Full wwPDB X-ray Structure Validation Report (i)

Jan 6, 2024 – 09:59 pm GMT

PDB ID	:	6EJK
Title	:	Structure of a glycosyltransferase
Authors	:	Ramirez, A.S.; Boilevin, J.; Mehdipour, A.R.; Hummer, G.; Darbre, T.; Reymond, J.L.; Locher, K.P.
Deposited on	:	2017-09-21
Resolution	:	3.30 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:

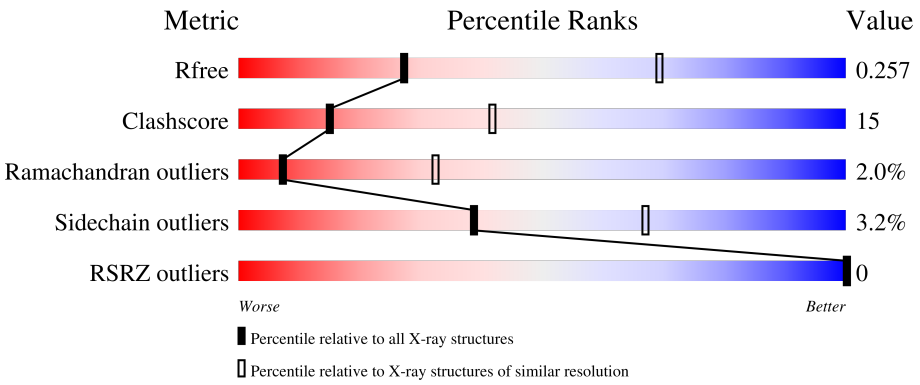
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	373	62% 33% • •
1	B	373	62% 32% • •
2	C	3	100%
2	D	3	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6012 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 WlaC protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	360	2914	1886	486	529	9	4	0	0	0
1	B	360	2914	1886	486	529	9	4	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP O86151
A	2	MSE	-	expression tag	UNP O86151
A	3	MSE	-	expression tag	UNP O86151
A	361	LEU	-	expression tag	UNP O86151
A	362	GLY	-	expression tag	UNP O86151
A	363	SER	-	expression tag	UNP O86151
A	364	HIS	-	expression tag	UNP O86151
A	365	HIS	-	expression tag	UNP O86151
A	366	HIS	-	expression tag	UNP O86151
A	367	HIS	-	expression tag	UNP O86151
A	368	HIS	-	expression tag	UNP O86151
A	369	HIS	-	expression tag	UNP O86151
A	370	HIS	-	expression tag	UNP O86151
A	371	HIS	-	expression tag	UNP O86151
A	372	HIS	-	expression tag	UNP O86151
A	373	HIS	-	expression tag	UNP O86151
B	1	MSE	-	initiating methionine	UNP O86151
B	2	MSE	-	expression tag	UNP O86151
B	3	MSE	-	expression tag	UNP O86151
B	361	LEU	-	expression tag	UNP O86151
B	362	GLY	-	expression tag	UNP O86151
B	363	SER	-	expression tag	UNP O86151
B	364	HIS	-	expression tag	UNP O86151
B	365	HIS	-	expression tag	UNP O86151
B	366	HIS	-	expression tag	UNP O86151

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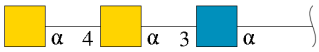
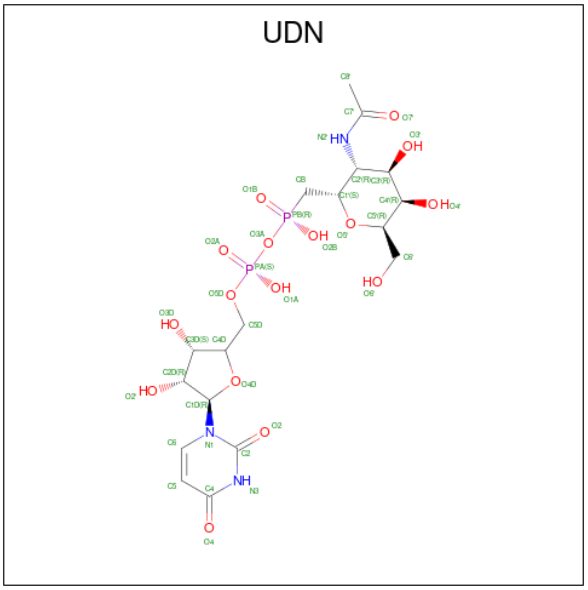
Chain	Residue	Modelled	Actual	Comment	Reference
B	367	HIS	-	expression tag	UNP O86151
B	368	HIS	-	expression tag	UNP O86151
B	369	HIS	-	expression tag	UNP O86151
B	370	HIS	-	expression tag	UNP O86151
B	371	HIS	-	expression tag	UNP O86151
B	372	HIS	-	expression tag	UNP O86151
B	373	HIS	-	expression tag	UNP O86151

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



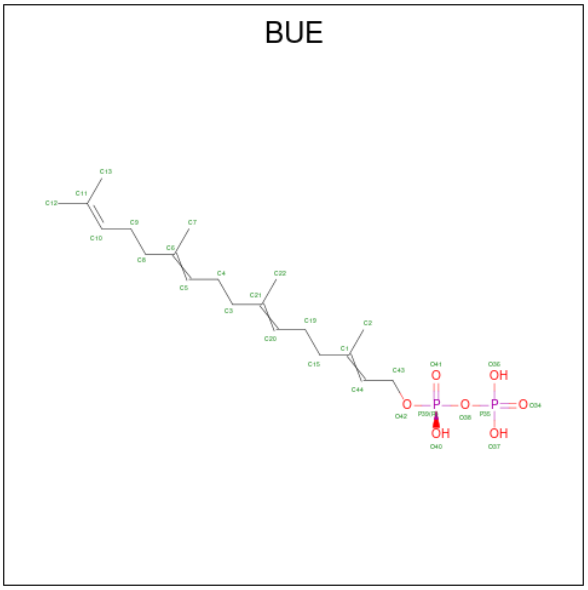
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	42	24	3	15	0	0	0
			Total	C	N	O			
2	D	3	42	24	3	15	0	0	0

- Molecule 3 is Uridine-Diphosphate-Methylene-N-acetyl-galactosamine (three-letter code: UDN) (formula: $C_{18}H_{29}N_3O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 39	C 18	N 3	O 16	P 2	0	0
3	B	1	Total 39	C 18	N 3	O 16	P 2	0	0

- Molecule 4 is NerylNeryl pyrophosphate (three-letter code: BUE) (formula: $C_{20}H_{36}O_7P_2$).



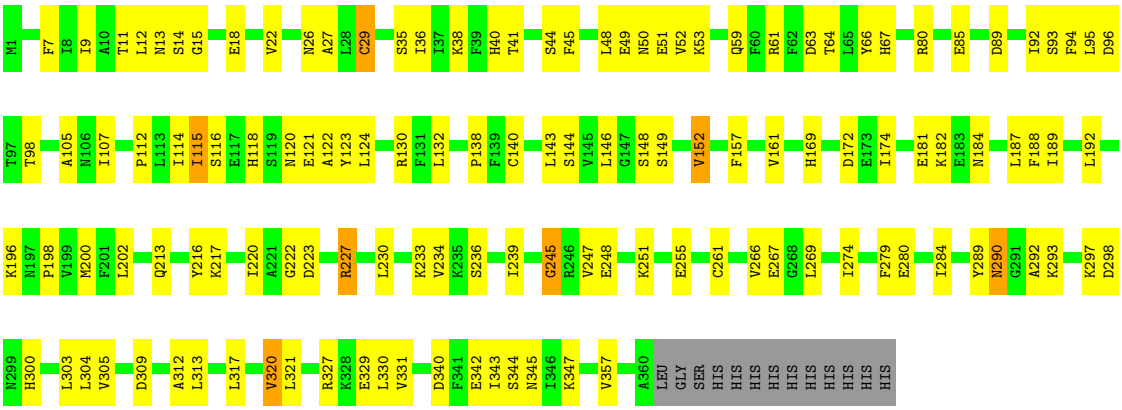
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 11	C 2	O 7	P 2	0	0
4	B	1	Total 11	C 2	O 7	P 2	0	0

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.

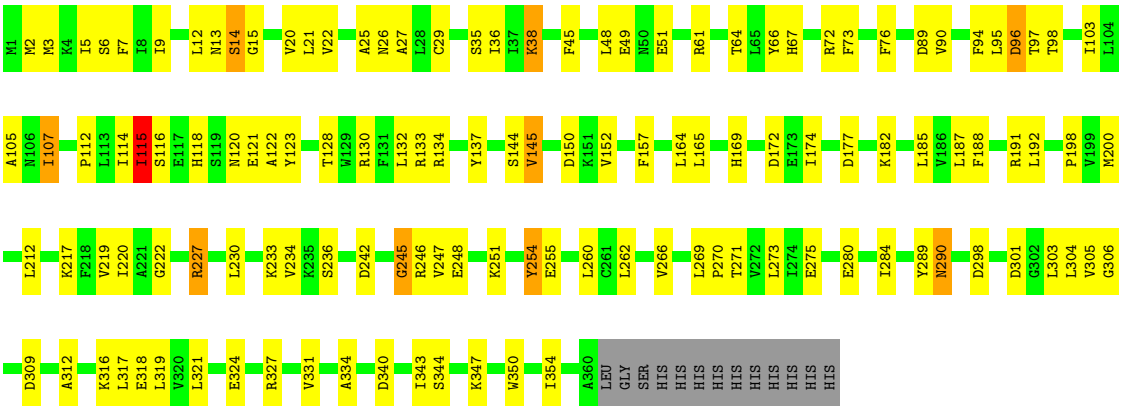
• Molecule 1: WlaC protein

Chain A: 62% 33%



• Molecule 1: WlaC protein

Chain B: 62% 32%



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

Chain C: 100%

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.87Å 126.91Å 71.09Å 90.00° 90.27° 90.00°	Depositor
Resolution (Å)	29.89 – 3.30 29.89 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.89-3.30) 87.1 (29.89-2.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.211 , 0.254 0.216 , 0.257	Depositor DCC
R_{free} test set	1016 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	75.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 4.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6012	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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: BUE, UDN, NDG, A2G

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	0.65	1/2965 (0.0%)	0.69	0/3983
1	B	0.61	0/2965	0.68	0/3983
All	All	0.63	1/5930 (0.0%)	0.69	0/7966

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	CYS	CB-SG	-6.47	1.71	1.82

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	2914	0	2992	91	0
1	B	2914	0	2992	84	0
2	C	42	0	34	6	0
2	D	42	0	34	8	0
3	A	39	0	0	3	0
3	B	39	0	0	2	0
4	A	11	0	0	0	0
4	B	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6012	0	6052	182	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 15.

