Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:03 AM GMT

PDB ID	:	2VS4
Title	:	THE BINDING OF UDP-GALACTOSE BY AN ACTIVE SITE MUTANT OF ALPHA-1,3 GALACTOSYLTRANSFERASE (ALPHA3GT)
Authors	:	Tumbale, P.; Jamaluddin, H.; Thiyagarajan, N.; Brew, K.; Acharya, K.R.
Deposited on	:	2008-04-18
Resolution	:	1.77 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

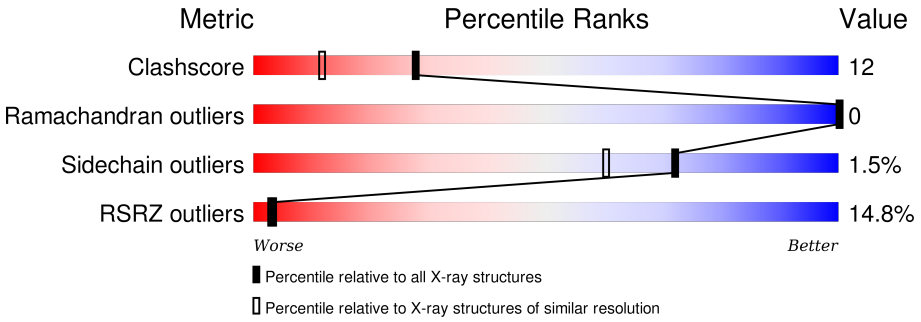
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 1.77 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))
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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. 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	289	16% 81% 18%
1	B	289	13% 80% 20%

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	NLC	A	1371	X	-	-	-
4	NLC	B	1371	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6170 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 N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	4	0
			2400	1568	396	424	12			
1	B	288	Total	C	N	O	S	0	3	0
			2400	1568	396	424	12			

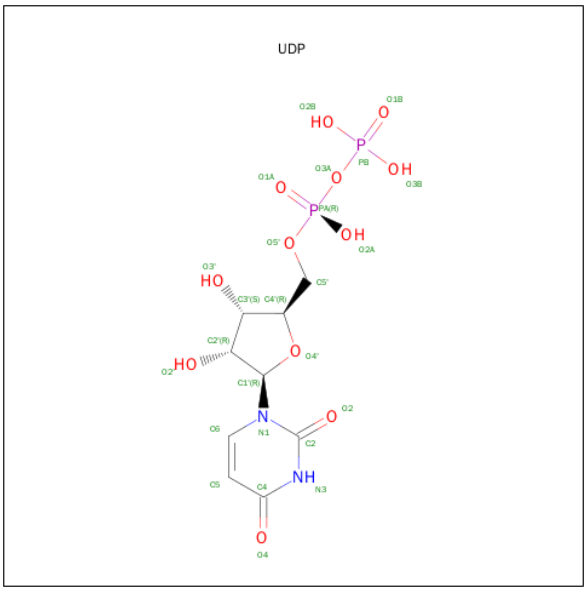
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	GLU	ASP	ENGINEERED MUTATION	UNP P14769
B	316	GLU	ASP	ENGINEERED MUTATION	UNP P14769

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

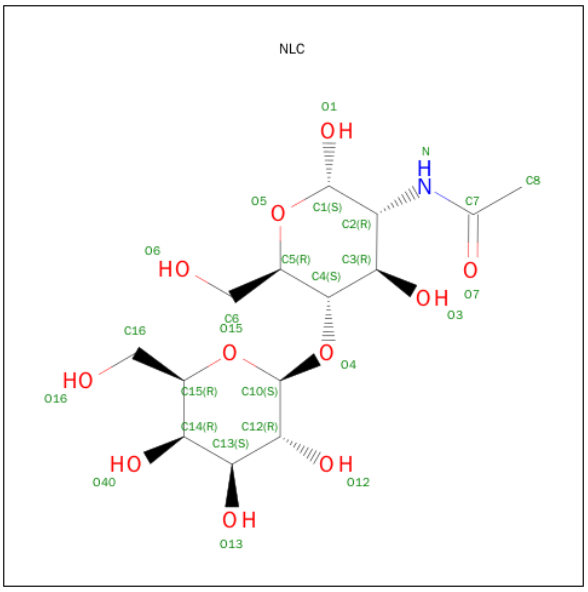
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



