Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 01:01 PM EDT

PDB ID	:	4NDZ
Title	:	Structure of Maltose Binding Protein fusion to 2-O-Sulfotransferase with bound heptasaccharide and PAP
Authors	:	Liu, C.; Sheng, J.; Krahn, J.M.; Perera, L.; Xu, Y.; Hsieh, P.; Liu, J.; Pedersen, L.C.
Deposited on	:	2013-10-28
Resolution	:	3.45 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 (i) 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 (i)) were used in the production of this report:

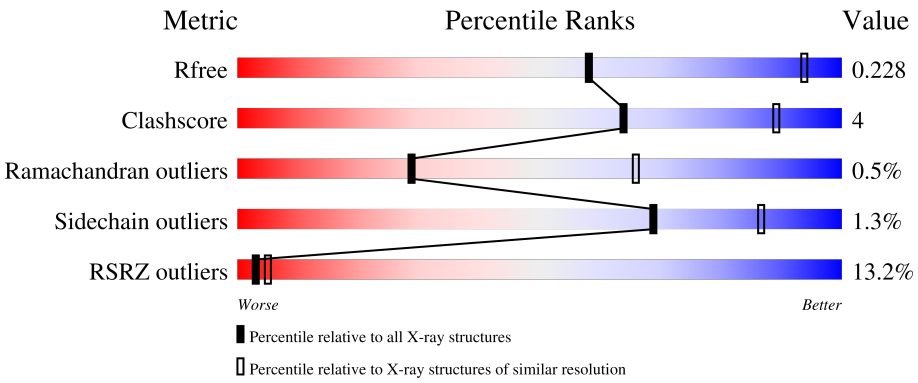
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	658	38% 6% 56%
1	B	658	27% 86% 14% •
1	C	658	10% 87% 12%
1	D	658	6% 86% 12% ••

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Mol	Chain	Length	Quality of chain
1	E	658	5% 87% 13%
1	F	658	23% 86% 13%
2	G	7	100%
2	I	7	86% 14%
2	L	7	14% 86%
2	N	7	71% 29%
2	P	7	71% 29%
3	H	2	100%
3	J	2	100%
3	K	2	50% 50%
3	M	2	50% 50%
3	O	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	BDP	N	5	-	-	-	X
2	BDP	N	7	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 28764 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 Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2352	1522	399	422	9	0	0	1
1	B	654	5136	3314	852	955	15	0	0	1
1	C	655	5128	3311	848	955	14	0	0	1
1	D	654	5136	3313	853	955	15	0	0	1
1	E	654	5110	3298	842	955	15	0	0	1
1	F	654	5124	3307	846	956	15	0	1	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ALA	GLU	engineered mutation	UNP P0AEX9
A	362	ALA	LYS	engineered mutation	UNP P0AEX9
A	363	ALA	ASP	engineered mutation	UNP P0AEX9
A	367	ASN	ARG	engineered mutation	UNP P0AEX9
A	368	ALA	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
B	359	ALA	GLU	engineered mutation	UNP P0AEX9
B	362	ALA	LYS	engineered mutation	UNP P0AEX9
B	363	ALA	ASP	engineered mutation	UNP P0AEX9
B	367	ASN	ARG	engineered mutation	UNP P0AEX9
B	368	ALA	-	linker	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
C	359	ALA	GLU	engineered mutation	UNP P0AEX9
C	362	ALA	LYS	engineered mutation	UNP P0AEX9

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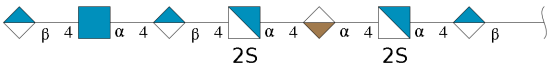
Chain	Residue	Modelled	Actual	Comment	Reference
C	363	ALA	ASP	engineered mutation	UNP P0AEX9
C	367	ASN	ARG	engineered mutation	UNP P0AEX9
C	368	ALA	-	linker	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9
D	359	ALA	GLU	engineered mutation	UNP P0AEX9
D	362	ALA	LYS	engineered mutation	UNP P0AEX9
D	363	ALA	ASP	engineered mutation	UNP P0AEX9
D	367	ASN	ARG	engineered mutation	UNP P0AEX9
D	368	ALA	-	linker	UNP P0AEX9
D	369	ALA	-	linker	UNP P0AEX9
D	370	ALA	-	linker	UNP P0AEX9
E	359	ALA	GLU	engineered mutation	UNP P0AEX9
E	362	ALA	LYS	engineered mutation	UNP P0AEX9
E	363	ALA	ASP	engineered mutation	UNP P0AEX9
E	367	ASN	ARG	engineered mutation	UNP P0AEX9
E	368	ALA	-	linker	UNP P0AEX9
E	369	ALA	-	linker	UNP P0AEX9
E	370	ALA	-	linker	UNP P0AEX9
F	359	ALA	GLU	engineered mutation	UNP P0AEX9
F	362	ALA	LYS	engineered mutation	UNP P0AEX9
F	363	ALA	ASP	engineered mutation	UNP P0AEX9
F	367	ASN	ARG	engineered mutation	UNP P0AEX9
F	368	ALA	-	linker	UNP P0AEX9
F	369	ALA	-	linker	UNP P0AEX9
F	370	ALA	-	linker	UNP P0AEX9

- Molecule 2 is an oligosaccharide called beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	7	92	44	3	43	2	0	0	0
			Total	C	N	O	S			
2	I	7	92	44	3	43	2	0	0	0

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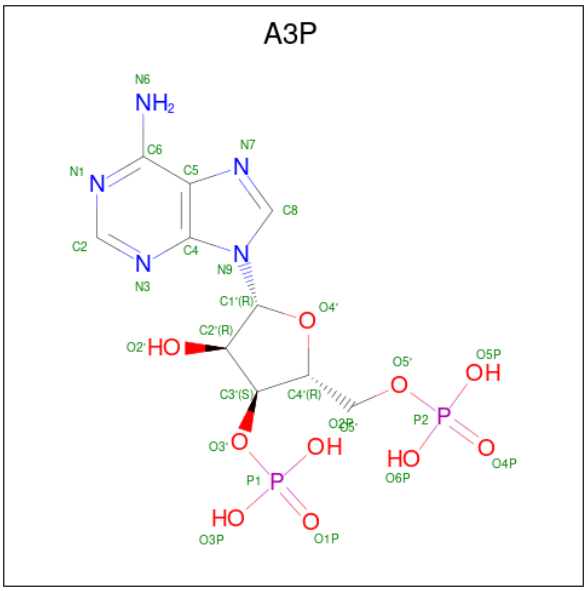
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	7	92	44	3	43	2	0	0	0
			Total	C	N	O	S			
2	N	7	92	44	3	43	2	0	0	0
			Total	C	N	O	S			
2	P	7	93	44	3	44	2	0	0	0

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

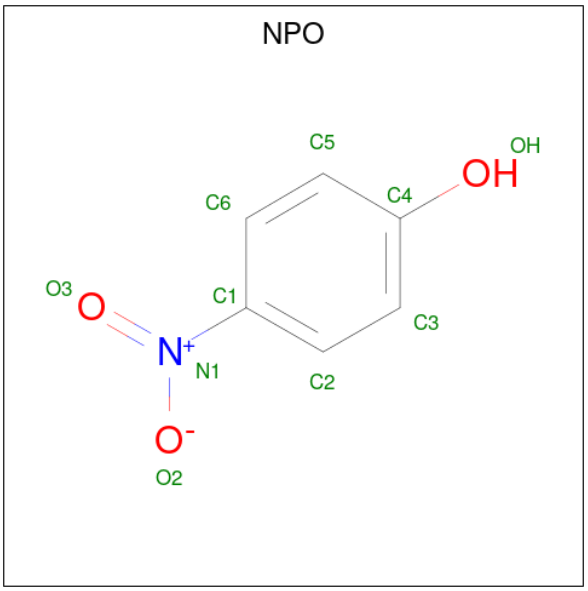
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	H	2	23	12	11	0	0	0
			Total	C	O			
3	J	2	23	12	11	0	0	0
			Total	C	O			
3	K	2	23	12	11	0	0	0
			Total	C	O			
3	M	2	23	12	11	0	0	0
			Total	C	O			
3	O	2	23	12	11	0	0	0

- Molecule 4 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is P-NITROPHENOL (three-letter code: NPO) (formula: $C_6H_5NO_3$).



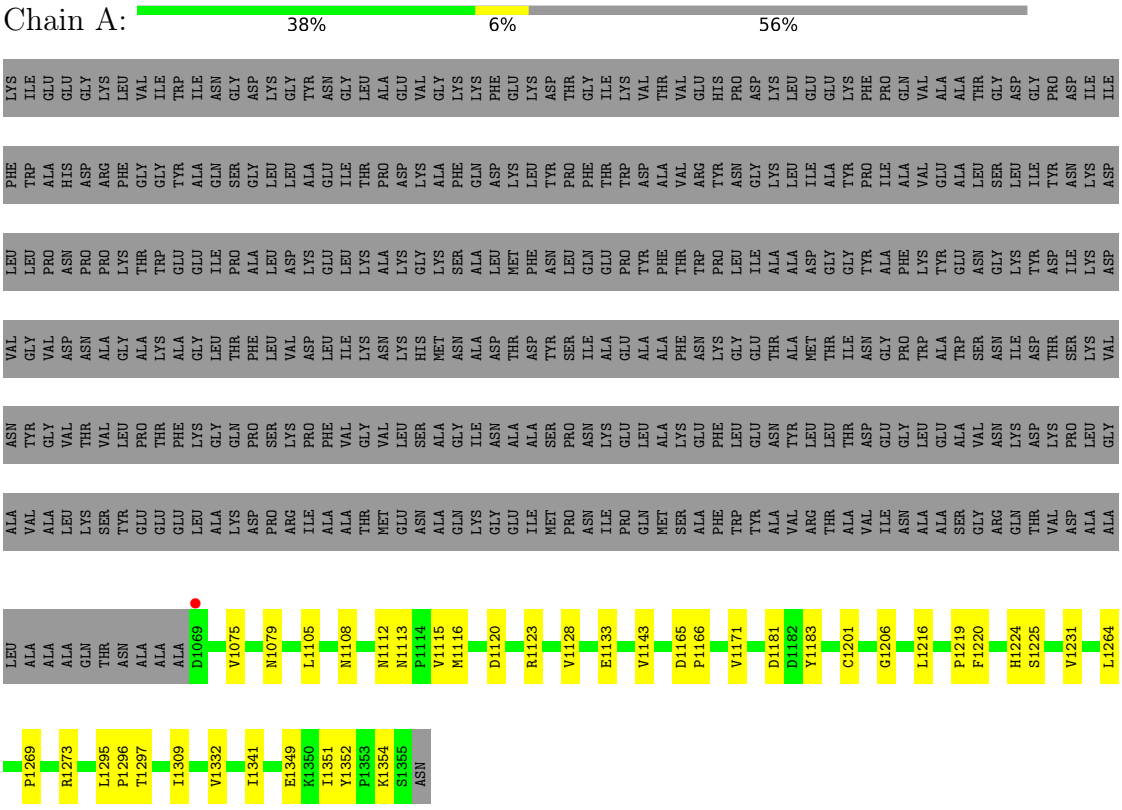
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	10	6	1	3	0	0
			Total	C	N	O		
5	B	1	10	6	1	3	0	0
			Total	C	N	O		
5	D	1	10	6	1	3	0	0
			Total	C	N	O		
5	E	1	10	6	1	3	0	0

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.

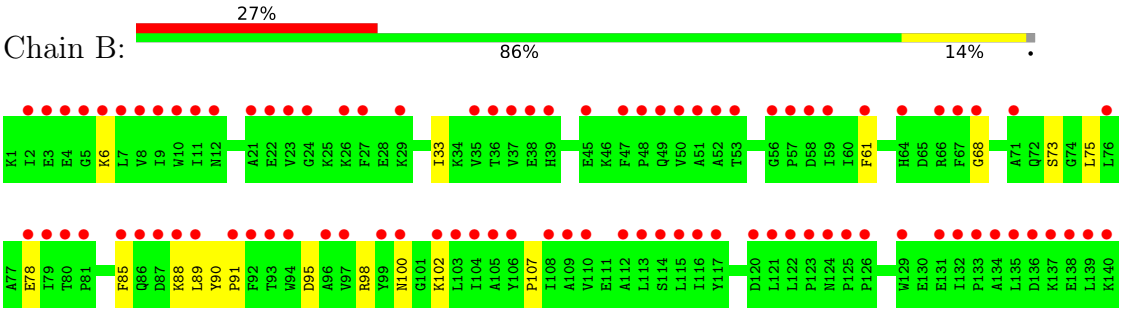
• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

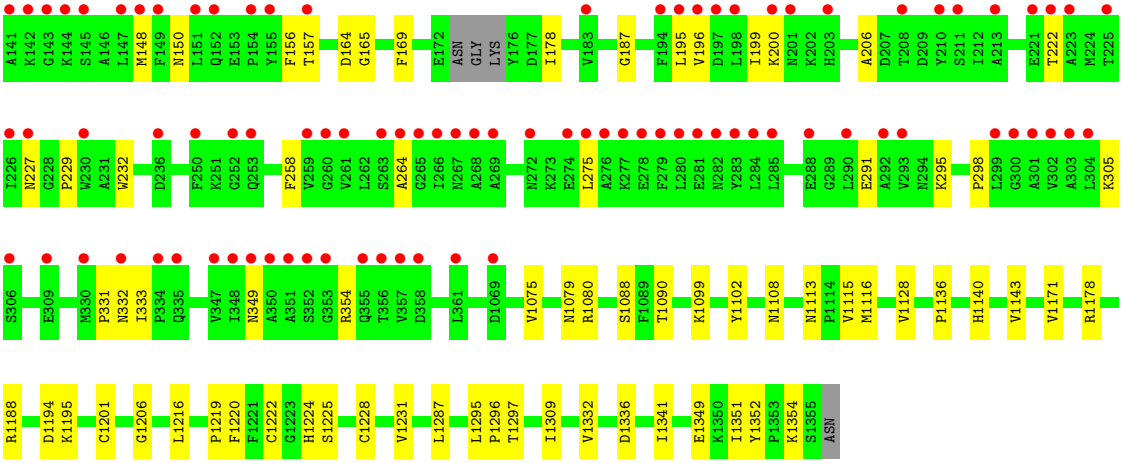
Chain A:



• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

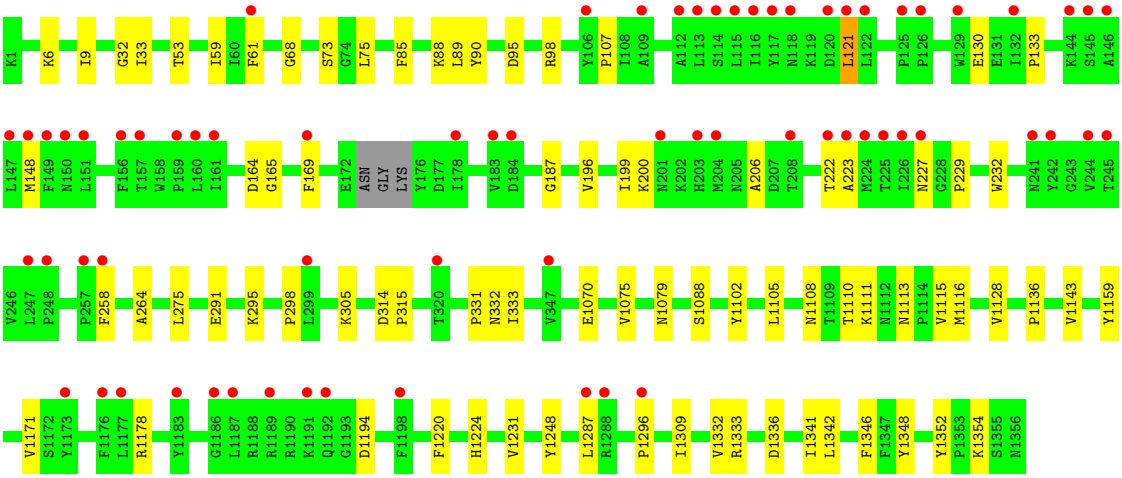
Chain B:





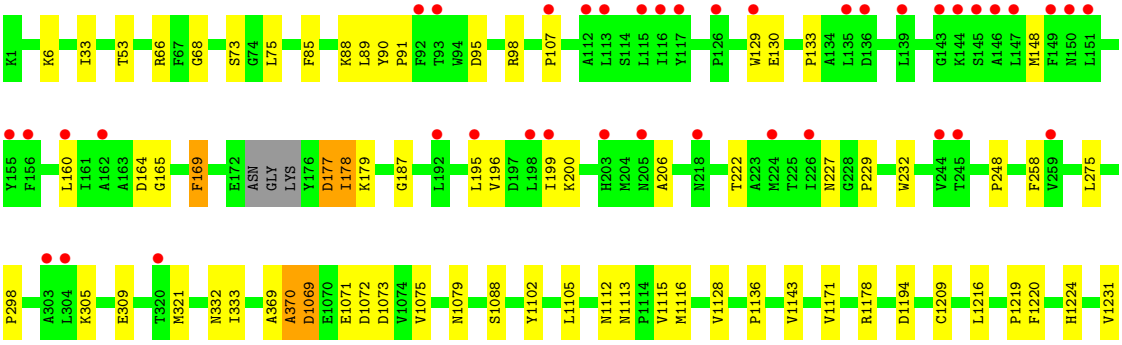
• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain C:



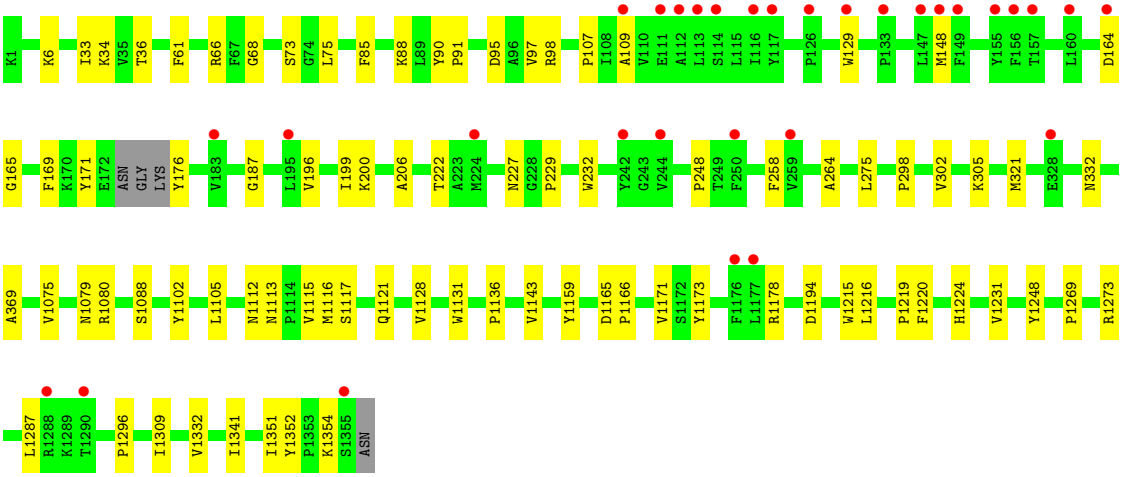
• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain D:



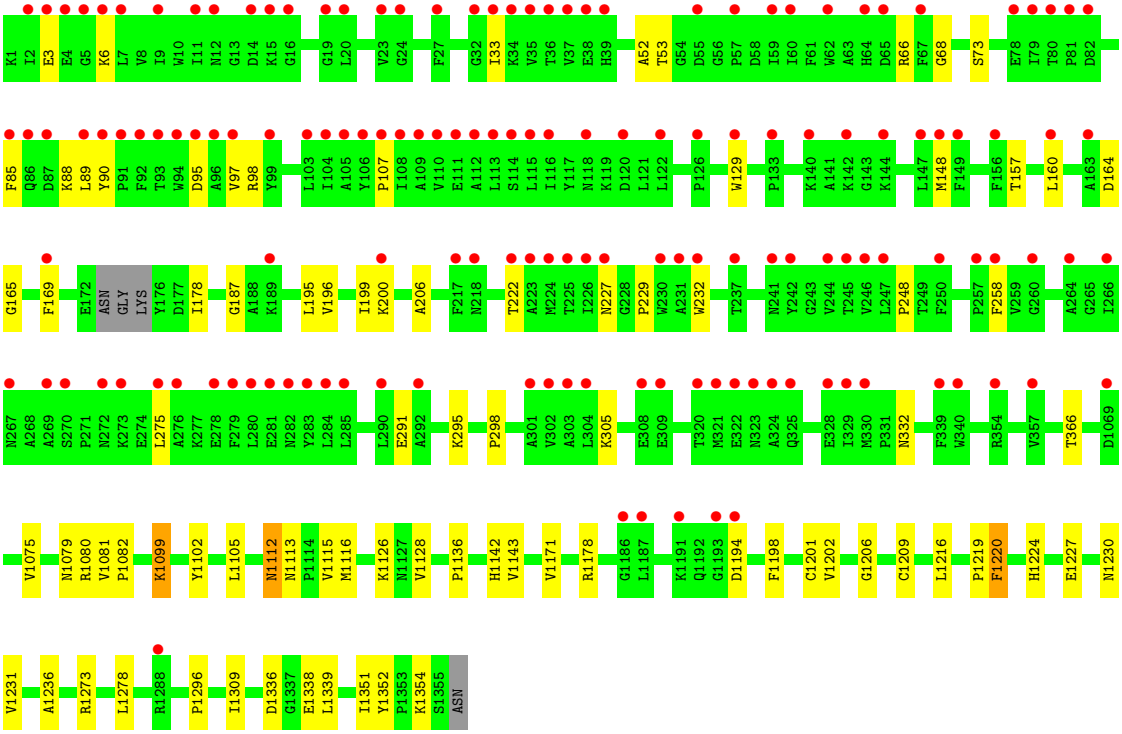
• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain E:



• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain F:



• Molecule 2: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain G: 100%

BDP1 GNS2 IDR3 GNS4 BDP5 NDG6 BDP7

• Molecule 2: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain I: 86% 14%

BDP1 GNS2 IDR3 GNS4 BDP5 NDG6 BDP7

• Molecule 2: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain L: 14% 86%

BDP1 GNS2 IDR3 GNS4 BDP5 NDG6 BDP7

• Molecule 2: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain N: 71% 29%

BDP1 GNS2 IDR3 GNS4 BDP5 NDG6 BDP7

• Molecule 2: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain P: 71% 29%

BDP1 GNS2 IDR3 GNS4 BDP5 NDG6 BDP7

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

Chain H: 100%

GLC1 GLC2

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

Chain J: 100%

GLC1 GLC2

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

Chain K: 50% 50%

GLC1 GLC2

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

Chain M: 50% 50%

GLC1 GLC2

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

Chain O: 50% 50%

GLC1 GLC2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	155.72Å 170.69Å 183.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 3.45 49.80 – 3.45	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.66-3.45) 91.1 (49.80-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.176 , 0.228 0.180 , 0.228	Depositor DCC
R_{free} test set	1962 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å^2)	88.5	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 85.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28764	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A3P, GNS, GLC, NPO, NDG, BDP, IDR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.38	0/2416	0.47	0/3270
1	B	0.30	0/5267	0.42	0/7153
1	C	0.29	0/5259	0.43	0/7144
1	D	0.30	0/5267	0.43	0/7152
1	E	0.30	0/5241	0.44	0/7123
1	F	0.29	0/5256	0.42	0/7142
All	All	0.30	0/28706	0.43	0/38984

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2352	0	2265	21	0
1	B	5136	0	4988	49	0
1	C	5128	0	4973	41	0
1	D	5136	0	4988	45	0
1	E	5110	0	4933	47	0
1	F	5124	0	4950	48	0
2	G	92	0	54	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	92	0	54	2	0
2	L	92	0	54	0	0
2	N	92	0	54	2	0
2	P	93	0	56	2	0
3	H	23	0	21	0	0
3	J	23	0	21	0	0
3	K	23	0	21	1	0
3	M	23	0	21	1	0
3	O	23	0	21	1	0
4	A	27	0	11	0	0
4	B	27	0	11	0	0
4	C	27	0	11	0	0
4	D	27	0	11	0	0
4	E	27	0	11	0	0
4	F	27	0	11	0	0
5	A	10	0	4	0	0
5	B	10	0	4	0	0
5	D	10	0	4	0	0
5	E	10	0	4	0	0
All	All	28764	0	27556	239	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 4.

