



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 12:29 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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

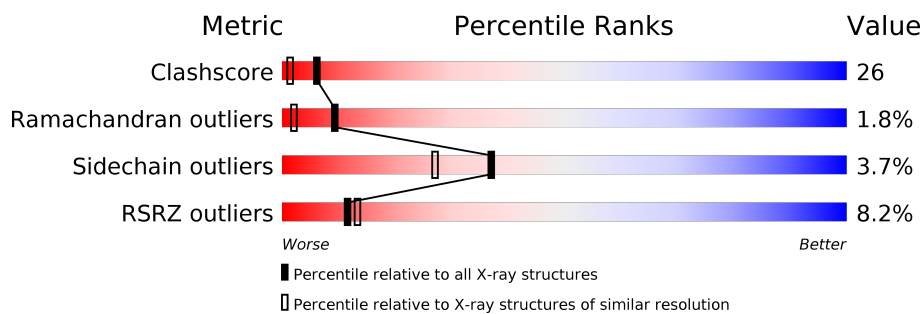
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (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 ≥ 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	122	<div> <div>25%</div> <div>54%</div> <div>41%</div> <div>• •</div> </div>
2	L	214	<div> <div>3%</div> <div>66%</div> <div>31%</div> <div>•</div> </div>
3	H	213	<div> <div>4%</div> <div>73%</div> <div>24%</div> <div>•</div> </div>
4	U	276	<div> <div>7%</div> <div>52%</div> <div>35%</div> <div>• 10%</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
10	FUC	U	453	X	-	-	-
12	PG4	U	402	-	-	X	-
6	ETX	L	401	-	-	X	-
9	NAG	U	452	X	-	-	-
9	NAG	U	472	-	-	X	-
9	NAG	U	473	X	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 6600 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	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:

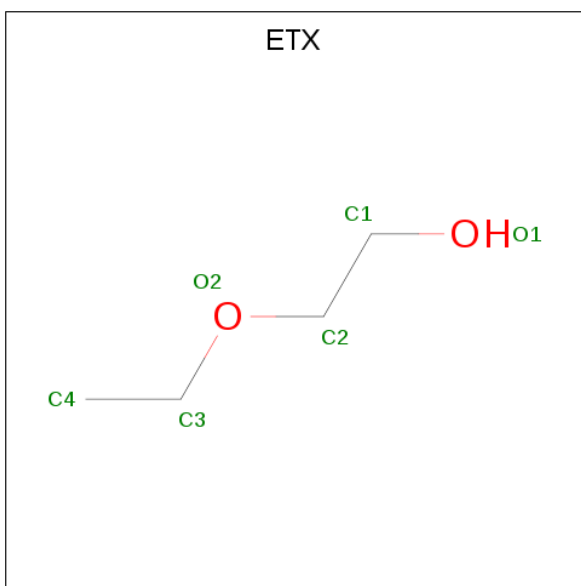
Chain	Residue	Modelled	Actual	Comment	Reference
U	1A	SER	-	CLONING ARTIFACT	UNP Q03405

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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: C₄H₁₀O₂).



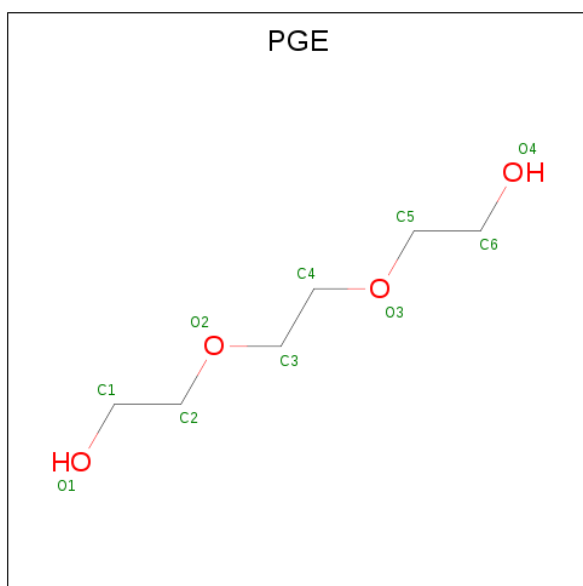
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			6	4	2		
6	L	1	Total	C	O	0	0
			6	4	2		
6	H	1	Total	C	O	0	0
			6	4	2		

