WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 02:32 AM EDT

PDB ID	:	3LAQ
Title	:	Structure-based engineering of species selectivity in the uPA-uPAR interaction
Authors	:	Huang, M.
Deposited on	:	2010-01-06
Resolution	:	3.20 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.20 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	Percentile Ranks	Value
Rfree		0.340
Clashscore		34
Ramachandran outliers		8.4%
Sidechain outliers		22.2%
RSRZ outliers		2.6%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
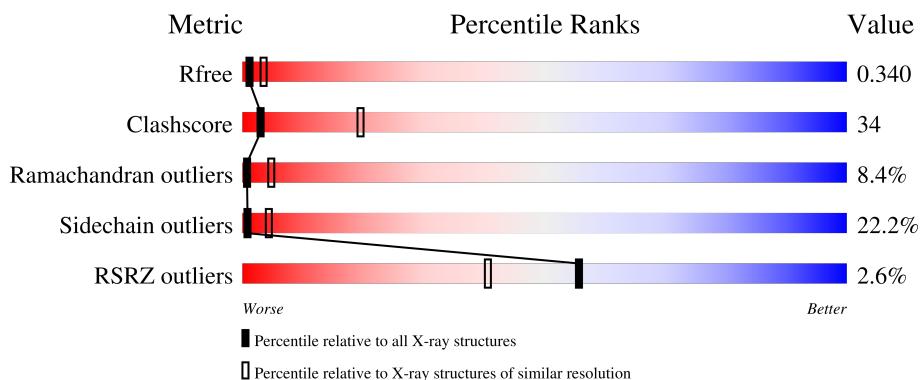
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	134	39% · 45% · 5% · 7%
1	B	134	% · 38% · 38% · 16% · 7%
2	U	277	4% · 39% · 39% · 15% · 7%
2	V	277	3% · 34% · 42% · 17% · 6%
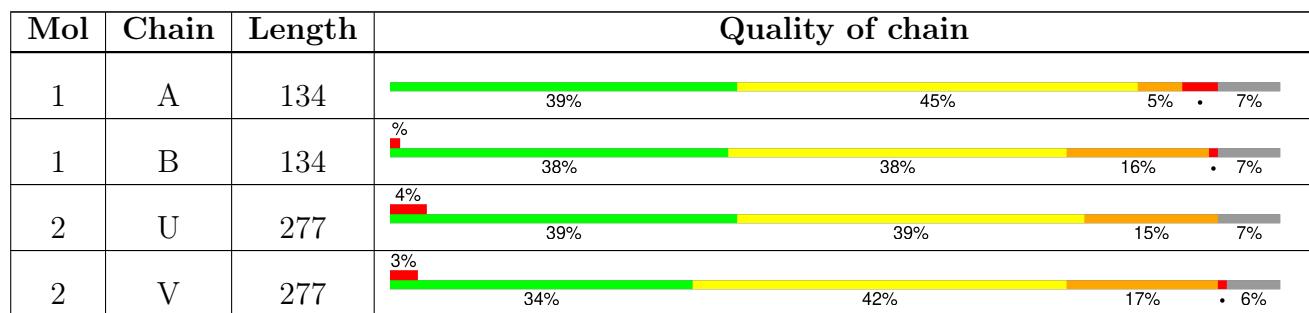
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	U	1160	-	-	-	X
3	NAG	V	1160	-	-	-	X
3	NAG	V	1259	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6035 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 981	C 601	N 190	O 177	S 13	0	0	0
1	B	125	Total 989	C 605	N 191	O 180	S 13	0	0	0

- Molecule 2 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	258	Total 1955	C 1173	N 355	O 394	S 33	0	0	0
2	V	260	Total 1970	C 1182	N 357	O 398	S 33	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
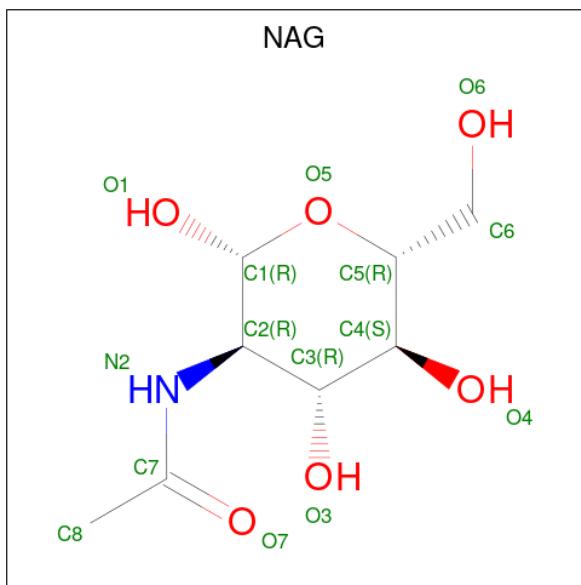
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	U	1	Total 14	C 8	N 1	O 5	0	0
3	U	1	Total 14	C 8	N 1	O 5	0	0
3	U	1	Total 14	C 8	N 1	O 5	0	0
3	U	1	Total 14	C 8	N 1	O 5	0	0
3	U	1	Total 14	C 8	N 1	O 5	0	0
3	V	1	Total 14	C 8	N 1	O 5	0	0
3	V	1	Total 14	C 8	N 1	O 5	0	0
3	V	1	Total 14	C 8	N 1	O 5	0	0
3	V	1	Total 14	C 8	N 1	O 5	0	0
3	V	1	Total 14	C 8	N 1	O 5	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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
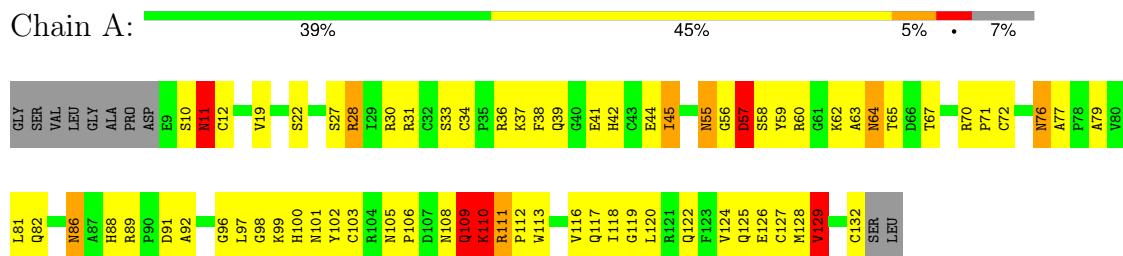
Chain A:

• Molecule 1: Urokinase-type plasminogen activator

Chain B:

• Molecule 2: Urokinase plasminogen activator surface receptor

Chain U:

