Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 10:32 PM EDT

PDB ID	:	2F8T
Title	:	Crystal structure of Aa-Ago with externally-bound siRNA
Authors	:	Yuan, Y.R.; Chen, H.Y.; Patel, D.J.
Deposited on	:	2005-12-03
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

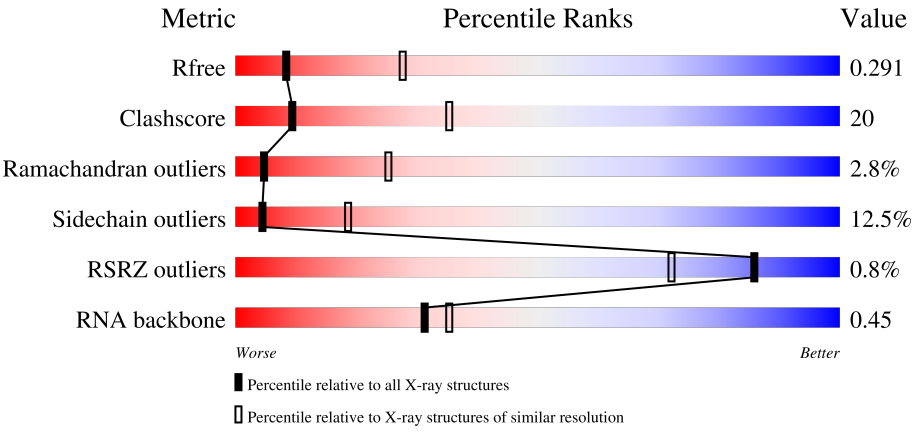
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	C	26	15% 46% 19% 19%
1	D	26	15% 38% 35% 8%
2	A	706	58% 36% 6%
2	B	706	% 52% 39% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12841 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 RNA chain called 26-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	26	Total	C	N	O	P	0	0	0
			551	246	94	185	26			
1	D	24	Total	C	N	O	P	0	0	0
			511	228	90	169	24			

- Molecule 2 is a protein called Argonaute protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	704	Total	C	N	O	S	0	0	0
			5864	3818	993	1042	11			
2	B	704	Total	C	N	O	S	0	0	0
			5864	3818	993	1042	11			

- Molecule 3 is water.

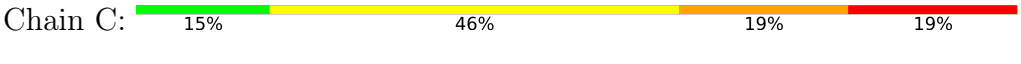
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	O	0	0
			2	2		
3	D	2	Total	O	0	0
			2	2		
3	A	24	Total	O	0	0
			24	24		
3	B	23	Total	O	0	0
			23	23		

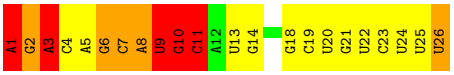
3 Residue-property plots (i)

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

- Molecule 1: 26-MER

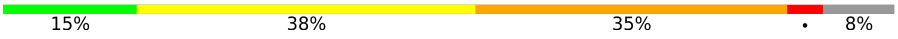
Chain C:

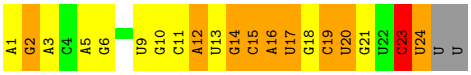




- Molecule 1: 26-MER

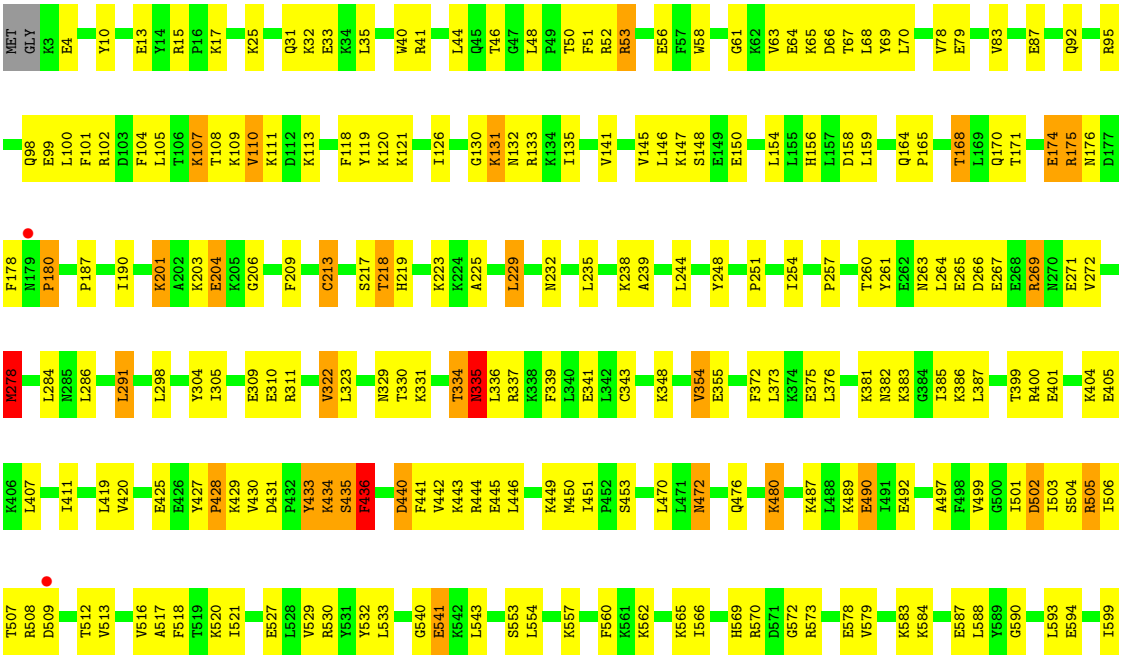
Chain D:

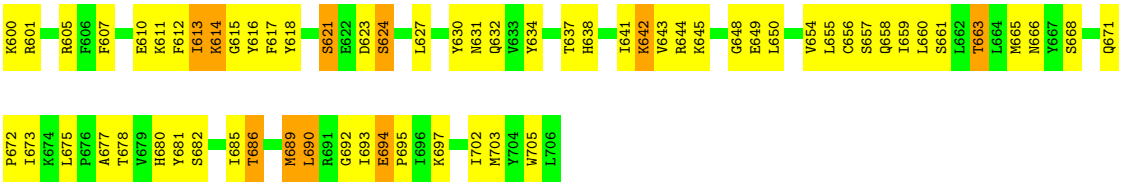




- Molecule 2: Argonaute protein

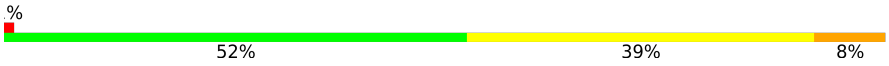
Chain A:

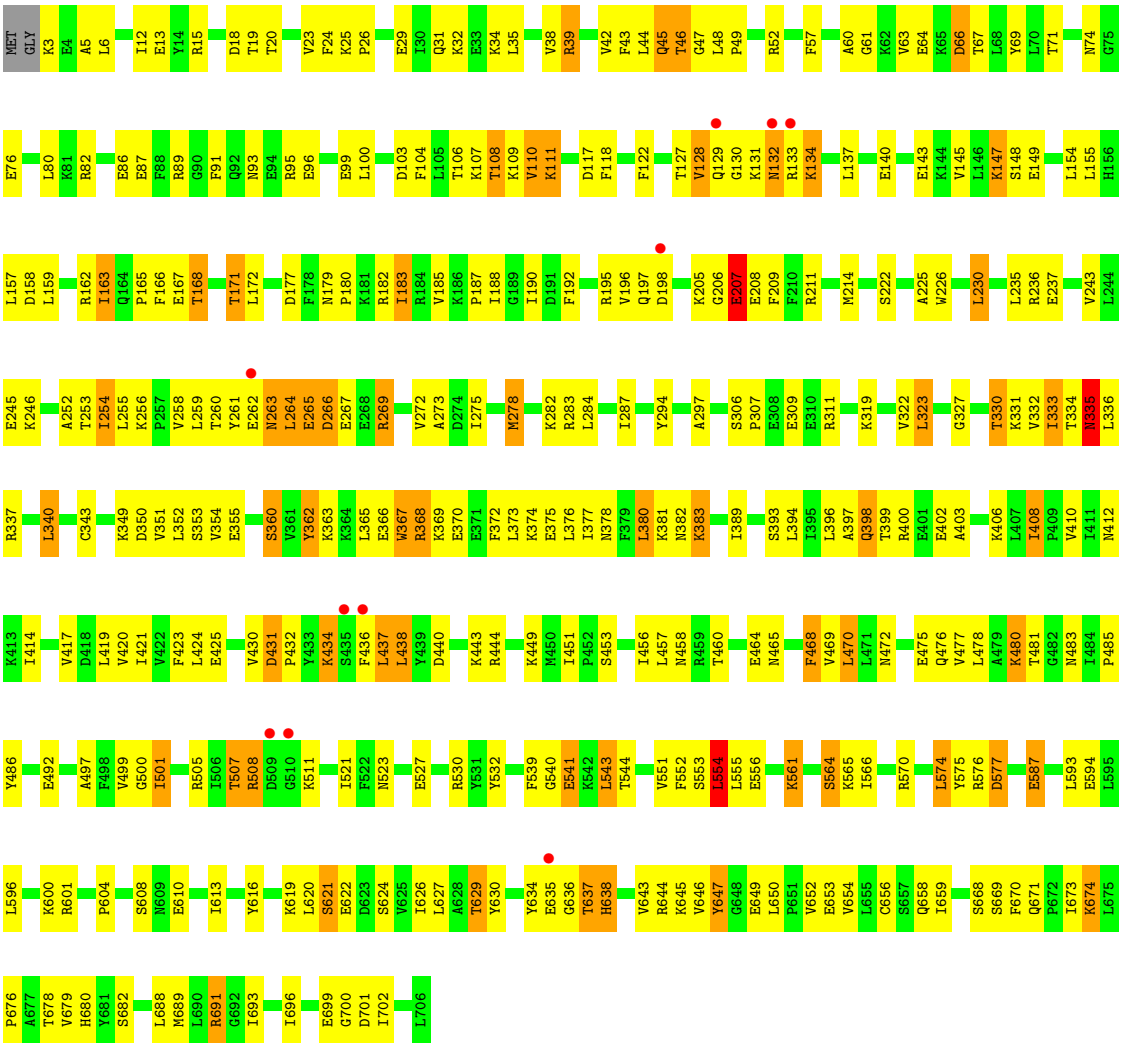




• Molecule 2: Argonaute protein

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.20Å 118.08Å 98.50Å 90.00° 99.57° 90.00°	Depositor
Resolution (Å)	40.00 – 3.10 32.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-3.10) 100.0 (32.44-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.71 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.297 0.201 , 0.291	Depositor DCC
R_{free} test set	1672 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	58.5	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12841	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	C	2.45	24/614 (3.9%)	2.20	31/952 (3.3%)
1	D	1.33	5/570 (0.9%)	1.75	14/884 (1.6%)
2	A	0.76	5/5979 (0.1%)	0.82	2/8027 (0.0%)
2	B	0.72	0/5979	0.81	2/8027 (0.0%)
All	All	0.93	34/13142 (0.3%)	1.00	49/17890 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	A	0	1
2	B	0	4
All	All	0	6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	G	N9-C8	21.71	1.53	1.37
1	C	2	G	C5-C4	16.53	1.50	1.38
1	C	1	A	N7-C5	16.30	1.49	1.39
1	C	1	A	N9-C4	14.03	1.46	1.37
1	C	2	G	N3-C4	13.16	1.44	1.35
1	C	3	A	N1-C2	11.84	1.45	1.34
1	C	2	G	C8-N7	11.76	1.38	1.30
1	C	2	G	N1-C2	11.57	1.47	1.37
1	C	1	A	N3-C4	10.91	1.41	1.34
1	C	9	U	N3-C4	10.82	1.48	1.38
1	C	9	U	N1-C6	10.64	1.47	1.38
1	D	1	A	OP3-P	-10.37	1.48	1.61
1	C	2	G	C6-O6	9.73	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	9	U	C4-C5	7.45	1.50	1.43
2	A	642	LYS	CD-CE	7.42	1.69	1.51
1	C	2	G	C2-N3	7.32	1.38	1.32
2	A	642	LYS	CG-CD	7.16	1.76	1.52
1	C	1	A	N9-C8	7.12	1.43	1.37
1	C	10	G	N1-C2	7.05	1.43	1.37
1	C	1	A	P-OP1	6.79	1.60	1.49
2	A	238	LYS	CD-CE	6.66	1.67	1.51
1	C	9	U	C2-O2	6.54	1.28	1.22
1	D	15	C	N1-C2	6.53	1.46	1.40
2	A	213	CYS	CB-SG	-6.44	1.71	1.82
2	A	238	LYS	CE-NZ	6.38	1.65	1.49
1	C	3	A	C5-C4	6.09	1.43	1.38
1	C	2	G	C2-N2	5.91	1.40	1.34
1	D	15	C	C2-N3	5.86	1.40	1.35
1	D	15	C	C1'-N1	5.70	1.57	1.48
1	C	2	G	C1'-N9	5.53	1.57	1.48
1	D	15	C	C4-C5	5.53	1.47	1.43
