



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:46 AM GMT

PDB ID : 3BT1
Title : Structure of urokinase receptor, urokinase and vitronectin complex
Authors : Huang, M.
Deposited on : 2007-12-27
Resolution : 2.80 Å(reported)

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

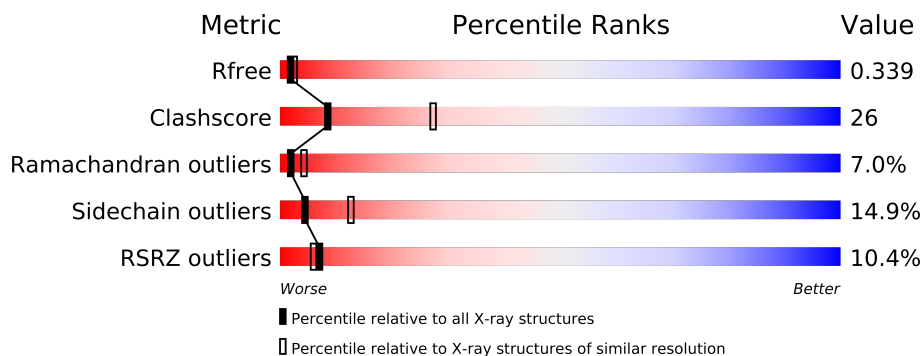
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	135	
2	B	40	
3	U	283	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3461 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			987	608	187	178	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	EXPRESSION TAG	UNP P00749
A	0	SER	-	EXPRESSION TAG	UNP P00749

- Molecule 2 is a protein called Vitronectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	S	0	0	0
			312	185	51	68	8			

- Molecule 3 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	U	273	Total	C	N	O	S	0	0	0
			2095	1253	388	420	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-1	ARG	-	EXPRESSION TAG	UNP Q03405
U	0	SER	-	EXPRESSION TAG	UNP Q03405

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	U	1	Total	C	N	O	0	0
			14	8	1	5		
4	U	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (N-ACETYL-D-GLUCOSAMINE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	U	3	Total	C	N	O	0	0
			39	22	2	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-1	ARG	-	EXPRESSION TAG	UNP Q03405
U	0	SER	-	EXPRESSION TAG	UNP Q03405

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.35Å 105.19Å 55.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.68 – 2.80 27.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.68-2.80) 99.6 (27.68-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.241 , 0.308 0.308 , 0.339	Depositor DCC
R_{free} test set	726 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	81.3	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14504 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3461	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.75	0/1015	0.81	0/1372
2	B	0.68	1/316 (0.3%)	0.73	0/421
3	U	0.81	2/2129 (0.1%)	0.91	2/2867 (0.1%)
All	All	0.79	3/3460 (0.1%)	0.87	2/4660 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	U	0	3
5	U	1	0
All	All	1	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	33	GLU	CB-CG	6.02	1.63	1.52
3	U	153	CYS	CB-SG	-5.79	1.72	1.81
2	B	31	CYS	CB-SG	-5.06	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	144	LEU	CA-CB-CG	6.28	129.75	115.30
3	U	54	THR	N-CA-C	5.20	125.03	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	U	1200	NAG	C1

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	U	16	GLU	Peptide
3	U	185	GLU	Peptide
3	U	230	GLU	Peptide

