



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:18 AM GMT

PDB ID : 1ON8
Title : Crystal structure of mouse alpha-1,4-N-acetylhexosaminyltransferase(EXTL2) with UDP and GlcUAb(1-3)Galb(1-O)-naphthalenelmethanolan acceptor substrate analog
Authors : Pedersen, L.C.; Dong, J.; Taniguchi, F.; Kitagawa, H.; Krahn, J.M.; Pedersen, L.G.; Sugahara, K.; Negishi, M.
Deposited on : 2003-02-27
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

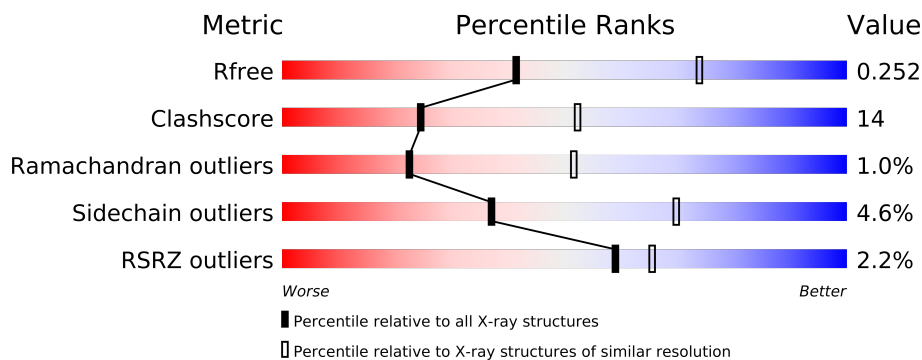
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	293	
1	B	293	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4393 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Alpha-1,4-N-acetylhexosaminyltransferaseEXTL2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2110	1362	354	383	11			
1	B	262	Total	C	N	O	S	0	0	0
			2078	1342	348	377	11			

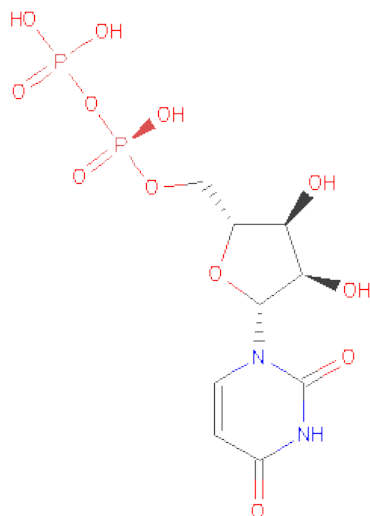
- Molecule 2 is a polymer of unknown type called SUGAR (GCU-GAL).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	0
			24	12	12		
2	B	2	Total	C	O	0	0
			24	12	12		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



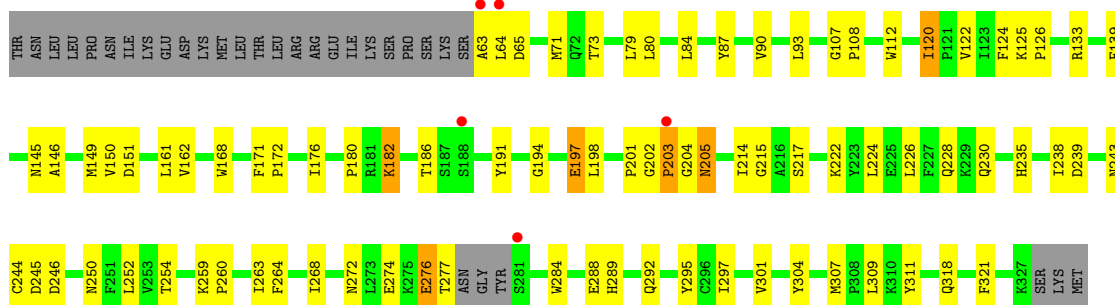
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	53	Total 53	O 53	0	0
6	B	44	Total 44	O 44	0	0

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Chain A:



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.16Å 125.16Å 83.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.70 19.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.98-2.70) 96.8 (19.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.71Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.254 0.192 , 0.252	Depositor DCC
R_{free} test set	889 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 20.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 18472 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4393	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, UDP, MN, EDO, BDP

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	0/2169	0.63	0/2949
1	B	0.36	0/2135	0.60	0/2906
All	All	0.37	0/4304	0.61	0/5855

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2110	0	2051	57	0
1	B	2078	0	2015	63	0
2	A	24	0	17	0	0
2	B	24	0	17	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	25	0	11	0	0
4	B	25	0	11	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	53	0	0	2	0
6	B	44	0	0	4	0
All	All	4393	0	4134	118	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (118) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288:GLU:O	1:A:292:GLN:HB2	1.75	0.86
1:B:71:MET:CE	1:B:80:LEU:HD12	2.19	0.72
1:A:318:GLN:HE22	1:B:205:ASN:HB3	1.56	0.71
1:B:238:ILE:HD12	1:B:245:ASP:HA	1.71	0.71
1:A:214:ILE:HG12	1:A:246:ASP:HB3	1.71	0.70
1:B:226:LEU:HD23	1:B:252:LEU:HD21	1.73	0.70
1:A:79:LEU:HD22	1:A:277:THR:HB	1.72	0.70
1:B:64:LEU:O	1:B:64:LEU:HD23	1.92	0.70
1:B:146:ALA:HB2	1:B:168:TRP:CZ3	2.27	0.69
1:B:71:MET:HE3	1:B:80:LEU:HD12	1.76	0.67
1:B:272:ASN:OD1	1:B:274:GLU:HB2	1.94	0.66
1:A:71:MET:CE	1:A:80:LEU:HD12	2.26	0.65
1:B:133:ARG:HG2	6:B:636:HOH:O	1.97	0.65
1:A:147:VAL:HG23	1:A:221:SER:HB3	1.77	0.65
1:B:133:ARG:HD3	1:B:239:ASP:OD1	1.96	0.64
1:B:64:LEU:HD12	1:B:145:ASN:ND2	2.13	0.64
1:A:199:GLN:HE21	1:A:200:THR:HG22	1.64	0.63
1:A:201:PRO:HG3	1:A:311:TYR:CE1	2.34	0.63
1:B:63:ALA:C	1:B:65:ASP:H	2.02	0.62
1:B:146:ALA:HB2	1:B:168:TRP:CH2	2.34	0.62
1:B:182:LYS:HD2	6:B:640:HOH:O	1.98	0.62
1:A:307:MET:HE1	1:A:309:LEU:HB2	1.81	0.61
1:B:90:VAL:HG21	1:B:161:LEU:HD12	1.82	0.61
1:A:238:ILE:HD12	1:A:245:ASP:HA	1.82	0.61
1:A:182:LYS:HG2	1:A:183:HIS:N	2.15	0.60