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

- Molecule 4 is 2-(ACETYLAMINO)-2-DEOXY-4-O-BETA-D-GALACTOPYRANOSYL-ALPHA-D-GLUCOPYRANOSE (three-letter code: NLC) (formula: $C_{14}H_{25}NO_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	14	1	11		

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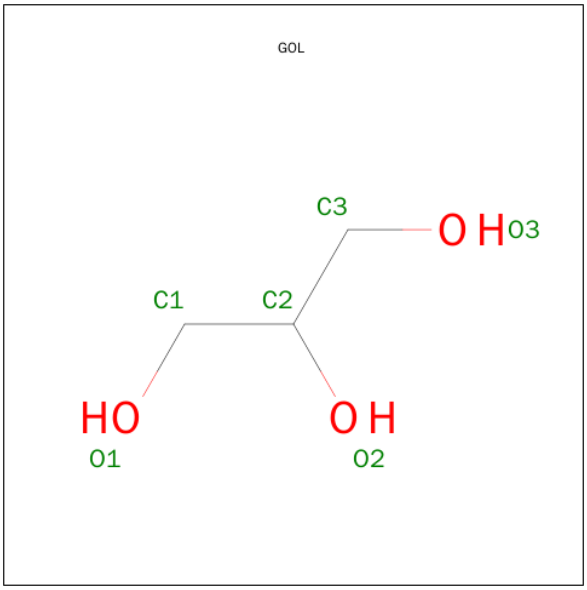
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			26	14	1	11		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

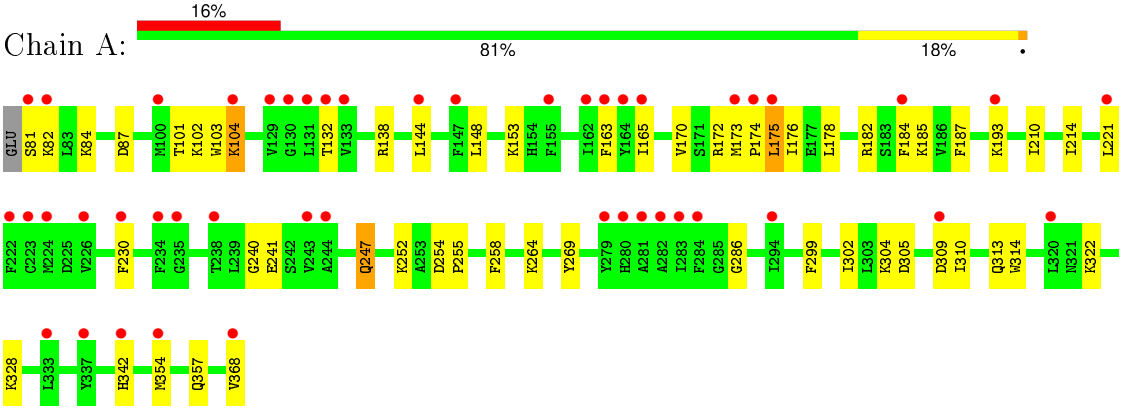
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	W	1254	Total	O	0	0
			1254	1254		

3 Residue-property plots (i)

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.

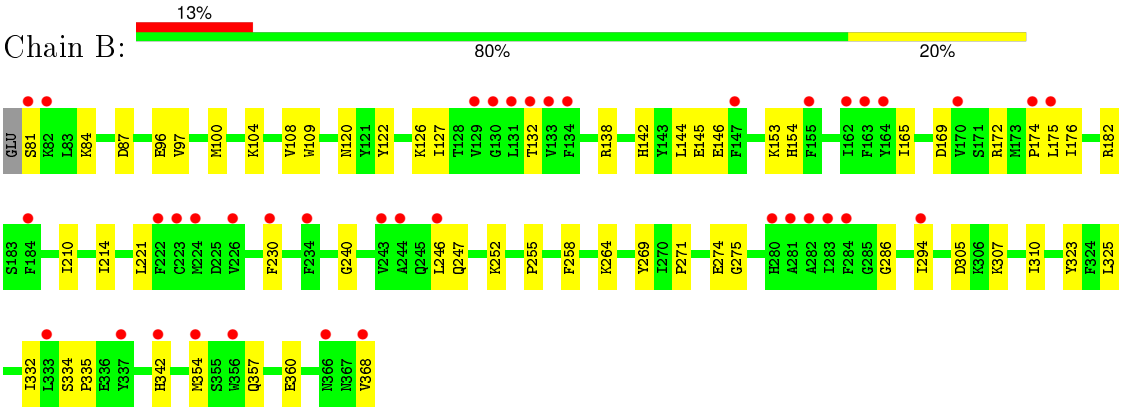
• Molecule 1: N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERAS E

