Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:25 PM GMT

PDB ID	:	1FGX
Title	:	CRYSTAL STRUCTURE OF THE BOVINE BETA 1,4 GALACTOSYLT RANSFERASE (B4GALT1) CATALYTIC DOMAIN COMPLEXED WITH UMP
Authors	:	Gastinel, L.N.; Cambillau, C.; Bourne, Y.
Deposited on	:	2000-07-29
Resolution	:	2.40 Å(reported)

The following versions of software and data (see references ⓘ) 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	Percentile Ranks	Value
Rfree		0.444
Clashscore		13
Ramachandran outliers		1.1%
Sidechain outliers		7.1%
RSRZ outliers		37.2%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
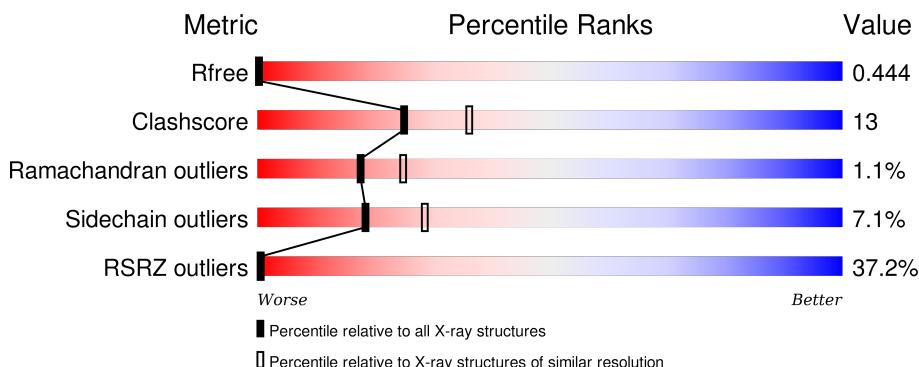
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	28% / 65% 26% • 6%
1	B	288	42% / 66% 25% • 5%
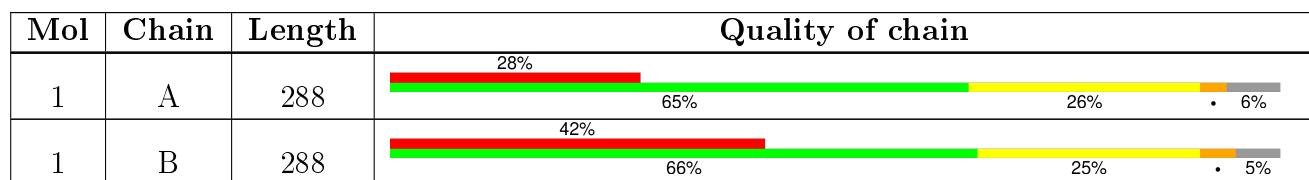
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4609 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	272	Total	C	N	O	S	0	0	0
			2219	1425	382	398	14			
1	B	273	Total	C	N	O	S	0	0	0
			2224	1428	383	399	14			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).
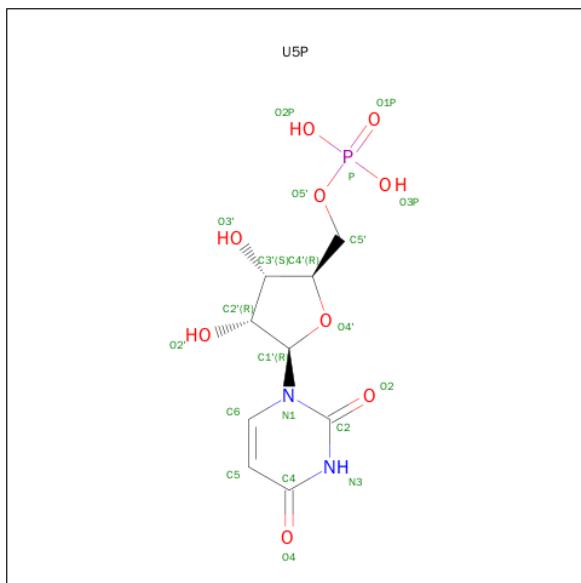
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total 73	O 73	0	0
3	B	72	Total 72	O 72	0	0