• Molecule 2: Urokinase plasminogen activator surface receptor

Chain V:
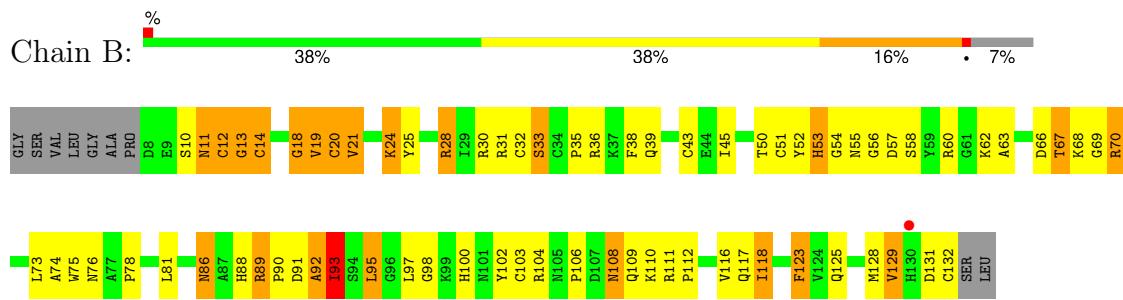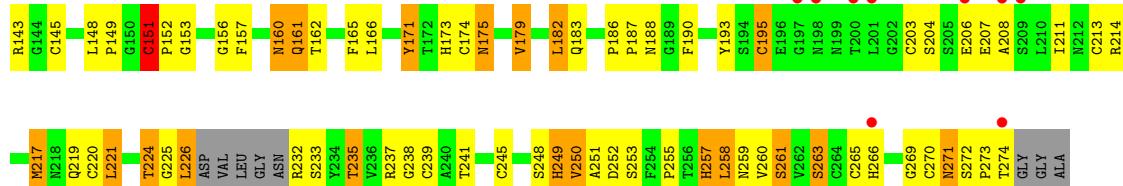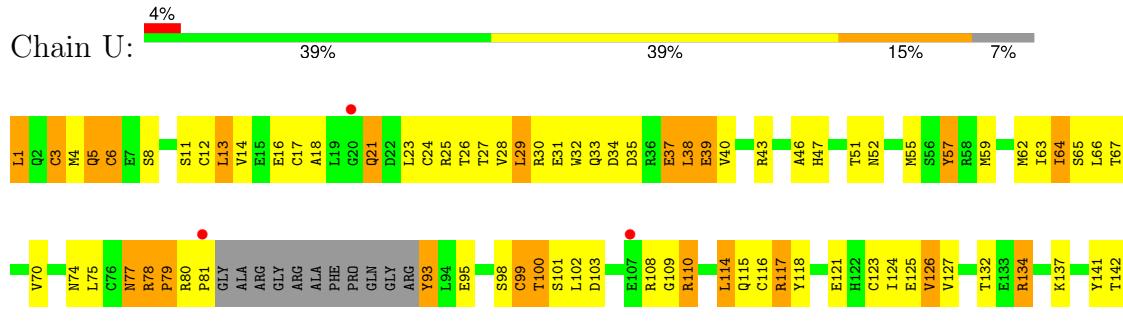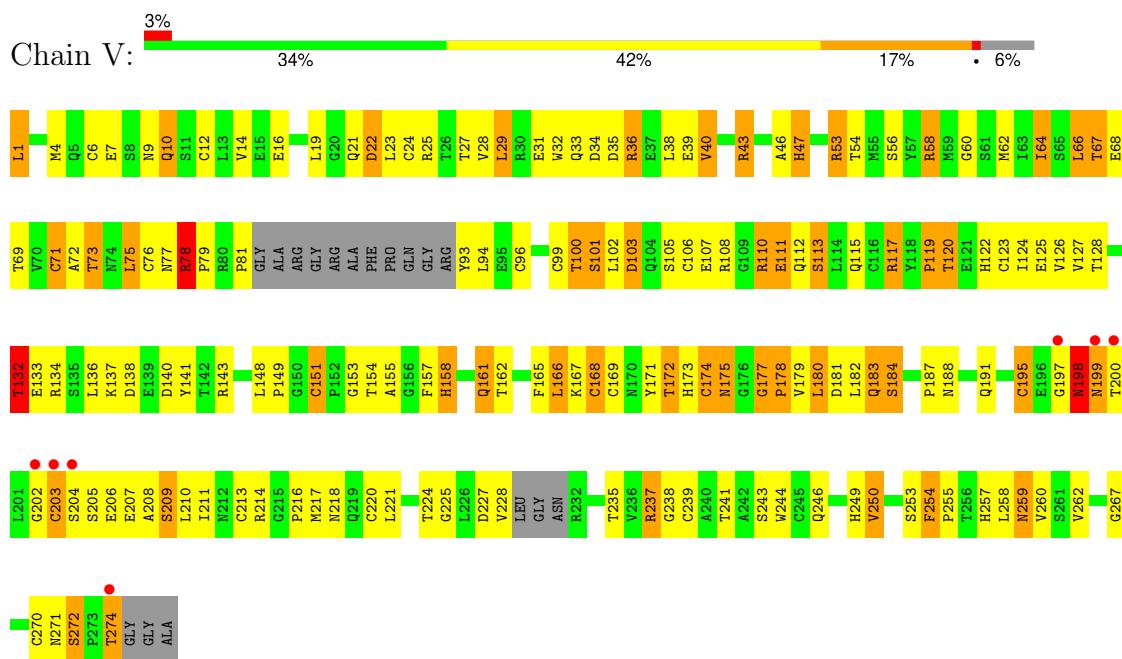
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.42Å 137.25Å 65.78Å 90.00° 106.17° 90.00°	Depositor
Resolution (Å)	44.74 – 3.20 44.73 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (44.74-3.20) 93.3 (44.73-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.231 , 0.341 0.234 , 0.340	Depositor DCC
R_{free} test set	853 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å^2)	66.7	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.3	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6035	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.72	1/1006 (0.1%)	0.82	1/1356 (0.1%)
1	B	0.65	0/1014	0.75	0/1367
2	U	0.68	2/1988 (0.1%)	0.85	2/2690 (0.1%)
2	V	0.69	0/2003	0.86	5/2711 (0.2%)
All	All	0.69	3/6011 (0.0%)	0.83	8/8124 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	V	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	24	CYS	CB-SG	-5.88	1.72	1.81
2	U	245	CYS	CB-SG	-5.37	1.73	1.81
1	A	103	CYS	CB-SG	-5.10	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	CYS	CA-CB-SG	-6.94	101.50	114.00
2	U	24	CYS	CA-CB-SG	-6.50	102.29	114.00
2	V	158	HIS	O-C-N	6.44	133.00	122.70
2	U	114	LEU	CA-CB-CG	5.60	128.17	115.30
2	V	168	CYS	CA-CB-SG	5.53	123.96	114.00
2	V	78	ARG	C-N-CD	-5.44	108.63	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	158	HIS	CA-C-N	-5.41	105.30	117.20
2	V	1	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	78	ARG	Peptide

5.2   Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	981	0	919	62	0
1	B	989	0	923	80	0
2	U	1955	0	1806	116	0
2	V	1970	0	1821	153	0
3	U	70	0	64	1	0
3	V	70	0	64	9	0
All	All	6035	0	5597	400	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 34.

