Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:37 PM GMT

PDB ID	:	3U73
Title	:	Crystal structure of stabilized human uPAR mutant in complex with ATF
Authors	:	Huang, M.D.; Xu, X.; Yuan, C.
Deposited on	:	2011-10-13
Resolution	:	3.19 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:

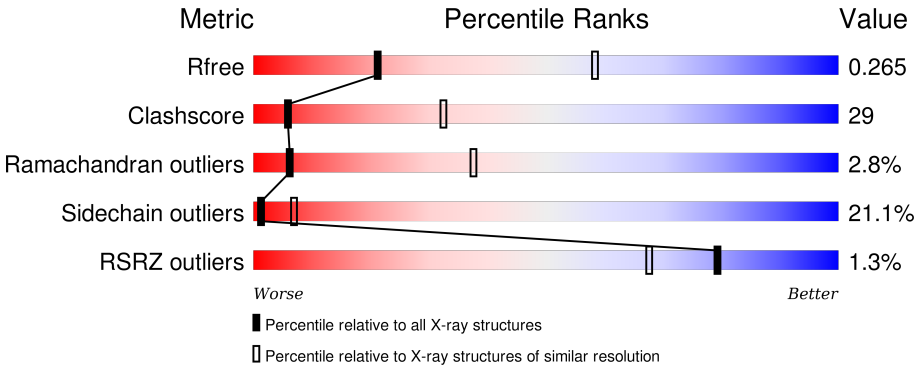
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.19 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	U	283	% 47% 37% 9% • 5%
2	A	132	% 45% 39% 8% 7%

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
3	NAG	U	501	-	-	X	-
4	NAG	U	502	-	-	X	-
5	NAG	U	506	-	-	X	-
5	NAG	U	507	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3133 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 plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	U	269	2063	1237	376	414	36	0	0	0

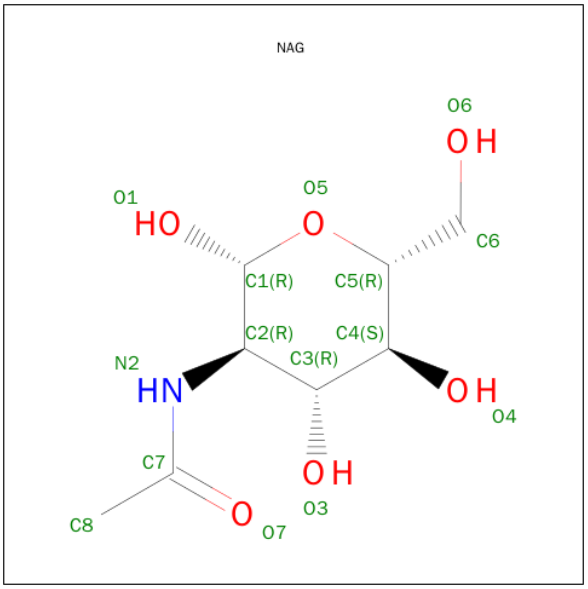
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	47	CYS	HIS	ENGINEERED MUTATION	UNP Q03405
U	259	CYS	ASN	ENGINEERED MUTATION	UNP Q03405

- Molecule 2 is a protein called Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	123	975	600	185	176	14	0	0	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	U	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

