



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:09 PM GMT

PDB ID : 2O26
Title : Structure of a class III RTK signaling assembly
Authors : Liu, H.; Chen, X.; Focia, P.J.; He, X.
Deposited on : 2006-11-29
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

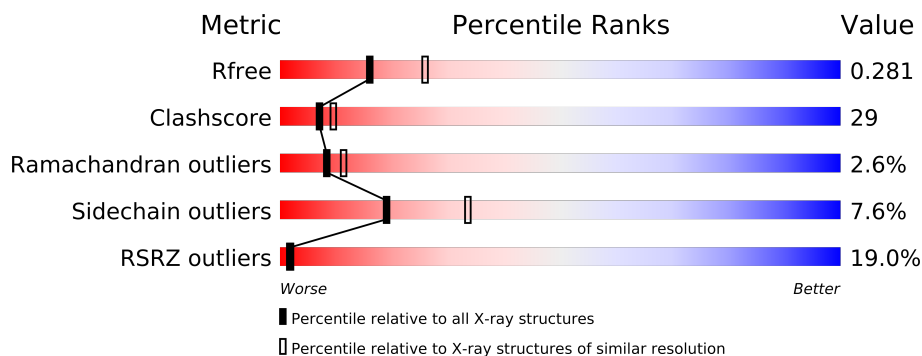
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	145	
1	B	145	
1	E	145	
1	F	145	
2	U	290	
2	W	290	
2	X	290	
2	Y	290	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15104 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 Kit ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1140	722	189	220	9			
1	B	139	Total	C	N	O	S	0	0	0
			1090	692	174	215	9			
1	E	139	Total	C	N	O	S	0	0	0
			1090	692	174	215	9			
1	F	139	Total	C	N	O	S	0	0	0
			1090	692	174	215	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	HIS	-	EXPRESSION TAG	UNP P20826
A	143	HIS	-	EXPRESSION TAG	UNP P20826
A	144	HIS	-	EXPRESSION TAG	UNP P20826
A	145	HIS	-	EXPRESSION TAG	UNP P20826
A	146	HIS	-	EXPRESSION TAG	UNP P20826
A	147	HIS	-	EXPRESSION TAG	UNP P20826
B	142	HIS	-	EXPRESSION TAG	UNP P20826
B	143	HIS	-	EXPRESSION TAG	UNP P20826
B	144	HIS	-	EXPRESSION TAG	UNP P20826
B	145	HIS	-	EXPRESSION TAG	UNP P20826
B	146	HIS	-	EXPRESSION TAG	UNP P20826
B	147	HIS	-	EXPRESSION TAG	UNP P20826
E	142	HIS	-	EXPRESSION TAG	UNP P20826
E	143	HIS	-	EXPRESSION TAG	UNP P20826
E	144	HIS	-	EXPRESSION TAG	UNP P20826
E	145	HIS	-	EXPRESSION TAG	UNP P20826
E	146	HIS	-	EXPRESSION TAG	UNP P20826
E	147	HIS	-	EXPRESSION TAG	UNP P20826
F	142	HIS	-	EXPRESSION TAG	UNP P20826
F	143	HIS	-	EXPRESSION TAG	UNP P20826
F	144	HIS	-	EXPRESSION TAG	UNP P20826

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Chain	Residue	Modelled	Actual	Comment	Reference
F	145	HIS	-	EXPRESSION TAG	UNP P20826
F	146	HIS	-	EXPRESSION TAG	UNP P20826
F	147	HIS	-	EXPRESSION TAG	UNP P20826

- Molecule 2 is a protein called Mast/stem cell growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	275	Total	C	N	O	S	0	0	0
			2164	1369	372	411	12			
2	Y	275	Total	C	N	O	S	0	0	0
			2164	1369	372	411	12			
2	U	275	Total	C	N	O	S	0	0	0
			2164	1369	372	411	12			
2	W	275	Total	C	N	O	S	0	0	0
			2164	1369	372	411	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	146	GLN	ASN	ENGINEERED	UNP P05532
Y	146	GLN	ASN	ENGINEERED	UNP P05532
U	146	GLN	ASN	ENGINEERED	UNP P05532
W	146	GLN	ASN	ENGINEERED	UNP P05532

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	X	3	Total	C	N	O	0	0
			38	22	2	14		
3	Y	3	Total	C	N	O	0	0
			38	22	2	14		
3	U	3	Total	C	N	O	0	0
			38	22	2	14		
3	W	3	Total	C	N	O	0	0
			38	22	2	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	146	GLN	ASN	ENGINEERED	UNP P05532
Y	146	GLN	ASN	ENGINEERED	UNP P05532
U	146	GLN	ASN	ENGINEERED	UNP P05532

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Chain	Residue	Modelled	Actual	Comment	Reference
W	146	GLN	ASN	ENGINEERED	UNP P05532

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	X	3	Total	C	N	O	0	0
			39	22	2	15		
4	Y	3	Total	C	N	O	0	0
			39	22	2	15		
4	U	3	Total	C	N	O	0	0
			39	22	2	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	146	GLN	ASN	ENGINEERED	UNP P05532
Y	146	GLN	ASN	ENGINEERED	UNP P05532
U	146	GLN	ASN	ENGINEERED	UNP P05532

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	W	3	Total	C	N	O	0	0
			39	22	2	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	146	GLN	ASN	ENGINEERED	UNP P05532

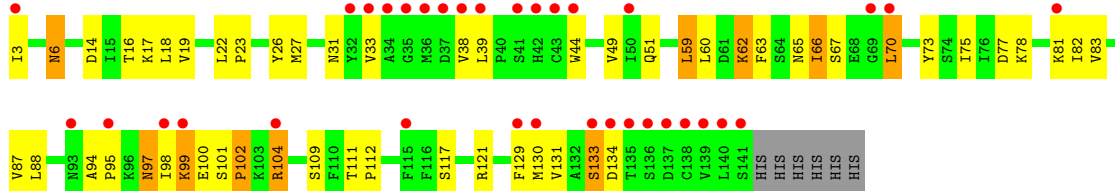
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	171	Total	O	0	0
			171	171		
6	B	144	Total	O	0	0
			144	144		
6	E	152	Total	O	0	0
			152	152		
6	F	143	Total	O	0	0
			143	143		

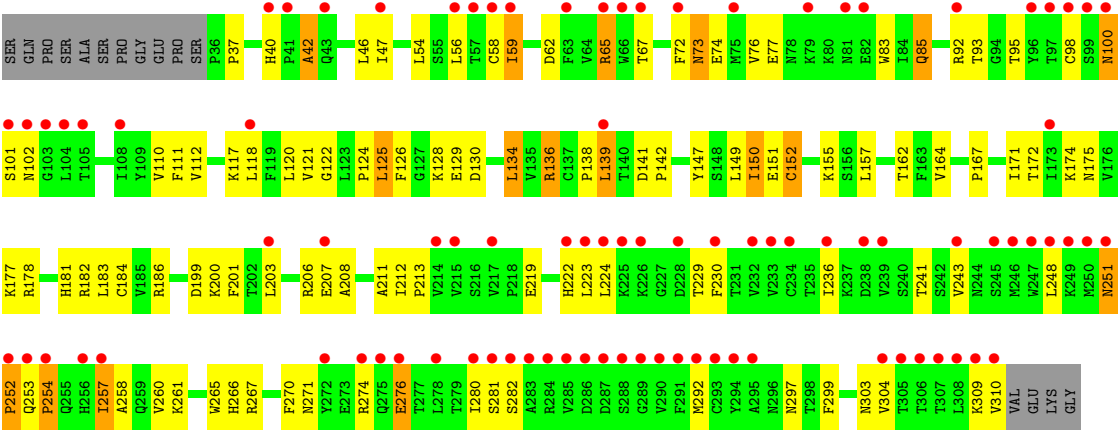
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	U	270	Total 270	O 270	0	0
6	W	267	Total 267	O 267	0	0
6	X	273	Total 273	O 273	0	0
6	Y	310	Total 310	O 310	0	0



Chain W: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.85Å 200.15Å 82.02Å 90.00° 91.42° 90.00°	Depositor
Resolution (Å)	19.93 – 2.50 48.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.93-2.50) 96.8 (48.46-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.270 0.251 , 0.281	Depositor DCC
R_{free} test set	4160 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 75.7	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 82592 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15104	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: FUL, NAG, NDG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/1164	0.70	1/1579 (0.1%)
1	B	0.48	1/1109 (0.1%)	0.67	0/1504
1	E	0.40	0/1109	0.64	1/1504 (0.1%)
1	F	0.41	0/1109	0.65	1/1504 (0.1%)
2	U	0.38	0/2214	0.72	1/3011 (0.0%)
2	W	0.35	0/2214	0.64	0/3011
2	X	0.37	0/2214	0.69	2/3011 (0.1%)
2	Y	0.36	0/2214	0.65	0/3011
All	All	0.39	1/13347 (0.0%)	0.67	6/18135 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	SER	CA-CB	7.77	1.64	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	138	PRO	CA-N-CD	-14.78	90.81	111.50
2	X	41	PRO	CA-N-CD	-12.45	94.08	111.50
1	A	102	PRO	CA-N-CD	-8.86	99.09	111.50
1	F	134	ASP	C-N-CA	-5.22	108.64	121.70
2	X	208	ALA	N-CA-C	-5.22	96.92	111.00
1	E	134	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

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	1140	0	1121	62	0
1	B	1090	0	1086	68	0
1	E	1090	0	1086	65	0
1	F	1090	0	1086	54	0
2	U	2164	0	2140	139	0
2	W	2164	0	2140	117	0
2	X	2164	0	2140	145	0
2	Y	2164	0	2140	125	0
3	U	38	0	34	3	0
3	W	38	0	34	0	0
3	X	38	0	34	1	0
3	Y	38	0	34	2	0
4	U	39	0	34	0	0
4	X	39	0	34	1	0
4	Y	39	0	34	1	0
5	W	39	0	34	2	0
6	A	171	0	0	24	0
6	B	144	0	0	32	0
6	E	152	0	0	24	0
6	F	143	0	0	23	0
6	U	270	0	0	37	0
6	W	267	0	0	35	0
6	X	273	0	0	50	0
6	Y	310	0	0	46	0
All	All	15104	0	13211	761	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 29.

