Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:45 AM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

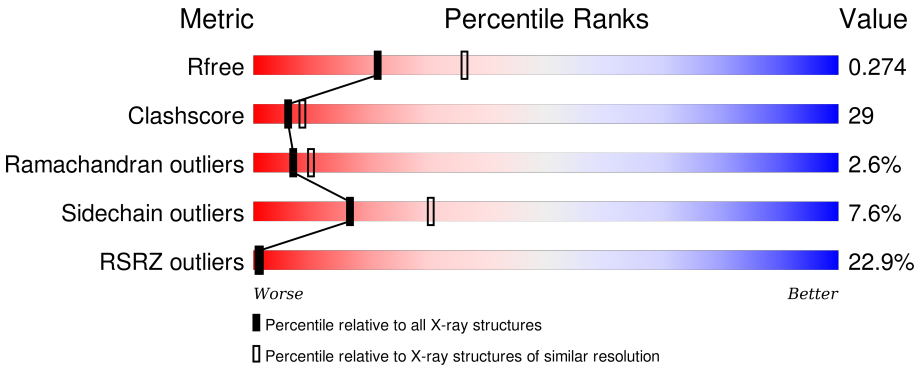
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	145	9% 62% 30% 7% ••
1	B	145	21% 55% 33% 7% • •
1	E	145	16% 54% 36% 6% • •
1	F	145	21% 59% 30% 7% •
2	U	290	23% 49% 39% 6% 5%

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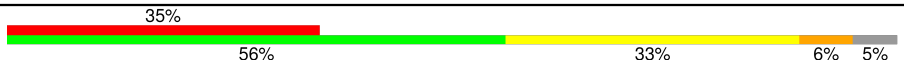
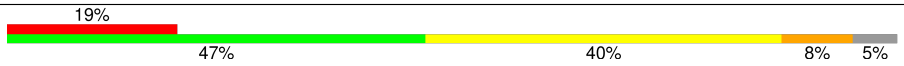
Mol	Chain	Length	Quality of chain
2	W	290	
2	X	290	
2	Y	290	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15104 atoms, of which 0 are 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 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
U	146	GLN	ASN	ENGINEERED	UNP P05532
W	146	GLN	ASN	ENGINEERED	UNP P05532
X	146	GLN	ASN	ENGINEERED	UNP P05532
Y	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		

- 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		

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

- 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 39 22 2 15	0	0

- Molecule 6 is water.

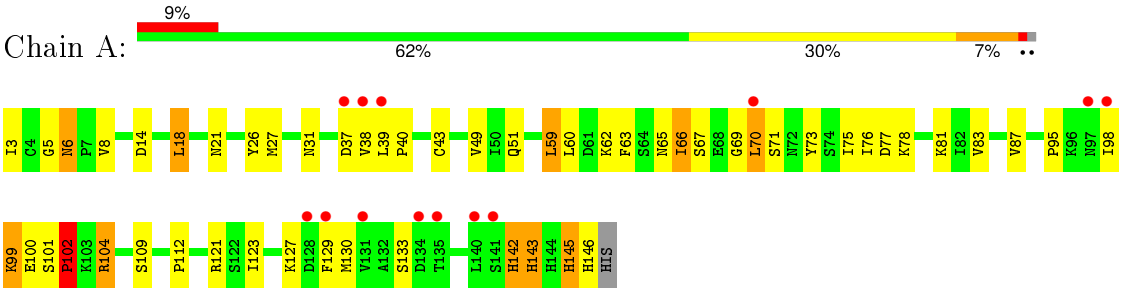
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	171	Total O 171 171	0	0
6	B	144	Total O 144 144	0	0
6	E	152	Total O 152 152	0	0
6	F	143	Total O 143 143	0	0
6	U	270	Total O 270 270	0	0
6	W	267	Total O 267 267	0	0
6	X	273	Total O 273 273	0	0
6	Y	310	Total O 310 310	0	0

3 Residue-property plots (i)

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

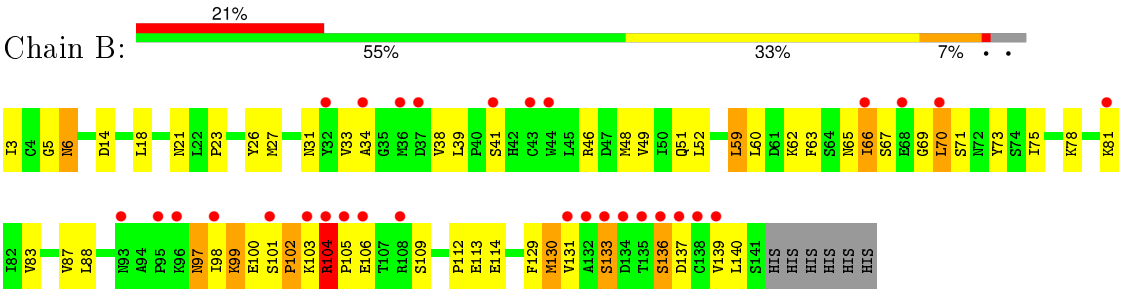
- Molecule 1: Kit ligand

Chain A:



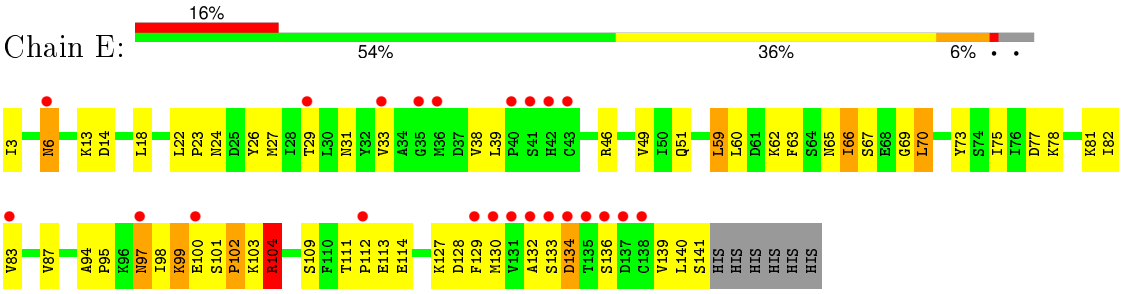
- Molecule 1: Kit ligand

Chain B:



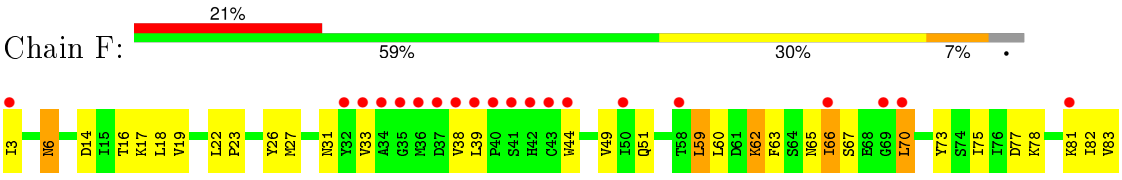
- Molecule 1: Kit ligand

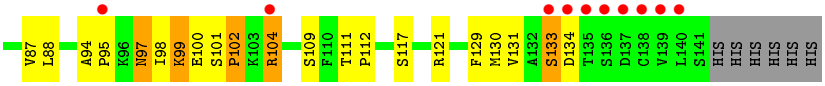
Chain E:



- Molecule 1: Kit ligand

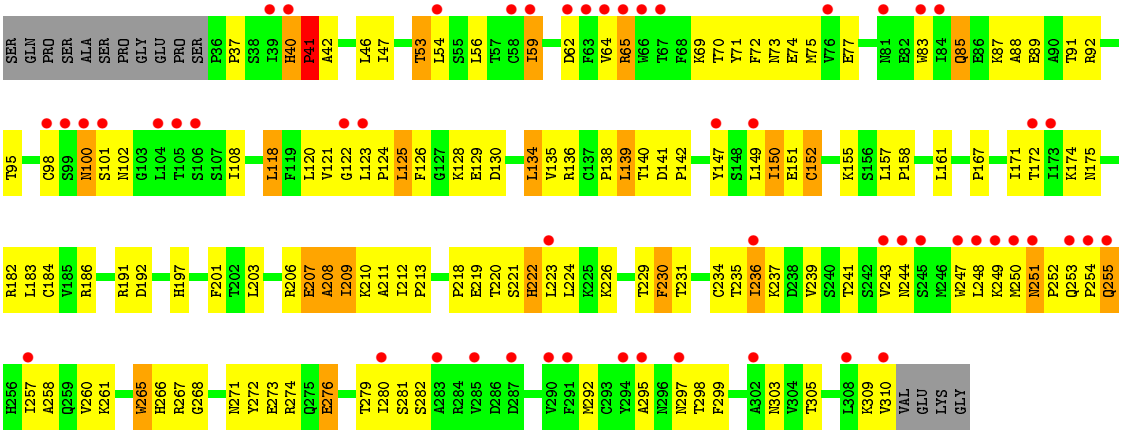
Chain F:





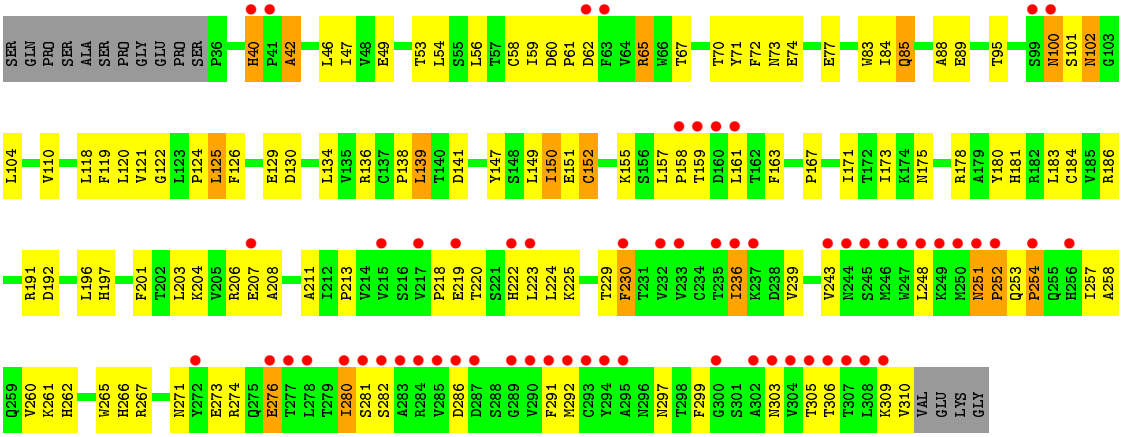
• Molecule 2: Mast/stem cell growth factor receptor

Chain X:



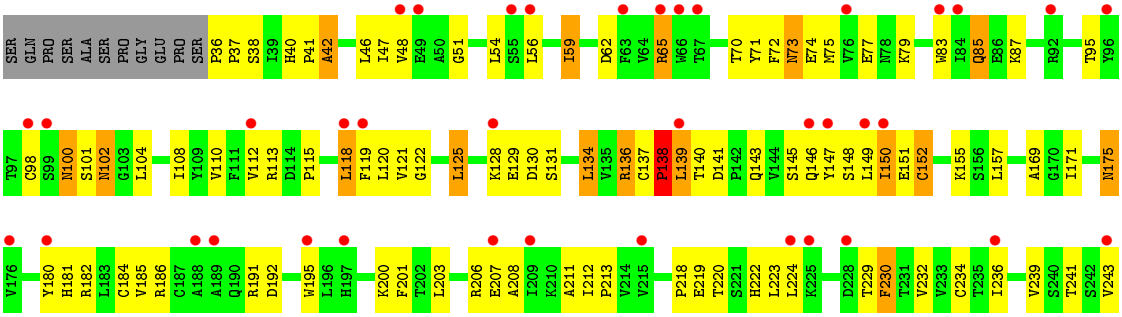
• Molecule 2: Mast/stem cell growth factor receptor

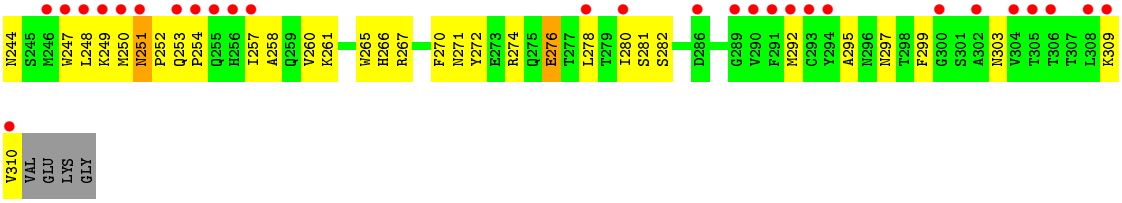
Chain Y:



• Molecule 2: Mast/stem cell growth factor receptor

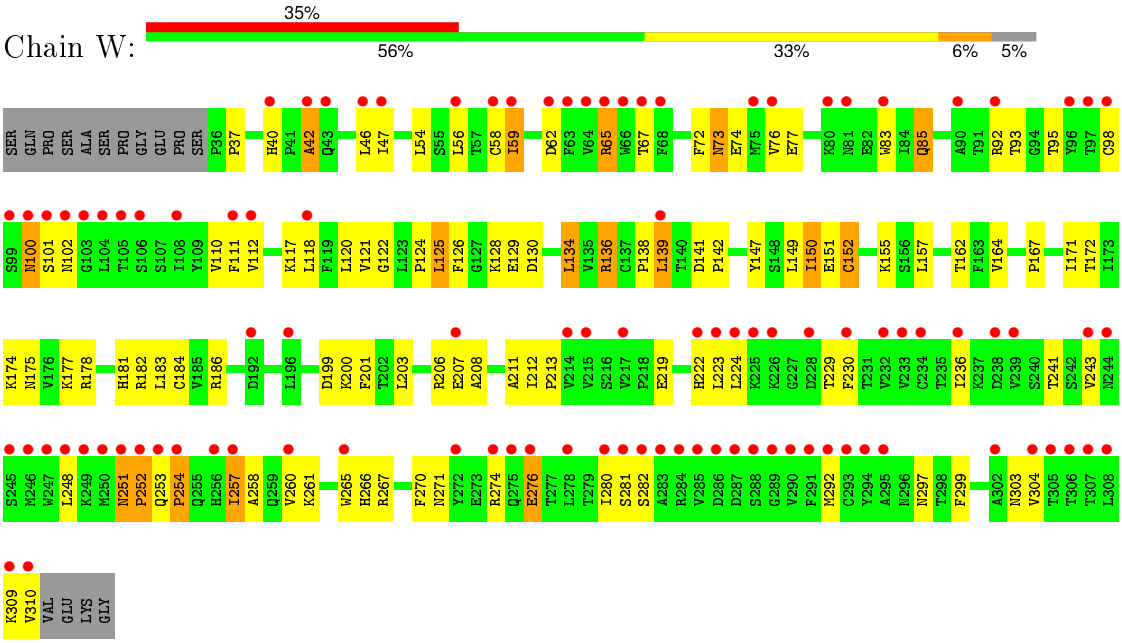
Chain U:





- Molecule 2: Mast/stem cell growth factor receptor

Chain W:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.38 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.270 0.242 , 0.274	Depositor DCC
R_{free} test set	4155 reflections (5.04%)	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 , 87.8	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 82592 reflections	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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 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	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

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 29.

All (761) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASP:HB3	1:B:75:ILE:HD12	1.65	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (i)

5.3.1 Protein backbone (i)

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%)	4	6
1	B	137/145 (94%)	122 (89%)	10 (7%)	5 (4%)	4	5
1	E	137/145 (94%)	124 (90%)	9 (7%)	4 (3%)	6	8
1	F	137/145 (94%)	121 (88%)	12 (9%)	4 (3%)	6	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	U	273/290 (94%)	252 (92%)	15 (6%)	6 (2%)	8 13
2	W	273/290 (94%)	255 (93%)	12 (4%)	6 (2%)	8 13
2	X	273/290 (94%)	253 (93%)	15 (6%)	5 (2%)	11 18
2	Y	273/290 (94%)	249 (91%)	16 (6%)	8 (3%)	6 8
All	All	1645/1740 (94%)	1500 (91%)	102 (6%)	43 (3%)	7 10

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
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

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Mol	Chain	Res	Type
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 (i)

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%)	15	27
1	B	130/136 (96%)	119 (92%)	11 (8%)	13	25
1	E	130/136 (96%)	120 (92%)	10 (8%)	16	30
1	F	130/136 (96%)	120 (92%)	10 (8%)	16	30
2	U	247/259 (95%)	231 (94%)	16 (6%)	21	39
2	W	247/259 (95%)	230 (93%)	17 (7%)	19	35
2	X	247/259 (95%)	224 (91%)	23 (9%)	11	21
2	Y	247/259 (95%)	230 (93%)	17 (7%)	19	35
All	All	1513/1580 (96%)	1398 (92%)	115 (8%)	16	30