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



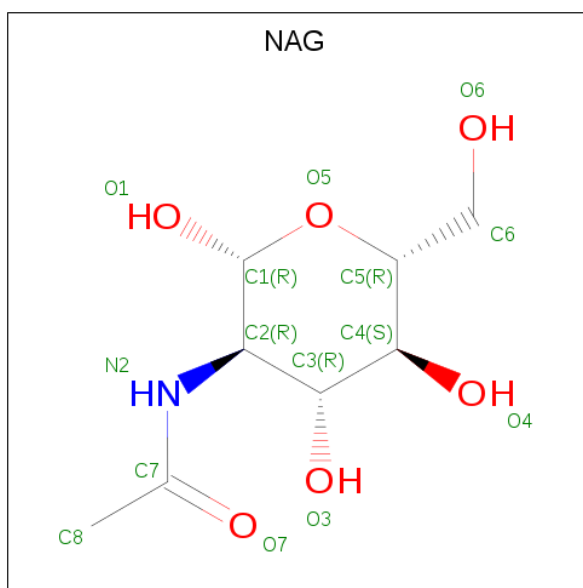
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		

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



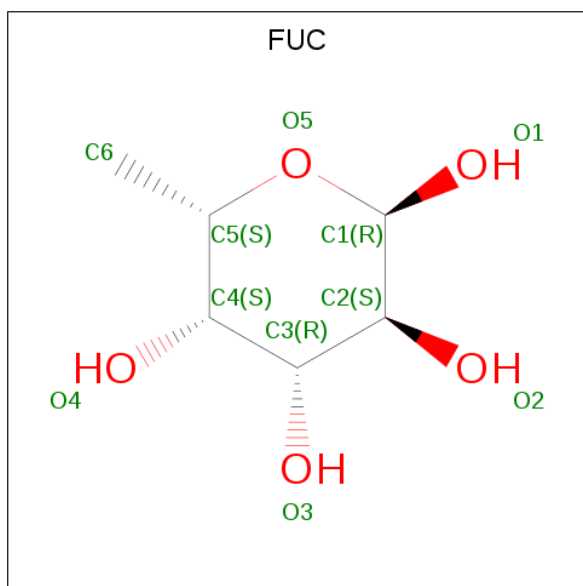
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



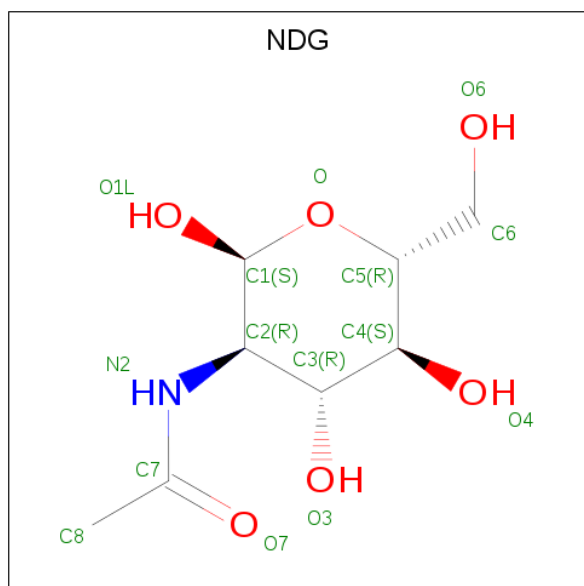
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	U	1	Total	C	N	O	0	0
			15	8	1	6		
9	U	1	Total	C	N	O	0	0
			15	8	1	6		
9	U	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 10 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