1:B:87:TYR:O	1:B:93:LEU:HD22	2.02	0.60
1:A:146:ALA:HB2	1:A:168:TRP:CH2	2.37	0.59
1:B:307:MET:HE1	1:B:309:LEU:HB2	1.84	0.59
1:A:95:LYS:HD3	1:A:123:ILE:HD12	1.85	0.58
1:B:243:ASN:O	1:B:244:CYS:HB2	2.03	0.58
1:B:197:GLU:H	1:B:197:GLU:CD	2.07	0.58
1:A:120:ILE:HD13	1:A:120:ILE:H	1.69	0.58
1:A:182:LYS:HE2	1:A:201:PRO:HD3	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:146:ALA:HB2	1:A:168:TRP:CZ3	2.41	0.56
1:B:120:ILE:H	1:B:120:ILE:HD13	1.70	0.55
1:B:71:MET:HE2	1:B:80:LEU:HD12	1.88	0.55
1:A:91:PRO:O	1:A:92:SER:HB2	2.08	0.54
1:A:274:GLU:O	1:A:277:THR:HG22	2.09	0.53
1:B:292:GLN:O	1:B:295:TYR:HB3	2.09	0.53
1:A:306:GLY:O	1:A:308:PRO:HD3	2.09	0.53
1:B:133:ARG:NH1	1:B:235:HIS:HB3	2.24	0.53
1:A:168:TRP:HA	1:A:176:ILE:HG13	1.91	0.52
1:B:214:ILE:HG12	1:B:246:ASP:HB3	1.91	0.52
1:B:73:THR:HB	1:B:80:LEU:HD13	1.90	0.52
1:A:201:PRO:HG2	1:A:202:GLY:N	2.25	0.52
1:B:243:ASN:OD1	1:B:244:CYS:N	2.43	0.51
1:A:71:MET:HE3	1:A:80:LEU:HD12	1.92	0.51
1:B:230:GLN:NE2	1:B:304:TYR:OH	2.42	0.51
1:B:272:ASN:OD1	1:B:274:GLU:CB	2.59	0.51
1:B:284:TRP:HA	1:B:289:HIS:CG	2.46	0.51
1:A:137:GLN:HA	1:A:228:GLN:NE2	2.25	0.50
1:A:95:LYS:HD3	1:A:123:ILE:CD1	2.42	0.49
1:A:252:LEU:C	1:A:252:LEU:HD23	2.32	0.49
1:A:252:LEU:HD23	1:A:253:VAL:N	2.27	0.49
1:B:112:TRP:CZ2	1:B:122:VAL:HG21	2.48	0.49
1:A:243:ASN:OD1	1:A:244:CYS:N	2.38	0.49
1:B:79:LEU:HD22	1:B:277:THR:HB	1.94	0.49
1:B:63:ALA:C	1:B:65:ASP:N	2.64	0.48
1:A:171:PHE:N	1:A:172:PRO:HD3	2.27	0.48
1:B:194:GLY:HA3	1:B:198:LEU:HD12	1.95	0.48
1:B:318:GLN:HB3	1:B:321:PHE:HB3	1.95	0.48
1:B:191:TYR:CZ	1:B:307:MET:HG3	2.49	0.47
1:B:168:TRP:HA	1:B:176:ILE:HG13	1.97	0.47
1:A:86:HIS:CD2	1:A:155:LEU:HD13	2.48	0.47
1:B:243:ASN:O	1:B:244:CYS:CB	2.61	0.47
1:A:120:ILE:HD13	1:A:120:ILE:N	2.30	0.47
1:A:150:VAL:HA	1:A:215:GLY:O	2.14	0.47
1:B:64:LEU:HD12	1:B:145:ASN:HD22	1.79	0.47
1:B:150:VAL:HA	1:B:215:GLY:O	2.14	0.47
1:A:297:ILE:O	1:A:301:VAL:HG23	2.15	0.47
1:A:227:PHE:HA	1:A:252:LEU:CD1	2.45	0.46
1:A:163:PHE:CD1	1:A:318:GLN:HG3	2.51	0.46
1:B:180:PRO:HD3	1:B:264:PHE:CE1	2.50	0.46
1:A:187:SER:O	1:A:188:SER:C	2.54	0.46
1:A:187:SER:HB3	1:A:190:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194:GLY:HA3	1:B:198:LEU:CD1	2.46	0.46
1:B:301:VAL:CG2	1:B:307:MET:HG2	2.46	0.46