All (761) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:W:184:CYS:HB2	6:W:321:HOH:O	1.50	1.08
2:U:251:ASN:HB2	2:U:252:PRO:HD3	1.36	1.06
2:Y:251:ASN:HB2	2:Y:252:PRO:HD3	1.34	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:W:251:ASN:HB2	2:W:252:PRO:HD3	1.37	1.06
2:X:251:ASN:HB2	2:X:252:PRO:HD3	1.35	1.03
1:B:48:MET:HB3	6:B:195:HOH:O	1.59	1.02
2:W:150:ILE:HD12	2:W:151:GLU:H	1.22	1.00
2:X:150:ILE:HD12	2:X:151:GLU:H	1.24	1.00
2:U:150:ILE:HD12	2:U:151:GLU:H	1.31	0.96
2:X:219:GLU:HB2	2:X:222:HIS:CE1	2.01	0.96
1:A:66:ILE:HG23	1:A:67:SER:H	1.31	0.96
1:F:19:VAL:HA	6:F:233:HOH:O	1.65	0.96
1:F:66:ILE:HG23	1:F:67:SER:H	1.30	0.95
2:U:200:LYS:HB3	6:U:331:HOH:O	1.66	0.94
2:U:184:CYS:HB2	6:U:331:HOH:O	1.65	0.94
1:E:66:ILE:HG23	1:E:67:SER:H	1.32	0.93
1:A:8:VAL:HB	6:A:162:HOH:O	1.66	0.93
1:A:76:ILE:HG13	6:A:261:HOH:O	1.67	0.92
2:X:53:THR:HG23	6:X:390:HOH:O	1.67	0.92
2:Y:150:ILE:HD12	2:Y:151:GLU:H	1.33	0.92
2:W:229:THR:HG22	2:W:281:SER:HA	1.53	0.91
1:B:66:ILE:HG23	1:B:67:SER:H	1.33	0.90
2:Y:229:THR:HG22	2:Y:281:SER:HA	1.54	0.90
2:U:146:GLN:OE1	2:U:195:TRP:CZ2	2.27	0.88
2:X:229:THR:HG22	2:X:281:SER:HA	1.56	0.87
2:U:110:VAL:HG21	6:U:415:HOH:O	1.73	0.87
2:W:200:LYS:HB3	6:W:321:HOH:O	1.75	0.87
2:U:229:THR:HG22	2:U:281:SER:HA	1.58	0.86
2:X:236:ILE:HD12	2:X:236:ILE:N	1.91	0.85
2:W:150:ILE:HD12	2:W:151:GLU:N	1.91	0.84
2:Y:150:ILE:HG21	6:Y:624:HOH:O	1.78	0.83
2:X:125:LEU:HD21	2:X:135:VAL:HA	1.58	0.83
2:Y:56:LEU:HG	6:Y:368:HOH:O	1.78	0.83
2:U:150:ILE:HD12	2:U:151:GLU:N	1.94	0.81
1:A:75:ILE:HB	6:A:261:HOH:O	1.81	0.81
2:X:276:GLU:HB2	6:X:511:HOH:O	1.82	0.80
1:F:22:LEU:HB2	6:F:233:HOH:O	1.80	0.80
2:W:157:LEU:HG	6:W:474:HOH:O	1.82	0.79
2:X:41:PRO:HD2	6:X:498:HOH:O	1.83	0.79
1:E:14:ASP:HB3	1:E:75:ILE:HD12	1.64	0.79
1:A:14:ASP:HB3	1:A:75:ILE:HD12	1.65	0.79
2:X:207:GLU:CD	2:X:207:GLU:H	1.87	0.78
2:U:138:PRO:HD3	2:U:169:ALA:O	1.82	0.78
2:X:310:VAL:HG12	6:X:397:HOH:O	1.82	0.78
1:B:14:ASP:HB3	1:B:75:ILE:HD12	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:150:ILE:HD12	2:X:151:GLU:N	2.00	0.77
1:F:14:ASP:HB3	1:F:75:ILE:HD12	1.66	0.77
2:U:260:VAL:HG11	2:U:276:GLU:HG3	1.66	0.77
1:A:76:ILE:HG22	6:A:199:HOH:O	1.84	0.77
1:E:99:LYS:HB3	2:U:77:GLU:HB3	1.66	0.76
2:W:260:VAL:HG11	2:W:276:GLU:HG3	1.67	0.76
1:A:6:ASN:HD22	1:A:6:ASN:N	1.83	0.76
1:F:130:MET:HE1	6:F:165:HOH:O	1.85	0.75
2:Y:125:LEU:HD13	2:Y:203:LEU:HB2	1.68	0.75
1:F:33:VAL:HB	6:F:273:HOH:O	1.86	0.74
2:Y:260:VAL:HG11	2:Y:276:GLU:HG3	1.69	0.74
2:U:185:VAL:HG12	6:U:574:HOH:O	1.86	0.74
2:W:174:LYS:HE2	6:W:417:HOH:O	1.87	0.74
2:W:172:THR:HB	6:W:417:HOH:O	1.86	0.74
1:E:97:ASN:OD1	2:U:75:MET:HG2	1.88	0.74
2:X:219:GLU:CB	2:X:222:HIS:CE1	2.71	0.73
2:U:125:LEU:HD13	2:U:203:LEU:HB2	1.71	0.73
2:X:260:VAL:HG11	2:X:276:GLU:HG3	1.71	0.72
2:Y:213:PRO:HB3	6:Y:383:HOH:O	1.89	0.72
1:E:6:ASN:N	1:E:6:ASN:HD22	1.87	0.72
2:W:206:ARG:HA	6:W:493:HOH:O	1.89	0.72
2:Y:121:VAL:HG12	2:Y:122:GLY:N	2.04	0.72
1:B:6:ASN:N	1:B:6:ASN:HD22	1.87	0.72
1:A:66:ILE:HG23	1:A:67:SER:N	2.05	0.72
1:F:66:ILE:HG23	1:F:67:SER:N	2.04	0.72
2:Y:236:ILE:N	2:Y:236:ILE:HD12	2.05	0.72
2:W:236:ILE:HD12	2:W:236:ILE:N	2.05	0.72
2:Y:121:VAL:HG12	2:Y:122:GLY:H	1.54	0.71
2:X:139:LEU:HB3	6:X:455:HOH:O	1.90	0.71
2:Y:70:THR:HG21	6:Y:340:HOH:O	1.90	0.70
1:B:139:VAL:HG12	1:B:140:LEU:H	1.56	0.70
1:E:23:PRO:HD3	6:E:182:HOH:O	1.91	0.70
2:U:261:LYS:HA	2:U:261:LYS:HE2	1.73	0.70
2:U:54:LEU:HD21	6:U:415:HOH:O	1.91	0.70
2:Y:40:HIS:O	2:Y:42:ALA:N	2.25	0.70
2:U:236:ILE:N	2:U:236:ILE:HD12	2.06	0.70
2:Y:150:ILE:HD12	2:Y:151:GLU:N	2.06	0.70
2:Y:183:LEU:HD21	6:Y:350:HOH:O	1.91	0.70
1:F:78:LYS:HE3	2:W:266:HIS:O	1.92	0.70
2:U:207:GLU:H	2:U:207:GLU:CD	1.95	0.69
1:A:5:GLY:C	1:A:6:ASN:HD22	1.97	0.69
1:E:66:ILE:HG23	1:E:67:SER:N	2.08	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:W:93:THR:HA	6:W:539:HOH:O	1.93	0.69
2:U:102:ASN:HB3	6:U:360:HOH:O	1.93	0.69
2:Y:261:LYS:HA	2:Y:261:LYS:HE2	1.74	0.69
2:X:292:MET:HE2	6:X:497:HOH:O	1.94	0.68
2:U:125:LEU:HB3	2:U:203:LEU:HA	1.76	0.68
2:W:136:ARG:HD3	6:W:381:HOH:O	1.94	0.68
2:X:142:PRO:HD2	6:X:501:HOH:O	1.93	0.68
2:U:243:VAL:HB	6:U:363:HOH:O	1.94	0.68
2:X:118:LEU:HD22	6:X:455:HOH:O	1.93	0.67
2:W:125:LEU:HD13	2:W:203:LEU:HB2	1.75	0.67
2:W:139:LEU:HD23	2:W:139:LEU:H	1.58	0.67
2:U:79:LYS:HE2	6:U:494:HOH:O	1.94	0.67
2:U:220:THR:HG23	6:U:481:HOH:O	1.94	0.67
1:E:99:LYS:HB3	2:U:77:GLU:CB	2.25	0.67
1:E:113:GLU:HB2	6:E:211:HOH:O	1.94	0.67
2:U:134:LEU:HD13	2:U:136:ARG:HG2	1.77	0.66
2:Y:139:LEU:N	2:Y:139:LEU:HD23	2.10	0.66
2:Y:139:LEU:H	2:Y:139:LEU:HD23	1.60	0.66
1:F:17:LYS:HD2	6:F:248:HOH:O	1.95	0.66
2:X:141:ASP:HB2	6:X:319:HOH:O	1.95	0.66
2:W:139:LEU:HD23	2:W:139:LEU:N	2.10	0.66
2:U:37:PRO:HB3	2:U:98:CYS:SG	2.36	0.66
1:B:106:GLU:HA	6:B:227:HOH:O	1.95	0.66
2:U:278:LEU:HD23	6:U:386:HOH:O	1.95	0.66
2:U:56:LEU:HD21	6:U:415:HOH:O	1.96	0.66
2:W:261:LYS:HE2	2:W:261:LYS:HA	1.77	0.66
2:X:236:ILE:N	2:X:236:ILE:CD1	2.59	0.66
1:B:5:GLY:C	1:B:6:ASN:HD22	1.99	0.66
3:U:3:NAG:H61	6:U:543:HOH:O	1.95	0.66
1:B:66:ILE:HG23	1:B:67:SER:N	2.09	0.66
2:U:206:ARG:HG3	6:U:375:HOH:O	1.95	0.65
2:Y:196:LEU:HG	6:Y:617:HOH:O	1.97	0.65
2:Y:207:GLU:H	2:Y:207:GLU:CD	1.98	0.65
2:U:40:HIS:O	2:U:42:ALA:N	2.29	0.65
2:X:261:LYS:HA	2:X:261:LYS:HE2	1.79	0.65
1:E:99:LYS:HD3	2:U:77:GLU:OE1	1.96	0.65
2:U:230:PHE:HB2	6:U:351:HOH:O	1.96	0.65
2:Y:54:LEU:HD11	6:Y:560:HOH:O	1.95	0.64
1:E:63:PHE:HE2	6:F:154:HOH:O	1.80	0.64
2:Y:292:MET:HE2	6:Y:407:HOH:O	1.97	0.64
1:A:69:GLY:HA3	6:B:261:HOH:O	1.95	0.64
2:U:129:GLU:HB3	2:U:208:ALA:HB2	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:W:257:ILE:HD12	2:W:258:ALA:H	1.62	0.64
2:Y:40:HIS:HA	6:Y:315:HOH:O	1.97	0.64
6:B:155:HOH:O	2:Y:74:GLU:HA	1.97	0.64
2:Y:251:ASN:CB	2:Y:252:PRO:HD3	2.20	0.64
2:W:151:GLU:HG2	2:W:155:LYS:HB2	1.80	0.64
1:A:66:ILE:HD12	1:A:66:ILE:C	2.18	0.64
2:Y:157:LEU:HG	6:Y:350:HOH:O	1.95	0.64
2:Y:110:VAL:HG21	6:Y:560:HOH:O	1.98	0.64
2:X:40:HIS:O	2:X:42:ALA:N	2.30	0.64
1:B:66:ILE:HD12	1:B:66:ILE:C	2.19	0.64
1:E:66:ILE:C	1:E:66:ILE:HD12	2.18	0.64
2:U:131:SER:HB2	6:U:330:HOH:O	1.98	0.64
2:Y:163:PHE:HB3	6:Y:486:HOH:O	1.97	0.64
1:B:99:LYS:HD3	2:Y:77:GLU:OE1	1.98	0.64
2:X:139:LEU:HD23	2:X:139:LEU:N	2.12	0.64
2:W:62:ASP:HB2	2:W:100:ASN:HD21	1.63	0.64
2:U:41:PRO:HD3	6:U:476:HOH:O	1.97	0.64
2:X:139:LEU:H	2:X:139:LEU:HD23	1.62	0.63
2:Y:46:LEU:HD23	2:Y:46:LEU:C	2.17	0.63
2:U:36:PRO:HG2	6:U:484:HOH:O	1.96	0.63
2:W:251:ASN:CB	2:W:252:PRO:HD3	2.23	0.63
2:Y:151:GLU:HG2	2:Y:155:LYS:HB2	1.79	0.63
1:F:66:ILE:C	1:F:66:ILE:HD12	2.18	0.63
2:W:124:PRO:HB2	2:W:126:PHE:CE1	2.33	0.63
1:E:82:ILE:HA	6:E:154:HOH:O	1.99	0.63
2:Y:151:GLU:N	2:Y:157:LEU:HD11	2.14	0.63
2:X:151:GLU:N	2:X:157:LEU:HD11	2.14	0.63
2:X:221:SER:C	2:X:222:HIS:ND1	2.52	0.63
2:U:253:GLN:HG2	2:U:254:PRO:HD2	1.81	0.63
1:E:6:ASN:ND2	1:E:6:ASN:N	2.46	0.63
1:A:130:MET:HG3	6:A:308:HOH:O	1.98	0.63
1:B:81:LYS:HB3	6:B:148:HOH:O	1.99	0.62
1:E:132:ALA:HB1	6:E:215:HOH:O	1.98	0.62
1:E:33:VAL:HG13	6:E:236:HOH:O	1.99	0.62
2:U:139:LEU:N	2:U:139:LEU:HD23	2.14	0.62
2:X:253:GLN:HG2	2:X:254:PRO:HD2	1.80	0.62
3:U:3:NAG:H82	3:U:3:NAG:H3	1.82	0.62
2:Y:305:THR:HG23	6:Y:407:HOH:O	1.99	0.62
2:X:250:MET:HB3	6:X:471:HOH:O	1.99	0.62
2:X:62:ASP:HB2	2:X:100:ASN:HD21	1.65	0.62
1:A:121:ARG:HD2	6:A:193:HOH:O	2.00	0.62
1:E:13:LYS:HE2	6:E:272:HOH:O	1.98	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:ILE:HG12	6:A:215:HOH:O	1.98	0.62
2:W:40:HIS:O	2:W:42:ALA:N	2.32	0.61
2:W:243:VAL:HB	6:W:458:HOH:O	2.00	0.61
2:W:120:LEU:HB2	2:W:138:PRO:HG2	1.80	0.61
1:A:143:HIS:C	1:A:145:HIS:H	2.04	0.61
2:U:151:GLU:N	2:U:157:LEU:HD11	2.15	0.61
1:F:117:SER:HA	6:F:261:HOH:O	1.99	0.61
1:A:37:ASP:HA	6:A:240:HOH:O	2.00	0.61
2:X:244:ASN:HB2	6:X:583:HOH:O	1.99	0.61
2:W:253:GLN:HG2	2:W:254:PRO:HD2	1.82	0.61
1:B:98:ILE:HD12	6:B:192:HOH:O	2.01	0.61
2:X:209:ILE:HG21	2:X:298:THR:OG1	2.00	0.61
2:U:121:VAL:HG12	2:U:122:GLY:N	2.15	0.61
2:X:140:THR:HA	6:X:371:HOH:O	2.01	0.61
1:B:66:ILE:HD13	6:B:200:HOH:O	1.99	0.61
2:U:100:ASN:HB3	6:U:360:HOH:O	2.01	0.61
1:B:103:LYS:HD3	6:B:265:HOH:O	2.00	0.61
1:E:127:LYS:HB3	6:E:188:HOH:O	2.00	0.61
2:W:98:CYS:HA	6:W:434:HOH:O	1.99	0.61
2:Y:243:VAL:HG23	2:Y:274:ARG:HH21	1.66	0.60
6:A:200:HOH:O	1:B:71:SER:HB2	2.01	0.60
2:X:62:ASP:HB3	2:X:101:SER:HB3	1.83	0.60
1:A:21:ASN:ND2	1:B:21:ASN:ND2	2.49	0.60
2:X:151:GLU:HG2	2:X:155:LYS:HB2	1.83	0.60
2:U:151:GLU:HG2	2:U:155:LYS:HB2	1.82	0.60
2:W:112:VAL:HG23	6:W:539:HOH:O	2.02	0.60
2:W:257:ILE:HD12	2:W:258:ALA:N	2.15	0.60
2:Y:102:ASN:HB2	6:Y:452:HOH:O	2.01	0.60
2:U:232:VAL:HB	6:U:386:HOH:O	2.00	0.60
2:W:117:LYS:HE2	2:W:120:LEU:HD23	1.82	0.60
1:A:21:ASN:HD21	1:B:21:ASN:ND2	2.00	0.60
2:X:251:ASN:CB	2:X:252:PRO:HD3	2.21	0.60
5:W:4:NDG:O3	5:W:5:NAG:H2	2.01	0.60
1:B:48:MET:HE2	6:B:157:HOH:O	2.01	0.60
2:U:251:ASN:CB	2:U:252:PRO:HD3	2.22	0.60
2:U:243:VAL:HG23	2:U:274:ARG:HH21	1.66	0.60
2:Y:273:GLU:HG2	6:Y:561:HOH:O	2.01	0.60
2:X:243:VAL:HG23	2:X:274:ARG:HH21	1.67	0.60
2:W:124:PRO:HB2	2:W:126:PHE:HE1	1.66	0.59
2:W:138:PRO:HD3	6:W:569:HOH:O	2.00	0.59
2:W:59:ILE:HD13	2:W:59:ILE:N	2.17	0.59
2:U:145:SER:HA	6:U:435:HOH:O	2.01	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Y:223:LEU:HD13	2:Y:309:LYS:HG3	1.84	0.59
2:W:243:VAL:HG23	2:W:274:ARG:HH21	1.67	0.59
1:A:143:HIS:CD2	1:A:143:HIS:H	2.20	0.59
2:W:149:LEU:HG	2:W:171:ILE:HG21	1.85	0.59
1:E:139:VAL:HG12	1:E:141:SER:H	1.66	0.59
2:W:62:ASP:HB3	2:W:101:SER:HB3	1.84	0.59
1:B:114:GLU:HA	6:B:255:HOH:O	2.03	0.59
1:A:98:ILE:HG22	1:A:99:LYS:HG2	1.85	0.59
2:W:292:MET:CE	2:W:303:ASN:HD22	2.15	0.59
2:X:249:LYS:HE3	6:X:405:HOH:O	2.00	0.59
2:Y:253:GLN:HG2	2:Y:254:PRO:HD2	1.85	0.59
2:U:258:ALA:HA	6:U:400:HOH:O	2.02	0.59
1:B:129:PHE:HA	6:B:173:HOH:O	2.02	0.59
1:F:112:PRO:HB3	6:F:233:HOH:O	2.02	0.59
2:X:129:GLU:HB3	2:X:208:ALA:HB2	1.85	0.58
2:Y:46:LEU:HD23	2:Y:47:ILE:N	2.18	0.58
1:E:46:ARG:HB3	6:E:276:HOH:O	2.04	0.58
2:U:143:GLN:HA	6:U:559:HOH:O	2.03	0.58
2:X:219:GLU:OE2	2:X:222:HIS:CG	2.57	0.58
2:X:100:ASN:HD22	2:X:101:SER:H	1.52	0.58
2:Y:62:ASP:HB2	2:Y:100:ASN:HD21	1.68	0.58
1:F:98:ILE:HG22	1:F:99:LYS:HG2	1.85	0.58
2:U:129:GLU:HB3	2:U:208:ALA:CB	2.34	0.58
2:Y:62:ASP:HB3	2:Y:101:SER:HB3	1.85	0.58
1:B:98:ILE:HG22	1:B:99:LYS:HG2	1.85	0.58
2:U:224:LEU:O	2:U:310:VAL:HG22	2.04	0.58
2:W:251:ASN:HB2	2:W:252:PRO:CD	2.24	0.58
2:W:117:LYS:HE2	2:W:120:LEU:CD2	2.33	0.58
2:Y:178:ARG:HH12	2:Y:239:VAL:HG11	1.69	0.58
1:F:133:SER:HB2	6:F:245:HOH:O	2.04	0.58
2:Y:84:ILE:HG12	6:Y:606:HOH:O	2.03	0.57
2:Y:223:LEU:HD23	2:Y:223:LEU:N	2.19	0.57
1:B:78:LYS:HE3	2:Y:266:HIS:O	2.04	0.57
2:W:151:GLU:N	2:W:157:LEU:HD11	2.18	0.57
1:A:123:ILE:HD12	6:A:162:HOH:O	2.03	0.57
2:W:76:VAL:HG11	6:W:387:HOH:O	2.04	0.57
2:U:46:LEU:C	2:U:46:LEU:HD23	2.25	0.57
2:X:46:LEU:HD23	2:X:46:LEU:C	2.25	0.57
2:X:253:GLN:HA	6:X:383:HOH:O	2.04	0.57
1:E:98:ILE:HG22	1:E:99:LYS:HG2	1.86	0.57
2:W:164:VAL:HB	6:W:417:HOH:O	2.03	0.57
2:U:223:LEU:N	2:U:223:LEU:HD23	2.19	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:223:LEU:HD13	2:X:309:LYS:HG3	1.85	0.57
