



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:32 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 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

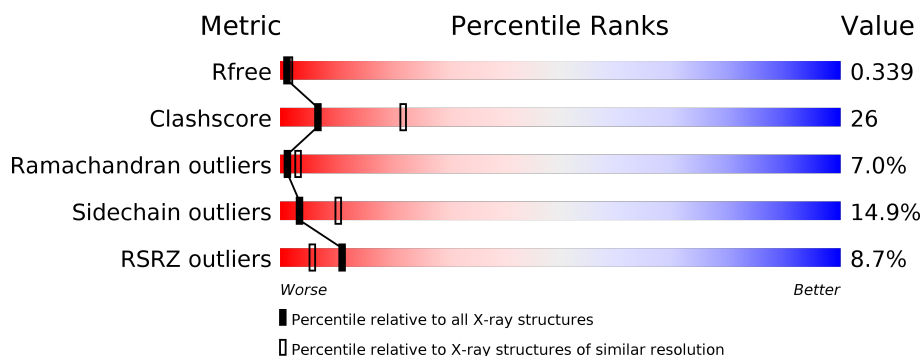
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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. 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 $\leq 5\%$. 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	135	
2	B	40	
3	U	283	

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	NAG	U	1172	X	-	-	-
5	NAG	U	1200	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3461 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 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		

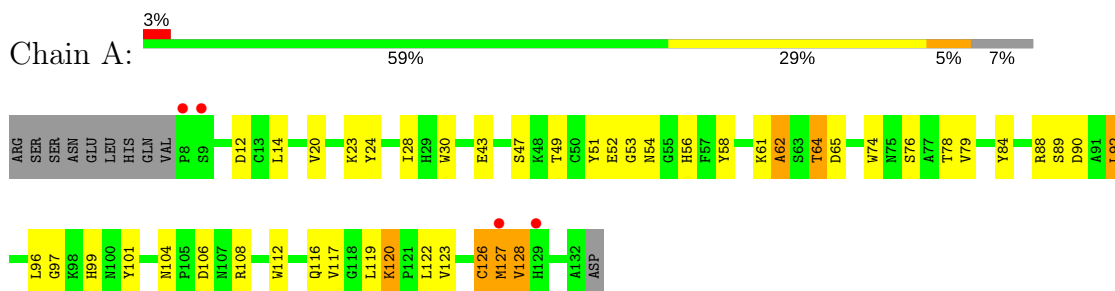
- Molecule 5 is a polymer of unknown type called SUGAR (N-ACETYL-D-GLUCOSAMINE).

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

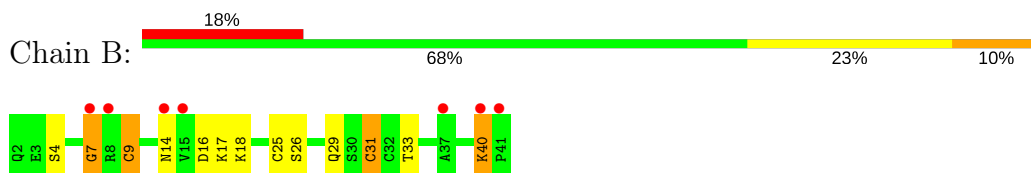
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

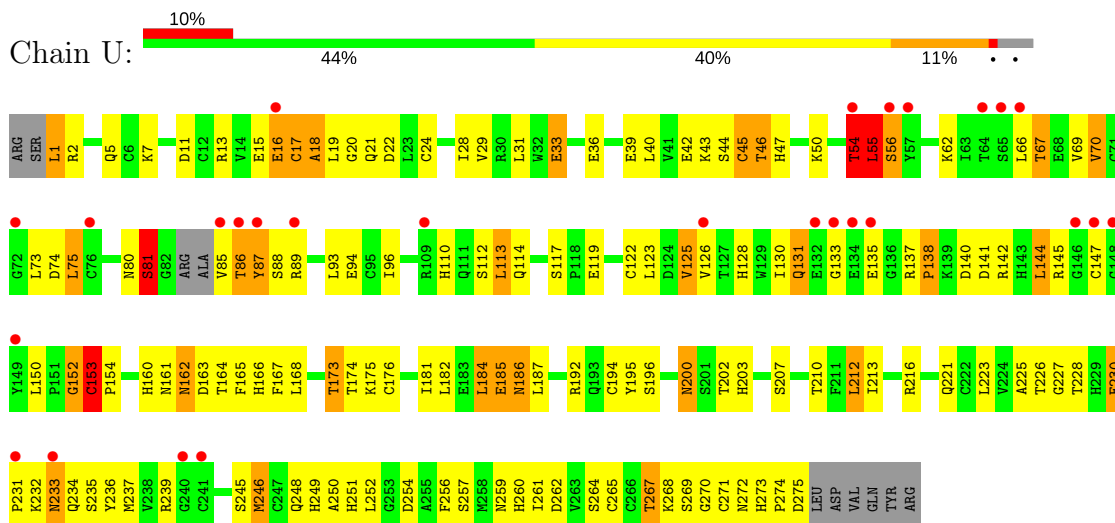
- Molecule 1: Urokinase-type plasminogen activator



- Molecule 2: Vitronectin



- Molecule 3: Urokinase plasminogen activator surface receptor



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 0.306 , 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 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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 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	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

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 26.

