OCS	CA-CB-SG-OD1
1	B	300	OCS	CA-CB-SG-OD2
1	A	300	OCS	CA-CB-SG-OD3
1	B	300	OCS	CA-CB-SG-OD3

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

17 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	C	1	1,2	14,14,15	0.40	0	17,19,21	0.57	0
2	NAG	C	2	2	14,14,15	0.54	0	17,19,21	0.41	0
2	MAN	C	3	2	11,11,12	0.98	0	15,15,17	1.33	3 (20%)
2	MAN	C	4	2	11,11,12	0.94	0	15,15,17	1.04	2 (13%)
2	MAN	C	5	2	11,11,12	0.91	0	15,15,17	1.00	0
2	MAN	C	6	2	11,11,12	1.22	1 (9%)	15,15,17	1.18	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	D	1[A]	1,3	14,14,15	0.42	0	17,19,21	0.67	1 (5%)
3	NAG	D	1[B]	1	14,14,15	1.54	1 (7%)	17,19,21	1.45	2 (11%)
3	NAG	D	2	3	14,14,15	0.41	0	17,19,21	0.42	0
2	NAG	E	1	1,2	14,14,15	0.34	0	17,19,21	0.51	0
2	NAG	E	2	2	14,14,15	0.65	1 (7%)	17,19,21	0.43	0
2	MAN	E	3	2	11,11,12	1.29	0	15,15,17	1.34	2 (13%)
2	MAN	E	4	2	11,11,12	0.82	0	15,15,17	1.12	2 (13%)
2	MAN	E	5	2	11,11,12	1.26	2 (18%)	15,15,17	1.23	3 (20%)
2	MAN	E	6	2	11,11,12	0.94	1 (9%)	15,15,17	1.04	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.62	0	17,19,21	1.03	2 (11%)
3	NAG	F	2	3	14,14,15	0.46	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	1/1/1/1
3	NAG	D	1[A]	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1[B]	1	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
2	MAN	E	5	2	-	1/2/19/22	0/1/1/1
2	MAN	E	6	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1[B]	NAG	O5-C1	-5.44	1.35	1.43
2	C	6	MAN	C1-C2	2.71	1.58	1.52
2	E	5	MAN	C4-C3	2.32	1.58	1.52
2	E	6	MAN	C1-C2	2.17	1.57	1.52
2	E	2	NAG	O5-C1	-2.02	1.40	1.43
2	E	5	MAN	C4-C5	2.01	1.57	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1[B]	NAG	C3-C4-C5	4.57	118.39	110.24
2	C	6	MAN	C1-O5-C5	3.01	116.27	112.19
2	E	4	MAN	C1-O5-C5	3.00	116.26	112.19
3	D	1[B]	NAG	C4-C3-C2	2.91	115.29	111.02
3	F	1	NAG	C1-O5-C5	2.79	115.97	112.19
2	E	6	MAN	C1-O5-C5	2.78	115.95	112.19
2	E	3	MAN	C1-C2-C3	2.76	113.06	109.67
2	E	3	MAN	C1-O5-C5	2.65	115.78	112.19
2	C	3	MAN	C1-C2-C3	2.56	112.82	109.67
2	E	5	MAN	C1-O5-C5	2.41	115.45	112.19
2	E	5	MAN	C1-C2-C3	-2.33	106.80	109.67
2	C	3	MAN	O2-C2-C3	-2.24	105.65	110.14
2	E	4	MAN	O2-C2-C3	-2.16	105.80	110.14
3	D	1[A]	NAG	C1-O5-C5	2.14	115.09	112.19
3	F	1	NAG	C1-C2-N2	2.09	114.06	110.49
2	C	6	MAN	O2-C2-C3	-2.08	105.98	110.14
2	E	5	MAN	O2-C2-C1	2.05	113.34	109.15
2	C	4	MAN	C1-O5-C5	2.05	114.96	112.19
2	C	3	MAN	C1-O5-C5	2.03	114.94	112.19
2	C	4	MAN	O2-C2-C3	-2.03	106.07	110.14

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	MAN	C4-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6
2	E	6	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	6	MAN	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
2	E	3	MAN	C4-C5-C6-O6
2	E	6	MAN	C4-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	E	3	MAN	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
3	D	1[B]	NAG	C4-C5-C6-O6
3	D	1[B]	NAG	O5-C5-C6-O6
3	D	1[B]	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7

All (1) ring outliers are listed below:

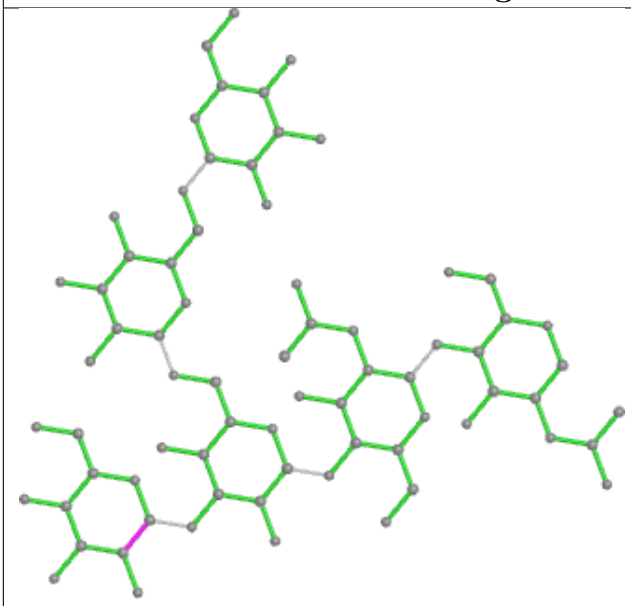
Mol	Chain	Res	Type	Atoms
2	C	6	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

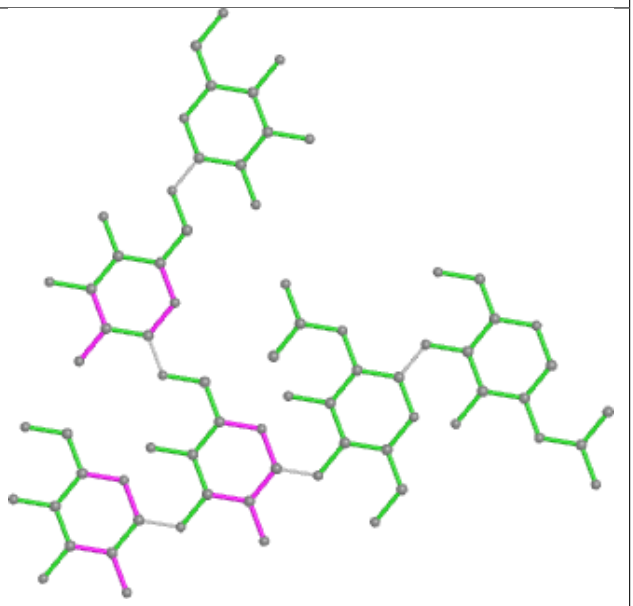
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
3	D	1[B]	NAG	1	0
3	D	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

