Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:28 PM GMT

PDB ID	:	1FR8
Title	:	CRYSTAL STRUCTURE OF THE BOVINE BETA 1,4 GALACTOSYLT RANSFERASE (B4GALT1) CATALYTIC DOMAIN COMPLEXED WITH URIDINE DIPHOSPHOGALACTOSE
Authors	:	Gastinel, L.N.; Cambillau, C.; Bourne, Y.
Deposited on	:	2000-09-07
Resolution	:	2.40 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:

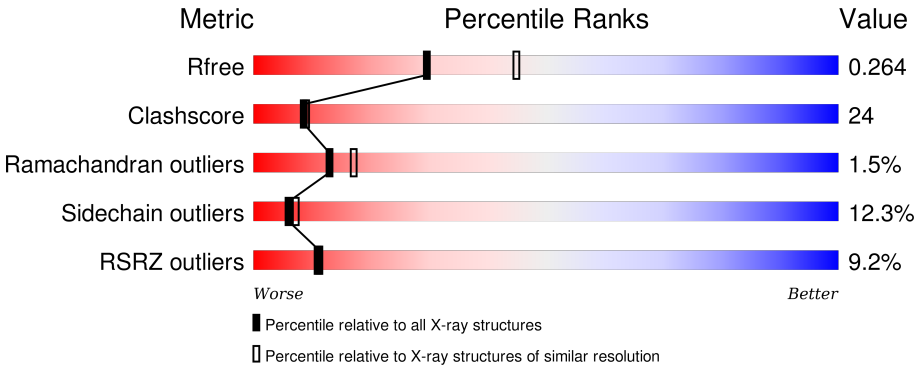
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	288	10% 51% 35% 8% • 6%
1	B	288	8% 57% 28% 8% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4549 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.

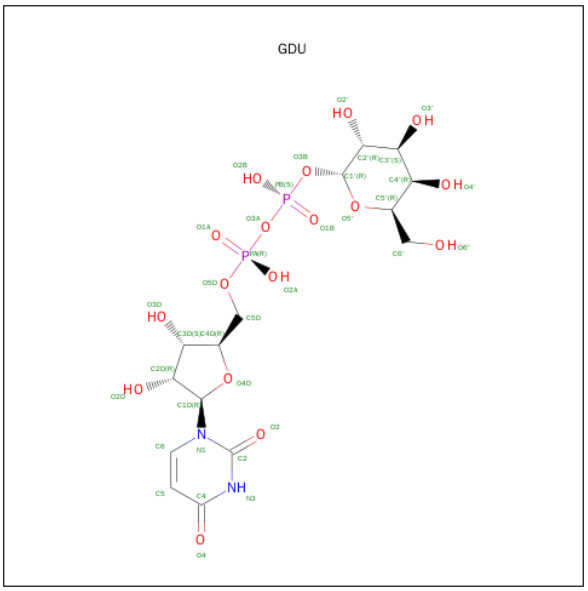
- Molecule 1 is a protein called BETA 1,4 GALACTOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2210	1418	381	397	14			
1	B	271	Total	C	N	O	S	0	0	0
			2210	1418	381	397	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	VAL	ILE	CONFLICT	UNP P08037
A	187	PRO	LEU	SEE REMARK 999	UNP P08037
B	158	VAL	ILE	CONFLICT	UNP P08037
B	187	PRO	LEU	SEE REMARK 999	UNP P08037

- Molecule 2 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (three-letter code: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



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

- Molecule 3 is water.