1	C	10	G	C5-C4	5.48	1.42	1.38
1	C	9	U	N1-C2	5.09	1.43	1.38
1	C	10	G	N9-C8	5.05	1.41	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2	G	C8-N9-C4	-17.28	99.49	106.40
1	C	2	G	C2-N3-C4	-13.63	105.08	111.90
1	C	2	G	N3-C2-N2	-11.04	112.17	119.90
1	C	2	G	N3-C4-N9	-10.15	119.91	126.00
1	C	2	G	N7-C8-N9	10.09	118.15	113.10
1	C	11	C	N1-C1'-C2'	-9.99	101.01	112.00
1	C	2	G	N9-C4-C5	9.62	109.25	105.40
1	C	13	U	P-O3'-C3'	-9.15	108.72	119.70
1	C	10	G	C5-C6-O6	-8.69	123.39	128.60
1	C	10	G	O4'-C1'-N9	8.30	114.84	108.20
1	C	20	U	O4'-C1'-N1	8.12	114.70	108.20
1	D	14	G	P-O3'-C3'	-7.96	110.15	119.70
1	C	11	C	O4'-C1'-N1	7.82	114.46	108.20
1	D	23	C	C3'-C2'-C1'	-7.50	95.50	101.50
1	D	12	A	O4'-C1'-N9	7.06	113.85	108.20
1	D	5	A	O4'-C4'-C3'	-7.00	97.00	104.00
1	D	21	G	O4'-C1'-N9	6.87	113.69	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2	G	N1-C2-N3	6.86	128.02	123.90
1	D	1	A	P-O3'-C3'	6.77	127.82	119.70
1	C	10	G	N9-C1'-C2'	-6.76	104.56	112.00
1	C	2	G	C5-N7-C8	-6.71	100.95	104.30
1	C	10	G	N1-C6-O6	6.70	123.92	119.90
1	C	1	A	C8-N9-C4	6.57	108.43	105.80
1	C	1	A	N7-C8-N9	-6.30	110.65	113.80
1	C	19	C	N3-C4-C5	6.16	124.36	121.90
2	A	238	LYS	CD-CE-NZ	-6.07	97.73	111.70
1	C	9	U	C5-C4-O4	-6.07	122.26	125.90
1	C	3	A	O4'-C1'-N9	6.03	113.03	108.20
1	C	7	C	O4'-C1'-N1	5.93	112.95	108.20
1	C	9	U	C4-C5-C6	-5.79	116.22	119.70
2	B	554	LEU	CB-CG-CD2	-5.74	101.25	111.00
2	B	380	LEU	CA-CB-CG	5.70	128.41	115.30
1	C	8	A	C4'-C3'-C2'	-5.66	96.94	102.60
1	D	19	C	C3'-C2'-C1'	-5.61	97.01	101.50
1	C	21	G	C4-C5-N7	5.60	113.04	110.80
1	C	21	G	C5-C6-O6	-5.58	125.25	128.60
1	C	9	U	C4'-C3'-C2'	-5.57	97.03	102.60
1	D	15	C	N3-C2-O2	-5.55	118.02	121.90
1	D	23	C	P-O3'-C3'	5.54	126.35	119.70
1	D	23	C	O4'-C1'-N1	5.51	112.61	108.20
1	D	15	C	O4'-C1'-N1	5.47	112.58	108.20
1	D	1	A	N9-C1'-C2'	-5.35	106.12	112.00
1	C	22	U	C2-N1-C1'	5.25	124.00	117.70
1	D	19	C	O4'-C4'-C3'	-5.20	98.80	104.00
2	A	291	LEU	CA-CB-CG	5.15	127.14	115.30
1	C	23	C	O4'-C1'-N1	5.14	112.31	108.20
1	C	23	C	C4'-C3'-C2'	-5.12	97.48	102.60
1	D	15	C	C2-N3-C4	-5.05	117.37	119.90
1	C	18	G	C3'-C2'-C1'	-5.01	97.49	101.50