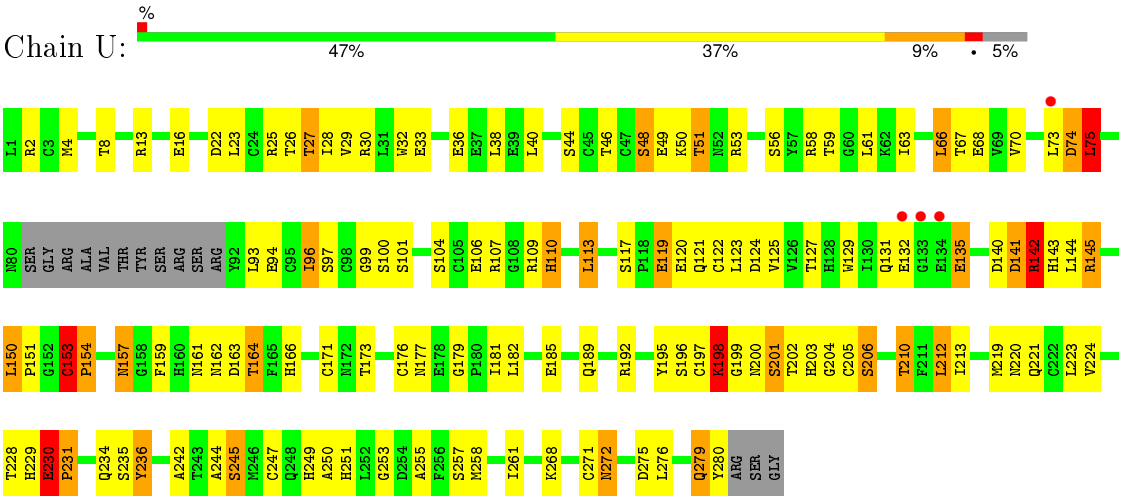
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		

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.

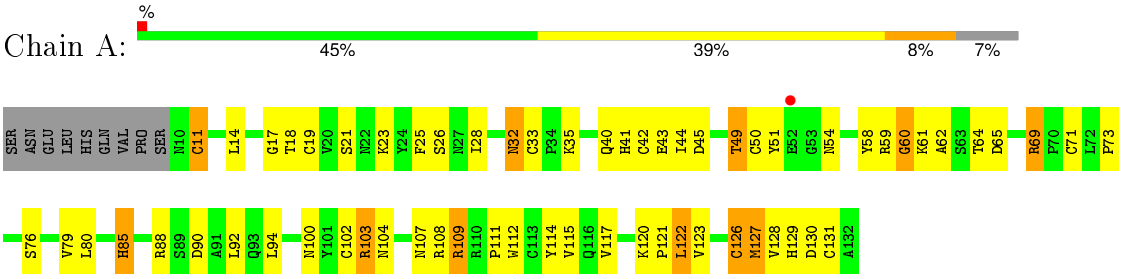
- Molecule 1: Urokinase plasminogen activator surface receptor

Chain U:



- Molecule 2: Urokinase-type plasminogen activator

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	130.90Å 130.90Å 105.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.76 – 3.19 47.76 – 3.19	Depositor EDS
% Data completeness (in resolution range)	96.2 (47.76-3.19) 96.3 (47.76-3.19)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.216 , 0.258 0.233 , 0.265	Depositor DCC
R_{free} test set	900 reflections (5.55%)	DCC
Wilson B-factor (Å^2)	95.0	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 93.6	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 17119 reflections (0.012%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3133	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: 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	U	0.85	2/2096 (0.1%)	0.95	3/2824 (0.1%)
2	A	0.88	1/1002 (0.1%)	0.91	2/1353 (0.1%)
All	All	0.86	3/3098 (0.1%)	0.94	5/4177 (0.1%)

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
1	U	0	1
2	A	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	114	TYR	CE1-CZ	-5.80	1.31	1.38
1	U	129	TRP	CD2-CE2	5.55	1.48	1.41
1	U	32	TRP	CD2-CE2	5.38	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	11	CYS	CA-CB-SG	6.65	125.97	114.00
1	U	75	LEU	CA-CB-CG	5.39	127.69	115.30
1	U	142	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	A	103	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	U	275	ASP	CB-CG-OD1	-5.02	113.78	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	11	CYS	Peptide
2	A	62	ALA	Peptide
1	U	153	CYS	Peptide

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	U	2063	0	1914	120	0
2	A	975	0	906	35	0
3	U	14	0	12	9	0
4	U	25	0	21	11	0
5	U	56	0	50	30	0
All	All	3133	0	2903	172	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 29.