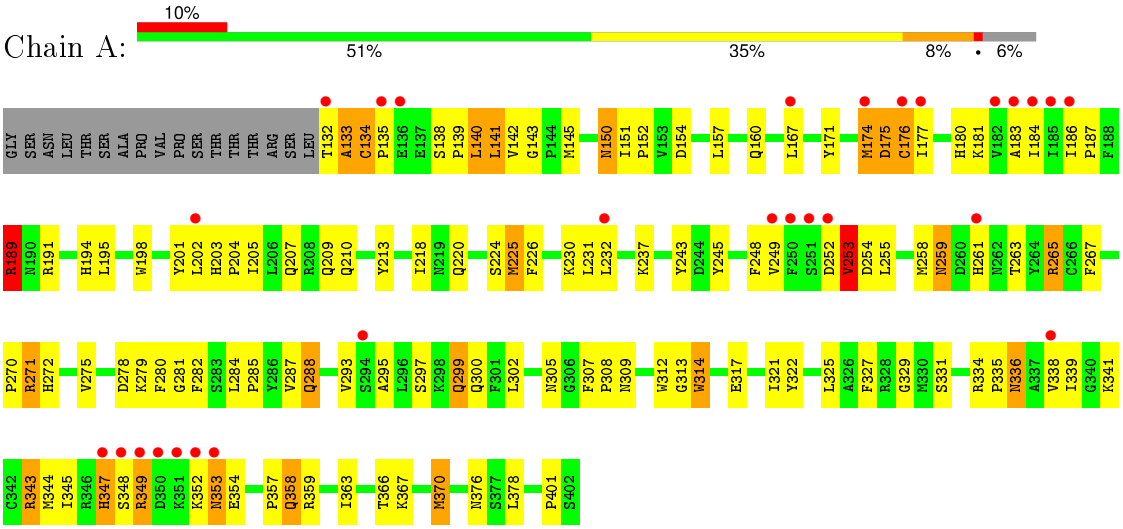
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	47	Total	O	0	0
			47	47		

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.

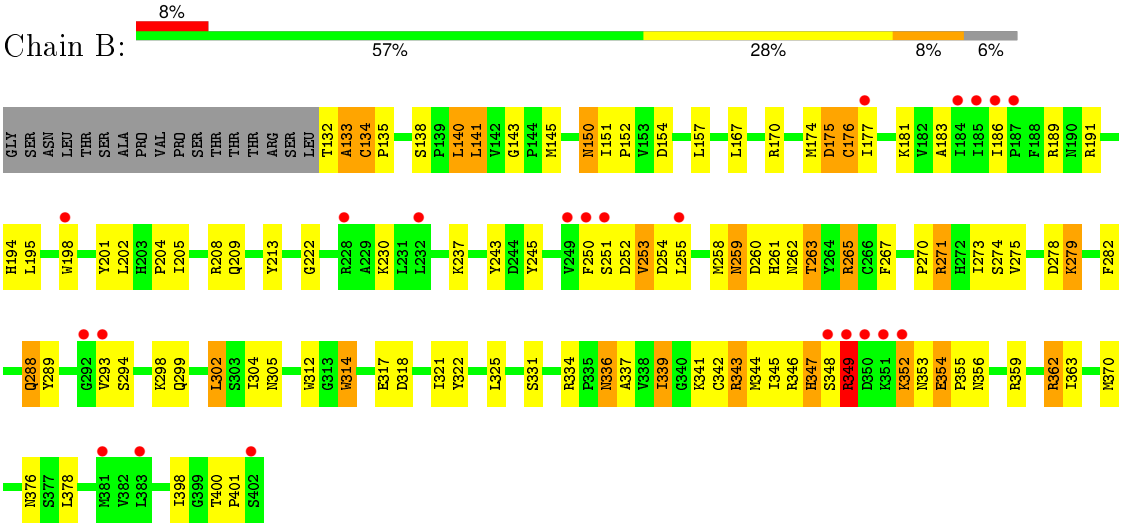
- Molecule 1: BETA 1,4 GALACTOSYLTRANSFERASE

Chain A:



- Molecule 1: BETA 1,4 GALACTOSYLTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	104.72Å 161.37Å 106.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.62 – 2.30	Depositor EDS
% Data completeness (in resolution range)	3.1 (30.00-2.40) 92.2 (29.62-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.31Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.237 , 0.262 0.235 , 0.264	Depositor DCC
R_{free} test set	1000 reflections (3.16%)	DCC
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 37161 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4549	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, 0.375 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: GDU

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	0.63	0/2270	0.81	2/3074 (0.1%)
1	B	0.69	0/2270	0.81	0/3074
All	All	0.66	0/4540	0.81	2/6148 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	253	VAL	CB-CA-C	-5.06	101.79	111.40

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	2210	0	2174	111	0
1	B	2210	0	2174	101	0
2	A	25	0	11	2	0
2	B	25	0	11	3	0
3	A	32	0	0	2	0
3	B	47	0	0	12	0
All	All	4549	0	4370	210	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 24.