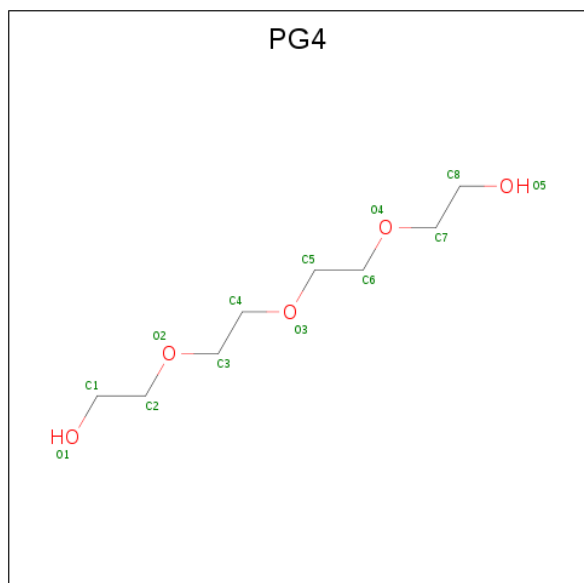
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	U	1	Total	C	O	0	0
			11	6	5		

- Molecule 11 is 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		

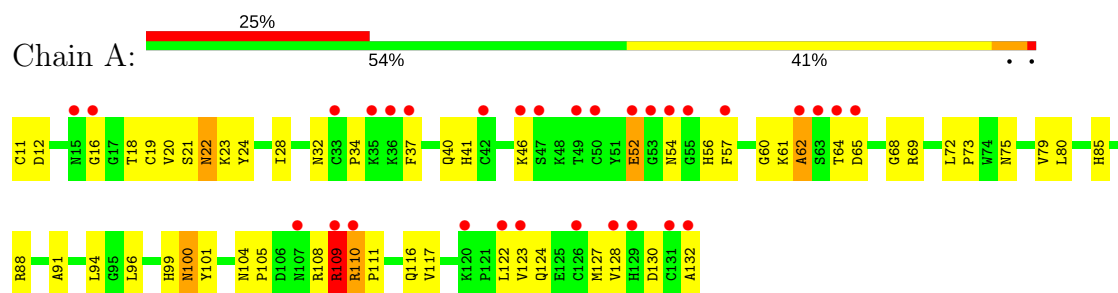
- Molecule 13 is water.

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

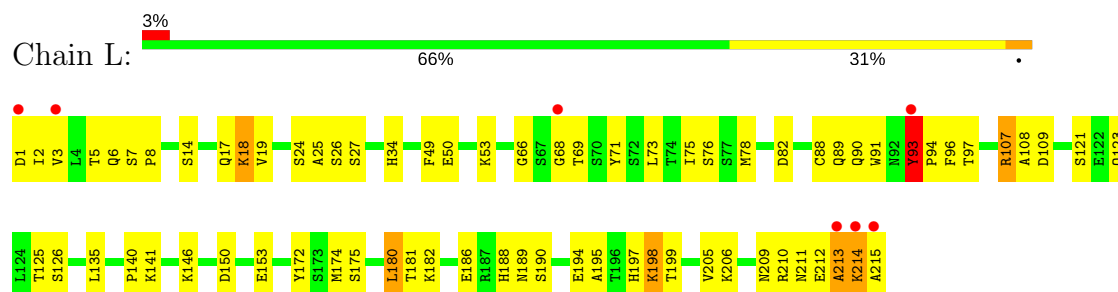
3 Residue-property plots [i](#)