All (172) 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)
5:U:506:NAG:H62	5:U:507:NAG:C7	1.34	1.53
5:U:506:NAG:H62	5:U:507:NAG:O7	1.27	1.30
1:U:50:LYS:O	1:U:51:THR:HG22	1.43	1.18
3:U:501:NAG:O6	4:U:502:NAG:H82	1.44	1.17
1:U:202:THR:HG21	5:U:506:NAG:C8	1.79	1.13
5:U:506:NAG:C6	5:U:507:NAG:C7	2.27	1.12
1:U:202:THR:HG21	5:U:506:NAG:H82	1.22	1.11
5:U:506:NAG:H62	5:U:507:NAG:C8	1.80	1.11
5:U:506:NAG:C6	5:U:507:NAG:C8	2.32	1.06
4:U:502:NAG:O3	4:U:503:MAN:H2	1.58	1.03
1:U:234:GLN:OE1	5:U:506:NAG:H61	1.59	1.02
1:U:202:THR:CG2	5:U:506:NAG:H82	1.89	1.02
1:U:202:THR:HG21	5:U:506:NAG:C7	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:198:LYS:O	1:U:198:LYS:HG2	1.65	0.96
1:U:157:ASN:HB3	1:U:245:SER:HB2	1.47	0.96
3:U:501:NAG:H62	4:U:502:NAG:N2	1.78	0.95
5:U:506:NAG:C6	5:U:507:NAG:O7	2.15	0.94
1:U:50:LYS:C	1:U:51:THR:HG22	1.79	0.92
1:U:198:LYS:N	1:U:205:CYS:SG	2.45	0.89
1:U:50:LYS:C	1:U:51:THR:CG2	2.39	0.88
3:U:501:NAG:HO6	4:U:502:NAG:H82	1.37	0.86
1:U:162:ASN:OD1	5:U:504:NAG:C7	2.26	0.83
1:U:202:THR:C	1:U:203:HIS:ND1	2.31	0.83
2:A:126:CYS:SG	2:A:127:MET:N	2.52	0.82
1:U:162:ASN:OD1	5:U:504:NAG:C2	2.17	0.81
5:U:506:NAG:C6	5:U:507:NAG:H81	2.11	0.80
2:A:69:ARG:HD2	2:A:115:VAL:HG11	1.65	0.79
1:U:50:LYS:O	1:U:51:THR:CG2	2.30	0.79
1:U:27:THR:HG23	1:U:68:GLU:HB2	1.65	0.78
1:U:198:LYS:O	1:U:198:LYS:CG	2.31	0.77
1:U:162:ASN:OD1	5:U:504:NAG:O7	2.05	0.75
1:U:230:GLU:HG2	1:U:231:PRO:HD3	1.68	0.74
5:U:506:NAG:H61	5:U:507:NAG:C8	2.17	0.74
1:U:202:THR:CG2	5:U:506:NAG:C8	2.58	0.74
1:U:162:ASN:OD1	5:U:504:NAG:H2	1.89	0.73
4:U:502:NAG:O3	4:U:503:MAN:C2	2.34	0.73
2:A:54:ASN:ND2	2:A:107:ASN:OD1	2.23	0.71
1:U:25:ARG:NH1	1:U:27:THR:OG1	2.23	0.71
1:U:51:THR:HG23	1:U:53:ARG:HH21	1.60	0.66
1:U:161:ASN:OD1	1:U:161:ASN:C	2.30	0.66
2:A:58:TYR:O	2:A:59:ARG:NH1	2.24	0.66
1:U:74:ASP:HB3	1:U:75:LEU:HD22	1.76	0.65
2:A:49:THR:OG1	2:A:50:CYS:N	2.29	0.65
1:U:234:GLN:NE2	5:U:506:NAG:H4	2.12	0.65
1:U:202:THR:OG1	1:U:203:HIS:ND1	2.29	0.65
1:U:162:ASN:OD1	5:U:504:NAG:N2	2.30	0.64
1:U:122:CYS:HB2	1:U:176:CYS:SG	2.38	0.64
1:U:200:ASN:O	1:U:202:THR:N	2.30	0.64
1:U:206:SER:O	1:U:210:THR:HG22	1.98	0.64
1:U:202:THR:O	1:U:203:HIS:ND1	2.30	0.64
5:U:506:NAG:H61	5:U:507:NAG:H82	1.78	0.63
3:U:501:NAG:H62	4:U:502:NAG:C7	2.29	0.61
1:U:197:CYS:CB	1:U:205:CYS:SG	2.88	0.61
3:U:501:NAG:H62	4:U:502:NAG:HN2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:71:CYS:HB2	2:A:100:ASN:HB2	1.83	0.61
2:A:17:GLY:HA2	2:A:32:ASN:O	2.00	0.60
2:A:73:PRO:O	2:A:76:SER:OG	2.16	0.60