3 Residue-property plots ⓘ

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
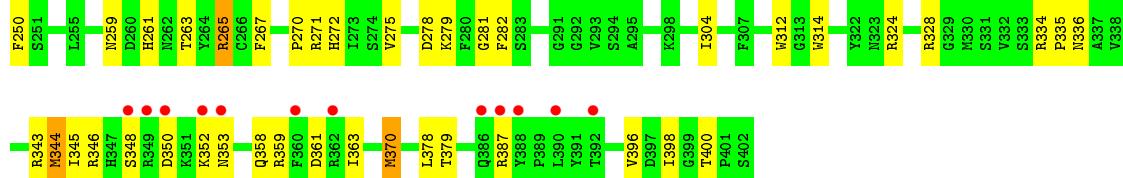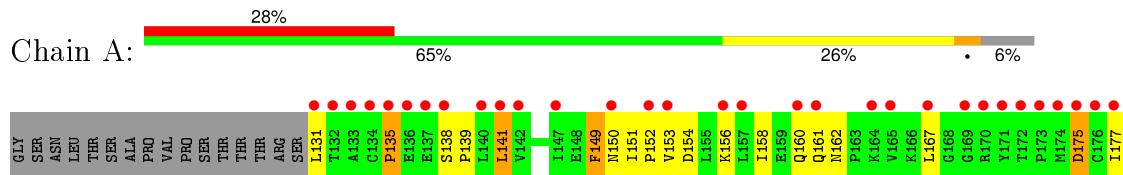
- Molecule 1: BETA 1,4 GALACTOSYLTRANSFERASE
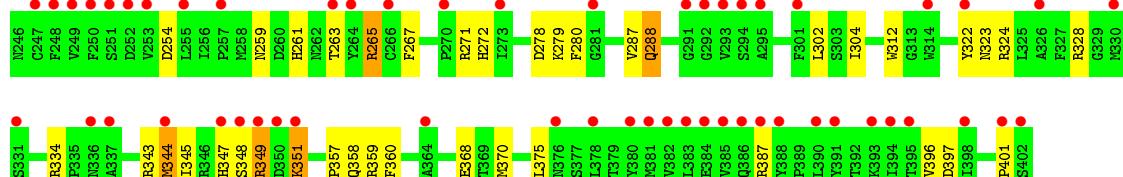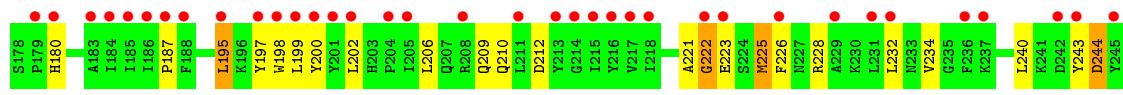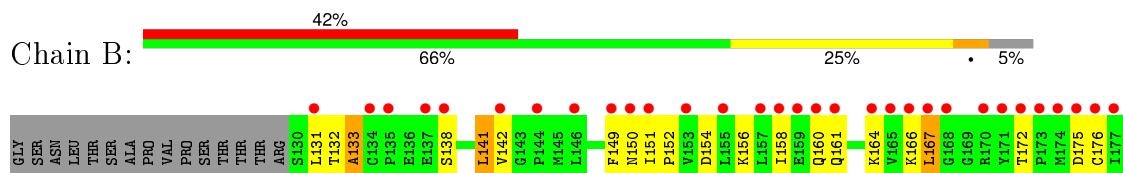
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	108.50Å 161.00Å 107.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.28 – 2.40 29.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	3.0 (29.28-2.40) 91.6 (29.88-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.33 (at 2.39Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.225 , 0.268 0.406 , 0.444	Depositor DCC
R_{free} test set	1026 reflections (3.10%)	DCC
Wilson B-factor (Å²)	55.3	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.32 , 76.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<\|L\|> = 0.48, <L^2> = 0.32$	Xtriage
Outliers	1 of 34096 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	4609	wwPDB-VP
Average B, all atoms (Å²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: U5P

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	0.70	0/2279	0.88	2/3086 (0.1%)
1	B	0.75	0/2284	0.88	2/3093 (0.1%)
All	All	0.72	0/4563	0.88	4/6179 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	222	GLY	N-CA-C	9.06	135.76	113.10
1	B	167	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	212	ASP	N-CA-C	-5.14	97.11	111.00
1	B	344	MET	CB-CG-SD	5.12	127.77	112.40

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	2219	0	2187	53	4
1	B	2224	0	2189	61	4
2	B	21	0	11	1	0
3	A	73	0	0	4	1
3	B	72	0	0	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4609	0	4387	112	5

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 13.