2:U:54:LEU:HD11	6:U:415:HOH:O	2.04	0.57
2:W:174:LYS:HD2	6:W:570:HOH:O	2.03	0.57
2:W:46:LEU:C	2:W:46:LEU:HD23	2.24	0.57
2:Y:251:ASN:HB2	2:Y:252:PRO:CD	2.22	0.57
2:X:223:LEU:HD23	2:X:223:LEU:N	2.18	0.57
2:W:128:LYS:HE2	6:W:469:HOH:O	2.05	0.57
2:Y:149:LEU:HG	2:Y:171:ILE:HG21	1.86	0.57
2:Y:59:ILE:N	2:Y:59:ILE:HD13	2.19	0.57
2:Y:257:ILE:HD12	2:Y:258:ALA:H	1.70	0.57
2:X:183:LEU:HD12	6:X:350:HOH:O	2.03	0.57
2:W:46:LEU:HD23	2:W:47:ILE:N	2.20	0.56
2:W:211:ALA:HA	6:W:385:HOH:O	2.04	0.56
2:X:251:ASN:HB2	2:X:252:PRO:CD	2.23	0.56
1:F:94:ALA:HB1	6:F:267:HOH:O	2.04	0.56
1:F:22:LEU:HD12	6:F:233:HOH:O	2.05	0.56
2:W:229:THR:CG2	2:W:281:SER:HA	2.30	0.56
2:W:224:LEU:O	2:W:310:VAL:HG22	2.05	0.56
1:E:99:LYS:N	2:U:75:MET:O	2.37	0.56
2:Y:121:VAL:CG1	2:Y:122:GLY:H	2.19	0.56
1:A:99:LYS:HD3	6:X:391:HOH:O	2.04	0.56
1:E:97:ASN:HB3	1:E:100:GLU:OE1	2.05	0.56
1:A:67:SER:HB2	6:A:253:HOH:O	2.06	0.56
2:U:118:LEU:HD13	2:U:119:PHE:CE1	2.41	0.56
2:U:62:ASP:HB2	2:U:100:ASN:HD21	1.70	0.56
2:W:223:LEU:N	2:W:223:LEU:HD23	2.21	0.56
2:Y:224:LEU:O	2:Y:310:VAL:HG22	2.06	0.56
1:E:78:LYS:HE3	2:U:266:HIS:O	2.06	0.56
2:W:223:LEU:HD13	2:W:309:LYS:HG3	1.88	0.55
3:Y:2:NAG:H61	6:Y:384:HOH:O	2.05	0.55
2:U:100:ASN:HD22	2:U:101:SER:H	1.53	0.55
2:Y:88:ALA:HA	6:Y:330:HOH:O	2.06	0.55
1:B:97:ASN:HB3	1:B:100:GLU:OE1	2.06	0.55
1:E:136:SER:HB3	6:E:258:HOH:O	2.06	0.55
2:U:292:MET:CE	2:U:303:ASN:HD22	2.20	0.55
1:B:105:PRO:HD2	6:B:201:HOH:O	2.06	0.55
1:B:33:VAL:HG12	6:B:196:HOH:O	2.06	0.55
2:U:46:LEU:HD23	2:U:47:ILE:N	2.22	0.55
2:X:229:THR:CG2	2:X:281:SER:HA	2.33	0.55
2:Y:100:ASN:HD22	2:Y:101:SER:H	1.54	0.55
2:W:83:TRP:HE1	2:W:85:GLN:HE22	1.55	0.55
1:E:22:LEU:HA	6:E:182:HOH:O	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:X:5:NAG:H83	6:X:582:HOH:O	2.06	0.55
2:W:213:PRO:HG3	2:W:297:ASN:ND2	2.21	0.55
2:U:139:LEU:H	2:U:139:LEU:HD23	1.72	0.55
1:F:97:ASN:HB3	1:F:100:GLU:OE1	2.07	0.55
2:U:223:LEU:HD13	2:U:309:LYS:HG3	1.88	0.55
1:F:82:ILE:HA	6:F:204:HOH:O	2.05	0.55
2:X:139:LEU:HD12	2:X:141:ASP:O	2.07	0.54
2:U:62:ASP:HB3	2:U:101:SER:HB3	1.90	0.54
2:U:251:ASN:HB2	2:U:252:PRO:CD	2.23	0.54
2:X:229:THR:HG22	2:X:282:SER:H	1.73	0.54
2:W:100:ASN:HD22	2:W:101:SER:H	1.55	0.54
2:X:280:ILE:HA	6:X:481:HOH:O	2.07	0.54
2:Y:159:THR:HA	6:Y:458:HOH:O	2.07	0.54
2:U:150:ILE:HG21	6:U:521:HOH:O	2.07	0.54
1:A:78:LYS:HE3	2:X:266:HIS:O	2.07	0.54
2:X:236:ILE:CD1	6:X:511:HOH:O	2.56	0.54
2:X:261:LYS:HG3	6:X:495:HOH:O	2.06	0.54
1:A:26:TYR:O	1:A:112:PRO:HD3	2.07	0.54
2:W:292:MET:HE2	6:W:422:HOH:O	2.08	0.54
2:W:207:GLU:CD	2:W:207:GLU:H	2.11	0.54
1:B:137:ASP:HB3	6:B:203:HOH:O	2.08	0.53
2:W:150:ILE:HD11	6:W:516:HOH:O	2.07	0.53
2:W:236:ILE:N	2:W:236:ILE:CD1	2.71	0.53
2:X:292:MET:CE	2:X:303:ASN:HD22	2.21	0.53
2:X:292:MET:HE2	2:X:303:ASN:HD22	1.73	0.53
1:B:98:ILE:HG23	6:Y:455:HOH:O	2.06	0.53
2:U:222:HIS:HD2	6:U:561:HOH:O	1.90	0.53
5:W:6:MAN:H3	6:W:376:HOH:O	2.08	0.53
2:X:276:GLU:OE1	2:X:276:GLU:HA	2.09	0.53
2:X:226:LYS:HB3	6:X:397:HOH:O	2.07	0.53
1:A:21:ASN:ND2	1:B:21:ASN:HD21	2.06	0.53
2:Y:225:LYS:HB2	6:Y:355:HOH:O	2.07	0.53
2:X:87:LYS:HD3	6:X:362:HOH:O	2.09	0.53
2:X:222:HIS:N	2:X:222:HIS:ND1	2.57	0.53
2:Y:54:LEU:HD11	2:Y:56:LEU:HD21	1.90	0.53
2:Y:236:ILE:N	2:Y:236:ILE:CD1	2.72	0.53
4:Y:5:NAG:H3	4:Y:5:NAG:H82	1.90	0.53
2:Y:229:THR:HG22	2:Y:282:SER:H	1.74	0.53
2:X:254:PRO:HD3	6:X:383:HOH:O	2.09	0.53
2:Y:211:ALA:HA	6:Y:562:HOH:O	2.09	0.53
2:X:257:ILE:HD12	2:X:258:ALA:H	1.74	0.53
2:X:92:ARG:HG3	6:X:367:HOH:O	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Y:229:THR:CG2	2:Y:281:SER:HA	2.33	0.52
1:B:103:LYS:HA	6:B:265:HOH:O	2.08	0.52
2:Y:130:ASP:HA	6:Y:548:HOH:O	2.08	0.52
1:B:69:GLY:HA3	6:B:225:HOH:O	2.08	0.52
2:Y:173:ILE:HA	6:Y:486:HOH:O	2.09	0.52
2:X:209:ILE:HG23	2:X:209:ILE:O	2.10	0.52
1:A:27:MET:HB3	1:A:109:SER:HB2	1.90	0.52
2:Y:276:GLU:OE1	2:Y:276:GLU:HA	2.09	0.52
1:E:140:LEU:HB2	6:E:270:HOH:O	2.09	0.52
1:A:133:SER:HB3	6:A:213:HOH:O	2.08	0.52
1:F:23:PRO:HD3	6:F:154:HOH:O	2.10	0.52
2:X:46:LEU:HD23	2:X:47:ILE:N	2.24	0.52
2:X:220:THR:HA	6:X:543:HOH:O	2.10	0.52
2:X:303:ASN:HB2	6:X:497:HOH:O	2.09	0.52
1:E:26:TYR:O	1:E:112:PRO:HD3	2.09	0.52
2:X:254:PRO:HB3	6:X:471:HOH:O	2.10	0.52
2:Y:180:TYR:O	2:Y:181:HIS:C	2.47	0.52
1:B:26:TYR:O	1:B:112:PRO:HD3	2.10	0.52
1:F:27:MET:HB3	1:F:109:SER:HB2	1.91	0.52
2:X:83:TRP:HE1	2:X:85:GLN:HE22	1.58	0.52
2:X:211:ALA:HB1	6:X:404:HOH:O	2.08	0.52
1:E:27:MET:HB3	1:E:109:SER:HB2	1.91	0.52
1:A:95:PRO:HG2	6:A:178:HOH:O	2.08	0.52
2:Y:121:VAL:CG1	2:Y:122:GLY:N	2.71	0.52
2:Y:158:PRO:HD3	6:Y:325:HOH:O	2.10	0.52
2:U:121:VAL:CG1	2:U:122:GLY:N	2.73	0.51
2:U:65:ARG:NH1	2:U:77:GLU:OE2	2.44	0.51
2:Y:139:LEU:HB3	6:Y:341:HOH:O	2.09	0.51
2:X:174:LYS:HG2	6:X:410:HOH:O	2.10	0.51
2:W:151:GLU:HG2	2:W:155:LYS:H	1.75	0.51
6:A:202:HOH:O	1:B:66:ILE:HG21	2.10	0.51
2:X:54:LEU:HD11	2:X:56:LEU:HD21	1.92	0.51
2:W:276:GLU:HA	2:W:276:GLU:OE1	2.11	0.51
1:A:6:ASN:N	1:A:6:ASN:ND2	2.55	0.51
1:B:27:MET:HB3	1:B:109:SER:HB2	1.93	0.51
2:X:149:LEU:HG	2:X:171:ILE:HG21	1.91	0.51
2:W:151:GLU:CG	2:W:155:LYS:H	2.23	0.51
1:E:14:ASP:CB	1:E:75:ILE:HD12	2.38	0.51
2:W:111:PHE:CG	2:W:142:PRO:HD3	2.46	0.51
2:U:212:ILE:HD12	2:U:212:ILE:H	1.76	0.51
2:Y:70:THR:HG22	2:Y:71:TYR:N	2.25	0.51
2:Y:139:LEU:HD13	6:Y:341:HOH:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Y:83:TRP:HE1	2:Y:85:GLN:HE22	1.58	0.51
1:A:18:LEU:HG	6:A:261:HOH:O	2.11	0.51
2:W:54:LEU:HD11	2:W:56:LEU:HD21	1.93	0.51
1:F:66:ILE:CG2	1:F:67:SER:H	2.13	0.51
2:X:235:THR:C	2:X:236:ILE:HD12	2.31	0.51
2:X:56:LEU:N	2:X:56:LEU:HD22	2.26	0.51
1:E:103:LYS:HB3	6:E:168:HOH:O	2.10	0.51
2:Y:118:LEU:HD12	2:Y:119:PHE:CE1	2.46	0.50
1:A:70:LEU:HD22	1:A:75:ILE:HD11	1.93	0.50
2:X:224:LEU:O	2:X:310:VAL:HG22	2.10	0.50
1:A:71:SER:HB2	6:A:211:HOH:O	2.10	0.50
2:U:37:PRO:CB	2:U:98:CYS:SG	3.00	0.50
1:F:14:ASP:CB	1:F:75:ILE:HD12	2.38	0.50
2:U:276:GLU:OE1	2:U:276:GLU:HA	2.11	0.50
2:U:229:THR:CG2	2:U:281:SER:HA	2.35	0.50
2:U:236:ILE:CD1	2:U:236:ILE:N	2.72	0.50
2:W:134:LEU:HD13	2:W:136:ARG:HG2	1.93	0.50
1:B:59:LEU:HD22	1:B:63:PHE:HE1	1.76	0.50
1:B:113:GLU:HB2	6:B:213:HOH:O	2.11	0.50
2:U:250:MET:HB3	6:U:324:HOH:O	2.11	0.50
2:W:67:THR:HG21	6:W:366:HOH:O	2.11	0.50
2:U:149:LEU:HG	2:U:171:ILE:HG21	1.94	0.50
1:F:26:TYR:O	1:F:112:PRO:HD3	2.12	0.50
1:F:67:SER:HB2	6:F:175:HOH:O	2.12	0.50
2:X:292:MET:HG3	6:X:497:HOH:O	2.11	0.50
2:X:212:ILE:HD12	2:X:212:ILE:N	2.26	0.50
2:X:77:GLU:HB3	6:X:391:HOH:O	2.11	0.50
2:U:46:LEU:HD22	2:U:110:VAL:HG13	1.94	0.50
2:X:118:LEU:HD13	6:X:455:HOH:O	2.11	0.50
2:U:139:LEU:HD12	2:U:141:ASP:O	2.12	0.50
2:U:191:ARG:O	2:U:192:ASP:HB2	2.12	0.50
2:X:248:LEU:N	2:X:248:LEU:HD22	2.27	0.50
2:U:146:GLN:OE1	2:U:195:TRP:HZ2	1.91	0.49
1:E:70:LEU:HD22	1:E:75:ILE:HD11	1.95	0.49
2:W:121:VAL:HG12	2:W:122:GLY:N	2.27	0.49
2:W:130:ASP:HA	6:W:351:HOH:O	2.10	0.49
2:X:273:GLU:HB2	6:X:411:HOH:O	2.11	0.49
1:A:142:HIS:N	1:A:142:HIS:ND1	2.58	0.49
2:U:151:GLU:HG2	2:U:155:LYS:CB	2.43	0.49
1:E:98:ILE:HG12	6:E:180:HOH:O	2.13	0.49
2:X:253:GLN:HG2	2:X:254:PRO:CD	2.43	0.49
2:W:65:ARG:NH1	2:W:77:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:U:297:ASN:HB3	2:U:299:PHE:H	1.77	0.49
2:U:72:PHE:O	2:U:74:GLU:HG3	2.12	0.49
2:W:40:HIS:HA	6:W:315:HOH:O	2.13	0.49
2:U:118:LEU:HD23	2:U:118:LEU:O	2.12	0.49
3:Y:2:NAG:H81	6:Y:566:HOH:O	2.11	0.49
2:U:38:SER:HB2	6:U:579:HOH:O	2.12	0.49
1:E:29:THR:HB	6:E:217:HOH:O	2.11	0.49
2:W:304:VAL:HA	6:W:423:HOH:O	2.10	0.49
2:U:180:TYR:O	2:U:181:HIS:C	2.49	0.49
2:X:151:GLU:HG2	2:X:155:LYS:CB	2.42	0.49
2:W:219:GLU:OE2	2:W:222:HIS:HB3	2.13	0.49
2:X:128:LYS:HE2	6:X:499:HOH:O	2.13	0.49
2:X:59:ILE:N	2:X:59:ILE:CD1	2.75	0.49
2:W:151:GLU:HG2	2:W:155:LYS:CB	2.41	0.49
2:Y:151:GLU:HG2	2:Y:155:LYS:CB	2.43	0.49
1:F:70:LEU:HD22	1:F:75:ILE:HD11	1.95	0.49
1:E:59:LEU:HD22	1:E:63:PHE:HE1	1.77	0.49
2:Y:219:GLU:OE2	2:Y:222:HIS:HB3	2.12	0.49
2:U:70:THR:HG22	2:U:71:TYR:N	2.28	0.49
2:U:211:ALA:HA	6:U:418:HOH:O	2.12	0.49
1:B:66:ILE:CG2	1:B:67:SER:H	2.16	0.48
2:Y:257:ILE:HD12	2:Y:258:ALA:N	2.27	0.48
2:W:175:ASN:HB3	6:W:351:HOH:O	2.13	0.48
2:U:229:THR:HG22	2:U:282:SER:H	1.77	0.48
2:X:209:ILE:CG2	2:X:298:THR:OG1	2.61	0.48
2:X:65:ARG:NH1	2:X:77:GLU:OE2	2.46	0.48
2:U:212:ILE:HD12	2:U:212:ILE:N	2.28	0.48
2:Y:213:PRO:HG3	2:Y:297:ASN:ND2	2.28	0.48
2:Y:65:ARG:NH1	2:Y:77:GLU:OE2	2.47	0.48
2:U:230:PHE:HE2	2:U:280:ILE:HG13	1.78	0.48
2:X:64:VAL:HG21	6:X:502:HOH:O	2.12	0.48
2:Y:152:CYS:HB2	2:Y:186:ARG:HG3	1.95	0.48
1:A:66:ILE:CG2	1:A:67:SER:H	2.13	0.48
1:E:66:ILE:CG2	1:E:67:SER:H	2.16	0.48
2:Y:129:GLU:HB3	2:Y:208:ALA:HB2	1.95	0.48
2:W:178:ARG:NH2	2:W:208:ALA:O	2.47	0.48
1:A:59:LEU:HD22	1:A:63:PHE:HE1	1.79	0.48
1:B:48:MET:HG3	6:B:157:HOH:O	2.14	0.48
2:W:260:VAL:HG21	6:W:499:HOH:O	2.14	0.48
2:U:219:GLU:OE2	2:U:222:HIS:HB3	2.12	0.48
2:W:248:LEU:HD22	2:W:248:LEU:N	2.29	0.48
2:W:162:THR:HA	6:W:532:HOH:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:ILE:CD1	1:A:66:ILE:C	2.82	0.48
2:W:229:THR:HG22	2:W:282:SER:H	1.77	0.48
2:U:54:LEU:HD11	2:U:56:LEU:HD21	1.95	0.48
1:B:6:ASN:N	1:B:6:ASN:ND2	2.59	0.48
2:U:257:ILE:HD12	2:U:258:ALA:H	1.79	0.48
2:W:139:LEU:HD12	2:W:141:ASP:O	2.14	0.48
2:X:243:VAL:O	2:X:274:ARG:NH2	2.47	0.48
2:Y:89:GLU:HB2	6:Y:550:HOH:O	2.13	0.48
1:B:136:SER:HB3	6:B:266:HOH:O	2.12	0.48
1:B:41:SER:HB3	6:B:246:HOH:O	2.14	0.48
2:Y:248:LEU:N	2:Y:248:LEU:HD22	2.29	0.48
2:U:248:LEU:N	2:U:248:LEU:HD22	2.28	0.48
2:W:252:PRO:HG3	6:W:563:HOH:O	2.12	0.48
1:B:66:ILE:C	1:B:66:ILE:CD1	2.82	0.48
2:Y:222:HIS:HD2	6:Y:517:HOH:O	1.96	0.48
2:X:120:LEU:HB2	2:X:138:PRO:HG2	1.94	0.48
2:W:267:ARG:HB2	2:W:271:ASN:ND2	2.28	0.48
1:B:48:MET:HE2	6:B:195:HOH:O	2.13	0.47
1:F:59:LEU:HD22	1:F:63:PHE:HE1	1.77	0.47
2:W:183:LEU:HD11	6:W:474:HOH:O	2.13	0.47
1:B:70:LEU:HD22	1:B:75:ILE:HD11	1.97	0.47
2:X:213:PRO:HG3	2:X:297:ASN:ND2	2.28	0.47
2:X:59:ILE:N	2:X:59:ILE:HD13	2.29	0.47
2:X:267:ARG:HB2	2:X:271:ASN:ND2	2.29	0.47
1:F:66:ILE:CD1	1:F:66:ILE:C	2.82	0.47
2:X:268:GLY:HA3	6:X:552:HOH:O	2.14	0.47
2:Y:286:ASP:HB2	6:Y:518:HOH:O	2.13	0.47
1:A:14:ASP:CB	1:A:75:ILE:HD12	2.39	0.47
1:F:70:LEU:HD22	1:F:75:ILE:CD1	2.45	0.47
2:Y:292:MET:CE	2:Y:303:ASN:HD22	2.27	0.47
2:U:253:GLN:HG2	2:U:254:PRO:CD	2.43	0.47
1:B:103:LYS:HB2	6:B:271:HOH:O	2.15	0.47
1:E:66:ILE:C	1:E:66:ILE:CD1	2.82	0.47
1:A:70:LEU:HD22	1:A:75:ILE:CD1	2.45	0.47
2:U:138:PRO:CD	2:U:169:ALA:O	2.58	0.47
1:A:98:ILE:HD13	6:X:544:HOH:O	2.14	0.47
2:X:297:ASN:HB3	2:X:299:PHE:H	1.78	0.47
2:X:70:THR:HG22	2:X:71:TYR:N	2.30	0.47
2:W:72:PHE:O	2:W:74:GLU:N	2.48	0.47
2:W:253:GLN:HG2	2:W:254:PRO:CD	2.44	0.47
2:Y:85:GLN:HG3	6:Y:454:HOH:O	2.15	0.47
1:E:49:VAL:HG12	1:E:87:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:49:VAL:HG12	1:F:87:VAL:CG2	2.45	0.47
2:U:59:ILE:N	2:U:59:ILE:CD1	2.78	0.47
1:F:129:PHE:HD2	1:F:130:MET:HE3	1.80	0.47
2:U:72:PHE:O	2:U:74:GLU:N	2.48	0.47
2:Y:262:HIS:HA	6:Y:441:HOH:O	2.14	0.47
2:Y:125:LEU:HB3	2:Y:203:LEU:HA	1.97	0.47
3:X:2:NAG:H61	3:X:3:NAG:O5	2.15	0.47