1:U:96:ILE:HD12	1:U:110:HIS:HB3	1.83	0.60
1:U:123:LEU:H	1:U:177:ASN:HD22	1.49	0.60
1:U:107:ARG:NH2	1:U:109:ARG:HH21	2.00	0.59
4:U:502:NAG:O3	4:U:503:MAN:C1	2.50	0.59
1:U:29:VAL:HG23	2:A:28:ILE:HD13	1.85	0.59
1:U:234:GLN:CD	5:U:506:NAG:H61	2.21	0.59
1:U:200:ASN:OD1	1:U:203:HIS:N	2.30	0.59
2:A:108:ARG:HG2	2:A:109:ARG:H	1.66	0.58
3:U:501:NAG:C6	4:U:502:NAG:H82	2.31	0.58
1:U:200:ASN:OD1	1:U:200:ASN:C	2.42	0.58
1:U:4:MET:HE2	1:U:75:LEU:HD12	1.85	0.57
2:A:120:LYS:HG2	2:A:121:PRO:HD2	1.86	0.57
2:A:117:VAL:HG21	2:A:122:LEU:HD22	1.86	0.56
1:U:197:CYS:HB3	1:U:210:THR:HB	1.87	0.56
2:A:111:PRO:O	2:A:126:CYS:HB3	2.06	0.56
1:U:196:SER:HB2	1:U:213:ILE:HD13	1.88	0.56
2:A:85:HIS:CE1	2:A:88:ARG:HB3	2.40	0.56
1:U:96:ILE:HB	1:U:177:ASN:OD1	2.06	0.55
2:A:58:TYR:O	2:A:59:ARG:HD3	2.06	0.55
1:U:200:ASN:OD1	1:U:202:THR:N	2.36	0.55
1:U:23:LEU:HD13	1:U:70:VAL:HB	1.87	0.55
1:U:29:VAL:CG2	2:A:28:ILE:HD13	2.37	0.55
1:U:166:HIS:CD2	1:U:255:ALA:HB1	2.43	0.54
1:U:234:GLN:NE2	5:U:507:NAG:H82	2.23	0.53
1:U:200:ASN:N	1:U:203:HIS:O	2.30	0.53
3:U:501:NAG:C6	4:U:502:NAG:C7	2.86	0.53
1:U:100:SER:OG	1:U:143:HIS:HB2	2.08	0.53
1:U:66:LEU:HD12	2:A:25:PHE:CG	2.44	0.53
1:U:249:HIS:HB2	1:U:251:HIS:CE1	2.43	0.52
1:U:117:SER:HB3	1:U:120:GLU:HG2	1.91	0.52
1:U:234:GLN:HE22	5:U:507:NAG:C7	2.23	0.52
1:U:127:THR:O	1:U:142:ARG:HB2	2.10	0.52
1:U:203:HIS:N	1:U:203:HIS:ND1	2.57	0.52
2:A:88:ARG:HG3	2:A:90:ASP:OD1	2.10	0.52
1:U:200:ASN:C	1:U:202:THR:N	2.63	0.51
1:U:200:ASN:O	1:U:203:HIS:N	2.44	0.51
1:U:195:TYR:CZ	1:U:212:LEU:HD22	2.45	0.51
5:U:506:NAG:O4	5:U:507:NAG:C7	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:202:THR:OG1	1:U:203:HIS:N	2.43	0.51
2:A:112:TRP:CE3	2:A:123:VAL:HG13	2.46	0.51
1:U:121:GLN:HB2	1:U:171:CYS:O	2.11	0.51
2:A:102:CYS:O	2:A:103:ARG:HD3	2.11	0.51
1:U:253:GLY:O	1:U:257:SER:N	2.43	0.51
1:U:202:THR:CG2	5:U:506:NAG:C7	2.80	0.50
2:A:79:VAL:O	2:A:85:HIS:HB3	2.12	0.50
2:A:43:GLU:HG2	2:A:44:ILE:N	2.26	0.50
1:U:200:ASN:C	1:U:202:THR:H	2.15	0.50
1:U:200:ASN:OD1	1:U:200:ASN:O	2.30	0.50
2:A:80:LEU:HD23	2:A:85:HIS:HB2	1.94	0.50
2:A:41:HIS:O	2:A:42:CYS:HB2	2.12	0.49
1:U:234:GLN:HE22	5:U:507:NAG:H82	1.75	0.49
1:U:26:THR:HG22	1:U:28:ILE:HD11	1.93	0.49
1:U:198:LYS:CA	1:U:205:CYS:SG	3.01	0.49
1:U:33:GLU:N	1:U:36:GLU:O	2.40	0.49
2:A:45:ASP:O	2:A:60:GLY:HA2	2.12	0.49
1:U:58:ARG:HG2	1:U:63:ILE:HG12	1.93	0.49
1:U:161:ASN:OD1	1:U:163:ASP:OD1	2.30	0.48
1:U:123:LEU:N	1:U:177:ASN:HD22	2.11	0.48
1:U:58:ARG:HG3	1:U:113:LEU:HD23	1.95	0.48
1:U:228:THR:HA	1:U:235:SER:HA	1.96	0.48