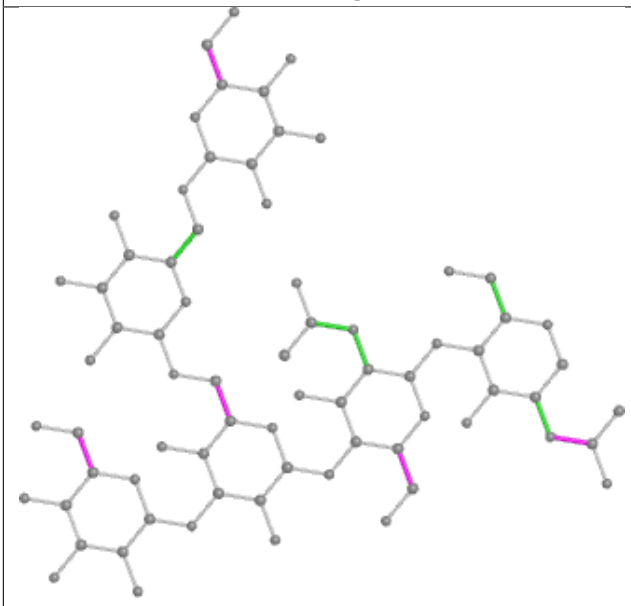
Oligosaccharide Chain C



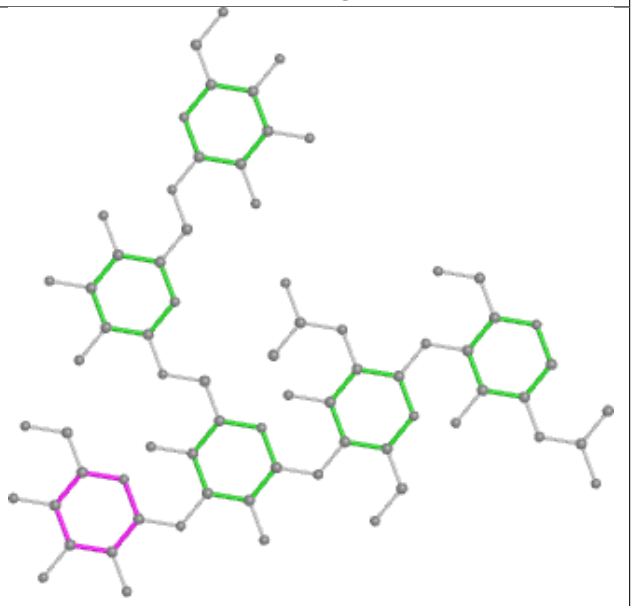
Bond lengths



Bond angles

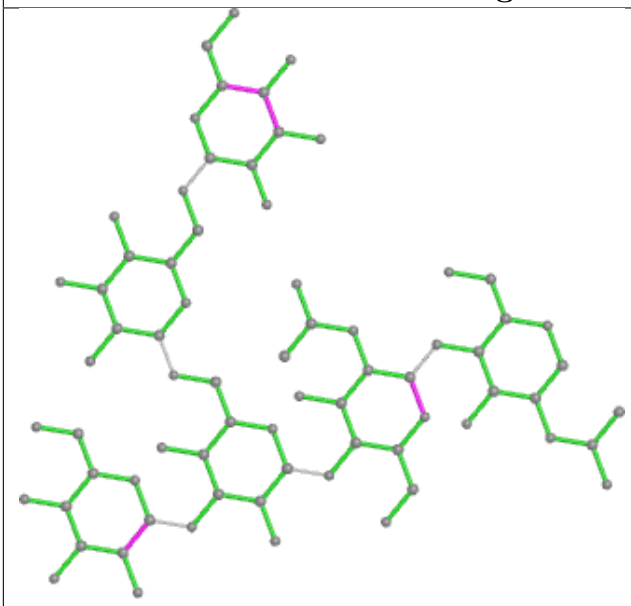


Torsions

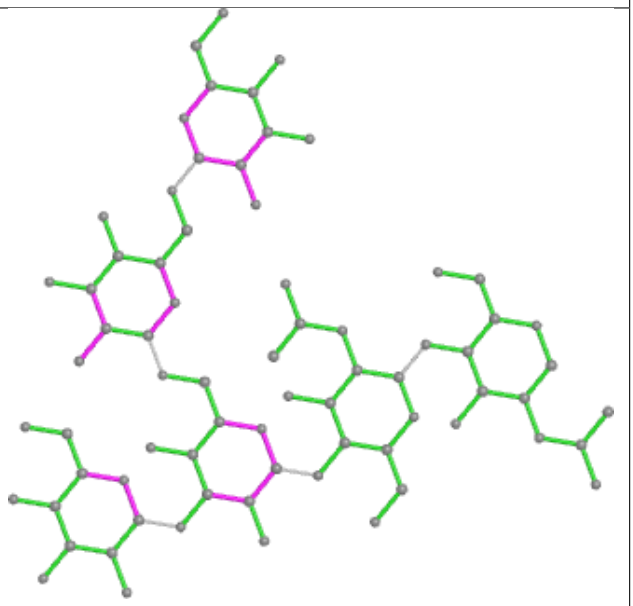


Rings

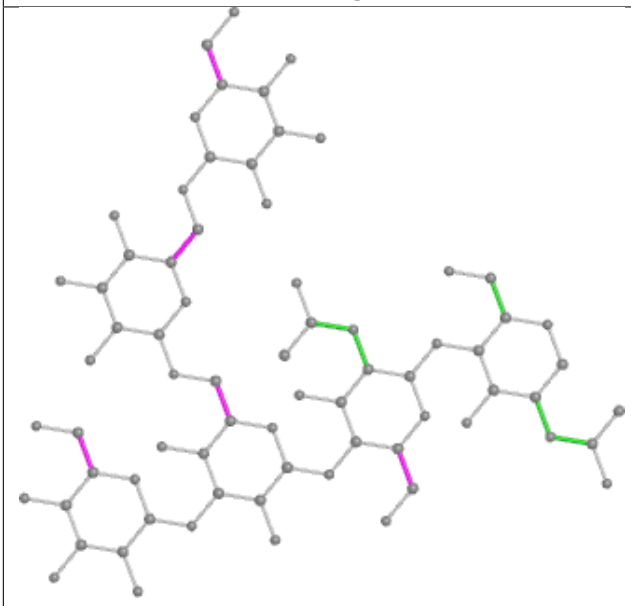
Oligosaccharide Chain E



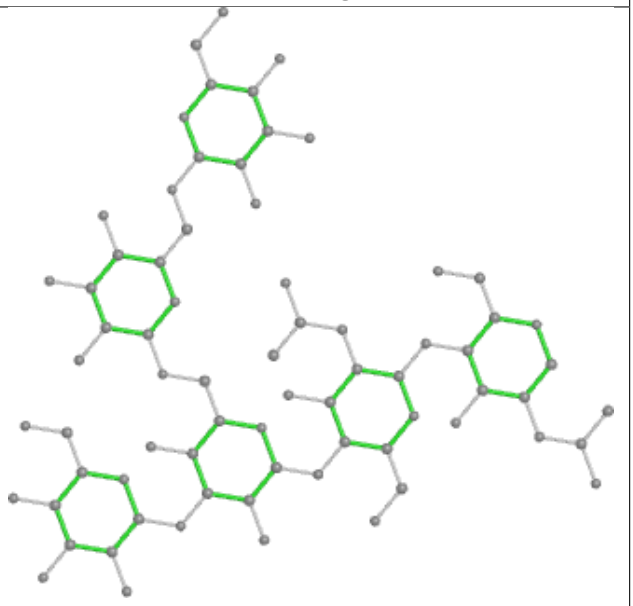
Bond lengths



Bond angles

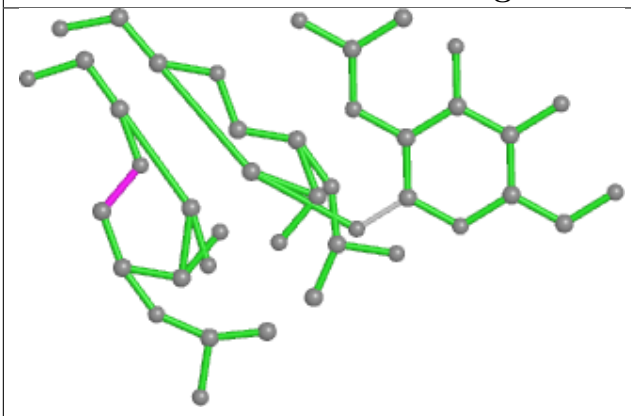


Torsions

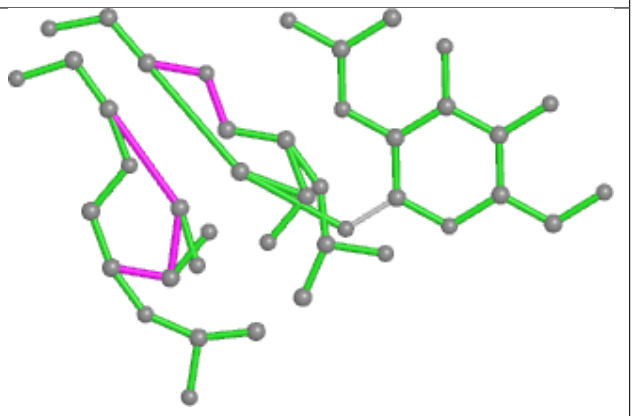


Rings

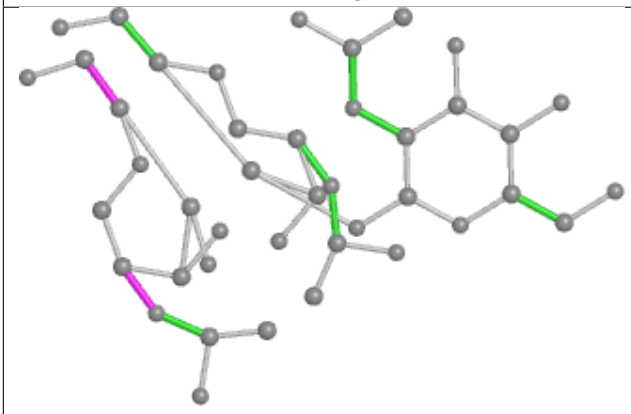
Oligosaccharide Chain D



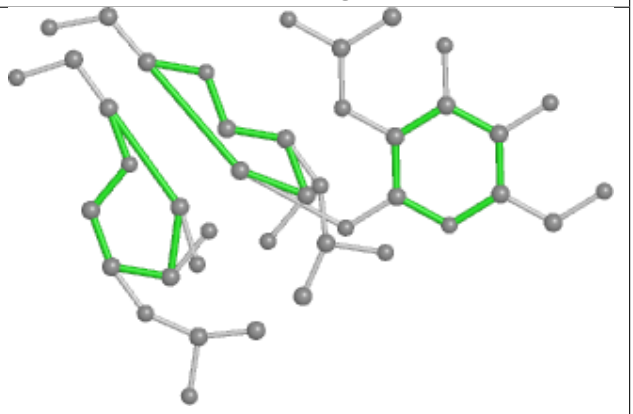
Bond lengths



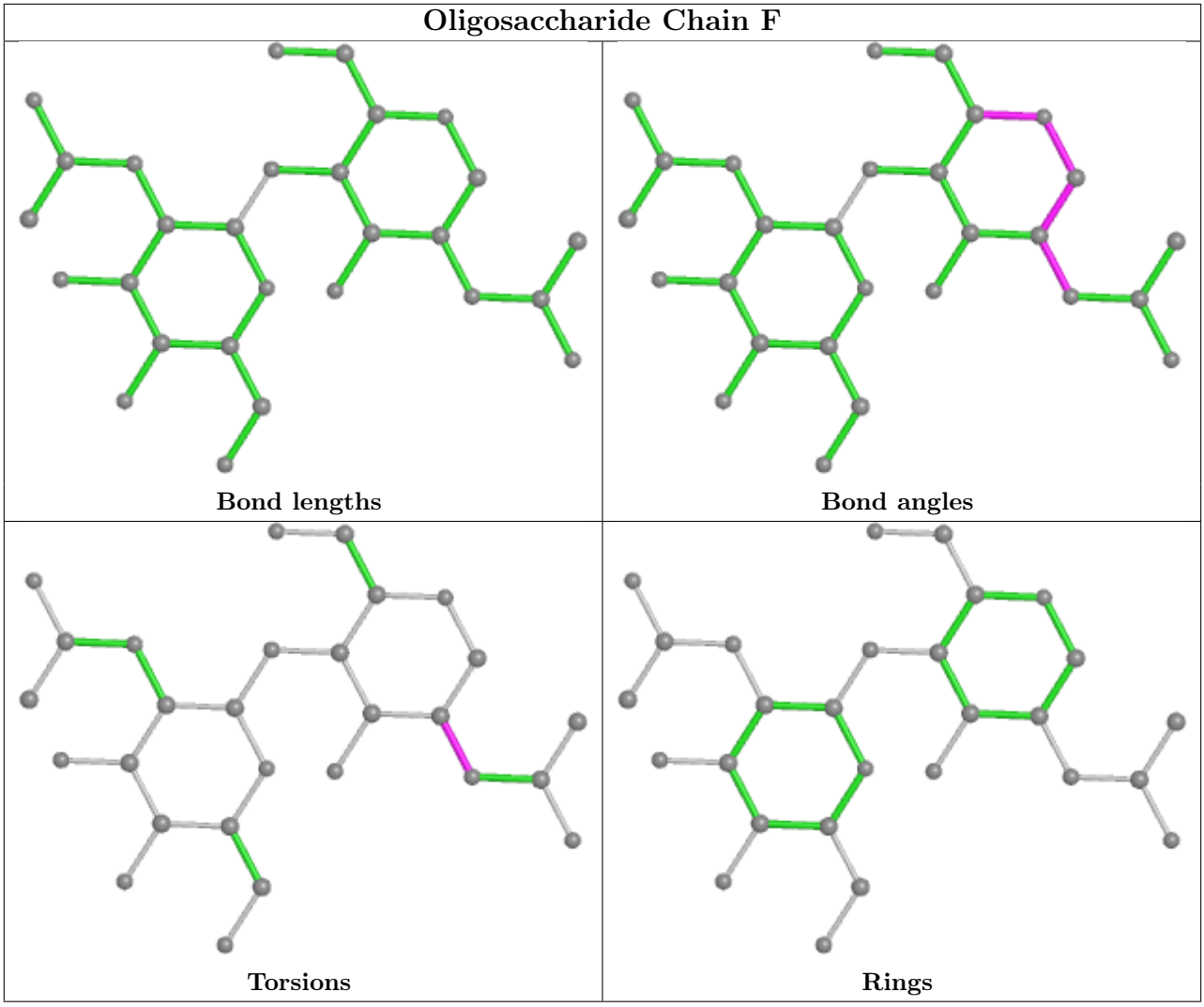
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
8	SO4	B	513	-	4,4,4	0.15	0	6,6,6	0.13	0
8	SO4	B	512	-	4,4,4	0.15	0	6,6,6	0.17	0
4	PST	B	502	4	18,18,22	5.08	13 (72%)	26,26,33	2.42	9 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	B	506	-	3,3,3	0.63	0	2,2,2	0.13	0
6	EDO	B	509	-	3,3,3	0.44	0	2,2,2	0.42	0
6	EDO	B	510	-	3,3,3	0.43	0	2,2,2	0.53	0
8	SO4	A	514	-	4,4,4	0.13	0	6,6,6	0.26	0
6	EDO	A	506	-	3,3,3	0.50	0	2,2,2	0.31	0
6	EDO	A	509	-	3,3,3	0.44	0	2,2,2	0.25	0
6	EDO	A	508	-	3,3,3	0.57	0	2,2,2	0.21	0
4	PST	B	503	4	0,3,22	-	-	0,3,33	-	-
6	EDO	A	505	-	3,3,3	0.52	0	2,2,2	0.18	0
5	PO4	A	503	-	4,4,4	0.96	0	6,6,6	0.46	0
4	PST	A	502	4	0,3,22	-	-	0,3,33	-	-
6	EDO	B	505	-	3,3,3	0.41	0	2,2,2	0.49	0
6	EDO	A	510	-	3,3,3	0.51	0	2,2,2	0.33	0
6	EDO	A	511	-	3,3,3	0.48	0	2,2,2	0.32	0
6	EDO	B	508	-	3,3,3	0.43	0	2,2,2	0.36	0
5	PO4	B	504	-	4,4,4	0.97	0	6,6,6	0.62	0