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

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	10,10,11	0.51	0	14,14,16	0.75	0
3	NAG	U	2	3,2	14,14,15	0.75	0	15,19,21	1.10	1 (6%)
3	NAG	U	3	3	14,14,15	0.59	0	15,19,21	0.78	1 (6%)
4	NAG	U	4	2,4	14,14,15	0.77	0	15,19,21	1.34	2 (13%)
4	NAG	U	5	4	14,14,15	0.71	0	15,19,21	0.76	0
4	MAN	U	6	4	11,11,12	0.65	0	14,15,17	0.82	1 (7%)
3	FUL	W	1	3	10,10,11	0.46	0	14,14,16	0.49	0
3	NAG	W	2	3,2	14,14,15	0.59	0	15,19,21	0.89	0
3	NAG	W	3	3	14,14,15	0.52	0	15,19,21	0.60	0
5	NDG	W	4	2,5	14,14,15	0.80	0	15,19,21	0.53	0
5	NAG	W	5	5	14,14,15	0.63	0	15,19,21	0.84	1 (6%)
5	MAN	W	6	5	11,11,12	0.71	0	14,15,17	0.74	1 (7%)
3	FUL	X	1	3	10,10,11	0.44	0	14,14,16	0.65	0
3	NAG	X	2	3,2	14,14,15	0.60	0	15,19,21	1.01	1 (6%)
3	NAG	X	3	3	14,14,15	0.55	0	15,19,21	0.72	1 (6%)
4	NAG	X	4	2,4	14,14,15	0.73	0	15,19,21	1.37	2 (13%)
4	NAG	X	5	4	14,14,15	0.70	0	15,19,21	0.79	1 (6%)
4	MAN	X	6	4	11,11,12	0.64	0	14,15,17	0.72	1 (7%)
3	FUL	Y	1	3	10,10,11	0.47	0	14,14,16	0.67	0
3	NAG	Y	2	3,2	14,14,15	0.71	0	15,19,21	1.16	2 (13%)
3	NAG	Y	3	3	14,14,15	0.61	0	15,19,21	0.65	0
4	NAG	Y	4	2,4	14,14,15	0.80	0	15,19,21	1.65	3 (20%)
4	NAG	Y	5	4	14,14,15	0.63	0	15,19,21	0.97	1 (6%)
4	MAN	Y	6	4	11,11,12	0.58	0	14,15,17	0.61	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	2	NAG	C2-N2-C7	-2.88	119.34	123.04
3	X	2	NAG	C2-N2-C7	-2.60	119.70	123.04
3	Y	2	NAG	C2-N2-C7	-2.37	120.00	123.04
4	Y	4	NAG	C2-N2-C7	-2.31	120.07	123.04
5	W	5	NAG	C2-N2-C7	-2.30	120.09	123.04
4	Y	5	NAG	C2-N2-C7	-2.29	120.09	123.04
3	U	3	NAG	C2-N2-C7	-2.23	120.18	123.04
3	X	3	NAG	C2-N2-C7	-2.09	120.36	123.04
4	X	5	NAG	C2-N2-C7	-2.02	120.44	123.04
3	Y	2	NAG	C3-C4-C5	2.05	113.77	110.20
4	X	6	MAN	C1-C2-C3	2.10	112.03	109.54
5	W	6	MAN	C1-C2-C3	2.45	112.44	109.54
4	U	6	MAN	C1-C2-C3	2.50	112.50	109.54
4	X	4	NAG	C3-C4-C5	2.87	115.20	110.20
4	U	4	NAG	C3-C4-C5	3.04	115.50	110.20
4	X	4	NAG	C4-C3-C2	3.10	116.05	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	4	NAG	C3-C4-C5	3.20	115.77	110.20
4	U	4	NAG	C4-C3-C2	3.48	116.63	111.23
4	Y	4	NAG	C4-C3-C2	4.53	118.27	111.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	1	FUL	1	0
3	U	3	NAG	3	0
5	W	4	NDG	1	0
5	W	5	NAG	1	0
5	W	6	MAN	1	0
3	X	2	NAG	1	0
3	X	3	NAG	1	0
4	X	5	NAG	1	0
3	Y	2	NAG	2	0
4	Y	5	NAG	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.82	13 (9%) 12 12	42, 68, 170, 188	0
1	B	139/145 (95%)	1.40	30 (21%) 1 1	39, 76, 187, 194	0
1	E	139/145 (95%)	1.60	23 (16%) 2 2	39, 69, 184, 200	0
1	F	139/145 (95%)	1.67	30 (21%) 1 1	45, 86, 185, 197	0
2	U	275/290 (94%)	1.19	66 (24%) 1 1	44, 85, 168, 187	0
2	W	275/290 (94%)	2.23	102 (37%) 0 0	59, 104, 183, 193	0
2	X	275/290 (94%)	1.26	54 (19%) 1 1	49, 90, 162, 189	0
2	Y	275/290 (94%)	1.64	62 (22%) 1 1	46, 81, 180, 191	0
All	All	1661/1740 (95%)	1.51	380 (22%) 1 1	39, 87, 177, 200	0

All (380) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	36	MET	16.0
2	W	224	LEU	13.6
1	B	133	SER	13.5
2	Y	248	LEU	13.3
2	Y	247	TRP	13.2
1	F	34	ALA	13.1
2	Y	290	VAL	13.0
2	W	96	TYR	12.7
2	W	246	MET	12.3
1	E	133	SER	12.0
2	W	247	TRP	11.9
1	F	39	LEU	11.5
2	X	63	PHE	11.5
1	F	35	GLY	11.2
1	E	134	ASP	10.3
2	U	290	VAL	10.2

