



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:41 AM GMT

PDB ID : 3BT2  
Title : Structure of urokinase receptor, urokinase and vitronectin complex  
Authors : Huang, M.  
Deposited on : 2007-12-27  
Resolution : 2.50 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](mailto: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.

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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

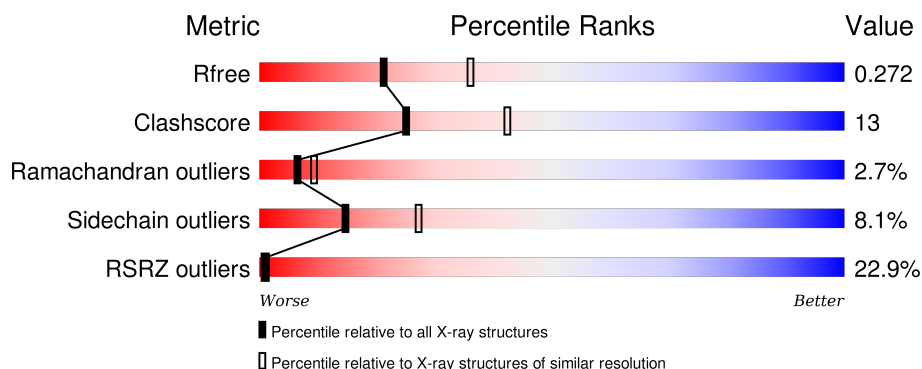
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 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	<div> <div>36%</div> <div>65%</div> <div>23%</div> <div>•</div> <div>8%</div> </div>
2	B	40	<div> <div>98%</div> <div>70%</div> <div>25%</div> <div>5%</div> </div>
3	L	212	<div> <div>7%</div> <div>77%</div> <div>19%</div> <div>•</div> </div>
4	H	214	<div> <div>8%</div> <div>86%</div> <div>11%</div> <div>••</div> </div>
5	U	283	<div> <div>26%</div> <div>64%</div> <div>21%</div> <div>6%</div> <div>8%</div> </div>

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
7	NAG	U	1200	-	-	X	-
7	NAG	U	1201	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6654 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	124	Total	C	N	O	S	0	0	0
			980	603	186	177	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 anti-uPAR antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1628	1020	268	333	7			

- Molecule 4 is a protein called anti-uPAR antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	212	Total	C	N	O	S	0	0	0
			1617	1035	262	314	6			

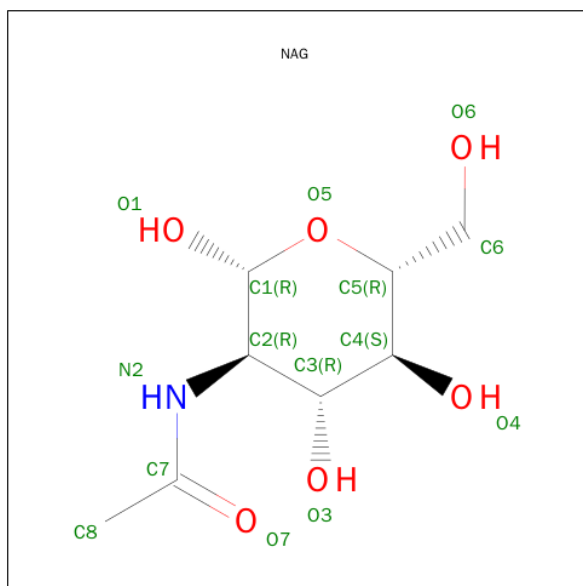
- Molecule 5 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	U	259	Total	C	N	O	S	0	0	0
			1990	1192	366	398	34			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	O	0	0
			4	4		
8	H	26	Total	O	0	0
			26	26		

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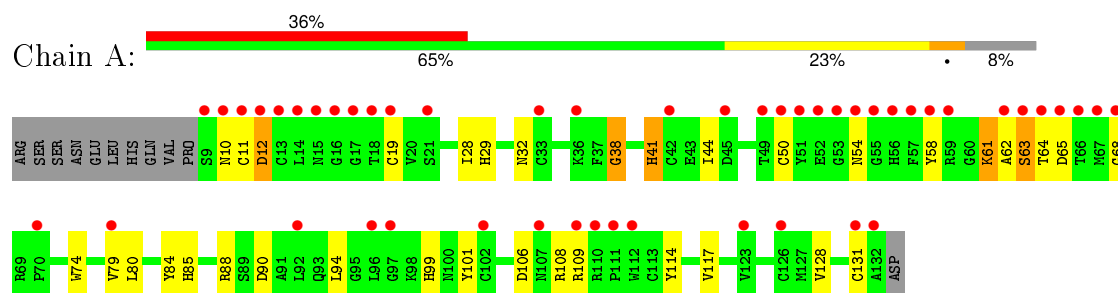
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	20	Total	O	0	0
			20	20		
8	U	7	Total	O	0	0
			7	7		

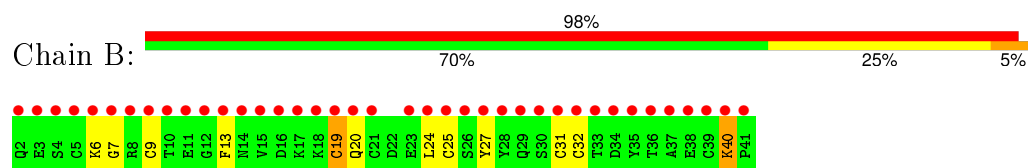
### 3 Residue-property plots

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.