All (400) 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)
2:V:259:ASN:OD1	3:V:1259:NAG:C7	1.89	1.20
2:V:259:ASN:OD1	3:V:1259:NAG:H2	1.42	1.19
2:V:259:ASN:OD1	3:V:1259:NAG:H83	1.45	1.16
2:V:259:ASN:OD1	3:V:1259:NAG:C8	1.93	1.14
2:V:259:ASN:OD1	3:V:1259:NAG:C2	1.96	1.12
2:V:259:ASN:OD1	3:V:1259:NAG:N2	1.84	1.09
2:U:78:ARG:HB3	2:U:79:PRO:HD3	1.27	1.09
2:V:6:CYS:HB3	2:V:12:CYS:HA	1.17	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:36:ARG:HG3	2:V:36:ARG:HH11	1.15	1.06
1:B:31:ARG:HG2	1:B:32:CYS:H	1.20	1.02
1:A:110:LYS:H	1:A:110:LYS:HD2	1.27	0.98
1:B:68:LYS:HB2	1:B:68:LYS:NZ	1.82	0.94
2:U:78:ARG:CB	2:U:79:PRO:HD3	2.00	0.92
2:U:5:GLN:NE2	1:B:36:ARG:HH22	1.69	0.91
2:V:148:LEU:HB3	2:V:149:PRO:HD2	1.53	0.90
1:A:39:GLN:HE22	1:A:62:LYS:NZ	1.70	0.90
2:V:123:CYS:HB2	2:V:169:CYS:SG	2.12	0.90
2:U:125:GLU:HG2	2:U:143:ARG:HG2	1.55	0.89
2:U:127:VAL:CG1	2:U:165:PHE:HB3	2.03	0.88
1:B:31:ARG:HG2	1:B:32:CYS:N	1.87	0.88
2:U:148:LEU:HB3	2:U:149:PRO:HD2	1.54	0.88
1:A:79:ALA:HB1	1:A:122:GLN:NE2	1.88	0.87
2:U:64:ILE:HD11	2:U:66:LEU:HG	1.58	0.86
2:V:39:GLU:OE1	2:V:81:PRO:HG2	1.74	0.86
1:B:86:ASN:H	1:B:89:ARG:HG3	1.41	0.85
2:V:108:ARG:HB2	2:V:110:ARG:HE	1.40	0.85
2:U:78:ARG:HB3	2:U:79:PRO:CD	2.05	0.85
2:V:220:CYS:HB3	2:V:271:ASN:ND2	1.92	0.85
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.42	0.85
2:V:224:THR:O	2:V:260:VAL:HB	1.77	0.85
2:V:148:LEU:HB3	2:V:149:PRO:CD	2.07	0.84
2:V:6:CYS:CB	2:V:12:CYS:HA	2.07	0.83
2:V:23:LEU:HB2	2:V:46:ALA:CB	2.07	0.83
2:U:31:GLU:OE2	2:U:38:LEU:HD23	1.79	0.83
1:A:79:ALA:HB1	1:A:122:GLN:HE21	1.43	0.82
2:U:121:GLU:OE1	2:U:145:CYS:HB3	1.80	0.81
2:V:195:CYS:HB2	2:V:208:ALA:HB1	1.61	0.81
2:U:30:ARG:HD3	2:U:39:GLU:HB2	1.62	0.81
2:V:36:ARG:HG3	2:V:36:ARG:NH1	1.91	0.79
2:V:250:VAL:O	2:V:253:SER:HB2	1.80	0.79
2:U:5:GLN:HE22	1:B:36:ARG:NH2	1.79	0.79
2:U:5:GLN:NE2	1:B:36:ARG:NH2	2.30	0.79
2:V:100:THR:O	2:V:105:SER:HB3	1.83	0.77
2:V:14:VAL:HG13	2:V:75:LEU:HD21	1.67	0.77
2:V:101:SER:HB3	2:V:141:TYR:H	1.49	0.77
1:A:22:SER:N	2:U:137:LYS:O	2.15	0.77
2:V:161:GLN:HE21	2:V:161:GLN:HA	1.49	0.77
1:B:68:LYS:HB2	1:B:68:LYS:HZ2	1.50	0.77
2:V:23:LEU:HB2	2:V:46:ALA:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:100:THR:CG2	2:V:102:LEU:HB3	2.15	0.76
2:V:100:THR:HG23	2:V:102:LEU:H	1.50	0.76
1:A:86:ASN:C	1:A:86:ASN:HD22	1.90	0.75
1:A:100:HIS:HD2	1:A:102:TYR:H	1.35	0.75
2:U:101:SER:HB3	2:U:141:TYR:H	1.52	0.75
1:B:86:ASN:H	1:B:89:ARG:CG	1.99	0.74
2:V:29:LEU:HB2	2:V:66:LEU:HG	1.69	0.74
2:U:160:ASN:HD22	2:U:161:GLN:HG3	1.52	0.74
2:U:220:CYS:HB2	2:U:270:CYS:HB3	1.70	0.74
2:V:119:PRO:O	2:V:120:THR:HG23	1.88	0.74
2:V:126:VAL:HG12	2:V:166:LEU:HD12	1.70	0.73
2:U:232:ARG:HD3	2:V:115:GLN:HB3	1.68	0.73
1:A:39:GLN:HE22	1:A:62:LYS:HZ2	1.33	0.73
2:V:171:TYR:O	2:V:174:CYS:SG	2.47	0.73
2:V:250:VAL:HG11	2:V:262:VAL:HG11	1.71	0.72
2:U:95:GLU:HG3	2:U:115:GLN:HG3	1.71	0.72
1:A:38:PHE:HA	1:A:45:ILE:O	1.90	0.72
2:U:114:LEU:HD23	2:U:115:GLN:H	1.54	0.72
1:B:98:GLY:H	1:B:100:HIS:CE1	2.08	0.72
2:U:77:ASN:O	2:U:78:ARG:HG2	1.90	0.72
1:B:100:HIS:HD2	1:B:102:TYR:H	1.36	0.71
1:A:108:ASN:O	1:A:109:GLN:HG2	1.88	0.71
2:V:227:ASP:O	2:V:228:VAL:HB	1.91	0.71
2:U:272:SER:O	2:U:274:THR:N	2.24	0.71
1:B:24:LYS:HD2	1:B:25:TYR:CE2	2.26	0.71
1:A:39:GLN:NE2	1:A:62:LYS:NZ	2.39	0.70
2:V:187:PRO:HD3	2:V:214:ARG:HH21	1.55	0.70
2:U:151:CYS:O	2:U:152:PRO:C	2.29	0.70
2:V:122:HIS:HD2	2:V:151:CYS:SG	2.13	0.70
2:U:93:TYR:HA	2:U:116:CYS:O	1.92	0.70
2:U:17:CYS:HB3	2:U:21:GLN:HB2	1.73	0.69
1:B:118:ILE:HG23	1:B:123:PHE:CD1	2.28	0.69
1:A:63:ALA:HB2	1:A:129:VAL:HG13	1.75	0.69
1:B:91:ASP:O	1:B:93:ILE:HG12	1.92	0.69
2:U:203:CYS:HB2	2:U:208:ALA:HB2	1.76	0.68
2:V:4:MET:HG2	2:V:75:LEU:HD22	1.75	0.68
2:V:205:SER:O	2:V:207:GLU:OE1	2.11	0.68
2:V:267:GLY:O	2:V:270:CYS:HB3	1.92	0.68
2:V:154:THR:HB	2:V:166:LEU:O	1.93	0.68
2:U:93:TYR:HD1	2:U:117:ARG:HD3	1.59	0.67
2:V:36:ARG:HH11	2:V:36:ARG:CG	1.98	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:122:HIS:CD2	2:V:151:CYS:SG	2.87	0.67
2:U:78:ARG:CB	2:U:79:PRO:CD	2.71	0.67
2:U:250:VAL:O	2:U:253:SER:HB3	1.94	0.67
2:V:220:CYS:HB2	2:V:270:CYS:SG	2.34	0.67
1:A:110:LYS:HD2	1:A:110:LYS:N	2.07	0.67
2:U:6:CYS:HB3	2:U:12:CYS:HA	1.77	0.66
1:A:41:GLU:HG2	1:A:41:GLU:O	1.95	0.66
2:V:151:CYS:O	2:V:168:CYS:HB2	1.96	0.65
2:U:190:PHE:O	2:U:213:CYS:HB2	1.97	0.65
2:U:156:GLY:O	2:U:241:THR:HG23	1.97	0.65
1:B:31:ARG:CG	1:B:32:CYS:H	2.03	0.64
1:B:57:ASP:OD2	1:B:58:SER:N	2.30	0.64
1:B:10:SER:HB3	1:B:20:CYS:H	1.62	0.64
1:B:68:LYS:HB2	1:B:68:LYS:HZ3	1.61	0.64
1:B:100:HIS:CD2	1:B:102:TYR:H	2.16	0.64
2:V:151:CYS:O	2:V:153:GLY:N	2.31	0.64
2:U:183:GLN:HA	2:U:214:ARG:HH12	1.62	0.63
2:V:208:ALA:O	2:V:209:SER:O	2.16	0.63
2:U:57:TYR:HE1	2:U:100:THR:HB	1.63	0.63
2:V:6:CYS:HB3	2:V:12:CYS:CA	2.10	0.63
2:V:270:CYS:SG	2:V:271:ASN:N	2.72	0.62
2:V:96:CYS:O	2:V:113:SER:HA	1.99	0.62
1:B:68:LYS:NZ	1:B:68:LYS:CB	2.59	0.62
1:A:109:GLN:HE21	1:A:109:GLN:HA	1.65	0.62
2:U:186:PRO:O	2:U:188:ASN:N	2.33	0.62
2:U:5:GLN:HE22	1:B:36:ARG:HH22	1.41	0.61
2:U:249:HIS:O	2:U:252:ASP:OD2	2.18	0.61
2:V:127:VAL:HG12	2:V:165:PHE:HB3	1.82	0.61
2:U:157:PHE:HD1	2:U:239:CYS:O	1.82	0.61
3:U:1052:NAG:H61	3:U:1053:NAG:O5	2.01	0.60
2:U:217:MET:HB3	2:U:239:CYS:SG	2.41	0.60
1:A:105:ASN:HB2	1:A:112:PRO:HA	1.84	0.60
1:A:39:GLN:HE22	1:A:62:LYS:HZ3	1.46	0.60
2:V:126:VAL:HG23	2:V:126:VAL:O	2.02	0.60
2:U:98:SER:O	2:U:99:CYS:HB3	2.02	0.59
2:V:105:SER:O	2:V:110:ARG:NH2	2.35	0.59
2:V:124:ILE:HA	2:V:167:LYS:O	2.01	0.59
1:A:19:VAL:HB	1:A:33:SER:OG	2.03	0.59
2:V:177:GLY:O	2:V:179:VAL:N	2.35	0.59
2:V:100:THR:CG2	2:V:102:LEU:H	2.16	0.59
2:V:102:LEU:O	2:V:102:LEU:HD12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:NE	1:B:90:PRO:HD2	2.18	0.59
2:V:127:VAL:CG1	2:V:165:PHE:HB3	2.33	0.59