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

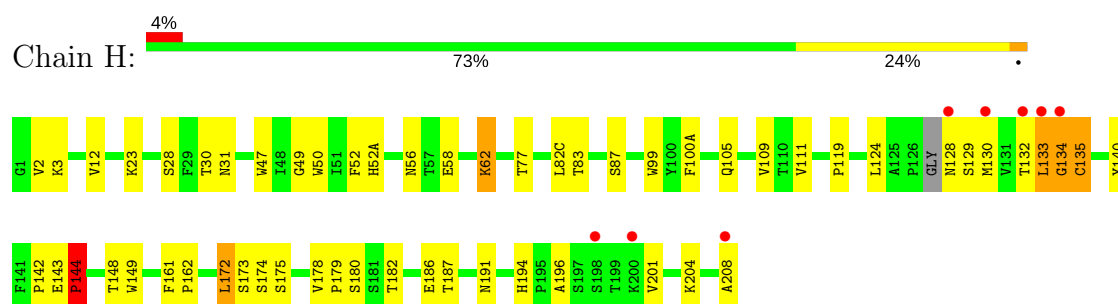
- Molecule 1: Urokinase-type plasminogen activator



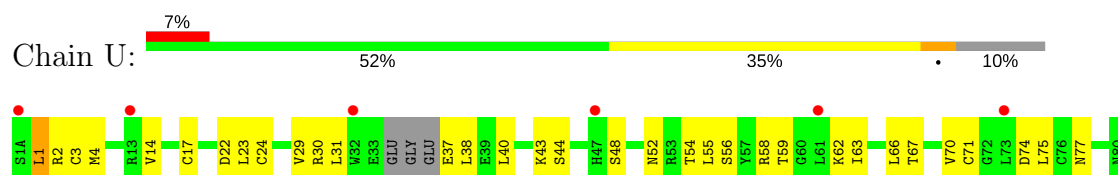
- Molecule 2: L chain of Fab of ATN-615 anti-uPAR antibody

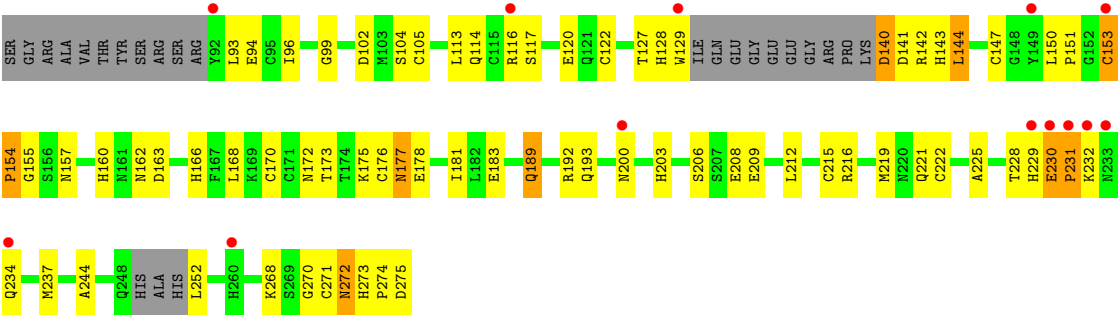


- Molecule 3: H chain of Fab of ATN-615 anti-uPAR antibody



- 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, α , β , γ	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) 92.4 (41.36-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.276 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6600	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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%)

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

There are no chirality outliers.

There are no planarity outliers.