1:A:110:GLU:HB3	6:A:647:HOH:O	2.16	0.46
1:B:149:MET:SD	1:B:214:ILE:HD12	2.56	0.46
1:B:297:ILE:O	1:B:301:VAL:HG23	2.16	0.46
1:A:201:PRO:CG	1:A:202:GLY:N	2.79	0.45
1:B:150:VAL:HG12	1:B:151:ASP:O	2.16	0.45
1:A:72:GLN:HA	1:A:99:VAL:HB	1.97	0.45
1:B:214:ILE:HA	1:B:217:SER:OG	2.17	0.45
1:B:125:LYS:HD3	1:B:139:PHE:CD2	2.51	0.45
1:A:272:ASN:OD1	1:A:274:GLU:HG3	2.17	0.44
1:A:125:LYS:HD3	1:A:139:PHE:CE2	2.53	0.44
1:B:222:LYS:HG3	6:B:621:HOH:O	2.18	0.43
1:A:134:ASN:O	1:A:137:GLN:HG3	2.18	0.43
1:B:171:PHE:N	1:B:172:PRO:HD3	2.34	0.43
1:B:162:VAL:HG13	6:B:616:HOH:O	2.17	0.43
1:A:149:MET:HB3	1:A:214:ILE:O	2.19	0.43
1:B:79:LEU:HD13	1:B:276:GLU:O	2.19	0.43
1:A:131:LYS:HB3	1:A:133:ARG:HG2	2.00	0.42
1:B:124:PHE:O	1:B:126:PRO:HD3	2.19	0.42
1:B:238:ILE:HD12	1:B:245:ASP:CA	2.47	0.42
1:B:252:LEU:HD23	1:B:252:LEU:C	2.40	0.42
1:A:182:LYS:CG	1:A:183:HIS:N	2.82	0.42
1:A:201:PRO:HG2	1:A:202:GLY:H	1.84	0.42
1:A:224:LEU:O	1:A:228:GLN:HG2	2.19	0.42
1:B:259:LYS:HB3	1:B:260:PRO:CD	2.50	0.42
1:B:120:ILE:HD13	1:B:120:ILE:N	2.33	0.42
1:A:251:PHE:O	1:A:255:ARG:HG3	2.19	0.42
1:A:228:GLN:HG3	6:A:617:HOH:O	2.19	0.42
1:A:133:ARG:HD2	1:A:239:ASP:OD1	2.20	0.42
1:A:155:LEU:HD12	1:A:155:LEU:C	2.40	0.41
1:A:201:PRO:CD	1:A:202:GLY:H	2.33	0.41
1:B:250:ASN:O	1:B:254:THR:HG22	2.20	0.41
1:A:73:THR:HG21	1:A:80:LEU:HD22	2.03	0.41
1:B:201:PRO:HG2	1:B:202:GLY:H	1.86	0.41
1:B:107:GLY:HA2	1:B:108:PRO:HD3	1.86	0.41
1:B:201:PRO:HG3	1:B:311:TYR:CE1	2.56	0.41
1:B:224:LEU:O	1:B:228:GLN:HG2	2.21	0.41
1:A:205:ASN:HB2	1:B:318:GLN:HE22	1.85	0.41
1:B:176:ILE:HD12	1:B:263:ILE:HB	2.02	0.40
1:A:133:ARG:NH1	1:A:239:ASP:OD2	2.53	0.40
1:A:112:TRP:CZ2	1:A:122:VAL:HG21	2.55	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:PRO:CG	1:A:202:GLY:H	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/293 (90%)	243 (92%)	18 (7%)	2 (1%)	27	58
1	B	258/293 (88%)	234 (91%)	21 (8%)	3 (1%)	19	45
All	All	521/586 (89%)	477 (92%)	39 (8%)	5 (1%)	22	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PRO
1	B	203	PRO
1	A	202	GLY
1	B	204	GLY
1	B	276	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/263 (88%)	218 (95%)	12 (5%)	32	63
1	B	227/263 (86%)	218 (96%)	9 (4%)	42	75
All	All	457/526 (87%)	436 (95%)	21 (5%)	37	70