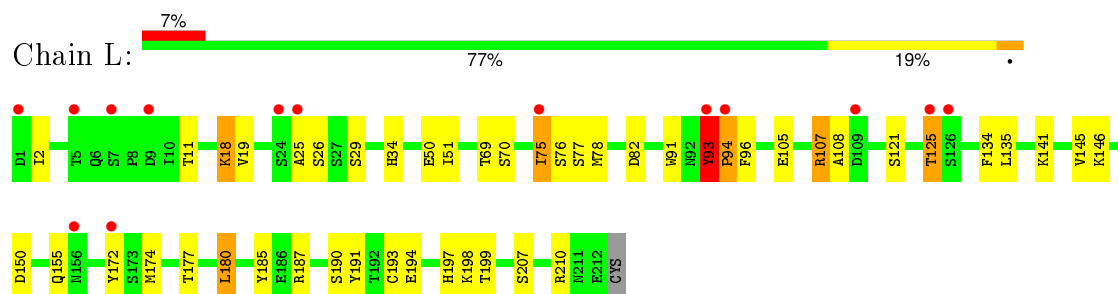
- Molecule 1: Urokinase-type plasminogen activator



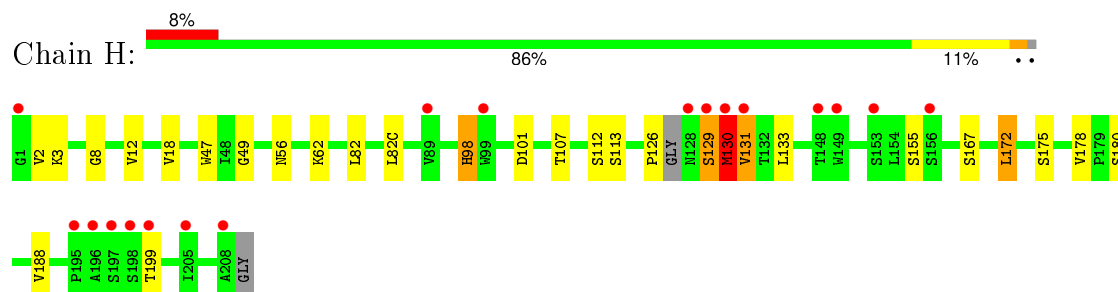
- Molecule 2: Vitronectin



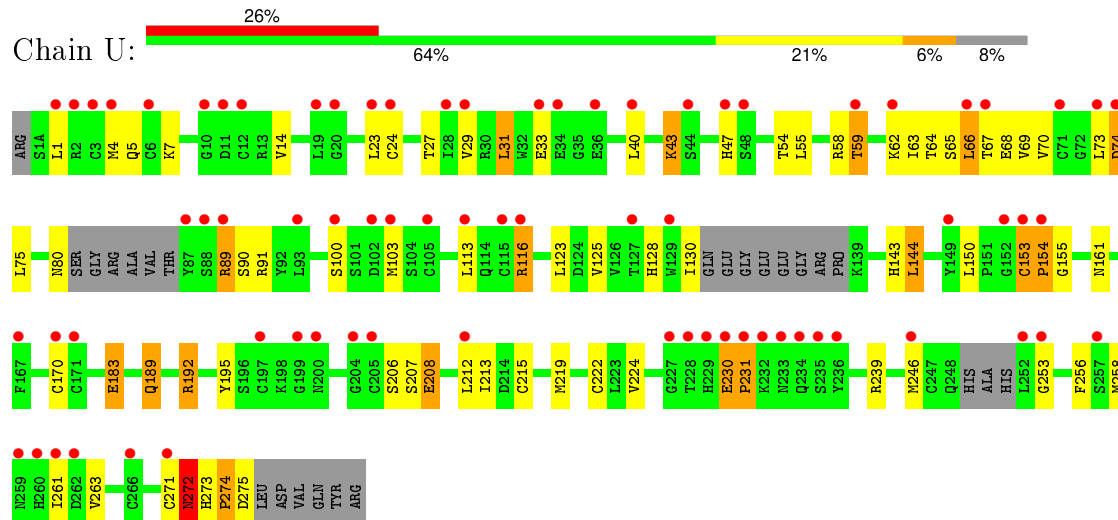
- Molecule 3: anti-uPAR antibody, light chain



- Molecule 4: anti-uPAR antibody, heavy chain



● Molecule 5: Urokinase plasminogen activator surface receptor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.10 Å 87.20 Å 124.27 Å 90.00° 94.31° 90.00°	Depositor
Resolution (Å)	42.88 – 2.50 42.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.88-2.50) 99.2 (42.88-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.229 , 0.272 0.232 , 0.272	Depositor DCC
$R_{free}$ test set	1191 reflections (3.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 64.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38222 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6654	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