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	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	45	0	40	15	0
10	U	11	0	11	0	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (319) 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)
4:U:230:GLU:HB3	4:U:231:PRO:HD2	1.36	1.06
9:U:472:NAG:H61	9:U:473:NAG:H82	1.37	1.05
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
9:U:472:NAG:C6	9:U:473:NAG:H82	1.91	1.00
4:U:172:ASN:ND2	9: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	9: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
3:H:56:ASN:HD22	12:U:402:PG4:H11	1.33	0.92
4:U:52:ASN:ND2	9:U:452:NAG:O1	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:U:472:NAG:H61	9: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
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
4:U:229:HIS:CD2	4:U:230:GLU:H	2.06	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:65:ASP:OD1	1:A:124:GLN:HB3	1.97	0.64
4:U:183:GLU:OE1	13:U:545:HOH:O	2.15	0.64
4:U:31:LEU:HD12	4:U:31:LEU:N	2.13	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
4:U:52:ASN:ND2	9:U:452:NAG:C2	2.60	0.64
9:U:472:NAG:H62	9: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:HG2	1:A:46:LYS:O	2.01	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:H11	1.83	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
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
4:U:4:MET:HE1	4:U:14:VAL:HG22	1.87	0.56
1:A:100:ASN:H	1:A:100:ASN:HD22	1.53	0.56
4:U:172:ASN:OD1	9:U:472:NAG:O5	2.24	0.56
3:H:77:THR:OG1	6:H:403:ETX:H21	2.05	0.56
9:U:472:NAG:C6	9:U:473:NAG:C8	2.73	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
1:A:18:THR:HB	1:A:32:ASN:HB2	1.88	0.55
2:L:19:VAL:HB	2:L:75:ILE:HG22	1.89	0.55
3:H:130:MET:CE	3:H:179:PRO:N	2.70	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:129:SER:O	3:H:179:PRO:HA	2.07	0.55
3:H:52(A):HIS:HB3	12:U:402:PG4:H12	1.89	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
3:H:142:PRO:HD2	3:H:196:ALA:HB1	1.90	0.54
4:U:129:TRP:O	4:U:163:ASP:O	2.24	0.54
1:A:94:LEU:HD23	1:A:105:PRO:HB3	1.88	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
2:L:69:THR:HG22	2:L:69:THR:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:LEU:HD23	2:L:180:LEU:N	2.23	0.53
2:L:93:TYR:O	2:L:96:PHE:CD2	2.62	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:150:LEU:HB3	4:U:151:PRO:HD2	1.92	0.52
4:U:177:ASN:H	4:U:177:ASN:HD22	1.58	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
1:A:61:LYS:O	1:A:62:ALA:HB2	2.11	0.51
4:U:43:LYS:HB3	4:U:77:ASN:OD1	2.11	0.51
1:A:108:ARG:HH12	1:A:123:VAL:HG21	1.75	0.51
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.45	0.51
2:L:146:LYS:HG3	2:L:153:GLU:OE2	2.11	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
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
1:A:64:THR:HG23	1:A:127:MET:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:214:LYS:HD3	3:H:208:ALA:OXT	2.12	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
1:A:109:ARG:NE	1:A:109:ARG:N	2.61	0.49
2:L:180:LEU:HD23	2:L:180:LEU:H	1.78	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:CD2	2:L:93:TYR:C	2.87	0.48
2:L:18:LYS:HD3	2:L:76:SER:HA	1.96	0.48
1:A:117:VAL:HG23	1:A:117:VAL:O	2.14	0.48
4:U:153:CYS:O	4:U:154:PRO:C	2.52	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:172:LEU:HD23	3:H:173:SER:N	2.30	0.47
3:H:187:THR:HG23	3:H:204:LYS:HE3	1.96	0.47
2:L:141:LYS:HB2	2:L:172:TYR:CE2	2.50	0.46
4:U:228:THR:HA	4:U:234:GLN:O	2.15	0.46
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:75:LEU:C	4:U:77:ASN:H	2.18	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