All (173) 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)
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	Interatomic distance (Å)	Clash overlap (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
3:U:141:ASP:HB2	3:U:144:LEU:HD13	1.73	0.71
1:A:23:LYS:NZ	3:U:166:HIS:ND1	2.39	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:130:ILE:HG23	3:U:131:GLN:H	1.56	0.70
3:U:16:GLU:O	3:U:18:ALA:N	2.24	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:96:ILE:HG23	3:U:110:HIS:HB3	1.78	0.66
3:U:130:ILE:CG2	3:U:163:ASP:HB2	2.24	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: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
1:A:99:HIS:CD2	1:A:101:TYR:H	2.19	0.60
3:U:250:ALA:HB1	3:U:261:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:46:THR:CG2	3:U:50:LYS:HG3	2.30	0.60
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:173:THR:HG23	3:U:176:CYS:CB	2.37	0.53
3:U:96:ILE:CG2	3:U:110:HIS:HB3	2.38	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
1:A:92:LEU:HD13	1:A:92:LEU:N	2.23	0.52
3:U:54:THR:O	3:U:55:LEU:O	2.28	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:128:HIS:CE1	3:U:142:ARG:CZ	2.93	0.51
3:U:153:CYS:HB3	3:U:154:PRO:CD	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:160:HIS:HE1	3:U:216:ARG:H	1.63	0.47
3:U:50:LYS:NZ	3:U:254:ASP:OD1	2.44	0.47
3:U:1:LEU:HD22	3:U:17:CYS:HB2	1.97	0.47
3:U:113:LEU:HD23	3:U:113:LEU:O	2.15	0.47
1:A:108:ARG:HG3	1:A:112:TRP:CD1	2.50	0.47
3:U:200:ASN:HB2	5:U:1200:NAG:H82	1.96	0.47
1:A:56:HIS:HD2	1:A:104:ASN:O	1.97	0.47
3:U:161:ASN:HA	3:U:213:ILE:CD1	2.45	0.47
3:U:94:GLU:CD	3:U:175:LYS:HZ1	2.18	0.46
3:U:184:LEU:CA	3:U:187:LEU:HD13	2.45	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
1:A:99:HIS:CG	1:A:101:TYR:CD2	3.03	0.46
3:U:162:ASN:ND2	3:U:163:ASP:CG	2.69	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:1:LEU:O	3:U:17:CYS:CB	2.64	0.45
3:U:200:ASN:N	3:U:200:ASN:OD1	2.50	0.45
3:U:87:TYR:C	3:U:87:TYR:CD1	2.89	0.45
3:U:126:VAL:O	3:U:166:HIS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:195:TYR:HB3	3:U:210:THR:CG2	2.47	0.45
1:A:117:VAL:HG13	1:A:117:VAL:O	2.17	0.44
1:A:12:ASP:O	1:A:14:LEU:HD13	2.18	0.44
3:U:1:LEU:CD2	3:U:1:LEU:C	2.85	0.44
3:U:200:ASN:HD22	5:U:1200:NAG:C8	2.22	0.44
3:U:2:ARG:HG2	3:U:16:GLU:HA	1.99	0.44
3:U:122:CYS:O	3:U:123:LEU:HD23	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: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:125:VAL:HA	3:U:167:PHE:O	2.19	0.42
3:U:226:THR:HG22	3:U:237:MET:HB2	2.00	0.42
3:U:28:ILE:HB	3:U:67:THR:HG23	2.00	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
1:A:76:SER:OG	1:A:79:VAL:HG23	2.20	0.42
3:U:54:THR:HG23	3:U:67:THR:HB	2.02	0.42
3:U:40:LEU:HD23	3:U:40:LEU:N	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
1:A:28:ILE:HA	1:A:28:ILE:HD12	1.82	0.41
3:U:259:ASN:O	3:U:260:HIS:C	2.59	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%)	4	15
2	B	38/40 (95%)	25 (66%)	9 (24%)	4 (10%)	0	1
3	U	269/283 (95%)	216 (80%)	31 (12%)	22 (8%)	1	2
All	All	430/458 (94%)	344 (80%)	56 (13%)	30 (7%)	1	3

