Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 08:41 AM EDT

PDB ID	:	4FRA
Title	:	Crystal Structure of ABBA+UDP+Gal at pH 5.0 with MPD as the cryoprotectant
Authors	:	Johal, A.R.; Alfaro, J.A.; Blackler, R.J.; Schuman, B.; Borisova, S.N.; Evans, S.V.
Deposited on	:	2012-06-26
Resolution	:	1.43 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:

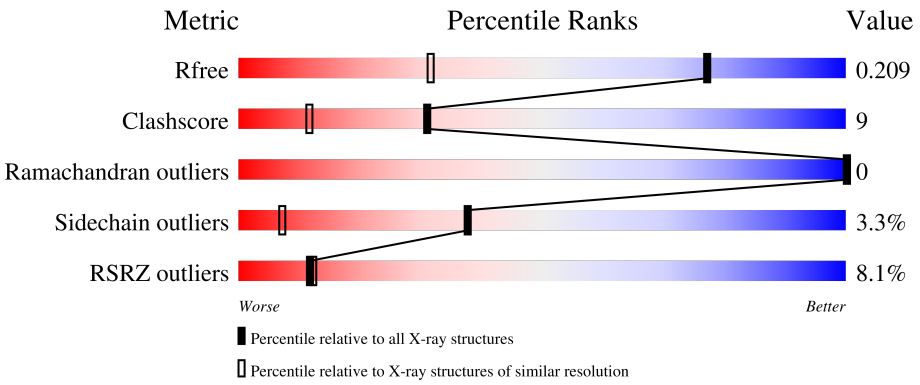
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.43 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	294	7% 72% 16% • 7%

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
4	PEG	A	403	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4942 atoms, of which 2323 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.

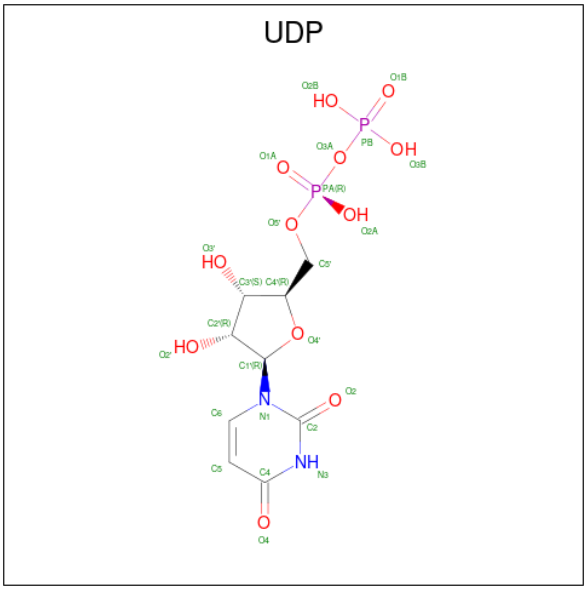
- Molecule 1 is a protein called Histo-blood group ABO system transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	272	4553	1470	2294	387	388	14	674	7	0

There are 5 discrepancies between the modelled and reference sequences:

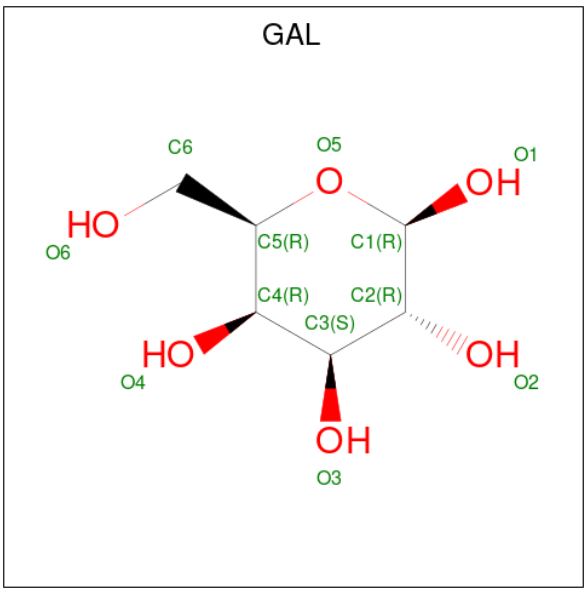
Chain	Residue	Modelled	Actual	Comment	Reference
A	62	PHE	-	expression tag	UNP H6A2X0
A	63	MET	-	expression tag	UNP H6A2X0
A	176	ARG	GLY	engineered mutation	UNP H6A2X0
A	268	GLY	ALA	engineered mutation	UNP H6A2X0
A	355	GLU	-	expression tag	UNP H6A2X0

