



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:33 AM GMT

PDB ID : 2FD6  
Title : Structure of Human Urokinase Plasminogen Activator in Complex with Urokinase Receptor and an anti-upar antibody at 1.9 Å  
Authors : Huang, M.; Huai, Q.; Li, Y.  
Deposited on : 2005-12-13  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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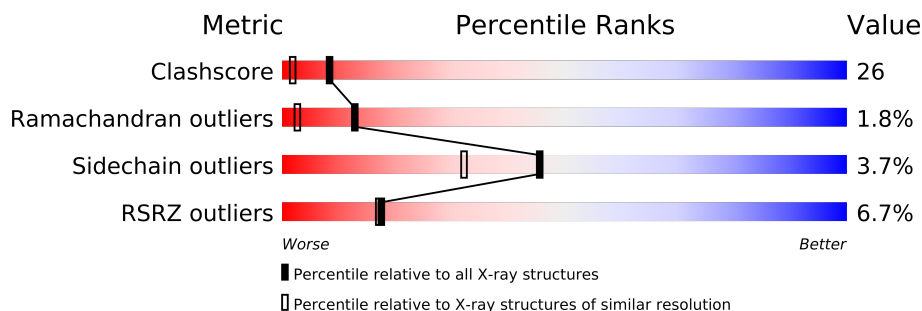
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 1.90 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))
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. 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	122	
2	L	214	
3	H	213	
4	U	276	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 6600 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	122	Total	C	N	O	S	0	0	0
			967	596	183	174	14			

- Molecule 2 is a protein called L chain of Fab of ATN-615 anti-uPAR antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1648	1032	272	337	7			

- Molecule 3 is a protein called H chain of Fab of ATN-615 anti-uPAR antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	212	Total	C	N	O	S	0	0	0
			1618	1035	262	315	6			

- Molecule 4 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	U	249	Total	C	N	O	S	0	0	0
			1906	1141	349	382	34			

There is a discrepancy between the modelled and reference sequences:

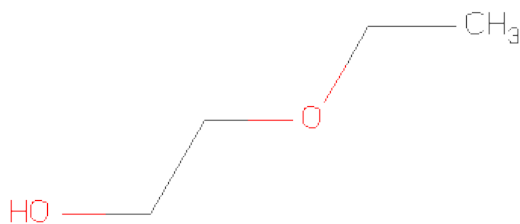
Chain	Residue	Modelled	Actual	Comment	Reference
U	1A	SER	-	CLONING ARTIFACT	UNP Q03405

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



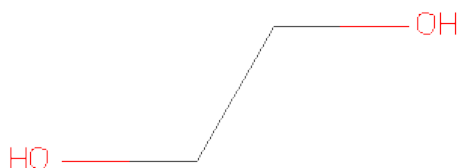
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



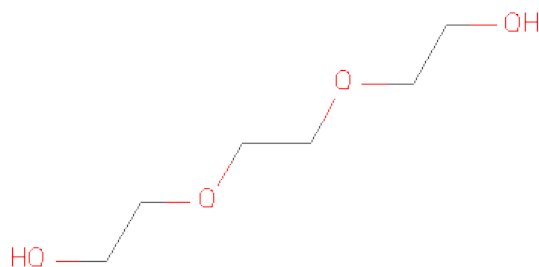
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			6	4	2		
6	L	1	Total	C	O	0	0
			6	4	2		
6	H	1	Total	C	O	0	0
			6	4	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	O	0	0
			10	6	4		

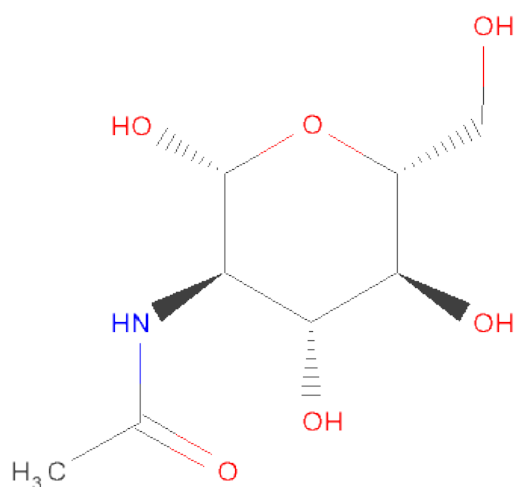
- Molecule 9 is a polymer of unknown type called SUGAR (N-ACETYL-D-GLUCOSAMINE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	U	2	Total	C	N	O	0	0
			26	14	1	11		

There is a discrepancy between the modelled and reference sequences:

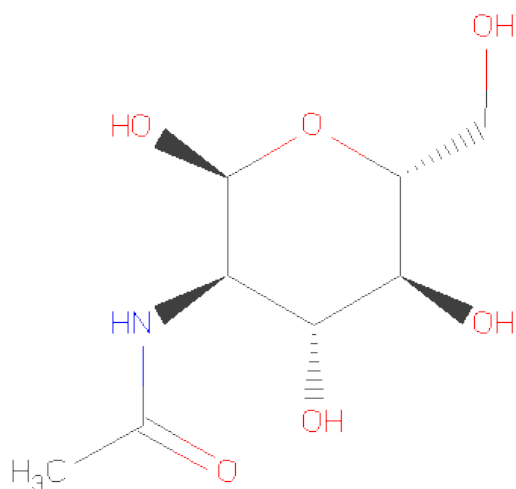
Chain	Residue	Modelled	Actual	Comment	Reference
U	1A	SER	-	CLONING ARTIFACT	UNP Q03405

- Molecule 10 is SUGAR (FUCOSE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



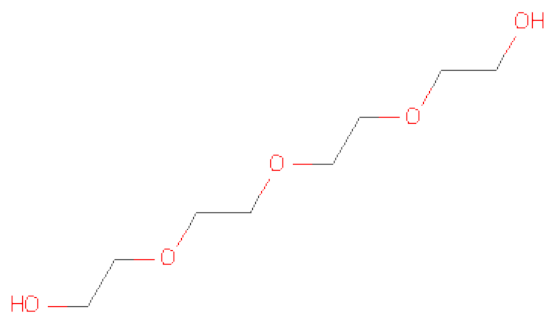
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	U	1	Total	C	N	O	0	0
			15	8	1	6		
10	U	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 11 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	U	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 12 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	U	1	Total	C	O	0	0
			13	8	5		

- Molecule 13 is water.