All (182) 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)
2:D:2:A2G:C6	2:D:2:A2G:O6	1.64	1.45
2:C:2:A2G:C6	2:C:2:A2G:O6	1.68	1.40
1:A:280:GLU:HA	1:A:331:VAL:HG11	1.33	1.08
1:B:324:GLU:OE2	1:B:327:ARG:NH1	1.86	1.08
1:B:324:GLU:CD	1:B:327:ARG:HH11	1.65	0.99
1:A:116:SER:HB3	1:A:144:SER:HB3	1.47	0.93
1:B:280:GLU:HA	1:B:331:VAL:HG11	1.48	0.93
1:B:22:VAL:HG13	1:B:48:LEU:HD13	1.56	0.87
2:D:2:A2G:O6	2:D:2:A2G:C5	2.33	0.75
1:A:22:VAL:HG13	1:A:48:LEU:HD13	1.70	0.74
1:B:29:CYS:SG	1:B:51:GLU:HB2	2.27	0.73
1:A:247:VAL:N	3:A:401:UDN:O4	2.20	0.73
1:B:116:SER:HB3	1:B:144:SER:HB3	1.74	0.69
2:C:1:NDG:O4	2:C:2:A2G:N2	2.26	0.69
1:B:191:ARG:NH1	2:D:3:A2G:H2	2.08	0.68
1:B:266:VAL:HG23	1:B:289:TYR:HB3	1.76	0.67
1:A:266:VAL:HG23	1:A:289:TYR:HB3	1.76	0.67
1:A:115:ILE:HD11	1:A:140:CYS:SG	2.35	0.67
1:A:188:PHE:HD2	1:A:220:ILE:HG23	1.61	0.66
1:B:247:VAL:N	3:B:401:UDN:O4	2.27	0.65
2:C:2:A2G:O6	2:C:2:A2G:C5	2.44	0.65
1:A:61:ARG:HH12	1:B:248:GLU:CD	2.00	0.64
1:A:280:GLU:CA	1:A:331:VAL:HG11	2.18	0.63
1:A:85:GLU:O	1:A:85:GLU:HG2	1.99	0.63
1:A:169:HIS:HA	1:A:343:ILE:HD11	1.81	0.62
1:A:309:ASP:HB3	1:A:312:ALA:HB3	1.80	0.62
1:B:309:ASP:HB3	1:B:312:ALA:HB3	1.81	0.62
1:B:121:GLU:OE1	1:B:130:ARG:NH2	2.31	0.61
1:A:342:GLU:CD	1:A:344:SER:OG	2.38	0.61
1:B:133:ARG:O	1:B:137:TYR:HB2	2.00	0.60
1:A:251:LYS:O	1:A:255:GLU:HG3	2.02	0.59
1:A:93:SER:OG	1:A:115:ILE:HG22	2.03	0.59
1:B:98:THR:OG1	2:D:2:A2G:H8	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:MSE:HE1	1:B:305:VAL:HG21	1.86	0.58
1:B:26:ASN:OD1	1:B:49:GLU:HB2	2.04	0.58
1:B:298:ASP:HB2	1:B:304:LEU:HD12	1.85	0.57
1:A:61:ARG:NH1	1:B:248:GLU:CD	2.57	0.57
2:C:2:A2G:C6	2:C:2:A2G:H15	2.11	0.57
1:A:64:THR:HG22	1:A:66:TYR:H	1.70	0.57
1:B:301:ASP:HB2	1:B:334:ALA:HB2	1.85	0.56
1:A:196:LYS:NZ	3:A:401:UDN:O2B	2.39	0.56
1:B:251:LYS:O	1:B:255:GLU:HG3	2.06	0.56
1:B:2:MSE:HG3	1:B:3:MSE:N	2.20	0.56
2:D:2:A2G:C6	2:D:2:A2G:H15	2.08	0.56
1:B:61:ARG:O	1:B:67:HIS:HB3	2.06	0.55
1:A:13:ASN:O	1:A:15:GLY:N	2.39	0.55
1:A:50:ASN:O	1:B:61:ARG:NH2	2.39	0.55
1:A:342:GLU:HB3	1:A:345:ASN:ND2	2.22	0.55
1:A:233:LYS:HA	1:A:236:SER:HB3	1.89	0.55
1:B:284:ILE:HG12	1:B:303:LEU:HB2	1.89	0.55
1:A:138:PRO:HB3	1:A:157:PHE:O	2.07	0.54
1:A:292:ALA:HB3	1:A:293:LYS:NZ	2.22	0.54
1:A:280:GLU:HA	1:A:331:VAL:CG1	2.22	0.54
1:A:187:LEU:HD13	1:A:189:ILE:HD11	1.90	0.54
1:A:342:GLU:HG2	1:A:344:SER:OG	2.07	0.53
1:A:223:ASP:OD1	1:A:227:ARG:HD3	2.07	0.53
1:A:181:GLU:OE1	1:A:181:GLU:N	2.41	0.53
1:B:217:LYS:NZ	1:B:217:LYS:HB3	2.23	0.53
1:B:222:GLY:O	1:B:245:GLY:HA2	2.08	0.53
1:B:192:LEU:HD13	1:B:230:LEU:HD12	1.91	0.53
1:B:145:VAL:HG21	1:B:150:ASP:HB3	1.91	0.52
1:A:9:ILE:O	1:A:38:LYS:HA	2.10	0.52
1:A:12:LEU:HD13	1:A:44:SER:HB2	1.91	0.52
1:B:96:ASP:CG	1:B:97:THR:H	2.14	0.52
1:A:22:VAL:HG12	1:A:26:ASN:ND2	2.25	0.52
1:B:6:SER:OG	1:B:35:SER:HB3	2.10	0.51
1:B:316:LYS:O	1:B:319:LEU:HB3	2.10	0.51
1:A:98:THR:OG1	2:C:2:A2G:H8	2.11	0.51
1:A:116:SER:HB3	1:A:144:SER:CB	2.30	0.51
1:B:191:ARG:HH12	2:D:3:A2G:H2	1.73	0.51
1:B:271:THR:O	1:B:275:GLU:HG3	2.11	0.51
3:B:401:UDN:O4'	3:B:401:UDN:O6'	2.27	0.51
1:B:7:PHE:HB2	1:B:36:ILE:HG12	1.93	0.51
1:B:96:ASP:OD1	1:B:97:THR:N	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:O	1:B:115:ILE:HG12	2.11	0.50
1:B:233:LYS:HA	1:B:236:SER:HB3	1.92	0.50
1:A:266:VAL:O	1:A:267:GLU:HG2	2.10	0.50
1:A:198:PRO:CG	1:A:230:LEU:HD11	2.42	0.50
1:A:11:THR:HG22	1:A:40:HIS:HB2	1.94	0.50
1:A:143:LEU:HD23	1:A:161:VAL:HG22	1.93	0.49
1:A:149:SER:HB3	1:A:290:ASN:HD21	1.78	0.49
1:B:9:ILE:O	1:B:38:LYS:HA	2.13	0.49
1:B:327:ARG:O	1:B:331:VAL:HG23	2.13	0.49
2:D:2:A2G:H6	2:D:3:A2G:C7	2.43	0.48
1:A:35:SER:HA	1:A:53:LYS:O	2.13	0.48
1:A:182:LYS:NZ	1:A:279:PHE:O	2.34	0.48
1:A:217:LYS:HB3	1:A:217:LYS:NZ	2.28	0.48
1:B:305:VAL:HG23	1:B:306:GLY:O	2.14	0.48
1:B:134:ARG:HD2	1:B:157:PHE:CD2	2.48	0.48
1:B:182:LYS:NZ	1:B:255:GLU:O	2.30	0.48
1:A:200:MSE:HE1	1:A:305:VAL:HG21	1.94	0.48
1:A:342:GLU:CG	1:A:344:SER:OG	2.60	0.48
1:A:92:ILE:HG23	1:A:114:ILE:HB	1.96	0.48
1:B:165:LEU:HD12	1:B:340:ASP:O	2.13	0.48
1:A:41:THR:HG21	1:A:59:GLN:HE21	1.79	0.48
1:A:222:GLY:O	1:A:245:GLY:HA2	2.14	0.48
1:B:133:ARG:HG3	1:B:137:TYR:CE1	2.47	0.48
1:B:324:GLU:CD	1:B:327:ARG:NH1	2.39	0.48
1:B:289:TYR:CE2	1:B:290:ASN:HB2	2.48	0.47
1:B:312:ALA:O	1:B:316:LYS:HG2	2.13	0.47
1:A:188:PHE:CD2	1:A:220:ILE:HG23	2.45	0.47
1:A:297:LYS:HB3	1:A:300:HIS:HB3	1.97	0.47
1:A:269:LEU:HG	1:A:274:ILE:HD11	1.96	0.47
1:B:172:ASP:OD2	1:B:343:ILE:HD12	2.14	0.47
1:B:254:TYR:HE1	1:B:260:LEU:HD13	1.80	0.47
1:A:289:TYR:CD2	1:A:290:ASN:HB2	2.50	0.47
1:A:7:PHE:HB2	1:A:36:ILE:HG12	1.95	0.47
1:A:18:GLU:O	1:A:22:VAL:HG23	2.15	0.47
1:A:118:HIS:HA	1:A:146:LEU:HD12	1.97	0.47
1:B:64:THR:HG22	1:B:66:TYR:H	1.80	0.47
1:A:298:ASP:HB2	1:A:304:LEU:HD12	1.96	0.46
1:A:202:LEU:HD13	1:A:234:VAL:HG23	1.98	0.46
1:A:320:VAL:HG12	1:A:321:LEU:HD23	1.97	0.46
1:B:289:TYR:CD2	1:B:290:ASN:HB2	2.51	0.46
1:A:114:ILE:O	1:A:115:ILE:CG1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:CYS:SG	1:A:51:GLU:HB2	2.56	0.46
1:A:27:ALA:HB1	1:A:347:LYS:HE2	1.98	0.46
1:A:121:GLU:O	1:A:130:ARG:NH1	2.46	0.46
1:A:174:ILE:HD11	1:A:251:LYS:HE2	1.97	0.45
1:B:103:ILE:O	1:B:107:ILE:HG13	2.17	0.45
1:B:5:ILE:HD12	1:B:354:ILE:HD13	1.98	0.45
1:A:149:SER:O	1:A:152:VAL:HG22	2.17	0.45
1:B:343:ILE:H	1:B:343:ILE:HG13	1.54	0.45
1:A:94:PHE:O	1:A:95:LEU:HB2	2.17	0.45
1:B:7:PHE:HB3	1:B:21:LEU:HD11	1.99	0.45
1:B:14:SER:O	1:B:14:SER:OG	2.25	0.45
1:B:76:PHE:CZ	1:B:105:ALA:HA	2.51	0.45
1:B:188:PHE:HD1	1:B:220:ILE:HG23	1.82	0.45
1:A:63:ASP:O	1:A:67:HIS:HB2	2.17	0.44
1:A:327:ARG:O	1:A:331:VAL:HG23	2.17	0.44
1:B:90:VAL:HG23	1:B:112:PRO:HB2	1.98	0.44
1:B:174:ILE:HD11	1:B:251:LYS:HE2	2.00	0.44
1:A:112:PRO:HB3	1:A:357:VAL:HG12	2.00	0.44
1:B:212:LEU:HD11	1:B:318:GLU:HG3	2.00	0.44
1:B:321:LEU:HA	1:B:321:LEU:HD23	1.70	0.44
1:A:12:LEU:HA	1:A:18:GLU:HG2	1.99	0.44
1:A:184:ASN:HB3	1:A:216:TYR:CG	2.53	0.44
1:A:200:MSE:HE2	1:A:313:LEU:HB2	1.99	0.43
1:B:219:VAL:HG22	1:B:242:ASP:HB2	2.00	0.43
2:D:1:NDG:H4	2:D:2:A2G:N2	2.33	0.43
1:B:262:LEU:HD22	1:B:273:LEU:HG	2.01	0.43
1:B:25:ALA:O	1:B:29:CYS:HB2	2.19	0.43
1:A:148:SER:O	1:A:152:VAL:HG13	2.19	0.43
1:A:289:TYR:CE2	1:A:290:ASN:HB2	2.54	0.42
1:B:132:LEU:HA	1:B:132:LEU:HD23	1.79	0.42
1:A:292:ALA:HB3	1:A:293:LYS:HZ2	1.82	0.42
1:A:26:ASN:OD1	1:A:49:GLU:HB2	2.20	0.42
1:A:85:GLU:O	1:A:85:GLU:CG	2.62	0.42
1:B:198:PRO:CG	1:B:230:LEU:HD11	2.49	0.42
3:A:401:UDN:C1'	2:C:3:A2G:O4	2.68	0.42
1:B:95:LEU:HD21	1:B:118:HIS:HB2	2.02	0.42
1:A:80:ARG:HG3	1:A:105:ALA:O	2.19	0.42
1:A:213:GLN:OE1	1:A:239:ILE:HG22	2.20	0.42
1:A:298:ASP:OD1	1:A:303:LEU:HA	2.20	0.42
1:B:13:ASN:O	1:B:15:GLY:N	2.53	0.42
1:B:120:ASN:HD22	1:B:122:ALA:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ALA:HB1	1:B:347:LYS:HE2	2.01	0.42
1:B:72:ARG:HA	1:B:72:ARG:HD2	1.77	0.42
1:B:262:LEU:HA	1:B:262:LEU:HD12	1.77	0.41
1:A:192:LEU:HD13	1:A:230:LEU:HD12	2.01	0.41
1:B:185:LEU:HD12	1:B:217:LYS:O	2.20	0.41
1:A:36:ILE:HD12	1:A:52:VAL:HG11	2.02	0.41
1:A:114:ILE:O	1:A:115:ILE:HG12	2.20	0.41
1:A:261:CYS:HA	1:A:284:ILE:O	2.20	0.41
1:B:164:LEU:HD13	1:B:350:TRP:CE2	2.55	0.41
1:B:73:PHE:N	1:B:73:PHE:CD1	2.88	0.41
1:B:269:LEU:HD12	1:B:269:LEU:HA	1.81	0.41
1:A:120:ASN:ND2	1:A:122:ALA:H	2.19	0.41
1:A:213:GLN:HE21	1:A:213:GLN:HB2	1.61	0.41
1:A:45:PHE:CZ	1:A:248:GLU:HG2	2.56	0.41
1:B:21:LEU:HD12	1:B:94:PHE:CD1	2.56	0.41
1:B:217:LYS:HB3	1:B:217:LYS:HZ3	1.85	0.41
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.78	0.41
1:B:192:LEU:HD12	1:B:227:ARG:HB2	2.03	0.41
1:A:61:ARG:HD3	1:B:45:PHE:CD1	2.56	0.40
1:A:172:ASP:OD2	1:A:343:ILE:HD12	2.21	0.40
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.68	0.40
1:A:48:LEU:HD12	1:A:49:GLU:H	1.86	0.40
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.85	0.40
1:A:329:GLU:O	1:A:330:LEU:C	2.60	0.40
1:B:12:LEU:HD23	1:B:12:LEU:HA	1.91	0.40
1:B:169:HIS:HA	1:B:343:ILE:HD11	2.03	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	358/373 (96%)	316 (88%)	35 (10%)	7 (2%)	7	32
1	B	358/373 (96%)	310 (87%)	41 (12%)	7 (2%)	7	32
All	All	716/746 (96%)	626 (87%)	76 (11%)	14 (2%)	7	32