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	0.77	2/1007 (0.2%)	0.77	3/1361 (0.2%)
2	B	0.41	0/316	0.68	1/421 (0.2%)
3	L	0.92	1/1668 (0.1%)	0.96	5/2267 (0.2%)
4	H	0.93	0/1667	0.82	2/2282 (0.1%)
5	U	0.90	6/2019 (0.3%)	0.86	4/2715 (0.1%)
All	All	0.88	9/6677 (0.1%)	0.86	15/9046 (0.2%)

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	A	0	1
2	B	1	0
4	H	0	1
5	U	0	1
All	All	1	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	183	GLU	CB-CG	13.87	1.78	1.52
5	U	7	LYS	C-O	10.18	1.42	1.23
1	A	38	GLY	C-O	8.25	1.36	1.23
3	L	193	CYS	CB-SG	-7.85	1.68	1.82
5	U	183	GLU	CD-OE2	6.97	1.33	1.25
5	U	183	GLU	CG-CD	5.88	1.60	1.51
5	U	7	LYS	C-N	5.69	1.47	1.34
5	U	43	LYS	C-O	5.39	1.33	1.23
1	A	41	HIS	CE1-NE2	5.06	1.44	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	192	ARG	NE-CZ-NH2	-10.53	115.04	120.30
3	L	187	ARG	NE-CZ-NH2	-9.25	115.67	120.30
3	L	93	TYR	CB-CG-CD1	-7.71	116.37	121.00
3	L	187	ARG	NE-CZ-NH1	6.95	123.77	120.30
3	L	93	TYR	CB-CG-CD2	6.73	125.04	121.00
5	U	192	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	88	ARG	NE-CZ-NH1	6.55	123.58	120.30
2	B	40	LYS	N-CA-C	6.41	128.30	111.00
4	H	101	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	12	ASP	CB-CG-OD1	-5.47	113.38	118.30
5	U	183	GLU	CG-CD-OE2	5.34	128.99	118.30
3	L	180	LEU	CA-CB-CG	5.28	127.44	115.30
4	H	101	ASP	CB-CG-OD1	5.02	122.82	118.30
5	U	272	ASN	N-CA-C	5.01	124.54	111.00
1	A	12	ASP	CB-CG-OD2	5.01	122.81	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	40	LYS	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	LYS	Peptide
4	H	130	MET	Peptide
5	U	271	CYS	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	980	0	911	28	0
2	B	312	0	272	5	0
3	L	1628	0	1554	32	0
4	H	1617	0	1558	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	U	1990	0	1856	74	0
6	U	14	0	13	0	0
7	U	56	0	50	12	0
8	A	4	0	0	0	0
8	H	26	0	0	0	0
8	L	20	0	0	1	0
8	U	7	0	0	0	0
All	All	6654	0	6214	162	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 13.