2:V:28:VAL:HG13	2:V:67:THR:HG23	1.85	0.59
2:V:171:TYR:CE2	2:V:174:CYS:HB3	2.38	0.59
2:V:27:THR:OG1	2:V:68:GLU:HG3	2.02	0.58
2:V:141:TYR:OH	2:V:181:ASP:HB3	2.04	0.58
2:U:232:ARG:HH22	2:V:117:ARG:HG2	1.68	0.58
1:B:123:PHE:CD1	1:B:123:PHE:N	2.71	0.58
2:U:29:LEU:HD12	2:U:66:LEU:CD2	2.33	0.57
1:B:93:ILE:HD13	1:B:93:ILE:H	1.69	0.57
2:U:64:ILE:CD1	2:U:66:LEU:HG	2.32	0.57
1:B:116:VAL:HG21	1:B:125:GLN:HB2	1.86	0.57
2:V:103:ASP:C	2:V:103:ASP:OD1	2.43	0.57
2:V:224:THR:HG23	2:V:235:THR:HG22	1.86	0.57
2:V:258:LEU:O	3:V:1259:NAG:H81	2.04	0.57
1:A:39:GLN:NE2	1:A:62:LYS:HZ2	1.99	0.57
2:U:100:THR:HG23	2:U:103:ASP:OD1	2.03	0.57
1:B:56:GLY:HA3	1:B:112:PRO:HD3	1.87	0.57
1:B:10:SER:HB3	1:B:19:VAL:HA	1.87	0.56
2:U:4:MET:CE	2:U:14:VAL:HG22	2.36	0.56
2:U:13:LEU:HD22	1:B:36:ARG:CZ	2.36	0.56
2:V:21:GLN:O	2:V:22:ASP:HB3	2.04	0.56
1:B:109:GLN:HG2	1:B:110:LYS:H	1.70	0.56
2:U:3:CYS:HA	2:U:75:LEU:HD23	1.87	0.56
2:V:188:ASN:OD1	2:V:213:CYS:O	2.24	0.56
2:U:182:LEU:HG	2:U:183:GLN:N	2.20	0.56
1:B:74:ALA:C	1:B:76:ASN:H	2.09	0.56
2:U:127:VAL:HG12	2:U:165:PHE:HB3	1.85	0.56
2:U:193:TYR:HD2	2:U:271:ASN:ND2	2.04	0.56
2:V:174:CYS:C	2:V:175:ASN:HD22	2.09	0.56
1:A:111:ARG:HH11	1:A:111:ARG:CG	2.17	0.56
1:B:73:LEU:HD21	1:B:117:GLN:HB2	1.88	0.56
2:V:254:PHE:CD1	2:V:254:PHE:N	2.72	0.56
2:V:43:ARG:NH1	2:V:78:ARG:O	2.39	0.55
2:V:258:LEU:O	2:V:260:VAL:HG13	2.06	0.55
1:A:59:TYR:CZ	1:A:129:VAL:HG11	2.41	0.55
1:A:96:GLY:O	1:A:100:HIS:HE1	1.89	0.55
1:B:55:ASN:CG	1:B:56:GLY:H	2.10	0.55
2:V:35:ASP:CG	2:V:35:ASP:O	2.44	0.55
2:U:220:CYS:CB	2:U:270:CYS:HB3	2.37	0.55
2:U:93:TYR:CD1	2:U:117:ARG:HD3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:HH21	1:B:91:ASP:HB3	1.72	0.55
2:U:221:LEU:HA	2:U:263:SER:O	2.07	0.54
2:U:237:ARG:NH1	2:U:271:ASN:O	2.40	0.54
2:V:258:LEU:O	2:V:260:VAL:N	2.40	0.54
2:U:4:MET:HE1	2:U:14:VAL:HG22	1.88	0.54
2:V:71:CYS:SG	2:V:72:ALA:N	2.80	0.54
1:B:18:GLY:HA2	1:B:33:SER:O	2.07	0.54
2:V:36:ARG:NH1	2:V:36:ARG:CG	2.61	0.54
2:V:71:CYS:SG	2:V:73:THR:HG23	2.48	0.54
2:V:227:ASP:O	2:V:228:VAL:CB	2.56	0.54
2:U:226:LEU:C	2:U:257:HIS:CD2	2.81	0.54
2:U:126:VAL:HG13	2:U:142:THR:HB	1.89	0.54
1:A:98:GLY:O	1:A:100:HIS:N	2.40	0.54
2:U:123:CYS:HB3	2:U:175:ASN:OD1	2.07	0.54
1:B:74:ALA:HA	1:B:100:HIS:O	2.07	0.54
2:U:249:HIS:O	2:U:250:VAL:C	2.47	0.54
1:A:110:LYS:H	1:A:110:LYS:CD	2.11	0.53
2:V:221:LEU:O	2:V:237:ARG:HA	2.08	0.53
2:U:183:GLN:HA	2:U:214:ARG:NH1	2.22	0.53
2:U:220:CYS:HB3	2:U:271:ASN:HB3	1.90	0.53
2:U:188:ASN:ND2	2:U:217:MET:O	2.41	0.53
2:V:161:GLN:OE1	3:V:1160:NAG:H83	2.08	0.53
1:A:42:HIS:ND1	1:A:44:GLU:OE1	2.42	0.53
1:B:116:VAL:CG2	1:B:125:GLN:HB2	2.38	0.53
2:V:58:ARG:HD2	2:V:112:GLN:HB3	1.91	0.53
2:V:220:CYS:HB3	2:V:271:ASN:CG	2.29	0.53
2:U:57:TYR:HE2	2:U:64:ILE:HG12	1.74	0.53
1:B:108:ASN:N	1:B:108:ASN:OD1	2.42	0.53
2:U:32:TRP:CH2	2:U:35:ASP:OD1	2.61	0.52
2:U:29:LEU:HD12	2:U:66:LEU:HD21	1.91	0.52
2:V:122:HIS:HB3	2:V:169:CYS:O	2.08	0.52
1:A:72:CYS:O	1:A:101:ASN:OD1	2.27	0.52
1:B:67:THR:HB	1:B:68:LYS:HG3	1.92	0.52
2:U:123:CYS:HB2	2:U:174:CYS:SG	2.50	0.52
2:V:258:LEU:O	3:V:1259:NAG:C8	2.57	0.52
1:B:68:LYS:HZ3	1:B:68:LYS:CB	2.22	0.52
1:A:10:SER:O	1:A:12:CYS:N	2.43	0.52
2:V:225:GLY:HA2	2:V:260:VAL:HG11	1.92	0.52
1:A:98:GLY:C	1:A:100:HIS:H	2.13	0.52
1:A:111:ARG:HD2	1:A:126:GLU:HB3	1.91	0.52
1:B:74:ALA:HB1	1:B:76:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:272:SER:HB2	2:V:274:THR:HG23	1.91	0.51
2:U:211:ILE:HD11	2:U:239:CYS:HB2	1.92	0.51
2:V:53:ARG:HB2	2:V:148:LEU:HD23	1.93	0.51
2:U:219:GLN:HG3	2:U:241:THR:O	2.11	0.51
1:A:79:ALA:O	1:A:82:GLN:HG2	2.10	0.50
1:A:100:HIS:CD2	1:A:102:TYR:H	2.21	0.50
2:U:217:MET:CE	2:U:241:THR:HG22	2.41	0.50
1:A:128:MET:O	1:A:129:VAL:C	2.49	0.50
1:B:98:GLY:N	1:B:100:HIS:CE1	2.78	0.50
1:B:100:HIS:CD2	1:B:102:TYR:CD2	2.99	0.50
2:V:250:VAL:CG1	2:V:262:VAL:HG11	2.41	0.50
1:B:39:GLN:O	1:B:43:CYS:HA	2.12	0.50
2:V:148:LEU:HD12	2:V:166:LEU:HD11	1.94	0.50
1:A:117:GLN:NE2	1:A:119:GLY:O	2.36	0.49
2:U:11:SER:O	1:B:36:ARG:NH1	2.46	0.49
2:U:151:CYS:O	2:U:153:GLY:N	2.45	0.49
2:V:206:GLU:O	2:V:206:GLU:HG3	2.11	0.49
1:B:51:CYS:SG	1:B:132:CYS:N	2.85	0.49
1:A:56:GLY:O	1:A:58:SER:N	2.46	0.49
2:U:59:MET:CE	2:U:102:LEU:HD23	2.43	0.49
1:B:51:CYS:SG	1:B:52:TYR:N	2.86	0.49
2:V:216:PRO:HD2	2:V:217:MET:HG3	1.94	0.49
1:A:34:CYS:HB3	1:A:38:PHE:O	2.13	0.49
1:B:38:PHE:HA	1:B:45:ILE:O	2.12	0.49
2:V:237:ARG:HB3	2:V:237:ARG:NH1	2.28	0.49
2:U:193:TYR:HE2	2:U:269:GLY:HA2	1.76	0.49
2:U:160:ASN:ND2	2:U:161:GLN:HG3	2.24	0.48
2:V:175:ASN:HD22	2:V:175:ASN:N	2.10	0.48
2:V:179:VAL:HG23	2:V:179:VAL:O	2.14	0.48
1:A:81:LEU:HA	1:A:86:ASN:OD1	2.14	0.48
2:V:177:GLY:O	2:V:178:PRO:C	2.52	0.48
1:A:70:ARG:NH2	1:A:125:GLN:OE1	2.47	0.48
2:U:80:ARG:HB3	2:U:81:PRO:HD2	1.96	0.48
2:V:60:GLY:HA2	2:V:112:GLN:NE2	2.29	0.48
1:A:109:GLN:O	1:A:110:LYS:C	2.51	0.47
2:V:158:HIS:NE2	2:V:211:ILE:HD12	2.29	0.47
2:V:255:PRO:O	2:V:257:HIS:HD2	1.97	0.47
1:A:96:GLY:O	1:A:100:HIS:CE1	2.67	0.47
2:U:118:TYR:HB2	2:U:121:GLU:HG3	1.96	0.47
1:A:42:HIS:HB2	1:A:44:GLU:OE1	2.15	0.47
2:V:124:ILE:HG22	2:V:168:CYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:250:VAL:O	2:V:253:SER:CB	2.57	0.47
1:A:39:GLN:NE2	1:A:62:LYS:HZ3	2.04	0.47
2:U:64:ILE:HD12	2:U:65:SER:N	2.29	0.47
1:B:89:ARG:HE	1:B:90:PRO:HD2	1.80	0.47
2:V:39:GLU:CD	2:V:81:PRO:HG2	2.32	0.47
2:U:271:ASN:H	2:U:271:ASN:HD22	1.62	0.47
1:A:105:ASN:OD1	1:A:109:GLN:HB2	2.15	0.47
1:A:108:ASN:O	1:A:109:GLN:CG	2.59	0.47
2:U:224:THR:HG23	2:U:235:THR:HB	1.96	0.47
2:V:33:GLN:HG3	2:V:62:MET:HB2	1.95	0.47
2:V:39:GLU:OE1	2:V:81:PRO:CG	2.54	0.47
2:V:128:THR:O	2:V:128:THR:HG22	2.14	0.47
1:A:89:ARG:HB2	1:A:92:ALA:HB2	1.96	0.47
1:B:78:PRO:HA	1:B:81:LEU:HD12	1.97	0.46
2:V:100:THR:HG21	2:V:102:LEU:HB3	1.96	0.46
2:U:127:VAL:HG11	2:U:165:PHE:HB3	1.94	0.46