All (239) 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:D:369:ALA:O	1:D:1069:ASP:N	2.24	0.71
1:E:1131:TRP:NE1	1:F:366:THR:HG21	2.08	0.68
1:E:1131:TRP:CD1	1:F:366:THR:HG21	2.30	0.66
1:D:1071:GLU:O	1:D:1073:ASP:N	2.30	0.65
1:A:1120:ASP:OD1	1:A:1123:ARG:NH1	2.31	0.63
1:B:349:ASN:OD1	1:B:354:ARG:NH1	2.32	0.62
1:C:32:GLY:O	1:D:1291:THR:HG22	2.00	0.62
1:B:1075:VAL:HG11	1:B:1128:VAL:HG13	1.82	0.61
1:D:6:LYS:HA	1:D:33:ILE:HG23	1.82	0.61
1:F:6:LYS:HA	1:F:33:ILE:HG23	1.85	0.59
1:B:6:LYS:HA	1:B:33:ILE:HG23	1.85	0.58
1:D:1071:GLU:C	1:D:1073:ASP:H	2.07	0.57
1:F:1075:VAL:HG11	1:F:1128:VAL:HG13	1.87	0.57
1:A:1349:GLU:OE2	1:C:1108:ASN:ND2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:VAL:HG11	1:A:1128:VAL:HG13	1.87	0.56
1:E:1173:TYR:OH	2:N:1:BDP:O6A	2.17	0.56
1:E:1075:VAL:HG11	1:E:1128:VAL:HG13	1.88	0.55
1:B:1352:TYR:CE1	1:B:1354:LYS:HE2	2.42	0.55
1:C:6:LYS:HA	1:C:33:ILE:HG23	1.87	0.55
1:D:68:GLY:HA3	1:D:332:ASN:O	2.07	0.55
1:F:68:GLY:HA3	1:F:332:ASN:O	2.08	0.54
1:B:1080:ARG:NH1	2:I:4:GNS:O2S	2.40	0.54
1:C:95:ASP:OD1	1:C:98:ARG:NH1	2.41	0.54
1:B:68:GLY:HA3	1:B:332:ASN:O	2.08	0.53
1:E:68:GLY:HA3	1:E:332:ASN:O	2.08	0.53
1:D:1075:VAL:HG11	1:D:1128:VAL:HG13	1.89	0.53
1:F:232:TRP:HB2	1:F:298:PRO:HG2	1.91	0.53
1:C:121:LEU:HD22	1:C:223:ALA:HB2	1.90	0.53
1:E:196:VAL:HG12	1:E:200:LYS:HE2	1.91	0.53
1:C:199:ILE:HG21	1:C:206:ALA:HB2	1.91	0.53
1:D:1079:ASN:HB2	1:D:1143:VAL:O	2.09	0.53
1:D:232:TRP:HB2	1:D:298:PRO:HG2	1.91	0.52
1:C:1075:VAL:HG11	1:C:1128:VAL:HG13	1.90	0.52
1:E:6:LYS:HA	1:E:33:ILE:HG23	1.91	0.52
1:E:199:ILE:HG21	1:E:206:ALA:HB2	1.91	0.52
1:F:1338:GLU:HG2	1:F:1339:LEU:H	1.74	0.52
1:F:1352:TYR:CE1	1:F:1354:LYS:HE2	2.45	0.52
1:E:1352:TYR:CE1	1:E:1354:LYS:HE2	2.45	0.52
1:F:148:MET:HB2	1:F:222:THR:HG21	1.92	0.52
1:C:68:GLY:HA3	1:C:332:ASN:O	2.10	0.52
1:F:1079:ASN:HB2	1:F:1143:VAL:O	2.10	0.52
1:B:95:ASP:OD1	1:B:98:ARG:NH1	2.43	0.51
1:F:291:GLU:HG2	1:F:295:LYS:HE3	1.92	0.51
1:C:1231:VAL:HG12	1:C:1309:ILE:HD12	1.91	0.51
1:F:52:ALA:HA	1:F:1099:LYS:CD	2.40	0.51
1:E:95:ASP:OD1	1:E:98:ARG:NH1	2.42	0.51
1:A:1079:ASN:HB2	1:A:1143:VAL:O	2.11	0.51
1:B:1195:LYS:CB	1:F:1230:ASN:HA	2.41	0.51
1:C:1352:TYR:CE1	1:C:1354:LYS:HE2	2.45	0.51
1:B:232:TRP:HB2	1:B:298:PRO:HG2	1.91	0.51
1:D:95:ASP:OD1	1:D:98:ARG:NH1	2.44	0.51
1:A:1352:TYR:CE1	1:A:1354:LYS:HE2	2.46	0.51
1:B:199:ILE:HG21	1:B:206:ALA:HB2	1.92	0.51
1:E:148:MET:HB2	1:E:222:THR:HG21	1.92	0.51
1:C:232:TRP:HB2	1:C:298:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:THR:HG22	1:D:1347:PHE:CE2	2.46	0.51
1:D:196:VAL:HG12	1:D:200:LYS:HE2	1.93	0.51
1:F:73:SER:HB3	1:F:1273:ARG:HH22	1.76	0.50
1:E:232:TRP:HB2	1:E:298:PRO:HG2	1.93	0.50
1:E:1332:VAL:HG12	1:E:1341:ILE:HD12	1.94	0.50
1:E:90:TYR:CE1	1:E:305:LYS:HG2	2.47	0.50
1:A:1171:VAL:HG21	1:A:1296:PRO:HG3	1.94	0.50
1:D:1352:TYR:CE1	1:D:1354:LYS:HE2	2.47	0.50
1:F:1113:ASN:ND2	1:F:1115:VAL:O	2.44	0.50
1:B:196:VAL:HG12	1:B:200:LYS:HE2	1.94	0.50
1:B:1079:ASN:HB2	1:B:1143:VAL:O	2.12	0.50
1:F:199:ILE:HG21	1:F:206:ALA:HB2	1.93	0.50
1:F:1112:ASN:HB2	2:P:1:BDP:H3	1.94	0.49
1:C:73:SER:HB2	1:C:75:LEU:HG	1.95	0.49
1:C:1079:ASN:HB2	1:C:1143:VAL:O	2.13	0.49
1:D:164:ASP:HB3	1:D:187:GLY:HA2	1.95	0.49
1:B:85:PHE:HA	1:B:88:LYS:HE3	1.95	0.49
1:B:1116:MET:H	1:B:1224:HIS:CD2	2.31	0.49
1:D:148:MET:HB2	1:D:222:THR:HG21	1.94	0.49
1:D:1113:ASN:ND2	1:D:1115:VAL:O	2.46	0.49
1:A:1351:ILE:HG23	1:C:1105:LEU:HG	1.95	0.48
1:D:85:PHE:O	1:D:88:LYS:HG2	2.12	0.48
1:D:199:ILE:HG21	1:D:206:ALA:HB2	1.94	0.48
1:B:33:ILE:HG12	1:B:275:LEU:HD13	1.95	0.48
1:F:196:VAL:HG12	1:F:200:LYS:HE2	1.95	0.48
1:B:164:ASP:HB3	1:B:187:GLY:HA2	1.95	0.48
1:B:1216:LEU:C	1:B:1219:PRO:HD2	2.34	0.48
1:E:1102:TYR:HB3	1:E:1136:PRO:HG2	1.96	0.48
1:E:1171:VAL:HG21	1:E:1296:PRO:HG3	1.95	0.48
1:B:148:MET:HB2	1:B:222:THR:HG21	1.95	0.48
1:D:179:LYS:HA	1:D:370:ALA:HB3	1.95	0.48
1:C:148:MET:HB2	1:C:222:THR:HG21	1.96	0.48
1:B:1332:VAL:HG12	1:B:1341:ILE:HD12	1.94	0.48
1:D:66:ARG:NH2	3:K:2:GLC:O4	2.40	0.47
1:D:1178:ARG:HD2	1:D:1194:ASP:HB3	1.96	0.47
1:D:1332:VAL:HG12	1:D:1341:ILE:HD12	1.95	0.47
1:A:1216:LEU:C	1:A:1219:PRO:HD2	2.35	0.47
1:F:164:ASP:HB3	1:F:187:GLY:HA2	1.95	0.47
1:D:1171:VAL:HG21	1:D:1296:PRO:HG3	1.96	0.47
1:E:97:VAL:HG21	1:E:107:PRO:HD3	1.96	0.47
1:C:164:ASP:HB3	1:C:187:GLY:HA2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:ASP:HB3	1:E:187:GLY:HA2	1.95	0.47
1:F:1171:VAL:HG21	1:F:1296:PRO:HG3	1.97	0.47
1:D:1351:ILE:HG23	1:F:1105:LEU:HG	1.97	0.47
1:E:34:LYS:NZ	1:E:36:THR:OG1	2.47	0.47
1:B:73:SER:HB2	1:B:75:LEU:HG	1.96	0.47
1:C:291:GLU:O	1:C:295:LYS:HG3	2.14	0.47
1:D:85:PHE:HA	1:D:88:LYS:HE3	1.97	0.47
1:B:1231:VAL:HG12	1:B:1309:ILE:HD12	1.97	0.47
1:A:1116:MET:H	1:A:1224:HIS:CD2	2.33	0.46
1:D:89:LEU:HD23	1:D:107:PRO:HG2	1.96	0.46
1:F:1102:TYR:HB3	1:F:1136:PRO:HG2	1.98	0.46
1:A:1105:LEU:HG	1:B:1351:ILE:HG23	1.97	0.46
1:D:73:SER:HB2	1:D:75:LEU:HG	1.97	0.46
1:E:229:PRO:HA	1:E:232:TRP:CE2	2.49	0.46
1:E:1105:LEU:HG	1:F:1351:ILE:HG23	1.96	0.46
1:E:1178:ARG:HD2	1:E:1194:ASP:HB3	1.97	0.46
1:E:1216:LEU:C	1:E:1219:PRO:HD2	2.35	0.46
1:A:1113:ASN:ND2	1:A:1115:VAL:O	2.48	0.46
1:D:1116:MET:H	1:D:1224:HIS:CD2	2.33	0.46
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.50	0.46
1:D:169:PHE:CD2	1:D:333:ILE:HD11	2.50	0.46
1:E:33:ILE:HG12	1:E:275:LEU:HD13	1.98	0.46
1:E:66:ARG:NH2	3:M:2:GLC:O4	2.44	0.46
1:C:85:PHE:HA	1:C:88:LYS:HE3	1.97	0.46
1:C:1171:VAL:HG21	1:C:1296:PRO:HG3	1.96	0.46
1:E:1231:VAL:HG12	1:E:1309:ILE:HD12	1.97	0.46
1:E:85:PHE:O	1:E:88:LYS:HG2	2.16	0.46
1:F:95:ASP:OD1	1:F:98:ARG:NH1	2.48	0.46
1:C:1113:ASN:ND2	1:C:1115:VAL:O	2.49	0.46
1:D:229:PRO:HA	1:D:232:TRP:CE2	2.51	0.46
1:D:129:TRP:CD1	1:D:248:PRO:HB2	2.51	0.45
1:E:1269:PRO:O	1:E:1273:ARG:HB2	2.15	0.45
1:C:1178:ARG:HD2	1:C:1194:ASP:HB3	1.98	0.45
1:F:1080:ARG:NH1	2:P:4:GNS:O2S	2.50	0.45
1:A:1332:VAL:HG12	1:A:1341:ILE:HD12	1.98	0.45
1:E:1216:LEU:O	1:E:1219:PRO:HD2	2.17	0.45
1:B:85:PHE:O	1:B:88:LYS:HG2	2.16	0.45
1:E:1079:ASN:HB2	1:E:1143:VAL:O	2.17	0.45
1:F:97:VAL:HG21	1:F:107:PRO:HD3	1.99	0.45
1:B:1178:ARG:HD2	1:B:1194:ASP:HB3	1.98	0.45
1:C:130:GLU:O	1:C:133:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:PRO:HB2	1:C:333:ILE:HG12	1.99	0.45
1:C:1110:THR:HG22	1:C:1111:LYS:HG3	1.99	0.45
1:C:1116:MET:H	1:C:1224:HIS:CD2	2.35	0.45
1:D:1088:SER:HA	1:D:1287:LEU:HD12	1.99	0.45
1:C:90:TYR:CE1	1:C:305:LYS:HG2	2.52	0.45
1:F:90:TYR:CE1	1:F:305:LYS:HG2	2.52	0.45
1:B:157:THR:HG23	1:B:195:LEU:HD22	1.99	0.45
1:B:1201:CYS:SG	1:B:1206:GLY:HA3	2.56	0.44
1:F:1116:MET:H	1:F:1224:HIS:CD2	2.35	0.44
1:B:1108:ASN:O	1:C:1346:PHE:HA	2.17	0.44
1:D:33:ILE:HG12	1:D:275:LEU:HD13	1.98	0.44
1:C:1332:VAL:HG12	1:C:1341:ILE:HD12	2.00	0.44
1:B:89:LEU:HD23	1:B:107:PRO:HG2	1.99	0.44
1:C:33:ILE:HG12	1:C:275:LEU:HD13	2.00	0.44
1:E:1215:TRP:NE1	1:E:1219:PRO:HG3	2.33	0.44
1:F:85:PHE:HA	1:F:88:LYS:HE3	1.99	0.44
1:E:85:PHE:HA	1:E:88:LYS:HE3	1.99	0.44
1:F:1216:LEU:C	1:F:1219:PRO:HD2	2.38	0.44
1:B:1295:LEU:HA	1:B:1296:PRO:HD3	1.84	0.44
1:D:1102:TYR:HB3	1:D:1136:PRO:HG2	2.00	0.44
1:B:1113:ASN:ND2	1:B:1115:VAL:O	2.51	0.44
1:D:90:TYR:CE1	1:D:305:LYS:HG2	2.53	0.44
1:F:229:PRO:HA	1:F:232:TRP:CE2	2.52	0.44
1:A:1231:VAL:HG12	1:A:1309:ILE:HD12	1.99	0.43
1:A:1295:LEU:HA	1:A:1296:PRO:HD3	1.85	0.43
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.53	0.43
1:F:85:PHE:O	1:F:88:LYS:HG2	2.18	0.43
1:E:1116:MET:H	1:E:1224:HIS:CD2	2.35	0.43
1:A:1216:LEU:O	1:A:1219:PRO:HD2	2.18	0.43
1:F:1178:ARG:HD2	1:F:1194:ASP:HB3	2.00	0.43
1:C:196:VAL:HG12	1:C:200:LYS:HE2	1.99	0.43
1:F:33:ILE:HG12	1:F:275:LEU:HD13	2.00	0.43
1:F:1201:CYS:SG	1:F:1206:GLY:HA3	2.58	0.43
1:B:291:GLU:O	1:B:295:LYS:HG3	2.19	0.43
1:B:1216:LEU:O	1:B:1219:PRO:HD2	2.19	0.43
1:E:129:TRP:CD1	1:E:248:PRO:HB2	2.54	0.43
1:A:1201:CYS:SG	1:A:1206:GLY:HA3	2.58	0.43
1:A:1269:PRO:O	1:A:1273:ARG:HB2	2.19	0.43
1:B:1188:ARG:NH2	1:D:1314:ASN:OD1	2.52	0.43
1:E:1080:ARG:H	1:E:1080:ARG:HG2	1.61	0.43
1:C:61:PHE:CE2	1:C:264:ALA:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1080:ARG:NH1	2:N:4:GNS:O2S	2.49	0.43
1:C:85:PHE:O	1:C:88:LYS:HG2	2.18	0.43
1:C:1102:TYR:HB3	1:C:1136:PRO:HG2	2.01	0.42
1:A:1264:LEU:HD23	1:A:1264:LEU:HA	1.90	0.42
1:B:1090:THR:HG21	1:B:1140:HIS:CE1	2.54	0.42
1:C:1333:ARG:HB2	1:C:1342:LEU:HD21	2.01	0.42
1:E:73:SER:HB2	1:E:75:LEU:HG	2.01	0.42
1:F:1216:LEU:O	1:F:1219:PRO:HD2	2.18	0.42
1:F:1231:VAL:HG12	1:F:1309:ILE:HD12	2.01	0.42
1:B:291:GLU:HG2	1:B:295:LYS:HE3	2.01	0.42
1:C:89:LEU:HD23	1:C:107:PRO:HG2	2.00	0.42
1:E:61:PHE:CE2	1:E:264:ALA:HB2	2.55	0.42
1:E:90:TYR:HA	1:E:91:PRO:HD3	1.87	0.42
1:E:1113:ASN:ND2	1:E:1115:VAL:O	2.52	0.42
1:E:1117:SER:O	1:E:1121:GLN:HG3	2.20	0.42
1:F:1080:ARG:H	1:F:1080:ARG:HG2	1.57	0.42
1:B:90:TYR:CE1	1:B:305:LYS:HG2	2.54	0.42
1:D:1216:LEU:C	1:D:1219:PRO:HD2	2.40	0.42
1:C:1159:TYR:HB3	1:C:1248:TYR:CD2	2.55	0.42
1:F:66:ARG:NH2	3:O:2:GLC:O4	2.45	0.42
2:I:6:NDG:O7	2:I:6:NDG:O3	2.33	0.42
1:A:1181:ASP:OD2	1:A:1183:TYR:N	2.53	0.41
1:D:130:GLU:O	1:D:133:PRO:HD2	2.20	0.41
1:D:169:PHE:HB3	1:D:177:ASP:HB3	2.00	0.41
1:C:53:THR:HB	1:C:1348:TYR:CE2	2.55	0.41
1:D:305:LYS:O	1:D:309:GLU:HG3	2.20	0.41
1:F:1081:VAL:HA	1:F:1082:PRO:HD3	1.91	0.41
1:E:1088:SER:HA	1:E:1287:LEU:HD12	2.02	0.41
1:F:160:LEU:HD23	1:F:195:LEU:HB2	2.01	0.41
1:C:314:ASP:HA	1:C:315:PRO:HD3	1.91	0.41
1:D:1295:LEU:HA	1:D:1296:PRO:HD3	1.88	0.41
1:A:1108:ASN:ND2	1:B:1349:GLU:OE2	2.42	0.41
1:B:1102:TYR:HB3	1:B:1136:PRO:HG2	2.03	0.41
1:B:1352:TYR:HE1	1:B:1354:LYS:HE2	1.85	0.41
1:E:171:TYR:HA	1:E:176:TYR:O	2.21	0.41
1:B:90:TYR:HA	1:B:91:PRO:HD3	1.90	0.41
1:C:1088:SER:HA	1:C:1287:LEU:HD12	2.03	0.41
1:D:160:LEU:HD23	1:D:195:LEU:HB2	2.03	0.41
1:D:1105:LEU:HG	1:E:1351:ILE:HG23	2.02	0.41
1:F:1198:PHE:O	1:F:1202:VAL:HG23	2.20	0.41
1:F:1227:GLU:O	1:F:1236:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PHE:CE2	1:B:264:ALA:HB2	2.56	0.41
1:B:150:ASN:HB3	1:B:156:PHE:CD1	2.55	0.41
1:E:109:ALA:HA	1:E:302:VAL:HA	2.03	0.41
1:F:53:THR:HB	1:F:1278:LEU:HD13	2.03	0.41
1:F:1142[B]:HIS:CD2	1:F:1220:PHE:HZ	2.38	0.41
1:B:331:PRO:HB2	1:B:333:ILE:HG12	2.03	0.41
1:B:1088:SER:HA	1:B:1287:LEU:HD12	2.02	0.40
1:B:1222:CYS:HB3	1:B:1228:CYS:HB3	2.02	0.40
1:F:129:TRP:CD1	1:F:248:PRO:HB2	2.57	0.40
1:D:1231:VAL:HG12	1:D:1309:ILE:HD12	2.02	0.40
1:B:1171:VAL:HG21	1:B:1296:PRO:HG3	2.03	0.40
1:F:89:LEU:HD23	1:F:107:PRO:HG2	2.03	0.40
1:C:9:ILE:HG12	1:C:59:ILE:HB	2.03	0.40
1:D:90:TYR:HA	1:D:91:PRO:HD3	1.90	0.40
1:E:1159:TYR:HB3	1:E:1248:TYR:CD2	2.57	0.40
1:E:1165:ASP:OD2	1:E:1166:PRO:HD2	2.21	0.40
1:A:1165:ASP:OD2	1:A:1166:PRO:HD2	2.22	0.40
1:B:78:GLU:HG3	1:B:102:LYS:HB3	2.04	0.40
1:B:100:ASN:OD1	1:B:1099:LYS:HE2	2.22	0.40
1:F:157:THR:HG23	1:F:195:LEU:HD22	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	285/658 (43%)	272 (95%)	13 (5%)	0	100	100
1	B	650/658 (99%)	616 (95%)	31 (5%)	3 (0%)	29	66
1	C	651/658 (99%)	619 (95%)	28 (4%)	4 (1%)	25	62
1	D	650/658 (99%)	614 (94%)	30 (5%)	6 (1%)	17	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	650/658 (99%)	619 (95%)	28 (4%)	3 (0%)	29	66
1	F	651/658 (99%)	619 (95%)	29 (4%)	3 (0%)	29	66
All	All	3537/3948 (90%)	3359 (95%)	159 (4%)	19 (0%)	29	66

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	370	ALA
1	D	1072	ASP
1	E	369	ALA
1	B	1336	ASP
1	B	169	PHE
1	D	1069	ASP
1	E	169	PHE
1	F	1336	ASP
1	C	1336	ASP
1	F	169	PHE
1	C	169	PHE
1	D	169	PHE
1	C	1070	GLU
1	B	165	GLY
1	C	165	GLY
1	F	165	GLY
1	D	165	GLY
1	E	165	GLY
1	D	178	ILE