2:A:65:ASP:C	2:A:65:ASP:OD1	2.51	0.48
1:U:104:SER:HB2	1:U:109:ARG:HB2	1.96	0.48
2:A:85:HIS:HE1	2:A:88:ARG:HB3	1.77	0.48
1:U:164:THR:HG21	1:U:166:HIS:NE2	2.29	0.47
1:U:202:THR:OG1	1:U:203:HIS:CG	2.68	0.47
1:U:199:GLY:HA3	1:U:204:GLY:HA3	1.96	0.47
1:U:97:SER:HB2	1:U:113:LEU:HB2	1.96	0.47
3:U:501:NAG:O6	4:U:502:NAG:C8	2.37	0.46
1:U:230:GLU:HG2	1:U:231:PRO:CD	2.39	0.46
1:U:271:CYS:O	1:U:272:ASN:CB	2.62	0.46
1:U:145:ARG:NH2	1:U:179:GLY:O	2.48	0.46
1:U:157:ASN:HB3	1:U:245:SER:CB	2.33	0.46
1:U:40:LEU:HD21	2:A:40:GLN:HG3	1.98	0.45
1:U:51:THR:HG23	1:U:53:ARG:NH2	2.31	0.45
1:U:117:SER:OG	1:U:119:GLU:OE1	2.34	0.45
1:U:106:GLU:OE1	1:U:106:GLU:N	2.43	0.45
1:U:255:ALA:HA	2:A:23:LYS:HD2	1.98	0.45
1:U:223:LEU:HD22	1:U:242:ALA:HB2	1.99	0.44
2:A:51:TYR:CE1	2:A:130:ASP:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:2:ARG:HG2	1:U:16:GLU:HA	1.99	0.44
1:U:250:ALA:HB1	1:U:261:ILE:HD11	1.99	0.44
1:U:161:ASN:O	1:U:163:ASP:N	2.51	0.44
1:U:150:LEU:HD23	1:U:151:PRO:HD2	1.98	0.44
1:U:234:GLN:NE2	5:U:506:NAG:H61	2.33	0.43
1:U:271:CYS:O	1:U:272:ASN:HB3	2.19	0.43
1:U:25:ARG:HD3	1:U:46:THR:HB	2.01	0.43
1:U:244:ALA:O	1:U:247:CYS:HB2	2.19	0.43
1:U:258:MET:HE2	1:U:261:ILE:HG22	2.01	0.42
2:A:64:THR:OG1	2:A:65:ASP:N	2.51	0.42
1:U:48:SER:O	1:U:49:GLU:HB2	2.19	0.42
2:A:51:TYR:H	2:A:130:ASP:HA	1.84	0.42
1:U:199:GLY:HA2	1:U:236:TYR:CE1	2.55	0.42
1:U:276:LEU:HD23	1:U:276:LEU:HA	1.75	0.42
2:A:104:ASN:HB2	2:A:111:PRO:HA	2.02	0.42
1:U:229:HIS:O	1:U:231:PRO:N	2.53	0.42
1:U:202:THR:HG1	1:U:203:HIS:N	2.18	0.41
5:U:506:NAG:O6	5:U:507:NAG:H81	2.20	0.41
1:U:279:GLN:O	1:U:280:TYR:HB2	2.21	0.41
1:U:70:VAL:O	3:U:501:NAG:N2	2.50	0.41
1:U:272:ASN:OD1	1:U:272:ASN:C	2.59	0.41
1:U:161:ASN:OD1	1:U:162:ASN:N	2.52	0.41
2:A:121:PRO:O	2:A:122:LEU:HD12	2.21	0.41
1:U:93:LEU:HD23	1:U:94:GLU:N	2.35	0.41
1:U:25:ARG:HG2	1:U:44:SER:O	2.21	0.41
1:U:204:GLY:O	1:U:205:CYS:SG	2.78	0.41
1:U:153:CYS:HB3	1:U:154:PRO:CD	2.51	0.41
1:U:197:CYS:CB	1:U:210:THR:HB	2.51	0.40
1:U:99:GLY:HA2	1:U:143:HIS:O	2.21	0.40
1:U:234:GLN:HE22	5:U:507:NAG:C8	2.34	0.40
1:U:163:ASP:OD1	1:U:163:ASP:N	2.51	0.40
2:A:64:THR:H	2:A:64:THR:HG22	1.62	0.40
1:U:124:ASP:HA	1:U:145:ARG:HG3	2.02	0.40
1:U:159:PHE:CD2	1:U:223:LEU:HD23	2.57	0.40
1:U:100:SER:HB2	1:U:141:ASP:O	2.21	0.40
1:U:200:ASN:OD1	1:U:202:THR:HG23	2.22	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	U	265/283 (94%)	223 (84%)	35 (13%)	7 (3%)	7 40
2	A	121/132 (92%)	111 (92%)	6 (5%)	4 (3%)	5 32
All	All	386/415 (93%)	334 (86%)	41 (11%)	11 (3%)	6 37