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	335	ASN	Peptide
2	B	507	THR	Peptide
2	B	576	ARG	Peptide
2	B	621	SER	Peptide
2	B	634	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	1	A	Sidechain

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	C	551	0	279	25	0
1	D	511	0	259	31	0
2	A	5864	0	6128	210	0
2	B	5864	0	6128	251	0
3	A	24	0	0	3	0
3	B	23	0	0	1	0
3	C	2	0	0	0	0
3	D	2	0	0	1	0
All	All	12841	0	12794	504	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 20.

All (504) 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:A:642:LYS:CD	2:A:642:LYS:CG	1.76	1.61
2:B:532:TYR:CZ	2:B:554:LEU:HD21	1.70	1.27
2:B:532:TYR:CE1	2:B:554:LEU:HD21	1.78	1.18
2:A:66:ASP:HB3	3:A:708:HOH:O	1.51	1.11
2:B:122:PHE:CZ	2:B:275:ILE:HG21	1.87	1.09
2:B:122:PHE:HZ	2:B:275:ILE:HG21	1.10	1.07
2:A:265:GLU:HB3	2:A:429:LYS:HG2	1.04	1.02
2:B:12:ILE:HD11	2:B:155:LEU:HB2	1.44	0.99
2:B:532:TYR:CE1	2:B:554:LEU:CD2	2.44	0.99
2:B:122:PHE:HZ	2:B:275:ILE:CG2	1.77	0.98
2:A:265:GLU:HB3	2:A:429:LYS:CG	1.94	0.98
2:A:265:GLU:CB	2:A:429:LYS:HG2	1.93	0.97
2:B:532:TYR:CZ	2:B:554:LEU:CD2	2.47	0.96
2:B:147:LYS:HG2	2:B:621:SER:HB3	1.46	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:629:THR:HG21	2:B:674:LYS:O	1.66	0.95
2:A:614:LYS:NZ	2:A:663:THR:HG21	1.81	0.94
2:B:343:CYS:O	2:B:383:LYS:HE2	1.69	0.93
2:A:404:LYS:HD2	2:A:436:PHE:CE2	2.04	0.92
2:B:266:ASP:HB3	3:B:718:HOH:O	1.70	0.91
2:A:624:SER:HB3	2:A:644:ARG:HG3	1.52	0.91
2:B:12:ILE:CD1	2:B:155:LEU:HB2	2.01	0.90
2:B:128:VAL:HG11	2:B:267:GLU:HB3	1.51	0.90
2:A:372:PHE:CE2	2:A:376:LEU:HD11	2.06	0.89
2:A:176:ASN:HB3	2:A:178:PHE:CD1	2.06	0.89
2:B:322:VAL:HG11	2:B:486:TYR:CD1	2.09	0.87
2:B:108:THR:O	2:B:109:LYS:HB2	1.73	0.87
2:A:164:GLN:HG2	2:A:257:PRO:O	1.75	0.86
2:B:197:GLN:OE1	2:B:245:GLU:HA	1.76	0.86
2:B:468:PHE:C	2:B:468:PHE:CD2	2.49	0.86
2:B:42:VAL:O	2:B:46:THR:HB	1.76	0.85
2:B:468:PHE:C	2:B:468:PHE:HD2	1.81	0.84
2:B:93:ASN:H	2:B:96:GLU:HG3	1.44	0.83
2:B:185:VAL:HG11	2:B:255:LEU:HB3	1.59	0.83
2:A:694:GLU:HG2	2:A:695:PRO:HD2	1.59	0.82
2:A:614:LYS:HZ2	2:A:663:THR:HG21	1.42	0.82
2:B:523:ASN:HD21	2:B:527:GLU:HB3	1.45	0.82
2:A:118:PHE:HE2	2:A:126:ILE:HD11	1.43	0.82
2:B:431:ASP:H	2:B:436:PHE:HE2	1.26	0.81
2:B:532:TYR:OH	2:B:554:LEU:HD21	1.81	0.81
2:B:523:ASN:ND2	2:B:527:GLU:HB3	1.96	0.81
2:A:642:LYS:CG	2:A:642:LYS:CE	2.60	0.80
2:A:642:LYS:CD	2:A:642:LYS:CB	2.60	0.79
2:A:697:LYS:O	2:A:697:LYS:HG3	1.82	0.79