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	245/548 (45%)	240 (98%)	5 (2%)	55	79
1	B	524/548 (96%)	518 (99%)	6 (1%)	73	88
1	C	522/548 (95%)	518 (99%)	4 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	524/548 (96%)	515 (98%)	9 (2%)	60	82
1	E	519/548 (95%)	514 (99%)	5 (1%)	76	89
1	F	521/548 (95%)	512 (98%)	9 (2%)	60	82
All	All	2855/3288 (87%)	2817 (99%)	38 (1%)	69	86

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1112	ASN
1	A	1133	GLU
1	A	1220	PHE
1	A	1225	SER
1	A	1297	THR
1	B	178	ILE
1	B	227	ASN
1	B	258	PHE
1	B	1220	PHE
1	B	1225	SER
1	B	1297	THR
1	C	121	LEU
1	C	227	ASN
1	C	258	PHE
1	C	1220	PHE
1	D	177	ASP
1	D	178	ILE
1	D	227	ASN
1	D	258	PHE
1	D	321	MET
1	D	1112	ASN
1	D	1209	CYS
1	D	1220	PHE
1	D	1336	ASP
1	E	227	ASN
1	E	258	PHE
1	E	321	MET
1	E	1112	ASN
1	E	1220	PHE
1	F	3	GLU
1	F	178	ILE
1	F	227	ASN
1	F	258	PHE

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Mol	Chain	Res	Type
1	F	1099	LYS
1	F	1112	ASN
1	F	1126	LYS
1	F	1209	CYS
1	F	1220	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1127	ASN
1	B	1127	ASN
1	C	1106	HIS
1	C	1127	ASN
1	D	1127	ASN
1	E	1127	ASN
1	F	1106	HIS
1	F	1127	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

45 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	BDP	G	1	2,5	12,12,13	2.70	8 (66%)	14,17,19	1.16	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GNS	G	2	2	14,15,16	2.56	7 (50%)	17,22,24	2.28	3 (17%)
2	IDR	G	3	2	12,12,13	2.54	6 (50%)	14,17,19	1.22	2 (14%)
2	GNS	G	4	2	14,15,16	2.38	9 (64%)	17,22,24	2.40	5 (29%)
2	BDP	G	5	2	12,12,13	2.52	6 (50%)	14,17,19	1.14	0
2	NDG	G	6	2	14,14,15	0.61	1 (7%)	17,19,21	0.50	0
2	BDP	G	7	2	12,12,13	2.58	7 (58%)	14,17,19	1.06	2 (14%)
3	GLC	H	1	3	12,12,12	0.53	0	17,17,17	0.63	0
3	GLC	H	2	3	11,11,12	0.63	0	15,15,17	0.71	0
2	BDP	I	1	2,5	12,12,13	2.75	8 (66%)	14,17,19	0.99	1 (7%)
2	GNS	I	2	2	14,15,16	2.51	7 (50%)	17,22,24	2.22	3 (17%)
2	IDR	I	3	2	12,12,13	2.51	6 (50%)	14,17,19	1.30	2 (14%)
2	GNS	I	4	2	14,15,16	2.55	8 (57%)	17,22,24	2.42	4 (23%)
2	BDP	I	5	2	12,12,13	2.53	6 (50%)	14,17,19	1.12	0
2	NDG	I	6	2	14,14,15	0.56	0	17,19,21	0.63	0
2	BDP	I	7	2	12,12,13	2.62	6 (50%)	14,17,19	0.81	0
3	GLC	J	1	3	12,12,12	0.52	0	17,17,17	0.59	0
3	GLC	J	2	3	11,11,12	0.60	0	15,15,17	0.78	0
3	GLC	K	1	3	12,12,12	0.52	0	17,17,17	0.61	0
3	GLC	K	2	3	11,11,12	0.66	0	15,15,17	0.77	0
2	BDP	L	1	2,5	12,12,13	2.52	7 (58%)	14,17,19	1.08	0
2	GNS	L	2	2	14,15,16	2.57	8 (57%)	17,22,24	2.36	6 (35%)
2	IDR	L	3	2	12,12,13	2.50	6 (50%)	14,17,19	1.12	2 (14%)
2	GNS	L	4	2	14,15,16	2.50	7 (50%)	17,22,24	2.51	3 (17%)
2	BDP	L	5	2	12,12,13	2.44	5 (41%)	14,17,19	1.07	0
2	NDG	L	6	2	14,14,15	0.50	0	17,19,21	0.66	0
2	BDP	L	7	2	12,12,13	2.55	7 (58%)	14,17,19	1.16	1 (7%)
3	GLC	M	1	3	12,12,12	0.53	0	17,17,17	0.63	0
3	GLC	M	2	3	11,11,12	0.65	0	15,15,17	0.84	0
2	BDP	N	1	2,5	12,12,13	2.62	7 (58%)	14,17,19	1.10	1 (7%)
2	GNS	N	2	2	14,15,16	2.52	7 (50%)	17,22,24	2.40	4 (23%)
2	IDR	N	3	2	12,12,13	2.44	6 (50%)	14,17,19	1.18	1 (7%)
2	GNS	N	4	2	14,15,16	2.40	8 (57%)	17,22,24	2.41	3 (17%)
2	BDP	N	5	2	12,12,13	2.59	5 (41%)	14,17,19	0.97	0
2	NDG	N	6	2	14,14,15	0.60	1 (7%)	17,19,21	0.49	0
2	BDP	N	7	2	12,12,13	2.59	8 (66%)	14,17,19	0.91	0
3	GLC	O	1	3	12,12,12	0.51	0	17,17,17	0.64	0
3	GLC	O	2	3	11,11,12	0.65	0	15,15,17	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BDP	P	1	2	13,13,13	2.24	4 (30%)	18,19,19	1.49	1 (5%)
2	GNS	P	2	2	14,15,16	2.52	8 (57%)	17,22,24	2.50	4 (23%)
2	IDR	P	3	2	12,12,13	2.44	6 (50%)	14,17,19	1.20	2 (14%)
2	GNS	P	4	2	14,15,16	2.43	8 (57%)	17,22,24	2.39	4 (23%)
2	BDP	P	5	2	12,12,13	2.57	5 (41%)	14,17,19	1.00	0
2	NDG	P	6	2	14,14,15	0.58	1 (7%)	17,19,21	0.49	0
2	BDP	P	7	2	12,12,13	2.55	7 (58%)	14,17,19	1.02	1 (7%)

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	BDP	G	1	2,5	-	0/4/21/24	0/1/1/1
2	GNS	G	2	2	-	0/7/24/27	0/1/1/1
2	IDR	G	3	2	-	2/4/21/24	0/1/1/1
2	GNS	G	4	2	-	1/7/24/27	0/1/1/1
2	BDP	G	5	2	-	0/4/21/24	0/1/1/1
2	NDG	G	6	2	-	0/6/23/26	0/1/1/1
2	BDP	G	7	2	-	2/4/21/24	0/1/1/1
3	GLC	H	1	3	-	0/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
2	BDP	I	1	2,5	-	0/4/21/24	0/1/1/1
2	GNS	I	2	2	-	0/7/24/27	0/1/1/1
2	IDR	I	3	2	-	2/4/21/24	0/1/1/1
2	GNS	I	4	2	-	0/7/24/27	0/1/1/1
2	BDP	I	5	2	-	0/4/21/24	0/1/1/1
2	NDG	I	6	2	-	4/6/23/26	0/1/1/1
2	BDP	I	7	2	-	2/4/21/24	0/1/1/1
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
2	BDP	L	1	2,5	-	2/4/21/24	0/1/1/1
2	GNS	L	2	2	-	0/7/24/27	0/1/1/1
2	IDR	L	3	2	-	2/4/21/24	0/1/1/1
2	GNS	L	4	2	-	1/7/24/27	0/1/1/1
2	BDP	L	5	2	-	0/4/21/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	L	6	2	-	2/6/23/26	0/1/1/1
2	BDP	L	7	2	-	1/4/21/24	0/1/1/1
3	GLC	M	1	3	-	0/2/22/22	0/1/1/1
3	GLC	M	2	3	-	0/2/19/22	0/1/1/1
2	BDP	N	1	2,5	-	0/4/21/24	0/1/1/1
2	GNS	N	2	2	-	0/7/24/27	0/1/1/1
2	IDR	N	3	2	-	3/4/21/24	0/1/1/1
2	GNS	N	4	2	-	0/7/24/27	0/1/1/1
2	BDP	N	5	2	-	2/4/21/24	0/1/1/1
2	NDG	N	6	2	-	0/6/23/26	0/1/1/1
2	BDP	N	7	2	-	2/4/21/24	0/1/1/1
3	GLC	O	1	3	-	0/2/22/22	0/1/1/1
3	GLC	O	2	3	-	0/2/19/22	0/1/1/1
2	BDP	P	1	2	-	0/4/24/24	0/1/1/1
2	GNS	P	2	2	-	0/7/24/27	0/1/1/1
2	IDR	P	3	2	-	3/4/21/24	0/1/1/1
2	GNS	P	4	2	-	0/7/24/27	0/1/1/1
2	BDP	P	5	2	-	0/4/21/24	0/1/1/1
2	NDG	P	6	2	-	0/6/23/26	0/1/1/1
2	BDP	P	7	2	-	1/4/21/24	0/1/1/1

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	5	BDP	O6A-C6	5.32	1.38	1.22
2	I	1	BDP	O6A-C6	5.32	1.38	1.22
2	N	3	IDR	O6A-C6	5.28	1.38	1.22
2	P	1	BDP	O6A-C6	5.27	1.38	1.22
2	L	3	IDR	O6A-C6	5.26	1.38	1.22
2	I	5	BDP	O6A-C6	5.26	1.38	1.22
2	G	1	BDP	O6A-C6	5.24	1.38	1.22
2	L	5	BDP	O6A-C6	5.23	1.38	1.22
2	P	3	IDR	O6A-C6	5.21	1.38	1.22
2	I	7	BDP	O6A-C6	5.19	1.38	1.22
2	P	7	BDP	O6A-C6	5.18	1.37	1.22
2	I	3	IDR	O6A-C6	5.18	1.37	1.22
2	G	3	IDR	O6A-C6	5.18	1.37	1.22
2	G	7	BDP	O6A-C6	5.17	1.37	1.22
2	L	1	BDP	O6A-C6	5.15	1.37	1.22
2	L	7	BDP	O6A-C6	5.12	1.37	1.22
2	N	7	BDP	O6A-C6	5.12	1.37	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	5	BDP	O6A-C6	5.11	1.37	1.22
2	P	5	BDP	O6A-C6	5.10	1.37	1.22
2	N	1	BDP	O6A-C6	5.06	1.37	1.22
2	L	2	GNS	O3S-S1	4.47	1.47	1.42
2	P	2	GNS	O3S-S1	4.39	1.47	1.42
2	N	2	GNS	O3S-S1	4.37	1.47	1.42
2	I	2	GNS	O3S-S1	4.35	1.47	1.42
2	I	4	GNS	O3S-S1	4.30	1.47	1.42
2	L	2	GNS	O2S-S1	4.26	1.47	1.42
2	G	2	GNS	O5-C1	-4.25	1.36	1.43
2	L	4	GNS	O3S-S1	4.24	1.47	1.42
2	I	4	GNS	O2S-S1	4.23	1.47	1.42
2	P	5	BDP	O5-C1	-4.22	1.37	1.43
2	P	4	GNS	O3S-S1	4.22	1.46	1.42
2	I	2	GNS	O5-C1	-4.21	1.37	1.43
2	N	5	BDP	O5-C1	-4.18	1.37	1.43
2	N	2	GNS	O2S-S1	4.16	1.46	1.42
2	G	4	GNS	O3S-S1	4.14	1.46	1.42
2	N	4	GNS	O3S-S1	4.13	1.46	1.42
2	P	2	GNS	O2S-S1	4.11	1.46	1.42
2	N	1	BDP	O5-C1	-4.09	1.37	1.43
2	G	2	GNS	O3S-S1	4.03	1.46	1.42
2	L	2	GNS	O5-C1	-4.00	1.37	1.43
2	I	7	BDP	O5-C1	-3.97	1.37	1.43
2	L	4	GNS	O2S-S1	3.94	1.46	1.42
2	P	2	GNS	O5-C1	-3.93	1.37	1.43
2	I	1	BDP	O5-C1	-3.88	1.37	1.43
2	N	7	BDP	O5-C1	-3.87	1.37	1.43
2	G	3	IDR	O5-C1	-3.86	1.37	1.43
2	G	7	BDP	O5-C1	-3.85	1.37	1.43
2	G	5	BDP	O5-C1	-3.82	1.37	1.43
2	L	7	BDP	O5-C1	-3.78	1.37	1.43
2	L	4	GNS	O5-C1	-3.77	1.37	1.43
2	I	5	BDP	O5-C1	-3.73	1.37	1.43
2	G	1	BDP	O5-C1	-3.71	1.37	1.43
2	P	4	GNS	O5-C1	-3.71	1.37	1.43
2	L	5	BDP	O5-C1	-3.69	1.37	1.43
2	P	7	BDP	O5-C1	-3.69	1.37	1.43
2	I	4	GNS	O5-C1	-3.65	1.37	1.43
2	N	2	GNS	O5-C1	-3.64	1.37	1.43
2	I	3	IDR	O5-C1	-3.63	1.37	1.43
2	G	2	GNS	O2S-S1	3.63	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	GNS	O2S-S1	3.59	1.46	1.42
2	N	4	GNS	O2S-S1	3.59	1.46	1.42
2	L	3	IDR	O5-C1	-3.59	1.38	1.43
2	N	4	GNS	O5-C1	-3.56	1.38	1.43
2	P	4	GNS	O2S-S1	3.54	1.46	1.42
2	N	3	IDR	O5-C1	-3.51	1.38	1.43
2	G	4	GNS	O2S-S1	3.41	1.46	1.42
2	G	4	GNS	O5-C1	-3.37	1.38	1.43
2	P	3	IDR	O5-C1	-3.37	1.38	1.43
2	L	1	BDP	O5-C1	-3.31	1.38	1.43
2	G	1	BDP	O5-C5	-3.23	1.36	1.43
2	N	4	GNS	S1-N2	3.22	1.63	1.59
2	P	4	GNS	S1-N2	3.22	1.63	1.59
2	P	1	BDP	O5-C5	-3.20	1.38	1.43
2	I	1	BDP	O5-C5	-3.06	1.37	1.43
2	N	1	BDP	O5-C5	-3.06	1.37	1.43
2	P	5	BDP	O5-C5	-3.04	1.37	1.43
2	G	2	GNS	O5-C5	-3.02	1.37	1.43
2	I	7	BDP	O5-C5	-3.02	1.37	1.43
2	G	2	GNS	S1-N2	2.99	1.63	1.59
2	I	2	GNS	O5-C5	-2.98	1.37	1.43
2	N	5	BDP	O5-C5	-2.95	1.37	1.43
2	I	4	GNS	S1-N2	2.86	1.63	1.59
2	N	7	BDP	O5-C5	-2.86	1.37	1.43
2	G	7	BDP	O5-C5	-2.81	1.37	1.43
2	L	4	GNS	O5-C5	-2.80	1.37	1.43
2	G	4	GNS	O5-C5	-2.76	1.37	1.43
2	I	4	GNS	O5-C5	-2.75	1.37	1.43
2	L	2	GNS	O5-C5	-2.75	1.37	1.43
2	L	4	GNS	S1-N2	2.73	1.63	1.59
2	I	5	BDP	O5-C5	-2.72	1.37	1.43
2	G	5	BDP	O5-C5	-2.70	1.37	1.43
2	L	7	BDP	O5-C5	-2.70	1.37	1.43
2	G	1	BDP	O2-C2	-2.69	1.37	1.43
2	G	5	BDP	O2-C2	-2.67	1.37	1.43
2	L	5	BDP	O5-C5	-2.66	1.38	1.43
2	N	2	GNS	S1-N2	2.66	1.63	1.59
2	L	1	BDP	O5-C5	-2.65	1.38	1.43
2	P	7	BDP	O5-C5	-2.64	1.38	1.43
2	I	1	BDP	O2-C2	-2.64	1.37	1.43
2	N	2	GNS	O5-C5	-2.64	1.38	1.43
2	G	4	GNS	C2-N2	-2.64	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	5	BDP	O2-C2	-2.62	1.37	1.43
2	L	2	GNS	C2-N2	-2.62	1.43	1.47
2	N	2	GNS	C2-N2	-2.62	1.43	1.47
2	I	1	BDP	C4-C5	-2.60	1.48	1.53
2	G	3	IDR	O2-C2	-2.59	1.37	1.43
2	L	1	BDP	O2-C2	-2.58	1.37	1.43
2	I	3	IDR	O2-C2	-2.56	1.37	1.43
2	G	7	BDP	O2-C2	-2.56	1.37	1.43
2	L	7	BDP	O2-C2	-2.55	1.37	1.43
2	P	2	GNS	O5-C5	-2.55	1.38	1.43
2	P	7	BDP	O2-C2	-2.54	1.38	1.43
2	N	1	BDP	O2-C2	-2.52	1.38	1.43
2	P	2	GNS	C2-N2	-2.52	1.43	1.47
2	I	4	GNS	C2-N2	-2.51	1.43	1.47
2	I	2	GNS	C2-N2	-2.50	1.43	1.47
2	I	7	BDP	O2-C2	-2.49	1.38	1.43
2	P	2	GNS	S1-N2	2.49	1.62	1.59
2	G	2	GNS	C2-N2	-2.48	1.43	1.47
2	L	4	GNS	C2-N2	-2.48	1.43	1.47
2	P	3	IDR	O2-C2	-2.48	1.38	1.43
2	N	3	IDR	O2-C2	-2.48	1.38	1.43
2	L	3	IDR	O5-C5	-2.47	1.38	1.43
2	N	4	GNS	O5-C5	-2.46	1.38	1.43
2	I	2	GNS	S1-N2	2.46	1.62	1.59
2	N	7	BDP	O2-C2	-2.45	1.38	1.43
2	L	3	IDR	O2-C2	-2.45	1.38	1.43
2	P	5	BDP	O2-C2	-2.45	1.38	1.43
2	G	1	BDP	C4-C5	-2.44	1.49	1.53
2	L	5	BDP	O2-C2	-2.43	1.38	1.43
2	P	1	BDP	O6B-C6	2.42	1.38	1.30
2	I	1	BDP	O3-C3	-2.41	1.37	1.43
2	I	3	IDR	O5-C5	-2.41	1.38	1.43
2	G	3	IDR	O5-C5	-2.41	1.38	1.43
2	I	5	BDP	O2-C2	-2.41	1.38	1.43
2	P	4	GNS	O5-C5	-2.40	1.38	1.43
2	L	5	BDP	O6B-C6	2.34	1.38	1.30
2	G	3	IDR	O3-C3	-2.32	1.37	1.43
2	P	3	IDR	O3-C3	-2.31	1.37	1.43
2	L	3	IDR	O6B-C6	2.31	1.38	1.30
2	I	3	IDR	O3-C3	-2.31	1.37	1.43
2	G	1	BDP	O3-C3	-2.30	1.37	1.43
2	L	1	BDP	O6B-C6	2.30	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	5	BDP	O6B-C6	2.29	1.38	1.30
2	I	7	BDP	O6B-C6	2.29	1.38	1.30
2	I	5	BDP	O6B-C6	2.28	1.38	1.30
2	P	3	IDR	O5-C5	-2.28	1.38	1.43
2	P	4	GNS	C2-N2	-2.27	1.44	1.47
2	N	5	BDP	O6B-C6	2.26	1.38	1.30
2	G	1	BDP	C5-C6	-2.26	1.48	1.53
2	G	7	BDP	O6B-C6	2.26	1.38	1.30
2	L	3	IDR	O3-C3	-2.24	1.37	1.43
2	G	3	IDR	O6B-C6	2.24	1.37	1.30
2	L	1	BDP	C4-C5	-2.24	1.49	1.53
2	N	3	IDR	O5-C5	-2.24	1.38	1.43
2	N	3	IDR	O6B-C6	2.24	1.37	1.30
2	P	3	IDR	O6B-C6	2.23	1.37	1.30
2	P	1	BDP	O3-C3	-2.23	1.37	1.43
2	I	3	IDR	O6B-C6	2.22	1.37	1.30
2	N	7	BDP	O6B-C6	2.22	1.37	1.30
2	L	7	BDP	O6B-C6	2.21	1.37	1.30
2	P	5	BDP	O6B-C6	2.21	1.37	1.30
2	G	4	GNS	O4-C4	-2.20	1.37	1.43
2	P	7	BDP	O6B-C6	2.20	1.37	1.30
2	N	4	GNS	C2-N2	-2.20	1.44	1.47
2	N	2	GNS	O3-C3	-2.20	1.37	1.43
2	I	1	BDP	O6B-C6	2.19	1.37	1.30
2	I	1	BDP	C5-C6	-2.19	1.48	1.53
2	G	1	BDP	O6B-C6	2.19	1.37	1.30
2	I	4	GNS	O3-C3	-2.19	1.37	1.43
2	N	1	BDP	O6B-C6	2.19	1.37	1.30
2	N	1	BDP	C4-C5	-2.18	1.49	1.53
2	N	7	BDP	O4-C4	-2.18	1.37	1.43
2	L	2	GNS	O4-C4	-2.17	1.37	1.43
2	G	7	BDP	O4-C4	-2.17	1.37	1.43
2	I	5	BDP	O3-C3	-2.17	1.37	1.43
2	N	1	BDP	O3-C3	-2.17	1.37	1.43
2	N	3	IDR	O3-C3	-2.17	1.37	1.43
2	P	2	GNS	O3-C3	-2.16	1.37	1.43
2	N	4	GNS	O3-C3	-2.15	1.37	1.43
2	L	2	GNS	S1-N2	2.15	1.62	1.59
2	G	2	GNS	O3-C3	-2.15	1.37	1.43
2	P	4	GNS	O3-C3	-2.14	1.37	1.43
2	G	4	GNS	S1-N2	2.13	1.62	1.59
2	L	2	GNS	O3-C3	-2.13	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	7	BDP	O4-C4	-2.12	1.38	1.43
2	I	4	GNS	O4-C4	-2.11	1.38	1.43
2	G	7	BDP	O3-C3	-2.11	1.38	1.43
2	G	6	NDG	O5-C1	-2.11	1.40	1.43
2	L	4	GNS	O3-C3	-2.11	1.38	1.43
2	L	7	BDP	O3-C3	-2.11	1.38	1.43
2	N	7	BDP	O3-C3	-2.10	1.38	1.43
2	I	7	BDP	O4-C4	-2.10	1.38	1.43
2	P	4	GNS	O4-C4	-2.10	1.38	1.43
2	N	4	GNS	O4-C4	-2.10	1.38	1.43
2	G	4	GNS	O3-C3	-2.10	1.38	1.43
2	N	6	NDG	O5-C1	-2.09	1.40	1.43
2	L	1	BDP	O3-C3	-2.08	1.38	1.43
2	P	6	NDG	O5-C1	-2.08	1.40	1.43
2	L	7	BDP	O4-C4	-2.07	1.38	1.43
2	I	2	GNS	O3-C3	-2.06	1.38	1.43
2	P	2	GNS	O4-C4	-2.05	1.38	1.43
2	P	7	BDP	O3-C3	-2.04	1.38	1.43
2	G	4	GNS	C4-C5	-2.04	1.48	1.53
2	G	5	BDP	O3-C3	-2.03	1.38	1.43
2	N	7	BDP	C4-C5	-2.02	1.49	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	4	GNS	O2S-S1-O3S	-7.14	103.30	120.16
2	L	4	GNS	O2S-S1-O3S	-7.11	103.37	120.16
2	N	4	GNS	O2S-S1-O3S	-7.07	103.45	120.16
2	L	2	GNS	O2S-S1-O3S	-6.79	104.11	120.16
2	I	4	GNS	O2S-S1-O3S	-6.77	104.15	120.16
2	N	2	GNS	O2S-S1-O3S	-6.74	104.22	120.16
2	G	4	GNS	O2S-S1-O3S	-6.74	104.24	120.16
2	P	2	GNS	O2S-S1-O3S	-6.72	104.28	120.16
2	I	2	GNS	O2S-S1-O3S	-6.70	104.33	120.16
2	G	2	GNS	O2S-S1-O3S	-6.68	104.36	120.16
2	P	2	GNS	O5-C1-C2	-5.91	101.96	111.29
2	L	4	GNS	C1-O5-C5	5.44	119.56	112.19
2	I	4	GNS	C1-O5-C5	5.29	119.36	112.19
2	G	4	GNS	C1-O5-C5	5.13	119.14	112.19
2	N	4	GNS	C1-O5-C5	5.09	119.09	112.19
2	P	4	GNS	C1-O5-C5	4.70	118.56	112.19
2	N	2	GNS	C1-O5-C5	4.67	118.52	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	2	GNS	O5-C1-C2	-4.31	104.48	111.29
2	G	2	GNS	O5-C1-C2	-4.23	104.61	111.29
2	L	2	GNS	O5-C1-C2	-4.15	104.73	111.29
2	P	1	BDP	C1-O5-C5	4.09	118.25	112.22
2	I	2	GNS	O5-C1-C2	-3.83	105.25	111.29
2	G	2	GNS	C1-O5-C5	3.69	117.19	112.19
2	N	4	GNS	O5-C1-C2	-3.44	105.86	111.29
2	I	2	GNS	C1-O5-C5	3.41	116.81	112.19
2	P	2	GNS	C1-O5-C5	3.35	116.73	112.19
2	P	4	GNS	O5-C1-C2	-3.32	106.04	111.29
2	I	4	GNS	O5-C1-C2	-3.21	106.22	111.29
2	L	4	GNS	O5-C1-C2	-3.06	106.45	111.29
2	L	2	GNS	O5-C5-C6	3.00	111.90	107.20
2	G	4	GNS	O5-C1-C2	-2.83	106.82	111.29
2	G	1	BDP	O5-C1-C2	-2.83	106.41	110.77
2	L	2	GNS	C1-O5-C5	2.81	116.00	112.19
2	I	3	IDR	O6B-C6-O6A	-2.68	118.00	124.09
2	L	7	BDP	O5-C1-C2	-2.60	106.76	110.77
2	G	3	IDR	O6B-C6-O6A	-2.55	118.30	124.09
2	L	3	IDR	O6B-C6-O6A	-2.48	118.45	124.09
2	P	3	IDR	O6B-C6-O6A	-2.47	118.48	124.09
2	N	1	BDP	O5-C1-C2	-2.44	107.00	110.77
2	L	2	GNS	O4-C4-C5	-2.34	103.49	109.30
2	N	3	IDR	O6B-C6-O6A	-2.33	118.79	124.09
2	I	1	BDP	O5-C1-C2	-2.26	107.28	110.77
2	P	4	GNS	O5-C5-C6	2.26	110.75	107.20
2	P	7	BDP	O5-C1-C2	-2.24	107.31	110.77
2	G	4	GNS	O5-C5-C6	2.21	110.66	107.20
2	P	2	GNS	O5-C5-C6	2.18	110.63	107.20
2	G	4	GNS	C3-C4-C5	-2.18	106.36	110.24
2	G	3	IDR	O6B-C6-C5	2.14	121.49	113.65
2	I	3	IDR	O6B-C6-C5	2.13	121.46	113.65
2	L	3	IDR	O6B-C6-C5	2.12	121.39	113.65
2	G	7	BDP	O5-C1-C2	-2.11	107.51	110.77
2	I	4	GNS	C3-C4-C5	-2.06	106.57	110.24
2	G	7	BDP	O6B-C6-O6A	-2.05	119.43	124.09
2	L	2	GNS	C6-C5-C4	-2.02	108.26	113.00
2	P	3	IDR	O6B-C6-C5	2.01	121.02	113.65
2	N	2	GNS	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	3	IDR	C4-C5-C6-O6A
2	G	3	IDR	C4-C5-C6-O6B
2	I	3	IDR	C4-C5-C6-O6A
2	I	3	IDR	C4-C5-C6-O6B
2	L	3	IDR	C4-C5-C6-O6A
2	L	3	IDR	C4-C5-C6-O6B
2	N	3	IDR	C4-C5-C6-O6A
2	N	3	IDR	C4-C5-C6-O6B
2	P	3	IDR	C4-C5-C6-O6A
2	P	3	IDR	C4-C5-C6-O6B
2	I	6	NDG	C1-C2-N2-C7
2	I	6	NDG	C4-C5-C6-O6
2	L	6	NDG	C4-C5-C6-O6
2	I	6	NDG	O5-C5-C6-O6
2	N	3	IDR	O5-C5-C6-O6A
2	L	6	NDG	O5-C5-C6-O6
2	I	6	NDG	C3-C2-N2-C7
2	G	7	BDP	O5-C5-C6-O6B
2	I	7	BDP	O5-C5-C6-O6A
2	I	7	BDP	O5-C5-C6-O6B
2	L	1	BDP	O5-C5-C6-O6A
2	L	1	BDP	O5-C5-C6-O6B
2	N	5	BDP	O5-C5-C6-O6A
2	N	5	BDP	O5-C5-C6-O6B
2	N	7	BDP	O5-C5-C6-O6B
2	P	3	IDR	O5-C5-C6-O6A
2	G	4	GNS	C2-N2-S1-O2S
2	L	4	GNS	C2-N2-S1-O2S
2	G	7	BDP	C4-C5-C6-O6B
2	L	7	BDP	C4-C5-C6-O6B
2	N	7	BDP	C4-C5-C6-O6B
2	P	7	BDP	C4-C5-C6-O6B