All (162) 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:183:GLU:CB	5:U:183:GLU:CG	1.78	1.57
7:U:1200:NAG:C3	7:U:1201:NAG:H82	1.85	1.07
5:U:128:HIS:NE2	5:U:183:GLU:OE2	1.92	1.02
5:U:116:ARG:CZ	5:U:116:ARG:HB2	1.86	1.02
4:H:131:VAL:CG1	4:H:178:VAL:O	2.12	0.98
5:U:143:HIS:NE2	5:U:183:GLU:OE2	1.96	0.98
3:L:93:TYR:O	3:L:96:PHE:CD2	2.19	0.96
3:L:105:GLU:OE1	3:L:172:TYR:OH	1.83	0.96
7:U:1200:NAG:H3	7:U:1201:NAG:H82	1.42	0.94
5:U:273:HIS:O	5:U:275:ASP:N	1.99	0.94
3:L:93:TYR:O	3:L:96:PHE:N	2.01	0.93
7:U:1200:NAG:H3	7:U:1201:NAG:C8	2.00	0.92
1:A:12:ASP:OD2	1:A:41:HIS:NE2	2.03	0.91
5:U:23:LEU:HD13	5:U:70:VAL:HG11	1.51	0.91
5:U:128:HIS:HE2	5:U:183:GLU:CD	1.73	0.90
5:U:4:MET:CE	5:U:75:LEU:HD22	2.04	0.88
3:L:93:TYR:HA	3:L:96:PHE:CZ	2.15	0.81
7:U:1200:NAG:O3	7:U:1201:NAG:C7	2.28	0.81
4:H:130:MET:O	4:H:130:MET:SD	2.40	0.79
3:L:25:ALA:O	3:L:69:THR:OG1	2.00	0.79
5:U:59:THR:CG2	5:U:59:THR:O	2.31	0.79
1:A:58:TYR:OH	1:A:61:LYS:O	2.01	0.79
3:L:93:TYR:O	3:L:94:PRO:C	2.17	0.78
4:H:131:VAL:HG13	4:H:178:VAL:O	1.84	0.77
3:L:50:GLU:OE2	4:H:98:HIS:ND1	2.19	0.76
4:H:130:MET:O	4:H:131:VAL:HG12	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:128:HIS:NE2	5:U:183:GLU:CD	2.38	0.75
1:A:117:VAL:O	1:A:117:VAL:HG23	1.87	0.74
1:A:12:ASP:OD2	1:A:29:HIS:NE2	2.13	0.73
3:L:75:ILE:HD11	3:L:78:MET:HA	1.70	0.73
5:U:23:LEU:HD22	5:U:70:VAL:CG1	2.18	0.73
7:U:1200:NAG:C3	7:U:1201:NAG:C8	2.62	0.73
5:U:23:LEU:HD22	5:U:70:VAL:HG12	1.71	0.72
5:U:4:MET:HE3	5:U:75:LEU:HD22	1.71	0.72
7:U:1200:NAG:H3	7:U:1201:NAG:N2	2.04	0.72
5:U:273:HIS:C	5:U:275:ASP:H	1.93	0.72
5:U:153:CYS:O	5:U:155:GLY:N	2.21	0.72
5:U:73:LEU:O	5:U:74:ASP:HB2	1.89	0.71
5:U:4:MET:HE2	5:U:75:LEU:HD22	1.72	0.70
7:U:1200:NAG:O3	7:U:1201:NAG:H82	1.91	0.70
5:U:128:HIS:NE2	5:U:183:GLU:OE1	2.25	0.70
5:U:189:GLN:H	5:U:189:GLN:HE21	1.40	0.69
1:A:12:ASP:CG	1:A:41:HIS:HE2	1.96	0.68
1:A:12:ASP:CG	1:A:29:HIS:HE2	1.95	0.68
7:U:1200:NAG:O3	7:U:1201:NAG:C8	2.42	0.68
4:H:130:MET:C	4:H:131:VAL:HG12	2.15	0.67
3:L:105:GLU:CD	3:L:172:TYR:OH	2.33	0.67
1:A:12:ASP:CG	1:A:41:HIS:NE2	2.49	0.66
1:A:80:LEU:HD23	1:A:85:HIS:HB2	1.77	0.66
3:L:93:TYR:O	3:L:96:PHE:CG	2.49	0.66
5:U:222:CYS:HB3	5:U:272:ASN:HB2	1.78	0.64
7:U:1200:NAG:H3	7:U:1201:NAG:C7	2.26	0.64
4:H:131:VAL:O	4:H:131:VAL:HG13	1.97	0.64
5:U:59:THR:HG22	5:U:62:LYS:HB3	1.79	0.64
5:U:153:CYS:O	5:U:154:PRO:C	2.35	0.64
5:U:230:GLU:HB3	5:U:231:PRO:HD2	1.79	0.63
5:U:59:THR:HG23	5:U:59:THR:O	1.99	0.62
7:U:1200:NAG:C3	7:U:1201:NAG:N2	2.63	0.62
5:U:256:PHE:HB2	5:U:258:MET:HE3	1.82	0.61
1:A:74:TRP:HA	1:A:79:VAL:HG11	1.83	0.60
1:A:61:LYS:HG2	1:A:62:ALA:N	2.16	0.60
4:H:56:ASN:OD1	5:U:192:ARG:NH2	2.31	0.60
7:U:1200:NAG:C3	7:U:1201:NAG:C7	2.79	0.60
5:U:23:LEU:HD13	5:U:70:VAL:CG1	2.30	0.59
3:L:75:ILE:CD1	3:L:82:ASP:OD2	2.51	0.58
3:L:107:ARG:HG2	3:L:108:ALA:N	2.18	0.58
5:U:116:ARG:NH1	5:U:116:ARG:HB2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:18:LYS:HD3	3:L:76:SER:HA	1.84	0.58
5:U:116:ARG:CZ	5:U:116:ARG:CB	2.72	0.58
5:U:73:LEU:O	5:U:74:ASP:CB	2.52	0.57
1:A:54:ASN:ND2	1:A:108:ARG:O	2.38	0.57
1:A:28:ILE:HD13	5:U:29:VAL:HG23	1.86	0.57
5:U:153:CYS:O	5:U:170:CYS:HB3	2.04	0.57
2:B:24:LEU:HD11	5:U:58:ARG:HH21	1.70	0.56
3:L:93:TYR:O	3:L:96:PHE:CE2	2.59	0.56
5:U:59:THR:HG22	5:U:59:THR:O	2.05	0.56
1:A:61:LYS:CG	1:A:62:ALA:N	2.69	0.55
2:B:27:TYR:CZ	5:U:63:ILE:HG21	2.42	0.55
5:U:4:MET:HE1	5:U:14:VAL:HA	1.89	0.54
1:A:61:LYS:HG2	1:A:62:ALA:H	1.73	0.54
5:U:89:ARG:HD2	5:U:90:SER:H	1.72	0.54
2:B:24:LEU:HD11	5:U:58:ARG:NH2	2.23	0.53
4:H:126:PRO:HD3	4:H:133:LEU:HD23	1.90	0.53
4:H:131:VAL:HG12	4:H:178:VAL:O	2.05	0.53