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



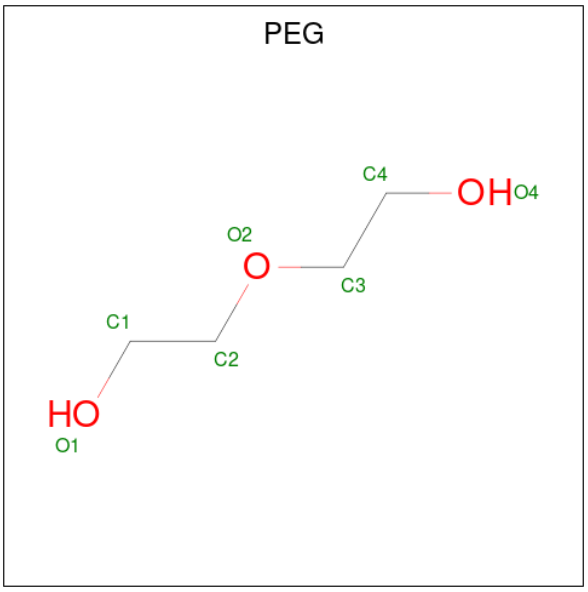
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	36	9	11	2	12	2	2	0

- Molecule 3 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	24	6	12	6	4	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	13	4	6	3	1	0

- Molecule 5 is water.

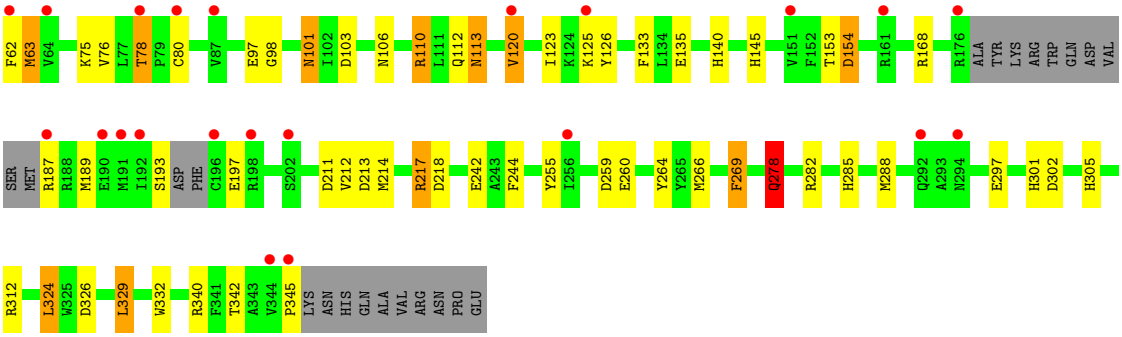
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	316	316	316	0	0

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: Histo-blood group ABO system transferase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	52.56Å 149.67Å 79.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.43 19.81 – 1.43	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-1.43) 94.8 (19.81-1.43)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.183 , 0.208 0.186 , 0.209	Depositor DCC
R_{free} test set	2804 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4942	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% 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: UDP, PEG, GAL