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	153	CYS
2	A	26	SER
2	A	60	GLY
2	A	127	MET
1	U	201	SER
1	U	135	GLU
1	U	230	GLU
1	U	198	LYS
2	A	128	VAL
1	U	154	PRO
1	U	231	PRO

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	U	239/250 (96%)	184 (77%)	55 (23%)	1 4
2	A	107/116 (92%)	89 (83%)	18 (17%)	2 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	346/366 (94%)	273 (79%)	73 (21%)	1 7

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	8	THR
1	U	13	ARG
1	U	22	ASP
1	U	27	THR
1	U	30	ARG
1	U	38	LEU
1	U	48	SER
1	U	51	THR
1	U	56	SER
1	U	59	THR
1	U	61	LEU
1	U	66	LEU
1	U	67	THR
1	U	73	LEU
1	U	74	ASP
1	U	75	LEU
1	U	96	ILE
1	U	101	SER
1	U	110	HIS
1	U	113	LEU
1	U	119	GLU
1	U	125	VAL
1	U	131	GLN
1	U	132	GLU
1	U	135	GLU
1	U	140	ASP
1	U	141	ASP
1	U	142	ARG
1	U	144	LEU
1	U	145	ARG
1	U	150	LEU
1	U	153	CYS
1	U	157	ASN
1	U	164	THR
1	U	173	THR
1	U	181	ILE
1	U	182	LEU