5:U:4:MET:CE	5:U:4:MET:HA	2.39	0.53
3:L:177:THR:HG22	8:L:230:HOH:O	2.08	0.53
5:U:195:TYR:O	5:U:272:ASN:ND2	2.43	0.52
3:L:150:ASP:HA	3:L:190:SER:HB3	1.91	0.52
4:H:82:LEU:HB3	4:H:82(C):LEU:HD21	1.92	0.51
1:A:90:ASP:OD2	1:A:94:LEU:HD22	2.10	0.51
5:U:161:ASN:HA	5:U:213:ILE:CD1	2.40	0.51
1:A:117:VAL:O	1:A:117:VAL:CG2	2.57	0.51
5:U:55:LEU:HD13	5:U:123:LEU:HD13	1.93	0.51
3:L:107:ARG:HG2	3:L:108:ALA:H	1.76	0.51
2:B:13:PHE:CE1	5:U:91:ARG:HD2	2.45	0.51
1:A:79:VAL:HG22	1:A:114:TYR:CD2	2.46	0.50
4:H:47:TRP:CZ2	4:H:49:GLY:HA2	2.46	0.50
5:U:273:HIS:C	5:U:275:ASP:N	2.59	0.50
1:A:12:ASP:OD1	1:A:12:ASP:N	2.41	0.50
5:U:29:VAL:HG12	5:U:31:LEU:HD13	1.94	0.50
1:A:28:ILE:HD13	5:U:29:VAL:CG2	2.42	0.49
3:L:135:LEU:HD12	3:L:135:LEU:N	2.27	0.49
4:H:18:VAL:HG12	4:H:82(C):LEU:HD11	1.94	0.49
5:U:31:LEU:CD1	5:U:64:THR:HG23	2.43	0.49
5:U:128:HIS:CD2	5:U:183:GLU:OE1	2.66	0.49
3:L:134:PHE:CE2	4:H:175:SER:HB3	2.48	0.49
5:U:23:LEU:HB3	5:U:70:VAL:HG13	1.95	0.48
5:U:5:GLN:HA	5:U:43:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:O	1:A:62:ALA:HB3	2.14	0.48
3:L:93:TYR:CG	3:L:94:PRO:N	2.81	0.48
3:L:93:TYR:HA	3:L:96:PHE:CE2	2.48	0.48
5:U:143:HIS:HE2	5:U:183:GLU:CD	2.09	0.47
1:A:61:LYS:HD2	1:A:63:SER:OG	2.14	0.47
5:U:4:MET:HE2	5:U:4:MET:N	2.28	0.47
1:A:38:GLY:O	1:A:44:ILE:HB	2.15	0.47
7:U:1200:NAG:C2	7:U:1201:NAG:H82	2.45	0.47
5:U:66:LEU:CD2	5:U:66:LEU:N	2.78	0.47
5:U:4:MET:CE	5:U:14:VAL:HG22	2.46	0.46
5:U:55:LEU:HD12	5:U:123:LEU:HD12	1.97	0.46
5:U:103:MET:HE2	5:U:103:MET:HA	1.96	0.46
3:L:185:TYR:CZ	3:L:210:ARG:HG3	2.50	0.46
1:A:12:ASP:CG	1:A:41:HIS:CD2	2.89	0.46
4:H:133:LEU:CD1	4:H:188:VAL:HG11	2.46	0.46
5:U:206:SER:OG	5:U:208:GLU:OE1	2.33	0.46
5:U:274:PRO:O	5:U:275:ASP:O	2.34	0.46
3:L:197:HIS:HD2	3:L:199:THR:OG1	1.99	0.45
3:L:141:LYS:HD2	3:L:172:TYR:CE1	2.51	0.45
5:U:150:LEU:O	5:U:153:CYS:HB2	2.16	0.45
4:H:8:GLY:O	4:H:107:THR:HG23	2.16	0.45
4:H:172:LEU:C	4:H:172:LEU:HD23	2.37	0.45
1:A:99:HIS:HD2	1:A:101:TYR:H	1.65	0.45
3:L:93:TYR:C	3:L:96:PHE:N	2.70	0.45
4:H:130:MET:O	4:H:131:VAL:CG1	2.62	0.44
5:U:261:ILE:HG23	5:U:261:ILE:O	2.18	0.44
5:U:222:CYS:HB3	5:U:272:ASN:CB	2.47	0.44
5:U:54:THR:HG23	5:U:66:LEU:O	2.18	0.44
4:H:130:MET:HA	4:H:180:SER:HB3	2.00	0.44
3:L:19:VAL:HB	3:L:75:ILE:HG23	2.00	0.44
1:A:61:LYS:CD	1:A:63:SER:OG	2.65	0.44
5:U:125:VAL:HG13	5:U:144:LEU:HB2	2.00	0.43
5:U:31:LEU:HD12	5:U:64:THR:HG23	2.01	0.43
5:U:215:CYS:HB3	5:U:219:MET:O	2.18	0.43
1:A:61:LYS:O	1:A:62:ALA:CB	2.66	0.43
5:U:116:ARG:NH1	5:U:116:ARG:CB	2.82	0.43
5:U:55:LEU:HD21	5:U:144:LEU:HD23	2.00	0.43
5:U:224:VAL:HG22	5:U:239:ARG:HG2	2.00	0.43
5:U:263:VAL:O	5:U:263:VAL:HG23	2.19	0.43
3:L:146:LYS:HB3	3:L:194:GLU:HB2	2.02	0.42
1:A:12:ASP:CG	1:A:29:HIS:NE2	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:CYS:C	2:B:31:CYS:SG	2.97	0.42
5:U:24:CYS:O	5:U:70:VAL:HA	2.20	0.42
3:L:75:ILE:CD1	3:L:78:MET:HA	2.44	0.42
5:U:89:ARG:NH1	5:U:116:ARG:O	2.52	0.42
5:U:27:THR:OG1	5:U:68:GLU:OE1	2.36	0.42
3:L:191:TYR:O	3:L:207:SER:HA	2.19	0.42
3:L:145:VAL:HG12	3:L:174:MET:HE1	2.03	0.41
3:L:34:HIS:HD2	3:L:50:GLU:H	1.67	0.41
4:H:133:LEU:HD12	4:H:188:VAL:HG11	2.03	0.41
3:L:121:SER:O	3:L:125:THR:HG23	2.20	0.41
5:U:274:PRO:C	5:U:275:ASP:O	2.57	0.40
5:U:23:LEU:HD12	5:U:47:HIS:O	2.20	0.40
1:A:84:TYR:OH	1:A:106:ASP:HB3	2.21	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	122/135 (90%)	104 (85%)	15 (12%)	3 (2%)	7	10
2	B	38/40 (95%)	28 (74%)	6 (16%)	4 (10%)	1	0
3	L	209/212 (99%)	195 (93%)	9 (4%)	5 (2%)	7	11
4	H	208/214 (97%)	200 (96%)	5 (2%)	3 (1%)	14	24
5	U	251/283 (89%)	229 (91%)	15 (6%)	7 (3%)	6	9
All	All	828/884 (94%)	756 (91%)	50 (6%)	22 (3%)	6	9