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

Mol	Chain	Res	Type
1	A	84	LEU
1	A	120	ILE
1	A	143	GLU
1	A	155	LEU
1	A	182	LYS
1	A	186	THR
1	A	197	GLU
1	A	252	LEU
1	A	268	ILE
1	A	280	TYR
1	A	283	MET
1	A	288	GLU
1	B	84	LEU
1	B	120	ILE
1	B	182	LYS
1	B	186	THR
1	B	197	GLU
1	B	203	PRO
1	B	205	ASN
1	B	268	ILE
1	B	288	GLU

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

Mol	Chain	Res	Type
1	A	199	GLN
1	A	292	GLN
1	A	318	GLN
1	B	75	ASN
1	B	145	ASN
1	B	199	GLN
1	B	230	GLN
1	B	292	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

4 carbohydrates 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	A	509	2	13,13,13	4.15	9 (69%)	19,19,19	1.68	5 (26%)
2	GAL	A	510	2	11,11,12	1.25	1 (9%)	10,15,17	0.80	0
2	BDP	B	519	2	13,13,13	4.10	8 (61%)	19,19,19	1.67	6 (31%)
2	GAL	B	520	2	11,11,12	1.20	2 (18%)	10,15,17	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BDP	A	509	2	-	0/4/24/24	0/1/1/1
2	GAL	A	510	2	-	0/2/18/22	0/1/1/1
2	BDP	B	519	2	-	0/4/24/24	0/1/1/1
2	GAL	B	520	2	-	0/2/18/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	509	BDP	O2-C2	-8.78	1.21	1.43
2	B	519	BDP	O2-C2	-8.28	1.23	1.43
2	B	519	BDP	C5-C6	-7.82	1.35	1.53
2	A	509	BDP	C5-C6	-7.48	1.36	1.53
2	A	509	BDP	O5-C5	5.50	1.52	1.43
2	B	519	BDP	O5-C5	4.92	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	519	BDP	O5-C1	4.59	1.52	1.43
2	A	509	BDP	O5-C1	4.41	1.51	1.43
2	B	519	BDP	O6A-C6	3.75	1.35	1.22
2	B	519	BDP	C4-C5	-3.69	1.46	1.53
2	A	509	BDP	O6A-C6	3.66	1.34	1.22
2	A	509	BDP	C4-C5	-3.54	1.46	1.53
2	A	510	GAL	C5-C4	3.11	1.57	1.52
2	B	520	GAL	C5-C4	2.54	1.56	1.52
2	A	509	BDP	O6B-C6	-2.21	1.22	1.30
2	B	519	BDP	O6B-C6	-2.21	1.22	1.30
2	B	519	BDP	O1-C1	2.19	1.47	1.39
2	B	520	GAL	C1-C2	2.18	1.54	1.53
2	A	509	BDP	O1-C1	2.05	1.47	1.39
2	A	509	BDP	C1-C2	2.03	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	519	BDP	C4-C5-C6	3.59	117.15	110.84
2	A	509	BDP	C4-C5-C6	3.38	116.78	110.84
2	B	519	BDP	O6B-C6-C5	3.01	124.46	113.49
2	A	509	BDP	O6B-C6-C5	2.95	124.24	113.49
2	A	509	BDP	C3-C4-C5	2.71	114.40	109.48
2	B	519	BDP	C3-C4-C5	2.48	113.98	109.48
2	A	509	BDP	O6B-C6-O6A	-2.27	118.94	124.07
2	A	509	BDP	C4-C3-C2	-2.12	106.89	110.82
2	B	519	BDP	O6B-C6-O6A	-2.11	119.31	124.07
2	B	519	BDP	C4-C3-C2	-2.07	106.99	110.82
2	B	519	BDP	C1-C2-C3	-2.04	107.30	110.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	UDP	A	351	3	26,26,26	1.61	7 (26%)	36,40,40	1.52	5 (13%)
5	EDO	A	401	-	3,3,3	2.12	2 (66%)	2,2,2	0.47	0
4	UDP	B	352	3	26,26,26	1.65	7 (26%)	36,40,40	1.56	6 (16%)