2:V:64:ILE:CD1	2:V:66:LEU:HD12	2.45	0.46
2:V:21:GLN:O	2:V:22:ASP:CB	2.63	0.46
2:V:143:ARG:NH1	2:V:175:ASN:O	2.48	0.46
1:B:104:ARG:C	1:B:106:PRO:HD3	2.35	0.46
2:V:29:LEU:HD23	2:V:40:VAL:HG22	1.96	0.46
2:V:195:CYS:HB3	2:V:237:ARG:HG3	1.96	0.46
1:B:118:ILE:CG2	1:B:123:PHE:CD1	2.99	0.46
2:V:32:TRP:O	2:V:33:GLN:HG3	2.16	0.46
1:A:67:THR:HA	1:A:128:MET:SD	2.56	0.46
2:U:157:PHE:CD1	2:U:239:CYS:O	2.67	0.46
1:B:66:ASP:OD2	1:B:70:ARG:N	2.49	0.46
2:V:155:ALA:HB2	2:V:243:SER:OG	2.15	0.46
2:U:225:GLY:O	2:U:233:SER:HA	2.16	0.46
1:B:13:GLY:O	1:B:14:CYS:O	2.33	0.46
1:B:123:PHE:N	1:B:123:PHE:HD1	2.12	0.46
1:A:86:ASN:C	1:A:86:ASN:ND2	2.63	0.46
2:U:1:LEU:HD23	2:U:74:ASN:OD1	2.16	0.46
2:V:198:ASN:HB2	2:V:203:CYS:HB2	1.98	0.46
2:V:25:ARG:N	2:V:77:ASN:HD22	2.14	0.45
2:U:148:LEU:CB	2:U:149:PRO:HD2	2.34	0.45
1:B:91:ASP:OD1	1:B:95:LEU:N	2.42	0.45
2:V:187:PRO:CD	2:V:214:ARG:HH21	2.25	0.45
2:V:69:THR:O	2:V:69:THR:HG23	2.17	0.45
2:U:31:GLU:O	2:U:37:GLU:HA	2.16	0.45
2:U:148:LEU:HB3	2:U:149:PRO:CD	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLY:O	1:B:14:CYS:C	2.55	0.45
2:V:225:GLY:HA2	2:V:260:VAL:CG1	2.46	0.45
1:B:86:ASN:O	1:B:89:ARG:HB2	2.17	0.45
2:V:101:SER:CB	2:V:141:TYR:H	2.25	0.45
2:V:136:LEU:HD21	2:V:254:PHE:HA	1.98	0.45
2:V:171:TYR:O	2:V:172:THR:C	2.55	0.45
2:V:175:ASN:N	2:V:175:ASN:ND2	2.65	0.45
1:A:60:ARG:HA	1:A:60:ARG:HD3	1.83	0.44
1:B:91:ASP:OD1	1:B:91:ASP:C	2.55	0.44
2:V:24:CYS:HB2	2:V:76:CYS:SG	2.57	0.44
2:V:198:ASN:HB3	2:V:199:ASN:H	1.64	0.44
2:V:137:LYS:HE2	2:V:137:LYS:HA	1.99	0.44
2:U:55:MET:HG2	2:U:66:LEU:HD12	1.99	0.44
2:U:260:VAL:O	2:U:261:SER:C	2.54	0.44
1:B:74:ALA:C	1:B:76:ASN:N	2.69	0.44
2:U:23:LEU:HB2	2:U:46:ALA:HB3	2.00	0.44
2:U:193:TYR:CE2	2:U:272:SER:HB2	2.52	0.44
1:B:28:ARG:HH12	2:V:136:LEU:HD22	1.83	0.44
2:V:7:GLU:HB2	2:V:10:GLN:OE1	2.18	0.44
1:A:55:ASN:OD1	1:A:105:ASN:ND2	2.50	0.44
2:U:25:ARG:NH1	2:U:27:THR:OG1	2.49	0.44
2:U:52:ASN:OD1	2:U:70:VAL:HG22	2.17	0.44
1:B:10:SER:CB	1:B:20:CYS:H	2.29	0.44
1:B:12:CYS:O	1:B:14:CYS:N	2.51	0.44
2:U:29:LEU:HD12	2:U:66:LEU:HD23	2.00	0.44
2:U:30:ARG:HD3	2:U:39:GLU:CB	2.39	0.43
1:B:66:ASP:OD2	1:B:69:GLY:N	2.51	0.43
1:A:64:ASN:ND2	1:A:65:THR:HG23	2.33	0.43
1:B:92:ALA:O	1:B:95:LEU:N	2.51	0.43
1:A:88:HIS:O	1:A:89:ARG:C	2.56	0.43
2:V:254:PHE:HB2	2:V:255:PRO:HD2	1.99	0.43
1:B:60:ARG:NH1	1:B:95:LEU:O	2.51	0.43
2:V:157:PHE:HA	2:V:239:CYS:O	2.18	0.43
2:U:98:SER:O	2:U:99:CYS:CB	2.64	0.43
1:B:10:SER:O	1:B:11:ASN:CB	2.65	0.43
1:B:18:GLY:N	1:B:35:PRO:HD3	2.33	0.43
2:V:60:GLY:CA	2:V:112:GLN:NE2	2.81	0.43
2:V:100:THR:HG23	2:V:102:LEU:HB3	1.97	0.43
2:V:157:PHE:CE1	2:V:238:GLY:HA3	2.54	0.43
2:U:204:SER:C	2:U:206:GLU:H	2.21	0.43
1:B:63:ALA:O	1:B:102:TYR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:198:ASN:OD1	2:V:202:GLY:HA3	2.19	0.43
2:V:60:GLY:O	2:V:112:GLN:NE2	2.51	0.43
2:U:14:VAL:O	1:B:62:LYS:HE3	2.19	0.43
2:U:114:LEU:HD23	2:U:115:GLN:N	2.29	0.43
2:V:203:CYS:HA	2:V:208:ALA:HB2	2.01	0.43
2:U:249:HIS:O	2:U:251:ALA:N	2.51	0.43
1:B:51:CYS:SG	1:B:131:ASP:C	2.97	0.43
1:A:33:SER:OG	1:A:33:SER:O	2.37	0.42
1:B:39:GLN:HE22	1:B:62:LYS:NZ	2.16	0.42
1:A:41:GLU:O	1:A:41:GLU:CG	2.66	0.42
2:U:5:GLN:HE21	2:U:5:GLN:C	2.23	0.42
1:A:76:ASN:HD22	1:A:76:ASN:HA	1.60	0.42
1:B:131:ASP:CG	1:B:132:CYS:H	2.22	0.42
2:V:178:PRO:O	2:V:180:LEU:HD23	2.19	0.42
1:A:111:ARG:HB2	1:A:112:PRO:CD	2.49	0.42
1:B:55:ASN:CG	1:B:56:GLY:N	2.72	0.42
2:V:75:LEU:HD23	2:V:75:LEU:HA	1.76	0.42
1:A:10:SER:O	1:A:11:ASN:C	2.58	0.42
2:V:126:VAL:O	2:V:126:VAL:CG2	2.68	0.42
2:U:18:ALA:HB2	2:V:35:ASP:OD1	2.19	0.42
2:V:221:LEU:N	2:V:271:ASN:HD22	2.18	0.42
2:U:26:THR:OG1	2:U:77:ASN:HB3	2.20	0.42
2:U:160:ASN:ND2	2:U:160:ASN:C	2.73	0.42
2:U:224:THR:O	2:U:260:VAL:HA	2.20	0.42
2:U:260:VAL:O	2:U:260:VAL:HG23	2.19	0.42
2:V:200:THR:C	2:V:204:SER:HB3	2.40	0.42
1:A:55:ASN:ND2	1:A:57:ASP:H	2.18	0.41
2:U:108:ARG:O	2:U:110:ARG:N	2.41	0.41
1:B:89:ARG:NH2	1:B:91:ASP:HB3	2.35	0.41
2:V:31:GLU:OE2	2:V:38:LEU:HD23	2.19	0.41
2:V:110:ARG:O	2:V:111:GLU:O	2.38	0.41
2:V:132:THR:O	2:V:133:GLU:C	2.58	0.41
1:B:21:VAL:O	1:B:21:VAL:HG22	2.20	0.41
1:B:92:ALA:O	1:B:95:LEU:HB2	2.21	0.41
1:B:89:ARG:HE	1:B:89:ARG:HB3	1.72	0.41
2:U:171:TYR:CD2	2:U:174:CYS:HB3	2.56	0.41
2:U:93:TYR:HE1	2:U:117:ARG:HE	1.68	0.41
2:V:211:ILE:O	2:V:211:ILE:HG13	2.20	0.41
1:A:56:GLY:O	1:A:59:TYR:N	2.42	0.41
1:A:116:VAL:HG21	1:A:125:GLN:HB2	2.02	0.41
2:U:117:ARG:C	2:U:117:ARG:HD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:125:GLU:CG	2:U:143:ARG:HG2	2.40	0.41
2:V:122:HIS:CD2	2:V:168:CYS:HB3	2.55	0.41
2:U:171:TYR:CG	2:U:174:CYS:HB3	2.56	0.41
2:V:46:ALA:O	2:V:47:HIS:HB2	2.21	0.41
2:V:244:TRP:CH2	2:V:250:VAL:HA	2.55	0.41
2:U:33:GLN:HG2	2:U:34:ASP:OD1	2.21	0.41
2:U:220:CYS:HB2	2:U:270:CYS:CB	2.46	0.41
2:V:125:GLU:CD	2:V:143:ARG:HH21	2.24	0.41
2:V:158:HIS:HE1	2:V:213:CYS:HA	1.85	0.41
1:A:37:LYS:HD2	1:A:38:PHE:CZ	2.56	0.41
1:B:57:ASP:O	1:B:60:ARG:NH2	2.54	0.41
2:V:111:GLU:HB3	2:V:112:GLN:H	1.70	0.41
2:V:207:GLU:CD	2:V:207:GLU:N	2.74	0.41
2:U:195:CYS:HB3	2:U:237:ARG:HG2	2.02	0.40
2:V:140:ASP:HB3	2:V:141:TYR:CD1	2.57	0.40
1:A:106:PRO:HD2	1:A:113:TRP:CZ2	2.56	0.40
2:U:193:TYR:HD2	2:U:271:ASN:HD21	1.68	0.40
1:B:95:LEU:HD22	1:B:106:PRO:CB	2.50	0.40
2:V:182:LEU:C	2:V:184:SER:N	2.73	0.40
1:A:70:ARG:HA	1:A:71:PRO:HD3	1.92	0.40
2:U:193:TYR:O	2:U:238:GLY:HA2	2.21	0.40
1:B:70:ARG:HE	1:B:70:ARG:HB2	1.66	0.40
2:V:198:ASN:HD22	2:V:198:ASN:HA	1.56	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	122/134 (91%)	91 (75%)	23 (19%)	8 (7%)	1	9
1	B	123/134 (92%)	86 (70%)	23 (19%)	14 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	U	252/277 (91%)	196 (78%)	41 (16%)	15 (6%)	1	12
2	V	254/277 (92%)	191 (75%)	37 (15%)	26 (10%)	0	3
All	All	751/822 (91%)	564 (75%)	124 (16%)	63 (8%)	1	5