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	115	ILE
1	B	115	ILE
1	A	340	ASP
1	B	14	SER
1	B	96	ASP
1	A	124	LEU
1	A	245	GLY
1	A	290	ASN
1	B	245	GLY
1	B	246	ARG
1	B	290	ASN
1	B	107	ILE
1	A	107	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	324/332 (98%)	318 (98%)	6 (2%)	57	77
1	B	324/332 (98%)	309 (95%)	15 (5%)	27	58
All	All	648/664 (98%)	627 (97%)	21 (3%)	39	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	96	ASP

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Mol	Chain	Res	Type
1	A	123	TYR
1	A	152	VAL
1	A	227	ARG
1	A	320	VAL
1	B	20	VAL
1	B	38	LYS
1	B	89	ASP
1	B	115	ILE
1	B	123	TYR
1	B	128	THR
1	B	145	VAL
1	B	152	VAL
1	B	177	ASP
1	B	227	ARG
1	B	234	VAL
1	B	254	TYR
1	B	270	PRO
1	B	317	LEU
1	B	344	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	120	ASN
1	A	213	GLN
1	A	290	ASN
1	A	332	ASN
1	A	345	ASN
1	B	120	ASN
1	B	213	GLN
1	B	332	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)

6 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	NDG	C	1	4,2	14,14,15	2.71	7 (50%)	17,19,21	1.99	5 (29%)
2	A2G	C	2	2	14,14,15	2.65	5 (35%)	17,19,21	1.59	5 (29%)
2	A2G	C	3	2	14,14,15	2.78	7 (50%)	17,19,21	2.02	9 (52%)
2	NDG	D	1	4,2	14,14,15	2.79	8 (57%)	17,19,21	2.85	9 (52%)
2	A2G	D	2	2	14,14,15	2.38	6 (42%)	17,19,21	2.35	7 (41%)
2	A2G	D	3	2	14,14,15	2.77	7 (50%)	17,19,21	1.79	6 (35%)