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ASN

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Mol	Chain	Res	Type
2	B	40	LYS
3	L	2	ILE
3	L	93	TYR
4	H	129	SER
5	U	74	ASP
5	U	272	ASN
5	U	274	PRO
1	A	68	GLY
2	B	6	LYS
2	B	7	GLY
2	B	19	CYS
3	L	26	SER
3	L	94	PRO
4	H	130	MET
5	U	231	PRO
5	U	253	GLY
4	H	131	VAL
1	A	128	VAL
3	L	51	ILE
5	U	154	PRO
5	U	230	GLU

### 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	108/119 (91%)	99 (92%)	9 (8%)	14	26
2	B	37/37 (100%)	33 (89%)	4 (11%)	8	15
3	L	185/186 (100%)	173 (94%)	12 (6%)	21	39
4	H	182/182 (100%)	169 (93%)	13 (7%)	18	34
5	U	232/251 (92%)	210 (90%)	22 (10%)	11	20
All	All	744/775 (96%)	684 (92%)	60 (8%)	15	27

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

Mol	Chain	Res	Type
1	A	11	CYS
1	A	19	CYS
1	A	32	ASN
1	A	50	CYS
1	A	63	SER
1	A	64	THR
1	A	65	ASP
1	A	109	ARG
1	A	131	CYS
2	B	9	CYS
2	B	19	CYS
2	B	20	GLN
2	B	32	CYS
3	L	11	THR
3	L	18	LYS
3	L	29	SER
3	L	70	SER
3	L	75	ILE
3	L	77	SER
3	L	91	TRP
3	L	107	ARG
3	L	125	THR
3	L	155	GLN
3	L	180	LEU
3	L	198	LYS
4	H	2	VAL
4	H	3	LYS
4	H	12	VAL
4	H	62	LYS
4	H	98	HIS
4	H	112	SER
4	H	113	SER
4	H	129	SER
4	H	130	MET
4	H	155	SER
4	H	167	SER
4	H	172	LEU
4	H	199	THR
5	U	1	LEU
5	U	31	LEU
5	U	33	GLU
5	U	40	LEU
5	U	59	THR

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Mol	Chain	Res	Type
5	U	65	SER
5	U	66	LEU
5	U	67	THR
5	U	69	VAL
5	U	80	ASN
5	U	89	ARG
5	U	100	SER
5	U	113	LEU
5	U	116	ARG
5	U	130	ILE
5	U	144	LEU
5	U	153	CYS
5	U	189	GLN
5	U	207	SER
5	U	208	GLU
5	U	212	LEU
5	U	246	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	40	GLN
1	A	85	HIS
1	A	99	HIS
3	L	34	HIS
3	L	37	GLN
3	L	137	ASN
3	L	197	HIS
4	H	52(A)	HIS
4	H	159	HIS
5	U	47	HIS
5	U	160	HIS
5	U	162	ASN
5	U	166	HIS
5	U	189	GLN
5	U	203	HIS
5	U	229	HIS
5	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 ⓘ