1:E:24:ASN:ND2	1:F:62:LYS:HA	2.30	0.47
2:X:209:ILE:HD12	2:X:299:PHE:HB2	1.96	0.46
2:Y:120:LEU:HB2	2:Y:138:PRO:HG2	1.97	0.46
2:W:152:CYS:HB2	2:W:186:ARG:HG3	1.96	0.46
2:U:249:LYS:HD2	6:U:570:HOH:O	2.14	0.46
2:U:87:LYS:HG3	6:U:525:HOH:O	2.14	0.46
2:Y:150:ILE:HD11	6:Y:588:HOH:O	2.15	0.46
1:E:70:LEU:HD22	1:E:75:ILE:CD1	2.46	0.46
2:Y:297:ASN:HB3	2:Y:299:PHE:H	1.81	0.46
2:X:139:LEU:HD22	2:X:147:TYR:CE1	2.51	0.46
2:U:207:GLU:HB3	2:U:270:PHE:CD2	2.50	0.46
2:W:56:LEU:HD22	2:W:56:LEU:N	2.31	0.46
2:X:69:LYS:HB3	6:X:574:HOH:O	2.16	0.46
1:B:88:LEU:HD13	2:Y:206:ARG:HD3	1.96	0.46
2:U:115:PRO:HA	6:U:442:HOH:O	2.16	0.46
2:Y:197:HIS:CE1	6:Y:624:HOH:O	2.67	0.46
2:U:56:LEU:HD22	2:U:56:LEU:N	2.31	0.46
2:U:139:LEU:HD22	2:U:147:TYR:CE1	2.50	0.46
2:Y:129:GLU:O	2:Y:130:ASP:HB2	2.15	0.46
1:F:60:LEU:HD11	1:F:73:TYR:CD1	2.51	0.46
1:B:14:ASP:CB	1:B:75:ILE:HD12	2.39	0.46
2:W:111:PHE:CD1	2:W:142:PRO:HD3	2.51	0.46
2:U:213:PRO:HG3	2:U:297:ASN:ND2	2.29	0.46
1:F:121:ARG:HD2	6:F:187:HOH:O	2.15	0.46
1:B:49:VAL:HG12	1:B:87:VAL:CG2	2.46	0.46
2:X:172:THR:HB	6:X:410:HOH:O	2.15	0.46
2:X:72:PHE:O	2:X:74:GLU:N	2.49	0.46
2:Y:267:ARG:HB2	2:Y:271:ASN:ND2	2.30	0.46
1:A:60:LEU:HB2	6:A:199:HOH:O	2.16	0.46
2:W:125:LEU:HB3	2:W:203:LEU:HA	1.98	0.46
1:E:129:PHE:HD2	1:E:130:MET:HE3	1.81	0.46
1:A:49:VAL:HG12	1:A:87:VAL:CG2	2.45	0.46
2:Y:220:THR:HA	6:Y:577:HOH:O	2.16	0.46
2:W:151:GLU:HG2	2:W:155:LYS:N	2.31	0.46
2:X:209:ILE:HD13	2:X:210:LYS:N	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:W:37:PRO:HB3	2:W:98:CYS:SG	2.56	0.46
2:X:91:THR:HG23	6:X:356:HOH:O	2.15	0.46
2:X:230:PHE:HE2	2:X:280:ILE:HG13	1.82	0.45
2:Y:158:PRO:HB2	2:Y:161:LEU:HB2	1.98	0.45
2:W:199:ASP:HB2	6:W:361:HOH:O	2.16	0.45
1:E:24:ASN:HD21	1:F:62:LYS:HA	1.80	0.45
1:A:81:LYS:HD2	6:A:151:HOH:O	2.16	0.45
1:F:88:LEU:HB2	6:F:226:HOH:O	2.16	0.45
2:X:305:THR:HG23	6:X:497:HOH:O	2.16	0.45
1:A:129:PHE:HD2	1:A:130:MET:HE3	1.81	0.45
2:X:209:ILE:HD13	2:X:209:ILE:C	2.36	0.45
2:Y:253:GLN:HG2	2:Y:254:PRO:CD	2.46	0.45
2:W:129:GLU:HB3	2:W:208:ALA:HB2	1.98	0.45
6:F:210:HOH:O	2:W:73:ASN:HB3	2.16	0.45
1:F:101:SER:N	1:F:102:PRO:HD3	2.31	0.45
2:Y:56:LEU:HD22	2:Y:56:LEU:N	2.32	0.45
2:Y:139:LEU:HD12	2:Y:141:ASP:O	2.16	0.45
1:B:103:LYS:HG3	6:B:182:HOH:O	2.15	0.45
2:W:58:CYS:C	2:W:59:ILE:HD13	2.37	0.45
2:W:46:LEU:HD22	2:W:110:VAL:HG13	1.99	0.45
2:U:119:PHE:N	2:U:119:PHE:CD1	2.84	0.45
1:E:101:SER:N	1:E:102:PRO:HD3	2.31	0.45
1:A:40:PRO:HG2	1:A:43:CYS:SG	2.57	0.45
1:B:70:LEU:HD22	1:B:75:ILE:CD1	2.47	0.45
2:X:209:ILE:HG22	6:X:361:HOH:O	2.15	0.45
1:A:142:HIS:HB2	1:A:146:HIS:CE1	2.51	0.45
2:Y:124:PRO:HB2	2:Y:126:PHE:CE1	2.52	0.45
1:F:131:VAL:HG11	6:F:166:HOH:O	2.15	0.45
2:X:257:ILE:HD12	2:X:258:ALA:N	2.30	0.45
1:A:66:ILE:HG23	6:A:253:HOH:O	2.16	0.45
1:E:97:ASN:ND2	2:U:73:ASN:O	2.49	0.45
1:E:38:VAL:HG23	1:E:39:LEU:N	2.32	0.45
1:B:101:SER:N	1:B:102:PRO:HD3	2.31	0.45
2:Y:291:PHE:HD1	6:Y:445:HOH:O	2.00	0.45
1:B:129:PHE:HD2	1:B:130:MET:CE	2.30	0.45
1:E:130:MET:H	1:E:130:MET:HG2	1.60	0.45
1:E:70:LEU:HA	6:E:226:HOH:O	2.17	0.44
2:U:254:PRO:HB3	6:U:324:HOH:O	2.16	0.44
2:X:129:GLU:O	2:X:130:ASP:HB2	2.17	0.44
1:F:38:VAL:HG23	1:F:39:LEU:N	2.32	0.44
2:Y:280:ILE:HA	6:Y:586:HOH:O	2.17	0.44
2:X:88:ALA:HA	6:X:352:HOH:O	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:3:ILE:HA	6:B:286:HOH:O	2.18	0.44
1:E:3:ILE:O	1:E:3:ILE:HG22	2.17	0.44
2:Y:72:PHE:O	2:Y:74:GLU:N	2.50	0.44
1:B:3:ILE:O	1:B:3:ILE:HG22	2.17	0.44
1:B:34:ALA:HB1	6:B:197:HOH:O	2.17	0.44
2:X:253:GLN:HB3	2:X:255:GLN:HE22	1.82	0.44
1:F:77:ASP:OD2	2:W:182:ARG:NH2	2.51	0.44
1:A:127:LYS:HG2	6:A:153:HOH:O	2.17	0.44
2:X:134:LEU:HD13	2:X:136:ARG:HG2	1.99	0.44
2:Y:257:ILE:HD11	6:Y:541:HOH:O	2.17	0.44
1:B:131:VAL:HG11	6:B:181:HOH:O	2.17	0.44
2:X:152:CYS:HB2	2:X:186:ARG:HG3	1.99	0.44
1:B:6:ASN:ND2	6:B:228:HOH:O	2.49	0.44
1:E:60:LEU:HD11	1:E:73:TYR:CD1	2.52	0.44
1:F:31:ASN:HB2	1:F:51:GLN:OE1	2.16	0.44
1:A:38:VAL:HG23	1:A:39:LEU:N	2.32	0.44
1:B:38:VAL:HG23	1:B:39:LEU:N	2.32	0.44
2:Y:184:CYS:HA	2:Y:201:PHE:O	2.18	0.44
2:U:108:ILE:HG23	2:U:108:ILE:O	2.18	0.44
2:W:213:PRO:HB3	6:W:393:HOH:O	2.18	0.44
2:W:212:ILE:N	2:W:212:ILE:HD12	2.32	0.44
2:X:151:GLU:HG2	2:X:155:LYS:H	1.81	0.44
2:Y:139:LEU:HD22	2:Y:147:TYR:CE1	2.53	0.44
2:Y:230:PHE:HE1	6:Y:477:HOH:O	2.01	0.44
2:X:191:ARG:O	2:X:192:ASP:HB2	2.17	0.44
6:F:199:HOH:O	2:W:181:HIS:HE1	2.01	0.44
1:A:60:LEU:HD11	1:A:73:TYR:CD1	2.53	0.44
2:X:89:GLU:HB3	6:X:356:HOH:O	2.17	0.44
1:E:81:LYS:HD3	6:E:165:HOH:O	2.18	0.44
1:A:3:ILE:O	1:A:3:ILE:HG22	2.18	0.44
2:X:237:LYS:HB3	6:X:335:HOH:O	2.18	0.43
1:F:38:VAL:HG21	6:F:176:HOH:O	2.18	0.43
1:F:3:ILE:O	1:F:3:ILE:HG22	2.18	0.43
2:U:128:LYS:HE3	2:U:208:ALA:HA	1.99	0.43
2:U:244:ASN:O	2:U:295:ALA:HA	2.18	0.43
2:U:260:VAL:CG1	2:U:276:GLU:HG3	2.45	0.43
2:Y:54:LEU:HD13	2:Y:54:LEU:O	2.18	0.43
1:F:94:ALA:HA	1:F:95:PRO:HD3	1.87	0.43
2:Y:118:LEU:HD22	2:Y:118:LEU:O	2.18	0.43
2:X:128:LYS:HA	2:X:206:ARG:HB2	2.00	0.43
1:F:6:ASN:O	2:W:241:THR:HB	2.18	0.43
1:B:46:ARG:NH2	6:B:216:HOH:O	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:ASP:HA	6:A:199:HOH:O	2.18	0.43
2:U:192:ASP:N	6:U:425:HOH:O	2.48	0.43
1:B:31:ASN:HB2	1:B:51:GLN:OE1	2.18	0.43
2:W:206:ARG:HB3	6:W:439:HOH:O	2.18	0.43
2:X:212:ILE:HD12	2:X:212:ILE:H	1.83	0.43
1:F:129:PHE:HD2	1:F:130:MET:CE	2.31	0.43
1:A:129:PHE:HD2	1:A:130:MET:CE	2.31	0.43
2:Y:178:ARG:NH1	2:Y:239:VAL:HG11	2.33	0.43
2:X:237:LYS:HG2	6:X:411:HOH:O	2.17	0.43
1:A:49:VAL:HG12	1:A:87:VAL:HG23	2.01	0.43
1:E:31:ASN:HB2	1:E:51:GLN:OE1	2.18	0.43
2:U:234:CYS:HB2	2:U:247:TRP:CZ2	2.54	0.43
2:W:260:VAL:CG1	2:W:276:GLU:HG3	2.45	0.43
1:B:100:GLU:CG	6:B:155:HOH:O	2.66	0.43
2:Y:46:LEU:CD2	2:Y:46:LEU:C	2.85	0.43
1:A:63:PHE:CZ	1:B:23:PRO:HG3	2.53	0.43
1:E:129:PHE:HD2	1:E:130:MET:CE	2.31	0.43
1:E:97:ASN:O	2:U:75:MET:CG	2.67	0.43
2:U:128:LYS:HA	2:U:206:ARG:HB2	2.01	0.43
2:Y:292:MET:HE2	2:Y:303:ASN:HD22	1.84	0.43
2:X:100:ASN:HD22	2:X:101:SER:N	2.17	0.43
2:W:292:MET:HE2	2:W:303:ASN:HD22	1.82	0.43
1:E:49:VAL:HG12	1:E:87:VAL:HG23	2.00	0.43
2:U:267:ARG:HB2	2:U:271:ASN:ND2	2.33	0.43
2:U:253:GLN:HG3	6:U:581:HOH:O	2.18	0.43
2:U:48:VAL:CG1	2:U:112:VAL:HG22	2.49	0.43
6:A:176:HOH:O	2:X:265:TRP:HZ3	2.01	0.43
2:X:151:GLU:CG	2:X:155:LYS:H	2.31	0.42
2:U:184:CYS:HA	2:U:201:PHE:O	2.19	0.42
2:Y:243:VAL:O	2:Y:274:ARG:NH2	2.51	0.42
2:Y:58:CYS:C	2:Y:59:ILE:HD13	2.38	0.42
2:U:59:ILE:N	2:U:59:ILE:HD13	2.34	0.42
1:E:102:PRO:HA	6:E:239:HOH:O	2.18	0.42
2:U:121:VAL:CG1	2:U:122:GLY:H	2.32	0.42
2:W:297:ASN:HB3	2:W:299:PHE:H	1.83	0.42
2:X:174:LYS:HE2	6:X:410:HOH:O	2.19	0.42
2:Y:191:ARG:O	2:Y:192:ASP:HB2	2.18	0.42
3:U:1:FUL:H61	3:U:3:NAG:H62	2.00	0.42
1:F:49:VAL:HG12	1:F:87:VAL:HG23	1.99	0.42
2:W:177:LYS:HA	6:W:430:HOH:O	2.19	0.42
2:W:129:GLU:O	2:W:130:ASP:HB2	2.19	0.42
2:X:237:LYS:HD3	6:X:439:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:U:182:ARG:O	2:U:182:ARG:HG2	2.20	0.42
2:X:108:ILE:O	2:X:108:ILE:HG23	2.18	0.42
2:X:151:GLU:HG2	2:X:155:LYS:N	2.34	0.42
1:F:44:TRP:HB2	6:F:273:HOH:O	2.20	0.42
2:W:92:ARG:NH1	6:W:317:HOH:O	2.50	0.42
2:U:175:ASN:HB3	6:U:384:HOH:O	2.19	0.42
1:B:60:LEU:HD11	1:B:73:TYR:CD1	2.54	0.42
2:Y:40:HIS:HD2	6:Y:401:HOH:O	2.01	0.42
2:U:83:TRP:HE1	2:U:85:GLN:HE22	1.66	0.42
1:E:94:ALA:HA	1:E:95:PRO:HD3	1.85	0.42
2:X:207:GLU:HG3	2:X:239:VAL:HG23	2.02	0.42
2:X:231:THR:HG22	2:X:279:THR:OG1	2.20	0.42
1:E:111:THR:OG1	1:E:114:GLU:CD	2.58	0.42
2:U:129:GLU:O	2:U:130:ASP:HB2	2.19	0.42
2:X:209:ILE:HD13	2:X:211:ALA:H	1.85	0.42
2:U:120:LEU:O	2:U:137:CYS:HA	2.19	0.42
2:Y:67:THR:HB	6:Y:585:HOH:O	2.20	0.42
2:U:152:CYS:HB2	2:U:186:ARG:HG3	2.01	0.42
1:F:16:THR:HB	6:F:153:HOH:O	2.19	0.42
2:W:184:CYS:HA	2:W:201:PHE:O	2.20	0.42
2:X:125:LEU:HB3	2:X:203:LEU:HA	2.01	0.42
2:W:139:LEU:HD22	2:W:147:TYR:CE1	2.55	0.42
2:Y:254:PRO:HD3	6:Y:498:HOH:O	2.20	0.42
1:E:46:ARG:HD3	6:E:228:HOH:O	2.20	0.42
2:U:241:THR:HG22	2:U:272:TYR:CE1	2.54	0.42
2:X:158:PRO:HB2	2:X:161:LEU:HB2	2.02	0.42
2:U:51:GLY:O	2:U:87:LYS:HA	2.20	0.42
1:E:112:PRO:HB2	6:E:148:HOH:O	2.20	0.41
1:E:104:ARG:NE	1:E:104:ARG:HA	2.34	0.41
1:B:81:LYS:HD2	6:B:148:HOH:O	2.20	0.41
1:B:104:ARG:HA	1:B:105:PRO:HD3	1.90	0.41
1:B:49:VAL:HG12	1:B:87:VAL:HG23	2.02	0.41
2:X:241:THR:HG22	2:X:272:TYR:CE1	2.55	0.41
2:X:184:CYS:HA	2:X:201:PHE:O	2.21	0.41
1:E:134:ASP:HB2	6:E:201:HOH:O	2.19	0.41
1:E:128:ASP:HB3	6:E:243:HOH:O	2.20	0.41
2:X:234:CYS:HB2	2:X:247:TRP:CZ2	2.56	0.41
1:A:6:ASN:OD1	6:A:290:HOH:O	2.22	0.41
2:X:139:LEU:HD21	2:X:167:PRO:HA	2.01	0.41
2:U:207:GLU:HG3	2:U:239:VAL:O	2.20	0.41
2:Y:139:LEU:HD21	2:Y:167:PRO:HA	2.02	0.41
2:W:121:VAL:HG11	2:W:199:ASP:HB2	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:66:ILE:CG2	1:B:67:SER:N	2.81	0.41
2:W:139:LEU:HD21	2:W:167:PRO:HA	2.02	0.41
1:A:98:ILE:N	1:A:100:GLU:OE2	2.52	0.41
2:X:37:PRO:HB3	2:X:98:CYS:SG	2.60	0.41
2:Y:53:THR:HG22	6:Y:601:HOH:O	2.19	0.41
2:Y:60:ASP:HA	2:Y:61:PRO:HD3	1.91	0.41
1:F:130:MET:HG2	1:F:130:MET:H	1.61	0.41
2:Y:203:LEU:HD12	2:Y:204:LYS:N	2.36	0.41
6:E:162:HOH:O	1:F:66:ILE:HG21	2.20	0.41
1:A:77:ASP:OD2	2:X:182:ARG:NH2	2.54	0.41
2:U:148:SER:HB3	6:U:329:HOH:O	2.20	0.41
2:W:128:LYS:HA	2:W:206:ARG:HB2	2.03	0.41
1:A:142:HIS:O	1:A:146:HIS:ND1	2.54	0.41
2:X:123:LEU:HA	2:X:124:PRO:HD3	1.91	0.41
1:B:97:ASN:HB2	6:B:155:HOH:O	2.21	0.41
2:X:244:ASN:O	2:X:295:ALA:HA	2.20	0.41
1:E:46:ARG:HD2	6:E:241:HOH:O	2.21	0.41
2:Y:100:ASN:HB3	2:Y:104:LEU:H	1.86	0.41
1:A:127:LYS:HE2	6:A:248:HOH:O	2.21	0.41
1:F:6:ASN:N	1:F:6:ASN:ND2	2.69	0.41
1:A:31:ASN:HB2	1:A:51:GLN:OE1	2.20	0.41
1:F:111:THR:HB	6:F:241:HOH:O	2.21	0.41
1:B:52:LEU:CD1	6:B:195:HOH:O	2.68	0.41
2:Y:70:THR:HG22	2:Y:71:TYR:H	1.86	0.41
2:U:261:LYS:CA	2:U:261:LYS:HE2	2.47	0.41
1:F:81:LYS:NZ	6:W:343:HOH:O	2.53	0.41
2:U:104:LEU:N	6:U:360:HOH:O	2.40	0.40
2:Y:222:HIS:HE1	6:Y:477:HOH:O	2.03	0.40
1:E:77:ASP:OD2	2:U:182:ARG:NH2	2.54	0.40
2:X:124:PRO:HB2	2:X:126:PHE:HE1	1.86	0.40
2:U:113:ARG:HA	2:U:140:THR:O	2.21	0.40
2:W:59:ILE:CD1	2:W:59:ILE:N	2.84	0.40
2:U:257:ILE:HD12	2:U:258:ALA:N	2.35	0.40
1:E:69:GLY:HA3	6:E:232:HOH:O	2.20	0.40
2:X:75:MET:HE1	6:X:433:HOH:O	2.21	0.40
2:U:151:GLU:HG2	2:U:155:LYS:H	1.85	0.40
2:X:125:LEU:HD22	2:X:125:LEU:HA	1.84	0.40
1:F:88:LEU:CD1	2:W:206:ARG:HG2	2.51	0.40
2:W:207:GLU:HB3	2:W:270:PHE:CD2	2.56	0.40
2:U:51:GLY:O	2:U:87:LYS:HD2	2.21	0.40
2:Y:306:THR:HA	6:Y:577:HOH:O	2.20	0.40
1:A:101:SER:N	1:A:102:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:197:HIS:HB2	6:X:322:HOH:O	2.21	0.40
2:X:121:VAL:HG12	2:X:122:GLY:N	2.37	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	142/145 (98%)	124 (87%)	13 (9%)	5 (4%)	6	7
1	B	137/145 (94%)	122 (89%)	10 (7%)	5 (4%)	5	6
1	E	137/145 (94%)	124 (90%)	9 (7%)	4 (3%)	7	9
1	F	137/145 (94%)	121 (88%)	12 (9%)	4 (3%)	7	9
2	U	273/290 (94%)	252 (92%)	15 (6%)	6 (2%)	10	15
2	W	273/290 (94%)	255 (93%)	12 (4%)	6 (2%)	10	15
2	X	273/290 (94%)	253 (93%)	15 (6%)	5 (2%)	13	20
2	Y	273/290 (94%)	249 (91%)	16 (6%)	8 (3%)	7	9
All	All	1645/1740 (94%)	1500 (91%)	102 (6%)	43 (3%)	8	11