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	6	NDG	1	0
3	M	2	GLC	1	0
2	P	4	GNS	1	0
2	P	1	BDP	1	0
3	O	2	GLC	1	0
3	K	2	GLC	1	0

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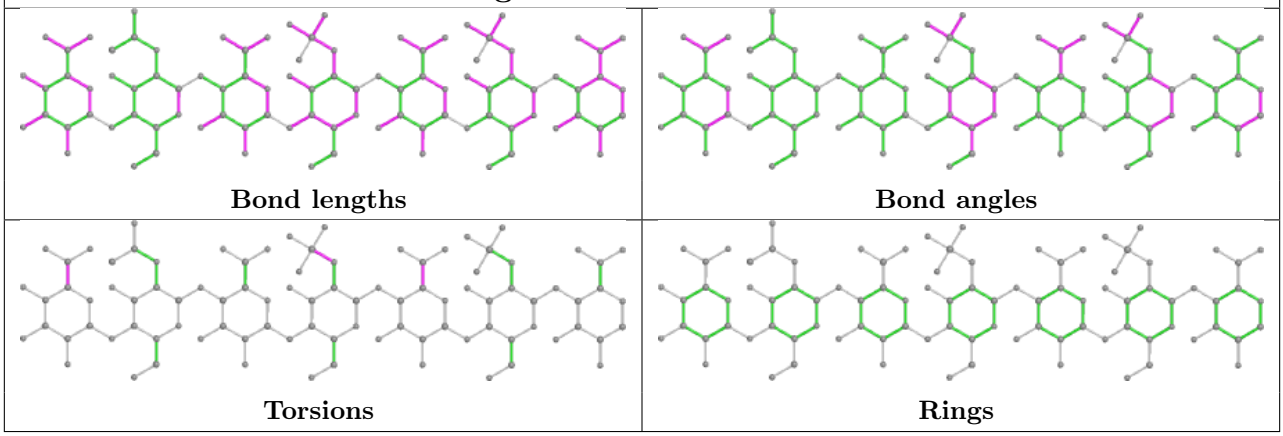
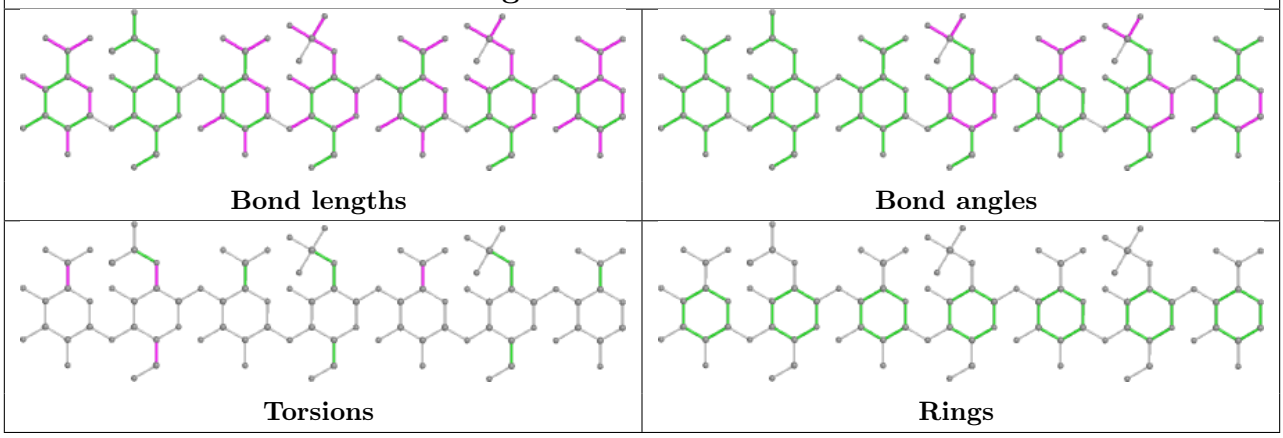
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	4	GNS	1	0
2	N	1	BDP	1	0
2	I	4	GNS	1	0

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

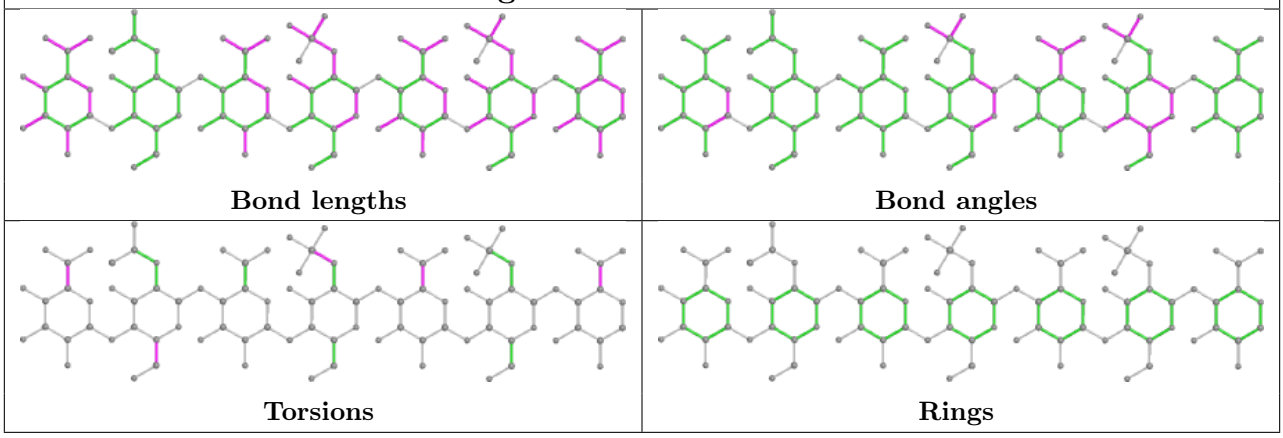
Oligosaccharide Chain G

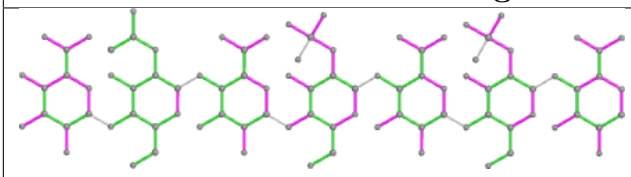
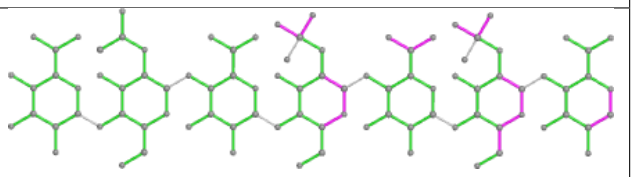
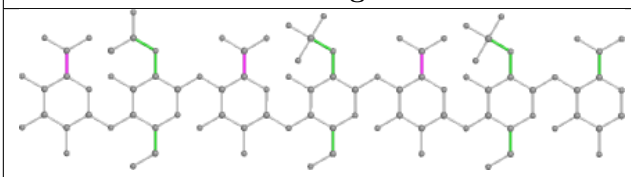
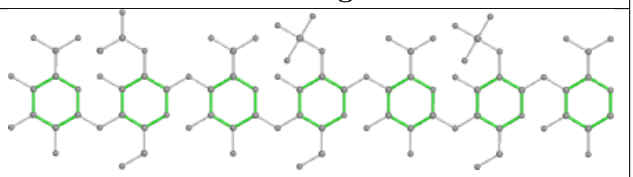


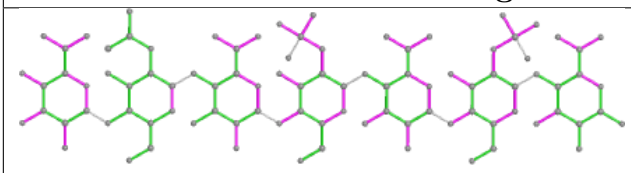
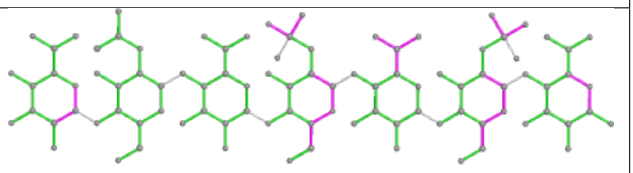
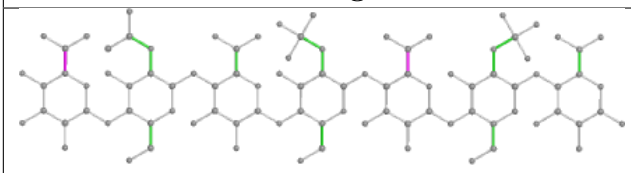
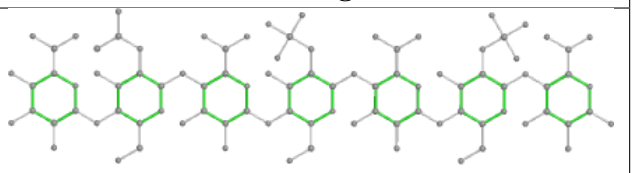
Oligosaccharide Chain I



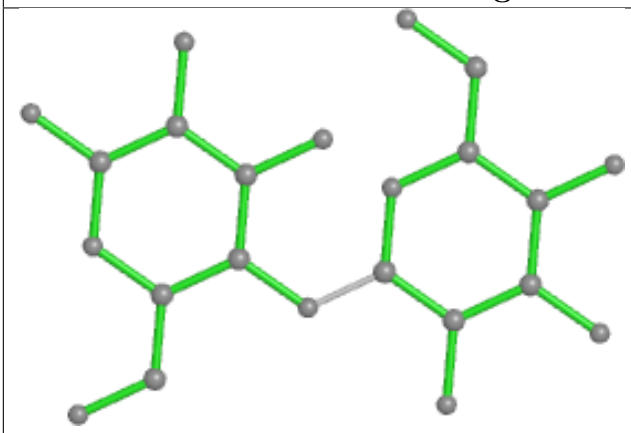
Oligosaccharide Chain L



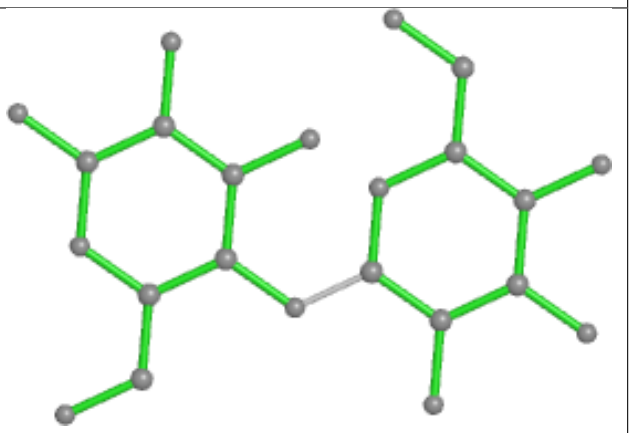
Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