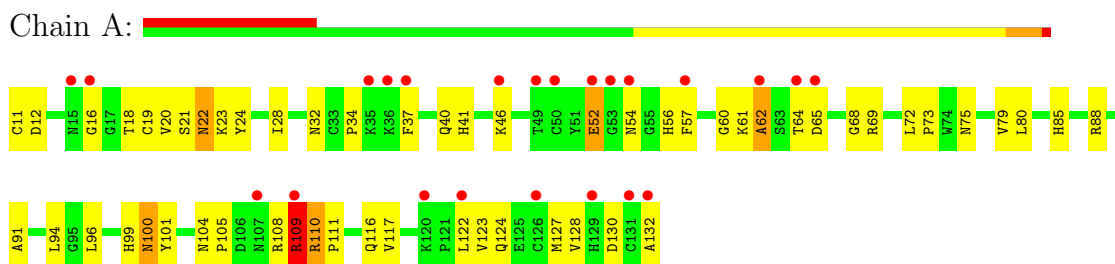
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	22	Total 22	O 22	0	0
13	L	121	Total 121	O 121	0	0
13	H	121	Total 121	O 121	0	0
13	U	72	Total 72	O 72	0	0



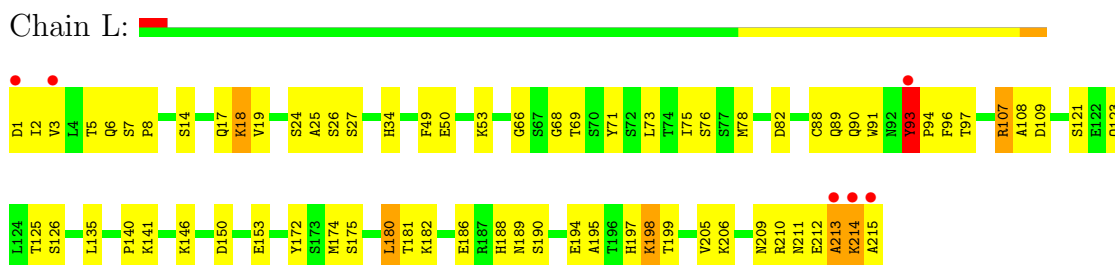
### 3 Residue-property plots

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

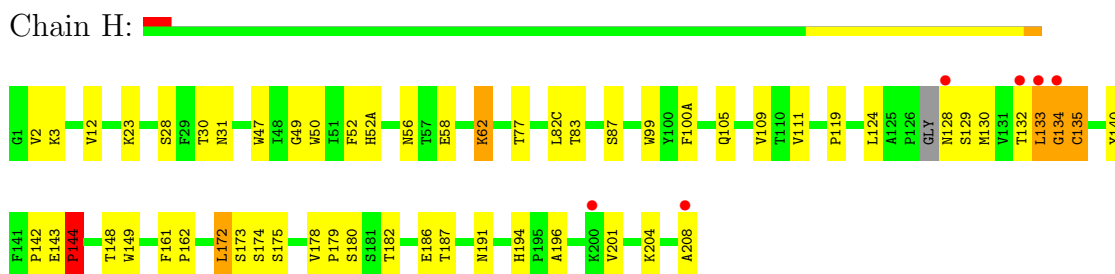
- Molecule 1: Urokinase-type plasminogen activator



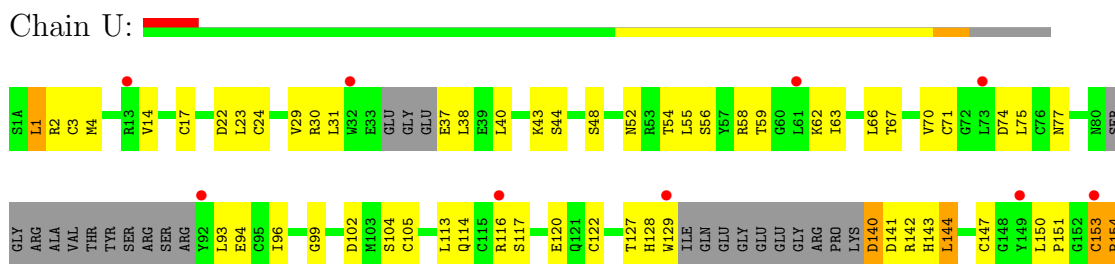
- Molecule 2: L chain of Fab of ATN-615 anti-uPAR antibody

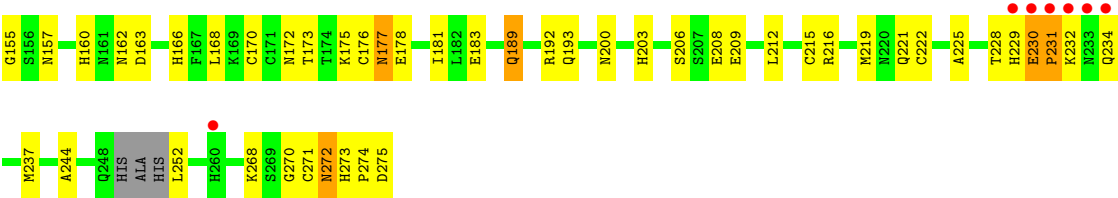


- Molecule 3: H chain of Fab of ATN-615 anti-uPAR antibody



- Molecule 4: 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, $\alpha$ , $\beta$ , $\gamma$	51.79Å 86.81Å 124.69Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	41.36 – 1.90 41.36 – 1.85	Depositor EDS
% Data completeness (in resolution range)	95.8 (41.36-1.90) 92.5 (41.36-1.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 1.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.276 0.246 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 86788 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: PGE, NAG, ETX, EDO, NDG, PG4, SO4, FUC

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	0.32	0/994	0.59	0/1342
2	L	0.40	0/1688	0.70	1/2292 (0.0%)
3	H	0.50	2/1668 (0.1%)	0.77	3/2282 (0.1%)
4	U	0.35	0/1933	0.66	0/2599
All	All	0.41	2/6283 (0.0%)	0.69	4/8515 (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
9	U	2	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	134	GLY	C-N	-8.55	1.14	1.34
3	H	134	GLY	N-CA	-5.83	1.37	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	134	GLY	CA-C-N	-7.82	100.00	117.20
3	H	133	LEU	C-N-CA	-7.25	107.08	122.30
3	H	134	GLY	O-C-N	6.50	133.11	122.70
2	L	93	TYR	N-CA-C	5.40	125.59	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	U	452	NAG	C1
9	U	453	FUC	C1

There are no planarity outliers.