All (112) 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:279:LYS:HZ2	1:B:344:MET:HB2	1.40	0.86
1:B:279:LYS:NZ	1:B:344:MET:HB2	1.99	0.77
1:A:230:LYS:HD3	1:A:398:ILE:HB	1.66	0.77
1:A:222:GLY:O	1:A:223:GLU:HB2	1.86	0.76
1:A:131:LEU:HD13	1:A:177:ILE:HD11	1.73	0.71
1:A:151:ILE:HG13	1:A:151:ILE:O	1.92	0.69
1:B:158:ILE:HD11	1:B:200:TYR:HB2	1.74	0.68
1:B:280:PHE:CZ	1:B:357:PRO:HD3	2.31	0.66
1:B:154:ASP:OD2	1:B:156:LYS:HB2	1.97	0.64
1:A:154:ASP:OD2	1:A:156:LYS:HB2	1.98	0.63
1:A:344:MET:HG2	1:A:346:ARG:HG2	1.80	0.63
1:B:259:ASN:OD1	1:B:261:HIS:HB2	2.00	0.61
1:A:158:ILE:HD11	1:A:200:TYR:HB2	1.83	0.60
1:B:150:ASN:O	1:B:152:PRO:HD3	2.01	0.60
1:B:225:MET:HA	1:B:225:MET:HE3	1.82	0.59
1:B:312:TRP:CD2	1:B:401:PRO:HG3	2.38	0.59
1:A:202:LEU:O	1:A:206:LEU:HG	2.03	0.59
1:B:234:VAL:HG11	1:B:396:VAL:HG11	1.84	0.58
1:A:232:LEU:HD22	1:A:250:PHE:HD2	1.69	0.58
1:B:132:THR:O	1:B:133:ALA:HB2	2.02	0.58
1:A:205:ILE:O	1:A:209:GLN:HG3	2.04	0.57
1:A:358:GLN:NE2	1:B:358:GLN:HG3	2.19	0.57
1:A:275:VAL:HG22	1:A:334:ARG:HD3	1.85	0.57
1:A:279:LYS:HD3	1:A:344:MET:SD	2.45	0.56
1:A:150:ASN:O	1:A:152:PRO:HD3	2.05	0.56
1:A:234:VAL:HG11	1:A:396:VAL:HG11	1.88	0.56
1:B:167:LEU:CD1	1:B:387:ARG:HB3	2.36	0.56
1:B:349:ARG:CZ	1:B:351:LYS:HB3	2.35	0.55
1:B:131:LEU:HD22	1:B:176:CYS:HA	1.88	0.55
1:B:132:THR:O	1:B:133:ALA:CB	2.54	0.55
1:A:358:GLN:HE21	1:B:358:GLN:HG3	1.73	0.54
1:B:138:SER:HB3	1:B:141:LEU:HD13	1.90	0.54
1:A:259:ASN:OD1	1:A:261:HIS:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:HB3	1:A:378:LEU:HD22	1.90	0.53
1:B:226:PHE:HB2	2:B:101:U5P:H1'	1.90	0.52
1:B:151:ILE:O	1:B:151:ILE:HD12	2.09	0.52
1:A:151:ILE:O	1:A:151:ILE:CG1	2.57	0.52
1:B:312:TRP:CG	1:B:401:PRO:HG3	2.45	0.52
1:A:278:ASP:OD2	1:A:279:LYS:N	2.43	0.52
1:B:141:LEU:HD23	1:B:261:HIS:CE1	2.45	0.52
1:B:267:PHE:CD1	1:B:271:ARG:HD3	2.45	0.52
1:B:225:MET:HA	1:B:225:MET:CE	2.39	0.51
1:A:187:PRO:HD3	1:A:232:LEU:HD21	1.92	0.51
1:B:272:HIS:HB3	1:B:334:ARG:HG2	1.93	0.51
1:B:221:ALA:O	1:B:222:GLY:O	2.28	0.51
1:A:281:GLY:O	1:A:282:PHE:HB2	2.10	0.51
1:B:167:LEU:HD11	1:B:387:ARG:HB3	1.92	0.51
1:B:197:TYR:CE1	1:B:347:HIS:HE1	2.29	0.51
1:A:228:ARG:HB2	3:A:509:HOH:O	2.10	0.50
1:B:328:ARG:NH2	3:B:522:HOH:O	2.06	0.50
1:B:278:ASP:OD2	1:B:279:LYS:N	2.45	0.50
1:B:280:PHE:CE1	1:B:357:PRO:HD3	2.47	0.50
1:B:244:ASP:CG	1:B:244:ASP:O	2.50	0.50
1:A:180:HIS:CE1	1:A:265:ARG:HD2	2.47	0.50
1:A:379:THR:N	3:A:549:HOH:O	2.13	0.49