4 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$
7	NAG	U	1172	5,7	14,14,15	0.63	0	15,19,21	0.92	1 (6%)
7	NAG	U	1173	7	14,14,15	0.45	0	15,19,21	1.78	4 (26%)
7	NAG	U	1200	5,7	14,14,15	0.54	0	15,19,21	3.16	7 (46%)
7	NAG	U	1201	7	14,14,15	0.54	0	15,19,21	3.16	7 (46%)

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
7	NAG	U	1172	5,7	-	0/6/23/26	0/1/1/1
7	NAG	U	1173	7	-	0/6/23/26	0/1/1/1
7	NAG	U	1200	5,7	-	0/6/23/26	0/1/1/1
7	NAG	U	1201	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	1200	NAG	C4-C3-C2	-6.35	101.36	111.23
7	U	1201	NAG	C4-C3-C2	-6.34	101.38	111.23
7	U	1173	NAG	C4-C3-C2	-3.83	105.27	111.23
7	U	1200	NAG	C3-C4-C5	-3.37	104.31	110.20
7	U	1201	NAG	C3-C4-C5	-3.37	104.33	110.20
7	U	1173	NAG	O7-C7-C8	-2.21	118.01	122.06
7	U	1173	NAG	C8-C7-N2	2.16	120.23	116.11
7	U	1172	NAG	O3-C3-C4	2.27	115.45	110.34
7	U	1200	NAG	O3-C3-C4	2.75	116.52	110.34
7	U	1201	NAG	O3-C3-C4	2.75	116.53	110.34
7	U	1200	NAG	O5-C5-C6	2.80	113.42	107.35
7	U	1201	NAG	O5-C5-C6	2.81	113.43	107.35
7	U	1201	NAG	O4-C4-C3	3.05	117.22	110.34
7	U	1200	NAG	O4-C4-C3	3.07	117.26	110.34
7	U	1173	NAG	C1-O5-C5	3.47	116.65	112.25
7	U	1200	NAG	O4-C4-C5	4.31	120.65	109.24
7	U	1201	NAG	O4-C4-C5	4.32	120.69	109.24
7	U	1201	NAG	C1-O5-C5	6.93	121.05	112.25
7	U	1200	NAG	C1-O5-C5	6.94	121.05	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	1200	NAG	12	0
7	U	1201	NAG	12	0

## 5.6 Ligand geometry

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
6	NAG	U	1052	5	14,14,15	0.52	0	15,19,21	1.32	1 (6%)

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
6	NAG	U	1052	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	1052	NAG	C1-O5-C5	4.10	117.45	112.25

There are no chirality outliers.

There are no torsion outliers.

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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	124/135 (91%)	2.23	49 (39%) 0 0	63, 74, 81, 83	0
2	B	40/40 (100%)	6.70	39 (97%) 0 0	84, 88, 89, 89	40 (100%)
3	L	211/212 (99%)	1.02	14 (6%) 22 24	51, 68, 80, 86	0
4	H	212/214 (99%)	1.07	18 (8%) 13 14	59, 70, 83, 88	0
5	U	259/283 (91%)	1.65	74 (28%) 1 0	57, 74, 91, 102	0
All	All	846/884 (95%)	1.67	194 (22%) 1 1	51, 72, 87, 102	40 (4%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	9	CYS	15.6
2	B	40	LYS	12.4
2	B	32	CYS	11.7
2	B	41	PRO	11.3
2	B	11	GLU	10.9
2	B	5	CYS	9.9
2	B	8	ARG	9.8
2	B	31	CYS	9.0
2	B	38	GLU	8.5
1	A	11	CYS	8.4
2	B	39	CYS	8.0
5	U	252	LEU	8.0
2	B	7	GLY	7.9
5	U	153	CYS	7.9
1	A	131	CYS	7.6
2	B	34	ASP	7.2
2	B	2	GLN	7.2
1	A	55	GLY	7.1
2	B	19	CYS	7.1
2	B	20	GLN	7.1