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Mol	Chain	Res	Type
1	U	185	GLU
1	U	189	GLN
1	U	192	ARG
1	U	198	LYS
1	U	201	SER
1	U	206	SER
1	U	210	THR
1	U	212	LEU
1	U	219	MET
1	U	220	ASN
1	U	221	GLN
1	U	224	VAL
1	U	230	GLU
1	U	236	TYR
1	U	245	SER
1	U	268	LYS
1	U	272	ASN
1	U	279	GLN
2	A	14	LEU
2	A	18	THR
2	A	19	CYS
2	A	21	SER
2	A	32	ASN
2	A	33	CYS
2	A	35	LYS
2	A	49	THR
2	A	61	LYS
2	A	69	ARG
2	A	85	HIS
2	A	92	LEU
2	A	94	LEU
2	A	109	ARG
2	A	122	LEU
2	A	126	CYS
2	A	129	HIS
2	A	131	CYS

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

Mol	Chain	Res	Type
1	U	234	GLN
1	U	251	HIS

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Mol	Chain	Res	Type
1	U	279	GLN
2	A	54	ASN
2	A	56	HIS
2	A	85	HIS
2	A	107	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

6 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	$\#\|Z\| > 2$
4	NAG	U	502	3,4	14,14,15	2.10	6 (42%)	15,19,21	1.73	4 (26%)
4	MAN	U	503	4	11,11,12	1.84	3 (27%)	14,15,17	2.12	5 (35%)
5	NAG	U	504	1,5	14,14,15	2.36	5 (35%)	15,19,21	3.03	10 (66%)
5	NAG	U	505	5	14,14,15	1.93	5 (35%)	15,19,21	1.58	5 (33%)
5	NAG	U	506	1,5	14,14,15	0.39	0	15,19,21	1.16	2 (13%)
5	NAG	U	507	5	14,14,15	0.39	0	15,19,21	1.15	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	502	3,4	-	0/6/23/26	0/1/1/1
4	MAN	U	503	4	-	0/2/19/22	0/1/1/1
5	NAG	U	504	1,5	-	0/6/23/26	0/1/1/1
5	NAG	U	505	5	-	0/6/23/26	0/1/1/1
5	NAG	U	506	1,5	-	0/6/23/26	0/1/1/1
5	NAG	U	507	5	-	0/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	503	MAN	C2-C3	-4.23	1.46	1.52
4	U	502	NAG	C3-C2	-3.67	1.43	1.52
5	U	505	NAG	C3-C2	-3.41	1.44	1.52
5	U	504	NAG	C4-C3	-2.59	1.45	1.52
4	U	503	MAN	O2-C2	-2.28	1.38	1.43
4	U	502	NAG	C4-C3	-2.14	1.46	1.52
5	U	505	NAG	C4-C3	-2.13	1.46	1.52
4	U	502	NAG	C1-C2	-2.07	1.49	1.52
4	U	503	MAN	O3-C3	2.07	1.47	1.43
5	U	505	NAG	O3-C3	2.14	1.48	1.43
5	U	504	NAG	O5-C1	2.16	1.47	1.43
5	U	505	NAG	C2-N2	2.65	1.51	1.46
4	U	502	NAG	O3-C3	2.81	1.49	1.43
4	U	502	NAG	C2-N2	2.88	1.51	1.46
5	U	504	NAG	O3-C3	3.03	1.50	1.43
5	U	504	NAG	C2-N2	4.09	1.53	1.46
5	U	505	NAG	C7-N2	4.25	1.50	1.34
4	U	502	NAG	C7-N2	4.26	1.50	1.34
5	U	504	NAG	C7-N2	5.18	1.54	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	U	504	NAG	O3-C3-C4	-4.72	99.70	110.34
5	U	504	NAG	C2-N2-C7	-4.35	117.44	123.04
4	U	502	NAG	C2-N2-C7	-4.01	117.88	123.04
5	U	504	NAG	C6-C5-C4	-2.74	106.24	113.02
5	U	504	NAG	O7-C7-C8	-2.48	117.51	122.06
5	U	506	NAG	C2-N2-C7	-2.39	119.97	123.04
5	U	507	NAG	C2-N2-C7	-2.35	120.02	123.04
5	U	505	NAG	C2-N2-C7	-2.29	120.10	123.04
5	U	505	NAG	O3-C3-C2	-2.27	104.61	109.11
5	U	506	NAG	C8-C7-N2	2.01	119.94	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	U	507	NAG	C8-C7-N2	2.01	119.95	116.11
5	U	505	NAG	O5-C5-C6	2.02	111.72	107.35
4	U	503	MAN	O6-C6-C5	2.10	118.25	111.33
4	U	503	MAN	C1-O5-C5	2.12	114.93	112.25
5	U	504	NAG	C8-C7-N2	2.21	120.33	116.11
5	U	505	NAG	C4-C3-C2	2.31	114.83	111.23
4	U	503	MAN	C2-C3-C4	2.33	114.99	111.04
4	U	502	NAG	C8-C7-N2	2.45	120.80	116.11
4	U	502	NAG	O5-C5-C6	2.52	112.81	107.35
5	U	504	NAG	C3-C2-N2	2.55	116.67	110.56
4	U	502	NAG	C4-C3-C2	2.60	115.27	111.23
5	U	505	NAG	O6-C6-C5	2.65	120.08	111.33
4	U	503	MAN	C3-C4-C5	3.36	116.06	110.20
5	U	504	NAG	O3-C3-C2	3.68	116.40	109.11
5	U	504	NAG	C3-C4-C5	3.80	116.81	110.20
5	U	504	NAG	C1-O5-C5	3.96	117.28	112.25
5	U	504	NAG	O5-C5-C6	4.96	118.09	107.35
4	U	503	MAN	C1-C2-C3	5.31	115.82	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	502	NAG	11	0
4	U	503	MAN	3	0
5	U	504	NAG	5	0
5	U	506	NAG	21	0
5	U	507	NAG	15	0