1:A:162:ASN:HD22	1:A:207:GLN:HE22	1.58	0.49
1:B:180:HIS:CE1	1:B:265:ARG:HD2	2.48	0.48
1:B:288:GLN:HB3	1:B:322:TYR:CZ	2.47	0.48
1:B:304:ILE:HB	1:B:324:ARG:HB3	1.95	0.48
1:B:279:LYS:CE	1:B:344:MET:HB2	2.44	0.48
1:A:324:ARG:HG2	1:A:370:MET:HG3	1.96	0.48
1:A:271:ARG:NH2	1:A:335:PRO:HB3	2.29	0.48
1:B:323:ASN:ND2	3:B:582:HOH:O	2.35	0.47
1:A:225:MET:SD	1:A:312:TRP:HB3	2.55	0.47
1:A:222:GLY:O	1:A:223:GLU:CB	2.56	0.47
1:A:281:GLY:N	1:A:353:ASN:OD1	2.47	0.47
1:A:138:SER:HB3	1:A:141:LEU:HD13	1.96	0.47
1:A:275:VAL:CG2	1:A:334:ARG:HD3	2.45	0.47
1:B:164:LYS:NZ	3:B:568:HOH:O	2.48	0.47
1:B:212:ASP:OD2	1:B:243:TYR:OH	2.22	0.47
1:B:167:LEU:HD11	1:B:387:ARG:CB	2.45	0.46
1:B:265:ARG:NH1	3:B:641:HOH:O	2.48	0.46
1:B:288:GLN:HG3	1:B:359:ARG:NH2	2.31	0.46
1:A:188:PHE:CD1	1:A:188:PHE:C	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASP:OD1	1:A:175:ASP:N	2.48	0.46
1:B:279:LYS:NZ	1:B:344:MET:CB	2.77	0.45
1:B:198:TRP:CZ2	1:B:202:LEU:HG	2.52	0.45
1:A:167:LEU:CD1	1:A:387:ARG:HB3	2.47	0.44
1:A:328:ARG:HE	1:A:328:ARG:HB3	1.55	0.44
1:A:218:ILE:HG22	1:A:231:LEU:HD22	2.00	0.44
1:B:288:GLN:OE1	1:B:288:GLN:N	2.52	0.43
1:A:153:VAL:HG23	1:A:196:LYS:HB3	2.00	0.43
1:B:187:PRO:HD3	1:B:232:LEU:HD21	2.00	0.43
1:B:360:PHE:HA	3:B:585:HOH:O	2.19	0.43
1:A:149:PHE:CE2	1:A:345:ILE:HG12	2.54	0.43
1:B:209:GLN:O	1:B:210:GLN:HB2	2.19	0.43
1:A:267:PHE:CD1	1:A:271:ARG:HD3	2.54	0.42
1:B:240:LEU:HD23	1:B:240:LEU:HA	1.86	0.42
1:B:195:LEU:HD22	1:B:199:LEU:HG	2.01	0.42
1:B:397:ASP:C	1:B:397:ASP:OD2	2.58	0.42
1:B:370:MET:HE3	1:B:370:MET:HB3	1.80	0.42
1:A:135:PRO:HG3	1:A:139:PRO:HD3	2.02	0.42
1:A:167:LEU:HD11	1:A:387:ARG:HB3	2.02	0.42
1:B:142:VAL:HG12	1:B:142:VAL:O	2.19	0.42
1:B:287:VAL:HG23	3:B:559:HOH:O	2.19	0.42
1:A:363:ILE:HG23	3:A:551:HOH:O	2.19	0.42
1:A:272:HIS:HB3	1:A:334:ARG:HG2	2.01	0.42
1:A:304:ILE:HB	1:A:324:ARG:HB3	2.02	0.42
1:B:375:LEU:HD12	1:B:375:LEU:HA	1.80	0.42
1:B:279:LYS:HD2	1:B:344:MET:HB2	2.01	0.42
1:A:344:MET:O	1:A:346:ARG:HG3	2.20	0.41
1:B:347:HIS:O	1:B:349:ARG:N	2.52	0.41
1:A:378:LEU:HA	3:A:549:HOH:O	2.19	0.41
1:A:361:ASP:OD1	1:A:363:ILE:HG22	2.20	0.41
1:B:254:ASP:HA	1:B:345:ILE:HD12	2.02	0.41
1:B:172:THR:HG23	1:B:212:ASP:CG	2.41	0.41
1:B:202:LEU:O	1:B:206:LEU:HG	2.21	0.41
1:A:198:TRP:CZ2	1:A:202:LEU:HG	2.56	0.41
1:A:167:LEU:HD13	1:A:167:LEU:C	2.41	0.41
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.93	0.40
1:B:228:ARG:O	1:B:232:LEU:HG	2.21	0.40
1:A:167:LEU:HD11	1:A:387:ARG:CB	2.51	0.40