2:B:47:GLY:O	2:B:107:LYS:HE3	1.81	0.79
2:A:330:THR:HG21	2:A:336:LEU:HD22	1.63	0.79
2:B:619:LYS:HE2	2:B:653:GLU:OE2	1.83	0.79
2:A:158:ASP:OD1	2:A:159:LEU:N	2.16	0.77
2:B:46:THR:HG22	2:B:48:LEU:H	1.49	0.77
2:B:437:LEU:HB3	2:B:440:ASP:HB2	1.65	0.77
2:B:481:THR:HG22	2:B:483:ASN:HD22	1.49	0.77
2:B:198:ASP:HB2	2:B:243:VAL:HB	1.64	0.77
2:B:481:THR:HG22	2:B:483:ASN:ND2	1.99	0.77
2:A:176:ASN:HB3	2:A:178:PHE:HD1	1.49	0.77
2:B:431:ASP:HB3	2:B:434:LYS:HB2	1.65	0.76
2:B:508:ARG:O	2:B:511:LYS:HD2	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:VAL:CG1	2:B:486:TYR:HB2	2.16	0.76
2:B:431:ASP:HB3	2:B:434:LYS:CB	2.16	0.76
2:B:539:PHE:HB3	2:B:543:LEU:HB3	1.66	0.76
2:B:180:PRO:HB3	2:B:183:ILE:HD12	1.66	0.76
2:B:360:SER:HB3	2:B:425:GLU:HG3	1.67	0.75
2:B:372:PHE:CE2	2:B:376:LEU:HD11	2.21	0.75
1:C:6:G:H1	1:D:19:C:H42	1.32	0.75
2:A:404:LYS:HD2	2:A:436:PHE:CZ	2.21	0.75
2:B:637:THR:HG23	2:B:638:HIS:N	2.02	0.74
1:D:15:C:H2'	1:D:16:A:H8	1.52	0.74
2:A:553:SER:O	2:A:557:LYS:HG3	1.87	0.74
2:A:689:MET:HA	2:A:689:MET:HE2	1.70	0.74
2:A:381:LYS:HA	2:A:385:ILE:O	1.88	0.73
2:A:689:MET:HA	2:A:689:MET:CE	2.18	0.72
2:A:594:GLU:HG2	2:A:655:LEU:HD21	1.71	0.72
2:B:691:ARG:HG3	2:B:691:ARG:HH11	1.55	0.71
2:A:118:PHE:CE2	2:A:126:ILE:HD11	2.26	0.70
2:B:187:PRO:HB2	2:B:190:ILE:HD12	1.73	0.70
2:A:605:ARG:HH21	2:A:637:THR:CG2	2.04	0.70
2:B:343:CYS:O	2:B:383:LYS:CE	2.38	0.70
1:C:1:A:H2'	1:C:2:G:H8	1.57	0.70
2:A:611:LYS:HD3	2:A:612:PHE:HE1	1.57	0.70
2:A:654:VAL:O	2:A:658:GLN:HG3	1.92	0.69
2:A:53:ARG:HE	2:A:92:GLN:HG3	1.57	0.69
1:C:1:A:H2'	1:C:2:G:C8	2.27	0.69
1:C:2:G:H2'	1:C:3:A:C8	2.28	0.69
2:B:530:ARG:HG3	2:B:700:GLY:O	1.93	0.69
2:B:530:ARG:CD	2:B:699:GLU:OE2	2.42	0.68
2:B:659:ILE:HG23	2:B:676:PRO:HG3	1.75	0.68
1:D:20:U:H6	1:D:20:U:O5'	1.77	0.68
2:A:614:LYS:HZ1	2:A:663:THR:HG21	1.56	0.68
2:B:476:GLN:O	2:B:480:LYS:HG2	1.93	0.68
2:A:131:LYS:HG3	2:A:132:ASN:N	2.09	0.68
2:A:660:LEU:O	2:A:663:THR:HB	1.94	0.68
2:B:180:PRO:CB	2:B:183:ILE:HD12	2.23	0.67
2:A:431:ASP:HB2	2:A:434:LYS:HB2	1.77	0.67
2:B:34:LYS:O	2:B:38:VAL:HG23	1.95	0.67
2:A:111:LYS:HE3	2:A:141:VAL:HB	1.75	0.66
2:A:610:GLU:HG3	2:A:612:PHE:H	1.59	0.66
2:B:431:ASP:CB	2:B:434:LYS:HB2	2.25	0.66
2:B:49:PRO:CB	2:B:100:LEU:HD12	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:443:LYS:HD3	2:B:453:SER:OG	1.96	0.66
2:B:629:THR:CG2	2:B:674:LYS:O	2.43	0.66
1:D:16:A:H2'	1:D:17:U:C6	2.31	0.66
2:A:147:LYS:HG2	2:A:621:SER:CB	2.26	0.66
1:C:25:U:OP1	1:C:25:U:H6	1.78	0.66