All (210) 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:258:MET:HE2	1:B:341:LYS:HB3	1.35	1.05
1:B:362:ARG:HD3	3:B:55:HOH:O	1.63	0.98
1:B:336:ASN:HD21	1:B:339:ILE:HG23	1.31	0.93
1:B:349:ARG:NE	1:B:349:ARG:HA	1.83	0.91
1:A:349:ARG:CZ	1:A:349:ARG:HA	2.05	0.85
1:B:250:PHE:HB2	3:B:35:HOH:O	1.75	0.84
1:A:267:PHE:CD1	1:A:271:ARG:HG3	2.11	0.84
1:B:258:MET:HE2	1:B:341:LYS:CB	2.07	0.83
1:B:134:CYS:SG	1:B:135:PRO:HD2	2.20	0.80
1:B:151:ILE:O	1:B:151:ILE:HD12	1.82	0.80
1:A:191:ARG:HD2	1:A:194:HIS:HD2	1.47	0.79
1:B:140:LEU:HD23	1:B:140:LEU:N	1.99	0.78
1:B:349:ARG:CZ	1:B:349:ARG:HA	2.12	0.78
1:A:349:ARG:NE	1:A:349:ARG:HA	2.01	0.76
1:B:259:ASN:HD22	1:B:259:ASN:C	1.90	0.75
1:A:336:ASN:C	1:A:336:ASN:HD22	1.91	0.75
1:B:336:ASN:HD21	1:B:339:ILE:H	1.31	0.74
1:B:230:LYS:HE2	1:B:398:ILE:HB	1.69	0.74
1:B:132:THR:HB	1:B:177:ILE:HG12	1.70	0.74
1:A:259:ASN:HD22	1:A:261:HIS:H	1.36	0.72
1:A:258:MET:HE2	1:A:341:LYS:HB3	1.70	0.71
1:A:279:LYS:HD3	1:A:344:MET:SD	2.31	0.71
1:A:134:CYS:SG	1:A:135:PRO:HD2	2.31	0.71
1:B:336:ASN:ND2	1:B:339:ILE:HG23	2.03	0.71
1:A:278:ASP:OD2	1:A:343:ARG:HA	1.92	0.70
1:B:305:ASN:HD21	1:B:376:ASN:H	1.38	0.70
1:A:225:MET:SD	1:A:312:TRP:O	2.50	0.70
1:A:132:THR:HB	1:A:177:ILE:HG12	1.74	0.69
1:A:174:MET:H	1:A:174:MET:CE	2.05	0.69
1:A:174:MET:HE3	1:A:174:MET:H	1.58	0.69
1:B:258:MET:HE1	1:B:341:LYS:HE2	1.74	0.68
1:B:259:ASN:ND2	1:B:261:HIS:H	1.92	0.68
1:B:336:ASN:ND2	1:B:339:ILE:H	1.93	0.67
1:A:140:LEU:HD23	1:A:140:LEU:N	2.08	0.67
1:B:259:ASN:HD22	1:B:261:HIS:H	1.42	0.66
1:A:252:ASP:HB3	2:A:100:GDU:H3D	1.76	0.66
1:A:151:ILE:O	1:A:151:ILE:HD12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASN:ND2	1:A:261:HIS:H	1.95	0.65
1:B:278:ASP:HA	1:B:282:PHE:CE1	2.32	0.65
1:B:344:MET:CE	1:B:346:ARG:HB3	2.27	0.65
1:B:198:TRP:CZ2	1:B:202:LEU:HG	2.32	0.65
1:B:344:MET:HE3	3:B:71:HOH:O	1.97	0.65
1:A:258:MET:HE2	1:A:341:LYS:CB	2.27	0.64
1:B:253:VAL:HG22	2:B:403:GDU:O2D	1.98	0.64
1:A:186:ILE:HG21	1:A:253:VAL:HG13	1.79	0.64
1:B:294:SER:OG	3:B:35:HOH:O	2.15	0.64
1:B:288:GLN:HG3	1:B:359:ARG:CZ	2.28	0.63
1:A:279:LYS:HD2	1:A:354:GLU:OE2	1.98	0.62
1:A:187:PRO:HD3	1:A:232:LEU:HD21	1.81	0.62
1:B:279:LYS:HB3	1:B:346:ARG:NH1	2.13	0.62
1:A:313:GLY:N	3:A:75:HOH:O	2.33	0.62
1:B:352:LYS:HE2	1:B:353:ASN:H	1.65	0.61
1:A:259:ASN:HD22	1:A:259:ASN:C	2.04	0.61
1:B:354:GLU:HG2	1:B:355:PRO:HD2	1.83	0.61
1:B:362:ARG:NH1	3:B:55:HOH:O	2.26	0.61