All (5) 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)
1:A:200:TYR:OH	1:B:160:GLN:OE1[6_554]	1.36	0.84
1:A:161:GLN:OE1	1:B:161:GLN:OE1[6_554]	1.63	0.57
1:A:161:GLN:NE2	1:B:161:GLN:OE1[6_554]	1.66	0.54
1:A:161:GLN:CD	1:B:161:GLN:OE1[6_554]	1.82	0.38
3:A:553:HOH:O	3:B:522:HOH:O[3_555]	2.10	0.10

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	270/288 (94%)	252 (93%)	15 (6%)	3 (1%)	17	25
1	B	271/288 (94%)	250 (92%)	18 (7%)	3 (1%)	17	25
All	All	541/576 (94%)	502 (93%)	33 (6%)	6 (1%)	17	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	LYS
1	B	133	ALA
1	B	222	GLY
1	B	348	SER
1	A	135	PRO
1	A	348	SER

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	245/259 (95%)	226 (92%)	19 (8%)	16	24
1	B	245/259 (95%)	229 (94%)	16 (6%)	21	33
All	All	490/518 (95%)	455 (93%)	35 (7%)	18	28

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LEU
1	A	149	PHE
1	A	160	GLN
1	A	175	ASP
1	A	188	PHE
1	A	195	LEU
1	A	223	GLU
1	A	224	SER
1	A	263	THR
1	A	265	ARG
1	A	270	PRO
1	A	314	TRP
1	A	336	ASN
1	A	343	ARG
1	A	344	MET
1	A	350	ASP
1	A	359	ARG
1	A	370	MET
1	A	400	THR
1	B	141	LEU
1	B	149	PHE
1	B	166	LYS
1	B	175	ASP
1	B	195	LEU
1	B	223	GLU
1	B	225	MET
1	B	244	ASP
1	B	263	THR
1	B	265	ARG
1	B	288	GLN
1	B	302	LEU
1	B	343	ARG
1	B	349	ARG
1	B	351	LYS
1	B	368	GLU

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

Mol	Chain	Res	Type
1	A	161	GLN
1	A	162	ASN
1	A	207	GLN
1	A	210	GLN
1	A	219	ASN
1	A	358	GLN
1	B	161	GLN
1	B	210	GLN
1	B	347	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	U5P	B	101	-	16,22,22	2.74	6 (37%)	21,33,33	3.65	10 (47%)