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Mol	Chain	Res	Type	RSRZ
5	U	87	TYR	6.9
1	A	9	SER	6.8
2	B	37	ALA	6.8
1	A	10	ASN	6.7
1	A	50	CYS	6.5
2	B	28	TYR	6.4
1	A	42	CYS	6.4
5	U	230	GLU	6.4
2	B	14	ASN	6.3
2	B	4	SER	6.3
2	B	33	THR	6.2
2	B	17	LYS	6.2
2	B	10	THR	6.1
2	B	27	TYR	6.0
2	B	35	TYR	5.9
2	B	15	VAL	5.7
5	U	88	SER	5.6
2	B	25	CYS	5.5
1	A	33	CYS	5.4
2	B	18	LYS	5.2
4	H	195	PRO	5.2
4	H	198	SER	5.2
1	A	54	ASN	5.2
2	B	6	LYS	5.2
2	B	21	CYS	5.1
5	U	152	GLY	5.1
4	H	130	MET	5.0
5	U	259	ASN	5.0
2	B	12	GLY	4.9
1	A	19	CYS	4.9
2	B	13	PHE	4.7
1	A	102	CYS	4.5
5	U	129	TRP	4.5
5	U	199	GLY	4.5
4	H	128	ASN	4.5
1	A	12	ASP	4.5
2	B	30	SER	4.5
2	B	26	SER	4.4
1	A	13	CYS	4.4
1	A	65	ASP	4.4
2	B	24	LEU	4.4
5	U	233	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
5	U	12	CYS	4.3
1	A	16	GLY	4.2
1	A	53	GLY	4.2
4	H	131	VAL	4.2
3	L	172	TYR	4.2
1	A	96	LEU	4.2
3	L	24	SER	4.1
5	U	3	CYS	4.0
1	A	66	THR	4.0
5	U	24	CYS	4.0
2	B	16	ASP	3.9
1	A	107	ASN	3.9
5	U	47	HIS	3.9
5	U	204	GLY	3.8
4	H	129	SER	3.7
1	A	36	LYS	3.7
5	U	73	LEU	3.7
5	U	105	CYS	3.6
1	A	49	THR	3.6
4	H	199	THR	3.6
2	B	23	GLU	3.6
1	A	123	VAL	3.5
2	B	3	GLU	3.5
5	U	231	PRO	3.4
5	U	116	ARG	3.4
5	U	235	SER	3.4
3	L	93	TYR	3.4
1	A	109	ARG	3.4
3	L	25	ALA	3.3
1	A	15	ASN	3.3
2	B	29	GLN	3.3
5	U	93	LEU	3.3
5	U	253	GLY	3.2
4	H	1	GLY	3.2
3	L	109	ASP	3.1
5	U	260	HIS	3.1
3	L	9	ASP	3.0
1	A	64	THR	3.0
1	A	14	LEU	3.0
5	U	228	THR	3.0
1	A	58	TYR	3.0
1	A	17	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	L	5	THR	2.9
1	A	126	CYS	2.9
5	U	102	ASP	2.9
1	A	52	GLU	2.9
2	B	36	THR	2.8
5	U	34	GLU	2.8
1	A	111	PRO	2.8
1	A	51	TYR	2.8
1	A	62	ALA	2.8
5	U	261	ILE	2.8
5	U	262	ASP	2.8
5	U	11	ASP	2.7
1	A	56	HIS	2.7
1	A	110	ARG	2.7
5	U	257	SER	2.7
1	A	57	PHE	2.7
1	A	59	ARG	2.7
1	A	18	THR	2.7
5	U	59	THR	2.7
5	U	71	CYS	2.7
1	A	63	SER	2.6
4	H	156	SER	2.6
4	H	197	SER	2.6
5	U	115	CYS	2.6
4	H	208	ALA	2.6
5	U	89	ARG	2.6
5	U	229	HIS	2.6
5	U	48	SER	2.6
5	U	29	VAL	2.5
3	L	126	SER	2.5
5	U	6	CYS	2.5
5	U	171	CYS	2.5
5	U	234	GLN	2.5
5	U	62	LYS	2.5
5	U	154	PRO	2.5
5	U	271	CYS	2.5
5	U	36	GLU	2.5
5	U	67	THR	2.5
5	U	227	GLY	2.4
5	U	149	TYR	2.4
5	U	236	TYR	2.4
1	A	45	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
5	U	74	ASP	2.4
5	U	246	MET	2.4
1	A	132	ALA	2.4
5	U	127	THR	2.4
5	U	100	SER	2.4
1	A	67	MET	2.4
5	U	205	CYS	2.4
5	U	10	GLY	2.4
1	A	70	PRO	2.3
4	H	148	THR	2.3
3	L	156	ASN	2.3
1	A	68	GLY	2.3
3	L	94	PRO	2.3
5	U	33	GLU	2.3
5	U	28	ILE	2.3
1	A	92	LEU	2.3
4	H	149	TRP	2.3
4	H	89	VAL	2.3
5	U	4	MET	2.3
1	A	21	SER	2.3
4	H	196	ALA	2.2
5	U	23	LEU	2.2
1	A	112	TRP	2.2
3	L	1	ASP	2.2
5	U	44	SER	2.2
5	U	19	LEU	2.2
5	U	266	CYS	2.2
3	L	75	ILE	2.2
5	U	113	LEU	2.2
5	U	212	LEU	2.2
1	A	79	VAL	2.2
5	U	197	CYS	2.2
5	U	200	ASN	2.1
1	A	97	GLY	2.1
5	U	232	LYS	2.1
5	U	66	LEU	2.1
3	L	125	THR	2.1
4	H	153	SER	2.1
5	U	170	CYS	2.1
5	U	1	LEU	2.1
4	H	205	ILE	2.1
5	U	103	MET	2.0

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Mol	Chain	Res	Type	RSRZ
5	U	20	GLY	2.0
4	H	99	TRP	2.0
3	L	7	SER	2.0
5	U	2	ARG	2.0
5	U	40	LEU	2.0
5	U	167	PHE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	NAG	U	1172	14/15	0.90	0.31	-	65,70,72,74	0
7	NAG	U	1201	14/15	0.69	0.50	-	92,96,98,101	0
7	NAG	U	1173	14/15	0.84	0.44	-	74,77,79,80	0
7	NAG	U	1200	14/15	0.70	0.27	-	82,86,88,91	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	NAG	U	1052	14/15	0.65	0.39	-	83,85,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.