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	1.34	7/2348 (0.3%)	1.46	32/3183 (1.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	GLU	CD-OE1	7.24	1.33	1.25
1	A	282	ARG	CZ-NH1	6.96	1.42	1.33
1	A	332	TRP	CD2-CE2	5.82	1.48	1.41
1	A	110	ARG	CZ-NH2	5.47	1.40	1.33
1	A	126	TYR	CE1-CZ	-5.42	1.31	1.38
1	A	260	GLU	CG-CD	-5.35	1.44	1.51
1	A	213	ASP	CB-CG	-5.11	1.41	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	282	ARG	NE-CZ-NH1	15.64	128.12	120.30
1	A	282	ARG	NE-CZ-NH2	-15.13	112.73	120.30
1	A	217	ARG	NE-CZ-NH1	-11.51	114.55	120.30
1	A	213	ASP	CB-CG-OD1	10.65	127.89	118.30
1	A	211	ASP	CB-CG-OD2	-9.92	109.38	118.30
1	A	312	ARG	NE-CZ-NH1	-9.82	115.39	120.30
1	A	217	ARG	NE-CZ-NH2	9.70	125.15	120.30
1	A	259	ASP	CB-CG-OD1	9.10	126.48	118.30
1	A	244	PHE	CB-CG-CD2	8.89	127.03	120.80
1	A	340	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	260	GLU	OE1-CD-OE2	-8.45	113.16	123.30
1	A	97	GLU	OE1-CD-OE2	-8.39	113.23	123.30
1	A	168	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	A	211	ASP	CB-CG-OD1	7.96	125.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	ASP	CB-CG-OD1	7.90	125.41	118.30
1	A	135	GLU	OE1-CD-OE2	7.70	132.54	123.30
1	A	269	PHE	CB-CG-CD2	6.98	125.69	120.80
1	A	120[A]	VAL	CG1-CB-CG2	-6.42	100.63	110.90
1	A	120[B]	VAL	CG1-CB-CG2	-6.42	100.63	110.90
1	A	63	MET	CG-SD-CE	6.05	109.88	100.20
1	A	244	PHE	CB-CG-CD1	-5.98	116.62	120.80
1	A	255	TYR	CB-CG-CD1	5.88	124.53	121.00
1	A	217	ARG	CB-CG-CD	5.83	126.76	111.60
1	A	213	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	326	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	189	MET	CG-SD-CE	5.68	109.29	100.20
1	A	264	TYR	CB-CG-CD1	5.53	124.31	121.00
1	A	278	GLN	CB-CG-CD	5.49	125.86	111.60
1	A	329	LEU	CB-CG-CD1	5.46	120.28	111.00
1	A	76	VAL	N-CA-CB	-5.32	99.79	111.50
1	A	154	ASP	OD1-CG-OD2	-5.31	113.21	123.30
1	A	218	ASP	CB-CG-OD2	5.11	122.89	118.30

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	2259	2294	2266	40	0
2	A	25	11	11	1	0
3	A	12	12	12	0	0
4	A	7	6	10	2	0
5	A	316	0	0	14	2
All	All	2619	2323	2299	42	2