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	109	GLN
1	A	129	VAL
2	U	78	ARG
2	U	134	ARG
2	U	151	CYS
2	U	249	HIS
2	U	250	VAL
2	U	255	PRO
2	U	258	LEU
2	U	273	PRO
1	B	11	ASN
1	B	13	GLY
1	B	14	CYS
1	B	24	LYS
1	B	93	ILE
1	B	95	LEU
1	B	128	MET
1	B	129	VAL
2	V	9	ASN
2	V	22	ASP
2	V	78	ARG
2	V	79	PRO
2	V	94	LEU
2	V	107	GLU
2	V	111	GLU
2	V	113	SER
2	V	120	THR
2	V	132	THR
2	V	177	GLY
2	V	178	PRO
2	V	199	ASN
2	V	209	SER
2	V	249	HIS

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Mol	Chain	Res	Type
2	V	259	ASN
1	A	99	LYS
2	U	6	CYS
2	U	8	SER
2	U	79	PRO
2	U	99	CYS
2	U	109	GLY
1	B	18	GLY
1	B	54	GLY
2	V	180	LEU
2	V	183	GLN
1	A	28	ARG
1	A	57	ASP
2	U	187	PRO
1	B	75	TRP
1	B	88	HIS
1	B	92	ALA
2	V	34	ASP
2	V	172	THR
2	V	197	GLY
1	A	77	ALA
1	A	110	LYS
1	B	53	HIS
2	V	47	HIS
2	V	75	LEU
2	V	119	PRO
2	V	198	ASN
2	V	117	ARG
2	U	179	VAL