8	SO4	A	515	-	4,4,4	0.13	0	6,6,6	0.18	0
4	PST	A	501	4	18,18,22	5.04	14 (77%)	26,26,33	2.33	9 (34%)
6	EDO	A	507	-	3,3,3	0.64	0	2,2,2	0.24	0
6	EDO	A	512	-	3,3,3	0.48	0	2,2,2	0.23	0
6	EDO	B	507	-	3,3,3	0.50	0	2,2,2	0.34	0
5	PO4	A	504	-	4,4,4	0.80	0	6,6,6	0.58	0
6	EDO	B	501	-	3,3,3	0.58	0	2,2,2	0.43	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
4	PST	B	502	4	-	2/6/18/22	0/2/2/2
4	PST	A	501	4	-	4/6/18/22	0/2/2/2
6	EDO	A	507	-	-	1/1/1/1	-
6	EDO	B	506	-	-	0/1/1/1	-
6	EDO	A	512	-	-	0/1/1/1	-
6	EDO	B	507	-	-	0/1/1/1	-
6	EDO	B	509	-	-	1/1/1/1	-
6	EDO	B	508	-	-	0/1/1/1	-
6	EDO	A	510	-	-	1/1/1/1	-
6	EDO	B	510	-	-	1/1/1/1	-
6	EDO	A	508	-	-	1/1/1/1	-
6	EDO	B	501	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	506	-	-	1/1/1/1	-
6	EDO	A	509	-	-	0/1/1/1	-
6	EDO	A	511	-	-	0/1/1/1	-
6	EDO	A	505	-	-	0/1/1/1	-
6	EDO	B	505	-	-	1/1/1/1	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	PST	C2'-C3'	-11.10	1.23	1.52
4	A	501	PST	C2'-C3'	-10.58	1.24	1.52
4	A	501	PST	C6-C5	8.82	1.49	1.34
4	B	502	PST	C6-C5	8.66	1.48	1.34
4	B	502	PST	C2-N1	7.94	1.51	1.38
4	A	501	PST	C2-N1	7.30	1.50	1.38
4	B	502	PST	C2-N3	6.94	1.50	1.38
4	A	501	PST	C2-N3	6.78	1.50	1.38
4	A	501	PST	O3'-C3'	6.73	1.57	1.43
4	B	502	PST	O3'-C3'	6.33	1.56	1.43
4	A	501	PST	C6-N1	4.86	1.46	1.38
4	B	502	PST	C2'-C1'	4.66	1.65	1.52
4	A	501	PST	C2'-C1'	4.46	1.64	1.52
4	B	502	PST	C4-N3	4.45	1.47	1.38
4	A	501	PST	C4-N3	4.42	1.47	1.38
4	B	502	PST	C6-N1	4.37	1.45	1.38
4	A	501	PST	O4'-C1'	-4.23	1.32	1.42
4	B	502	PST	O4'-C1'	-4.10	1.33	1.42
4	A	501	PST	C3'-C4'	3.84	1.63	1.53