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 9.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:HE2	1:A:324:LEU:HG	1.23	1.12
1:A:266:MET:HE2	1:A:324:LEU:CG	1.89	1.02
1:A:302:ASP:OD2	5:A:722:HOH:O	1.99	0.81
1:A:197:GLU:HA	1:A:278:GLN:OE1	1.80	0.80
1:A:214[A]:MET:HE2	5:A:740:HOH:O	1.83	0.78
1:A:63:MET:HE2	5:A:723:HOH:O	1.86	0.76
2:A:401:UDP:O1A	5:A:816:HOH:O	2.06	0.73
1:A:75:LYS:HB2	1:A:78[A]:THR:HG23	1.73	0.71
1:A:112:GLN:NE2	5:A:745:HOH:O	2.29	0.66
1:A:345:PRO:HD2	5:A:784:HOH:O	1.98	0.64
1:A:266:MET:HE2	1:A:324:LEU:CD2	2.27	0.64
1:A:123:ILE:CD1	1:A:153:THR:HA	2.29	0.62
1:A:120[A]:VAL:HG21	1:A:133:PHE:CZ	2.35	0.62
1:A:101:ASN:HD22	1:A:101:ASN:C	2.06	0.59
1:A:266:MET:CE	1:A:324:LEU:CD2	2.82	0.57
1:A:266:MET:CE	1:A:324:LEU:HD21	2.34	0.57
1:A:193:SER:HA	1:A:278:GLN:NE2	2.20	0.57
1:A:305:HIS:HE1	5:A:550:HOH:O	1.87	0.56
1:A:110:ARG:HH22	1:A:113:ASN:HD22	1.54	0.56
4:A:403:PEG:H22	5:A:811:HOH:O	2.05	0.56
1:A:106:ASN:OD1	1:A:145:HIS:HE1	1.90	0.55
1:A:217:ARG:HD3	1:A:342:THR:OG1	2.07	0.55
1:A:140:HIS:HA	4:A:403:PEG:H12	1.89	0.55
1:A:123:ILE:HD13	1:A:153:THR:HA	1.90	0.54
1:A:285:HIS:HA	1:A:288:MET:HE3	1.90	0.54
1:A:101:ASN:HD21	1:A:103:ASP:HB2	1.74	0.53
1:A:62:PHE:N	5:A:706:HOH:O	2.42	0.52
1:A:120[A]:VAL:HG11	1:A:212:VAL:HG23	1.91	0.52
1:A:266:MET:HE1	1:A:324:LEU:HD21	1.92	0.52
1:A:305:HIS:HD2	5:A:542:HOH:O	1.92	0.51
1:A:120[A]:VAL:CG1	1:A:212:VAL:HB	2.44	0.48
1:A:242:GLU:H	1:A:242:GLU:CD	2.17	0.47
1:A:120[A]:VAL:HG21	1:A:133:PHE:CE2	2.50	0.46
1:A:80:CYS:SG	5:A:566:HOH:O	2.23	0.46
1:A:145:HIS:HD2	5:A:512:HOH:O	1.98	0.45
1:A:110:ARG:HH22	1:A:113:ASN:ND2	2.13	0.45
1:A:125:LYS:H	1:A:125:LYS:HE2	1.84	0.43
1:A:297:GLU:OE2	1:A:301:HIS:HD2	2.02	0.43
1:A:285:HIS:HD2	5:A:711:HOH:O	2.01	0.43
1:A:123:ILE:HD12	1:A:154:ASP:H	1.83	0.42
1:A:80:CYS:HB3	1:A:98:GLY:O	2.19	0.41
1:A:214[A]:MET:CE	5:A:740:HOH:O	2.54	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:579:HOH:O	5:A:647:HOH:O[3_455]	2.09	0.11
5:A:647:HOH:O	5:A:647:HOH:O[3_455]	2.14	0.06

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	273/294 (93%)	267 (98%)	6 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	250/263 (95%)	241 (96%)	9 (4%)	35 5

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

Mol	Chain	Res	Type
1	A	78[A]	THR
1	A	78[B]	THR
1	A	101	ASN
1	A	113	ASN
1	A	187	ARG

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Mol	Chain	Res	Type
1	A	269	PHE
1	A	278	GLN
1	A	324	LEU
1	A	329	LEU

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	101	ASN
1	A	113	ASN
1	A	145	HIS
1	A	275	GLN
1	A	285	HIS
1	A	286	GLN
1	A	294	ASN
1	A	301	HIS
1	A	305	HIS

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
2	UDP	A	401	-	24,26,26	1.81	6 (25%)	37,40,40	2.12	12 (32%)
4	PEG	A	403	-	6,6,6	0.98	0	5,5,5	3.21	4 (80%)
3	GAL	A	402	-	12,12,12	1.40	3 (25%)	17,17,17	1.65	4 (23%)