1:D:12:A:H2'	1:D:13:U:C6	2.31	0.65
1:D:15:C:H2'	1:D:16:A:C8	2.32	0.65
2:A:187:PRO:HB2	2:A:190:ILE:HD12	1.77	0.65
2:B:372:PHE:CZ	2:B:376:LEU:HD11	2.32	0.65
1:C:5:A:H61	1:D:20:U:H3	1.45	0.65
2:B:45:GLN:NE2	2:B:69:TYR:O	2.30	0.65
2:B:322:VAL:HG11	2:B:486:TYR:HD1	1.59	0.64
2:A:98:GLN:HE21	2:A:145:VAL:H	1.44	0.64
2:B:481:THR:CG2	2:B:483:ASN:HD22	2.10	0.64
2:B:39:ARG:HB2	2:B:57:PHE:HE2	1.60	0.64
2:A:605:ARG:NH2	2:A:637:THR:HG21	2.12	0.64
2:A:40:TRP:CZ2	2:A:44:LEU:HD21	2.32	0.64
2:A:504:SER:OG	2:A:686:THR:CG2	2.45	0.64
2:B:501:ILE:HG22	2:B:570:ARG:HD2	1.79	0.64
2:A:605:ARG:HH21	2:A:637:THR:HG23	1.63	0.64
2:B:147:LYS:HG2	2:B:621:SER:CB	2.24	0.63
2:B:431:ASP:OD2	2:B:434:LYS:HB2	1.97	0.63
2:A:540:GLY:O	2:A:541:GLU:HB3	1.99	0.63
2:B:230:LEU:HA	2:B:236:ARG:HH21	1.63	0.63
2:A:147:LYS:HG2	2:A:621:SER:HB3	1.81	0.63
1:D:17:U:H2'	1:D:18:G:H8	1.64	0.63
2:B:475:GLU:OE1	2:B:669:SER:HB3	1.98	0.62
2:A:573:ARG:HG3	2:A:599:ILE:HD11	1.82	0.62
2:B:499:VAL:HG22	2:B:521:ILE:HG12	1.80	0.62
2:B:19:THR:HG22	2:B:19:THR:O	1.98	0.62
2:B:185:VAL:CG1	2:B:255:LEU:HB3	2.29	0.62
2:A:697:LYS:O	2:A:697:LYS:CG	2.48	0.62
2:B:398:GLN:HG3	2:B:402:GLU:OE1	1.98	0.62
2:A:148:SER:HB3	2:A:154:LEU:HD11	1.80	0.62
2:B:530:ARG:HD3	2:B:699:GLU:OE2	1.99	0.62
2:A:497:ALA:HB2	2:A:560:PHE:CZ	2.35	0.61
2:A:504:SER:CB	2:A:686:THR:HG23	2.30	0.61
2:B:334:THR:O	2:B:335:ASN:HB3	1.99	0.61
2:B:335:ASN:HA	2:B:669:SER:OG	2.00	0.61
2:B:49:PRO:HB2	2:B:100:LEU:CD1	2.31	0.61
2:B:530:ARG:HD2	2:B:699:GLU:OE2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:G:H2'	1:C:3:A:H8	1.65	0.61
2:A:67:THR:HG22	2:A:68:LEU:N	2.16	0.61
2:A:168:THR:HG22	2:A:171:THR:H	1.66	0.61
2:A:171:THR:O	2:A:175:ARG:HB2	1.99	0.61
1:C:3:A:H2	1:D:23:C:H1'	1.65	0.60
2:B:49:PRO:HB2	2:B:100:LEU:HD12	1.83	0.60
2:A:187:PRO:HA	2:A:254:ILE:O	2.00	0.60
2:B:25:LYS:HG2	2:B:26:PRO:HD2	1.83	0.60
2:A:613:ILE:HD11	2:A:632:GLN:HG3	1.84	0.60
2:A:35:LEU:HD22	2:A:52:ARG:HD2	1.83	0.59
2:A:431:ASP:CB	2:A:434:LYS:HB2	2.32	0.59
2:B:52:ARG:HB3	2:B:95:ARG:HH21	1.68	0.59
2:B:48:LEU:HD13	2:B:61:GLY:HA3	1.83	0.59
2:B:128:VAL:HG12	2:B:129:GLN:H	1.67	0.59
2:B:322:VAL:HG11	2:B:486:TYR:HB2	1.83	0.59
2:A:450:MET:CE	2:A:533:LEU:HD23	2.33	0.59
2:B:52:ARG:HB3	2:B:95:ARG:NH2	2.18	0.59
2:A:51:PHE:HD2	2:A:100:LEU:HD13	1.67	0.58
1:D:12:A:H2'	1:D:13:U:H6	1.67	0.58
2:A:323:LEU:HB3	2:A:329:ASN:HB3	1.84	0.58
1:C:8:A:H2'	1:C:9:U:H6	1.68	0.58
2:A:506:ILE:HG13	2:A:690:LEU:HD13	1.84	0.58