## 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	967	0	902	61	0
2	L	1648	0	1577	70	0
3	H	1618	0	1557	62	0
4	U	1906	0	1773	124	0
5	A	5	0	0	0	0
6	H	6	0	10	3	0
6	L	12	0	20	8	0
7	H	4	0	6	0	0
7	L	4	0	6	0	0
8	H	10	0	14	1	0
9	U	26	0	24	6	0
10	U	30	0	27	9	0
11	U	15	0	15	2	0
12	U	13	0	18	11	0
13	A	22	0	0	2	0
13	H	121	0	0	3	0
13	L	121	0	0	5	0
13	U	72	0	0	14	0
All	All	6600	0	5949	319	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 (319) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:U:230:GLU:HB3	4:U:231:PRO:HD2	1.36	1.06
10:U:472:NAG:H61	10:U:473:NAG:H82	1.37	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:U:452:NAG:H83	13:U:530:HOH:O	1.57	1.02
4:U:221:GLN:HE21	12:U:402:PG4:H32	1.25	1.01
10:U:472:NAG:C6	10:U:473:NAG:H82	1.91	1.00
4:U:172:ASN:ND2	10:U:472:NAG:C7	2.25	0.99
3:H:134:GLY:O	3:H:149:TRP:HH2	1.45	0.98
4:U:244:ALA:HB2	12:U:402:PG4:H31	1.46	0.96
4:U:232:LYS:HB2	4:U:234:GLN:HE22	1.28	0.96
3:H:132:THR:O	3:H:133:LEU:HD23	1.67	0.94
4:U:172:ASN:ND2	10:U:472:NAG:O7	2.01	0.93
4:U:23:LEU:HD13	4:U:70:VAL:HG11	1.49	0.93
4:U:4:MET:HE3	4:U:75:LEU:HD22	1.52	0.92
4:U:189:GLN:HE21	4:U:189:GLN:H	1.07	0.92
4:U:52:ASN:ND2	9:U:452:NAG:O1	2.00	0.92
3:H:56:ASN:HD22	12:U:402:PG4:H11	1.33	0.92
3:H:134:GLY:O	3:H:149:TRP:CH2	2.22	0.92
1:A:99:HIS:HD2	1:A:101:TYR:H	1.21	0.88
4:U:99:GLY:H	4:U:104:SER:HB3	1.38	0.86
4:U:96:ILE:H	4:U:177:ASN:HD21	1.23	0.85
10:U:472:NAG:H61	10:U:473:NAG:C8	2.05	0.85
3:H:132:THR:O	3:H:133:LEU:CD2	2.25	0.84
3:H:128:ASN:O	3:H:180:SER:OG	1.95	0.84
4:U:94:GLU:OE2	4:U:175:LYS:HE2	1.78	0.83
4:U:232:LYS:HB2	4:U:234:GLN:NE2	1.95	0.81
1:A:110:ARG:HD3	1:A:111:PRO:HD2	1.62	0.81
1:A:54:ASN:ND2	1:A:56:HIS:HB2	1.96	0.81
3:H:23:LYS:HD2	6:H:403:ETX:H12	1.62	0.81
3:H:119:PRO:HB3	3:H:140:TYR:HB3	1.63	0.81
3:H:12:VAL:HG21	3:H:82(C):LEU:CD1	2.11	0.80
4:U:221:GLN:HE21	12:U:402:PG4:C3	1.96	0.78
2:L:25:ALA:O	2:L:69:THR:HG23	1.85	0.77
3:H:182:THR:O	3:H:186:GLU:HB2	1.85	0.76
2:L:107:ARG:HG2	2:L:108:ALA:N	2.00	0.75
2:L:19:VAL:HB	2:L:75:ILE:CG2	2.17	0.75
4:U:230:GLU:HB3	4:U:231:PRO:CD	2.14	0.74
2:L:3:VAL:H	2:L:26:SER:CB	2.00	0.74
4:U:229:HIS:CD2	4:U:230:GLU:H	2.06	0.74
1:A:22:ASN:HD22	1:A:24:TYR:H	1.36	0.74
1:A:23:LYS:NZ	4:U:166:HIS:HD2	1.86	0.74
1:A:99:HIS:CD2	1:A:101:TYR:H	2.06	0.73
4:U:153:CYS:O	4:U:170:CYS:HB3	1.87	0.73
4:U:4:MET:CE	4:U:75:LEU:HD22	2.18	0.73
2:L:194:GLU:HG3	2:L:205:VAL:HG22	1.69	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:56:ASN:HD22	12:U:402:PG4:C1	2.03	0.72
1:A:34:PRO:HG2	1:A:37:PHE:HD2	1.54	0.72
4:U:229:HIS:CG	4:U:230:GLU:H	2.07	0.72
4:U:59:THR:HG22	13:U:481:HOH:O	1.90	0.71
1:A:122:LEU:HD12	1:A:123:VAL:H	1.55	0.71
4:U:221:GLN:NE2	12:U:402:PG4:H32	2.03	0.71
4:U:206:SER:HB3	4:U:209:GLU:HG3	1.73	0.70
4:U:128:HIS:NE2	13:U:545:HOH:O	1.96	0.70
4:U:273:HIS:O	4:U:275:ASP:N	2.23	0.70
1:A:23:LYS:HZ1	4:U:166:HIS:HD2	1.40	0.69
4:U:52:ASN:HD22	9:U:452:NAG:C1	2.00	0.69
3:H:12:VAL:HG21	3:H:82(C):LEU:HD12	1.73	0.69
4:U:3:CYS:HB3	4:U:77:ASN:HD22	1.56	0.69
3:H:132:THR:HG22	3:H:133:LEU:H	1.58	0.68
12:U:402:PG4:H62	13:U:475:HOH:O	1.93	0.68
2:L:3:VAL:H	2:L:26:SER:HB3	1.59	0.67
1:A:54:ASN:HD22	1:A:56:HIS:HB2	1.58	0.67
3:H:130:MET:HE2	3:H:178:VAL:C	2.15	0.66
1:A:108:ARG:O	1:A:110:ARG:N	2.28	0.66
2:L:1:ASP:HA	6:L:401:ETX:H12	1.78	0.66
4:U:22:ASP:OD1	4:U:48:SER:HB3	1.96	0.66
3:H:132:THR:O	3:H:133:LEU:CG	2.43	0.66
4:U:189:GLN:HE21	4:U:189:GLN:N	1.88	0.64
4:U:30:ARG:C	4:U:31:LEU:HD12	2.17	0.64
4:U:183:GLU:OE1	13:U:545:HOH:O	2.15	0.64
1:A:65:ASP:OD1	1:A:124:GLN:HB3	1.97	0.64
4:U:31:LEU:HD12	4:U:31:LEU:N	2.13	0.64
4:U:52:ASN:ND2	9:U:452:NAG:C2	2.60	0.64
4:U:102:ASP:OD1	4:U:104:SER:HB2	1.97	0.64
4:U:117:SER:HB2	4:U:120:GLU:HG3	1.78	0.64
10:U:472:NAG:H62	10:U:473:NAG:H82	1.77	0.63