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	U5P	B	101	-	-	0/6/26/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	U5P	C5'-C4'	2.16	1.58	1.51
2	B	101	U5P	O3'-C3'	2.67	1.49	1.43
2	B	101	U5P	P-O3P	4.12	1.69	1.54
2	B	101	U5P	O4'-C1'	4.25	1.46	1.41
2	B	101	U5P	C4-N3	4.85	1.42	1.33
2	B	101	U5P	C6-N1	5.78	1.43	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	U5P	C5-C4-N3	-3.75	113.49	123.12
2	B	101	U5P	O2P-P-O1P	-2.28	103.23	110.58
2	B	101	U5P	O3P-P-O5'	-2.20	100.24	106.56
2	B	101	U5P	C2'-C3'-C4'	-2.16	98.17	102.61
2	B	101	U5P	C6-C5-C4	2.01	121.05	117.28
2	B	101	U5P	O3P-P-O1P	2.54	118.76	110.58
2	B	101	U5P	O5'-C5'-C4'	2.55	118.53	109.12
2	B	101	U5P	O4'-C1'-N1	4.31	117.17	108.08
2	B	101	U5P	O5'-P-O1P	4.33	118.16	107.14
2	B	101	U5P	C4-N3-C2	13.53	127.54	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	101	U5P	1	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 (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	272/288 (94%)	1.65	82 (30%)	1	1	39, 57, 94, 98	0
1	B	273/288 (94%)	2.01	121 (44%)	0	0	34, 54, 90, 98	0
All	All	545/576 (94%)	1.83	203 (37%)	0	0	34, 56, 93, 98	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	LEU	10.8
1	A	176	CYS	7.4
1	B	383	LEU	6.9
1	B	388	TYR	6.1
1	B	138	SER	5.8
1	B	391	TYR	5.8
1	A	175	ASP	5.7
1	A	353	ASN	5.4
1	B	175	ASP	5.4
1	A	138	SER	5.1
1	A	174	MET	5.1
1	B	165	VAL	5.1
1	B	211	LEU	4.9
1	B	158	ILE	4.9
1	B	155	LEU	4.9
1	A	245	TYR	4.8
1	B	197	TYR	4.7
1	B	200	TYR	4.7
1	B	242	ASP	4.7
1	B	281	GLY	4.7
1	A	134	CYS	4.6
1	B	166	LYS	4.6
1	A	173	PRO	4.5
1	B	185	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	245	TYR	4.4
1	B	131	LEU	4.4
1	B	386	GLN	4.2
1	A	141	LEU	4.2
1	B	171	TYR	4.2
1	B	186	ILE	4.2
1	B	243	TYR	4.2
1	A	178	SER	4.1
1	B	348	SER	4.1
1	B	198	TRP	4.1
1	A	240	LEU	4.1
1	A	251	SER	4.1
1	B	384	GLU	4.1
1	B	347	HIS	4.1
1	B	314	TRP	4.0
1	B	385	VAL	4.0
1	B	170	ARG	4.0
1	A	153	VAL	4.0
1	B	223	GLU	3.9
1	B	137	GLU	3.9
1	A	164	LYS	3.9
1	B	393	LYS	3.9
1	A	142	VAL	3.9
1	B	394	ILE	3.9
1	B	229	ALA	3.8
1	A	157	LEU	3.8
1	A	350	ASP	3.7
1	A	267	PHE	3.7
1	A	180	HIS	3.7
1	B	179	PRO	3.7
1	A	332	VAL	3.7
1	A	349	ARG	3.7
1	B	213	TYR	3.6
1	B	217	VAL	3.6
1	A	243	TYR	3.6
1	A	177	ILE	3.6
1	A	186	ILE	3.5
1	B	349	ARG	3.5
1	B	264	TYR	3.5
1	B	237	LYS	3.5
1	A	200	TYR	3.4
1	B	236	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	398	ILE	3.4
1	B	253	VAL	3.4
1	B	202	LEU	3.4
1	A	266	CYS	3.4
1	A	248	PHE	3.4
1	B	150	ASN	3.4
1	B	157	LEU	3.4