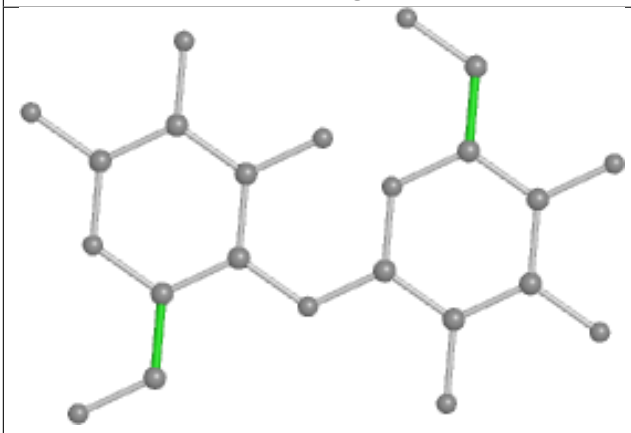
Oligosaccharide Chain H



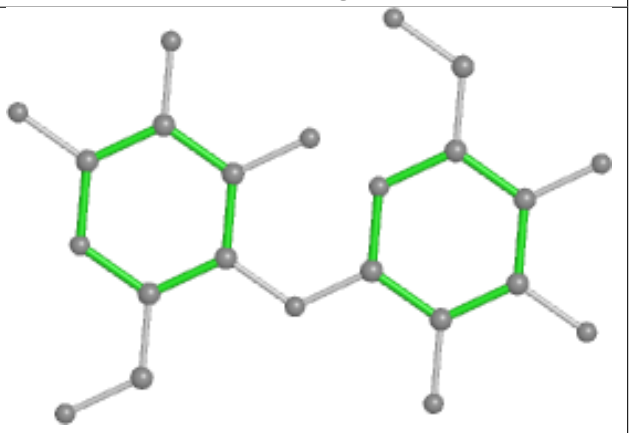
Bond lengths



Bond angles

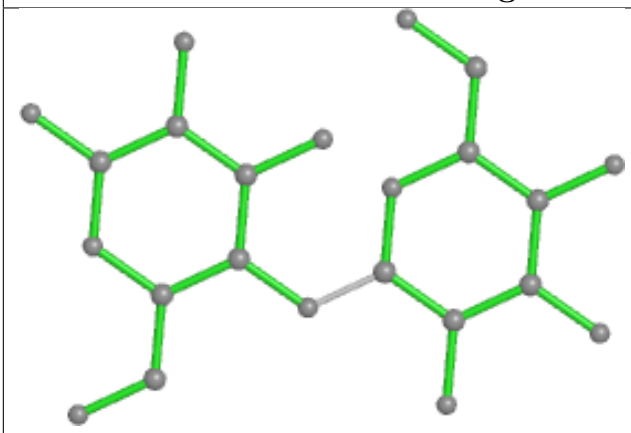


Torsions

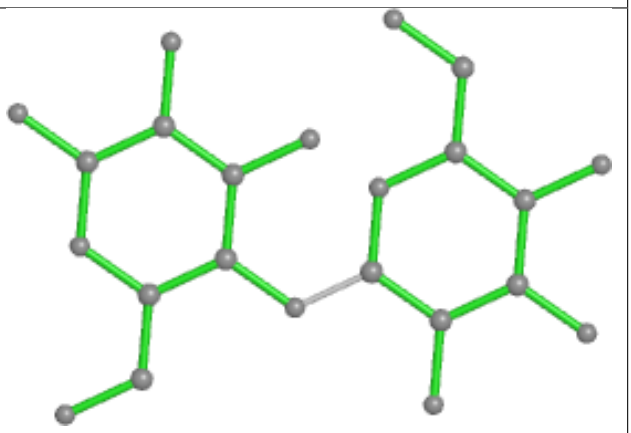


Rings

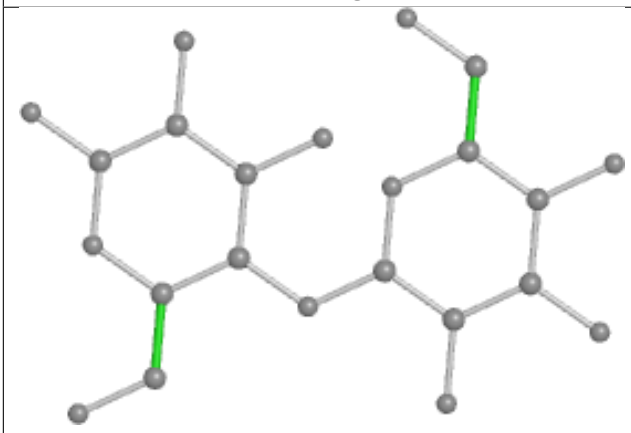
Oligosaccharide Chain J



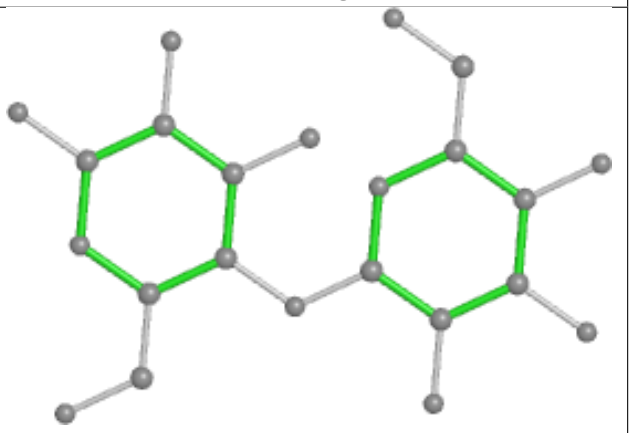
Bond lengths



Bond angles

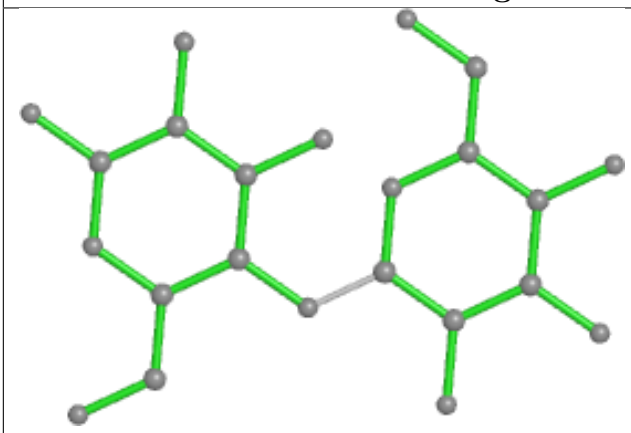


Torsions

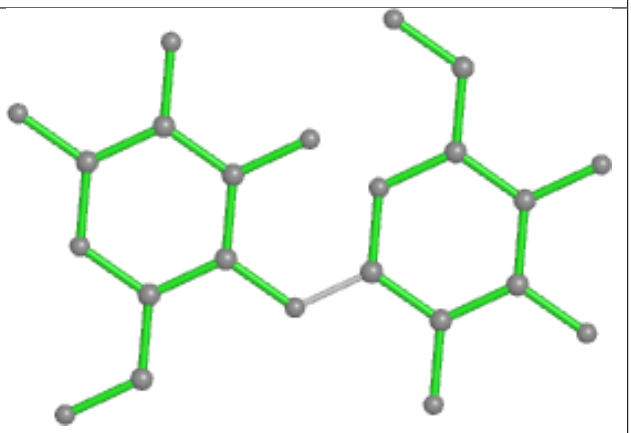


Rings

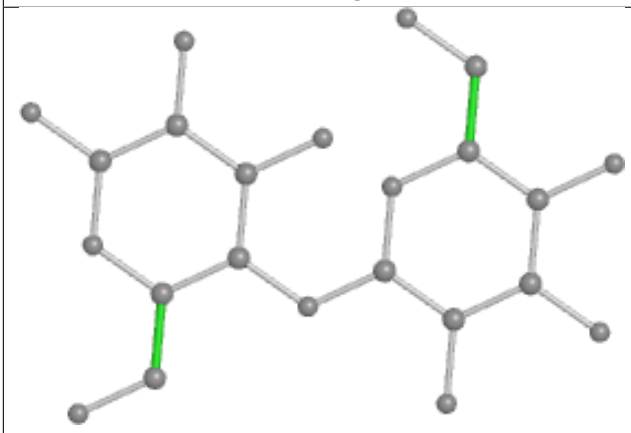
Oligosaccharide Chain K



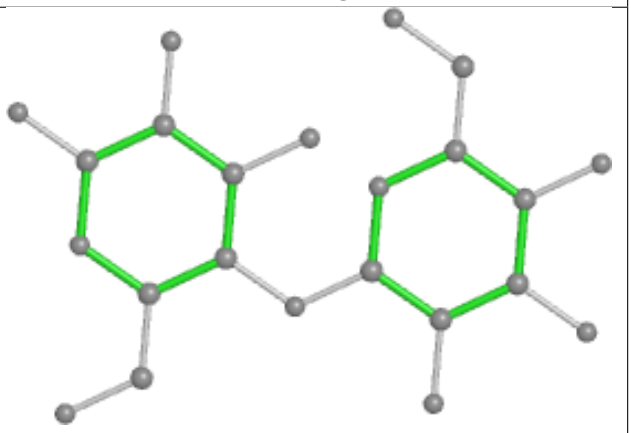
Bond lengths



Bond angles

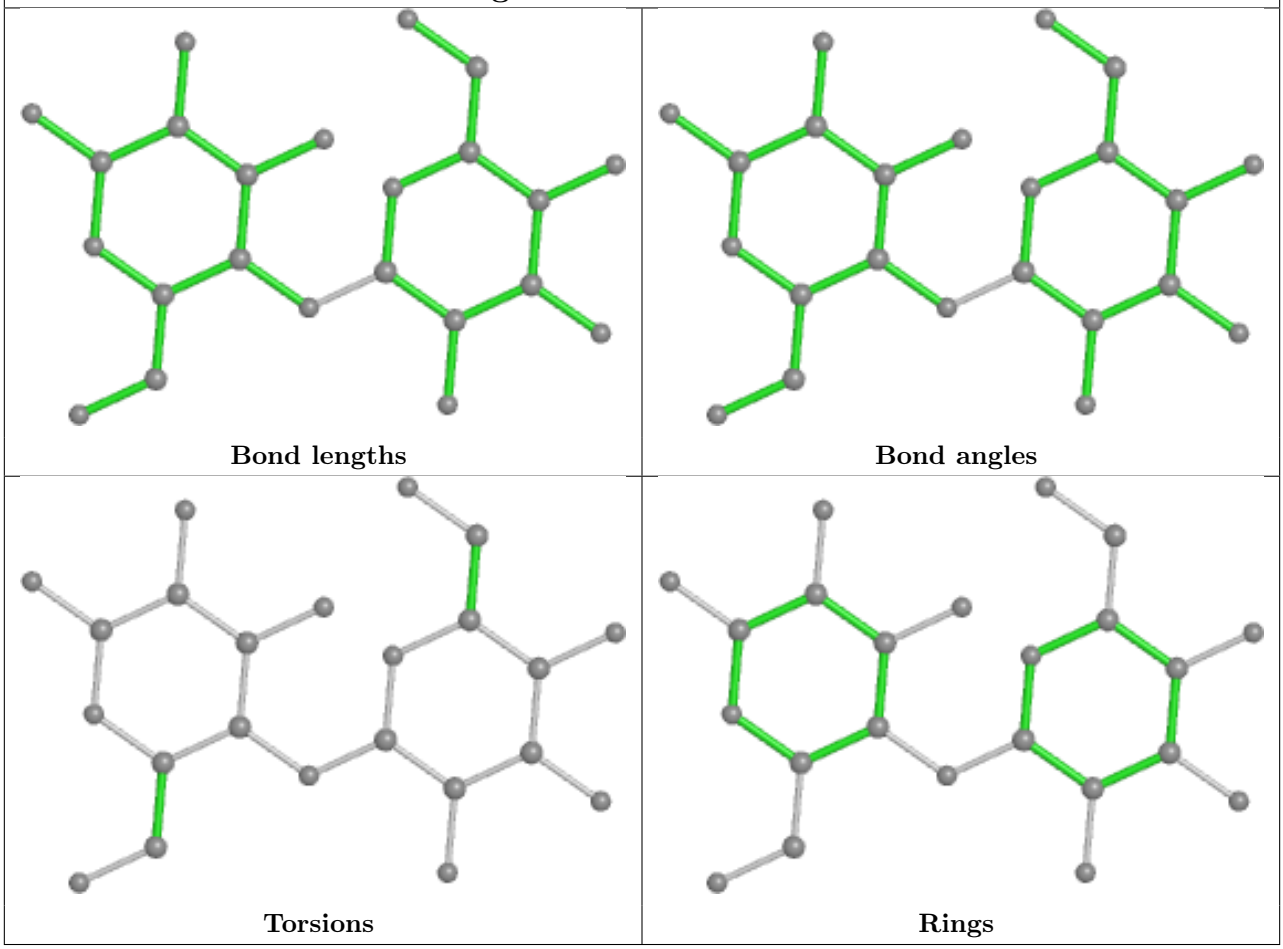


Torsions

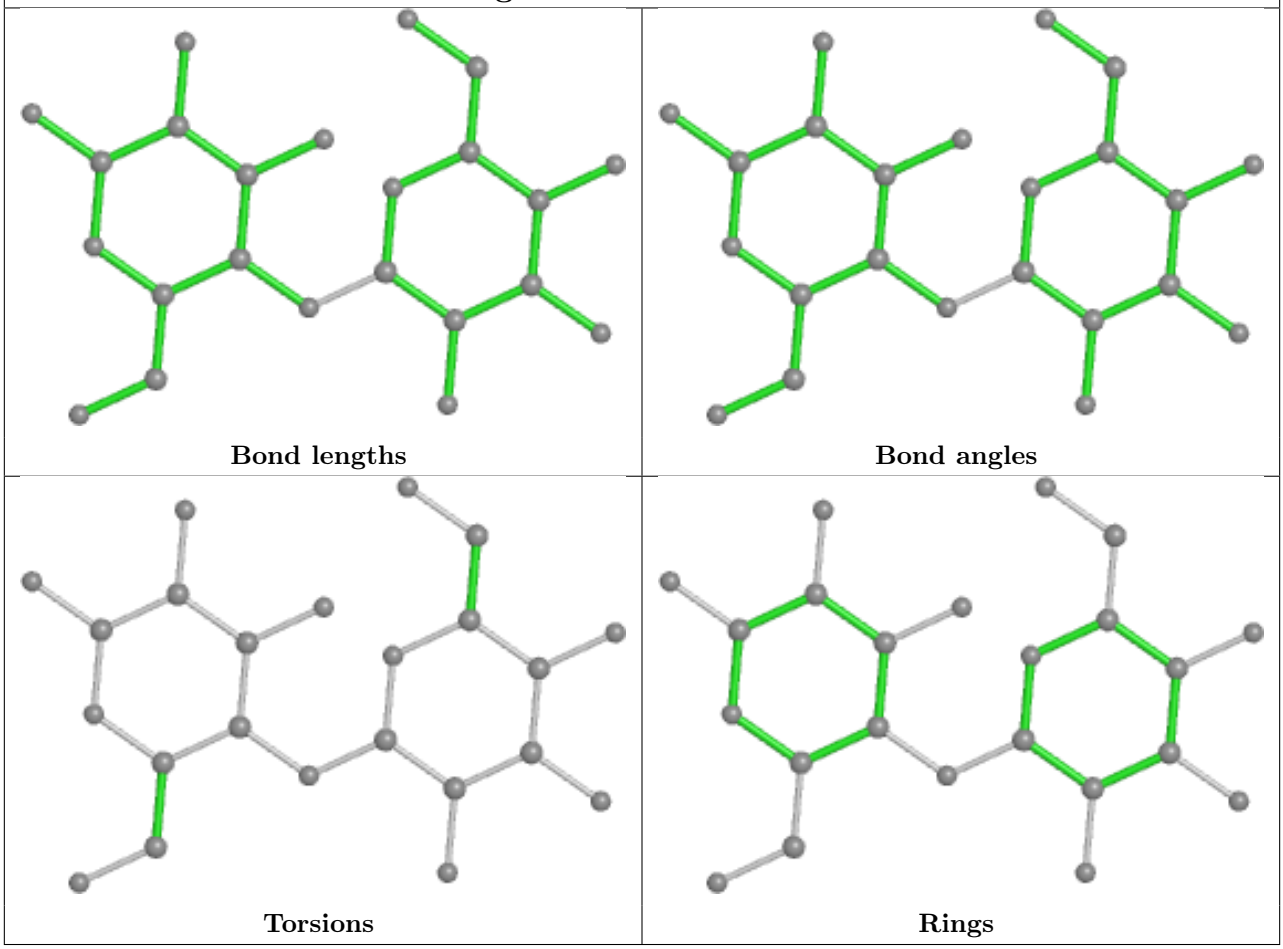


Rings

Oligosaccharide Chain M



Oligosaccharide Chain O



5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
4	A3P	D	2003	-	26,29,29	2.77	11 (42%)	31,45,45	1.16	1 (3%)
4	A3P	C	2003	-	26,29,29	2.82	10 (38%)	31,45,45	1.13	2 (6%)
4	A3P	E	2003	-	26,29,29	2.80	10 (38%)	31,45,45	1.18	1 (3%)
4	A3P	B	2003	-	26,29,29	2.74	11 (42%)	31,45,45	1.18	1 (3%)
4	A3P	F	2003	-	26,29,29	2.84	11 (42%)	31,45,45	1.16	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NPO	E	2011	2	9,10,10	0.40	0	11,13,13	0.58	0
5	NPO	A	2011	2	9,10,10	0.48	0	11,13,13	0.95	1 (9%)
5	NPO	B	2011	2	9,10,10	0.45	0	11,13,13	0.79	1 (9%)
5	NPO	D	2011	2	9,10,10	0.40	0	11,13,13	0.60	0
4	A3P	A	2003	-	26,29,29	2.78	12 (46%)	31,45,45	1.14	2 (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
4	A3P	D	2003	-	-	0/11/31/31	0/3/3/3
4	A3P	C	2003	-	-	0/11/31/31	0/3/3/3
4	A3P	E	2003	-	-	0/11/31/31	0/3/3/3
4	A3P	B	2003	-	-	0/11/31/31	0/3/3/3
4	A3P	F	2003	-	-	1/11/31/31	0/3/3/3
5	NPO	E	2011	2	-	0/2/4/4	0/1/1/1
5	NPO	A	2011	2	-	0/2/4/4	0/1/1/1
5	NPO	B	2011	2	-	0/2/4/4	0/1/1/1
5	NPO	D	2011	2	-	0/2/4/4	0/1/1/1
4	A3P	A	2003	-	-	0/11/31/31	0/3/3/3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2003	A3P	C2-N3	7.26	1.43	1.32
4	E	2003	A3P	C2-N3	7.16	1.43	1.32
4	D	2003	A3P	C2-N3	7.09	1.43	1.32
4	C	2003	A3P	C2-N3	7.01	1.43	1.32
4	A	2003	A3P	C2-N3	6.95	1.43	1.32
4	B	2003	A3P	C2-N3	6.81	1.43	1.32
4	E	2003	A3P	C4-N3	5.50	1.43	1.35
4	C	2003	A3P	C4-N3	5.46	1.43	1.35
4	F	2003	A3P	C4-N3	5.40	1.43	1.35
4	F	2003	A3P	C2-N1	5.25	1.43	1.33
4	A	2003	A3P	C4-N3	5.25	1.42	1.35
4	B	2003	A3P	C4-N3	5.25	1.42	1.35
4	D	2003	A3P	C2-N1	5.24	1.43	1.33
4	E	2003	A3P	C2-N1	5.18	1.43	1.33
4	D	2003	A3P	C4-N3	5.16	1.42	1.35
4	C	2003	A3P	C2-N1	5.12	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2003	A3P	C2-N1	5.07	1.43	1.33
4	B	2003	A3P	C2-N1	5.04	1.43	1.33
4	C	2003	A3P	C8-N7	4.95	1.43	1.34
4	E	2003	A3P	C8-N7	4.92	1.43	1.34
4	A	2003	A3P	C8-N7	4.92	1.43	1.34
4	B	2003	A3P	C8-N7	4.89	1.43	1.34
4	F	2003	A3P	C8-N7	4.83	1.43	1.34
4	D	2003	A3P	C8-N7	4.81	1.43	1.34
4	C	2003	A3P	C2'-C1'	-3.87	1.47	1.53
4	B	2003	A3P	C2'-C1'	-3.74	1.48	1.53
4	D	2003	A3P	C2'-C1'	-3.56	1.48	1.53
4	F	2003	A3P	C2'-C1'	-3.51	1.48	1.53
4	A	2003	A3P	C2'-C1'	-3.35	1.48	1.53
4	B	2003	A3P	O4'-C4'	-3.33	1.37	1.45
4	A	2003	A3P	O4'-C4'	-3.29	1.37	1.45
4	E	2003	A3P	C2'-C1'	-3.14	1.49	1.53
4	C	2003	A3P	O4'-C4'	-3.12	1.38	1.45
4	F	2003	A3P	O4'-C4'	-3.12	1.38	1.45
4	D	2003	A3P	O4'-C4'	-3.10	1.38	1.45
4	E	2003	A3P	O4'-C4'	-3.02	1.38	1.45
4	F	2003	A3P	C5-C4	2.88	1.48	1.40
4	E	2003	A3P	C5-C4	2.87	1.48	1.40
4	C	2003	A3P	C5-C4	2.84	1.48	1.40
4	A	2003	A3P	C5-C4	2.83	1.48	1.40
4	B	2003	A3P	C5-C4	2.77	1.48	1.40
4	D	2003	A3P	C5-C4	2.72	1.48	1.40
4	A	2003	A3P	P1-O3'	-2.58	1.54	1.59
4	F	2003	A3P	C6-N6	2.54	1.43	1.34
4	E	2003	A3P	C6-N6	2.53	1.43	1.34
4	C	2003	A3P	C6-N6	2.51	1.43	1.34
4	B	2003	A3P	C6-N6	2.48	1.43	1.34
4	D	2003	A3P	C6-N6	2.46	1.43	1.34
4	E	2003	A3P	O2'-C2'	-2.45	1.37	1.43
4	A	2003	A3P	C6-N6	2.41	1.42	1.34
4	D	2003	A3P	O2'-C2'	-2.38	1.37	1.43
4	C	2003	A3P	O2'-C2'	-2.33	1.37	1.43
4	F	2003	A3P	O2'-C2'	-2.32	1.37	1.43
4	A	2003	A3P	O2'-C2'	-2.32	1.37	1.43
4	D	2003	A3P	O4'-C1'	-2.26	1.37	1.41
4	A	2003	A3P	C2'-C3'	-2.26	1.47	1.52
4	F	2003	A3P	O4'-C1'	-2.24	1.38	1.41
4	E	2003	A3P	C2'-C3'	-2.23	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2003	A3P	C2'-C3'	-2.18	1.48	1.52
4	B	2003	A3P	O2'-C2'	-2.17	1.37	1.43
4	B	2003	A3P	C2'-C3'	-2.16	1.48	1.52
4	C	2003	A3P	C2'-C3'	-2.15	1.48	1.52
4	A	2003	A3P	O4'-C1'	-2.11	1.38	1.41
4	D	2003	A3P	C2'-C3'	-2.07	1.48	1.52
4	B	2003	A3P	O4'-C1'	-2.06	1.38	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	2003	A3P	N3-C2-N1	-4.81	121.16	128.68
4	B	2003	A3P	N3-C2-N1	-4.69	121.34	128.68
4	D	2003	A3P	N3-C2-N1	-4.64	121.42	128.68
4	C	2003	A3P	N3-C2-N1	-4.58	121.52	128.68
4	F	2003	A3P	N3-C2-N1	-4.49	121.66	128.68
4	A	2003	A3P	N3-C2-N1	-4.31	121.95	128.68
5	A	2011	NPO	C2-C1-N1	2.57	121.31	119.38
4	C	2003	A3P	C4-C5-N7	-2.46	106.84	109.40
4	A	2003	A3P	C4-C5-N7	-2.29	107.02	109.40
4	F	2003	A3P	C4-C5-N7	-2.08	107.23	109.40
5	B	2011	NPO	C2-C1-N1	2.07	120.94	119.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2003	A3P	C3'-C4'-C5'-O5'

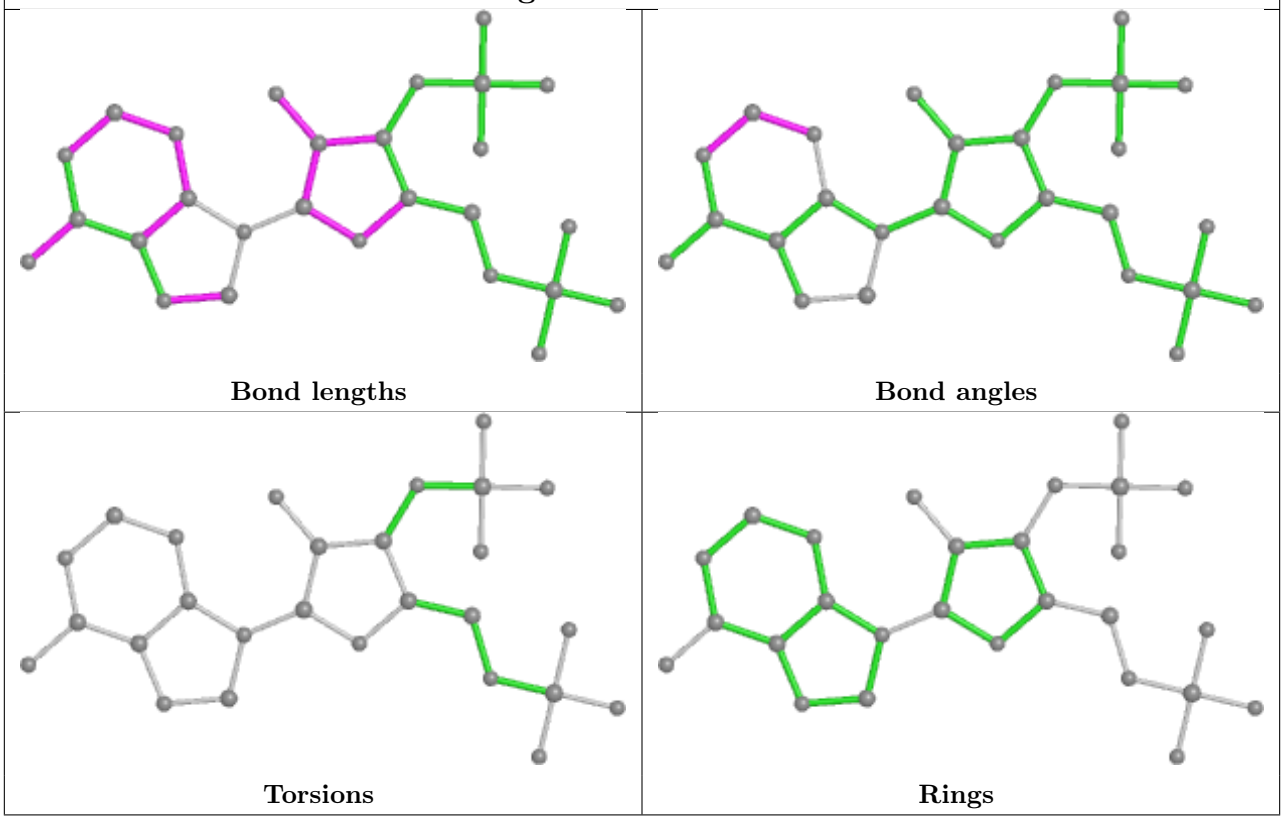
There are no ring outliers.

No monomer is involved in short contacts.