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	987	0	919	36	0
2	B	312	0	272	5	0
3	U	2095	0	1947	136	0
4	U	28	0	26	0	0
5	U	39	0	34	5	0
All	All	3461	0	3198	173	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (173) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:113:LEU:CD2	3:U:147:CYS:SG	2.55	0.94
3:U:182:LEU:HD22	3:U:187:LEU:HD11	1.48	0.92
3:U:113:LEU:HD21	3:U:147:CYS:SG	2.09	0.92
3:U:113:LEU:HD23	3:U:113:LEU:C	1.94	0.89
1:A:61:LYS:O	1:A:62:ALA:CB	2.22	0.86
3:U:259:ASN:O	3:U:261:ILE:HG23	1.83	0.79
3:U:46:THR:HG21	3:U:50:LYS:HG3	1.65	0.79
3:U:200:ASN:HD22	5:U:1200:NAG:H82	1.47	0.77
3:U:93:LEU:HD11	3:U:174:THR:HA	1.68	0.76
3:U:29:VAL:HG22	3:U:66:LEU:CD1	2.14	0.76
1:A:28:ILE:HD13	3:U:42:GLU:CD	2.06	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:VAL:HG21	1:A:30:TRP:CE2	2.22	0.74
3:U:1:LEU:O	3:U:17:CYS:N	2.19	0.74
3:U:195:TYR:CD1	3:U:212:LEU:HD13	2.23	0.74
3:U:46:THR:HG23	3:U:47:HIS:N	2.03	0.73
3:U:246:MET:HE3	3:U:246:MET:HA	1.71	0.72
1:A:23:LYS:NZ	3:U:166:HIS:ND1	2.39	0.71
3:U:141:ASP:HB2	3:U:144:LEU:HD13	1.73	0.71
3:U:17:CYS:C	3:U:45:CYS:SG	2.69	0.70
2:B:40:LYS:O	2:B:40:LYS:HG3	1.91	0.70
3:U:16:GLU:O	3:U:18:ALA:N	2.24	0.70
3:U:130:ILE:HG23	3:U:131:GLN:H	1.56	0.70
3:U:195:TYR:CE2	3:U:212:LEU:HD11	2.29	0.68
1:A:20:VAL:CG2	1:A:30:TRP:CE2	2.77	0.68
1:A:64:THR:HG23	1:A:127:MET:HB3	1.75	0.68
3:U:29:VAL:HG22	3:U:66:LEU:HD12	1.74	0.67
3:U:153:CYS:O	3:U:154:PRO:C	2.32	0.67
3:U:1:LEU:HD12	3:U:22:ASP:HA	1.76	0.67
1:A:61:LYS:O	1:A:62:ALA:HB2	1.94	0.67
3:U:200:ASN:ND2	5:U:1200:NAG:H82	2.09	0.67
3:U:200:ASN:CB	5:U:1200:NAG:H82	2.24	0.66
3:U:192:ARG:NH2	3:U:267:THR:HG23	2.10	0.66
3:U:259:ASN:O	3:U:261:ILE:CG2	2.43	0.66
3:U:54:THR:O	3:U:66:LEU:O	2.13	0.66
3:U:130:ILE:CG2	3:U:163:ASP:HB2	2.24	0.66
3:U:96:ILE:HG23	3:U:110:HIS:HB3	1.78	0.66
3:U:153:CYS:HB3	3:U:154:PRO:HD3	1.78	0.66
3:U:246:MET:CE	3:U:251:HIS:HB2	2.27	0.64
3:U:141:ASP:CB	3:U:144:LEU:HD13	2.28	0.64
3:U:173:THR:HG23	3:U:176:CYS:HB3	1.79	0.64
3:U:246:MET:HE1	3:U:252:LEU:N	2.14	0.63
1:A:64:THR:HG23	1:A:127:MET:CB	2.29	0.63
3:U:130:ILE:HG23	3:U:131:GLN:N	2.14	0.63
3:U:113:LEU:C	3:U:113:LEU:CD2	2.67	0.62
1:A:61:LYS:O	1:A:62:ALA:HB3	1.97	0.62
3:U:273:HIS:C	3:U:275:ASP:H	2.04	0.61
1:A:74:TRP:CD2	1:A:96:LEU:HD22	2.36	0.61
3:U:46:THR:CG2	3:U:47:HIS:N	2.63	0.61
3:U:195:TYR:CE1	3:U:212:LEU:HD13	2.36	0.61
3:U:246:MET:HE3	3:U:251:HIS:HB2	1.82	0.61
3:U:250:ALA:HB1	3:U:261:ILE:HD11	1.82	0.60
1:A:99:HIS:CD2	1:A:101:TYR:H	2.19	0.60
3:U:46:THR:CG2	3:U:50:LYS:HG3	2.30	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:184:LEU:O	3:U:186:ASN:N	2.34	0.60