Chain A:



• Molecule 1: N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERAS E

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.25Å 94.63Å 94.69Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	32.50 – 1.77 32.50 – 1.77	Depositor EDS
% Data completeness (in resolution range)	91.3 (32.50-1.77) 91.4 (32.50-1.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 1.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.263 , 0.278 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 71608 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6170	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.99 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6740e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, UDP, MN, NLC

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	0.45	2/2473 (0.1%)	0.63	0/3349
1	B	0.37	0/2473	0.63	0/3349
All	All	0.41	2/4946 (0.0%)	0.63	0/6698

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	GLN	C-O	-8.91	1.06	1.23
1	A	247	GLN	CD-OE1	-8.39	1.05	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2400	0	2355	61	0
1	B	2400	0	2356	55	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	11	0	0
3	B	25	0	11	0	0
4	A	26	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	26	0	24	0	0
5	A	6	0	7	0	0
5	B	6	0	7	0	0
6	W	1254	0	0	61	3
All	All	6170	0	4795	115	3

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 12.

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:SER:HB2	6:W:734:HOH:O	1.46	1.13
1:B:335:PRO:HD2	6:W:734:HOH:O	1.58	1.03
1:B:145:GLU:HG3	6:W:1171:HOH:O	1.69	0.90
1:B:368:VAL:HA	6:W:1014:HOH:O	1.75	0.85
1:B:342[B]:HIS:ND1	6:W:1249:HOH:O	2.01	0.85
1:B:368:VAL:HG12	6:W:119:HOH:O	1.77	0.83
1:B:120:ASN:HB2	6:W:437:HOH:O	1.80	0.80
1:B:360:GLU:CD	6:W:591:HOH:O	2.20	0.80
1:A:176:ILE:HA	6:W:264:HOH:O	1.82	0.79
1:A:172:ARG:NH2	6:W:413:HOH:O	2.14	0.78
1:B:252:LYS:HD2	6:W:1220:HOH:O	1.83	0.78
1:A:101:THR:O	6:W:945:HOH:O	2.01	0.78
1:A:153:LYS:HD3	6:W:962:HOH:O	1.86	0.74
1:A:254:ASP:HB3	6:W:491:HOH:O	1.86	0.74
1:A:132:THR:HG23	1:A:221:LEU:HD11	1.71	0.73
1:A:82:LYS:NZ	1:A:84:LYS:HD3	2.04	0.73