4	B	502	PST	C3'-C4'	3.37	1.62	1.53
4	A	501	PST	C4-C5	2.92	1.49	1.44
4	B	502	PST	C4-C5	2.81	1.49	1.44
4	B	502	PST	C5'-C4'	-2.69	1.42	1.51
4	A	501	PST	O2-C2	-2.36	1.18	1.23
4	B	502	PST	O4-C4	-2.32	1.19	1.23
4	A	501	PST	C5'-C4'	-2.31	1.44	1.51
4	A	501	PST	O4-C4	-2.27	1.19	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	PST	C4-N3-C2	-5.22	120.59	127.35
4	B	502	PST	C5-C4-N3	5.14	119.70	115.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	PST	C5-C4-N3	4.84	119.45	115.31
4	B	502	PST	C4-N3-C2	-4.77	121.18	127.35
4	B	502	PST	O4-C4-C5	-4.56	119.61	124.90
4	A	501	PST	O4-C4-C5	-4.37	119.84	124.90
4	A	501	PST	N3-C2-N1	3.90	120.07	114.89
4	B	502	PST	C1'-N1-C2	3.86	125.24	117.64
4	B	502	PST	O4'-C1'-N1	3.41	113.96	107.86
4	B	502	PST	C1'-N1-C6	-3.26	115.14	120.77
4	A	501	PST	C1'-N1-C2	2.86	123.27	117.64
4	A	501	PST	O4'-C1'-N1	2.86	112.97	107.86
4	B	502	PST	C4'-O4'-C1'	-2.82	102.64	109.45
4	A	501	PST	C6-N1-C2	-2.77	118.49	121.30
4	B	502	PST	N3-C2-N1	2.68	118.45	114.89
4	A	501	PST	C2'-C1'-N1	2.53	119.59	113.77
4	B	502	PST	C5M-C5-C6	-2.18	119.94	122.85
4	A	501	PST	C4'-O4'-C1'	-2.06	104.47	109.45

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	PST	O4'-C4'-C5'-O5'
6	B	501	EDO	O1-C1-C2-O2
4	A	501	PST	C3'-C4'-C5'-O5'
4	A	501	PST	O4'-C1'-N1-C6
4	A	501	PST	O4'-C1'-N1-C2
4	B	502	PST	O4'-C1'-N1-C6
4	B	502	PST	O4'-C1'-N1-C2
6	A	508	EDO	O1-C1-C2-O2
6	B	505	EDO	O1-C1-C2-O2
6	A	507	EDO	O1-C1-C2-O2
6	B	509	EDO	O1-C1-C2-O2
6	B	510	EDO	O1-C1-C2-O2
6	A	506	EDO	O1-C1-C2-O2
6	A	510	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	PST	5	0