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	NDG	C	1	4,2	-	2/6/23/26	0/1/1/1
2	A2G	C	2	2	-	0/6/23/26	0/1/1/1
2	A2G	C	3	2	-	2/6/23/26	0/1/1/1
2	NDG	D	1	4,2	-	4/6/23/26	0/1/1/1
2	A2G	D	2	2	-	1/6/23/26	0/1/1/1
2	A2G	D	3	2	-	2/6/23/26	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	A2G	O6-C6	6.17	1.68	1.42
2	D	1	NDG	O5-C5	5.82	1.55	1.43
2	C	1	NDG	O5-C5	5.65	1.54	1.43
2	C	3	A2G	O5-C5	5.25	1.54	1.43
2	D	3	A2G	O5-C5	5.25	1.54	1.43
2	D	2	A2G	O6-C6	5.21	1.64	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	A2G	C2-N2	5.00	1.54	1.46
2	D	3	A2G	C2-N2	4.82	1.54	1.46
2	D	1	NDG	C2-N2	4.16	1.53	1.46
2	C	2	A2G	C7-N2	4.13	1.48	1.34
2	C	1	NDG	C2-N2	4.05	1.53	1.46
2	C	3	A2G	C7-N2	4.05	1.48	1.34
2	D	3	A2G	C7-N2	3.98	1.48	1.34
2	C	2	A2G	O5-C1	3.73	1.49	1.43
2	D	1	NDG	C7-N2	3.68	1.47	1.34
2	D	2	A2G	C7-N2	3.66	1.46	1.34
2	C	1	NDG	C7-N2	3.61	1.46	1.34
2	D	2	A2G	O5-C1	3.27	1.48	1.43
2	D	3	A2G	C6-C5	-3.19	1.41	1.51
2	C	3	A2G	C6-C5	-3.17	1.41	1.51
2	D	1	NDG	C6-C5	-3.09	1.41	1.51
2	D	3	A2G	O5-C1	3.02	1.48	1.43
2	C	3	A2G	O5-C1	3.01	1.48	1.43
2	C	1	NDG	C6-C5	-2.98	1.41	1.51
2	C	1	NDG	O3-C3	2.98	1.50	1.43
2	C	2	A2G	C2-N2	2.97	1.51	1.46
2	D	1	NDG	O3-C3	2.71	1.49	1.43
2	D	1	NDG	C1-C2	-2.64	1.48	1.52
2	D	3	A2G	O3-C3	2.47	1.48	1.43
2	C	3	A2G	C3-C2	-2.41	1.47	1.52
2	C	2	A2G	O5-C5	2.34	1.48	1.43
2	C	1	NDG	O5-C1	2.31	1.47	1.43
2	D	1	NDG	C3-C2	-2.27	1.47	1.52
2	D	2	A2G	C2-N2	2.24	1.50	1.46
2	D	2	A2G	C3-C2	-2.24	1.47	1.52
2	D	3	A2G	C3-C2	-2.19	1.47	1.52
2	C	1	NDG	C3-C2	-2.16	1.47	1.52
2	D	2	A2G	O5-C5	2.15	1.47	1.43
2	C	3	A2G	O3-C3	2.10	1.47	1.43
2	D	1	NDG	O7-C7	-2.05	1.18	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	A2G	C1-O5-C5	-5.47	104.78	112.19
2	D	1	NDG	C3-C4-C5	5.44	119.95	110.24
2	D	1	NDG	O3-C3-C2	-4.67	99.81	109.47
2	D	2	A2G	O6-C6-C5	-4.40	96.19	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NDG	O3-C3-C4	-4.13	100.80	110.35
2	C	1	NDG	C3-C4-C5	4.12	117.59	110.24
2	D	1	NDG	O5-C1-C2	-4.09	104.82	111.29
2	D	1	NDG	C6-C5-C4	-4.02	103.58	113.00
2	D	3	A2G	O5-C1-C2	3.45	116.73	111.29
2	D	3	A2G	O5-C5-C4	-3.40	102.56	110.83
2	C	2	A2G	O6-C6-C5	-3.35	99.81	111.29
2	C	3	A2G	C3-C4-C5	3.27	116.06	110.24
2	C	1	NDG	O3-C3-C2	-3.23	102.78	109.47
2	C	3	A2G	C1-O5-C5	3.19	116.51	112.19
2	D	2	A2G	C1-C2-N2	3.00	115.62	110.49
2	D	1	NDG	C8-C7-N2	2.97	121.12	116.10
2	D	1	NDG	C4-C3-C2	2.92	115.30	111.02
2	C	2	A2G	C1-C2-N2	2.87	115.40	110.49
2	C	3	A2G	C6-C5-C4	-2.80	106.44	113.00
2	D	2	A2G	O5-C1-C2	-2.80	106.87	111.29
2	C	1	NDG	O3-C3-C4	-2.79	103.90	110.35
2	D	2	A2G	O5-C5-C6	2.79	111.57	107.20
2	D	2	A2G	C4-C3-C2	-2.78	106.94	111.02
2	C	3	A2G	O4-C4-C5	-2.69	102.61	109.30
2	C	1	NDG	C8-C7-N2	2.65	120.58	116.10
2	C	2	A2G	O5-C5-C6	2.62	111.31	107.20
2	D	3	A2G	O5-C5-C6	2.55	111.21	107.20
2	C	3	A2G	O5-C1-C2	2.41	115.09	111.29
2	C	3	A2G	C8-C7-N2	2.40	120.16	116.10
2	D	3	A2G	C1-O5-C5	2.35	115.38	112.19
2	D	2	A2G	C3-C4-C5	-2.35	106.05	110.24
2	D	3	A2G	C8-C7-N2	2.34	120.07	116.10
2	C	1	NDG	C4-C3-C2	2.30	114.40	111.02
2	C	2	A2G	O5-C1-C2	-2.25	107.74	111.29
2	D	1	NDG	O4-C4-C5	-2.12	104.03	109.30
2	C	3	A2G	O3-C3-C4	-2.09	105.53	110.35
2	D	3	A2G	C1-C2-N2	-2.08	106.93	110.49
2	C	2	A2G	C3-C4-C5	-2.08	106.53	110.24
2	C	3	A2G	O5-C5-C4	-2.08	105.77	110.83
2	D	1	NDG	C2-N2-C7	-2.08	119.95	122.90
2	C	3	A2G	C4-C3-C2	2.04	114.00	111.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

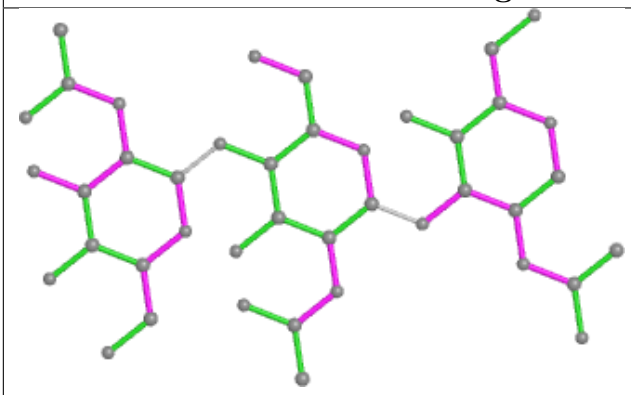
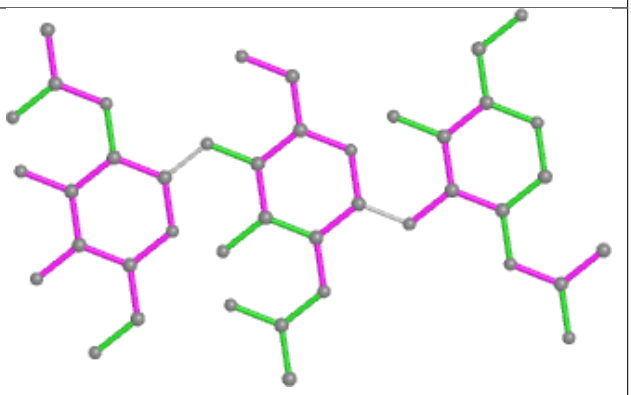
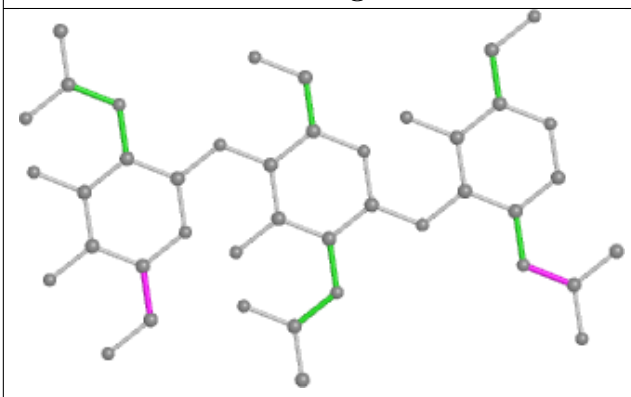
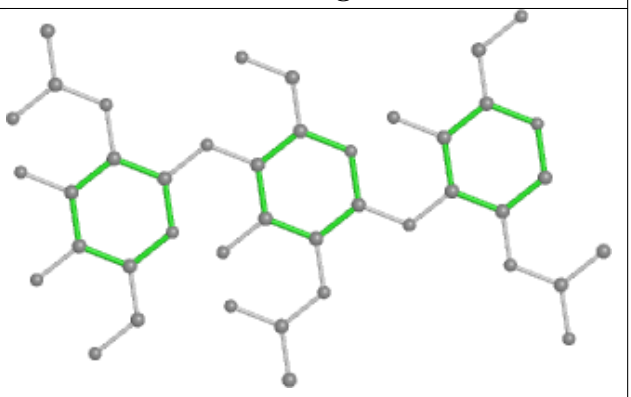
Mol	Chain	Res	Type	Atoms
2	C	3	A2G	O5-C5-C6-O6
2	D	1	NDG	O5-C5-C6-O6
2	C	3	A2G	C4-C5-C6-O6
2	D	1	NDG	C4-C5-C6-O6
2	D	3	A2G	O5-C5-C6-O6
2	D	3	A2G	C4-C5-C6-O6
2	C	1	NDG	C8-C7-N2-C2
2	C	1	NDG	O7-C7-N2-C2
2	D	1	NDG	C8-C7-N2-C2
2	D	1	NDG	O7-C7-N2-C2
2	D	2	A2G	C4-C5-C6-O6