1:A:175:LEU:HD23	1:B:175:LEU:HD11	1.73	0.70
1:B:146:GLU:OE1	6:W:1124:HOH:O	2.09	0.70
1:B:81:SER:N	6:W:840:HOH:O	2.24	0.70
1:A:104:LYS:N	6:W:945:HOH:O	1.96	0.68
1:B:342[B]:HIS:CE1	6:W:1249:HOH:O	2.44	0.68
1:A:252:LYS:HD2	6:W:319:HOH:O	1.94	0.68
1:A:193:LYS:HD3	6:W:1244:HOH:O	1.94	0.67
1:B:210:ILE:HA	1:B:214:ILE:HB	1.75	0.67
1:B:104:LYS:HB3	6:W:1062:HOH:O	1.98	0.64
1:B:271:PRO:HG2	1:B:274:GLU:HG3	1.80	0.64
1:A:368:VAL:HG12	6:W:200:HOH:O	1.96	0.63
1:A:255:PRO:HA	1:A:258:PHE:CD1	2.33	0.63
1:A:304:LYS:CE	6:W:727:HOH:O	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HE3	6:W:442:HOH:O	2.01	0.60
1:B:109:TRP:CH2	6:W:734:HOH:O	2.51	0.60
1:B:108:VAL:O	1:B:334:SER:HB3	2.01	0.60
1:A:104:LYS:CA	6:W:945:HOH:O	2.47	0.59
1:B:81:SER:HB2	6:W:1119:HOH:O	2.03	0.59
1:A:313:GLN:HG2	1:A:314:TRP:CD1	2.38	0.58
1:A:185:LYS:HG2	1:A:187:PHE:CE1	2.39	0.58
1:A:174:PRO:CA	6:W:367:HOH:O	2.51	0.57
1:A:252:LYS:NZ	6:W:1190:HOH:O	2.38	0.57
1:B:230:PHE:HA	1:B:354[B]:MET:HG2	1.87	0.56
1:A:84:LYS:O	1:A:87:ASP:HB2	2.06	0.56
1:B:109:TRP:CZ2	6:W:734:HOH:O	2.58	0.56
1:A:174:PRO:HA	6:W:367:HOH:O	2.05	0.56
1:B:142:HIS:HD2	6:W:731:HOH:O	1.88	0.56
1:A:313:GLN:HG3	6:W:196:HOH:O	2.05	0.55
1:A:342[A]:HIS:CG	6:W:287:HOH:O	2.58	0.55
1:B:368:VAL:HG21	6:W:1216:HOH:O	2.06	0.55
1:A:175:LEU:N	6:W:367:HOH:O	2.39	0.55
1:B:255:PRO:HA	1:B:258:PHE:CD1	2.42	0.54
1:B:138:ARG:NH1	6:W:583:HOH:O	2.41	0.54
1:A:309:ASP:CB	6:W:1114:HOH:O	2.56	0.54
1:A:210:ILE:HA	1:A:214:ILE:HB	1.88	0.54
1:A:176:ILE:N	6:W:264:HOH:O	2.40	0.53
1:B:153:LYS:HE3	1:B:154:HIS:CE1	2.44	0.53
1:A:102:LYS:HE3	6:W:337:HOH:O	2.08	0.53
1:A:104:LYS:HA	6:W:945:HOH:O	2.07	0.52
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.75	0.52
1:A:170:VAL:O	1:A:173:MET:HB3	2.10	0.52
1:B:172:ARG:NH2	6:W:585:HOH:O	2.43	0.52
1:A:148:LEU:HD11	1:A:165:ILE:HD13	1.92	0.50
1:A:81:SER:O	1:A:82:LYS:HB3	2.11	0.50
1:A:230:PHE:HA	1:A:354[A]:MET:HG2	1.94	0.50
1:B:335:PRO:CD	6:W:734:HOH:O	2.35	0.49
1:A:138:ARG:NE	6:W:542:HOH:O	2.45	0.49
1:A:368:VAL:HG22	1:A:368:VAL:OXT	2.12	0.49
1:B:307:LYS:HE2	6:W:181:HOH:O	2.12	0.49
1:A:309:ASP:HB2	6:W:1114:HOH:O	2.11	0.49