1:B:198:TRP:HZ2	3:B:40:HOH:O	1.83	0.60
1:A:218:ILE:HG22	1:A:231:LEU:HD22	1.84	0.60
1:A:255:LEU:HD12	1:A:293:VAL:HG23	1.82	0.60
1:A:275:VAL:HG22	1:A:334:ARG:HD3	1.82	0.59
1:B:237:LYS:HD2	1:B:378:LEU:HD23	1.84	0.59
1:B:312:TRP:CD2	1:B:401:PRO:HG3	2.38	0.59
1:B:255:LEU:HD12	1:B:293:VAL:HG23	1.82	0.59
1:A:275:VAL:HG21	1:A:335:PRO:HD2	1.85	0.59
1:A:189:ARG:HB3	1:A:226:PHE:CE1	2.38	0.58
1:A:305:ASN:HD21	1:A:376:ASN:H	1.50	0.58
1:B:150:ASN:HD22	1:B:151:ILE:N	2.02	0.58
1:A:203:HIS:O	1:A:207:GLN:HG3	2.02	0.58
1:B:344:MET:O	1:B:346:ARG:HG2	2.03	0.58
1:A:258:MET:HE1	1:A:341:LYS:HE2	1.87	0.57
1:B:186:ILE:HG21	1:B:253:VAL:HG13	1.86	0.57
1:B:258:MET:CE	1:B:341:LYS:HB3	2.22	0.57
1:A:154:ASP:O	1:A:157:LEU:HB3	2.04	0.57
1:A:150:ASN:O	1:A:152:PRO:HD3	2.05	0.56
1:A:285:PRO:HB3	1:A:357:PRO:HG2	1.87	0.56
1:B:175:ASP:N	1:B:175:ASP:OD1	2.37	0.56
1:B:138:SER:HB3	1:B:141:LEU:HD13	1.87	0.56
1:B:279:LYS:HB2	1:B:354:GLU:HB2	1.87	0.56
1:A:180:HIS:CE1	1:A:265:ARG:HD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASP:N	1:A:175:ASP:OD1	2.39	0.56
1:B:336:ASN:HD22	1:B:336:ASN:C	2.08	0.55
1:A:336:ASN:ND2	1:A:339:ILE:H	2.04	0.55
1:A:259:ASN:ND2	1:A:261:HIS:HB2	2.22	0.55
1:B:317:GLU:O	1:B:321:ILE:HG13	2.06	0.55
1:B:150:ASN:O	1:B:152:PRO:HD3	2.08	0.54
1:A:205:ILE:O	1:A:209:GLN:HG3	2.08	0.54
1:B:258:MET:CE	1:B:341:LYS:HE2	2.38	0.54
1:B:279:LYS:HB3	1:B:346:ARG:CZ	2.37	0.54
1:A:358:GLN:HG2	1:A:359:ARG:N	2.22	0.54
1:A:201:TYR:O	1:A:204:PRO:HD2	2.08	0.54
1:B:267:PHE:CD1	1:B:271:ARG:HG3	2.43	0.54
1:A:271:ARG:HH12	1:A:335:PRO:HB3	1.73	0.53
1:A:272:HIS:HB3	1:A:334:ARG:HG2	1.90	0.53
1:A:347:HIS:C	1:A:348:SER:O	2.45	0.53
1:B:254:ASP:HA	1:B:345:ILE:HD12	1.90	0.53
1:B:181:LYS:HD3	1:B:243:TYR:CE2	2.44	0.53
1:A:132:THR:O	1:A:133:ALA:CB	2.56	0.53
1:A:288:GLN:HG3	1:A:359:ARG:HD2	1.91	0.53
1:A:336:ASN:ND2	1:A:338:VAL:H	2.07	0.52
1:A:307:PHE:HB3	1:A:308:PRO:HD2	1.91	0.52
1:B:132:THR:O	1:B:133:ALA:CB	2.57	0.52
1:B:134:CYS:HA	1:B:176:CYS:HB2	1.91	0.52
1:A:132:THR:HB	1:A:177:ILE:CG1	2.40	0.52
1:B:312:TRP:CG	1:B:401:PRO:HG3	2.45	0.52
1:B:259:ASN:HB2	3:B:36:HOH:O	2.10	0.51
1:A:282:PHE:HE2	1:A:341:LYS:HB3	1.74	0.51
1:A:189:ARG:HG3	1:A:189:ARG:O	2.09	0.51
1:B:354:GLU:CG	1:B:355:PRO:HD2	2.40	0.51
1:A:133:ALA:H	1:A:177:ILE:H	1.58	0.51
1:B:263:THR:HB	1:B:265:ARG:HG2	1.92	0.51
1:B:154:ASP:O	1:B:157:LEU:HB3	2.11	0.51
1:B:273:ILE:HB	1:B:293:VAL:HG12	1.92	0.50