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Mol	Chain	Res	Type	RSRZ
2	Y	232	VAL	10.2
2	W	249	LYS	10.0
1	B	135	THR	10.0
2	Y	249	LYS	9.9
2	W	280	ILE	9.9
2	W	99	SER	9.6
2	X	287	ASP	9.5
1	F	33	VAL	9.3
2	Y	293	CYS	9.3
2	W	66	TRP	9.2
1	B	132	ALA	9.2
2	Y	246	MET	9.1
1	B	134	ASP	9.1
2	W	291	PHE	8.9
2	W	215	VAL	8.8
2	X	65	ARG	8.8
2	Y	304	VAL	8.6
1	B	36	MET	8.5
2	W	98	CYS	8.5
2	W	287	ASP	8.4
2	U	291	PHE	8.3
2	Y	286	ASP	8.1
2	Y	295	ALA	8.1
2	Y	291	PHE	8.1
2	W	283	ALA	8.1
1	F	38	VAL	7.9
2	W	248	LEU	7.8
2	Y	294	TYR	7.8
1	E	130	MET	7.7
2	W	308	LEU	7.7
2	X	99	SER	7.6
1	F	138	CYS	7.6
2	W	304	VAL	7.6
2	W	236	ILE	7.6
2	W	292	MET	7.6
2	W	290	VAL	7.5
2	X	66	TRP	7.4
1	E	136	SER	7.4
2	U	248	LEU	7.3
2	Y	278	LEU	7.1
2	W	293	CYS	7.0
1	B	131	VAL	7.0