1:A:20:VAL:HG21	1:A:30:TRP:NE1	2.16	0.60
3:U:39:GLU:C	3:U:40:LEU:HD23	2.21	0.59
3:U:29:VAL:HG12	3:U:31:LEU:CD1	2.32	0.59
3:U:94:GLU:CD	3:U:175:LYS:NZ	2.56	0.59
3:U:152:GLY:HA3	3:U:251:HIS:NE2	2.17	0.58
3:U:113:LEU:HD22	3:U:147:CYS:SG	2.40	0.58
3:U:195:TYR:HB3	3:U:210:THR:HG22	1.85	0.58
3:U:137:ARG:HB3	3:U:138:PRO:HD2	1.86	0.57
1:A:116:GLN:OE1	1:A:119:LEU:O	2.23	0.57
1:A:99:HIS:HD2	1:A:101:TYR:H	1.53	0.56
3:U:39:GLU:O	3:U:40:LEU:HD23	2.05	0.55
3:U:248:GLN:C	3:U:249:HIS:HD1	2.10	0.55
3:U:192:ARG:CZ	3:U:267:THR:HG23	2.37	0.55
3:U:184:LEU:HA	3:U:187:LEU:HD13	1.89	0.54
3:U:1:LEU:HD12	3:U:22:ASP:CA	2.36	0.54
3:U:1:LEU:HD13	3:U:17:CYS:HB3	1.89	0.54
3:U:122:CYS:C	3:U:123:LEU:HD23	2.29	0.54
3:U:46:THR:HG23	3:U:47:HIS:H	1.71	0.53
3:U:128:HIS:CE1	3:U:142:ARG:NH1	2.76	0.53
3:U:96:ILE:CG2	3:U:110:HIS:HB3	2.38	0.53
3:U:173:THR:HG23	3:U:176:CYS:CB	2.37	0.53
1:A:65:ASP:HA	1:A:126:CYS:HA	1.90	0.53
1:A:58:TYR:OH	1:A:61:LYS:O	2.26	0.53
1:A:88:ARG:O	1:A:90:ASP:N	2.42	0.52
3:U:54:THR:O	3:U:55:LEU:O	2.28	0.52
1:A:92:LEU:HD13	1:A:92:LEU:N	2.23	0.52
3:U:194:CYS:C	3:U:212:LEU:HD12	2.30	0.52
3:U:259:ASN:C	3:U:261:ILE:HG23	2.30	0.52
3:U:153:CYS:HB3	3:U:154:PRO:CD	2.40	0.51
3:U:128:HIS:CE1	3:U:142:ARG:CZ	2.93	0.51
3:U:248:GLN:C	3:U:249:HIS:ND1	2.64	0.51
3:U:250:ALA:CB	3:U:261:ILE:HD11	2.40	0.51
3:U:55:LEU:HD23	3:U:56:SER:N	2.26	0.51
3:U:270:GLY:C	3:U:272:ASN:H	2.13	0.51
3:U:113:LEU:HD23	3:U:114:GLN:N	2.26	0.50
3:U:165:PHE:CE1	3:U:184:LEU:HB2	2.46	0.50
3:U:43:LYS:O	3:U:44:SER:HB3	2.10	0.50
3:U:69:VAL:HG22	3:U:70:VAL:N	2.26	0.50
3:U:227:GLY:HA3	3:U:261:ILE:HG22	1.94	0.50
3:U:273:HIS:C	3:U:275:ASP:N	2.63	0.49
3:U:162:ASN:HD22	3:U:163:ASP:N	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:17:CYS:O	3:U:18:ALA:HB3	2.12	0.49
3:U:7:LYS:HE2	3:U:11:ASP:HB3	1.94	0.49
3:U:225:ALA:CB	3:U:252:LEU:HD23	2.42	0.49
3:U:85:VAL:O	3:U:86:THR:HB	2.12	0.49
3:U:80:ASN:OD1	3:U:81:SER:N	2.44	0.49
3:U:162:ASN:HD22	3:U:163:ASP:CG	2.16	0.48
1:A:119:LEU:O	1:A:120:LYS:C	2.52	0.48
3:U:195:TYR:CD2	3:U:212:LEU:HD11	2.48	0.48
1:A:24:TYR:CD2	3:U:150:LEU:HD22	2.48	0.48
1:A:74:TRP:HB2	1:A:97:GLY:O	2.14	0.48
3:U:123:LEU:O	3:U:145:ARG:HB2	2.14	0.48
3:U:128:HIS:HE1	3:U:142:ARG:NH1	2.11	0.47
1:A:74:TRP:CE3	1:A:96:LEU:HD22	2.50	0.47
2:B:7:GLY:O	2:B:9:CYS:N	2.46	0.47
3:U:223:LEU:HD12	3:U:265:CYS:SG	2.54	0.47
3:U:50:LYS:NZ	3:U:254:ASP:OD1	2.44	0.47
3:U:160:HIS:HE1	3:U:216:ARG:H	1.63	0.47
3:U:1:LEU:HD22	3:U:17:CYS:HB2	1.97	0.47
3:U:113:LEU:O	3:U:113:LEU:HD23	2.15	0.47
3:U:200:ASN:HB2	5:U:1200:NAG:H82	1.96	0.47
1:A:108:ARG:HG3	1:A:112:TRP:CD1	2.50	0.47