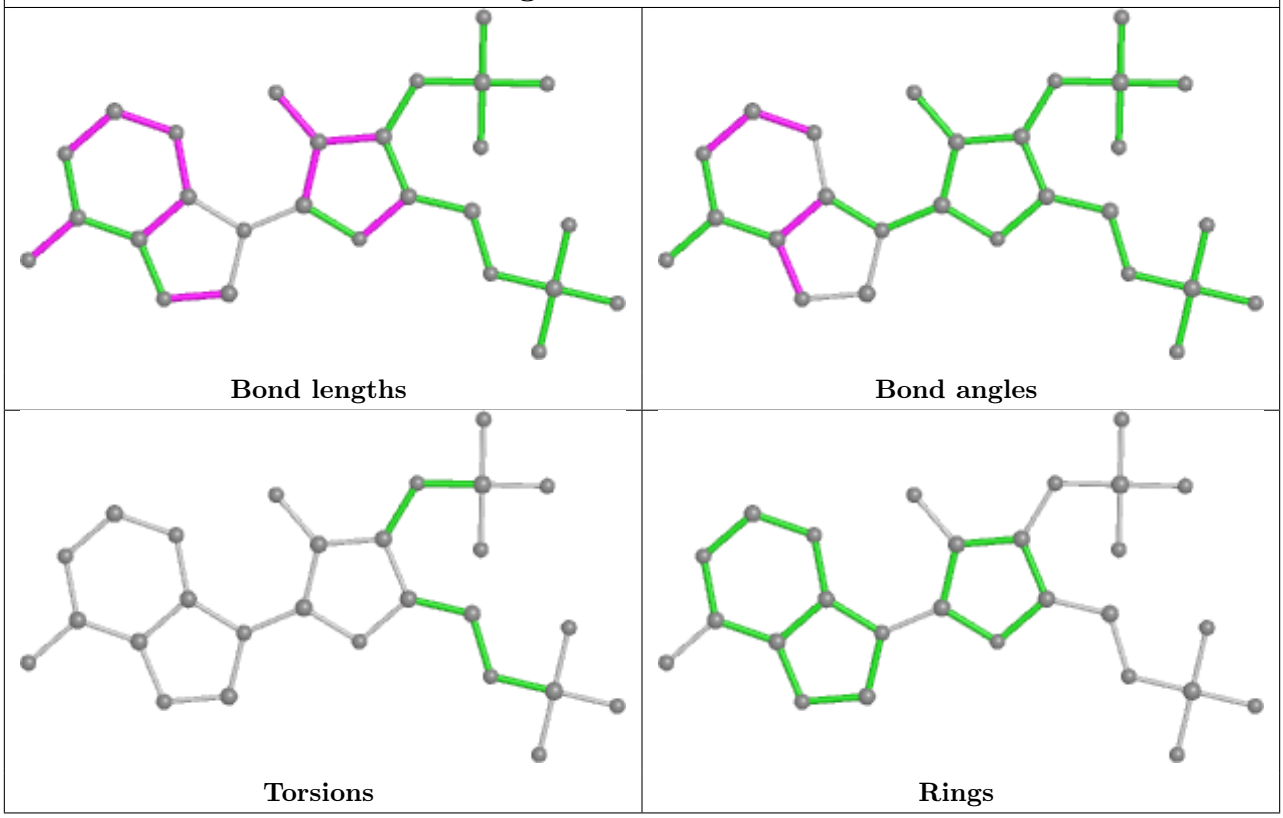
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

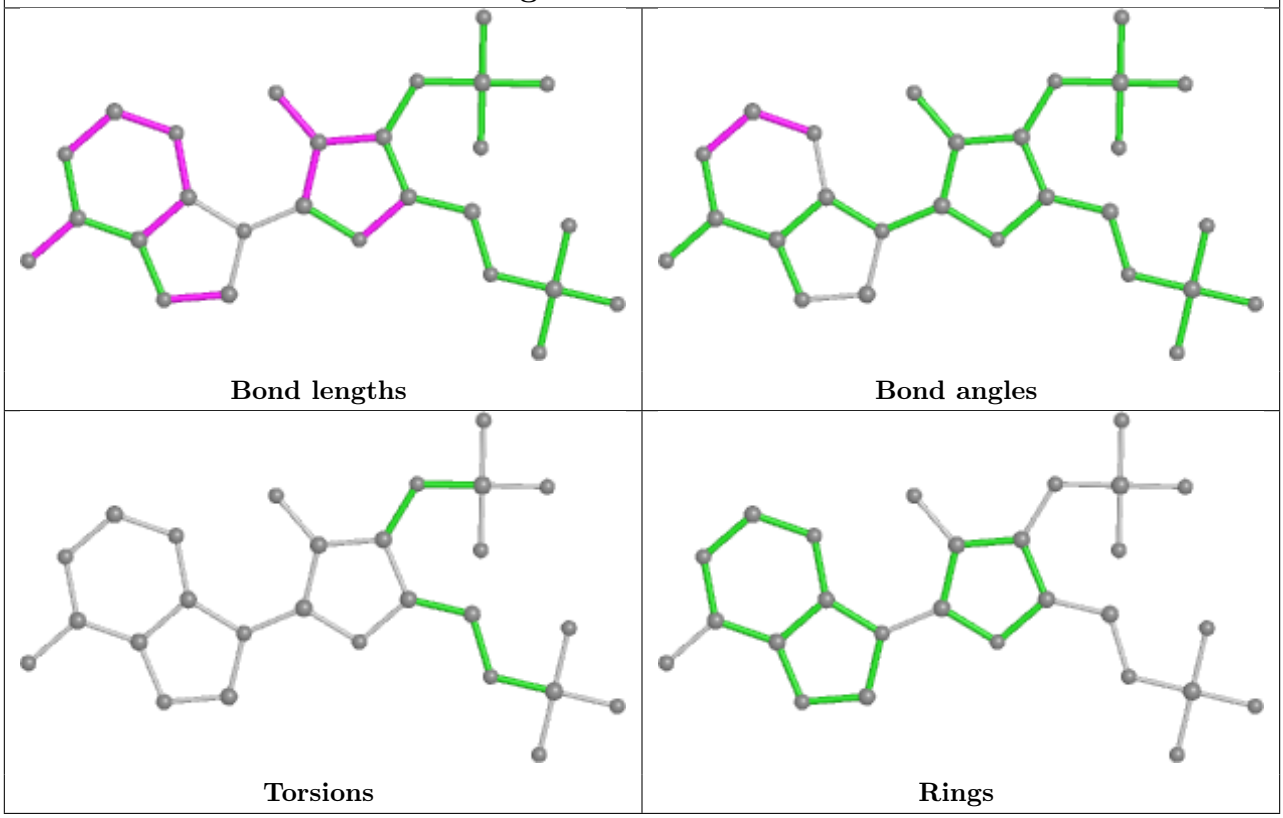
Ligand A3P D 2003



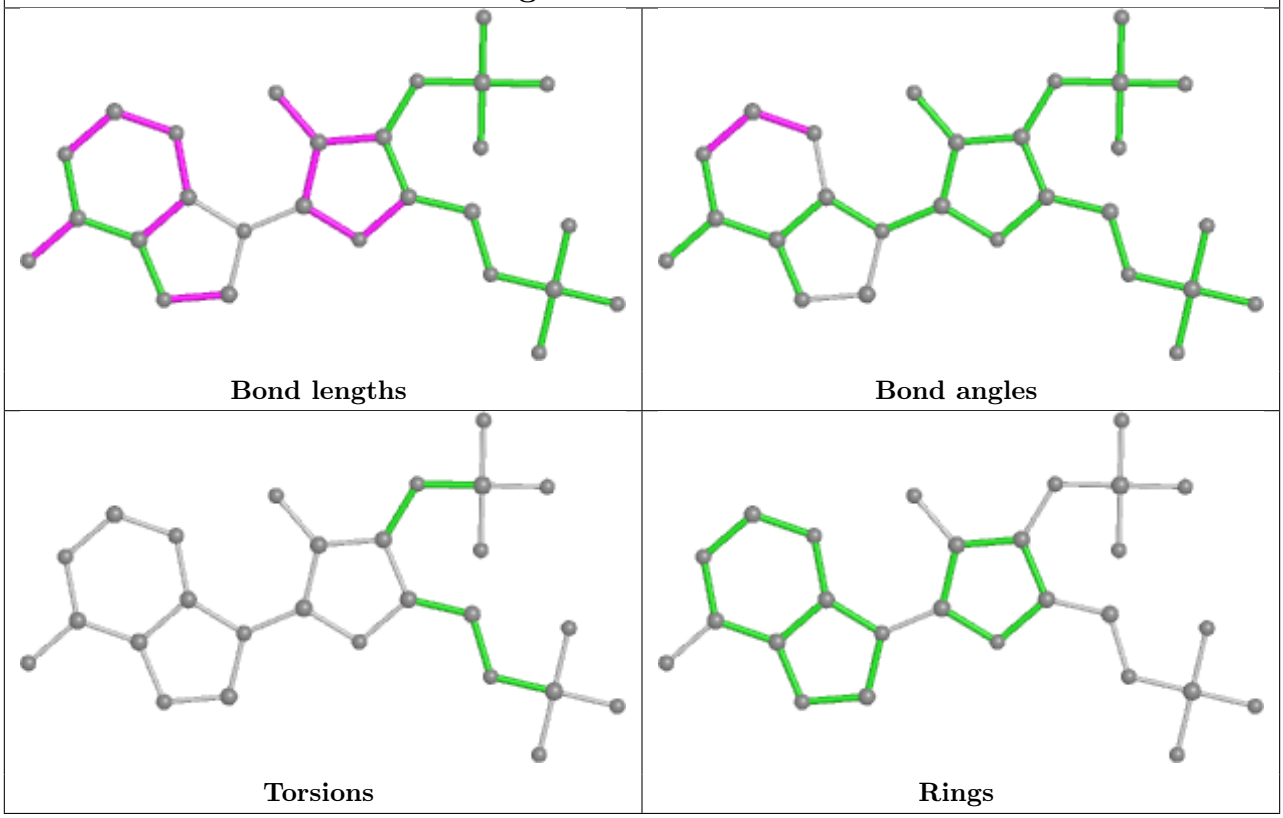
Ligand A3P C 2003



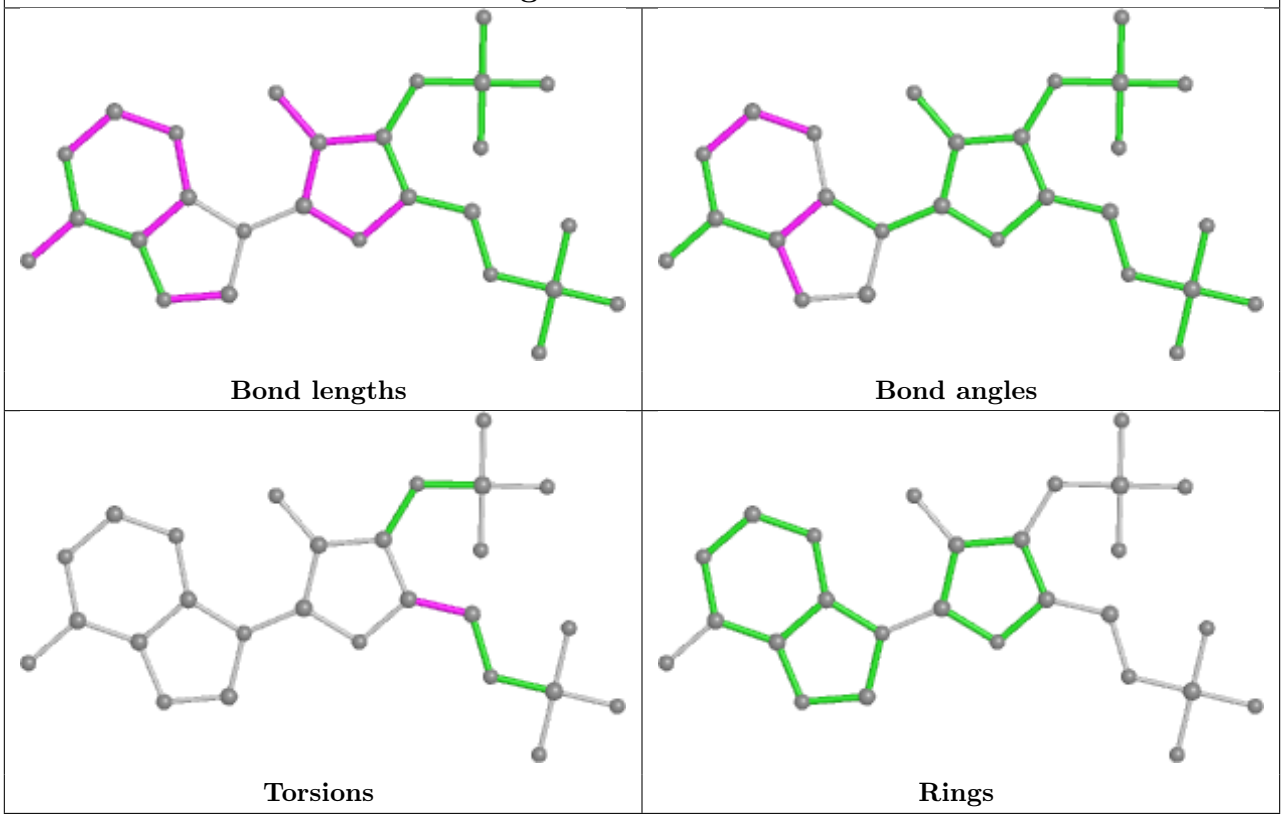
Ligand A3P E 2003



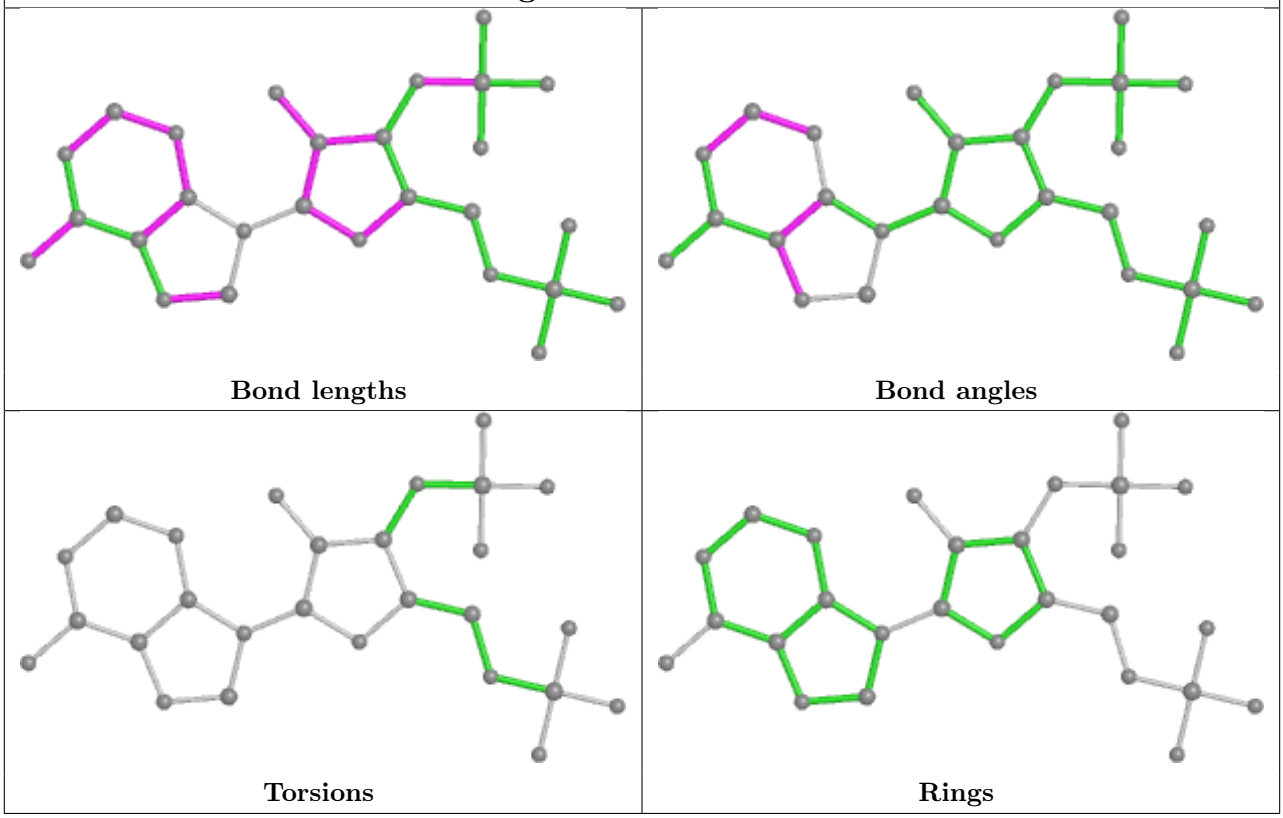
Ligand A3P B 2003



Ligand A3P F 2003



Ligand A3P A 2003



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	287/658 (43%)	-0.09	1 (0%)	94	92	48, 83, 133, 185	0
1	B	654/658 (99%)	1.41	180 (27%)	0	0	54, 196, 294, 399	0
1	C	655/658 (99%)	0.46	68 (10%)	6	8	63, 129, 207, 293	0
1	D	654/658 (99%)	0.34	41 (6%)	20	20	54, 128, 195, 252	0
1	E	654/658 (99%)	0.25	31 (4%)	31	31	58, 122, 191, 274	0
1	F	654/658 (99%)	1.06	150 (22%)	0	1	57, 170, 263, 333	0
All	All	3558/3948 (90%)	0.64	471 (13%)	3	5	48, 127, 250, 399	0

All (471) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	ILE	24.8
1	B	7	LEU	17.5
1	B	51	ALA	16.0
1	B	35	VAL	11.6
1	F	111	GLU	9.9
1	B	50	VAL	9.4
1	F	94	TRP	9.3
1	B	148	MET	9.3
1	B	52	ALA	9.2
1	B	48	PRO	8.9
1	B	64	HIS	8.8
1	F	285	LEU	8.8
1	B	11	ILE	8.7
1	B	5	GLY	8.5
1	B	59	ILE	8.3
1	B	67	PHE	8.2
1	B	104	ILE	8.1
1	F	110	VAL	8.1
1	B	269	ALA	7.8