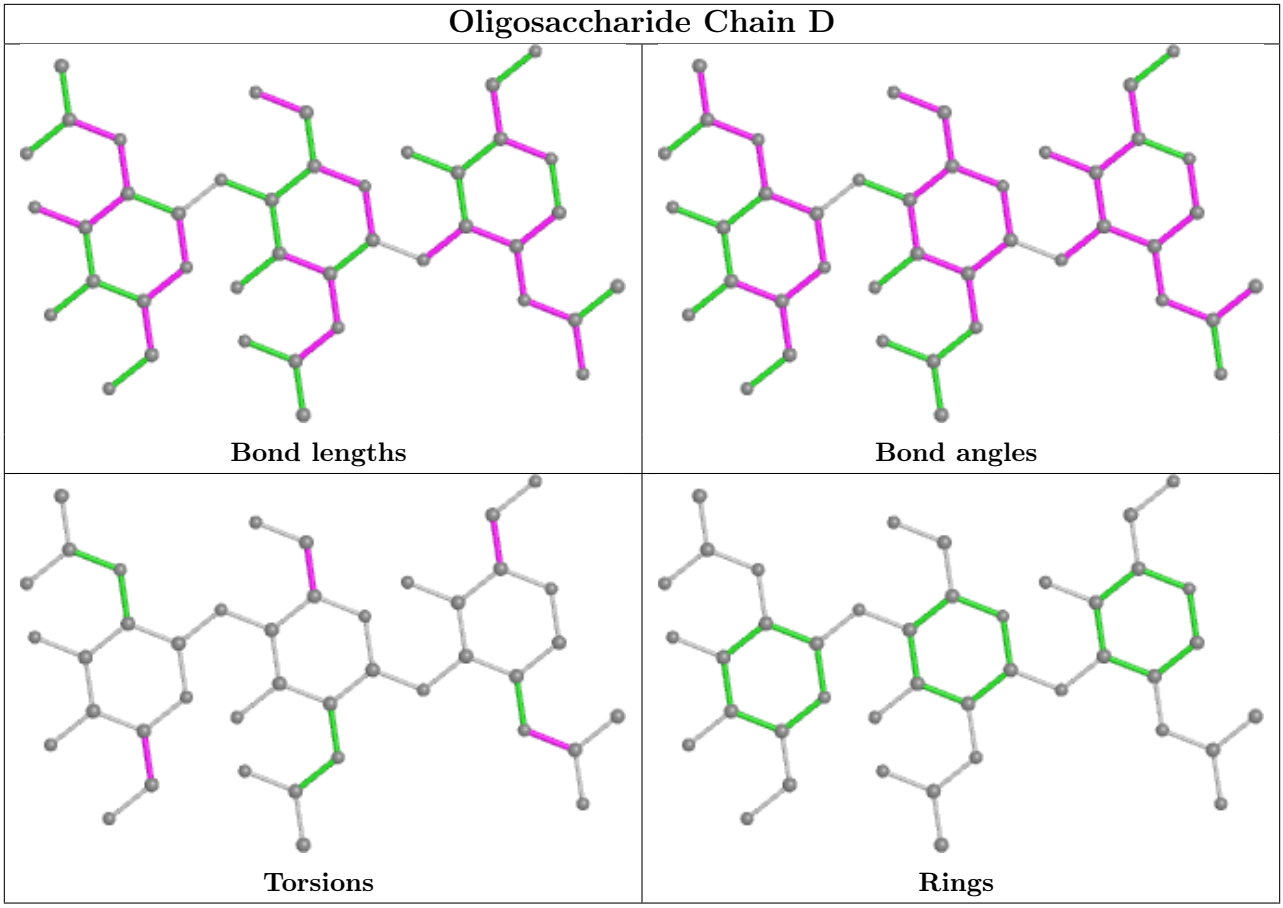
There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NDG	1	0
2	D	2	A2G	6	0
2	C	3	A2G	1	0
2	C	2	A2G	5	0
2	C	1	NDG	1	0
2	D	3	A2G	3	0

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

Oligosaccharide Chain C	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	UDN	A	401	-	39,41,41	3.06	15 (38%)	51,62,62	2.46	17 (33%)
4	BUE	B	405	2	8,10,28	1.79	1 (12%)	12,15,37	1.42	2 (16%)
4	BUE	A	405	2	8,10,28	1.81	1 (12%)	12,15,37	1.79	4 (33%)
3	UDN	B	401	-	39,41,41	2.86	15 (38%)	51,62,62	2.53	20 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDN	A	401	-	-	10/24/63/63	0/3/3/3
4	BUE	B	405	2	-	4/10/10/31	-
4	BUE	A	405	2	-	2/10/10/31	-
3	UDN	B	401	-	-	8/24/63/63	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	UDN	PB-O3A	8.76	1.68	1.58
3	A	401	UDN	PB-CB	-8.05	1.68	1.80
3	B	401	UDN	PB-CB	-8.05	1.68	1.80
3	A	401	UDN	C5D-C4D	-7.98	1.26	1.51
3	A	401	UDN	PB-O3A	6.84	1.66	1.58
3	B	401	UDN	O4D-C1D	-5.43	1.29	1.42
3	A	401	UDN	C3D-C2D	-5.31	1.38	1.53
3	B	401	UDN	O3D-C3D	-5.27	1.30	1.43
3	A	401	UDN	O4D-C1D	-5.10	1.29	1.42
3	B	401	UDN	PB-O2B	-4.50	1.45	1.56
3	A	401	UDN	PB-O2B	-4.38	1.46	1.56
3	A	401	UDN	O5D-C5D	-4.38	1.27	1.44
4	B	405	BUE	P35-O36	3.54	1.68	1.54
3	B	401	UDN	C2D-C1D	-3.52	1.42	1.53
4	A	405	BUE	P35-O36	3.49	1.68	1.54
3	B	401	UDN	C4-N3	-3.39	1.32	1.38
3	A	401	UDN	C7'-N2'	3.23	1.45	1.34
3	A	401	UDN	C2D-C1D	-3.19	1.43	1.53
3	A	401	UDN	C2'-N2'	3.19	1.50	1.45
3	A	401	UDN	O5'-C5'	2.96	1.51	1.44
3	A	401	UDN	PB-O1B	-2.80	1.44	1.51
3	A	401	UDN	C4-N3	-2.74	1.33	1.38
3	B	401	UDN	C7'-N2'	2.72	1.43	1.34
3	B	401	UDN	O5'-C5'	2.71	1.50	1.44
3	A	401	UDN	O4D-C4D	2.51	1.50	1.45
3	B	401	UDN	C5D-C4D	-2.35	1.44	1.51
3	B	401	UDN	O2'-C2D	-2.34	1.37	1.43
3	B	401	UDN	PB-O1B	-2.27	1.46	1.51
3	A	401	UDN	O2'-C2D	-2.25	1.37	1.43
3	B	401	UDN	O4-C4	-2.17	1.20	1.24
3	B	401	UDN	C2'-N2'	2.12	1.49	1.45
3	B	401	UDN	C2-N3	-2.03	1.34	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	UDN	O4D-C1D-N1	7.55	125.63	108.36
3	B	401	UDN	O3D-C3D-C4D	7.31	132.18	111.05
3	A	401	UDN	O3D-C3D-C4D	6.75	130.56	111.05
3	A	401	UDN	O4D-C4D-C3D	-5.84	93.55	105.11
3	A	401	UDN	O4D-C1D-N1	4.96	119.70	108.36
3	A	401	UDN	O4D-C4D-C5D	4.69	124.81	109.37
3	A	401	UDN	O2'-C2D-C1D	4.67	125.65	110.02
3	A	401	UDN	C2D-C1D-N1	4.42	125.73	113.22
3	B	401	UDN	C3D-C2D-C1D	4.18	109.37	101.43
3	B	401	UDN	C4-N3-C2	-4.02	121.27	126.58
3	B	401	UDN	C5-C4-N3	4.02	120.86	114.84
3	A	401	UDN	C4-N3-C2	-4.00	121.30	126.58
3	A	401	UDN	C5-C4-N3	3.89	120.66	114.84
3	B	401	UDN	C2D-C3D-C4D	-3.88	95.10	102.64
3	A	401	UDN	O4-C4-C5	-3.62	118.80	125.16
4	A	405	BUE	O37-P35-O34	-3.47	97.09	110.68
3	A	401	UDN	O2B-PB-CB	3.47	113.36	105.72
3	B	401	UDN	O4D-C4D-C5D	3.42	120.61	109.37
3	B	401	UDN	O2'-C2D-C3D	3.39	122.78	111.82
3	B	401	UDN	N3-C2-N1	3.32	119.30	114.89
4	A	405	BUE	O36-P35-O38	3.26	115.58	104.64
3	A	401	UDN	N3-C2-N1	3.03	118.91	114.89
3	B	401	UDN	O2B-PB-O1B	-2.98	100.13	110.07
4	A	405	BUE	O40-P39-O41	-2.96	97.62	112.24
3	B	401	UDN	O4-C4-C5	-2.96	119.96	125.16
3	B	401	UDN	C2D-C1D-N1	2.94	121.55	113.22
3	A	401	UDN	C4'-C3'-C2'	2.93	114.63	110.34
3	B	401	UDN	C1'-C2'-N2'	-2.84	104.46	110.62
3	B	401	UDN	O2'-C2D-C1D	2.84	119.50	110.02
3	B	401	UDN	O2B-PB-CB	2.77	111.81	105.72
3	B	401	UDN	C6'-C5'-C4'	-2.66	106.78	113.00
3	B	401	UDN	PB-O3A-PA	-2.64	124.17	132.56
4	B	405	BUE	O40-P39-O41	-2.64	99.18	112.24
3	A	401	UDN	O2B-PB-O1B	-2.58	101.46	110.07
3	A	401	UDN	PB-O3A-PA	-2.55	124.46	132.56
4	B	405	BUE	O37-P35-O34	-2.55	100.69	110.68
3	B	401	UDN	O1A-PA-O2A	-2.26	101.05	112.24
3	A	401	UDN	O1B-PB-CB	2.17	114.94	108.99
3	A	401	UDN	O3D-C3D-C2D	2.11	118.63	111.82
3	B	401	UDN	PA-O5D-C5D	-2.08	109.48	121.68
4	A	405	BUE	O37-P35-O38	2.06	111.54	104.64
3	B	401	UDN	O6'-C6'-C5'	-2.04	104.29	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	UDN	O2'-C2D-C3D	2.00	118.30	111.82