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

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Mol	Chain	Res	Type
3	U	18	ALA
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%)	9	25
2	B	37/37 (100%)	34 (92%)	3 (8%)	14	37
3	U	242/251 (96%)	198 (82%)	44 (18%)	2	6
All	All	388/407 (95%)	330 (85%)	58 (15%)	3	10

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

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Mol	Chain	Res	Type
3	U	19	LEU
3	U	33	GLU
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 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 ⓘ

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	14,14,15	0.85	0	15,19,21	1.74	3 (20%)
5	NAG	U	1201	5	14,14,15	0.98	0	15,19,21	1.48	4 (26%)
5	MAN	U	1202	5	11,11,12	0.70	0	13,15,17	2.96	4 (30%)

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	1200	NAG	O7-C7-C8	-3.09	116.43	122.06
5	U	1202	MAN	C6-C5-C4	-2.28	107.67	113.00
5	U	1201	NAG	C2-N2-C7	2.03	125.90	122.94
5	U	1201	NAG	O4-C4-C5	2.16	114.73	109.28
5	U	1200	NAG	O4-C4-C3	2.18	115.10	110.36
5	U	1202	MAN	O5-C1-C2	2.52	114.74	110.79
5	U	1201	NAG	C1-O5-C5	2.88	116.13	112.17
5	U	1201	NAG	C4-C3-C2	3.01	115.43	111.02
5	U	1200	NAG	C1-O5-C5	4.56	118.45	112.17
5	U	1202	MAN	C1-C2-C3	4.92	115.88	109.65
5	U	1202	MAN	C1-O5-C5	8.43	123.78	112.17

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.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	U	1200	NAG	5	0

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	14,14,15	0.50	0	15,19,21	1.21	2 (13%)
4	NAG	U	1172	3	14,14,15	0.77	1 (7%)	15,19,21	1.62	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	-	0/6/23/26	0/1/1/1
4	NAG	U	1172	3	1/1/5/7	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	1172	NAG	C1-C2	2.04	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	1052	NAG	O5-C1-C2	-2.58	107.88	111.47
4	U	1172	NAG	O3-C3-C2	2.25	114.20	109.39
4	U	1052	NAG	C2-N2-C7	2.61	126.75	122.94
4	U	1172	NAG	C1-O5-C5	4.14	117.87	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	U	1172	NAG	C1

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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	125/135 (92%)	0.29	4 (3%) 48 37	49, 55, 61, 64	0
2	B	40/40 (100%)	0.87	7 (17%) 2 1	60, 63, 70, 71	0
3	U	273/283 (96%)	0.65	27 (9%) 8 4	41, 63, 76, 100	0
All	All	438/458 (95%)	0.57	38 (8%) 11 6	41, 61, 74, 100	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	PRO	6.9
3	U	134	GLU	6.0
1	A	9	SER	5.3
3	U	72	GLY	4.3
3	U	133	GLY	4.3
2	B	37	ALA	4.1
2	B	8	ARG	4.0
3	U	56	SER	3.9
3	U	54	THR	3.5
3	U	89	ARG	3.4
1	A	129	HIS	3.4
3	U	109	ARG	3.2
2	B	41	PRO	3.2
3	U	135	GLU	3.1
3	U	241	CYS	3.0
3	U	231	PRO	3.0
2	B	15	VAL	2.9
3	U	233	ASN	2.8
3	U	132	GLU	2.7
3	U	65	SER	2.7
3	U	146	GLY	2.7
3	U	76	CYS	2.6
3	U	240	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	40	LYS	2.5
3	U	57	TYR	2.5
3	U	16	GLU	2.5
3	U	148	GLY	2.4
3	U	126	VAL	2.3
2	B	14	ASN	2.3
3	U	64	THR	2.2
1	A	127	MET	2.2
3	U	66	LEU	2.2
3	U	147	CYS	2.2
3	U	86	THR	2.1
2	B	7	GLY	2.1
3	U	87	TYR	2.1
3	U	149	TYR	2.0
3	U	85	VAL	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](#)

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
5	MAN	U	1202	11/12	0.65	0.35	-	115,116,117,118	0
5	NAG	U	1200	14/15	0.67	0.18	-	92,94,98,101	0
5	NAG	U	1201	14/15	0.75	0.34	-	101,106,110,113	0

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(\AA^2)	Q<0.9
4	NAG	U	1172	14/15	0.73	0.30	0.70	93,97,100,100	0
4	NAG	U	1052	14/15	0.73	0.34	-	109,112,115,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.