4:U:56:SER:HB2	13:U:544:HOH:O	1.99	0.63
2:L:2:ILE:H	6:L:401:ETX:H12	1.62	0.63
3:H:187:THR:HG23	3:H:204:LYS:HG3	1.79	0.63
1:A:60:GLY:O	1:A:101:TYR:HB3	1.98	0.63
1:A:52:GLU:OE2	1:A:57:PHE:HB2	1.99	0.62
3:H:124:LEU:HB2	3:H:134:GLY:H	1.61	0.62
2:L:107:ARG:HG2	2:L:108:ALA:H	1.63	0.62
4:U:58:ARG:HB2	13:U:532:HOH:O	1.98	0.62
3:H:132:THR:O	3:H:133:LEU:HG	1.99	0.62
9:U:452:NAG:C8	13:U:530:HOH:O	2.30	0.62
1:A:22:ASN:ND2	1:A:24:TYR:H	1.96	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:U:232:LYS:CB	4:U:234:GLN:HE22	2.10	0.62
3:H:56:ASN:ND2	12:U:402:PG4:H11	2.11	0.61
3:H:142:PRO:HD2	3:H:196:ALA:CB	2.30	0.61
2:L:2:ILE:HG13	6:L:401:ETX:H21	1.82	0.61
2:L:49:PHE:HD1	2:L:50:GLU:HG3	1.66	0.61
4:U:215:CYS:HB3	4:U:219:MET:O	2.01	0.61
1:A:108:ARG:C	1:A:110:ARG:H	2.04	0.60
2:L:34:HIS:HD2	2:L:50:GLU:H	1.49	0.60
2:L:213:ALA:O	2:L:214:LYS:HG2	2.01	0.60
4:U:160:HIS:HE1	4:U:216:ARG:H	1.50	0.60
2:L:188:HIS:O	2:L:210:ARG:NH1	2.34	0.60
4:U:29:VAL:HG12	4:U:31:LEU:HD11	1.84	0.60
1:A:46:LYS:HG2	1:A:46:LYS:O	2.01	0.59
2:L:94:PRO:HG2	6:L:401:ETX:H11	1.83	0.59
1:A:11:CYS:SG	1:A:19:CYS:HB2	2.42	0.59
2:L:94:PRO:HG2	6:L:401:ETX:C1	2.33	0.59
4:U:274:PRO:O	4:U:275:ASP:O	2.20	0.59
3:H:58:GLU:OE2	4:U:192:ARG:NH1	2.36	0.59
2:L:34:HIS:CD2	2:L:50:GLU:H	2.21	0.59
3:H:132:THR:HG22	3:H:133:LEU:N	2.18	0.58
4:U:160:HIS:HD2	13:U:495:HOH:O	1.86	0.57
2:L:75:ILE:CD1	2:L:78:MET:HA	2.34	0.56
4:U:4:MET:HE1	4:U:14:VAL:HG22	1.87	0.56
1:A:34:PRO:CG	1:A:37:PHE:HD2	2.17	0.56
2:L:121:SER:O	2:L:125:THR:HG23	2.05	0.56
1:A:100:ASN:H	1:A:100:ASN:HD22	1.53	0.56
4:U:172:ASN:OD1	10:U:472:NAG:O5	2.24	0.56
10:U:472:NAG:C6	10:U:473:NAG:C8	2.73	0.56
3:H:77:THR:OG1	6:H:403:ETX:H21	2.05	0.56
4:U:59:THR:HG23	4:U:59:THR:O	2.06	0.56
2:L:5:THR:OG1	2:L:24:SER:HB3	2.05	0.56
2:L:3:VAL:H	2:L:26:SER:HB2	1.70	0.56
3:H:134:GLY:CA	3:H:174:SER:O	2.53	0.56
4:U:54:THR:HG22	4:U:55:LEU:N	2.21	0.56
4:U:275:ASP:HA	13:U:536:HOH:O	2.05	0.56
3:H:134:GLY:HA2	3:H:174:SER:O	2.07	0.55
2:L:19:VAL:HB	2:L:75:ILE:HG22	1.89	0.55
1:A:18:THR:HB	1:A:32:ASN:HB2	1.88	0.55
2:L:107:ARG:NH1	2:L:108:ALA:O	2.39	0.55
4:U:143:HIS:NE2	13:U:545:HOH:O	1.87	0.55
3:H:130:MET:CE	3:H:179:PRO:N	2.70	0.55
3:H:52(A):HIS:HB3	12:U:402:PG4:H12	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:129:SER:O	3:H:179:PRO:HA	2.07	0.55
2:L:14:SER:O	2:L:17:GLN:HB3	2.06	0.55
4:U:140:ASP:N	13:U:502:HOH:O	2.39	0.55
4:U:1:LEU:HD22	4:U:2:ARG:N	2.21	0.55
1:A:122:LEU:HD12	1:A:123:VAL:N	2.23	0.54
4:U:129:TRP:O	4:U:163:ASP:O	2.24	0.54
3:H:142:PRO:HD2	3:H:196:ALA:HB1	1.90	0.54
4:U:153:CYS:O	4:U:155:GLY:N	2.40	0.54
4:U:105:CYS:HB3	4:U:181:ILE:HG21	1.89	0.54
1:A:94:LEU:HD23	1:A:105:PRO:HB3	1.88	0.54
2:L:69:THR:HG22	2:L:69:THR:O	2.07	0.54
2:L:93:TYR:HA	2:L:96:PHE:CZ	2.43	0.54
1:A:12:ASP:CG	13:A:523:HOH:O	2.46	0.53
2:L:109:ASP:OD2	2:L:198:LYS:HD2	2.09	0.53
1:A:104:ASN:HD21	1:A:108:ARG:H	1.54	0.53
4:U:62:LYS:HG2	4:U:63:ILE:N	2.24	0.53
2:L:93:TYR:O	2:L:96:PHE:CD2	2.62	0.53
2:L:180:LEU:HD23	2:L:180:LEU:N	2.23	0.53
3:H:56:ASN:OD1	4:U:192:ARG:NH2	2.41	0.52
4:U:268:LYS:O	4:U:271:CYS:SG	2.67	0.52
4:U:177:ASN:H	4:U:177:ASN:HD22	1.58	0.52
4:U:150:LEU:HB3	4:U:151:PRO:HD2	1.92	0.52
1:A:109:ARG:HG3	1:A:109:ARG:HH11	1.75	0.51
3:H:105:GLN:CD	3:H:105:GLN:H	2.13	0.51
4:U:200:ASN:ND2	11:U:400:NDG:C1	2.73	0.51
4:U:113:LEU:HD22	4:U:147:CYS:SG	2.50	0.51
4:U:173:THR:OG1	4:U:176:CYS:HB3	2.10	0.51
4:U:229:HIS:CG	4:U:230:GLU:N	2.76	0.51
1:A:99:HIS:HE1	13:A:503:HOH:O	1.93	0.51
4:U:43:LYS:HB3	4:U:77:ASN:OD1	2.11	0.51
1:A:61:LYS:O	1:A:62:ALA:HB2	2.11	0.51
1:A:108:ARG:HH12	1:A:123:VAL:HG21	1.75	0.51
2:L:146:LYS:HG3	2:L:153:GLU:OE2	2.11	0.51
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.45	0.51