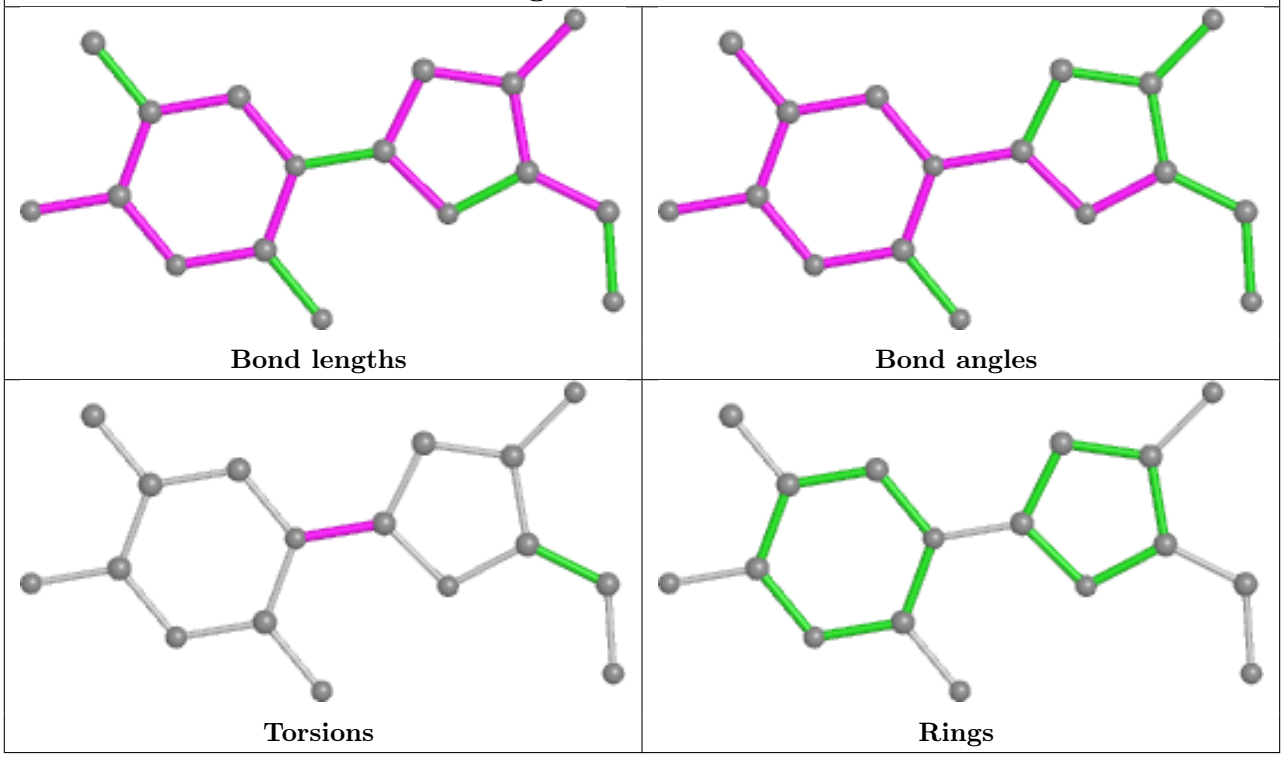
Continued on next page...

Continued from previous page...

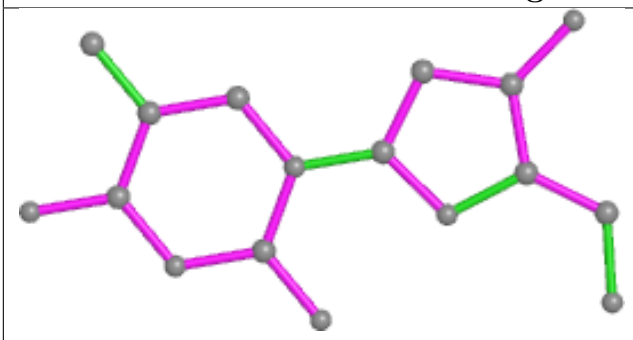
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	509	EDO	2	0
6	B	510	EDO	1	0
8	A	514	SO4	1	0
6	A	509	EDO	2	0
4	B	503	PST	4	0
4	A	502	PST	3	0
6	A	511	EDO	1	0

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 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.

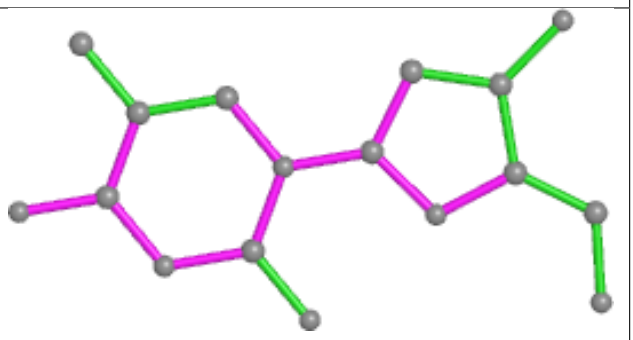
Ligand PST B 502



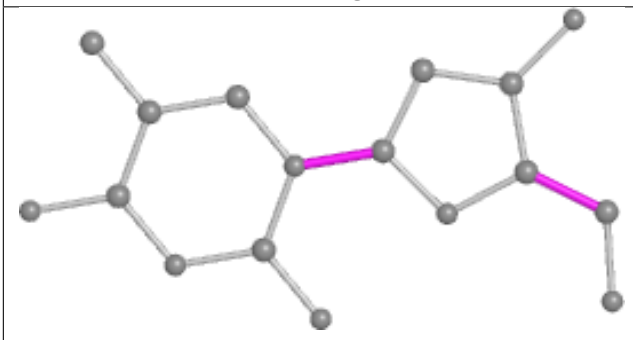
Ligand PST A 501



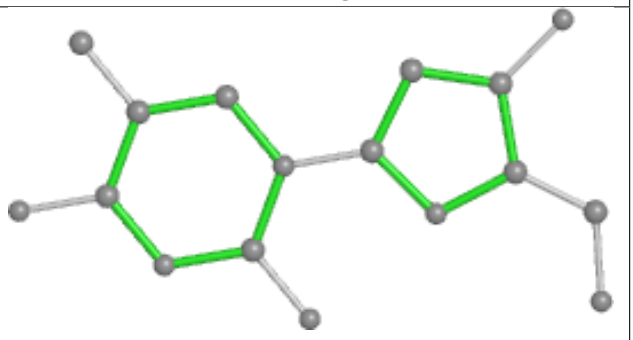
Bond lengths



Bond angles



Torsions



Rings

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	419/433 (96%)	-0.29	12 (2%)	51	50	21, 33, 70, 117	0
1	B	418/433 (96%)	-0.23	15 (3%)	42	40	22, 33, 63, 121	0
All	All	837/866 (96%)	-0.26	27 (3%)	47	45	21, 33, 69, 121	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	PHE	5.9
1	B	337	HIS	5.2
1	B	338	PRO	4.2
1	B	388	HIS	4.1
1	A	335	PHE	4.1
1	B	97	ASN	4.0
1	A	338	PRO	3.9
1	A	337	HIS	3.8
1	A	171	PRO	3.6
1	B	98	ALA	3.6
1	A	336	SER	3.4
1	B	336	SER	3.4
1	B	96	PRO	3.4
1	A	492	ALA	3.4
1	A	388	HIS	3.2
1	B	453	ARG	3.1
1	B	171	PRO	3.1
1	B	339	HIS	2.9
1	A	389	THR	2.9
1	B	387	ASN	2.8
1	B	390	HIS	2.7
1	A	390	HIS	2.3
1	A	100	THR	2.2
1	A	339	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	389	THR	2.2
1	A	493	GLN	2.1
1	B	117	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	OCS	A	300	9/10	0.98	0.09	25,28,33,37	3
1	OCS	B	300	9/10	0.98	0.07	28,29,33,37	4