3:H:130:MET:CE	3:H:179:PRO:CA	2.93	0.46
4:U:70:VAL:CG1	4:U:71:CYS:N	2.79	0.46
2:L:69:THR:CG2	2:L:69:THR:O	2.64	0.46
4:U:229:HIS:CD2	4:U:230:GLU:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:U:74:ASP:OD1	4:U:75:LEU:HG	2.16	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:100(A):PHE:CD1	3:H:100(A):PHE:N	2.85	0.45
3:H:130:MET:HE3	3:H:179:PRO:HA	1.99	0.45
2:L:7:SER:HA	2:L:8:PRO:C	2.36	0.45
2:L:206:LYS:HD2	13:L:433:HOH:O	2.16	0.45
4:U:128:HIS:ND1	4:U:142:ARG:NH1	2.65	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
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:206:SER:HB3	4:U:209:GLU:OE2	2.17	0.45
2:L:75:ILE:HD11	2:L:82:ASP:OD2	2.17	0.44
4:U:96:ILE:HG13	4:U:178:GLU:HB3	1.99	0.44
1:A:109:ARG:HG3	1:A:109:ARG:NH1	2.32	0.44
2:L:50:GLU:CD	13:H:408:HOH:O	2.55	0.44
4:U:29:VAL:HG13	4:U:66:LEU:HD23	1.99	0.44
1:A:91:ALA:HB1	1:A:96:LEU:O	2.17	0.44
4:U:183:GLU:CD	13:U:545:HOH:O	2.55	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
4:U:52:ASN:CG	9:U:452:NAG:O1	2.56	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
1:A:65:ASP:HB3	1:A:69:ARG:HB3	2.00	0.44
4:U:270:GLY:C	4:U:272:ASN:H	2.21	0.44
4:U:268:LYS:HB3	4:U:271:CYS:HB3	1.99	0.44
4:U:43:LYS:O	4:U:44:SER:HB3	2.18	0.44
3:H:87:SER:HA	3:H:109:VAL:O	2.18	0.44
4:U:128:HIS:O	4:U:129:TRP:C	2.56	0.44
2:L:73:LEU:HD23	2:L:73:LEU:C	2.38	0.44
4:U:230:GLU:CB	4:U:231:PRO:HD2	2.25	0.44
2:L:89:GLN:HG2	2:L:90:GLN:O	2.17	0.43
4:U:177:ASN:H	4:U:177:ASN:ND2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:3:CYS:HB3	4:U:77:ASN:ND2	2.30	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
3:H:172:LEU:C	3:H:172:LEU:HD23	2.38	0.43
6:L:401:ETX:H32	13:L:444:HOH:O	2.18	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:123:GLN:O	2:L:126:SER:HB2	2.18	0.43
2:L:150:ASP:HA	2:L:190:SER:HB3	1.99	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
1:A:20:VAL:HG22	1:A:21:SER:N	2.34	0.42
2:L:181:THR:HA	13:L:473:HOH:O	2.19	0.42
3:H:30:THR:HB	3:H:52(A):HIS:CD2	2.54	0.42
3:H:62:LYS:HA	3:H:62:LYS:HE3	2.01	0.42
2:L:188:HIS:CE1	13:L:522:HOH:O	2.72	0.42
1:A:23:LYS:NZ	4:U:166:HIS:CD2	2.77	0.42
1:A:80:LEU:HD23	1:A:85:HIS:HB2	2.02	0.42
4:U:160:HIS:CE1	4:U:216:ARG:H	2.31	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
2:L:135:LEU:CD2	2:L:195:ALA:HB2	2.50	0.42
4:U:206:SER:CB	4:U:209:GLU:OE2	2.67	0.42
2:L:189:ASN:OD1	2:L:211:ASN:ND2	2.53	0.42
4:U:208:GLU:N	4:U:208:GLU:OE1	2.53	0.42
3:H:130:MET:CE	3:H:179:PRO:HA	2.50	0.42
4:U:273:HIS:CE1	4:U:274:PRO:HD2	2.55	0.42
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
2:L:209:ASN:ND2	13:L:475:HOH:O	2.52	0.41
4:U:221:GLN:NE2	12:U:402:PG4:H22	2.35	0.41
1:A:73:PRO:C	1:A:75:ASN:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:23:LEU:HD13	4:U:70:VAL:CG1	2.35	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
9:U:472:NAG:C7	9:U:472:NAG:O1	2.48	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
4:U:122:CYS:HB2	4:U:176:CYS:SG	2.61	0.40
1:A:100:ASN:N	1:A:100:ASN:HD22	2.13	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
3:H:161:PHE:HA	3:H:162:PRO:HD3	1.94	0.40
2:L:141:LYS:HD2	2:L:172:TYR:CE1	2.57	0.40
4:U:172:ASN:N	4:U:172:ASN:OD1	2.50	0.40
4:U:230:GLU:CB	4:U:231:PRO:CD	2.89	0.40
4:U:200:ASN:ND2	11:U:400:NDG:O1L	2.54	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%)	4	0
2	L	212/214 (99%)	204 (96%)	4 (2%)	4 (2%)	9	2
3	H	208/213 (98%)	199 (96%)	7 (3%)	2 (1%)	17	7
4	U	239/276 (87%)	215 (90%)	20 (8%)	4 (2%)	10	2
All	All	779/825 (94%)	716 (92%)	49 (6%)	14 (2%)	9	2