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Mol	Chain	Res	Type	RSRZ
2	W	232	VAL	7.0
2	Y	250	MET	7.0
1	F	134	ASP	7.0
2	W	295	ALA	6.9
2	W	225	LYS	6.8
2	W	234	CYS	6.8
1	E	42	HIS	6.8
1	F	43	CYS	6.8
2	U	250	MET	6.8
2	X	81	ASN	6.7
2	X	291	PHE	6.7
1	F	41	SER	6.7
2	U	249	LYS	6.6
2	X	250	MET	6.6
2	Y	307	THR	6.6
2	W	254	PRO	6.6
2	W	233	VAL	6.5
1	F	136	SER	6.5
2	W	284	ARG	6.5
2	W	222	HIS	6.5
2	W	100	ASN	6.5
2	W	67	THR	6.5
1	F	37	ASP	6.5
2	W	286	ASP	6.4
2	Y	236	ILE	6.4
2	W	226	LYS	6.4
2	X	249	LYS	6.3
2	Y	283	ALA	6.3
2	Y	302	ALA	6.3
1	F	44	TRP	6.3
1	E	131	VAL	6.3
2	W	243	VAL	6.3
1	F	42	HIS	6.2
2	W	288	SER	6.2
2	X	285	VAL	6.2
2	Y	305	THR	6.1
2	W	245	SER	6.1
2	X	58	CYS	6.0
2	X	64	VAL	6.0
1	A	38	VAL	5.9
2	W	63	PHE	5.9
2	Y	252	PRO	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	138	CYS	5.8
2	U	66	TRP	5.8
2	W	59	ILE	5.7
1	E	137	ASP	5.7
2	W	274	ARG	5.7
1	E	132	ALA	5.6
2	W	310	VAL	5.5
2	Y	292	MET	5.5
2	Y	306	THR	5.4
1	B	93	ASN	5.4
2	X	100	ASN	5.4
2	U	56	LEU	5.4
1	A	134	ASP	5.4
1	E	135	THR	5.3
2	W	75	MET	5.3
2	X	98	CYS	5.2
2	W	294	TYR	5.2
1	B	32	TYR	5.2
1	F	70	LEU	5.2
2	W	56	LEU	5.1
1	E	41	SER	5.1
2	W	108	ILE	5.1
2	W	217	VAL	5.1
2	W	278	LEU	5.1
2	Y	230	PHE	5.1
2	X	254	PRO	5.0
2	X	104	LEU	5.0
2	Y	308	LEU	5.0
1	B	95	PRO	5.0
2	W	223	LEU	4.9
2	U	255	GLN	4.9
1	F	140	LEU	4.9
2	Y	100	ASN	4.9
2	U	304	VAL	4.9
1	B	98	ILE	4.8
2	W	256	HIS	4.8
2	W	214	VAL	4.7
2	W	305	THR	4.7
2	W	285	VAL	4.7
2	X	67	THR	4.7
2	Y	285	VAL	4.7
2	X	248	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	41	SER	4.6
2	U	243	VAL	4.6
2	Y	289	GLY	4.5
2	Y	219	GLU	4.5
2	W	230	PHE	4.5
1	F	3	ILE	4.4
2	W	253	GLN	4.4
2	X	310	VAL	4.4
2	W	97	THR	4.4
2	W	102	ASN	4.4
2	U	189	ALA	4.3
2	Y	309	LYS	4.3
2	W	244	ASN	4.3
2	U	292	MET	4.3
2	Y	245	SER	4.3
2	W	101	SER	4.3
2	U	251	ASN	4.2
2	W	282	SER	4.2
2	W	92	ARG	4.2
1	B	66	ILE	4.2
2	W	47	ILE	4.2
2	Y	280	ILE	4.1
2	X	255	GLN	4.1
2	X	294	TYR	4.0
2	W	65	ARG	4.0
2	W	105	THR	4.0
1	B	105	PRO	4.0
1	A	128	ASP	4.0
1	E	97	ASN	4.0
2	Y	217	VAL	4.0
2	W	58	CYS	3.9
2	W	309	LYS	3.9
2	Y	222	HIS	3.9
2	Y	256	HIS	3.9
2	X	59	ILE	3.9
2	U	83	TRP	3.9
2	U	112	VAL	3.9
2	X	236	ILE	3.9
2	X	302	ALA	3.8
1	F	137	ASP	3.8
2	W	289	GLY	3.8
2	Y	303	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	X	105	THR	3.8
2	U	246	MET	3.8
2	U	118	LEU	3.8
2	W	76	VAL	3.7
2	Y	254	PRO	3.7
1	A	129	PHE	3.7
2	W	104	LEU	3.7
1	B	43	CYS	3.7
2	Y	159	THR	3.7
2	U	67	THR	3.7
2	W	306	THR	3.7
2	W	281	SER	3.7
1	A	131	VAL	3.6
1	E	40	PRO	3.6
2	U	256	HIS	3.6
1	F	40	PRO	3.5
2	U	309	LYS	3.5
1	B	37	ASP	3.5
2	W	252	PRO	3.5
2	W	250	MET	3.5
2	Y	40	HIS	3.4
2	U	254	PRO	3.4
2	X	106	SER	3.4
2	W	207	GLU	3.4
1	F	135	THR	3.3
2	X	283	ALA	3.3
1	F	32	TYR	3.3
2	U	48	VAL	3.3
1	E	129	PHE	3.3
2	Y	276	GLU	3.3
1	B	70	LEU	3.3
2	U	76	VAL	3.3
1	A	37	ASP	3.3
2	Y	287	ASP	3.3
2	X	295	ALA	3.3
1	F	104	ARG	3.3
2	X	54	LEU	3.2
1	F	95	PRO	3.2
1	B	138	CYS	3.2
2	Y	158	PRO	3.2
2	W	275	GLN	3.2
1	A	98	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	X	280	ILE	3.2
2	Y	300	GLY	3.2
2	U	55	SER	3.2
2	W	118	LEU	3.2
1	B	44	TRP	3.2
2	Y	282	SER	3.2
2	W	43	GLN	3.1
2	W	111	PHE	3.1
2	Y	237	LYS	3.1
2	W	68	PHE	3.1
2	X	247	TRP	3.1
2	X	251	ASN	3.1
1	E	35	GLY	3.1
2	X	223	LEU	3.1
2	U	294	TYR	3.1
2	W	307	THR	3.0
1	B	34	ALA	3.0
2	X	290	VAL	3.0
2	Y	99	SER	3.0
2	U	188	ALA	3.0
2	Y	235	THR	3.0
2	W	239	VAL	3.0
2	X	147	TYR	3.0
2	U	176	VAL	3.0
2	U	63	PHE	3.0
2	W	251	ASN	3.0
1	E	43	CYS	2.9