3:U:161:ASN:HA	3:U:213:ILE:CD1	2.45	0.47
1:A:56:HIS:HD2	1:A:104:ASN:O	1.97	0.47
3:U:184:LEU:CA	3:U:187:LEU:HD13	2.45	0.46
3:U:94:GLU:CD	3:U:175:LYS:HZ1	2.18	0.46
3:U:182:LEU:HD22	3:U:187:LEU:CD1	2.34	0.46
3:U:267:THR:HG22	3:U:268:LYS:N	2.30	0.46
1:A:24:TYR:CG	3:U:150:LEU:HD22	2.50	0.46
1:A:53:GLY:O	1:A:54:ASN:HB3	2.16	0.46
3:U:162:ASN:ND2	3:U:163:ASP:CG	2.69	0.46
1:A:99:HIS:CG	1:A:101:TYR:CD2	3.03	0.46
3:U:246:MET:HE3	3:U:246:MET:CA	2.41	0.45
3:U:165:PHE:CD1	3:U:184:LEU:HB2	2.52	0.45
3:U:235:SER:O	3:U:236:TYR:C	2.54	0.45
3:U:230:GLU:O	3:U:233:ASN:ND2	2.50	0.45
3:U:200:ASN:N	3:U:200:ASN:OD1	2.50	0.45
3:U:1:LEU:O	3:U:17:CYS:CB	2.64	0.45
3:U:87:TYR:C	3:U:87:TYR:CD1	2.89	0.45
3:U:195:TYR:HB3	3:U:210:THR:CG2	2.47	0.45
3:U:126:VAL:O	3:U:166:HIS:HA	2.17	0.45
1:A:117:VAL:HG13	1:A:117:VAL:O	2.17	0.44
3:U:200:ASN:HD22	5:U:1200:NAG:C8	2.22	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:2:ARG:HG2	3:U:16:GLU:HA	1.99	0.44
3:U:1:LEU:CD2	3:U:1:LEU:C	2.85	0.44
1:A:12:ASP:O	1:A:14:LEU:HD13	2.18	0.44
3:U:130:ILE:HG21	3:U:163:ASP:HB2	1.98	0.44
3:U:94:GLU:CD	3:U:175:LYS:HZ3	2.20	0.44
3:U:122:CYS:O	3:U:123:LEU:HD23	2.18	0.44
3:U:1:LEU:HD21	3:U:24:CYS:SG	2.57	0.44
3:U:5:GLN:HB2	3:U:15:GLU:HG2	2.00	0.44
1:A:20:VAL:O	1:A:20:VAL:HG23	2.15	0.43
3:U:195:TYR:CZ	3:U:212:LEU:HD11	2.53	0.43
3:U:256:PHE:O	3:U:257:SER:C	2.55	0.43
2:B:26:SER:N	2:B:31:CYS:SG	2.92	0.43
3:U:246:MET:HE1	3:U:251:HIS:HB2	2.01	0.43
3:U:18:ALA:HB3	3:U:21:GLN:HG3	2.01	0.43
3:U:28:ILE:HB	3:U:67:THR:HG23	2.00	0.42
3:U:226:THR:HG22	3:U:237:MET:HB2	2.00	0.42
3:U:125:VAL:HA	3:U:167:PHE:O	2.19	0.42
3:U:137:ARG:CB	3:U:138:PRO:HD2	2.49	0.42
1:A:84:TYR:CE1	1:A:106:ASP:HB3	2.55	0.42
3:U:162:ASN:CG	3:U:196:SER:HG	2.23	0.42
1:A:20:VAL:HG22	1:A:30:TRP:O	2.20	0.42
3:U:54:THR:HG23	3:U:67:THR:HB	2.02	0.42
1:A:76:SER:OG	1:A:79:VAL:HG23	2.20	0.42
3:U:40:LEU:N	3:U:40:LEU:HD23	2.35	0.42
3:U:128:HIS:CD2	3:U:142:ARG:HG3	2.54	0.42
1:A:51:TYR:CD2	1:A:128:VAL:HG13	2.55	0.41
2:B:25:CYS:O	2:B:29:GLN:N	2.52	0.41
2:B:14:ASN:OD1	2:B:17:LYS:HB2	2.20	0.41
3:U:130:ILE:CG2	3:U:131:GLN:H	2.30	0.41
3:U:73:LEU:O	3:U:75:LEU:N	2.53	0.41
3:U:18:ALA:CB	3:U:21:GLN:OE1	2.69	0.41
3:U:160:HIS:CE1	3:U:216:ARG:H	2.39	0.41
3:U:259:ASN:O	3:U:260:HIS:C	2.59	0.41
1:A:28:ILE:HD12	1:A:28:ILE:HA	1.82	0.41
1:A:53:GLY:O	1:A:54:ASN:CB	2.69	0.40
3:U:195:TYR:CG	3:U:212:LEU:CD1	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	123/135 (91%)	103 (84%)	16 (13%)	4 (3%)	6	19
2	B	38/40 (95%)	25 (66%)	9 (24%)	4 (10%)	1	1
3	U	269/283 (95%)	216 (80%)	31 (12%)	22 (8%)	1	3
All	All	430/458 (94%)	344 (80%)	56 (13%)	30 (7%)	2	4