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	UDN	C1'-CB-PB-O3A
3	A	401	UDN	C1'-CB-PB-O1B
3	A	401	UDN	C5D-O5D-PA-O3A
3	B	401	UDN	C1'-CB-PB-O3A
3	B	401	UDN	C1'-CB-PB-O1B
3	B	401	UDN	C1'-CB-PB-O2B
3	B	401	UDN	C5D-O5D-PA-O3A
4	A	405	BUE	P35-O38-P39-O42
4	A	405	BUE	C43-O42-P39-O38
3	B	401	UDN	O4D-C4D-C5D-O5D
3	A	401	UDN	C4'-C5'-C6'-O6'
3	A	401	UDN	O5'-C5'-C6'-O6'
3	B	401	UDN	C3D-C4D-C5D-O5D
3	A	401	UDN	O4D-C4D-C5D-O5D
4	B	405	BUE	P39-O38-P35-O36
4	B	405	BUE	C43-O42-P39-O38
3	A	401	UDN	C5D-O5D-PA-O1A
3	A	401	UDN	C5D-O5D-PA-O2A
3	B	401	UDN	C5D-O5D-PA-O1A
3	B	401	UDN	C5D-O5D-PA-O2A
4	B	405	BUE	C43-O42-P39-O40
4	B	405	BUE	P39-O38-P35-O34
3	A	401	UDN	C2'-C1'-CB-PB
3	A	401	UDN	O5'-C1'-CB-PB

There are no ring outliers.

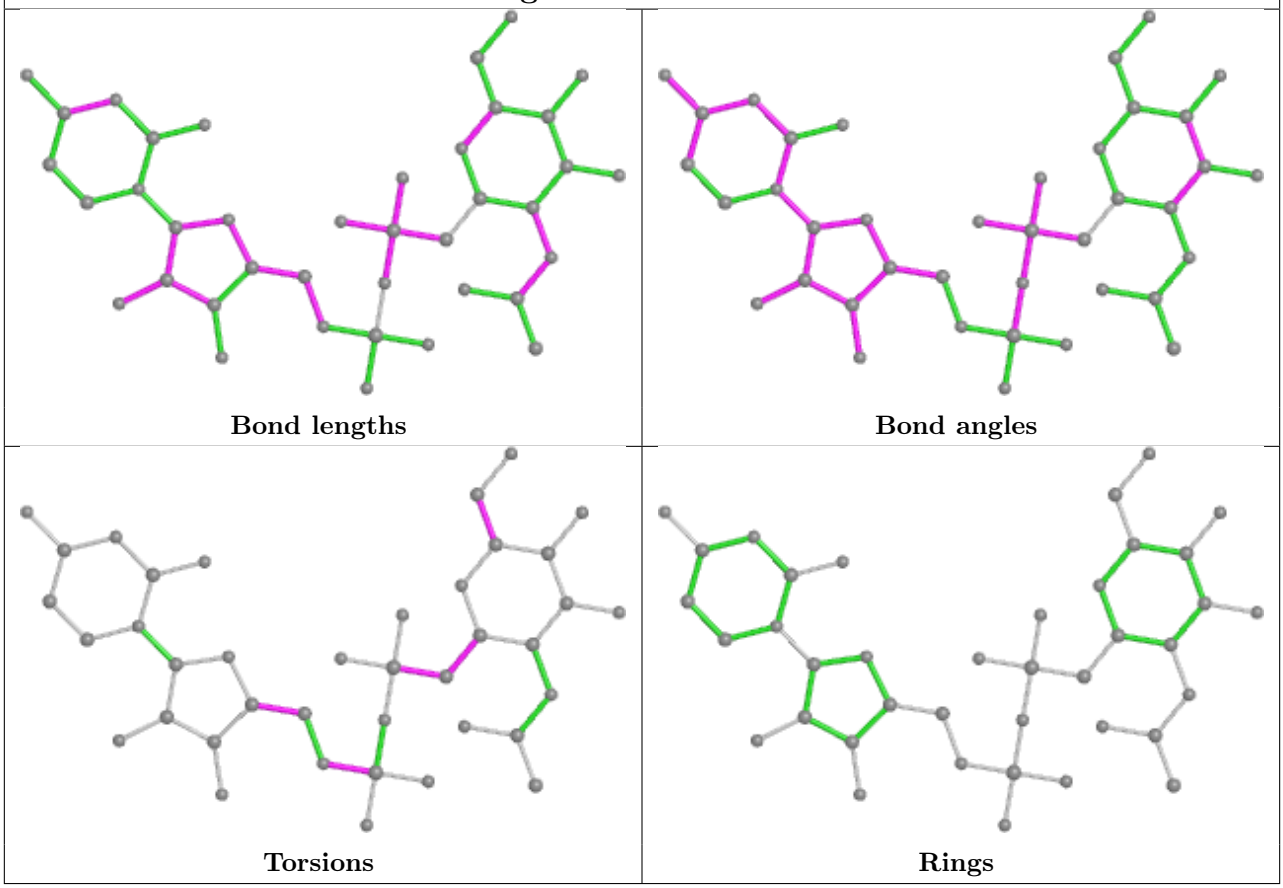
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	UDN	3	0
3	B	401	UDN	2	0

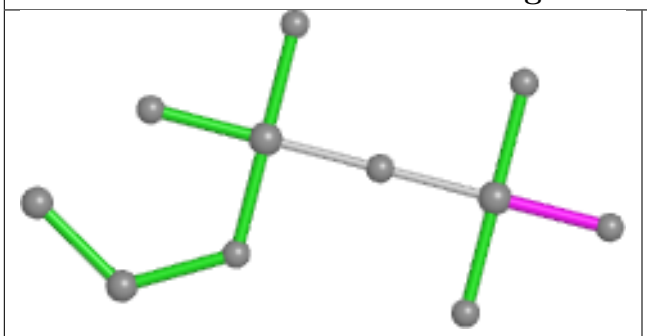
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