6.3 Carbohydrates (i)

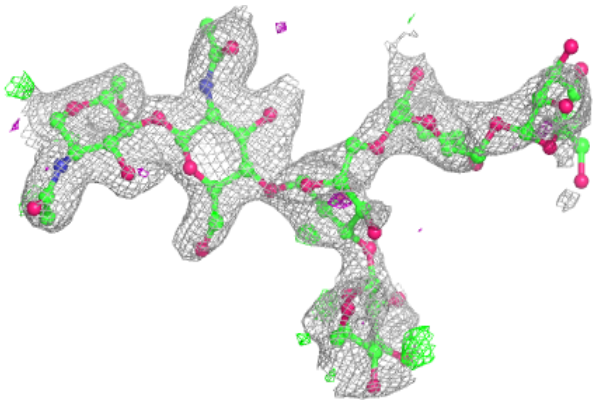
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

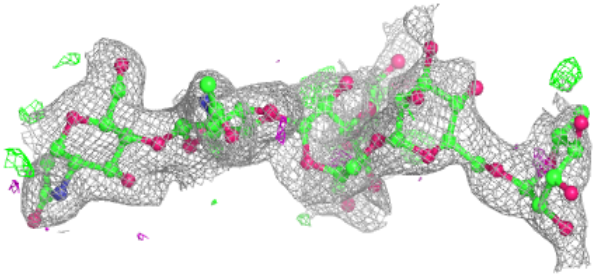
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	E	3	11/12	0.41	0.32	97,101,109,109	0
2	MAN	C	6	11/12	0.48	0.34	94,107,111,114	0
2	MAN	C	3	11/12	0.48	0.29	78,85,96,101	11
2	MAN	C	5	11/12	0.55	0.35	86,94,99,102	11
2	MAN	E	5	11/12	0.60	0.24	96,106,112,113	0
2	MAN	E	6	11/12	0.69	0.42	102,109,111,112	0
2	MAN	E	4	11/12	0.73	0.32	96,102,107,110	0
2	MAN	C	4	11/12	0.81	0.24	78,84,90,92	0
3	NAG	D	2	14/15	0.81	0.39	67,80,102,109	0
3	NAG	F	1	14/15	0.85	0.17	51,59,68,81	0
3	NAG	F	2	14/15	0.85	0.35	82,95,103,109	0
2	NAG	E	2	14/15	0.87	0.21	44,59,80,88	0
2	NAG	E	1	14/15	0.90	0.18	39,45,50,58	0
3	NAG	D	1[A]	14/15	0.90	0.15	39,48,54,60	14
3	NAG	D	1[B]	14/15	0.90	0.15	42,48,55,57	14
2	NAG	C	2	14/15	0.92	0.17	38,58,76,84	0
2	NAG	C	1	14/15	0.94	0.15	45,51,60,66	0

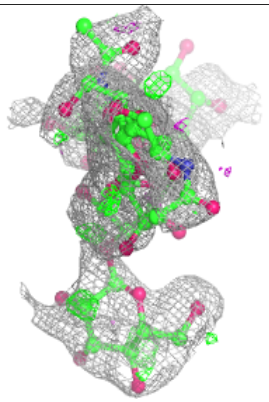
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

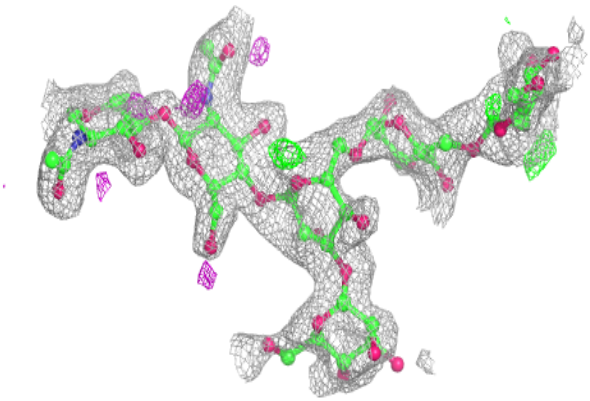


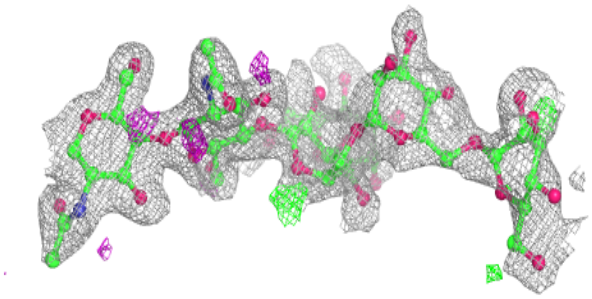


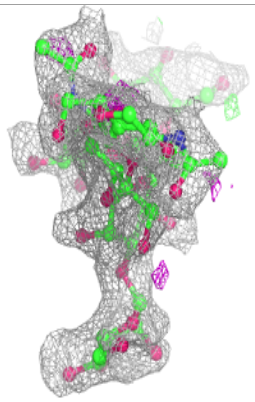


Electron density around Chain E:

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

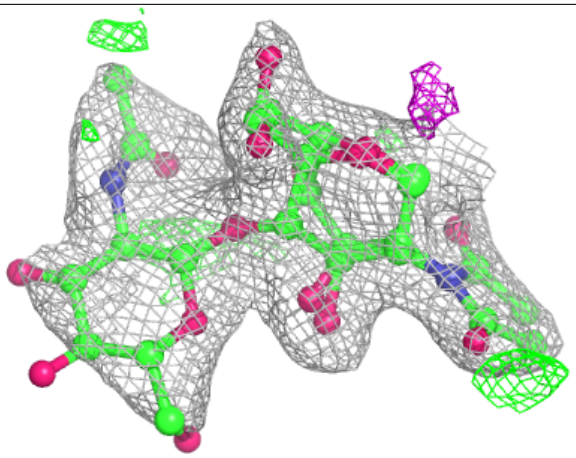


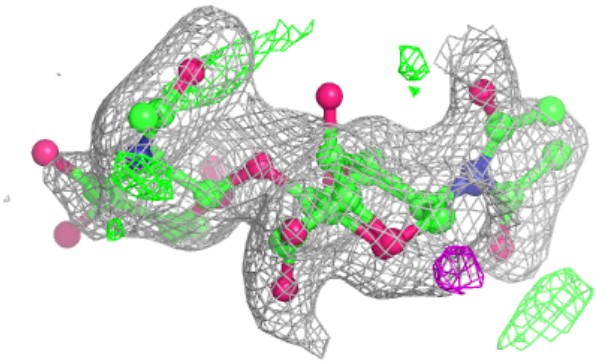


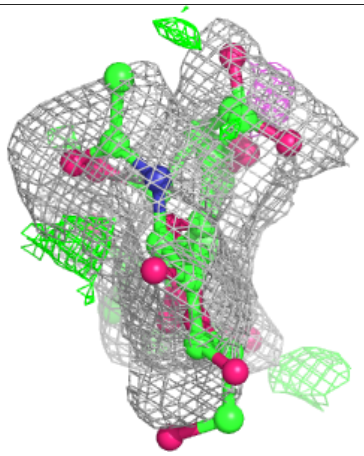


Electron density around Chain D:

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

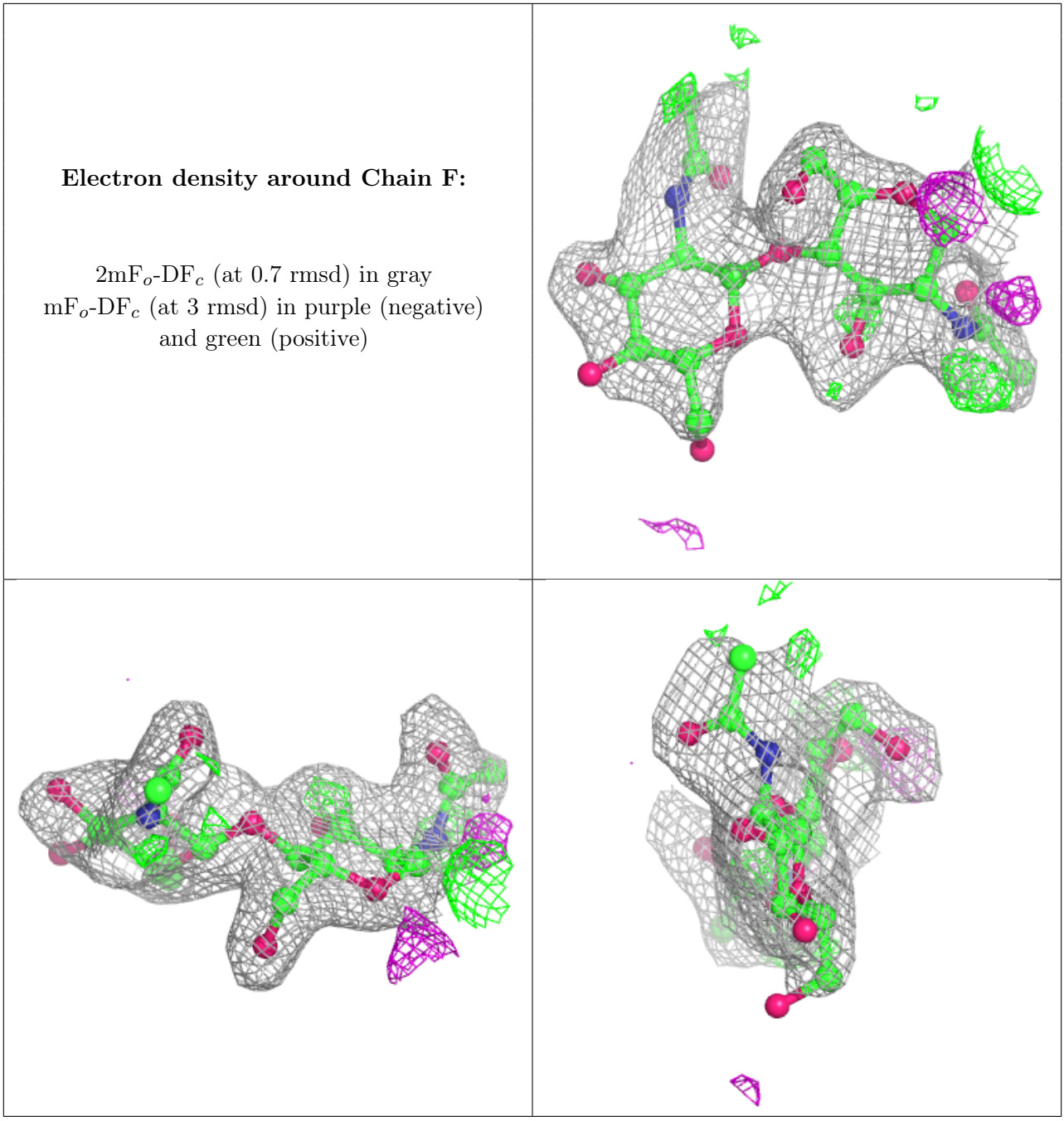






Electron density around Chain F:

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



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
6	EDO	A	505	4/4	0.38	0.26	74,80,84,86	0

Continued on next page...