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ALA
1	A	127	MET
2	B	4	SER
2	B	18	LYS
3	U	17	CYS
3	U	20	GLY
3	U	55	LEU
3	U	86	THR
3	U	135	GLU
3	U	185	GLU
3	U	186	ASN
3	U	203	HIS
3	U	231	PRO
1	A	89	SER
3	U	74	ASP
3	U	131	GLN
3	U	133	GLY
3	U	153	CYS
3	U	271	CYS
2	B	7	GLY
3	U	152	GLY
2	B	40	LYS
3	U	45	CYS
3	U	138	PRO
3	U	18	ALA

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Mol	Chain	Res	Type
3	U	75	LEU
3	U	81	SER
1	A	120	LYS
3	U	184	LEU
3	U	274	PRO

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/119 (92%)	98 (90%)	11 (10%)	11	30
2	B	37/37 (100%)	34 (92%)	3 (8%)	17	43
3	U	242/251 (96%)	198 (82%)	44 (18%)	2	7
All	All	388/407 (95%)	330 (85%)	58 (15%)	4	12

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	47	SER
1	A	49	THR
1	A	52	GLU
1	A	64	THR
1	A	78	THR
1	A	92	LEU
1	A	122	LEU
1	A	123	VAL
1	A	126	CYS
1	A	128	VAL
2	B	9	CYS
2	B	16	ASP
2	B	33	THR
3	U	1	LEU
3	U	13	ARG
3	U	19	LEU
3	U	33	GLU

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Mol	Chain	Res	Type
3	U	36	GLU
3	U	46	THR
3	U	54	THR
3	U	55	LEU
3	U	56	SER
3	U	62	LYS
3	U	67	THR
3	U	70	VAL
3	U	81	SER
3	U	87	TYR
3	U	88	SER
3	U	89	ARG
3	U	112	SER
3	U	113	LEU
3	U	117	SER
3	U	119	GLU
3	U	125	VAL
3	U	140	ASP
3	U	153	CYS
3	U	162	ASN
3	U	164	THR
3	U	168	LEU
3	U	173	THR
3	U	181	ILE
3	U	200	ASN
3	U	202	THR
3	U	207	SER
3	U	212	LEU
3	U	221	GLN
3	U	228	THR
3	U	232	LYS
3	U	233	ASN
3	U	234	GLN
3	U	239	ARG
3	U	245	SER
3	U	246	MET
3	U	262	ASP
3	U	264	SER
3	U	267	THR
3	U	269	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	85	HIS
1	A	99	HIS
1	A	107	ASN
1	A	116	GLN
3	U	128	HIS
3	U	160	HIS
3	U	162	ASN
3	U	229	HIS
3	U	272	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

3 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	U	1200	3,5	12,14,15	1.04	1 (8%)	15,19,21	1.68	4 (26%)
5	NAG	U	1201	5	12,14,15	0.94	0	15,19,21	1.42	2 (13%)
5	MAN	U	1202	5	10,11,12	0.54	0	11,15,17	1.92	3 (27%)