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Mol	Chain	Res	Type	RSRZ
1	F	113	LEU	7.7
1	B	38	GLU	7.5
1	B	6	LYS	7.5
1	B	267	ASN	7.4
1	B	284	LEU	7.4
1	B	303	ALA	6.8
1	B	304	LEU	6.8
1	B	56	GLY	6.7
1	F	225	THR	6.7
1	B	227	ASN	6.6
1	B	103	LEU	6.5
1	F	276	ALA	6.5
1	F	37	VAL	6.5
1	B	47	PHE	6.4
1	F	106	TYR	6.3
1	B	226	ILE	6.2
1	F	244	VAL	6.2
1	B	351	ALA	6.1
1	F	280	LEU	6.1
1	F	104	ILE	6.1
1	B	114	SER	6.0
1	B	358	ASP	6.0
1	B	94	TRP	5.9
1	B	285	LEU	5.9
1	B	149	PHE	5.8
1	B	281	GLU	5.8
1	C	1189	ARG	5.7
1	B	87	ASP	5.7
1	F	92	PHE	5.6
1	B	4	GLU	5.6
1	B	306	SER	5.6
1	F	226	ILE	5.6
1	F	93	THR	5.5
1	B	9	ILE	5.4
1	B	124	ASN	5.4
1	F	301	ALA	5.4
1	D	146	ALA	5.4
1	F	91	PRO	5.3
1	B	141	ALA	5.3
1	B	280	LEU	5.3
1	B	225	THR	5.3
1	B	80	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	302	VAL	5.2
1	B	265	GLY	5.1
1	B	282	ASN	5.1
1	B	143	GLY	5.1
1	F	279	PHE	5.1
1	B	8	VAL	5.1
1	B	97	VAL	5.1
1	F	245	THR	5.0
1	B	122	LEU	5.0
1	B	99	TYR	5.0
1	D	112	ALA	5.0
1	F	112	ALA	4.9
1	B	78	GLU	4.9
1	B	299	LEU	4.9
1	B	134	ALA	4.9
1	B	350	ALA	4.9
1	F	304	LEU	4.8
1	F	284	LEU	4.8
1	F	324	ALA	4.8
1	B	61	PHE	4.6
1	B	106	TYR	4.6
1	F	35	VAL	4.6
1	F	224	MET	4.6
1	F	103	LEU	4.6
1	B	37	VAL	4.6
1	B	352	SER	4.5
1	B	10	TRP	4.5
1	F	115	LEU	4.5
1	B	133	PRO	4.5
1	F	105	ALA	4.5
1	F	80	THR	4.5
1	F	258	PHE	4.5
1	C	116	ILE	4.4
1	C	226	ILE	4.4
1	C	257	PRO	4.4
1	B	105	ALA	4.4
1	F	16	GLY	4.4
1	B	49	GLN	4.4
1	B	132	ILE	4.4
1	C	160	LEU	4.4
1	F	81	PRO	4.3
1	F	33	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	302	VAL	4.3
1	B	123	PRO	4.3
1	C	1177	LEU	4.3
1	F	15	LYS	4.2
1	E	244	VAL	4.2
1	C	224	MET	4.1
1	B	135	LEU	4.1
1	F	118	ASN	4.1
1	F	67	PHE	4.1
1	B	39	HIS	4.1
1	F	4	GLU	4.1
1	C	114	SER	4.0
1	B	195	LEU	4.0
1	B	100	ASN	4.0
1	B	93	THR	4.0
1	C	113	LEU	4.0
1	B	142	LYS	4.0
1	C	1173	TYR	4.0
1	C	157	THR	4.0
1	C	225	THR	3.9
1	F	275	LEU	3.9
1	C	120	ASP	3.9
1	F	330	MET	3.9
1	E	112	ALA	3.9
1	C	129	TRP	3.8
1	B	292	ALA	3.8
1	B	139	LEU	3.8
1	D	156	PHE	3.8
1	F	140	LYS	3.8
1	B	348	ILE	3.8
1	F	60	ILE	3.8
1	F	109	ALA	3.8
1	B	27	PHE	3.8
1	B	68	GLY	3.8
1	F	309	GLU	3.8
1	F	232	TRP	3.8
1	C	121	LEU	3.8
1	B	279	PHE	3.8
1	B	126	PRO	3.7
1	B	277	LYS	3.7
1	D	1355	SER	3.7
1	B	29	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	58	ASP	3.7
1	C	147	LEU	3.7
1	C	1187	LEU	3.7
1	B	272	ASN	3.7
1	D	113	LEU	3.7
1	F	20	LEU	3.7
1	B	198	LEU	3.7
1	C	126	PRO	3.7
1	D	226	ILE	3.7
1	F	329	ILE	3.6
1	B	131	GLU	3.6
1	F	231	ALA	3.6
1	B	129	TRP	3.6
1	F	323	ASN	3.6
1	F	59	ILE	3.6
1	C	115	LEU	3.6
1	F	247	LEU	3.6
1	B	278	GLU	3.6
1	F	122	LEU	3.6
1	B	293	VAL	3.6
1	B	102	LYS	3.6
1	C	149	PHE	3.6
1	F	281	GLU	3.6
1	B	208	THR	3.6
1	B	355	GLN	3.5
1	F	129	TRP	3.5
1	F	90	TYR	3.5
1	B	332	ASN	3.5
1	B	194	PHE	3.5
1	B	221	GLU	3.5
1	F	149	PHE	3.5
1	B	140	LYS	3.4
1	F	147	LEU	3.4
1	B	276	ALA	3.4
1	F	267	ASN	3.4
1	B	203	HIS	3.4
1	D	198	LEU	3.4
1	F	79	ILE	3.4
1	F	108	ILE	3.4
1	D	143	GLY	3.4
1	F	230	TRP	3.4
1	C	148	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	183	VAL	3.4
1	B	26	LYS	3.4
1	F	107	PRO	3.4
1	B	89	LEU	3.4
1	F	241	ASN	3.4
1	F	1187	LEU	3.4
1	D	126	PRO	3.4
1	F	160	LEU	3.4
1	B	138	GLU	3.4
1	B	3	GLU	3.3
1	B	144	LYS	3.3
1	F	278	GLU	3.3
1	F	142	LYS	3.3
1	B	79	ILE	3.3
1	B	357	VAL	3.3
1	F	1186	GLY	3.3
1	E	1288	ARG	3.3
1	B	92	PHE	3.3
1	E	224	MET	3.3
1	C	242	TYR	3.3
1	E	113	LEU	3.3
1	B	86	GLN	3.3
1	B	250	PHE	3.3
1	C	145	SER	3.2
1	B	283	TYR	3.2
1	B	125	PRO	3.2
1	F	96	ALA	3.2
1	B	113	LEU	3.2
1	F	19	GLY	3.2
1	F	114	SER	3.2
1	F	36	THR	3.2
1	F	7	LEU	3.2
1	B	24	GLY	3.2
1	E	147	LEU	3.2
1	B	121	LEU	3.2
1	D	144	LYS	3.1
1	D	244	VAL	3.1
1	E	114	SER	3.1
1	B	137	LYS	3.1
1	B	330	MET	3.1
1	F	163	ALA	3.1
1	C	112	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	222	THR	3.1
1	E	129	TRP	3.1
1	C	1191	LYS	3.1
1	F	2	ILE	3.1
1	F	227	ASN	3.1
1	B	36	THR	3.1
1	B	108	ILE	3.1
1	B	147	LEU	3.1
1	B	300	GLY	3.1
1	B	309	GLU	3.1
1	D	203	HIS	3.1
1	D	129	TRP	3.0
1	C	223	ALA	3.0
1	D	303	ALA	3.0
1	F	250	PHE	3.0
1	B	211	SER	3.0
1	F	272	ASN	3.0
1	F	273	LYS	3.0
1	F	246	VAL	3.0
1	F	322	GLU	3.0
1	C	241	ASN	3.0
1	B	210	TYR	3.0
1	F	97	VAL	3.0
1	B	261	VAL	2.9
1	F	257	PRO	2.9
1	C	244	VAL	2.9
1	F	340	TRP	2.9
1	B	145	SER	2.9
1	B	109	ALA	2.9
1	F	200	LYS	2.9
1	E	117	TYR	2.9
1	F	242	TYR	2.9
1	D	92	PHE	2.9
1	D	205	ASN	2.9
1	B	259	VAL	2.9
1	F	82	ASP	2.9
1	F	95	ASP	2.9
1	B	81	PRO	2.9
1	C	201	ASN	2.9
1	D	135	LEU	2.9
1	B	223	ALA	2.9
1	B	290	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	156	PHE	2.9
1	B	353	GLY	2.9
1	D	150	ASN	2.8
1	F	217	PHE	2.8
1	F	290	LEU	2.8
1	D	199	ILE	2.8
1	F	64	HIS	2.8
1	C	258	PHE	2.8
1	B	183	VAL	2.8
1	E	183	VAL	2.8
1	E	250	PHE	2.8
1	F	62	TRP	2.8
1	B	110	VAL	2.8
1	F	12	ASN	2.8
1	C	227	ASN	2.8
1	C	122	LEU	2.8
1	B	66	ARG	2.8
1	C	247	LEU	2.8
1	F	320	THR	2.8
1	B	112	ALA	2.7
1	F	303	ALA	2.7
1	F	1194	ASP	2.7
1	B	356	THR	2.7
1	D	245	THR	2.7
1	F	6	LYS	2.7
1	E	1290	THR	2.7
1	F	27	PHE	2.7
1	F	144	LYS	2.7
1	F	189	LYS	2.7
1	B	196	VAL	2.7
1	C	118	ASN	2.7
1	B	347	VAL	2.7
1	B	2	ILE	2.7
1	B	275	LEU	2.6
1	D	115	LEU	2.6
1	C	159	PRO	2.6
1	F	65	ASP	2.6
1	C	146	ALA	2.6
1	C	151	LEU	2.6
1	C	169	PHE	2.6
1	F	11	ILE	2.6
1	D	116	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	301	ALA	2.6
1	D	117	TYR	2.6
1	C	222	THR	2.6
1	B	45	GLU	2.6
1	C	144	LYS	2.6
1	B	334	PRO	2.6
1	E	126	PRO	2.6
1	F	38	GLU	2.5
1	D	162	ALA	2.5
1	E	242	TYR	2.5
1	C	156	PHE	2.5
1	B	57	PRO	2.5
1	B	201	ASN	2.5
1	C	109	ALA	2.5
1	F	3	GLU	2.5
1	F	89	LEU	2.5
1	F	85	PHE	2.5
1	D	107	PRO	2.5
1	E	1355	SER	2.5
1	D	195	LEU	2.5
1	B	22	GLU	2.5
1	F	14	ASP	2.5
1	B	335	GLN	2.5
1	B	23	VAL	2.5
1	F	126	PRO	2.5
1	B	85	PHE	2.5
1	B	151	LEU	2.5
1	B	136	ASP	2.5
1	F	120	ASP	2.5
1	F	34	LYS	2.5
1	F	57	PRO	2.5
1	D	259	VAL	2.4
1	C	245	THR	2.4
1	B	91	PRO	2.4
1	C	1183	TYR	2.4
1	F	270	SER	2.4
1	A	1069	ASP	2.4
1	F	260	GLY	2.4
1	F	1069	ASP	2.4
1	C	178	ILE	2.4
1	B	197	ASP	2.4
1	B	274	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	152	GLN	2.4
1	D	147	LEU	2.4
1	C	125	PRO	2.4
1	C	248	PRO	2.4
1	F	148	MET	2.4
1	B	263	SER	2.4
1	F	116	ILE	2.4
1	C	208	THR	2.4
1	F	218	ASN	2.4
1	B	96	ALA	2.4
1	C	203	HIS	2.4
1	F	269	ALA	2.4
1	F	308	GLU	2.4
1	F	354	ARG	2.4
1	F	5	GLY	2.4
1	F	24	GLY	2.4
1	F	169	PHE	2.4
1	D	192	LEU	2.3
1	E	116	ILE	2.3
1	F	133	PRO	2.3
1	C	117	TYR	2.3
1	B	53	THR	2.3
1	B	200	LYS	2.3
1	C	184	ASP	2.3
1	D	224	MET	2.3
1	F	222	THR	2.3
1	C	132	ILE	2.3
1	D	151	LEU	2.3
1	B	12	ASN	2.3
1	F	325	GLN	2.3
1	E	195	LEU	2.3
1	B	154	PRO	2.3
1	E	328	GLU	2.3
1	B	21	ALA	2.3
1	B	116	ILE	2.3
1	C	1186	GLY	2.3
1	E	160	LEU	2.3
1	E	1177	LEU	2.3
1	F	339	PHE	2.3
1	F	328	GLU	2.3
1	F	282	ASN	2.3
1	C	1296	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	259	VAL	2.2
1	B	71	ALA	2.2
1	E	111	GLU	2.2
1	B	76	LEU	2.2
1	E	148	MET	2.2
1	D	218	ASN	2.2
1	E	133	PRO	2.2
1	C	1198	PHE	2.2
1	E	1176	PHE	2.2
1	C	320	THR	2.2
1	D	149	PHE	2.2
1	B	1069	ASP	2.2
1	F	283	TYR	2.2
1	F	292	ALA	2.2
1	B	361	LEU	2.2
1	C	204	MET	2.2
1	F	78	GLU	2.2
1	C	299	LEU	2.2
1	D	139	LEU	2.2
1	F	321	MET	2.2
1	F	223	ALA	2.2
1	B	236	ASP	2.2
1	F	87	ASP	2.2
1	B	230	TRP	2.2
1	F	32	GLY	2.2
1	F	86	GLN	2.2
1	F	9	ILE	2.2
1	B	155	TYR	2.2
1	F	237	THR	2.2
1	E	157	THR	2.1
1	B	252	GLY	2.1
1	C	1288	ARG	2.1
1	E	164	ASP	2.1
1	E	109	ALA	2.1
1	B	157	THR	2.1
1	F	23	VAL	2.1
1	B	120	ASP	2.1
1	B	264	ALA	2.1
1	F	39	HIS	2.1
1	C	61	PHE	2.1
1	C	1176	PHE	2.1
1	C	161	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	136	ASP	2.1
1	C	106	TYR	2.1
1	F	264	ALA	2.1
1	D	145	SER	2.1
1	B	253	GLN	2.1
1	C	1287	LEU	2.1
1	F	55	ASP	2.1
1	F	156	PHE	2.1
1	D	93	THR	2.0
1	F	357	VAL	2.0
1	D	304	LEU	2.0
1	F	1191	LYS	2.0
1	B	260	GLY	2.0
1	B	349	ASN	2.0
1	D	320	THR	2.0
1	D	160	LEU	2.0
1	E	149	PHE	2.0
1	C	1192	GLN	2.0
1	E	155	TYR	2.0
1	B	115	LEU	2.0
1	B	213	ALA	2.0
1	B	268	ALA	2.0
1	F	1193	GLY	2.0
1	C	150	ASN	2.0
1	B	88	LYS	2.0
1	F	99	TYR	2.0
1	F	266	ILE	2.0
1	F	1288	ARG	2.0
1	B	288	GLU	2.0
1	B	117	TYR	2.0
1	C	347	VAL	2.0
1	D	155	TYR	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BDP	P	5	12/13	0.68	0.24	136,206,212,214	0
2	BDP	P	1	13/13	0.69	0.39	120,143,173,179	0
2	BDP	P	7	12/13	0.72	0.39	195,218,230,230	0
3	GLC	H	2	11/12	0.72	0.35	218,235,256,257	0
2	BDP	N	5	12/13	0.75	0.44	145,194,213,217	0
3	GLC	H	1	12/12	0.77	0.27	197,218,230,239	0
2	BDP	N	7	12/13	0.77	0.45	186,205,213,218	0
2	BDP	G	7	12/13	0.78	0.39	179,197,225,229	0
2	BDP	L	7	12/13	0.81	0.25	172,199,213,219	0
2	NDG	P	6	14/15	0.83	0.22	145,173,202,210	0
2	BDP	L	5	12/13	0.83	0.20	126,144,163,173	0
2	BDP	N	1	12/13	0.85	0.18	146,191,216,218	0
2	IDR	P	3	12/13	0.87	0.23	142,162,187,200	0
2	NDG	N	6	14/15	0.87	0.30	139,188,202,212	0
2	BDP	I	7	12/13	0.88	0.16	148,161,172,176	0
2	BDP	G	5	12/13	0.88	0.15	95,130,153,167	0
3	GLC	O	2	11/12	0.89	0.31	149,166,181,185	0
2	NDG	L	6	14/15	0.90	0.18	104,145,162,178	0
3	GLC	K	1	12/12	0.90	0.28	135,142,153,154	0
2	GNS	P	4	15/16	0.90	0.28	112,150,186,198	0
2	GNS	P	2	15/16	0.91	0.53	177,183,197,203	0
3	GLC	O	1	12/12	0.91	0.24	165,176,181,186	0
2	BDP	I	5	12/13	0.91	0.14	108,137,152,153	0
2	NDG	G	6	14/15	0.92	0.17	107,132,150,170	0
3	GLC	K	2	11/12	0.93	0.25	92,109,127,127	0
2	BDP	L	1	12/13	0.93	0.14	103,127,150,155	0
2	NDG	I	6	14/15	0.93	0.13	109,128,158,160	0
2	GNS	L	2	15/16	0.94	0.18	100,120,139,152	0
2	GNS	N	2	15/16	0.94	0.28	150,164,191,196	0
2	IDR	I	3	12/13	0.94	0.20	100,112,121,124	0
2	IDR	N	3	12/13	0.95	0.31	128,148,209,213	0
3	GLC	J	1	12/12	0.96	0.30	95,124,137,149	0
2	BDP	G	1	12/13	0.96	0.15	68,93,105,108	0
2	GNS	I	2	15/16	0.96	0.18	84,89,108,118	0
3	GLC	M	1	12/12	0.96	0.33	88,98,112,113	0
2	GNS	L	4	15/16	0.96	0.19	88,117,142,145	0
2	GNS	N	4	15/16	0.96	0.24	123,144,168,187	0
2	IDR	G	3	12/13	0.97	0.24	68,88,103,113	0
2	IDR	L	3	12/13	0.97	0.19	103,126,151,165	0
2	GNS	G	2	15/16	0.97	0.17	63,75,99,100	0
2	BDP	I	1	12/13	0.97	0.18	77,94,107,109	0

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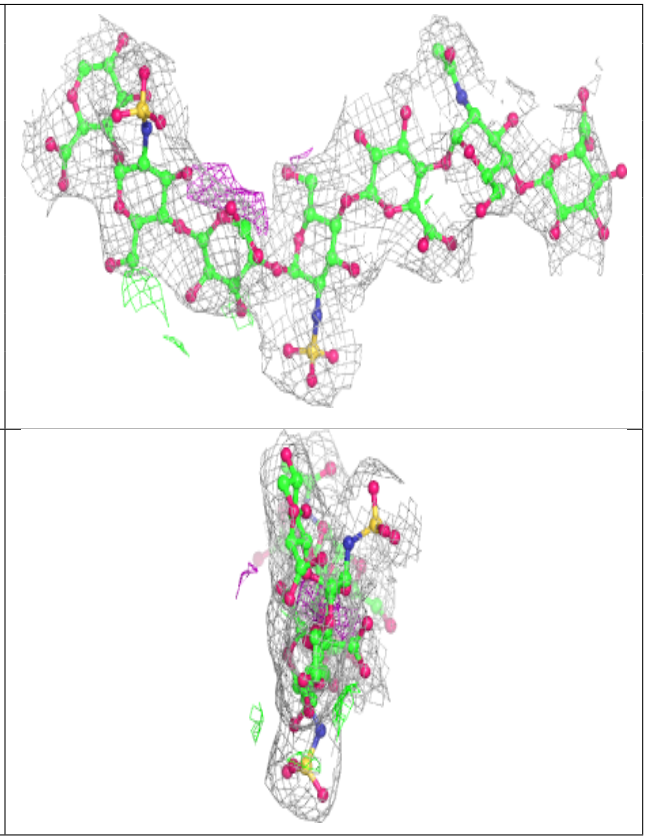
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	J	2	11/12	0.98	0.13	93,97,110,112	0
3	GLC	M	2	11/12	0.98	0.20	79,95,124,133	0
2	GNS	I	4	15/16	0.98	0.18	79,93,110,133	0
2	GNS	G	4	15/16	0.98	0.20	72,78,98,101	0

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.

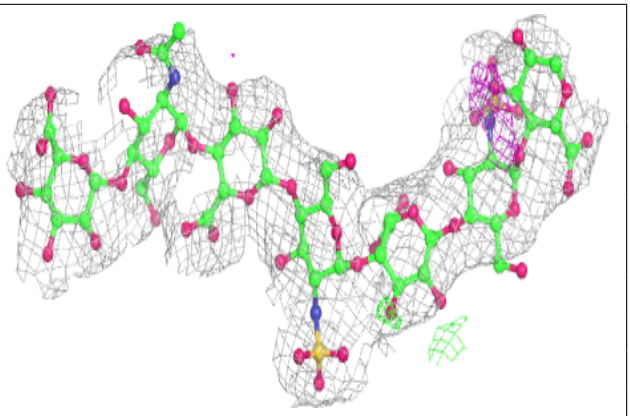
Electron density around Chain G:

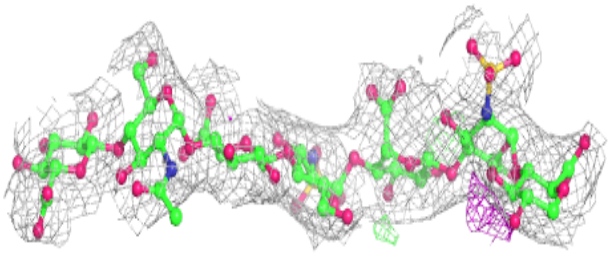
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

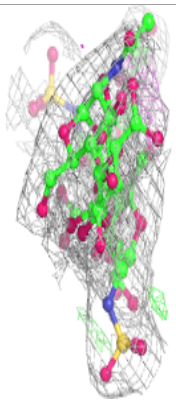


Electron density around Chain I:

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

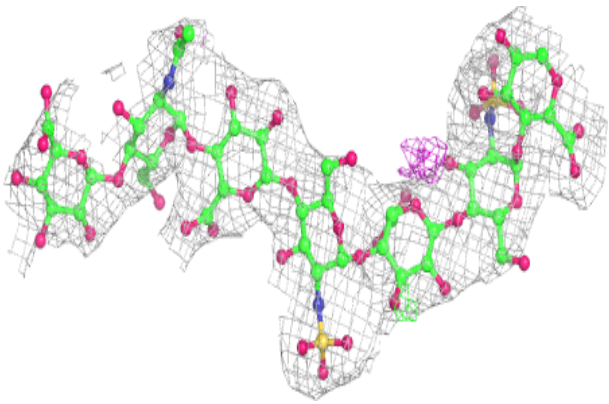


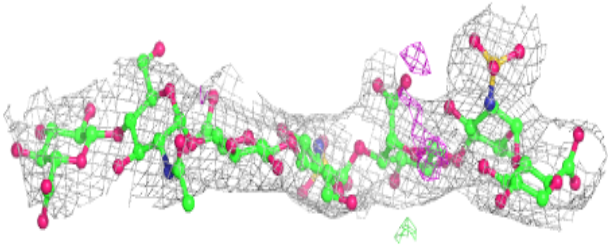


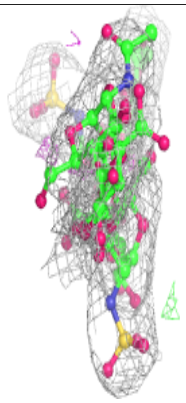


Electron density around Chain L:

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

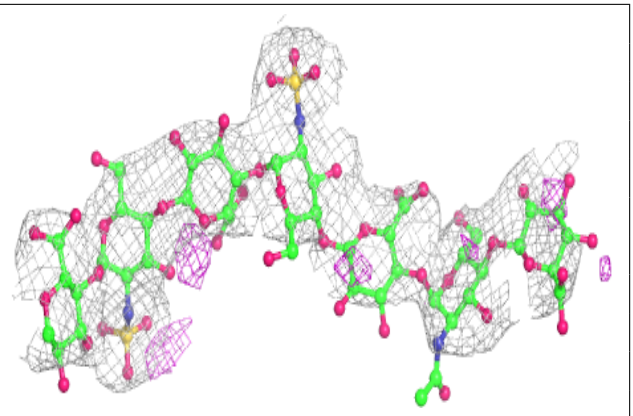


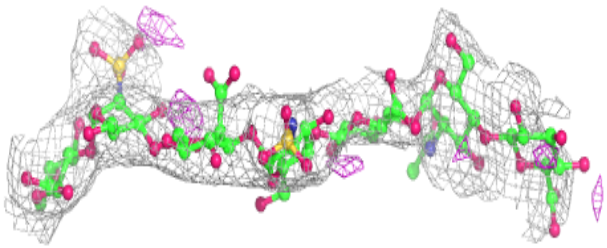


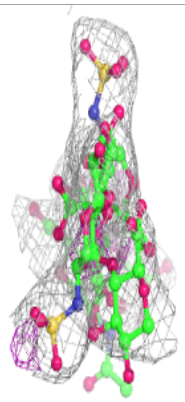


Electron density around Chain N:

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

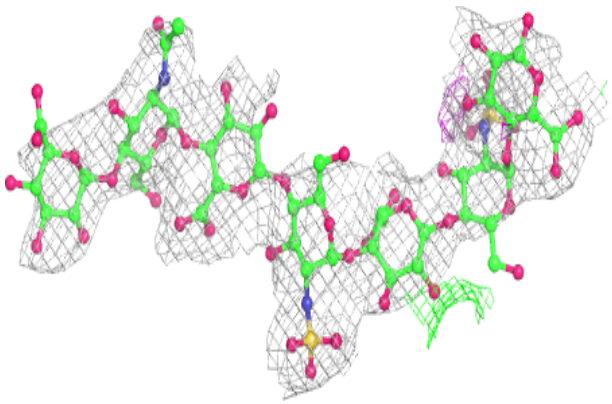


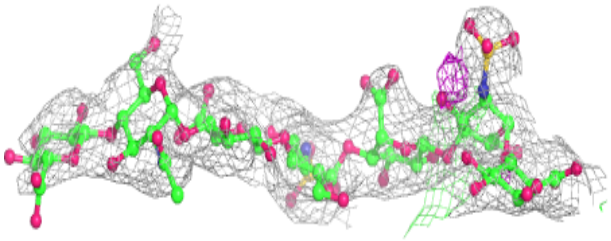




Electron density around Chain P:

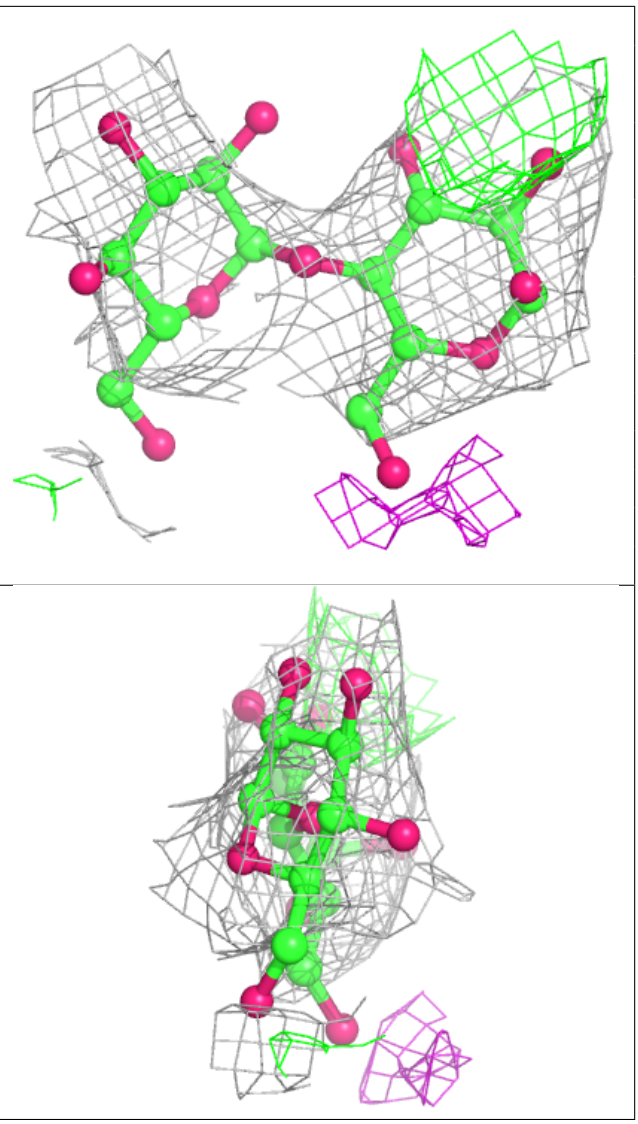
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