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	PRO
1	E	102	PRO
1	F	102	PRO
2	X	73	ASN
2	Y	73	ASN
2	W	73	ASN
1	A	70	LEU
1	A	102	PRO
1	B	70	LEU
1	E	70	LEU

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Mol	Chain	Res	Type
1	F	70	LEU
2	Y	42	ALA
2	U	73	ASN
2	U	136	ARG
2	W	42	ALA
2	W	136	ARG
2	X	251	ASN
2	Y	175	ASN
2	Y	251	ASN
2	U	251	ASN
2	W	251	ASN
1	A	99	LYS
1	B	99	LYS
1	E	99	LYS
1	F	99	LYS
2	Y	136	ARG
2	U	42	ALA
1	A	145	HIS
1	B	136	SER
2	X	41	PRO
2	X	175	ASN
1	B	104	ARG
1	F	104	ARG
2	U	175	ASN
2	X	218	PRO
2	U	218	PRO
1	A	104	ARG
1	E	104	ARG
2	Y	218	PRO
2	Y	252	PRO
2	W	254	PRO
2	Y	254	PRO
2	W	252	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	135/136 (99%)	124 (92%)	11 (8%)	17	30
1	B	130/136 (96%)	119 (92%)	11 (8%)	15	28
1	E	130/136 (96%)	120 (92%)	10 (8%)	18	33
1	F	130/136 (96%)	120 (92%)	10 (8%)	18	33
2	U	247/259 (95%)	231 (94%)	16 (6%)	24	42
2	W	247/259 (95%)	230 (93%)	17 (7%)	22	39
2	X	247/259 (95%)	224 (91%)	23 (9%)	13	23
2	Y	247/259 (95%)	230 (93%)	17 (7%)	22	39
All	All	1513/1580 (96%)	1398 (92%)	115 (8%)	19	33