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	106/113 (94%)	83 (78%)	23 (22%)	1	5
1	B	107/113 (95%)	86 (80%)	21 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	U	228/238 (96%)	173 (76%)	55 (24%)	0	3	
2	V	230/238 (97%)	180 (78%)	50 (22%)	1	5	
All	All	671/702 (96%)	522 (78%)	149 (22%)	1	4	

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	27	SER
1	A	28	ARG
1	A	30	ARG
1	A	31	ARG
1	A	36	ARG
1	A	45	ILE
1	A	55	ASN
1	A	57	ASP
1	A	64	ASN
1	A	76	ASN
1	A	86	ASN
1	A	91	ASP
1	A	97	LEU
1	A	109	GLN
1	A	110	LYS
1	A	111	ARG
1	A	118	ILE
1	A	120	LEU
1	A	124	VAL
1	A	127	CYS
1	A	129	VAL
1	A	132	CYS
2	U	1	LEU
2	U	3	CYS
2	U	5	GLN
2	U	13	LEU
2	U	16	GLU
2	U	21	GLN
2	U	28	VAL
2	U	29	LEU
2	U	37	GLU
2	U	38	LEU
2	U	39	GLU

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Mol	Chain	Res	Type
2	U	40	VAL
2	U	43	ARG
2	U	47	HIS
2	U	51	THR
2	U	57	TYR
2	U	62	MET
2	U	63	ILE
2	U	64	ILE
2	U	67	THR
2	U	77	ASN
2	U	93	TYR
2	U	100	THR
2	U	110	ARG
2	U	117	ARG
2	U	124	ILE
2	U	126	VAL
2	U	132	THR
2	U	134	ARG
2	U	151	CYS
2	U	160	ASN
2	U	161	GLN
2	U	162	THR
2	U	166	LEU
2	U	171	TYR
2	U	173	HIS
2	U	175	ASN
2	U	179	VAL
2	U	182	LEU
2	U	195	CYS
2	U	207	GLU
2	U	217	MET
2	U	221	LEU
2	U	224	THR
2	U	226	LEU
2	U	235	THR
2	U	248	SER
2	U	257	HIS
2	U	258	LEU
2	U	259	ASN
2	U	261	SER
2	U	263	SER
2	U	265	CYS

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Mol	Chain	Res	Type
2	U	266	HIS
2	U	271	ASN
1	B	12	CYS
1	B	19	VAL
1	B	20	CYS
1	B	21	VAL
1	B	28	ARG
1	B	30	ARG
1	B	33	SER
1	B	50	THR
1	B	53	HIS
1	B	67	THR
1	B	70	ARG
1	B	86	ASN
1	B	89	ARG
1	B	93	ILE
1	B	97	LEU
1	B	103	CYS
1	B	108	ASN
1	B	111	ARG
1	B	118	ILE
1	B	123	PHE
1	B	129	VAL
2	V	1	LEU
2	V	10	GLN
2	V	16	GLU
2	V	19	LEU
2	V	29	LEU
2	V	36	ARG
2	V	40	VAL
2	V	43	ARG
2	V	53	ARG
2	V	54	THR
2	V	56	SER
2	V	58	ARG
2	V	64	ILE
2	V	66	LEU
2	V	67	THR
2	V	71	CYS
2	V	73	THR
2	V	78	ARG
2	V	93	TYR

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Mol	Chain	Res	Type
2	V	99	CYS
2	V	100	THR
2	V	101	SER
2	V	103	ASP
2	V	106	CYS
2	V	110	ARG
2	V	132	THR
2	V	134	ARG
2	V	138	ASP
2	V	151	CYS
2	V	161	GLN
2	V	162	THR
2	V	166	LEU
2	V	173	HIS
2	V	174	CYS
2	V	175	ASN
2	V	183	GLN
2	V	184	SER
2	V	191	GLN
2	V	195	CYS
2	V	198	ASN
2	V	203	CYS
2	V	210	LEU
2	V	218	ASN
2	V	237	ARG
2	V	241	THR
2	V	246	GLN
2	V	250	VAL
2	V	254	PHE
2	V	272	SER
2	V	274	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	55	ASN
1	A	64	ASN
1	A	76	ASN
1	A	86	ASN
1	A	88	HIS
1	A	100	HIS