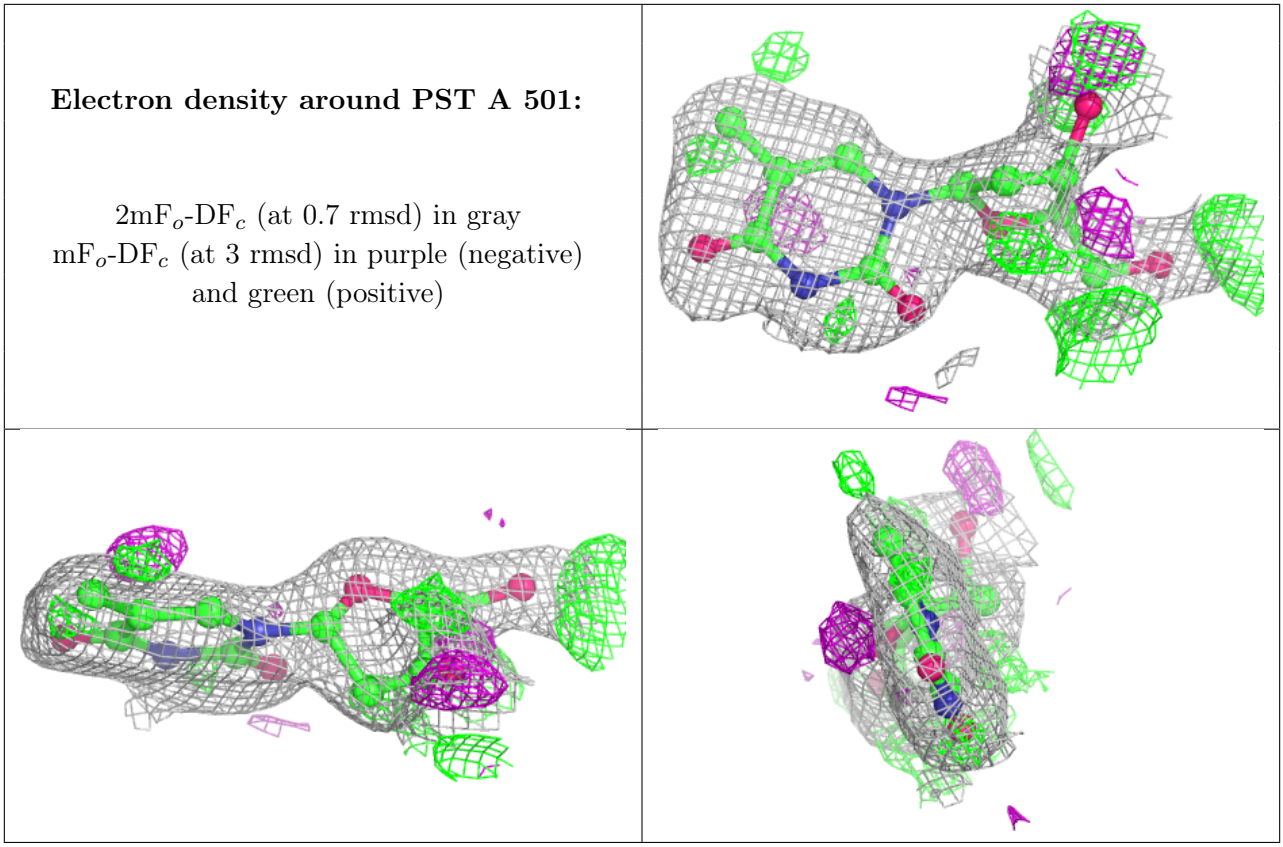
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	B	506	4/4	0.61	0.20	52,55,60,65	0
4	PST	A	501	17/21	0.78	0.14	49,54,65,69	0
4	PST	B	502	17/21	0.78	0.28	51,59,70,74	0
6	EDO	A	506	4/4	0.84	0.23	60,66,68,72	0
6	EDO	A	510	4/4	0.85	0.11	46,50,56,57	0
6	EDO	B	507	4/4	0.85	0.25	58,62,64,66	0
6	EDO	B	509	4/4	0.85	0.10	44,56,57,60	0
6	EDO	A	512	4/4	0.87	0.14	72,77,78,78	0
8	SO4	A	515	5/5	0.87	0.17	97,101,102,108	0
6	EDO	B	510	4/4	0.88	0.17	73,76,77,78	0
6	EDO	A	508	4/4	0.89	0.15	41,56,61,65	0
4	PST	A	502	4/21	0.89	0.13	42,45,52,53	0
6	EDO	A	511	4/4	0.89	0.12	52,61,63,71	0
6	EDO	A	509	4/4	0.90	0.13	46,56,56,63	0
5	PO4	B	504	5/5	0.91	0.23	69,74,79,95	0
8	SO4	A	514	5/5	0.92	0.16	76,77,90,103	0
4	PST	B	503	4/21	0.92	0.15	45,48,55,56	0
6	EDO	B	505	4/4	0.93	0.20	45,55,57,63	0
6	EDO	B	508	4/4	0.93	0.08	47,57,58,65	0
6	EDO	A	507	4/4	0.93	0.08	34,38,44,46	0
8	SO4	B	513	5/5	0.93	0.11	81,82,91,98	0
8	SO4	B	512	5/5	0.94	0.16	67,84,86,90	0
5	PO4	A	503	5/5	0.96	0.20	67,69,81,85	0
5	PO4	A	504	5/5	0.97	0.14	57,67,77,77	0
6	EDO	B	501	4/4	0.97	0.07	29,34,40,44	0
7	MN	A	513	1/1	0.99	0.08	34,34,34,34	0
7	MN	B	511	1/1	0.99	0.10	31,31,31,31	0
9	MG	A	516	1/1	1.00	0.20	20,20,20,20	0
9	MG	B	514	1/1	1.00	0.20	15,15,15,15	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.

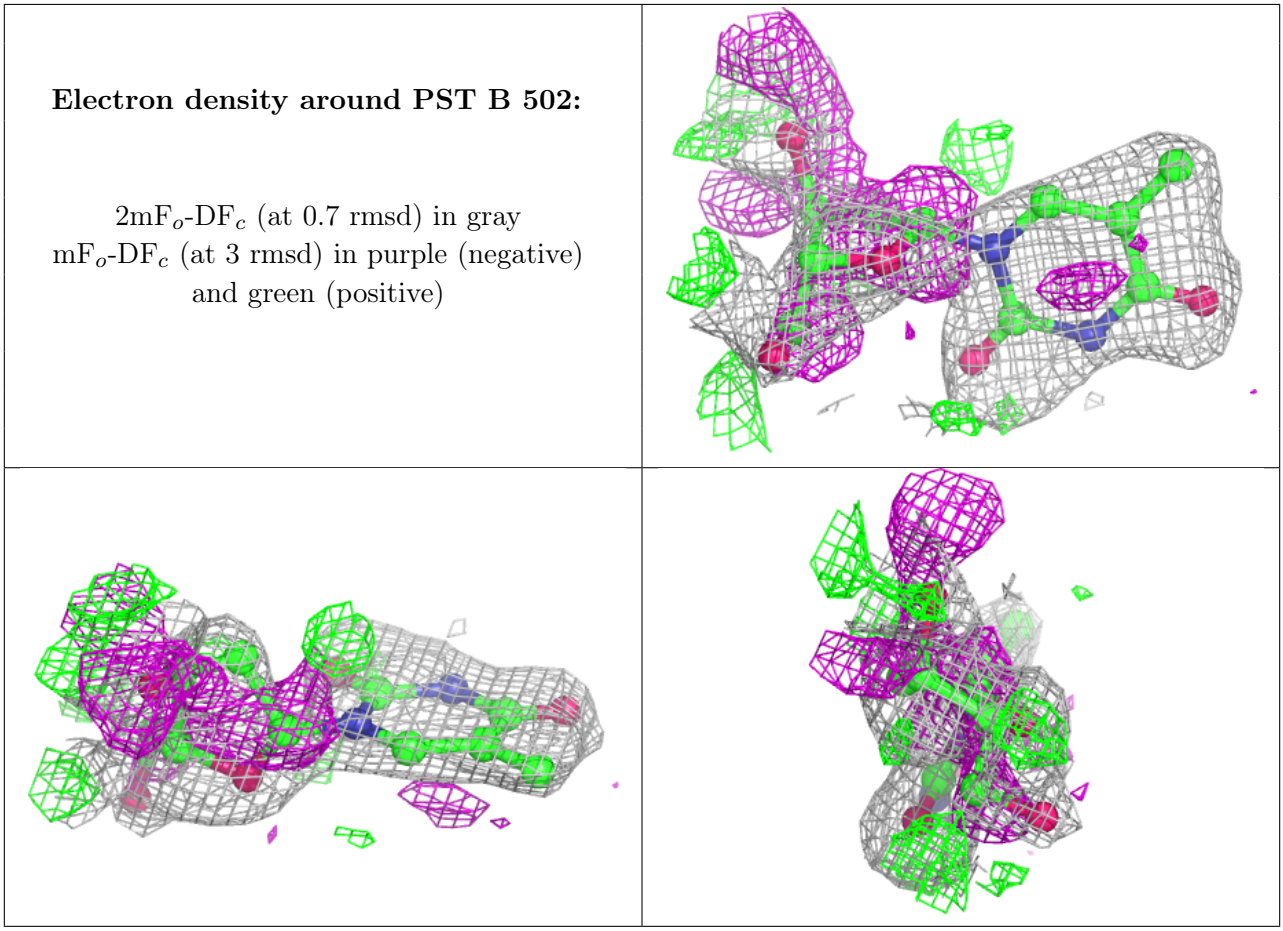
Electron density around PST A 501:

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



Electron density around PST B 502:

$2mF_o$-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.