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
5	NAG	U	1200	3,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	U	1201	5	-	0/6/23/26	0/1/1/1
5	MAN	U	1202	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	1200	NAG	O5-C5	-2.30	1.41	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	1202	MAN	O5-C5-C6	4.64	111.85	106.98
5	U	1201	NAG	O5-C5-C4	3.72	115.37	110.65
5	U	1200	NAG	C3-C2-N2	3.68	117.36	111.76
5	U	1200	NAG	O7-C7-C8	-2.87	116.43	122.04
5	U	1202	MAN	O5-C5-C4	2.74	114.13	110.65
5	U	1202	MAN	C6-C5-C4	-2.20	107.67	113.00
5	U	1200	NAG	O5-C5-C6	-2.15	104.73	106.98
5	U	1200	NAG	O4-C4-C3	2.12	115.10	110.35
5	U	1201	NAG	O4-C4-C5	2.07	114.73	109.28

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	U	1200	NAG	C1

There are no torsion outliers.

There are no ring outliers.

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
4	NAG	U	1052	3	12,14,15	0.64	0	15,19,21	1.19	2 (13%)
4	NAG	U	1172	3	12,14,15	0.60	0	15,19,21	1.35	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	U	1052	3	-	1/6/23/26	0/1/1/1
4	NAG	U	1172	3	1/1/5/7	1/6/23/26	1/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	1172	NAG	O5-C5-C4	2.67	114.04	110.65
4	U	1052	NAG	C3-C2-N2	2.50	115.57	111.76
4	U	1172	NAG	O3-C3-C2	2.44	114.20	109.09
4	U	1052	NAG	C2-N2-C7	2.18	126.75	123.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	U	1172	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	1052	NAG	C3-C2-N2-C7
4	U	1172	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	1172	NAG	C1-C2-C3-C4-C5-O5

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	125/135 (92%)	0.34	6 (4%) 29 30	49, 55, 61, 64	0
2	B	40/40 (100%)	0.84	7 (17%) 2 2	60, 63, 70, 71	0
3	U	273/283 (96%)	0.74	33 (12%) 5 4	41, 63, 76, 100	0
All	All	438/458 (95%)	0.64	46 (10%) 7 6	41, 61, 74, 100	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	U	72	GLY	6.0
1	A	8	PRO	5.8
3	U	134	GLU	5.2
1	A	9	SER	4.7
3	U	56	SER	4.1
3	U	89	ARG	4.0
3	U	54	THR	3.8
3	U	109	ARG	3.7
2	B	8	ARG	3.6
2	B	37	ALA	3.4
1	A	129	HIS	3.2
3	U	87	TYR	3.2
3	U	132	GLU	3.2
2	B	15	VAL	3.1
3	U	133	GLY	3.0
3	U	126	VAL	3.0
3	U	57	TYR	2.9
3	U	241	CYS	2.9
3	U	65	SER	2.8
3	U	16	GLU	2.8
2	B	7	GLY	2.7
3	U	146	GLY	2.7
3	U	135	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	41	PRO	2.6
3	U	67	THR	2.6
3	U	166	HIS	2.6
3	U	64	THR	2.6
2	B	14	ASN	2.4
3	U	66	LEU	2.4
2	B	40	LYS	2.3
3	U	55	LEU	2.3
3	U	76	CYS	2.3
1	A	127	MET	2.3
3	U	19	LEU	2.3
1	A	109	ARG	2.3
1	A	67	MET	2.2
3	U	148	GLY	2.2
3	U	127	THR	2.2
3	U	85	VAL	2.2
3	U	149	TYR	2.1
3	U	31	LEU	2.1
3	U	231	PRO	2.1
3	U	167	PHE	2.1
3	U	233	ASN	2.1
3	U	158	GLY	2.1
3	U	147	CYS	2.1

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	U	1201	14/15	0.30	12.33	101,106,110,113	0
5	MAN	U	1202	11/12	0.25	-0.17	115,116,117,118	0
5	NAG	U	1200	14/15	0.18	-0.74	92,94,98,101	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	U	1052	14/15	0.30	1.28	109,112,115,117	0
4	NAG	U	1172	14/15	0.30	0.62	93,97,100,100	0

6.5 Other polymers

There are no such residues in this entry.