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Mol	Chain	Res	Type
1	A	105	ASN
1	A	109	GLN
2	U	2	GLN
2	U	5	GLN
2	U	10	GLN
2	U	271	ASN
1	B	39	GLN
1	B	55	ASN
1	B	76	ASN
1	B	100	HIS
1	B	122	GLN
2	V	104	GLN
2	V	112	GLN
2	V	122	HIS
2	V	161	GLN
2	V	173	HIS
2	V	175	ASN
2	V	199	ASN
2	V	218	ASN
2	V	246	GLN
2	V	249	HIS
2	V	257	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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
3	NAG	U	1259	2	14,14,15	0.68	1 (7%)	17,19,21	2.56	5 (29%)
3	NAG	U	1053	-	14,14,15	1.06	1 (7%)	17,19,21	1.57	3 (17%)
3	NAG	U	1170	2	14,14,15	0.77	0	17,19,21	1.42	3 (17%)
3	NAG	U	1052	2	14,14,15	0.80	1 (7%)	17,19,21	1.72	4 (23%)
3	NAG	V	1160	2	14,14,15	0.96	1 (7%)	17,19,21	2.13	6 (35%)
3	NAG	V	1259	2	14,14,15	1.10	1 (7%)	17,19,21	1.85	5 (29%)
3	NAG	V	1170	2	14,14,15	0.46	0	17,19,21	1.28	2 (11%)
3	NAG	U	1160	-	14,14,15	0.79	1 (7%)	17,19,21	1.91	2 (11%)
3	NAG	V	1053	-	14,14,15	0.63	0	17,19,21	1.31	3 (17%)
3	NAG	V	1052	2	14,14,15	0.40	0	17,19,21	1.78	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	U	1259	2	-	4/6/23/26	0/1/1/1
3	NAG	U	1053	-	-	0/6/23/26	0/1/1/1
3	NAG	U	1170	2	-	3/6/23/26	0/1/1/1
3	NAG	U	1052	2	-	2/6/23/26	0/1/1/1
3	NAG	V	1160	2	-	4/6/23/26	0/1/1/1
3	NAG	V	1259	2	-	4/6/23/26	0/1/1/1
3	NAG	V	1170	2	-	0/6/23/26	0/1/1/1
3	NAG	U	1160	-	-	2/6/23/26	0/1/1/1
3	NAG	V	1053	-	-	4/6/23/26	0/1/1/1
3	NAG	V	1052	2	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	1160	NAG	C1-C2	3.08	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1053	NAG	C1-C2	2.98	1.56	1.52
3	U	1052	NAG	C1-C2	2.46	1.55	1.52
3	V	1259	NAG	C1-C2	2.45	1.55	1.52
3	U	1160	NAG	C1-C2	2.24	1.55	1.52
3	U	1259	NAG	C1-C2	2.14	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	1259	NAG	C1-O5-C5	7.51	122.25	112.19
3	U	1160	NAG	C1-O5-C5	6.37	120.73	112.19
3	U	1052	NAG	C3-C4-C5	-4.81	101.52	110.23
3	U	1259	NAG	O5-C1-C2	4.59	118.40	111.29
3	V	1052	NAG	C4-C3-C2	-4.58	104.30	111.02
3	V	1160	NAG	C2-N2-C7	4.24	128.58	122.90
3	V	1170	NAG	C1-O5-C5	4.14	117.74	112.19
3	U	1053	NAG	C2-N2-C7	3.96	128.21	122.90
3	V	1259	NAG	C1-O5-C5	3.85	117.35	112.19
3	V	1259	NAG	C2-N2-C7	3.74	127.92	122.90
3	V	1160	NAG	C1-C2-N2	3.70	116.26	110.43
3	V	1160	NAG	C4-C3-C2	-3.49	105.91	111.02
3	V	1160	NAG	C8-C7-N2	3.33	121.64	116.12
3	V	1052	NAG	C1-O5-C5	3.19	116.46	112.19
3	U	1160	NAG	C4-C3-C2	-2.90	106.77	111.02
3	U	1259	NAG	C4-C3-C2	-2.83	106.88	111.02
3	V	1053	NAG	O5-C1-C2	-2.69	107.13	111.29
3	V	1052	NAG	O7-C7-C8	-2.60	117.42	122.05
3	U	1170	NAG	O5-C1-C2	-2.59	107.28	111.29
3	U	1170	NAG	C4-C3-C2	2.55	114.75	111.02
3	U	1259	NAG	C1-C2-N2	2.35	114.13	110.43
3	V	1052	NAG	C8-C7-N2	2.33	119.98	116.12
3	V	1053	NAG	C8-C7-N2	2.33	119.98	116.12
3	U	1053	NAG	C1-C2-N2	2.25	113.98	110.43
3	V	1160	NAG	O5-C1-C2	-2.23	107.83	111.29
3	V	1259	NAG	C1-C2-N2	2.19	113.89	110.43
3	U	1052	NAG	O4-C4-C5	2.19	114.72	109.32
3	U	1170	NAG	C2-N2-C7	2.16	125.80	122.90
3	V	1259	NAG	O7-C7-C8	-2.15	118.22	122.05
3	U	1052	NAG	O5-C5-C4	-2.15	105.60	110.83
3	V	1259	NAG	C8-C7-N2	2.14	119.67	116.12
3	V	1170	NAG	O5-C5-C6	2.12	111.79	107.66
3	U	1259	NAG	C8-C7-N2	2.09	119.58	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	1053	NAG	O7-C7-C8	-2.08	118.35	122.05
3	U	1052	NAG	C6-C5-C4	2.07	118.11	113.02
3	U	1053	NAG	C4-C3-C2	2.05	114.03	111.02
3	V	1160	NAG	O5-C5-C6	2.02	111.60	107.66

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	U	1160	NAG	O5-C5-C6-O6
3	U	1052	NAG	O5-C5-C6-O6
3	V	1160	NAG	O5-C5-C6-O6
3	V	1053	NAG	O5-C5-C6-O6
3	U	1160	NAG	C4-C5-C6-O6
3	U	1259	NAG	O5-C5-C6-O6
3	U	1259	NAG	C4-C5-C6-O6
3	U	1052	NAG	C4-C5-C6-O6
3	V	1053	NAG	C4-C5-C6-O6
3	U	1259	NAG	C8-C7-N2-C2
3	U	1259	NAG	O7-C7-N2-C2
3	V	1052	NAG	C8-C7-N2-C2
3	V	1052	NAG	O7-C7-N2-C2
3	V	1053	NAG	C8-C7-N2-C2
3	V	1053	NAG	O7-C7-N2-C2
3	V	1160	NAG	C8-C7-N2-C2
3	V	1160	NAG	O7-C7-N2-C2
3	V	1259	NAG	C8-C7-N2-C2
3	V	1259	NAG	O7-C7-N2-C2
3	U	1170	NAG	O5-C5-C6-O6
3	V	1259	NAG	O5-C5-C6-O6
3	V	1160	NAG	C4-C5-C6-O6
3	U	1170	NAG	C4-C5-C6-O6
3	V	1259	NAG	C4-C5-C6-O6
3	U	1170	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	1053	NAG	1	0
3	U	1052	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	V	1160	NAG	1	0
3	V	1259	NAG	8	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	124/134 (92%)	-0.23	0	100	100	24, 34, 49, 72	0
1	B	125/134 (93%)	-0.16	1 (0%)	86	78	18, 31, 51, 77	0
2	U	258/277 (93%)	0.19	12 (4%)	31	19	11, 35, 48, 56	0
2	V	260/277 (93%)	0.08	7 (2%)	54	39	2, 34, 43, 50	0
All	All	767/822 (93%)	0.03	20 (2%)	56	40	2, 34, 47, 77	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	201	LEU	6.0
2	V	199	ASN	5.6
2	U	274	THR	4.8
2	V	200	THR	4.8
2	V	202	GLY	4.2
2	V	274	THR	3.9
2	U	206	GLU	3.2
2	U	209	SER	2.8
2	V	197	GLY	2.8
2	U	266	HIS	2.6
1	B	130	HIS	2.6
2	U	200	THR	2.5
2	U	107	GLU	2.4
2	U	81	PRO	2.3
2	U	198	ASN	2.3
2	U	208	ALA	2.2
2	V	203	CYS	2.2
2	U	20	GLY	2.2
2	U	197	GLY	2.1
2	V	204	SER	2.1

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 ⓘ

There are no monosaccharides in this entry.

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. 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
3	NAG	U	1052	14/15	0.62	0.28	60,66,67,72	0
3	NAG	U	1053	14/15	0.62	0.28	78,81,82,83	0
3	NAG	V	1259	14/15	0.68	0.28	71,78,85,85	0
3	NAG	V	1053	14/15	0.69	0.23	78,80,83,84	0
3	NAG	V	1160	14/15	0.69	0.44	62,67,73,74	0
3	NAG	U	1160	14/15	0.69	0.46	70,77,79,80	0
3	NAG	U	1259	14/15	0.85	0.30	69,77,78,78	0
3	NAG	U	1170	14/15	0.86	0.19	61,67,69,71	0
3	NAG	V	1052	14/15	0.90	0.14	59,66,68,73	0
3	NAG	V	1170	14/15	0.93	0.15	58,63,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

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