1:B:109:TRP:CZ3	6:W:734:HOH:O	2.64	0.49
1:B:255:PRO:HA	1:B:258:PHE:CE1	2.48	0.49
1:B:96:GLU:HG2	1:B:97:VAL:HG13	1.95	0.48
1:B:144:LEU:HD23	1:B:174:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ASP:HB3	1:B:310:ILE:O	2.14	0.48
1:A:322:LYS:HE2	6:W:827:HOH:O	2.13	0.48
1:B:126:LYS:CE	6:W:477:HOH:O	2.63	0.46
1:B:334:SER:CB	6:W:734:HOH:O	2.28	0.46
1:A:82:LYS:HZ1	1:A:84:LYS:HD3	1.79	0.46
1:A:138:ARG:HA	1:A:138:ARG:HD3	1.79	0.45
1:A:82:LYS:HE2	1:A:84:LYS:CG	2.47	0.45
1:B:100:MET:HE1	6:W:1062:HOH:O	2.15	0.45
1:B:264:LYS:HG2	1:B:269:TYR:CZ	2.52	0.45
1:B:165:ILE:N	1:B:165:ILE:HD12	2.30	0.45
1:A:144:LEU:HD23	1:A:174:PRO:HD2	1.99	0.45
1:B:252:LYS:CD	6:W:1220:HOH:O	2.54	0.44
1:B:169:ASP:HB3	1:B:172:ARG:HD3	1.99	0.44
1:B:132:THR:HG23	1:B:221:LEU:HD11	1.99	0.44
1:B:145:GLU:CG	6:W:1171:HOH:O	2.47	0.44
1:A:305:ASP:HB3	1:A:310:ILE:O	2.18	0.43
1:B:240:GLY:O	1:B:286:GLY:HA2	2.18	0.43
1:A:163:PHE:HB2	1:A:184[A]:PHE:HD2	1.83	0.43
1:A:103:TRP:O	1:A:104:LYS:HB2	2.17	0.43
1:A:103:TRP:CE2	1:A:328:LYS:HB3	2.52	0.43
1:A:304:LYS:CD	6:W:727:HOH:O	2.66	0.43
1:A:342[A]:HIS:CD2	6:W:287:HOH:O	2.72	0.43
1:B:122:TYR:CD2	1:B:127:ILE:HD13	2.54	0.42
1:A:304:LYS:HE2	6:W:727:HOH:O	2.17	0.42
1:A:264:LYS:HA	1:A:269:TYR:CG	2.53	0.42
1:A:82:LYS:HZ3	1:A:84:LYS:HD3	1.83	0.42
1:A:82:LYS:CE	1:A:84:LYS:HD3	2.49	0.42
1:B:275:GLY:HA2	1:B:325:LEU:HD13	2.02	0.42
1:A:138:ARG:NH2	6:W:851:HOH:O	2.51	0.42
1:A:255:PRO:HA	1:A:258:PHE:CE1	2.54	0.42
1:B:176:ILE:C	1:B:176:ILE:HD12	2.40	0.42
1:B:175:LEU:N	6:W:1153:HOH:O	2.53	0.41
1:B:252:LYS:HE2	6:W:187:HOH:O	2.19	0.41
1:A:165:ILE:HG21	1:A:173:MET:CE	2.50	0.41
1:B:174:PRO:CA	6:W:1153:HOH:O	2.68	0.41
1:B:294:ILE:HG12	1:B:323:TYR:CE1	2.56	0.41
1:B:84:LYS:O	1:B:87:ASP:HB2	2.20	0.41
1:A:299:PHE:HA	1:A:302:ILE:HD12	2.01	0.41
1:A:82:LYS:HE2	1:A:84:LYS:HG2	2.02	0.41
1:B:176:ILE:HG13	1:B:176:ILE:H	1.73	0.41
1:A:241:GLU:O	1:A:286:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLY:O	1:A:286:GLY:HA2	2.20	0.40
1:A:176:ILE:CA	6:W:264:HOH:O	2.51	0.40
1:A:178:LEU:HD11	1:A:184[A]:PHE:CD1	2.56	0.40
1:B:246:LEU:HG	1:B:332:ILE:CG2	2.51	0.40