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	18	LEU
1	A	59	LEU
1	A	62	LYS
1	A	65	ASN
1	A	66	ILE
1	A	83	VAL
1	A	102	PRO
1	A	104	ARG
1	A	142	HIS
1	A	143	HIS
1	B	6	ASN
1	B	18	LEU
1	B	59	LEU
1	B	62	LYS
1	B	65	ASN
1	B	66	ILE
1	B	83	VAL
1	B	97	ASN
1	B	104	ARG
1	B	130	MET
1	B	133	SER
1	E	6	ASN
1	E	18	LEU
1	E	59	LEU
1	E	62	LYS
1	E	65	ASN

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Mol	Chain	Res	Type
1	E	66	ILE
1	E	83	VAL
1	E	97	ASN
1	E	104	ARG
1	E	133	SER
1	F	6	ASN
1	F	18	LEU
1	F	59	LEU
1	F	62	LYS
1	F	65	ASN
1	F	66	ILE
1	F	83	VAL
1	F	97	ASN
1	F	104	ARG
1	F	133	SER
2	X	40	HIS
2	X	41	PRO
2	X	53	THR
2	X	59	ILE
2	X	65	ARG
2	X	85	GLN
2	X	95	THR
2	X	100	ASN
2	X	102	ASN
2	X	118	LEU
2	X	125	LEU
2	X	134	LEU
2	X	139	LEU
2	X	150	ILE
2	X	152	CYS
2	X	207	GLU
2	X	209	ILE
2	X	222	HIS
2	X	230	PHE
2	X	236	ILE
2	X	255	GLN
2	X	265	TRP
2	X	276	GLU
2	Y	40	HIS
2	Y	49	GLU
2	Y	65	ARG
2	Y	85	GLN