2:L:146:LYS:HE3	2:L:153:GLU:CD	2.31	0.51
4:U:252:LEU:HB2	13:U:494:HOH:O	2.11	0.51
1:A:12:ASP:OD1	1:A:41:HIS:CD2	2.64	0.51
2:L:93:TYR:CD2	2:L:93:TYR:O	2.64	0.50
4:U:70:VAL:HG12	4:U:71:CYS:N	2.26	0.50
2:L:75:ILE:HD13	2:L:78:MET:HA	1.94	0.50
4:U:4:MET:CE	4:U:14:VAL:HG22	2.40	0.50
3:H:128:ASN:ND2	13:H:452:HOH:O	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:U:1:LEU:HD13	4:U:17:CYS:SG	2.52	0.50
1:A:28:ILE:HD13	4:U:29:VAL:HG23	1.92	0.50
4:U:157:ASN:OD1	4:U:166:HIS:HE1	1.95	0.49
4:U:222:CYS:HB3	4:U:272:ASN:HB2	1.94	0.49
4:U:31:LEU:CD1	4:U:31:LEU:N	2.76	0.49
3:H:143:GLU:OE2	3:H:144:PRO:HA	2.12	0.49
1:A:110:ARG:NH1	1:A:128:VAL:O	2.45	0.49
1:A:22:ASN:HD22	1:A:24:TYR:N	2.08	0.49
6:L:407:ETX:H43	4:U:193:GLN:OE1	2.13	0.49
2:L:214:LYS:HD3	3:H:208:ALA:OXT	2.12	0.49
1:A:64:THR:HG23	1:A:127:MET:HB3	1.93	0.49
3:H:50:TRP:CE2	3:H:58:GLU:HB2	2.47	0.49
2:L:140:PRO:O	2:L:197:HIS:HE1	1.95	0.49
3:H:130:MET:CE	3:H:178:VAL:C	2.81	0.49
2:L:180:LEU:HD23	2:L:180:LEU:H	1.78	0.49
1:A:109:ARG:NE	1:A:109:ARG:N	2.61	0.49
4:U:225:ALA:O	4:U:237:MET:HA	2.13	0.49
4:U:153:CYS:HB3	4:U:154:PRO:HD3	1.95	0.48
1:A:85:HIS:O	1:A:88:ARG:HG2	2.14	0.48
3:H:134:GLY:O	3:H:135:CYS:HB2	2.12	0.48
4:U:75:LEU:C	4:U:77:ASN:N	2.67	0.48
3:H:130:MET:HE2	3:H:178:VAL:O	2.13	0.48
3:H:12:VAL:HG21	3:H:82(C):LEU:HD13	1.90	0.48
2:L:214:LYS:HG3	2:L:215:ALA:O	2.13	0.48
2:L:93:TYR:C	2:L:93:TYR:CD2	2.87	0.48
2:L:18:LYS:HD3	2:L:76:SER:HA	1.96	0.48
4:U:153:CYS:O	4:U:154:PRO:C	2.52	0.48
1:A:117:VAL:HG23	1:A:117:VAL:O	2.14	0.48
1:A:64:THR:HG23	1:A:127:MET:CB	2.43	0.48
2:L:6:GLN:HG3	2:L:88:CYS:SG	2.54	0.47
4:U:24:CYS:HB3	4:U:77:ASN:ND2	2.28	0.47
3:H:99:TRP:CH2	8:H:406:PGE:H4	2.49	0.47
4:U:29:VAL:HG12	4:U:31:LEU:CD1	2.44	0.47
4:U:200:ASN:HD22	4:U:203:HIS:HB2	1.78	0.47
4:U:127:THR:O	4:U:142:ARG:HA	2.13	0.47
1:A:28:ILE:HD13	4:U:29:VAL:CG2	2.44	0.47
3:H:83:THR:O	3:H:111:VAL:HG21	2.15	0.47
3:H:187:THR:HG23	3:H:204:LYS:HE3	1.96	0.47
3:H:172:LEU:HD23	3:H:173:SER:N	2.30	0.47
4:U:228:THR:HA	4:U:234:GLN:O	2.15	0.46
2:L:141:LYS:HB2	2:L:172:TYR:CE2	2.50	0.46
4:U:75:LEU:C	4:U:77:ASN:H	2.18	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:LEU:HD23	1:A:105:PRO:CB	2.45	0.46
2:L:66:GLY:HA3	2:L:71:TYR:HA	1.97	0.46
4:U:37:GLU:HG2	4:U:38:LEU:N	2.29	0.46
4:U:177:ASN:N	4:U:177:ASN:HD22	2.11	0.46
4:U:62:LYS:HG2	4:U:63:ILE:H	1.80	0.46
4:U:70:VAL:CG1	4:U:71:CYS:N	2.79	0.46
3:H:130:MET:CE	3:H:179:PRO:CA	2.93	0.46
4:U:229:HIS:CD2	4:U:230:GLU:N	2.79	0.46
2:L:69:THR:CG2	2:L:69:THR:O	2.64	0.46
4:U:74:ASP:OD1	4:U:75:LEU:HG	2.16	0.46
2:L:75:ILE:HD11	2:L:78:MET:HA	1.98	0.46
4:U:141:ASP:CB	4:U:144:LEU:HD13	2.46	0.46
1:A:61:LYS:HG2	1:A:62:ALA:N	2.31	0.46
6:H:403:ETX:H32	13:H:427:HOH:O	2.15	0.46
3:H:134:GLY:O	3:H:149:TRP:CZ2	2.66	0.45
1:A:72:LEU:HD21	1:A:116:GLN:HB2	1.99	0.45
3:H:130:MET:HE3	3:H:179:PRO:HA	1.99	0.45
3:H:100(A):PHE:CD1	3:H:100(A):PHE:N	2.85	0.45
2:L:7:SER:HA	2:L:8:PRO:C	2.36	0.45
4:U:128:HIS:ND1	4:U:142:ARG:NH1	2.65	0.45
2:L:206:LYS:HD2	13:L:433:HOH:O	2.16	0.45
1:A:123:VAL:HG23	1:A:123:VAL:O	2.17	0.45
2:L:182:LYS:O	2:L:186:GLU:HG2	2.16	0.45
4:U:206:SER:HB3	4:U:209:GLU:OE2	2.17	0.45
1:A:79:VAL:O	1:A:85:HIS:HB3	2.17	0.45
2:L:174:MET:HG2	2:L:175:SER:N	2.32	0.45
4:U:96:ILE:HG13	4:U:178:GLU:HB3	1.99	0.44
2:L:75:ILE:HD11	2:L:82:ASP:OD2	2.17	0.44
4:U:29:VAL:HG13	4:U:66:LEU:HD23	1.99	0.44
2:L:50:GLU:CD	13:H:408:HOH:O	2.55	0.44
1:A:109:ARG:HG3	1:A:109:ARG:NH1	2.32	0.44
4:U:183:GLU:CD	13:U:545:HOH:O	2.55	0.44
1:A:91:ALA:HB1	1:A:96:LEU:O	2.17	0.44
4:U:52:ASN:CG	9:U:452:NAG:O1	2.56	0.44
1:A:61:LYS:HA	1:A:101:TYR:CD1	2.53	0.44
2:L:49:PHE:CE1	2:L:53:LYS:HD2	2.53	0.44
4:U:113:LEU:HD23	4:U:114:GLN:N	2.32	0.44
3:H:132:THR:CG2	3:H:133:LEU:H	2.29	0.44
2:L:180:LEU:N	2:L:180:LEU:CD2	2.81	0.44