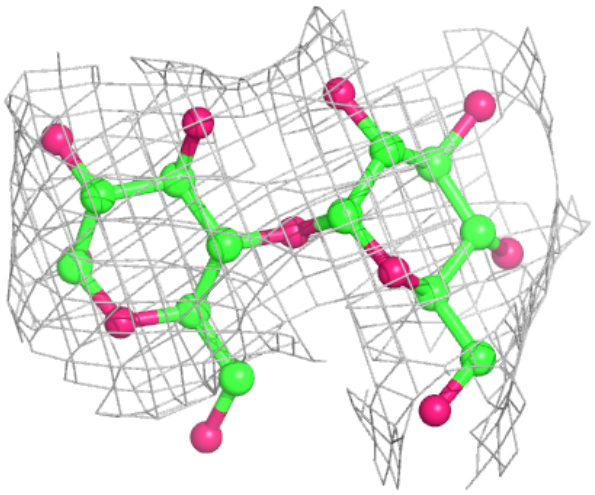
Electron density around Chain H:

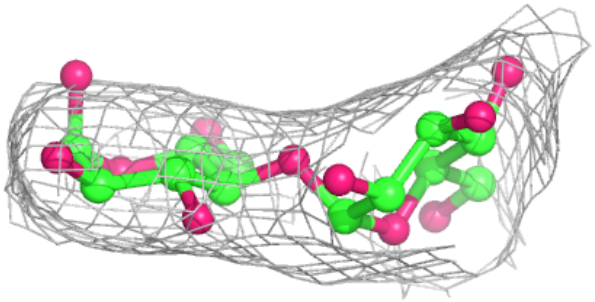
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

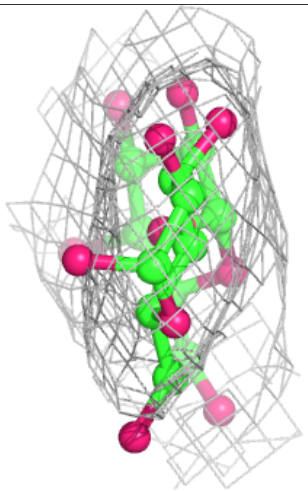


Electron density around Chain J:

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

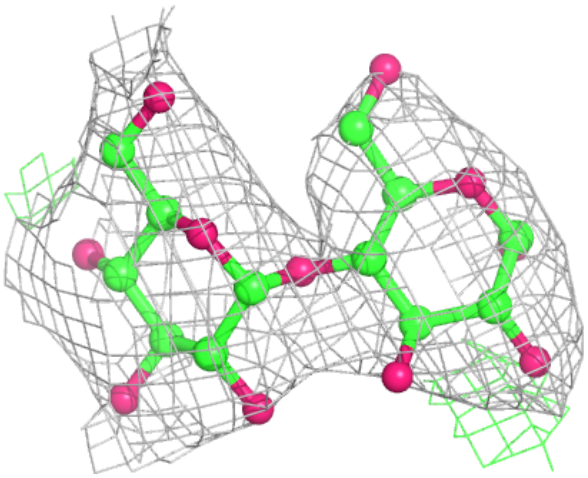


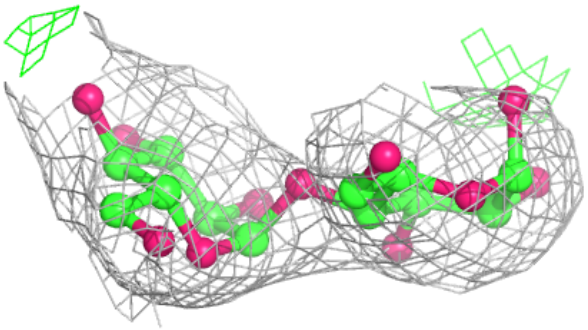


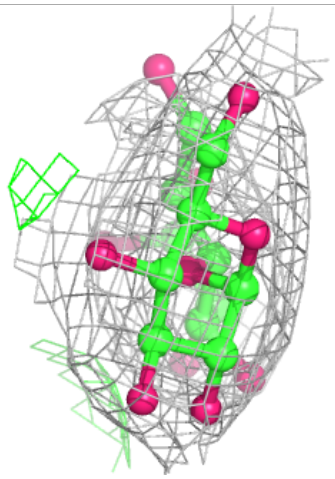


Electron density around Chain K:

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

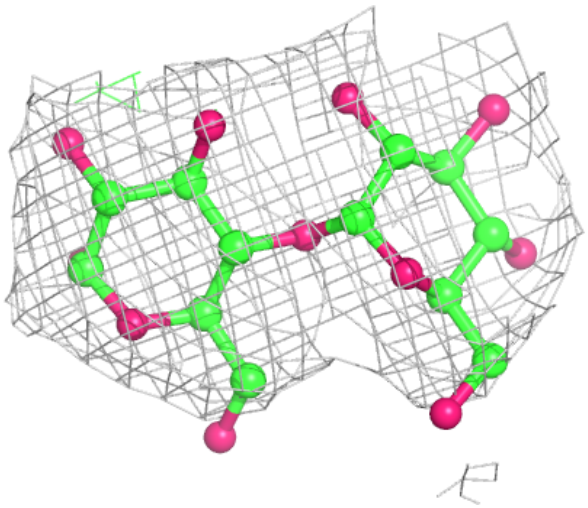


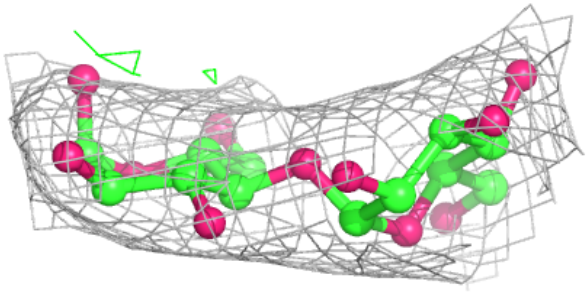


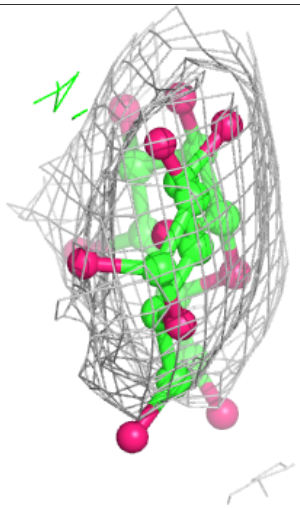


Electron density around Chain M:

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

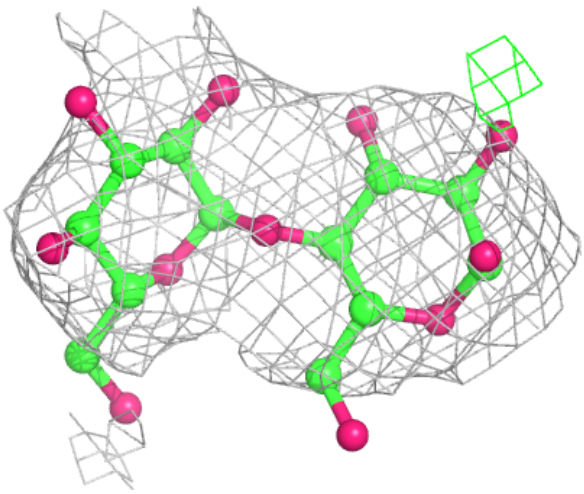


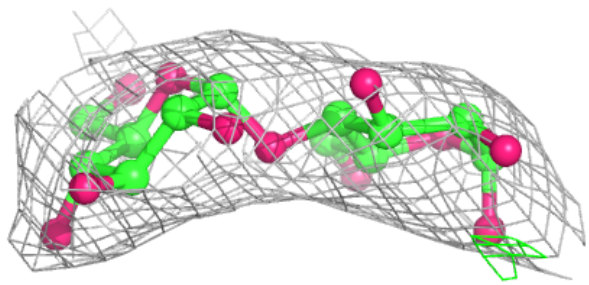


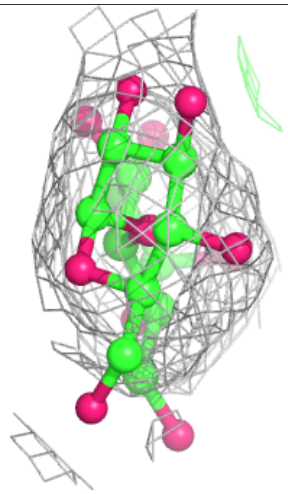


Electron density around Chain O:

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







6.4 Ligands (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
5	NPO	E	2011	10/10	0.73	0.37	157,172,185,189	0
5	NPO	D	2011	10/10	0.89	0.29	159,170,199,200	0
5	NPO	A	2011	10/10	0.92	0.31	103,138,146,154	0
4	A3P	C	2003	27/27	0.93	0.21	74,106,135,145	0
4	A3P	E	2003	27/27	0.94	0.27	80,104,114,119	0
4	A3P	F	2003	27/27	0.96	0.20	67,89,104,115	0
5	NPO	B	2011	10/10	0.96	0.30	105,120,169,173	0
4	A3P	B	2003	27/27	0.97	0.18	66,80,103,148	0
4	A3P	A	2003	27/27	0.97	0.18	53,68,87,93	0

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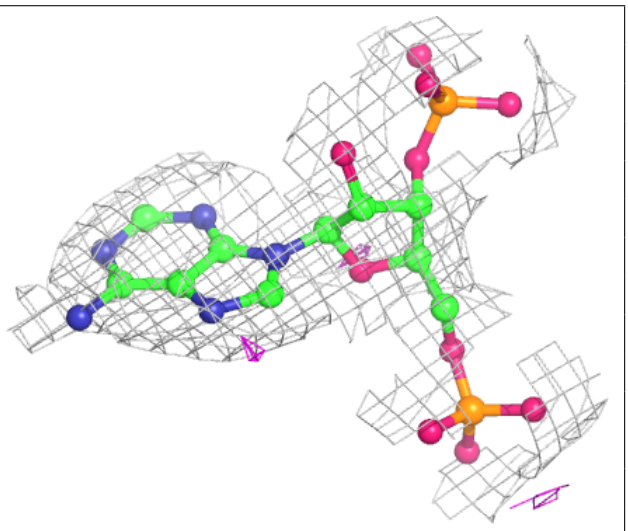
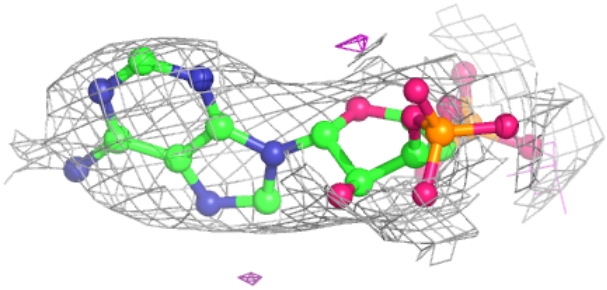
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	A3P	D	2003	27/27	0.97	0.20	57,83,108,112	0

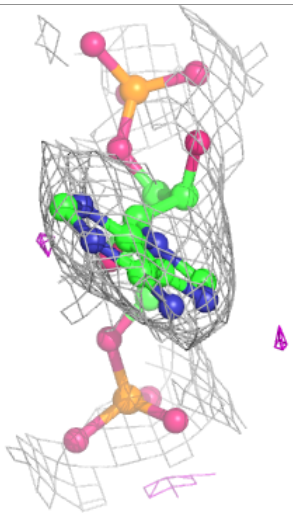
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A3P C 2003:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

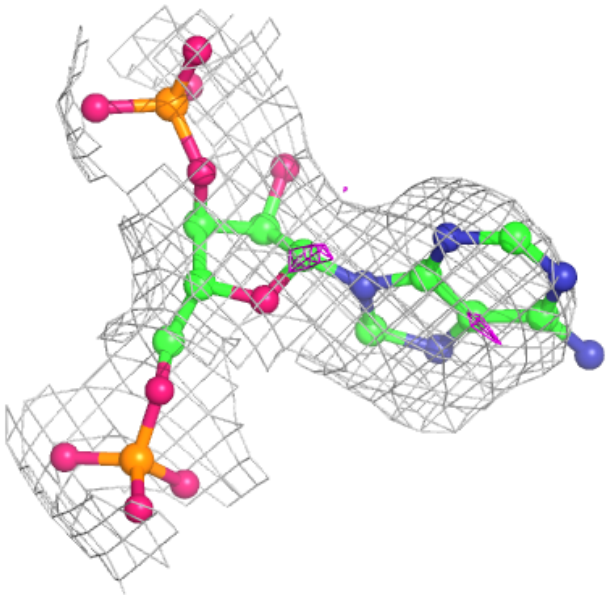


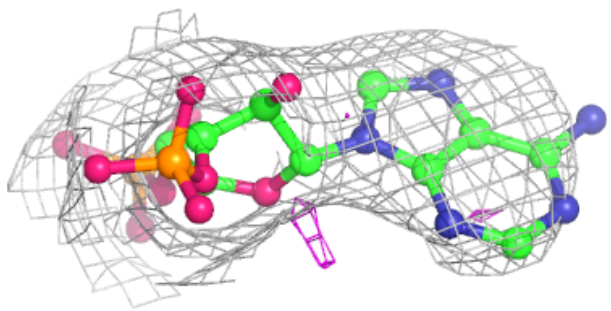


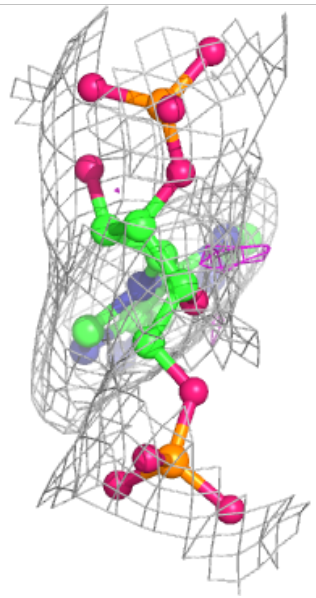


Electron density around A3P E 2003:

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

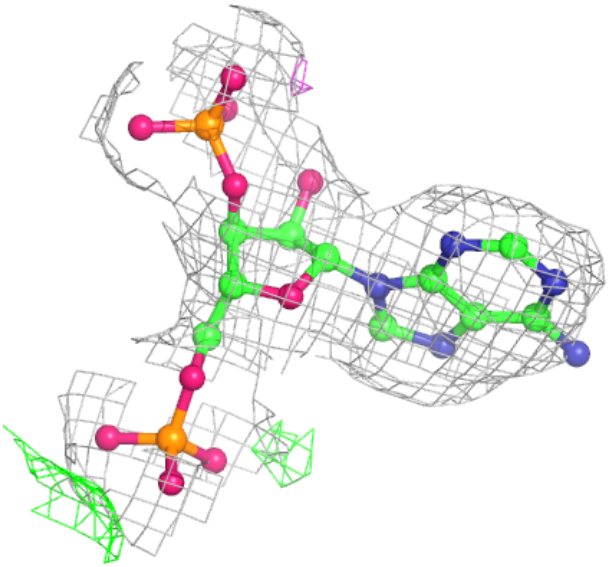


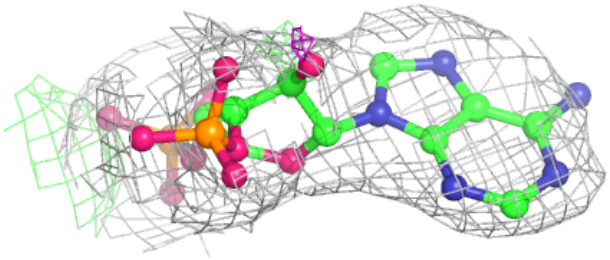


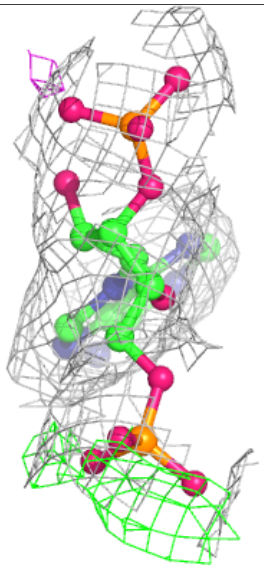


Electron density around A3P F 2003:

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

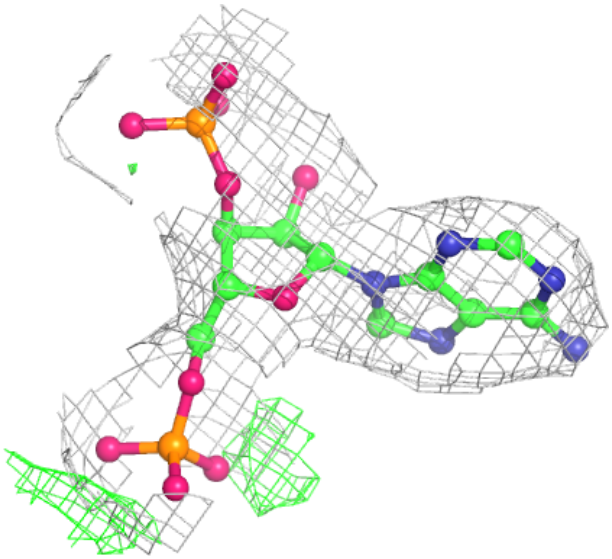


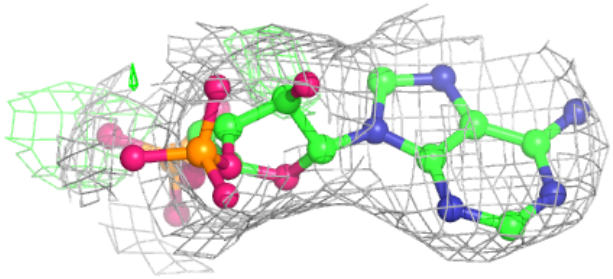


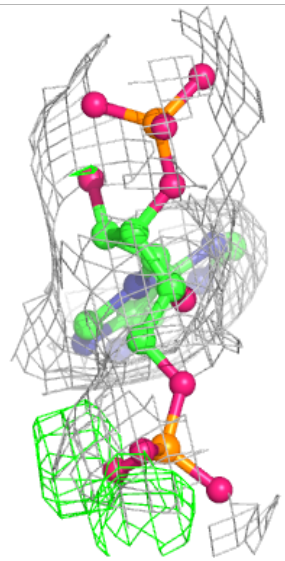


Electron density around A3P B 2003:

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

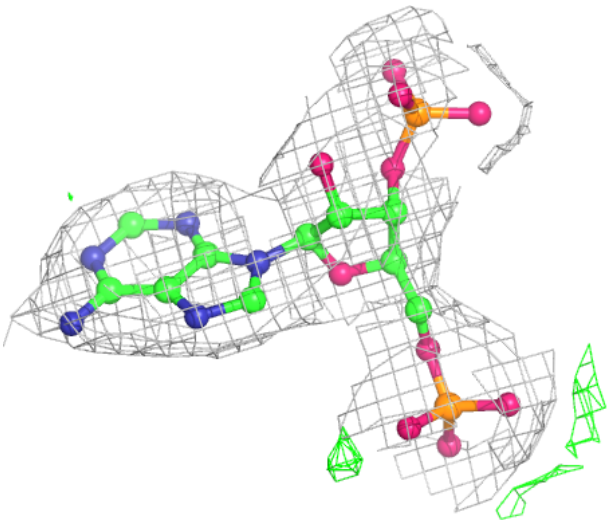


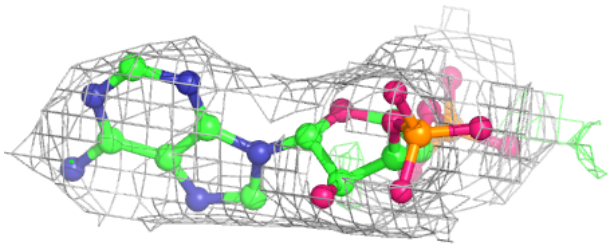


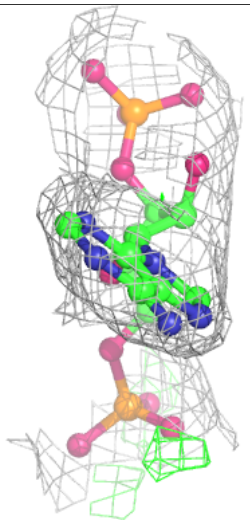


Electron density around A3P A 2003:

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

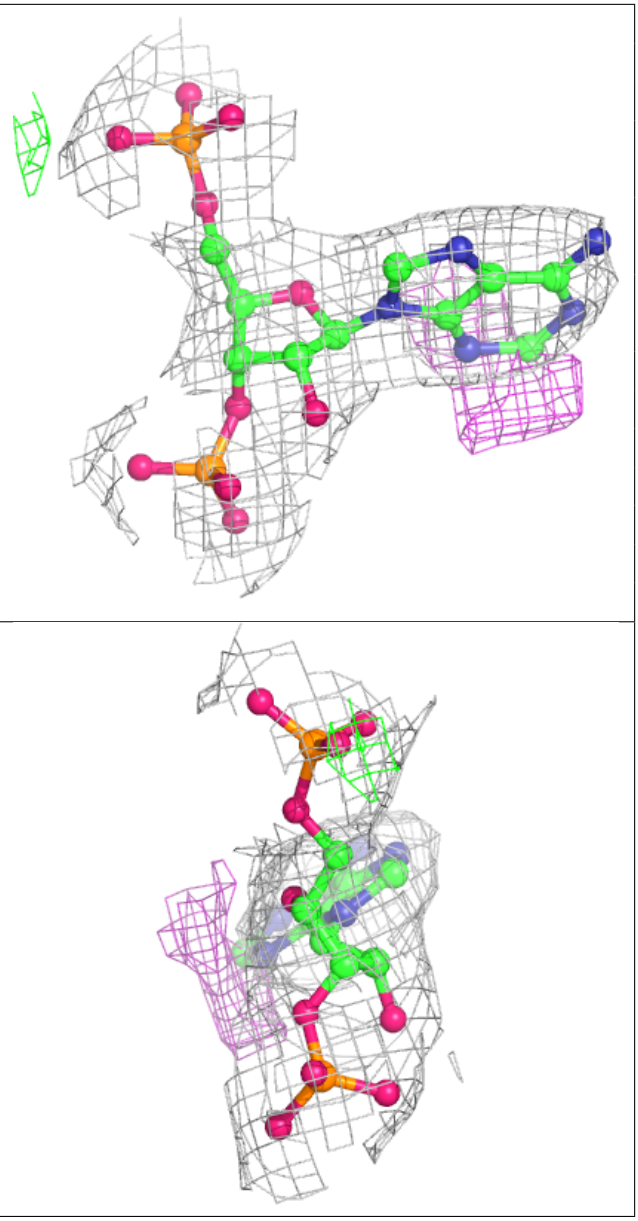






Electron density around A3P D 2003:

$2mF_o$-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.