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Mol	Chain	Res	Type
2	Y	95	THR
2	Y	100	ASN
2	Y	102	ASN
2	Y	125	LEU
2	Y	134	LEU
2	Y	139	LEU
2	Y	150	ILE
2	Y	152	CYS
2	Y	230	PHE
2	Y	236	ILE
2	Y	265	TRP
2	Y	276	GLU
2	Y	280	ILE
2	U	59	ILE
2	U	65	ARG
2	U	85	GLN
2	U	95	THR
2	U	100	ASN
2	U	102	ASN
2	U	118	LEU
2	U	125	LEU
2	U	134	LEU
2	U	138	PRO
2	U	139	LEU
2	U	150	ILE
2	U	152	CYS
2	U	230	PHE
2	U	265	TRP
2	U	276	GLU
2	W	59	ILE
2	W	65	ARG
2	W	85	GLN
2	W	95	THR
2	W	100	ASN
2	W	102	ASN
2	W	118	LEU
2	W	125	LEU
2	W	134	LEU
2	W	139	LEU
2	W	150	ILE
2	W	152	CYS
2	W	230	PHE

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Mol	Chain	Res	Type
2	W	257	ILE
2	W	265	TRP
2	W	276	GLU
2	W	280	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	65	ASN
1	A	120	ASN
1	A	143	HIS
1	B	6	ASN
1	B	21	ASN
1	B	65	ASN
1	B	120	ASN
1	E	6	ASN
1	E	65	ASN
1	E	120	ASN
1	F	65	ASN
1	F	120	ASN
2	X	85	GLN
2	X	100	ASN
2	X	102	ASN
2	X	251	ASN
2	X	255	GLN
2	X	259	GLN
2	X	297	ASN
2	Y	85	GLN
2	Y	100	ASN
2	Y	102	ASN
2	Y	251	ASN
2	Y	259	GLN
2	Y	297	ASN
2	U	85	GLN
2	U	100	ASN
2	U	102	ASN
2	U	251	ASN
2	U	259	GLN
2	U	297	ASN
2	W	85	GLN
2	W	100	ASN

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Mol	Chain	Res	Type
2	W	102	ASN
2	W	251	ASN
2	W	259	GLN
2	W	297	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 ⓘ

24 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	$\# Z > 2$
3	FUL	U	1	3	9,10,11	0.44	0	10,14,16	0.39	0
3	NAG	U	2	3,2	12,14,15	0.71	0	15,19,21	1.07	1 (6%)
3	NAG	U	3	3	12,14,15	0.48	0	15,19,21	0.79	0
4	NAG	U	4	2,4	12,14,15	0.79	0	15,19,21	1.13	2 (13%)
4	NAG	U	5	4	12,14,15	0.71	0	15,19,21	0.68	0
4	MAN	U	6	4	10,11,12	0.46	0	11,15,17	0.52	0
3	FUL	W	1	3	9,10,11	0.41	0	10,14,16	0.38	0
3	NAG	W	2	3,2	12,14,15	0.60	0	15,19,21	0.84	0
3	NAG	W	3	3	12,14,15	0.45	0	15,19,21	0.53	0
5	NDG	W	4	2,5	12,14,15	0.65	0	15,19,21	0.50	0
5	NAG	W	5	5	12,14,15	0.63	0	15,19,21	0.77	0
5	MAN	W	6	5	10,11,12	0.50	0	11,15,17	0.51	0
3	FUL	X	1	3	9,10,11	0.40	0	10,14,16	0.34	0
3	NAG	X	2	3,2	12,14,15	0.60	0	15,19,21	0.97	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	X	3	3	12,14,15	0.48	0	15,19,21	0.63	0
4	NAG	X	4	2,4	12,14,15	0.72	0	15,19,21	1.22	1 (6%)
4	NAG	X	5	4	12,14,15	0.71	0	15,19,21	0.67	0
4	MAN	X	6	4	10,11,12	0.46	0	11,15,17	0.48	0
3	FUL	Y	1	3	9,10,11	0.39	0	10,14,16	0.36	0
3	NAG	Y	2	3,2	12,14,15	0.68	0	15,19,21	1.12	0
3	NAG	Y	3	3	12,14,15	0.46	0	15,19,21	0.68	0
4	NAG	Y	4	2,4	12,14,15	0.83	0	15,19,21	1.36	2 (13%)
4	NAG	Y	5	4	12,14,15	0.62	0	15,19,21	0.89	0
4	MAN	Y	6	4	10,11,12	0.37	0	11,15,17	0.31	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
3	FUL	U	1	3	-	0/0/17/20	0/1/1/1
3	NAG	U	2	3,2	-	0/6/23/26	0/1/1/1
3	NAG	U	3	3	-	0/6/23/26	0/1/1/1
4	NAG	U	4	2,4	-	1/6/23/26	0/1/1/1
4	NAG	U	5	4	-	0/6/23/26	0/1/1/1
4	MAN	U	6	4	-	0/2/19/22	0/1/1/1
3	FUL	W	1	3	-	0/0/17/20	0/1/1/1
3	NAG	W	2	3,2	-	0/6/23/26	0/1/1/1
3	NAG	W	3	3	-	0/6/23/26	0/1/1/1
5	NDG	W	4	2,5	-	0/6/23/26	0/1/1/1
5	NAG	W	5	5	-	0/6/23/26	0/1/1/1
5	MAN	W	6	5	-	0/2/19/22	0/1/1/1
3	FUL	X	1	3	-	0/0/17/20	0/1/1/1
3	NAG	X	2	3,2	-	0/6/23/26	0/1/1/1
3	NAG	X	3	3	-	0/6/23/26	0/1/1/1
4	NAG	X	4	2,4	-	0/6/23/26	0/1/1/1
4	NAG	X	5	4	-	0/6/23/26	0/1/1/1
4	MAN	X	6	4	-	0/2/19/22	0/1/1/1
3	FUL	Y	1	3	-	0/0/17/20	0/1/1/1
3	NAG	Y	2	3,2	-	0/6/23/26	0/1/1/1
3	NAG	Y	3	3	-	0/6/23/26	0/1/1/1
4	NAG	Y	4	2,4	-	1/6/23/26	0/1/1/1
4	NAG	Y	5	4	-	0/6/23/26	0/1/1/1
4	MAN	Y	6	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	4	NAG	C3-C4-C5	3.12	115.77	110.20
4	U	4	NAG	C3-C4-C5	2.97	115.50	110.20
4	Y	4	NAG	C4-C3-C2	2.84	118.27	111.32
4	X	4	NAG	C3-C4-C5	2.80	115.20	110.20
3	U	2	NAG	C2-N2-C7	-2.23	119.34	123.09
4	U	4	NAG	C4-C3-C2	2.17	116.63	111.32
3	X	2	NAG	C2-N2-C7	-2.02	119.70	123.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	4	NAG	O7-C7-N2-C2
4	U	4	NAG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	144/145 (99%)	0.67	11 (7%) 14 13	42, 68, 170, 188	0
1	B	139/145 (95%)	1.24	25 (17%) 2 2	39, 76, 187, 194	0
1	E	139/145 (95%)	1.40	20 (14%) 3 3	39, 69, 184, 200	0
1	F	139/145 (95%)	1.49	34 (24%) 1 1	45, 86, 185, 197	0
2	U	275/290 (94%)	0.82	41 (14%) 3 3	44, 85, 168, 187	0
2	W	275/290 (94%)	1.67	91 (33%) 1 1	59, 104, 183, 193	0
2	X	275/290 (94%)	0.95	43 (15%) 3 2	49, 90, 162, 189	0
2	Y	275/290 (94%)	1.24	55 (20%) 2 1	46, 81, 180, 191	0
All	All	1661/1740 (95%)	1.18	320 (19%) 2 1	39, 87, 177, 200	0

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34	ALA	12.2
2	W	96	TYR	11.3
2	W	246	MET	10.9
1	F	36	MET	10.7
2	W	224	LEU	10.0
2	Y	247	TRP	9.9
1	F	35	GLY	9.7
1	E	133	SER	9.6
1	F	38	VAL	9.4
1	B	133	SER	9.4
2	W	247	TRP	9.3
1	E	134	ASP	8.9
2	Y	232	VAL	8.8
1	B	93	ASN	8.7
2	Y	248	LEU	8.2
1	F	39	LEU	8.0