4:U:54:THR:CG2	4:U:55:LEU:N	2.80	0.44
4:U:43:LYS:O	4:U:44:SER:HB3	2.18	0.44
1:A:65:ASP:HB3	1:A:69:ARG:HB3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:U:268:LYS:HB3	4:U:271:CYS:HB3	1.99	0.44
4:U:270:GLY:C	4:U:272:ASN:H	2.21	0.44
4:U:128:HIS:O	4:U:129:TRP:C	2.56	0.44
3:H:87:SER:HA	3:H:109:VAL:O	2.18	0.44
4:U:230:GLU:CB	4:U:231:PRO:HD2	2.25	0.44
2:L:73:LEU:HD23	2:L:73:LEU:C	2.38	0.44
4:U:3:CYS:HB3	4:U:77:ASN:ND2	2.30	0.43
4:U:177:ASN:H	4:U:177:ASN:ND2	2.16	0.43
2:L:89:GLN:HG2	2:L:90:GLN:O	2.17	0.43
4:U:113:LEU:HD23	4:U:113:LEU:C	2.39	0.43
3:H:119:PRO:CB	3:H:140:TYR:HB3	2.42	0.43
6:L:401:ETX:H32	13:L:444:HOH:O	2.18	0.43
3:H:172:LEU:HD23	3:H:172:LEU:C	2.38	0.43
1:A:40:GLN:HG3	4:U:40:LEU:HD21	2.01	0.43
1:A:128:VAL:O	1:A:128:VAL:HG13	2.18	0.43
2:L:2:ILE:HG12	2:L:27:SER:HB2	2.00	0.43
2:L:90:GLN:HE21	2:L:97:THR:HB	1.83	0.43
4:U:116:ARG:HG3	4:U:116:ARG:HH11	1.82	0.43
2:L:150:ASP:HA	2:L:190:SER:HB3	1.99	0.43
2:L:123:GLN:O	2:L:126:SER:HB2	2.18	0.43
1:A:104:ASN:HB2	1:A:111:PRO:HA	2.00	0.43
3:H:148:THR:OG1	3:H:191:ASN:HB2	2.18	0.43
1:A:16:GLY:O	1:A:34:PRO:HD3	2.19	0.43
2:L:135:LEU:HD12	2:L:135:LEU:N	2.34	0.43
2:L:181:THR:HA	13:L:473:HOH:O	2.19	0.42
1:A:20:VAL:HG22	1:A:21:SER:N	2.34	0.42
3:H:30:THR:HB	3:H:52(A):HIS:CD2	2.54	0.42
2:L:188:HIS:CE1	13:L:522:HOH:O	2.72	0.42
3:H:62:LYS:HA	3:H:62:LYS:HE3	2.01	0.42
1:A:23:LYS:NZ	4:U:166:HIS:CD2	2.77	0.42
4:U:160:HIS:CE1	4:U:216:ARG:H	2.31	0.42
1:A:80:LEU:HD23	1:A:85:HIS:HB2	2.02	0.42
3:H:134:GLY:HA2	3:H:175:SER:HA	2.00	0.42
3:H:194:HIS:CE1	3:H:196:ALA:HB3	2.53	0.42
2:L:2:ILE:N	6:L:401:ETX:H12	2.33	0.42
4:U:200:ASN:HB2	4:U:203:HIS:H	1.85	0.42
4:U:206:SER:CB	4:U:209:GLU:OE2	2.67	0.42
2:L:135:LEU:CD2	2:L:195:ALA:HB2	2.50	0.42
4:U:208:GLU:N	4:U:208:GLU:OE1	2.53	0.42
2:L:189:ASN:OD1	2:L:211:ASN:ND2	2.53	0.42
4:U:273:HIS:CE1	4:U:274:PRO:HD2	2.55	0.42
3:H:130:MET:CE	3:H:179:PRO:HA	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:146:LYS:HE3	2:L:153:GLU:OE1	2.20	0.41
2:L:212:GLU:O	2:L:213:ALA:HB2	2.20	0.41
2:L:93:TYR:O	2:L:96:PHE:CE2	2.73	0.41
3:H:52:PHE:CE2	12:U:402:PG4:H42	2.55	0.41
4:U:221:GLN:NE2	12:U:402:PG4:H22	2.35	0.41
2:L:209:ASN:ND2	13:L:475:HOH:O	2.52	0.41
4:U:23:LEU:HD13	4:U:70:VAL:CG1	2.35	0.41
1:A:73:PRO:C	1:A:75:ASN:H	2.24	0.41
1:A:109:ARG:H	1:A:109:ARG:NE	2.19	0.41
1:A:56:HIS:HA	1:A:104:ASN:HB3	2.02	0.41
2:L:197:HIS:HD2	2:L:199:THR:OG1	2.04	0.41
10:U:472:NAG:C7	10:U:472:NAG:O1	2.48	0.40
4:U:122:CYS:HB2	4:U:176:CYS:SG	2.61	0.40
1:A:130:ASP:C	1:A:132:ALA:H	2.24	0.40
3:H:28:SER:HB3	3:H:31:ASN:HD22	1.87	0.40
1:A:22:ASN:ND2	1:A:24:TYR:HB2	2.36	0.40
3:H:130:MET:HE3	3:H:179:PRO:CA	2.51	0.40
1:A:100:ASN:N	1:A:100:ASN:HD22	2.13	0.40
3:H:161:PHE:HA	3:H:162:PRO:HD3	1.94	0.40
4:U:230:GLU:CB	4:U:231:PRO:CD	2.89	0.40
4:U:172:ASN:N	4:U:172:ASN:OD1	2.50	0.40
4:U:200:ASN:ND2	11:U:400:NDG:O1L	2.54	0.40
2:L:141:LYS:HD2	2:L:172:TYR:CE1	2.57	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	120/122 (98%)	98 (82%)	18 (15%)	4 (3%)	6	1
2	L	212/214 (99%)	204 (96%)	4 (2%)	4 (2%)	12	2
3	H	208/213 (98%)	199 (96%)	7 (3%)	2 (1%)	22	8
4	U	239/276 (87%)	215 (90%)	20 (8%)	4 (2%)	14	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	779/825 (94%)	716 (92%)	49 (6%)	14 (2%)	13	3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	62	ALA
1	A	109	ARG
2	L	93	TYR
4	U	230	GLU
2	L	213	ALA
4	U	154	PRO
4	U	162	ASN
1	A	68	GLY
2	L	68	GLY
2	L	214	LYS
3	H	135	CYS
4	U	231	PRO
3	H	144	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	106/106 (100%)	102 (96%)	4 (4%)	44	31
2	L	186/186 (100%)	181 (97%)	5 (3%)	57	47
3	H	182/182 (100%)	176 (97%)	6 (3%)	50	37
4	U	223/244 (91%)	212 (95%)	11 (5%)	35	21
All	All	697/718 (97%)	671 (96%)	26 (4%)	45	32