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	UDP	A	401	-	-	1/16/32/32	0/2/2/2
4	PEG	A	403	-	-	3/4/4/4	-
3	GAL	A	402	-	-	0/2/22/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	UDP	PB-O1B	3.45	1.61	1.50
2	A	401	UDP	O4'-C1'	3.27	1.49	1.42
2	A	401	UDP	C6-C5	2.97	1.41	1.35
3	A	402	GAL	O5-C1	2.81	1.49	1.42
2	A	401	UDP	O3'-C3'	2.52	1.48	1.43
2	A	401	UDP	C3'-C2'	-2.41	1.46	1.53
2	A	401	UDP	C6-N1	2.38	1.43	1.38
3	A	402	GAL	O5-C5	-2.19	1.39	1.44
3	A	402	GAL	O3-C3	-2.10	1.38	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	UDP	O2'-C2'-C3'	-4.79	96.31	111.82
2	A	401	UDP	N3-C2-N1	4.43	120.77	114.89
4	A	403	PEG	O1-C1-C2	4.28	136.65	111.81
4	A	403	PEG	O2-C2-C1	4.12	128.16	110.07
2	A	401	UDP	PA-O3A-PB	-3.79	119.82	132.83
2	A	401	UDP	O4'-C1'-N1	-3.78	99.73	108.36
3	A	402	GAL	O5-C5-C4	3.67	116.36	109.69
2	A	401	UDP	C4-N3-C2	-3.33	122.19	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	UDP	C1'-N1-C6	3.32	128.09	120.84
2	A	401	UDP	O4'-C4'-C3'	-3.07	99.03	105.11
3	A	402	GAL	C1-O5-C5	-2.77	108.44	113.66
2	A	401	UDP	O3'-C3'-C2'	-2.74	102.97	111.82
4	A	403	PEG	C3-O2-C2	2.56	124.40	113.29
4	A	403	PEG	O2-C3-C4	2.55	121.29	110.07
3	A	402	GAL	O1-C1-C2	2.51	116.09	109.03
2	A	401	UDP	O2'-C2'-C1'	2.49	118.36	110.02
3	A	402	GAL	O1-C1-O5	-2.47	102.98	110.38
2	A	401	UDP	C1'-N1-C2	-2.33	113.36	117.57
2	A	401	UDP	O2B-PB-O1B	-2.31	101.64	110.68
2	A	401	UDP	C2'-C3'-C4'	2.01	106.55	102.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

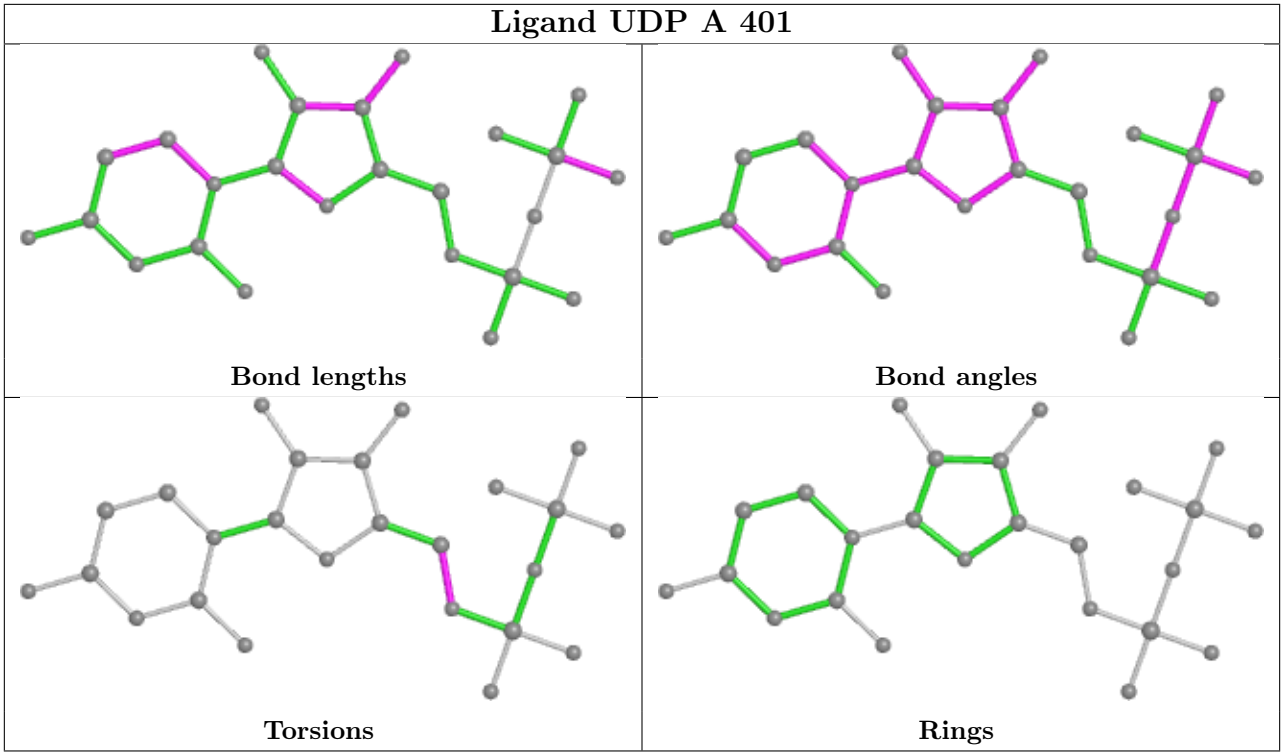
Mol	Chain	Res	Type	Atoms
4	A	403	PEG	O1-C1-C2-O2
4	A	403	PEG	O2-C3-C4-O4
2	A	401	UDP	C4'-C5'-O5'-PA
4	A	403	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	UDP	1	0
4	A	403	PEG	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.