1:A:336:ASN:HD22	1:A:338:VAL:H	1.58	0.50
1:A:347:HIS:O	1:A:348:SER:HB2	2.12	0.50
1:B:278:ASP:OD2	1:B:343:ARG:HD3	2.12	0.50
1:B:204:PRO:O	1:B:208:ARG:HG3	2.11	0.50
1:B:278:ASP:OD1	1:B:279:LYS:N	2.43	0.50
1:B:134:CYS:HB2	1:B:177:ILE:O	2.12	0.49
1:B:262:ASN:HB2	1:B:339:ILE:HD12	1.94	0.49
1:B:344:MET:HE2	1:B:346:ARG:HB3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:CYS:HA	1:A:176:CYS:HB2	1.94	0.49
1:A:150:ASN:HD22	1:A:151:ILE:N	2.11	0.49
1:A:363:ILE:HD13	1:B:314:TRP:CG	2.48	0.49
1:A:275:VAL:CG2	1:A:334:ARG:HD3	2.43	0.49
1:A:143:GLY:O	1:A:145:MET:HG3	2.13	0.49
1:A:189:ARG:HB3	1:A:226:PHE:HE1	1.77	0.49
1:A:280:PHE:CE2	1:A:357:PRO:HD3	2.48	0.49
1:A:181:LYS:HD3	1:A:243:TYR:CE2	2.48	0.49
2:A:100:GDU:O5D	2:A:100:GDU:H2D	2.12	0.49
1:B:253:VAL:CG2	2:B:403:GDU:O2D	2.60	0.48
1:A:138:SER:HB3	1:A:141:LEU:HD13	1.94	0.48
1:A:160:GLN:HE21	1:A:160:GLN:HA	1.78	0.48
1:B:252:ASP:HA	2:B:403:GDU:O3D	2.14	0.48
1:A:191:ARG:HD2	1:A:194:HIS:CD2	2.38	0.48
1:A:270:PRO:HD2	1:A:331:SER:O	2.14	0.47
1:A:270:PRO:HG2	1:A:325:LEU:HD22	1.96	0.47
1:A:184:ILE:HG13	1:A:249:VAL:HB	1.96	0.47
1:B:251:SER:CB	1:B:293:VAL:HG22	2.44	0.47
1:B:304:ILE:HG21	1:B:325:LEU:HD23	1.95	0.47
1:A:336:ASN:HD21	1:A:339:ILE:H	1.61	0.47
1:A:151:ILE:H	1:A:151:ILE:HG13	1.62	0.47
1:B:317:GLU:HG2	1:B:318:ASP:N	2.31	0.46
1:A:281:GLY:N	1:A:353:ASN:HD21	2.13	0.46
1:A:297:SER:OG	1:A:300:GLN:HG3	2.16	0.46
1:A:186:ILE:CG2	1:A:253:VAL:HG13	2.45	0.46
1:A:366:THR:HG22	1:A:370:MET:HE2	1.98	0.46
1:A:336:ASN:C	1:A:336:ASN:ND2	2.63	0.46
1:A:259:ASN:HD21	1:A:261:HIS:HB2	1.81	0.45
1:B:259:ASN:ND2	1:B:259:ASN:C	2.62	0.45
1:B:273:ILE:O	1:B:275:VAL:N	2.50	0.45
1:A:138:SER:HA	1:A:139:PRO:HD3	1.85	0.45
1:B:209:GLN:NE2	1:B:263:THR:HA	2.32	0.45
1:B:261:HIS:C	1:B:339:ILE:HD13	2.37	0.44
1:A:198:TRP:CZ2	1:A:202:LEU:HG	2.53	0.44
1:B:259:ASN:HD22	1:B:260:ASP:N	2.15	0.44
1:A:363:ILE:HD13	1:B:314:TRP:HB2	1.99	0.44
1:A:248:PHE:O	1:A:295:ALA:HA	2.17	0.44
1:A:312:TRP:CG	1:A:401:PRO:HB3	2.52	0.44
1:A:317:GLU:O	1:A:321:ILE:HG13	2.18	0.44
1:B:258:MET:SD	1:B:343:ARG:HG2	2.58	0.44
1:B:151:ILE:CD1	1:B:151:ILE:O	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLY:HA2	3:B:22:HOH:O	2.18	0.44
1:B:289:TYR:O	1:B:334:ARG:NH2	2.49	0.44
1:B:288:GLN:HB3	1:B:322:TYR:CE2	2.53	0.43
1:B:288:GLN:HB3	1:B:288:GLN:HE21	1.55	0.43
1:A:254:ASP:HA	1:A:345:ILE:HD12	2.00	0.43
1:A:299:GLN:HB2	3:A:17:HOH:O	2.18	0.43