All (3) 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)
6:W:706:HOH:O	6:W:859:HOH:O[2_545]	2.17	0.03
6:W:620:HOH:O	6:W:1059:HOH:O[2_555]	2.18	0.02
6:W:269:HOH:O	6:W:904:HOH:O[2_646]	2.19	0.01

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	286/289 (99%)	276 (96%)	10 (4%)	0	100	100
1	B	286/289 (99%)	280 (98%)	6 (2%)	0	100	100
All	All	572/578 (99%)	556 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	259/260 (100%)	254 (98%)	5 (2%)	65 49
1	B	259/260 (100%)	256 (99%)	3 (1%)	78 69
All	All	518/520 (100%)	510 (98%)	8 (2%)	72 60

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	175	LEU
1	A	182	ARG
1	A	247	GLN
1	A	357	GLN
1	B	182	ARG
1	B	247	GLN
1	B	357	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	313	GLN
1	A	357	GLN
1	B	120	ASN
1	B	296	GLN
1	B	313	GLN
1	B	357	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	UDP	A	1370	-	18,26,26	3.12	8 (44%)	26,40,40	2.60	7 (26%)
4	NLC	A	1371	-	27,27,27	1.86	5 (18%)	34,39,39	1.19	3 (8%)
5	GOL	A	1372	-	5,5,5	1.21	0	5,5,5	0.79	0
3	UDP	B	1370	-	18,26,26	3.18	9 (50%)	26,40,40	2.60	6 (23%)
4	NLC	B	1371	-	27,27,27	1.84	4 (14%)	34,39,39	1.23	3 (8%)
5	GOL	B	1372	-	5,5,5	1.38	0	5,5,5	0.68	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
3	UDP	A	1370	-	-	0/12/32/32	0/2/2/2
4	NLC	A	1371	-	1/1/11/12	0/12/52/52	0/2/2/2
5	GOL	A	1372	-	-	0/4/4/4	0/0/0/0
3	UDP	B	1370	-	-	0/12/32/32	0/2/2/2
4	NLC	B	1371	-	1/1/11/12	0/12/52/52	0/2/2/2
5	GOL	B	1372	-	-	0/4/4/4	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1370	UDP	PB-O2B	-7.99	1.26	1.54
3	A	1370	UDP	PB-O2B	-7.70	1.27	1.54
4	B	1371	NLC	C8-C7	-6.24	1.38	1.50
4	A	1371	NLC	C8-C7	-6.18	1.38	1.50
3	A	1370	UDP	PB-O3B	-5.48	1.35	1.54
3	B	1370	UDP	PB-O3B	-5.24	1.35	1.54
3	A	1370	UDP	PB-O1B	-4.83	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1370	UDP	PB-O1B	-4.73	1.35	1.51
3	A	1370	UDP	PA-O1A	-4.60	1.34	1.51
3	B	1370	UDP	PA-O1A	-4.33	1.35	1.51
3	B	1370	UDP	PA-O2A	-3.60	1.39	1.54
3	A	1370	UDP	PA-O2A	-3.50	1.40	1.54
4	B	1371	NLC	O3-C3	-3.42	1.34	1.43
4	A	1371	NLC	O3-C3	-3.38	1.34	1.43
4	B	1371	NLC	O15-C15	-3.13	1.36	1.44
4	A	1371	NLC	O15-C15	-3.00	1.36	1.44
3	B	1370	UDP	O4'-C1'	-2.85	1.37	1.41
3	B	1370	UDP	O4'-C4'	-2.60	1.39	1.45
4	A	1371	NLC	C1-C2	-2.51	1.50	1.53
3	A	1370	UDP	O4'-C1'	-2.49	1.38	1.41
3	A	1370	UDP	O4'-C4'	-2.22	1.39	1.45
3	B	1370	UDP	C3'-C2'	-2.19	1.47	1.53
3	A	1370	UDP	C4-N3	2.59	1.37	1.33
3	B	1370	UDP	C4-N3	2.68	1.38	1.33
4	B	1371	NLC	C14-C15	2.80	1.59	1.53
4	A	1371	NLC	C14-C15	2.88	1.59	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1370	UDP	PA-O3A-PB	-2.46	124.42	132.67
3	B	1370	UDP	C5-C4-N3	-2.18	117.52	123.12
3	A	1370	UDP	C5-C4-N3	-2.14	117.63	123.12
3	B	1370	UDP	PA-O3A-PB	-2.13	125.51	132.67
3	A	1370	UDP	O2A-PA-O3A	2.01	114.20	105.09
3	B	1370	UDP	C5-C6-N1	2.04	125.58	120.58
3	A	1370	UDP	C5-C6-N1	2.08	125.68	120.58
4	A	1371	NLC	O12-C12-C10	2.36	115.20	110.02
3	B	1370	UDP	O4'-C1'-N1	2.42	113.18	108.08
3	A	1370	UDP	O4'-C1'-N1	2.51	113.38	108.08
4	B	1371	NLC	O12-C12-C10	2.53	115.56	110.02
3	A	1370	UDP	C4'-O4'-C1'	2.60	112.57	109.72
4	A	1371	NLC	O4-C4-C3	2.75	114.28	107.17
4	B	1371	NLC	O4-C4-C3	2.77	114.33	107.17
4	B	1371	NLC	O5-C5-C6	2.89	113.67	106.36
3	B	1370	UDP	C4'-O4'-C1'	2.94	112.95	109.72
4	A	1371	NLC	O5-C5-C6	3.11	114.22	106.36
3	A	1370	UDP	C4-N3-C2	11.19	125.23	114.14
3	B	1370	UDP	C4-N3-C2	11.20	125.24	114.14