5	EDO	B	402	-	3,3,3	2.21	2 (66%)	2,2,2	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UDP	A	351	3	-	0/14/32/32	0/2/2/2
5	EDO	A	401	-	-	0/1/1/1	0/0/0/0
4	UDP	B	352	3	-	0/14/32/32	0/2/2/2
5	EDO	B	402	-	-	0/1/1/1	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	352	UDP	PA-O3A	3.57	1.66	1.59
4	A	351	UDP	PA-O3A	3.21	1.65	1.59
4	B	352	UDP	PB-O1B	3.14	1.61	1.51
4	A	351	UDP	PB-O1B	3.05	1.61	1.51
5	B	402	EDO	O2-C2	2.97	1.57	1.42
4	B	352	UDP	C6-N1	2.95	1.40	1.35
4	A	351	UDP	C6-N1	2.88	1.40	1.35
4	A	351	UDP	C4-N3	2.83	1.42	1.37
4	B	352	UDP	C2'-C1'	-2.81	1.49	1.53
5	A	401	EDO	O2-C2	2.76	1.56	1.42
4	A	351	UDP	PB-O3A	-2.63	1.55	1.60
4	B	352	UDP	C2-N1	2.62	1.41	1.38
4	B	352	UDP	C4-N3	2.57	1.41	1.37
4	A	351	UDP	C2-N1	2.54	1.41	1.38
4	B	352	UDP	PB-O3A	-2.30	1.56	1.60
5	B	402	EDO	O1-C1	2.19	1.53	1.42
5	A	401	EDO	O1-C1	2.16	1.53	1.42
4	A	351	UDP	C2'-C1'	-2.11	1.50	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	351	UDP	O3B-PB-O1B	4.74	125.95	110.44
4	B	352	UDP	O3B-PB-O1B	4.60	125.47	110.44
4	B	352	UDP	C2'-C1'-N1	3.75	122.92	113.26
4	A	351	UDP	C2'-C1'-N1	3.56	122.44	113.26
4	B	352	UDP	C2-N1-C1'	-3.03	116.31	118.21
4	B	352	UDP	O5'-C5'-C4'	2.81	119.25	108.94
4	A	351	UDP	O5'-C5'-C4'	2.62	118.55	108.94
4	A	351	UDP	C5-C6-N1	2.43	123.96	121.21
4	A	351	UDP	C2-N1-C1'	-2.39	116.71	118.21
4	B	352	UDP	C4'-O4'-C1'	2.15	112.08	109.75
4	B	352	UDP	C5-C6-N1	2.03	123.51	121.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/293 (90%)	-0.54	7 (2%) 53 59	13, 25, 50, 63	0
1	B	262/293 (89%)	-0.40	5 (1%) 64 70	16, 32, 52, 69	0
All	All	527/586 (89%)	-0.47	12 (2%) 59 64	13, 28, 51, 69	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	PRO	4.0
1	B	63	ALA	3.7
1	B	281	SER	3.1
1	A	279	GLY	3.1
1	A	188	SER	2.7
1	B	188	SER	2.6
1	B	64	LEU	2.6
1	A	64	LEU	2.5
1	B	203	PRO	2.4
1	A	202	GLY	2.3
1	A	280	TYR	2.1
1	A	128	THR	2.0

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

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

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GAL	A	510	11/12	0.17	0.94	45,46,49,52	0
2	BDP	A	509	13/13	0.15	0.83	35,39,43,44	0
2	GAL	B	520	11/12	0.16	0.44	52,55,57,61	0
2	BDP	B	519	13/13	0.14	0.10	45,48,50,52	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	B	402	4/4	0.14	1.37	25,25,26,28	0
5	EDO	A	401	4/4	0.11	0.05	17,17,19,20	0
4	UDP	A	351	25/25	0.11	-0.83	25,28,32,35	0
4	UDP	B	352	25/25	0.10	-0.99	27,33,35,36	0
3	MN	B	601	1/1	0.04	-2.41	41,41,41,41	0
3	MN	A	600	1/1	0.03	-3.16	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.