1:B:209:GLN:HG2	3:B:37:HOH:O	2.17	0.43
1:B:143:GLY:O	1:B:145:MET:HG3	2.18	0.43
1:A:312:TRP:HB2	1:A:314:TRP:CZ3	2.53	0.43
1:A:230:LYS:HD2	1:A:309:ASN:HB3	1.99	0.43
1:A:237:LYS:HD2	1:A:378:LEU:HD23	2.01	0.43
1:A:275:VAL:CG2	1:A:335:PRO:HD2	2.47	0.43
1:B:337:ALA:O	1:B:341:LYS:HG3	2.18	0.43
1:A:258:MET:CE	1:A:341:LYS:HB3	2.44	0.42
1:A:142:VAL:HG12	1:A:142:VAL:O	2.18	0.42
1:A:278:ASP:OD2	1:A:343:ARG:HD3	2.19	0.42
1:A:220:GLN:HB2	1:A:231:LEU:HD11	2.02	0.42
1:A:336:ASN:HD21	1:A:339:ILE:HG23	1.85	0.42
1:A:142:VAL:CG1	1:A:142:VAL:O	2.68	0.42
1:A:327:PHE:CZ	1:A:367:LYS:HB2	2.55	0.42
1:B:151:ILE:HG13	1:B:151:ILE:H	1.64	0.42
1:A:183:ALA:HB2	1:A:245:TYR:CD1	2.55	0.42
1:A:135:PRO:HG2	1:A:210:GLN:HE22	1.85	0.41
1:B:170:ARG:NH1	1:B:213:TYR:O	2.43	0.41
1:B:342:CYS:SG	3:B:60:HOH:O	2.34	0.41
1:A:171:TYR:HD2	1:A:213:TYR:CE2	2.39	0.41
1:A:278:ASP:OD1	1:A:279:LYS:N	2.54	0.41
1:B:288:GLN:HG2	1:B:288:GLN:H	1.57	0.41
1:B:271:ARG:NH1	3:B:39:HOH:O	2.39	0.41
1:A:370:MET:HB3	1:A:370:MET:HE3	1.74	0.41
1:A:157:LEU:O	1:A:160:GLN:HB3	2.20	0.41
1:A:258:MET:SD	1:A:343:ARG:HG2	2.61	0.41
1:A:284:LEU:HD21	1:A:334:ARG:CZ	2.50	0.41
1:B:339:ILE:HD12	1:B:339:ILE:O	2.21	0.41
1:A:281:GLY:O	1:A:282:PHE:HB2	2.21	0.41
1:B:198:TRP:CE2	1:B:202:LEU:HG	2.56	0.41
1:A:359:ARG:HH12	1:B:314:TRP:CA	2.34	0.41
1:B:191:ARG:HD2	1:B:194:HIS:HD2	1.85	0.41
1:B:222:GLY:HA3	3:B:32:HOH:O	2.20	0.41
1:B:349:ARG:NE	1:B:349:ARG:CA	2.67	0.41
1:A:145:MET:HE2	1:A:259:ASN:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:TYR:O	1:B:205:ILE:HG13	2.21	0.41
1:B:305:ASN:ND2	1:B:376:ASN:H	2.14	0.40
1:A:258:MET:CE	1:A:341:LYS:HE2	2.51	0.40
1:A:189:ARG:NH2	1:A:224:SER:O	2.47	0.40
1:A:288:GLN:HB3	1:A:322:TYR:CZ	2.55	0.40
1:B:270:PRO:HD2	1:B:331:SER:O	2.21	0.40
1:B:183:ALA:HB2	1:B:245:TYR:CD1	2.56	0.40
1:B:298:LYS:HG2	1:B:302:LEU:HD22	2.04	0.40
1:B:336:ASN:ND2	1:B:336:ASN:C	2.73	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	269/288 (93%)	248 (92%)	19 (7%)	2 (1%)	26 38
1	B	269/288 (93%)	244 (91%)	19 (7%)	6 (2%)	8 9
All	All	538/576 (93%)	492 (91%)	38 (7%)	8 (2%)	13 17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	ALA
1	B	133	ALA
1	B	274	SER
1	B	349	ARG
1	A	189	ARG
1	B	348	SER
1	B	347	HIS
1	B	363	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	244/259 (94%)	215 (88%)	29 (12%)	6 8
1	B	244/259 (94%)	213 (87%)	31 (13%)	5 6
All	All	488/518 (94%)	428 (88%)	60 (12%)	6 7