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	$\#\|Z\|>2$
3	NAG	U	501	1,4	14,14,15	2.12	6 (42%)	15,19,21	2.76	6 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	U	501	1,4	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	501	NAG	C3-C2	-3.20	1.44	1.52
3	U	501	NAG	C1-C2	-2.74	1.48	1.52
3	U	501	NAG	C4-C3	-2.05	1.47	1.52
3	U	501	NAG	O3-C3	2.23	1.48	1.43
3	U	501	NAG	C2-N2	3.31	1.52	1.46
3	U	501	NAG	C7-N2	4.44	1.51	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	501	NAG	C2-N2-C7	-6.07	115.24	123.04
3	U	501	NAG	O7-C7-N2	-2.82	116.12	121.86
3	U	501	NAG	C3-C2-N2	2.23	115.90	110.56
3	U	501	NAG	C3-C4-C5	2.47	114.51	110.20
3	U	501	NAG	C8-C7-N2	4.01	123.78	116.11
3	U	501	NAG	C1-O5-C5	5.73	119.51	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	501	NAG	9	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	U	269/283 (95%)	0.06	4 (1%)	76	63	62, 98, 143, 204	0
2	A	123/132 (93%)	0.04	1 (0%)	87	80	69, 97, 144, 183	0
All	All	392/415 (94%)	0.06	5 (1%)	79	67	62, 97, 146, 204	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	134	GLU	4.1
1	U	132	GLU	3.0
1	U	133	GLY	2.2
2	A	52	GLU	2.1
1	U	73	LEU	2.0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	U	507	14/15	0.68	0.40	-	20,20,20,20	0
4	MAN	U	503	11/12	0.76	0.26	-	183,210,233,236	0
5	NAG	U	506	14/15	0.76	0.40	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	U	505	14/15	0.91	0.27	-	130,155,179,187	0
4	NAG	U	502	14/15	0.82	0.16	-	191,203,223,232	0
5	NAG	U	504	14/15	0.86	0.20	-	128,155,179,187	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, 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
3	NAG	U	501	14/15	0.81	0.23	0.19	143,163,198,216	0

6.5 Other polymers (i)

There are no such residues in this entry.