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%)	36	26
2	L	186/186 (100%)	181 (97%)	5 (3%)	48	40
3	H	182/182 (100%)	176 (97%)	6 (3%)	41	32
4	U	223/244 (91%)	212 (95%)	11 (5%)	27	17
All	All	697/718 (97%)	671 (96%)	26 (4%)	37	27

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

Mol	Chain	Res	Type
1	A	22	ASN
1	A	100	ASN
1	A	109	ARG
1	A	110	ARG
2	L	18	LYS
2	L	91	TRP
2	L	107	ARG
2	L	180	LEU

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	0.27	0	6,6,6	0.13	0
6	ETX	H	403	-	5,5,5	1.11	0	4,4,4	2.51	1 (25%)
7	EDO	H	404	-	3,3,3	0.49	0	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PGE	H	406	-	9,9,9	1.14	0	8,8,8	1.88	2 (25%)
6	ETX	L	401	-	5,5,5	1.16	0	4,4,4	2.51	1 (25%)
7	EDO	L	405	-	3,3,3	0.57	0	2,2,2	0.60	0
6	ETX	L	407	-	5,5,5	1.12	0	4,4,4	2.45	1 (25%)
11	NDG	U	400	-	15,15,15	0.41	0	21,21,21	0.63	0
12	PG4	U	402	-	12,12,12	1.09	1 (8%)	11,11,11	0.81	0
9	NAG	U	452	10,4	15,15,15	0.45	0	21,21,21	0.80	1 (4%)
10	FUC	U	453	9	11,11,11	0.39	0	15,16,16	0.32	0
9	NAG	U	472	9,4	15,15,15	0.41	0	21,21,21	0.61	0
9	NAG	U	473	9	15,15,15	0.45	0	21,21,21	0.55	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
9	NAG	U	452	10,4	1/1/6/7	0/6/26/26	0/1/1/1
10	FUC	U	453	9	1/1/5/5	0/0/20/20	0/1/1/1
9	NAG	U	472	9,4	-	0/6/26/26	0/1/1/1
9	NAG	U	473	9	1/1/6/7	0/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	402	PG4	O2-C3	2.14	1.51	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	452	NAG	O5-C1-C2	2.06	111.58	109.52
8	H	406	PGE	O2-C2-C1	2.64	121.92	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	406	PGE	C5-O3-C4	3.93	130.56	113.30
6	L	407	ETX	C3-O2-C2	4.62	129.94	112.92
6	L	401	ETX	C3-O2-C2	4.64	130.01	112.92
6	H	403	ETX	C3-O2-C2	4.71	130.26	112.92

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	U	473	NAG	C1
9	U	452	NAG	C1
10	U	453	FUC	C1

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	403	ETX	3	0
8	H	406	PGE	1	0
6	L	401	ETX	7	0
6	L	407	ETX	1	0
11	U	400	NDG	2	0
12	U	402	PG4	11	0
9	U	452	NAG	6	0
9	U	472	NAG	9	0
9	U	473	NAG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	134:GLY	C	135:CYS	N	1.14