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	CYS
1	A	140	LEU
1	A	141	LEU
1	A	150	ASN
1	A	167	LEU
1	A	174	MET
1	A	175	ASP
1	A	176	CYS
1	A	189	ARG
1	A	195	LEU
1	A	225	MET
1	A	253	VAL
1	A	259	ASN
1	A	263	THR
1	A	265	ARG
1	A	271	ARG
1	A	287	VAL
1	A	288	GLN
1	A	299	GLN
1	A	302	LEU
1	A	314	TRP
1	A	336	ASN
1	A	343	ARG
1	A	347	HIS
1	A	349	ARG
1	A	352	LYS
1	A	353	ASN

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Mol	Chain	Res	Type
1	A	358	GLN
1	A	370	MET
1	B	134	CYS
1	B	140	LEU
1	B	141	LEU
1	B	150	ASN
1	B	167	LEU
1	B	174	MET
1	B	175	ASP
1	B	176	CYS
1	B	189	ARG
1	B	195	LEU
1	B	253	VAL
1	B	259	ASN
1	B	263	THR
1	B	265	ARG
1	B	271	ARG
1	B	279	LYS
1	B	288	GLN
1	B	299	GLN
1	B	302	LEU
1	B	314	TRP
1	B	336	ASN
1	B	339	ILE
1	B	343	ARG
1	B	347	HIS
1	B	349	ARG
1	B	352	LYS
1	B	354	GLU
1	B	356	ASN
1	B	362	ARG
1	B	370	MET
1	B	400	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	160	GLN
1	A	162	ASN
1	A	190	ASN
1	A	207	GLN