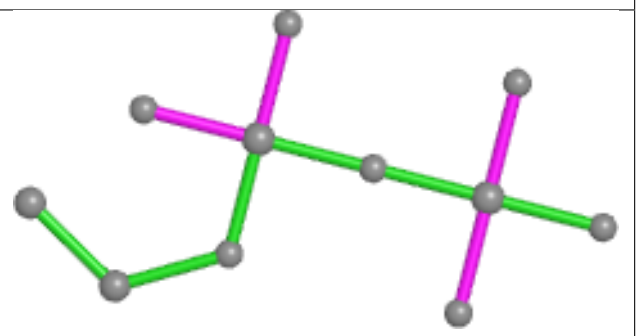
Ligand UDN A 401



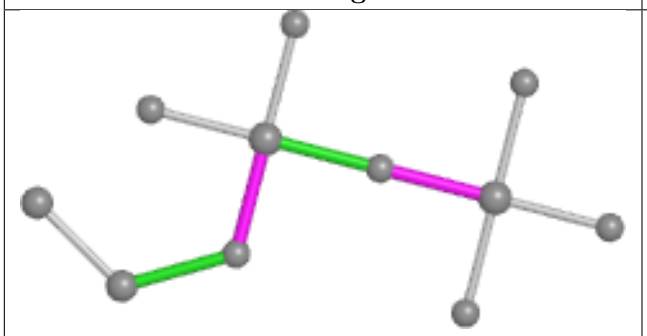
Ligand BUE B 405



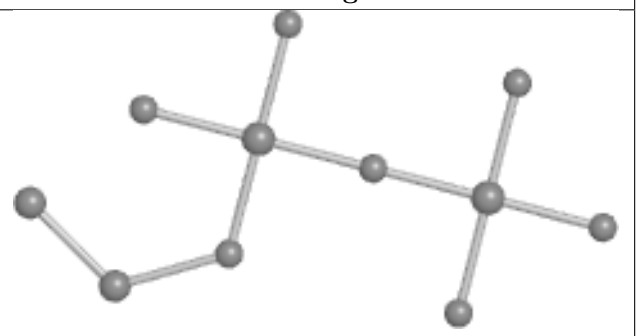
Bond lengths



Bond angles

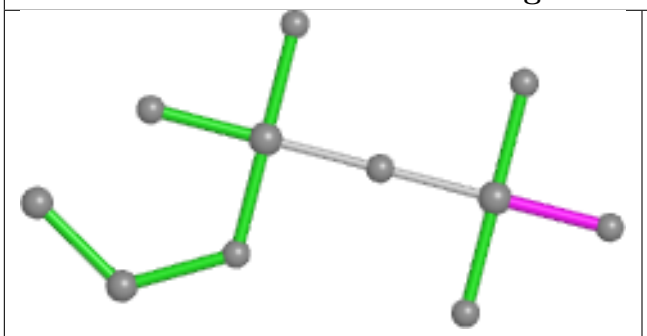


Torsions

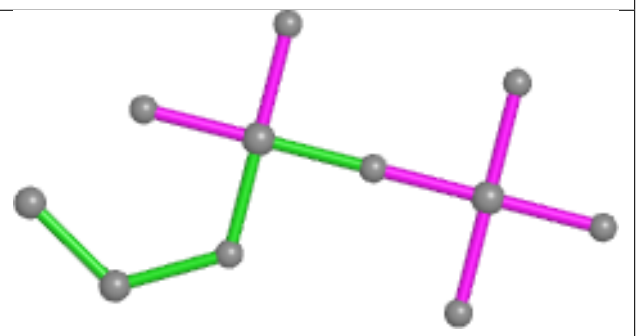


Rings

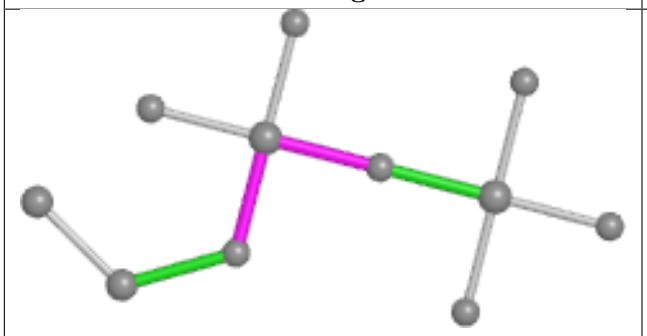
Ligand BUE A 405



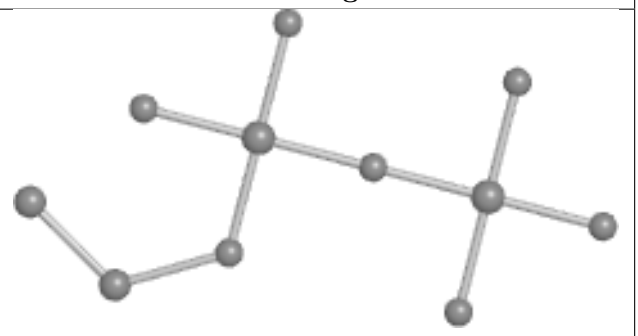
Bond lengths



Bond angles

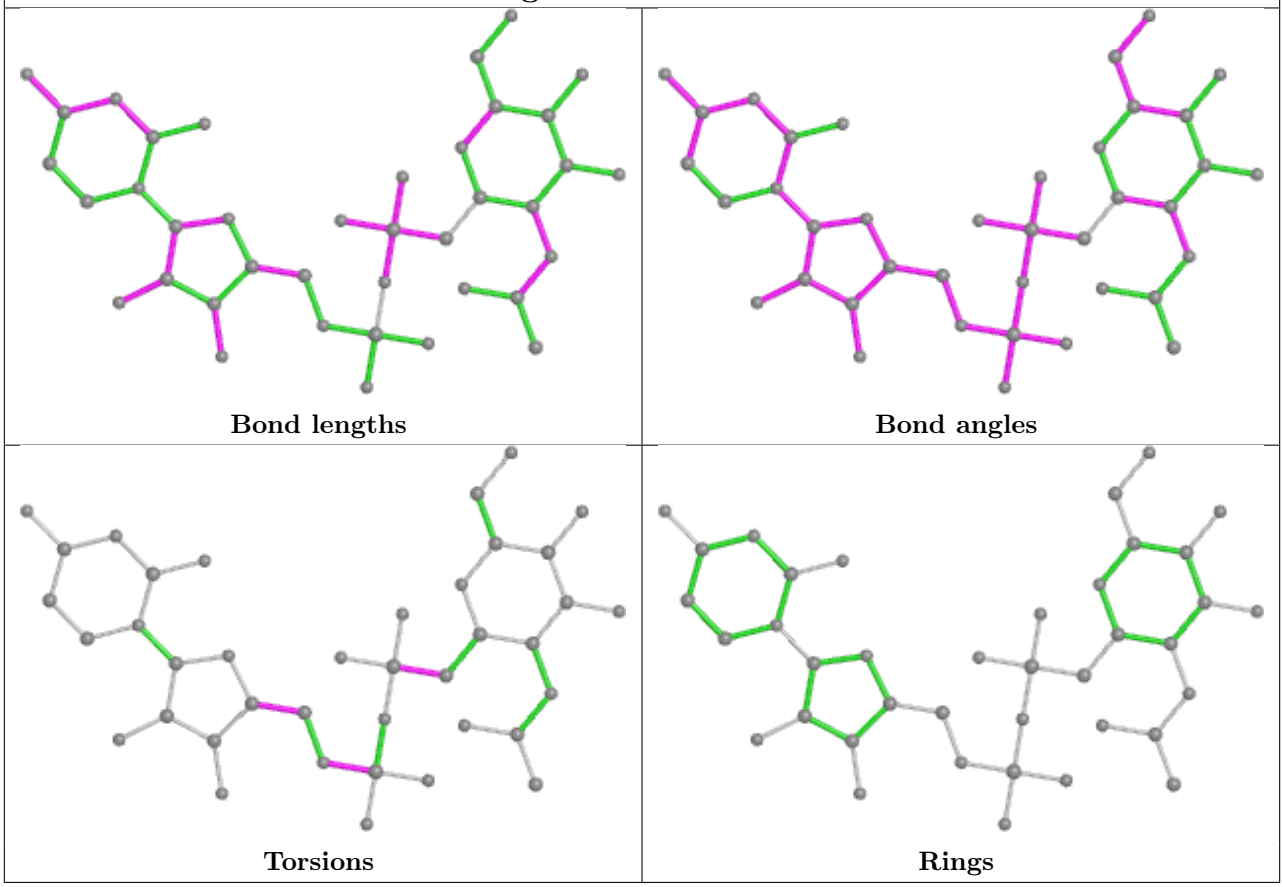


Torsions



Rings

Ligand UDN B 401



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	356/373 (95%)	-0.45	0	100	100	48, 64, 88, 106	0
1	B	356/373 (95%)	-0.41	0	100	100	48, 69, 89, 107	0
All	All	712/746 (95%)	-0.43	0	100	100	48, 67, 89, 107	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

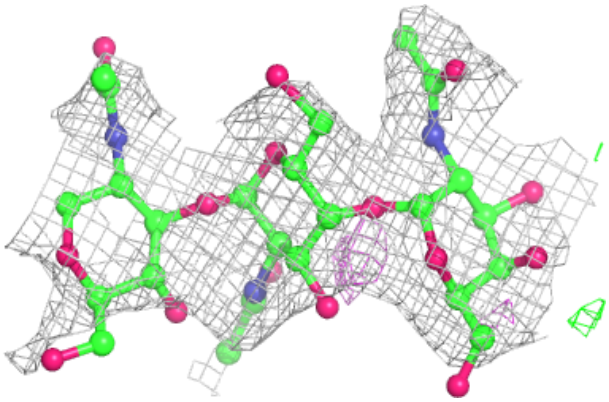
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

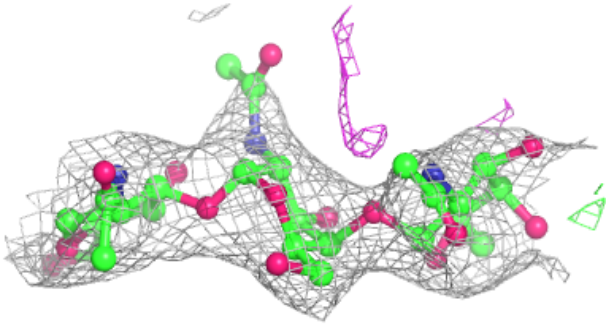
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NDG	D	1	14/15	0.82	0.15	129,131,132,132	0
2	NDG	C	1	14/15	0.85	0.18	124,127,129,130	0
2	A2G	D	2	14/15	0.89	0.23	126,128,130,130	0
2	A2G	D	3	14/15	0.89	0.16	126,129,132,132	0
2	A2G	C	3	14/15	0.90	0.21	124,126,128,129	0
2	A2G	C	2	14/15	0.90	0.28	122,124,127,128	0

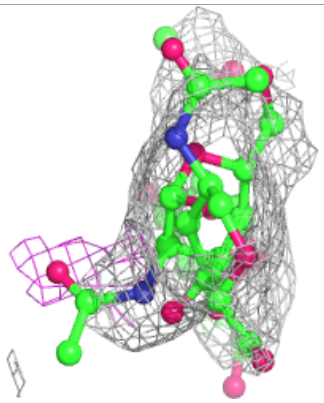
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

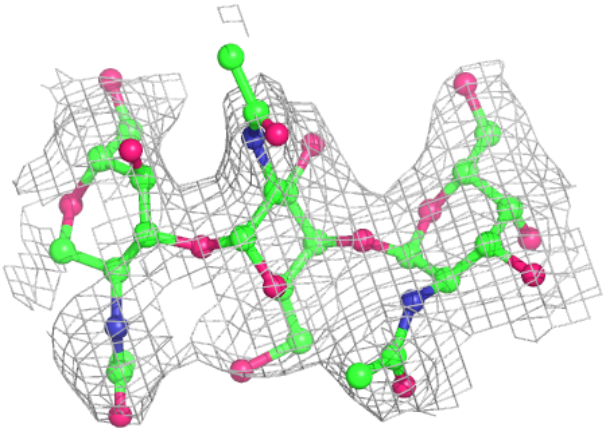


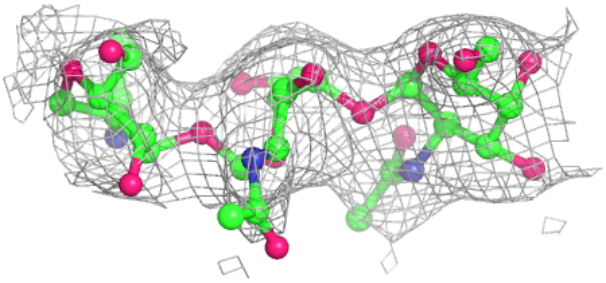


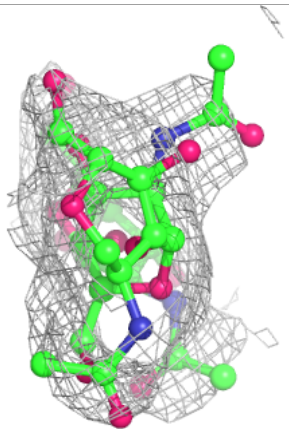


Electron density around Chain D:

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







6.4 Ligands (i)

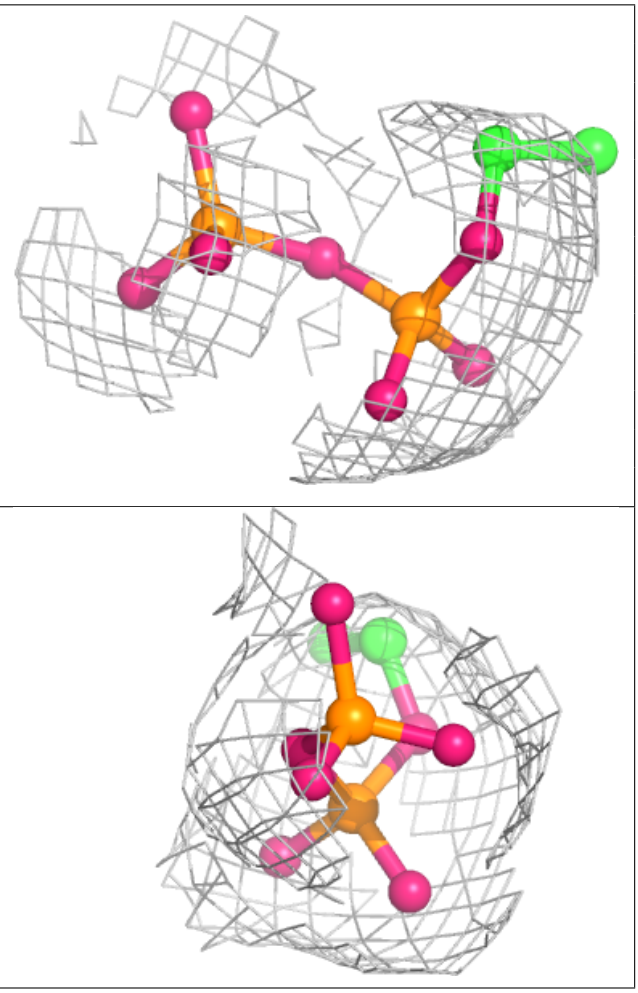
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BUE	B	405	11/29	0.88	0.11	134,139,145,146	0
4	BUE	A	405	11/29	0.90	0.14	128,131,132,133	0
3	UDN	B	401	39/39	0.92	0.20	94,96,99,99	0
3	UDN	A	401	39/39	0.94	0.20	80,87,94,96	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.

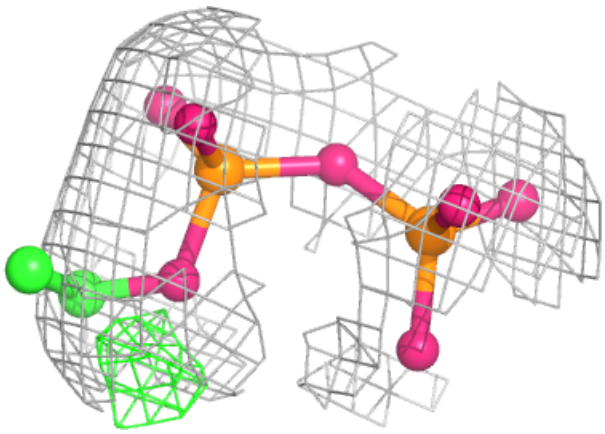
Electron density around BUE B 405:

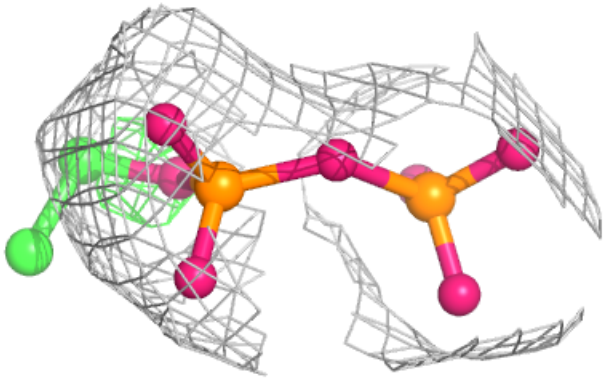
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

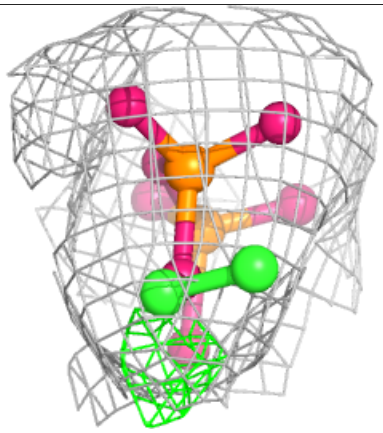


Electron density around BUE A 405:

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

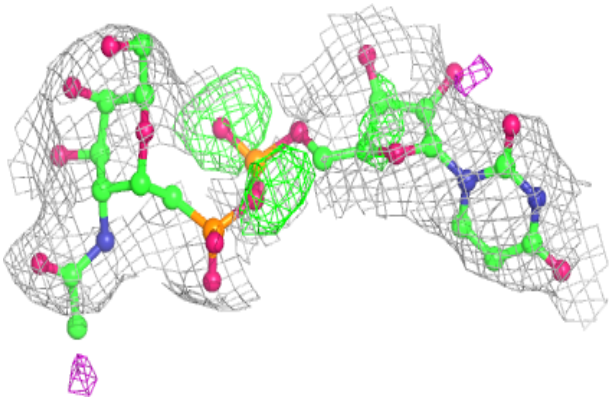


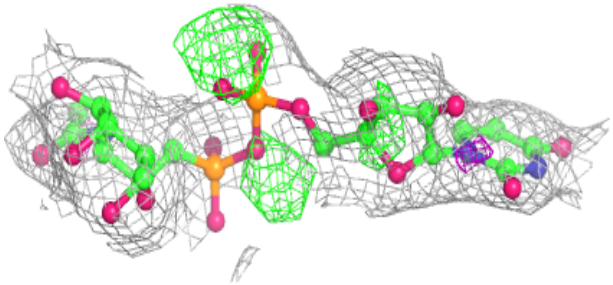


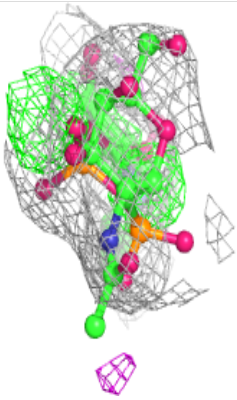


Electron density around UDN B 401:

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

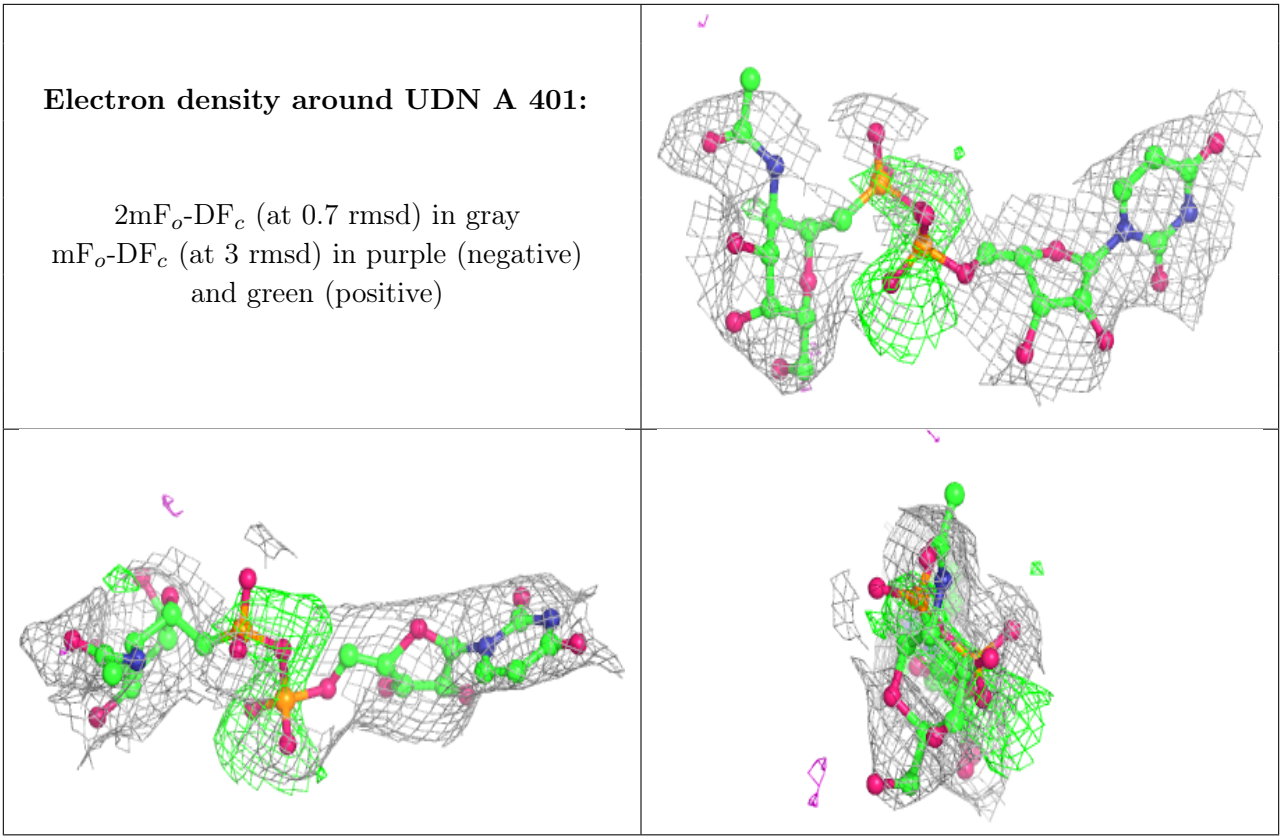






Electron density around UDN A 401:

$2mF_o$-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.