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	100	ASN

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Mol	Chain	Res	Type
1	A	109	ARG
1	A	110	ARG
2	L	18	LYS
2	L	91	TRP
2	L	107	ARG
2	L	180	LEU
2	L	198	LYS
3	H	2	VAL
3	H	3	LYS
3	H	62	LYS
3	H	144	PRO
3	H	172	LEU
3	H	201	VAL
4	U	1	LEU
4	U	67	THR
4	U	93	LEU
4	U	140	ASP
4	U	144	LEU
4	U	153	CYS
4	U	168	LEU
4	U	177	ASN
4	U	189	GLN
4	U	212	LEU
4	U	272	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	40	GLN
1	A	82	GLN
1	A	85	HIS
1	A	99	HIS
1	A	100	ASN
1	A	116	GLN
2	L	34	HIS
2	L	90	GLN
2	L	144	ASN
2	L	197	HIS
2	L	209	ASN
2	L	211	ASN
3	H	31	ASN

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Mol	Chain	Res	Type
3	H	52(A)	HIS
3	H	128	ASN
3	H	166	GLN
4	U	78	GLN
4	U	160	HIS
4	U	166	HIS
4	U	172	ASN
4	U	177	ASN
4	U	189	GLN
4	U	193	GLN
4	U	200	ASN
4	U	203	HIS
4	U	221	GLN
4	U	229	HIS
4	U	248	GLN
4	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 ⓘ