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Mol	Chain	Res	Type
1	A	210	GLN
1	A	259	ASN
1	A	288	GLN
1	A	305	ASN
1	A	310	ASN
1	A	336	ASN
1	A	353	ASN
1	B	150	ASN
1	B	160	GLN
1	B	190	ASN
1	B	210	GLN
1	B	259	ASN
1	B	288	GLN
1	B	305	ASN
1	B	310	ASN
1	B	336	ASN
1	B	356	ASN

5.3.3 RNA

There are no RNA molecules 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

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	GDU	A	100	-	18,26,38	1.97	4 (22%)	26,40,58	4.31	14 (53%)
2	GDU	B	403	-	18,26,38	1.93	4 (22%)	26,40,58	4.34	14 (53%)

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	GDU	A	100	-	-	0/12/32/59	0/2/2/3
2	GDU	B	403	-	-	0/12/32/59	0/2/2/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	GDU	C6-C5	-2.77	1.32	1.38
2	A	100	GDU	C3D-C2D	-2.18	1.47	1.53
2	A	100	GDU	PB-O1B	3.53	1.62	1.51
2	B	403	GDU	PB-O1B	3.61	1.63	1.51
2	A	100	GDU	C6-N1	4.32	1.41	1.35
2	B	403	GDU	C6-N1	4.43	1.42	1.35
2	B	403	GDU	C4-N3	4.45	1.41	1.33
2	A	100	GDU	C4-N3	4.60	1.41	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	403	GDU	O3A-PA-O5D	-10.29	75.63	102.94
2	A	100	GDU	O3A-PA-O5D	-9.90	76.67	102.94
2	A	100	GDU	O3B-PB-O2B	-9.03	72.99	107.38
2	B	403	GDU	O3B-PB-O2B	-8.60	74.63	107.38
2	B	403	GDU	O3B-PB-O3A	-4.68	83.85	105.09
2	B	403	GDU	O2A-PA-O3A	-4.59	84.27	105.09
2	A	100	GDU	O2A-PA-O3A	-3.90	87.40	105.09
2	A	100	GDU	O3B-PB-O3A	-3.89	87.44	105.09
2	A	100	GDU	O3B-PB-O1B	-3.79	98.37	110.58
2	A	100	GDU	O4D-C4D-C3D	-3.62	97.85	105.15
2	A	100	GDU	C5-C4-N3	-3.58	113.95	123.12
2	B	403	GDU	O3B-PB-O1B	-3.17	100.36	110.58
2	B	403	GDU	C5-C4-N3	-3.15	115.05	123.12
2	A	100	GDU	C2D-C3D-C4D	-2.41	97.67	102.61
2	B	403	GDU	O5D-PA-O1A	2.12	117.84	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	403	GDU	C2D-C3D-C4D	2.15	107.04	102.61
2	A	100	GDU	O5D-PA-O1A	2.28	118.48	109.62
2	A	100	GDU	O5D-C5D-C4D	2.45	118.16	109.12
2	A	100	GDU	O2A-PA-O5D	2.67	121.92	108.46
2	B	403	GDU	O2A-PA-O5D	3.02	123.67	108.46
2	B	403	GDU	O5D-C5D-C4D	3.28	121.20	109.12
2	B	403	GDU	C4D-O4D-C1D	3.40	113.45	109.72
2	B	403	GDU	O2B-PB-O1B	3.53	121.95	110.58
2	A	100	GDU	O2B-PB-O3A	3.60	121.40	105.09
2	B	403	GDU	O2B-PB-O3A	4.00	123.22	105.09
2	A	100	GDU	O2B-PB-O1B	4.28	124.35	110.58
2	A	100	GDU	C4-N3-C2	12.98	127.00	114.14
2	B	403	GDU	C4-N3-C2	13.11	127.12	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	100	GDU	2	0
2	B	403	GDU	3	0

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

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	271/288 (94%)	0.28	28 (10%) 9 8	29, 53, 94, 99	0
1	B	271/288 (94%)	0.17	22 (8%) 15 14	25, 49, 83, 99	0
All	All	542/576 (94%)	0.22	50 (9%) 11 11	25, 51, 90, 99	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	ARG	5.9
1	B	348	SER	5.8
1	A	184	ILE	4.7
1	A	177	ILE	4.7
1	B	251	SER	4.4
1	B	349	ARG	4.3
1	B	293	VAL	4.2
1	A	348	SER	4.2
1	A	347	HIS	3.8
1	A	338	VAL	3.8
1	A	352	LYS	3.7
1	B	184	ILE	3.7
1	B	351	LYS	3.5
1	A	249	VAL	3.3
1	A	261	HIS	3.3
1	B	185	ILE	3.2
1	A	251	SER	3.2
1	A	186	ILE	3.2
1	A	183	ALA	3.2
1	B	352	LYS	3.2
1	A	351	LYS	3.1
1	A	185	ILE	3.1
1	A	132	THR	3.1
1	B	177	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	402	SER	3.0
1	A	294	SER	3.0
1	A	202	LEU	2.9
1	A	176	CYS	2.9
1	B	250	PHE	2.9
1	A	250	PHE	2.8
1	B	292	GLY	2.7
1	A	174	MET	2.7
1	B	249	VAL	2.6
1	B	186	ILE	2.5
1	A	232	LEU	2.4
1	B	198	TRP	2.4
1	A	136	GLU	2.4
1	A	350	ASP	2.4
1	A	353	ASN	2.4
1	B	187	PRO	2.3
1	A	135	PRO	2.3
1	A	252	ASP	2.3
1	B	381	MET	2.2
1	B	255	LEU	2.2
1	B	383	LEU	2.2
1	B	350	ASP	2.1
1	A	182	VAL	2.1
1	B	232	LEU	2.1
1	A	167	LEU	2.0
1	B	228	ARG	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
2	GDU	A	100	25/36	0.90	0.18	-0.32	40,58,99,99	0
2	GDU	B	403	25/36	0.91	0.16	-0.70	40,67,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.