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1371	NLC	C1
4	A	1371	NLC	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	288/289 (99%)	0.91	46 (15%)	3 2	16, 20, 23, 26	4 (1%)
1	B	288/289 (99%)	0.83	39 (13%)	4 4	16, 20, 22, 25	3 (1%)
All	All	576/578 (99%)	0.87	85 (14%)	3 3	16, 20, 23, 26	7 (1%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354[A]	MET	21.9
1	B	354[B]	MET	19.8
1	A	184[A]	PHE	18.0
1	B	184[B]	PHE	15.0
1	A	368	VAL	9.0
1	A	81	SER	7.9
1	B	368	VAL	7.6
1	A	100[A]	MET	6.4
1	B	283	ILE	5.3
1	B	342[B]	HIS	5.2
1	B	81	SER	5.0
1	A	283	ILE	4.9
1	A	131	LEU	4.7
1	A	342[A]	HIS	4.7
1	A	175	LEU	4.7
1	B	284	PHE	4.6
1	A	284	PHE	4.2
1	A	82	LYS	4.2
1	B	131	LEU	4.2
1	B	147	PHE	3.7
1	B	174	PRO	3.6
1	B	282	ALA	3.5
1	A	155	PHE	3.5
1	A	133	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	280	HIS	3.4
1	B	175	LEU	3.4
1	A	222	PHE	3.4
1	B	226	VAL	3.3
1	B	162	ILE	3.3
1	A	226	VAL	3.2
1	A	234	PHE	3.2
1	A	164	TYR	3.2
1	B	82	LYS	3.0
1	B	281	ALA	3.0
1	A	333	LEU	3.0
1	B	134	PHE	3.0
1	B	155	PHE	2.9
1	B	170	VAL	2.9
1	B	333	LEU	2.9
1	B	294	ILE	2.9
1	B	133	VAL	2.9
1	A	174	PRO	2.8
1	A	132	THR	2.7
1	A	230	PHE	2.7
1	B	222	PHE	2.7
1	A	162	ILE	2.7
1	B	130	GLY	2.6
1	A	163	PHE	2.6
1	B	230	PHE	2.6
1	A	238	THR	2.6
1	A	147	PHE	2.6
1	B	129	VAL	2.5
1	B	234	PHE	2.5
1	B	243	VAL	2.5
1	A	235	GLY	2.5
1	B	356	TRP	2.5
1	A	224	MET	2.5
1	A	281	ALA	2.5
1	A	337	TYR	2.4
1	A	282	ALA	2.4
1	A	243	VAL	2.4
1	B	164	TYR	2.4
1	A	244	ALA	2.4
1	A	223	CYS	2.3
1	B	132	THR	2.3
1	B	163	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	223	CYS	2.3
1	A	129	VAL	2.3
1	A	280	HIS	2.3
1	A	144	LEU	2.3
1	A	221	LEU	2.3
1	A	320	LEU	2.2
1	B	244	ALA	2.2
1	A	173	MET	2.2
1	B	246	LEU	2.2
1	B	337	TYR	2.2
1	A	130	GLY	2.2
1	B	366	ASN	2.2
1	A	165	ILE	2.2
1	A	193	LYS	2.2
1	A	309	ASP	2.2
1	B	224	MET	2.1
1	A	104	LYS	2.1
1	A	294	ILE	2.1
1	A	279	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	GOL	A	1372	6/6	0.86	0.17	1.66	21,23,25,26	0
4	NLC	A	1371	26/26	0.84	0.15	0.50	20,23,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NLC	B	1371	26/26	0.86	0.14	0.03	19,22,25,25	0
3	UDP	B	1370	25/25	0.94	0.14	-0.35	8,18,20,22	0
3	UDP	A	1370	25/25	0.96	0.12	-0.75	12,19,21,22	0
5	GOL	B	1372	6/6	0.82	0.41	-	23,23,23,25	0
2	MN	A	1369	1/1	0.97	0.13	-	1,1,1,1	0
2	MN	B	1369	1/1	1.00	0.10	-	1,1,1,1	0

6.5 Other polymers

There are no such residues in this entry.