2:B:481:THR:CG2	2:B:483:ASN:ND2	2.65	0.58
2:B:497:ALA:HB3	2:B:566:ILE:HG12	1.85	0.58
2:A:372:PHE:HE2	2:A:376:LEU:HD11	1.68	0.58
2:A:693:ILE:HG22	2:A:693:ILE:O	2.04	0.58
1:D:17:U:H2'	1:D:18:G:C8	2.38	0.58
2:B:108:THR:HB	2:B:110:VAL:HG22	1.86	0.58
2:B:354:VAL:HG22	2:B:419:LEU:HB3	1.85	0.58
2:B:630:TYR:N	2:B:630:TYR:CD2	2.72	0.57
2:A:492:GLU:HG3	2:A:657:SER:OG	2.05	0.57
2:B:206:GLY:O	2:B:208:GLU:N	2.37	0.57
1:C:2:G:N2	1:D:24:U:O2	2.37	0.57
2:B:468:PHE:HD2	2:B:469:VAL:N	2.02	0.57
2:A:562:LYS:HD3	3:A:727:HOH:O	2.05	0.57
2:A:104:PHE:HB3	2:A:298:LEU:CD2	2.34	0.57
2:B:362:TYR:HB2	2:B:365:LEU:HD12	1.86	0.57
2:B:624:SER:HB3	2:B:644:ARG:HG3	1.86	0.57
2:A:504:SER:HB2	2:A:686:THR:HG23	1.86	0.57
2:A:613:ILE:HG22	2:A:616:TYR:CG	2.40	0.57
2:B:417:VAL:HG13	2:B:419:LEU:H	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:620:LEU:O	2:B:621:SER:C	2.42	0.57
2:A:331:LYS:HD3	2:B:89:ARG:NH2	2.19	0.56
2:A:435:SER:O	2:A:436:PHE:HB2	2.05	0.56
2:A:104:PHE:HB3	2:A:298:LEU:HD21	1.87	0.56
2:B:265:GLU:HA	2:B:430:VAL:HG11	1.86	0.56
1:C:3:A:H2'	1:C:4:C:H6	1.71	0.56
2:A:67:THR:HG22	2:A:68:LEU:H	1.70	0.56
2:B:206:GLY:C	2:B:208:GLU:H	2.09	0.55
2:B:378:ASN:O	2:B:381:LYS:HB2	2.06	0.55
2:B:49:PRO:HG2	2:B:104:PHE:CE1	2.41	0.55
2:A:504:SER:OG	2:A:686:THR:HG23	2.06	0.55
2:B:66:ASP:N	2:B:66:ASP:OD1	2.39	0.55
2:B:637:THR:CG2	2:B:638:HIS:N	2.68	0.55
2:A:48:LEU:HD13	2:A:61:GLY:HA3	1.89	0.55
2:A:381:LYS:C	2:A:383:LYS:H	2.10	0.55
2:A:373:LEU:HA	2:A:376:LEU:HD12	1.89	0.55
2:A:442:VAL:HG12	2:A:446:LEU:HD12	1.88	0.55
2:B:39:ARG:HB2	2:B:57:PHE:CE2	2.41	0.55
2:A:694:GLU:CG	2:A:695:PRO:HD2	2.35	0.54
2:A:605:ARG:NH2	2:A:637:THR:CG2	2.70	0.54
2:A:630:TYR:OH	2:A:638:HIS:HA	2.08	0.54
2:A:170:GLN:NE2	2:A:239:ALA:HA	2.23	0.54
2:B:19:THR:O	2:B:19:THR:CG2	2.54	0.54
2:B:555:LEU:HD13	2:B:566:ILE:HD13	1.89	0.54
2:A:334:THR:HG22	2:A:335:ASN:H	1.73	0.54
2:A:566:ILE:HB	2:A:593:LEU:CD2	2.38	0.54
2:B:336:LEU:HB2	2:B:340:LEU:HD12	1.90	0.54
2:B:434:LYS:HD3	2:B:436:PHE:HB3	1.89	0.54
1:C:7:C:O2'	1:C:8:A:H5'	2.07	0.53
1:C:8:A:H2'	1:C:9:U:C6	2.43	0.53
1:D:14:G:N2	1:D:15:C:C2	2.77	0.53
1:C:3:A:C2	1:D:23:C:H1'	2.43	0.53
2:B:261:TYR:HA	2:B:264:LEU:HD11	1.90	0.53
2:B:18:ASP:OD1	2:B:20:THR:HB	2.07	0.53
2:B:332:VAL:HG22	2:B:336:LEU:HD21	1.91	0.53
2:B:532:TYR:CE1	2:B:554:LEU:HD22	2.41	0.53
2:A:502:ASP:C	2:A:503:ILE:HG13	2.29	0.53
2:A:15:ARG:HH12	2:B:587:GLU:CG	2.22	0.53
2:B:91:PHE:HB3	2:B:96:GLU:HB2	1.90	0.53