1	B	382	VAL	3.4
1	A	242	ASP	3.4
1	A	150	ASN	3.4
1	A	184	ILE	3.4
1	B	293	VAL	3.3
1	A	250	PHE	3.3
1	B	214	GLY	3.3
1	B	153	VAL	3.3
1	A	352	LYS	3.2
1	A	387	ARG	3.2
1	B	146	LEU	3.2
1	B	249	VAL	3.2
1	B	168	GLY	3.2
1	B	337	ALA	3.2
1	B	326	ALA	3.2
1	B	174	MET	3.1
1	A	264	TYR	3.1
1	A	137	GLU	3.1
1	A	165	VAL	3.1
1	B	257	PRO	3.1
1	B	387	ARG	3.1
1	A	140	LEU	3.1
1	B	247	CYS	3.1
1	B	151	ILE	3.1
1	B	164	LYS	3.1
1	B	351	LYS	3.1
1	B	381	MET	3.0
1	B	255	LEU	3.0
1	A	185	ILE	3.0
1	B	295	ALA	3.0
1	B	167	LEU	3.0
1	B	177	ILE	3.0
1	B	273	ILE	3.0
1	B	250	PHE	3.0
1	A	170	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	136	GLU	3.0
1	B	231	LEU	2.9
1	A	295	ALA	2.9
1	A	236	PHE	2.9
1	B	188	PHE	2.9
1	A	132	THR	2.9
1	A	183	ALA	2.9
1	A	171	TYR	2.8
1	A	249	VAL	2.8
1	B	204	PRO	2.8
1	B	380	TYR	2.8
1	B	134	CYS	2.8
1	A	293	VAL	2.8
1	B	390	LEU	2.8
1	B	248	PHE	2.8
1	B	180	HIS	2.7
1	A	214	GLY	2.7
1	A	338	VAL	2.7
1	B	226	PHE	2.7
1	B	292	GLY	2.7
1	A	388	TYR	2.7
1	A	198	TRP	2.7
1	B	199	LEU	2.7
1	A	216	TYR	2.7
1	B	161	GLN	2.6
1	B	215	ILE	2.6
1	B	336	ASN	2.6
1	B	364	ALA	2.6
1	B	142	VAL	2.5
1	A	152	PRO	2.5
1	A	167	LEU	2.5
1	B	205	ILE	2.5
1	B	159	GLU	2.5
1	A	161	GLN	2.5
1	A	390	LEU	2.5
1	B	195	LEU	2.5
1	B	322	TYR	2.5
1	B	344	MET	2.5
1	B	135	PRO	2.5
1	B	144	PRO	2.5
1	A	160	GLN	2.5
1	B	187	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	201	TYR	2.4
1	A	133	ALA	2.4
1	A	156	LYS	2.4
1	A	211	LEU	2.4
1	A	215	ILE	2.4
1	B	184	ILE	2.4
1	B	160	GLN	2.4
1	A	273	ILE	2.4
1	B	294	SER	2.4
1	B	208	ARG	2.4
1	B	222	GLY	2.3
1	B	266	CYS	2.3
1	A	199	LEU	2.3
1	B	263	THR	2.3
1	B	395	THR	2.3
1	B	331	SER	2.3
1	B	183	ALA	2.3
1	B	251	SER	2.3
1	B	252	ASP	2.3
1	A	135	PRO	2.3
1	B	402	SER	2.3
1	A	298	LYS	2.3
1	A	360	PHE	2.2
1	B	378	LEU	2.2
1	A	291	GLY	2.2
1	A	255	LEU	2.2
1	A	172	THR	2.2
1	B	376	ASN	2.2
1	A	330	MET	2.2
1	A	348	SER	2.2
1	B	232	LEU	2.2
1	B	350	ASP	2.2
1	A	362	ARG	2.2
1	A	169	GLY	2.1
1	B	330	MET	2.1
1	A	147	ILE	2.1
1	B	176	CYS	2.1
1	B	301	PHE	2.1
1	A	392	THR	2.1
1	A	283	SER	2.1
1	A	322	TYR	2.1
1	B	216	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	291	GLY	2.1
1	B	218	ILE	2.1
1	A	307	PHE	2.1
1	A	179	PRO	2.1
1	B	270	PRO	2.1
1	B	172	THR	2.1
1	A	386	GLN	2.0
1	B	173	PRO	2.0
1	B	149	PHE	2.0
1	A	247	CYS	2.0
1	B	401	PRO	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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	U5P	B	101	21/21	0.67	0.31	0.71	92,98,98,98	0

6.5 Other polymers (i)

There are no such residues in this entry.