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	122/122 (100%)	1.32	31 (25%) 0 0	33, 56, 82, 86	0
2	L	214/214 (100%)	0.24	7 (3%) 46 50	21, 33, 54, 91	0
3	H	212/213 (99%)	0.22	8 (3%) 40 44	17, 33, 52, 64	0
4	U	249/276 (90%)	0.61	19 (7%) 14 15	22, 43, 70, 99	0
All	All	797/825 (96%)	0.52	65 (8%) 11 13	17, 39, 72, 99	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	215	ALA	6.4
1	A	53	GLY	6.1
2	L	213	ALA	6.0
1	A	131	CYS	5.9
4	U	230	GLU	5.8
1	A	109	ARG	5.6
1	A	35	LYS	5.4
4	U	129	TRP	5.2
4	U	153	CYS	5.1
4	U	92	TYR	5.1
4	U	231	PRO	5.0
4	U	233	ASN	5.0
1	A	57	PHE	4.7
1	A	62	ALA	4.7
1	A	52	GLU	4.4
4	U	32	TRP	4.3
1	A	122	LEU	4.2
3	H	128	ASN	4.0
4	U	116	ARG	3.8
1	A	16	GLY	3.8
4	U	61	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
3	H	134	GLY	3.7
1	A	50	CYS	3.6
1	A	36	LYS	3.6
1	A	64	THR	3.2
1	A	126	CYS	3.2
1	A	15	ASN	3.1
1	A	37	PHE	3.1
2	L	1	ASP	3.1
4	U	229	HIS	3.1
1	A	132	ALA	3.0
1	A	49	THR	3.0
1	A	54	ASN	3.0
4	U	232	LYS	3.0
1	A	107	ASN	3.0
4	U	234	GLN	2.9
1	A	65	ASP	2.9
1	A	129	HIS	2.8
1	A	120	LYS	2.8
4	U	149	TYR	2.6
3	H	208	ALA	2.6
4	U	73	LEU	2.6
2	L	93	TYR	2.6
3	H	133	LEU	2.6
3	H	132	THR	2.6
3	H	198	SER	2.4
1	A	128	VAL	2.4
4	U	13	ARG	2.4
1	A	46	LYS	2.3
2	L	3	VAL	2.3
3	H	200	LYS	2.3
2	L	214	LYS	2.3
1	A	33	CYS	2.2
1	A	42	CYS	2.2
4	U	260	HIS	2.2
1	A	55	GLY	2.2
3	H	130	MET	2.2
1	A	123	VAL	2.2
4	U	1(A)	SER	2.1
1	A	63	SER	2.1
1	A	110	ARG	2.1
4	U	200	ASN	2.0
2	L	68	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	47	SER	2.0
4	U	47	HIS	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](#)

There are no carbohydrates in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ETX	L	401	6/6	0.51	0.35	41,48,52,61	0
6	ETX	H	403	6/6	0.52	0.38	43,48,49,52	0
6	ETX	L	407	6/6	0.54	0.25	52,56,59,59	0
9	NAG	U	473	15/15	0.58	0.52	98,102,104,105	0
9	NAG	U	472	15/15	0.64	0.26	71,76,79,80	0
8	PGE	H	406	10/10	0.68	0.23	38,61,63,64	0
9	NAG	U	452	15/15	0.70	0.25	78,81,84,86	0
11	NDG	U	400	15/15	0.70	0.20	71,81,83,85	0
12	PG4	U	402	13/13	0.73	0.29	44,48,54,58	0
7	EDO	L	405	4/4	0.85	0.12	47,49,49,50	0
7	EDO	H	404	4/4	0.89	0.14	42,46,50,53	0
10	FUC	U	453	11/11	0.90	0.29	98,99,101,102	0
5	SO4	A	501	5/5	0.98	0.13	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.