2 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	$\# Z  > 2$
9	NAG	U	452	9,4	15,15,15	0.43	0	21,21,21	0.77	0
9	FUC	U	453	9	11,11,11	0.35	0	16,16,16	0.37	0



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
9	NAG	U	452	9,4	1/1/6/7	0/6/26/26	0/1/1/1
9	FUC	U	453	9	1/1/5/5	0/0/20/20	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	U	453	FUC	C1
9	U	452	NAG	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

11 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	$\# Z  > 2$
5	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.10	0
6	ETX	H	403	-	5,5,5	1.08	0	4,4,4	2.49	1 (25%)
7	EDO	H	404	-	3,3,3	0.56	0	2,2,2	0.52	0
8	PGE	H	406	-	9,9,9	1.14	1 (11%)	8,8,8	1.79	2 (25%)
6	ETX	L	401	-	5,5,5	1.13	0	4,4,4	2.49	1 (25%)
7	EDO	L	405	-	3,3,3	0.64	0	2,2,2	0.60	0
6	ETX	L	407	-	5,5,5	1.09	0	4,4,4	2.44	1 (25%)
11	NDG	U	400	-	15,15,15	0.41	0	21,21,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	PG4	U	402	-	12,12,12	1.12	1 (8%)	11,11,11	0.79	0
10	NAG	U	472	10,4	15,15,15	0.40	0	21,21,21	0.58	0
10	NAG	U	473	10	15,15,15	0.44	0	21,21,21	0.51	0

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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
6	ETX	H	403	-	-	0/3/3/3	0/0/0/0
7	EDO	H	404	-	-	0/1/1/1	0/0/0/0
8	PGE	H	406	-	-	0/7/7/7	0/0/0/0
6	ETX	L	401	-	-	0/3/3/3	0/0/0/0
7	EDO	L	405	-	-	0/1/1/1	0/0/0/0
6	ETX	L	407	-	-	0/3/3/3	0/0/0/0
11	NDG	U	400	-	-	0/6/26/26	0/1/1/1
12	PG4	U	402	-	-	0/10/10/10	0/0/0/0
10	NAG	U	472	10,4	-	0/6/26/26	0/1/1/1
10	NAG	U	473	10	1/1/6/7	0/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	402	PG4	O2-C3	2.23	1.51	1.42
8	H	406	PGE	C4-C3	2.04	1.59	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	403	ETX	C3-O2-C2	4.74	130.26	112.88
6	L	401	ETX	C3-O2-C2	4.68	130.01	112.88
6	L	407	ETX	C3-O2-C2	4.66	129.94	112.88
8	H	406	PGE	C5-O3-C4	3.91	130.56	113.38
8	H	406	PGE	O2-C2-C1	2.35	121.92	110.61

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	U	473	NAG	C1

There are no torsion outliers.

There are no ring outliers.

## 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<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	122/122 (100%)	1.10	23 (18%) 2 2	33, 56, 82, 86	0
2	L	214/214 (100%)	0.17	6 (2%) 50 51	21, 33, 54, 91	0
3	H	212/213 (99%)	0.15	6 (2%) 50 51	17, 33, 52, 64	0
4	U	249/276 (90%)	0.51	16 (6%) 19 18	22, 43, 70, 99	0
All	All	797/825 (96%)	0.42	51 (6%) 17 18	17, 39, 72, 99	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	GLY	6.5
4	U	230	GLU	5.7
2	L	213	ALA	5.3
2	L	215	ALA	5.2
4	U	129	TRP	5.0
1	A	35	LYS	4.7
1	A	109	ARG	4.7
4	U	92	TYR	4.6
4	U	231	PRO	4.5
1	A	131	CYS	4.3
1	A	52	GLU	4.1
3	H	128	ASN	4.0
4	U	153	CYS	4.0
1	A	57	PHE	4.0
4	U	32	TRP	3.9
1	A	62	ALA	3.9
1	A	122	LEU	3.6
1	A	16	GLY	3.6
4	U	233	ASN	3.6
3	H	134	GLY	3.4
2	L	1	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
4	U	116	ARG	3.1
1	A	15	ASN	3.0
1	A	36	LYS	2.9
4	U	61	LEU	2.9
4	U	229	HIS	2.8
1	A	120	LYS	2.8
4	U	232	LYS	2.8
1	A	37	PHE	2.7
1	A	132	ALA	2.6
1	A	64	THR	2.5
1	A	107	ASN	2.4
1	A	65	ASP	2.4
1	A	126	CYS	2.4
1	A	49	THR	2.4
4	U	234	GLN	2.3
4	U	73	LEU	2.3
3	H	208	ALA	2.3
3	H	133	LEU	2.3
3	H	132	THR	2.3
1	A	129	HIS	2.3
1	A	50	CYS	2.3
1	A	46	LYS	2.3
4	U	260	HIS	2.2
3	H	200	LYS	2.2
2	L	93	TYR	2.2
1	A	54	ASN	2.1
4	U	149	TYR	2.1
4	U	13	ARG	2.0
2	L	3	VAL	2.0
2	L	214	LYS	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<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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	FUC	U	453	11/11	0.27	-	98,99,101,102	0
9	NAG	U	452	15/15	0.22	-	78,81,84,86	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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	L	405	4/4	0.11	-	47,49,49,50	0
6	ETX	H	403	6/6	0.39	-	43,48,49,52	0
7	EDO	H	404	4/4	0.13	-	42,46,50,53	0
6	ETX	L	407	6/6	0.24	-	52,56,59,59	0
10	NAG	U	473	15/15	0.50	-	98,102,104,105	0
10	NAG	U	472	15/15	0.27	-	71,76,79,80	0
5	SO4	A	501	5/5	0.13	-	47,47,47,47	0
12	PG4	U	402	13/13	0.31	-	44,48,54,58	0
11	NDG	U	400	15/15	0.22	-	71,81,83,85	0
8	PGE	H	406	10/10	0.22	-	38,61,63,64	0
6	ETX	L	401	6/6	0.34	-	41,48,52,61	0

## 6.5 Other polymers

There are no such residues in this entry.