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Mol	Chain	Res	Type	RSRZ
2	Y	236	ILE	7.6
1	B	36	MET	7.5
2	Y	290	VAL	7.5
1	F	140	LEU	7.4
2	W	236	ILE	7.4
2	Y	293	CYS	7.3
2	W	59	ILE	7.3
2	W	254	PRO	7.2
1	B	134	ASP	7.1
2	W	226	LYS	7.0
1	F	3	ILE	6.9
2	X	63	PHE	6.8
2	Y	294	TYR	6.8
2	Y	295	ALA	6.8
2	W	283	ALA	6.7
2	W	225	LYS	6.5
2	U	291	PHE	6.4
2	W	234	CYS	6.3
1	F	134	ASP	6.3
2	X	99	SER	6.3
2	W	308	LEU	6.3
2	W	280	ILE	6.2
2	W	249	LYS	6.1
1	F	138	CYS	6.1
2	W	66	TRP	6.1
2	W	99	SER	6.0
2	U	290	VAL	6.0
2	W	293	CYS	6.0
2	Y	246	MET	5.9
2	W	253	GLN	5.9
2	X	65	ARG	5.8
1	B	98	ILE	5.8
1	A	38	VAL	5.8
1	E	131	VAL	5.8
1	F	33	VAL	5.7
1	F	136	SER	5.7
2	W	294	TYR	5.7
2	Y	283	ALA	5.7
2	W	292	MET	5.7
2	X	66	TRP	5.7
1	B	95	PRO	5.6
1	B	135	THR	5.6

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Mol	Chain	Res	Type	RSRZ
2	W	239	VAL	5.6
2	W	215	VAL	5.5
2	W	108	ILE	5.5
1	B	131	VAL	5.5
2	Y	304	VAL	5.4
1	F	37	ASP	5.4
2	W	304	VAL	5.4
1	E	132	ALA	5.4
2	W	245	SER	5.4
2	Y	302	ALA	5.4
2	W	287	ASP	5.3
1	E	130	MET	5.3
2	W	291	PHE	5.3
2	W	56	LEU	5.3
2	W	248	LEU	5.3
2	W	233	VAL	5.3
2	X	291	PHE	5.2
1	E	69	GLY	5.1
2	X	100	ASN	5.1
2	Y	278	LEU	5.1
1	E	135	THR	5.1
1	B	138	CYS	5.1
2	U	66	TRP	5.1
2	Y	237	LYS	5.0
2	Y	249	LYS	5.0
1	E	136	SER	5.0
2	U	248	LEU	4.9
2	W	274	ARG	4.9
2	W	98	CYS	4.9
2	W	295	ALA	4.8
2	Y	256	HIS	4.8
1	F	70	LEU	4.8
2	W	290	VAL	4.7
2	Y	219	GLU	4.7
1	B	132	ALA	4.6
2	W	67	THR	4.5
2	Y	291	PHE	4.5
1	B	96	LYS	4.5
2	W	232	VAL	4.4
1	B	32	TYR	4.4
2	W	238	ASP	4.4
1	A	134	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
2	W	252	PRO	4.3
2	Y	285	VAL	4.2
2	W	222	HIS	4.2
2	U	250	MET	4.2
2	W	243	VAL	4.2
2	Y	286	ASP	4.2
2	Y	309	LYS	4.1
1	E	35	GLY	4.1
2	Y	226	LYS	4.1
2	Y	250	MET	4.1
2	X	104	LEU	4.0
1	B	68	GLU	4.0
2	U	56	LEU	4.0
2	U	189	ALA	4.0
2	Y	252	PRO	4.0
2	X	285	VAL	4.0
2	X	250	MET	4.0
2	W	65	ARG	4.0
2	W	256	HIS	4.0
2	X	295	ALA	3.9
1	F	93	ASN	3.9
2	X	81	ASN	3.9
2	X	98	CYS	3.9
2	W	286	ASP	3.9
2	W	288	SER	3.8
2	W	305	THR	3.8
2	W	40	HIS	3.8
2	Y	230	PHE	3.8
2	W	100	ASN	3.8
1	F	44	TRP	3.7
2	X	294	TYR	3.7
1	A	37	ASP	3.7
2	X	84	ILE	3.7
2	Y	305	THR	3.7
2	W	217	VAL	3.7
1	E	97	ASN	3.7
2	U	246	MET	3.7
2	Y	40	HIS	3.6
2	Y	222	HIS	3.6
1	B	43	CYS	3.6
2	Y	223	LEU	3.6
1	B	99	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
2	X	287	ASP	3.5
2	X	236	ILE	3.5
2	W	104	LEU	3.5
1	E	137	ASP	3.5
2	U	247	TRP	3.5
2	W	284	ARG	3.5
1	E	138	CYS	3.5
2	Y	217	VAL	3.5
1	B	41	SER	3.5
2	Y	308	LEU	3.5
2	X	302	ALA	3.4
2	W	250	MET	3.4
2	U	304	VAL	3.4
1	F	41	SER	3.4
2	X	249	LYS	3.4
2	Y	307	THR	3.4
2	W	105	THR	3.4
2	X	244	ASN	3.4
2	U	278	LEU	3.4
1	B	139	VAL	3.3
2	W	310	VAL	3.3
2	Y	306	THR	3.3
2	X	257	ILE	3.3
1	F	135	THR	3.3
2	X	64	VAL	3.3
2	X	54	LEU	3.3
2	W	57	THR	3.3
2	W	282	SER	3.3
2	W	81	ASN	3.3
2	W	223	LEU	3.2
1	F	139	VAL	3.2
1	F	50	ILE	3.2
2	U	236	ILE	3.1
2	U	249	LYS	3.1
2	W	278	LEU	3.1
1	E	93	ASN	3.1
1	F	99	LYS	3.1
1	B	101	SER	3.1
2	W	63	PHE	3.1
2	W	102	ASN	3.1
1	B	44	TRP	3.1
1	E	42	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	X	83	TRP	3.0
1	A	131	VAL	3.0
2	U	118	LEU	3.0
2	W	275	GLN	3.0
2	Y	292	MET	3.0
1	F	137	ASP	3.0
1	B	70	LEU	2.9
2	X	280	ILE	2.9
2	U	280	ILE	2.9
2	X	56	LEU	2.9
2	W	309	LYS	2.9
2	W	207	GLU	2.9
2	X	310	VAL	2.9
2	Y	245	SER	2.9
2	X	58	CYS	2.9
1	E	129	PHE	2.9
1	F	141	SER	2.9
2	W	82	GLU	2.8
2	X	62	ASP	2.8
2	Y	215	VAL	2.8
2	W	306	THR	2.8
2	W	230	PHE	2.8
2	X	247	TRP	2.8
1	F	42	HIS	2.8
2	Y	235	THR	2.7
1	F	129	PHE	2.7
2	W	118	LEU	2.7
2	U	257	ILE	2.7
2	U	147	TYR	2.7
1	B	37	ASP	2.7
2	W	47	ILE	2.7
2	W	276	GLU	2.7
2	W	285	VAL	2.7
2	X	278	LEU	2.7
2	U	195	TRP	2.7
1	B	34	ALA	2.7
1	F	104	ARG	2.7
2	Y	284	ARG	2.7
1	E	34	ALA	2.7
2	W	272	TYR	2.6
2	W	75	MET	2.6
1	F	43	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	W	58	CYS	2.6
2	U	139	LEU	2.6
2	W	289	GLY	2.6
2	Y	272	TYR	2.6
2	Y	243	VAL	2.6
2	W	281	SER	2.6
2	Y	233	VAL	2.6
2	W	214	VAL	2.6
1	A	129	PHE	2.5
2	W	173	ILE	2.5
2	X	283	ALA	2.5
2	U	149	LEU	2.5
2	X	245	SER	2.5
2	Y	140	THR	2.5
2	Y	159	THR	2.5
1	B	105	PRO	2.5
1	F	81	LYS	2.5
2	X	223	LEU	2.5
2	X	297	ASN	2.5
2	Y	214	VAL	2.5
2	U	161	LEU	2.5
1	F	95	PRO	2.5
2	W	251	ASN	2.5
2	U	255	GLN	2.4
1	E	98	ILE	2.4
1	F	98	ILE	2.4
2	X	106	SER	2.4
2	Y	59	ILE	2.4
2	Y	144	VAL	2.4
2	X	59	ILE	2.4
2	U	253	GLN	2.4
2	X	67	THR	2.4
2	U	225	LYS	2.4
2	W	92	ARG	2.4
2	U	76	VAL	2.3
2	U	256	HIS	2.3
1	A	70	LEU	2.3
2	X	248	LEU	2.3
2	W	97	THR	2.3
2	Y	224	LEU	2.3
2	W	257	ILE	2.3
2	X	105	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	W	139	LEU	2.3
2	U	63	PHE	2.3
2	W	41	PRO	2.3
2	U	294	TYR	2.3
2	Y	257	ILE	2.3
2	U	243	VAL	2.3
2	U	196	LEU	2.2
2	X	254	PRO	2.2
2	Y	158	PRO	2.2
1	F	115	PHE	2.2
1	F	32	TYR	2.2
2	U	67	THR	2.2
2	U	228	ASP	2.2
2	U	212	ILE	2.2
2	W	101	SER	2.2
1	F	69	GLY	2.2
2	Y	276	GLU	2.2
2	Y	41	PRO	2.2
2	Y	242	SER	2.2
2	W	203	LEU	2.2
2	W	103	GLY	2.2
2	U	254	PRO	2.2
2	Y	280	ILE	2.2
2	W	72	PHE	2.2
1	F	130	MET	2.1
1	B	66	ILE	2.1
2	U	83	TRP	2.1
2	W	79	LYS	2.1
1	A	98	ILE	2.1
1	E	70	LEU	2.1
2	Y	244	ASN	2.1
2	U	215	VAL	2.1
2	W	307	THR	2.1
2	W	43	GLN	2.1
1	A	39	LEU	2.1
2	U	98	CYS	2.1
2	U	232	VAL	2.1
1	E	6	ASN	2.1
1	A	86	LEU	2.1
1	E	118	ILE	2.1
1	F	133	SER	2.1
1	B	94	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	141	SER	2.0
2	X	172	THR	2.0
2	X	243	VAL	2.0
2	U	306	THR	2.0
2	U	309	LYS	2.0
2	U	292	MET	2.0
2	W	228	ASP	2.0
1	A	135	THR	2.0
2	Y	277	THR	2.0
2	X	173	ILE	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	FUL	U	1	10/11	0.40	1.16	124,131,139,141	0
4	NAG	X	4	14/15	0.20	-0.49	112,143,156,171	0
3	NAG	Y	2	14/15	0.23	-0.50	156,169,179,192	0
3	FUL	W	1	10/11	0.27	-0.83	160,171,172,173	0
3	NAG	W	2	14/15	0.12	-0.96	145,156,169,178	0
5	NDG	W	4	14/15	0.23	-1.37	164,180,187,190	0
3	NAG	U	2	14/15	0.16	-1.61	97,118,131,148	0
3	NAG	X	2	14/15	0.15	-1.64	111,124,133,143	0
4	NAG	U	4	14/15	0.15	-1.94	151,162,169,171	0
3	FUL	X	1	10/11	0.18	-2.14	112,119,127,129	0
4	NAG	Y	4	14/15	0.19	-4.53	137,150,160,170	0
3	FUL	Y	1	10/11	0.39	-146.00	154,171,175,177	0
4	NAG	X	5	14/15	0.22	-	183,193,195,196	0
3	NAG	W	3	14/15	0.18	-	185,191,194,196	0
3	NAG	U	3	14/15	0.23	-	170,189,193,194	0
4	NAG	Y	5	14/15	0.18	-	180,190,198,198	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	U	5	14/15	0.21	-	179,186,194,197	0
3	NAG	Y	3	14/15	0.19	-	185,191,194,196	0
3	NAG	X	3	14/15	0.17	-	156,163,170,171	0
4	MAN	X	6	11/12	0.12	-	193,197,198,198	0
4	MAN	U	6	11/12	0.10	-	191,196,198,198	0
5	MAN	W	6	11/12	0.23	-	190,196,198,198	0
5	NAG	W	5	14/15	0.26	-	187,195,198,198	0
4	MAN	Y	6	11/12	0.11	-	161,171,175,177	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.