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	272/294 (92%)	0.62	22 (8%)	12	12	10, 17, 34, 69	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	ARG	6.3
1	A	80	CYS	6.2
1	A	345	PRO	6.2
1	A	191	MET	4.8
1	A	161	ARG	4.4
1	A	292	GLN	3.7
1	A	187	ARG	3.6
1	A	192	ILE	3.5
1	A	256	ILE	3.2
1	A	198	ARG	3.1
1	A	120[A]	VAL	2.9
1	A	62	PHE	2.8
1	A	344	VAL	2.7
1	A	78[A]	THR	2.6
1	A	64	VAL	2.6
1	A	151	VAL	2.6
1	A	196	CYS	2.4
1	A	202	SER	2.4
1	A	190	GLU	2.3
1	A	294	ASN	2.2
1	A	87[A]	VAL	2.2
1	A	125	LYS	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)

There are no monosaccharides in this entry.

6.4 Ligands (i)

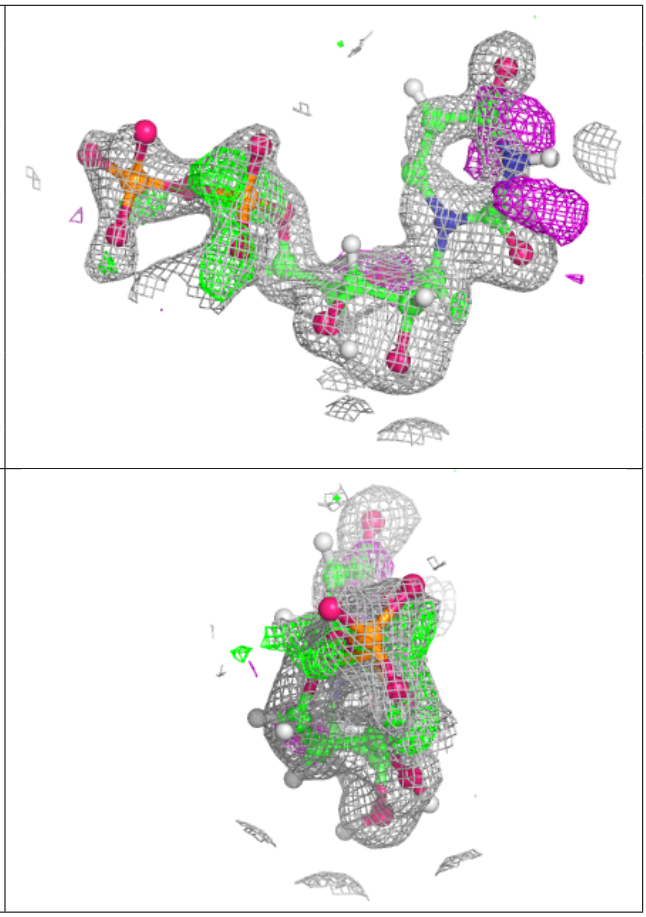
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UDP	A	401	25/25	0.58	0.29	16,26,36,39	11
4	PEG	A	403	7/7	0.82	0.20	19,34,42,42	1
3	GAL	A	402	12/12	0.93	0.12	8,16,21,21	16

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 UDP 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.