2	U	147	TYR	2.9
2	U	280	ILE	2.9
1	A	39	LEU	2.9
2	U	92	ARG	2.9
2	Y	272	TYR	2.9
1	B	139	VAL	2.9
2	W	40	HIS	2.9
2	U	257	ILE	2.9
2	X	257	ILE	2.8
2	Y	251	ASN	2.8
2	U	236	ILE	2.8
2	W	276	GLU	2.8
2	U	253	GLN	2.8
1	F	139	VAL	2.8
2	Y	41	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	141	SER	2.8
2	W	302	ALA	2.7
2	Y	277	THR	2.7
2	U	305	THR	2.7
2	W	238	ASP	2.7
1	F	81	LYS	2.7
2	Y	160	ASP	2.7
2	W	80	LYS	2.7
2	U	225	LYS	2.7
2	X	253	GLN	2.7
2	Y	284	ARG	2.6
2	U	247	TRP	2.6
2	U	149	LEU	2.6
1	B	104	ARG	2.6
2	X	40	HIS	2.6
2	W	106	SER	2.6
2	X	62	ASP	2.6
1	E	6	ASN	2.6
2	W	90	ALA	2.6
2	U	215	VAL	2.5
1	A	140	LEU	2.5
1	A	135	THR	2.5
2	Y	243	VAL	2.5
1	B	101	SER	2.5
2	X	149	LEU	2.5
2	U	278	LEU	2.5
2	U	306	THR	2.5
2	Y	63	PHE	2.5
1	E	29	THR	2.5
1	A	97	ASN	2.5
2	Y	244	ASN	2.5
2	Y	215	VAL	2.5
2	W	139	LEU	2.5
2	X	39	ILE	2.5
1	B	96	LYS	2.5
1	B	108	ARG	2.4
2	U	289	GLY	2.4
2	W	260	VAL	2.4
2	U	146	GLN	2.4
2	X	244	ASN	2.4
2	U	139	LEU	2.4
2	W	103	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	U	65	ARG	2.4
2	U	300	GLY	2.4
1	F	133	SER	2.4
2	U	293	CYS	2.4
2	U	119	PHE	2.4
2	W	64	VAL	2.4
1	F	50	ILE	2.4
2	X	122	GLY	2.4
2	X	243	VAL	2.4
2	U	308	LEU	2.4
2	Y	161	LEU	2.3
2	U	207	GLU	2.3
2	U	197	HIS	2.3
1	B	137	ASP	2.3
2	Y	281	SER	2.3
2	X	297	ASN	2.3
2	W	42	ALA	2.3
2	W	228	ASP	2.3
2	W	272	TYR	2.3
1	E	33	VAL	2.3
1	E	83	VAL	2.3
1	F	66	ILE	2.3
2	U	84	ILE	2.3
1	F	58	THR	2.3
2	U	310	VAL	2.3
2	W	83	TRP	2.3
2	W	62	ASP	2.3
2	X	101	SER	2.3
2	U	49	GLU	2.2
1	B	136	SER	2.2
2	W	81	ASN	2.2
2	U	286	ASP	2.2
1	F	69	GLY	2.2
1	B	103	LYS	2.2
2	U	195	TRP	2.2
2	W	265	TRP	2.2
1	A	70	LEU	2.2
2	X	83	TRP	2.2
2	X	76	VAL	2.2
2	U	98	CYS	2.2
1	E	36	MET	2.2
1	B	68	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	X	172	THR	2.2
2	X	84	ILE	2.2
2	Y	207	GLU	2.2
2	W	112	VAL	2.1
2	X	245	SER	2.1
2	Y	62	ASP	2.1
2	X	308	LEU	2.1
2	Y	223	LEU	2.1
2	Y	233	VAL	2.1
2	U	209	ILE	2.1
1	E	112	PRO	2.1
2	U	96	TYR	2.1
2	U	150	ILE	2.1
2	W	257	ILE	2.1
2	X	123	LEU	2.1
2	W	196	LEU	2.1
2	U	224	LEU	2.1
1	B	106	GLU	2.1
2	U	180	TYR	2.1
2	W	46	LEU	2.1
2	U	99	SER	2.1
2	X	173	ILE	2.0
2	W	192	ASP	2.0
2	U	302	ALA	2.0
1	B	81	LYS	2.0
2	U	228	ASP	2.0
2	U	128	LYS	2.0
1	E	100	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	Y	2	14/15	0.81	0.27	-0.47	156,169,179,192	0
3	NAG	W	2	14/15	0.73	0.15	-0.98	145,156,169,178	0
3	NAG	X	2	14/15	0.92	0.13	-1.74	111,124,133,143	0
3	NAG	Y	3	14/15	0.74	0.18	-	185,191,194,196	0
3	FUL	X	1	10/11	0.93	0.19	-	112,119,127,129	0
5	NAG	W	5	14/15	0.68	0.31	-	187,195,198,198	0
4	NAG	Y	5	14/15	0.78	0.16	-	180,190,198,198	0
4	NAG	U	5	14/15	0.77	0.22	-	179,186,194,197	0
3	FUL	U	1	10/11	0.84	0.31	-	124,131,139,141	0
5	NDG	W	4	14/15	0.76	0.30	-	164,180,187,190	0
4	NAG	U	4	14/15	0.86	0.17	-	151,162,169,171	0
4	MAN	Y	6	11/12	0.81	0.11	-	161,171,175,177	0
4	NAG	X	5	14/15	0.66	0.20	-	183,193,195,196	0
3	NAG	W	3	14/15	0.78	0.18	-	185,191,194,196	0
3	NAG	U	3	14/15	0.84	0.14	-	170,189,193,194	0
3	NAG	U	2	14/15	0.91	0.15	-	97,118,131,148	0
3	FUL	W	1	10/11	0.72	0.26	-	160,171,172,173	0
4	NAG	X	4	14/15	0.81	0.20	-	112,143,156,171	0
3	NAG	X	3	14/15	0.92	0.14	-	156,163,170,171	0
4	MAN	X	6	11/12	0.80	0.12	-	193,197,198,198	0
4	MAN	U	6	11/12	0.84	0.10	-	191,196,198,198	0
5	MAN	W	6	11/12	0.51	0.29	-	190,196,198,198	0
4	NAG	Y	4	14/15	0.88	0.24	-	137,150,160,170	0
3	FUL	Y	1	10/11	0.85	0.44	-	154,171,175,177	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.