2:B:373:LEU:HA	2:B:376:LEU:HD12	1.90	0.53
2:A:540:GLY:O	2:A:541:GLU:CB	2.56	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:472:ASN:OD1	2:B:671:GLN:NE2	2.33	0.52
2:B:165:PRO:C	2:B:167:GLU:H	2.13	0.52
2:B:654:VAL:O	2:B:658:GLN:HG3	2.09	0.52
2:A:15:ARG:HH12	2:B:587:GLU:HG2	1.74	0.52
2:A:645:LYS:NZ	2:A:648:GLY:O	2.38	0.52
2:B:367:TRP:HZ3	2:B:368:ARG:CZ	2.23	0.52
2:B:264:LEU:HB2	2:B:269:ARG:HG3	1.91	0.52
2:B:437:LEU:CB	2:B:440:ASP:HB2	2.37	0.52
2:B:52:ARG:O	2:B:95:ARG:NH2	2.42	0.52
2:B:575:TYR:HB3	2:B:577:ASP:HB3	1.91	0.52
2:A:201:LYS:HB3	2:A:204:GLU:OE2	2.10	0.52
2:B:540:GLY:O	2:B:541:GLU:HB2	2.09	0.52
2:B:180:PRO:O	2:B:196:VAL:HG11	2.09	0.52
2:B:330:THR:HB	2:B:331:LYS:O	2.10	0.52
2:B:149:GLU:HA	2:B:621:SER:HA	1.92	0.51
2:B:222:SER:O	2:B:226:TRP:CD1	2.63	0.51
2:A:400:ARG:NH1	2:A:436:PHE:O	2.43	0.51
2:B:93:ASN:HB3	2:B:95:ARG:H	1.75	0.51
2:B:168:THR:HG22	2:B:171:THR:H	1.75	0.51
1:D:14:G:C2	1:D:15:C:C2	2.98	0.51
2:A:450:MET:HE3	2:A:533:LEU:HD23	1.91	0.51
2:B:431:ASP:CG	2:B:434:LYS:HB2	2.31	0.51
2:A:217:SER:HB2	2:A:223:LYS:HG3	1.92	0.51
2:A:616:TYR:O	2:A:617:PHE:HB3	2.10	0.51
2:B:673:ILE:HG21	2:B:680:HIS:CD2	2.45	0.51
1:C:10:G:C2	1:D:16:A:C2	2.99	0.51
2:A:579:VAL:HG12	2:A:583:LYS:HE2	1.91	0.51
2:B:363:LYS:HE2	2:B:396:LEU:HD11	1.93	0.51
2:B:637:THR:HG23	2:B:638:HIS:H	1.74	0.51
2:A:680:HIS:CE1	2:A:681:TYR:CD2	2.98	0.51
2:B:198:ASP:HB2	2:B:243:VAL:CB	2.37	0.51
2:B:408:ILE:O	2:B:412:ASN:HB2	2.10	0.51
2:B:485:PRO:HG2	2:B:486:TYR:CD2	2.46	0.51
2:B:366:GLU:O	2:B:370:GLU:HG2	2.11	0.51
1:C:3:A:H2'	1:C:4:C:C6	2.46	0.50
2:A:570:ARG:HG2	2:A:572:GLY:H	1.76	0.50
2:A:69:TYR:CE2	2:A:79:GLU:HG3	2.46	0.50
2:A:420:VAL:HG23	2:A:451:ILE:HG21	1.92	0.50
2:B:32:LYS:HA	2:B:35:LEU:HD12	1.92	0.50
2:B:5:ALA:HA	2:B:608:SER:HB2	1.93	0.50
2:B:273:ALA:C	2:B:275:ILE:H	2.14	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:575:TYR:CB	2:B:577:ASP:HB3	2.41	0.50
2:A:67:THR:CG2	2:A:68:LEU:H	2.24	0.50
2:B:74:ASN:HB2	2:B:76:GLU:H	1.76	0.50
2:B:49:PRO:HB3	2:B:100:LEU:HD12	1.94	0.50
2:B:554:LEU:O	2:B:554:LEU:HG	2.11	0.50
2:B:561:LYS:O	2:B:564:SER:OG	2.27	0.50
2:A:505:ARG:NH1	2:A:543:LEU:HD23	2.27	0.50
2:B:252:ALA:C	2:B:254:ILE:H	2.13	0.50
2:A:46:THR:CG2	2:A:48:LEU:HB2	2.42	0.49
2:B:278:MET:HG3	2:B:282:LYS:HB3	1.94	0.49
2:B:363:LYS:HE2	2:B:396:LEU:CD1	2.42	0.49
1:D:10:G:H2'	1:D:11:C:C6	2.48	0.49
2:A:569:HIS:HD2	2:A:678:THR:OG1	1.95	0.49
2:B:163:ILE:H	2:B:163:ILE:HD12	1.77	0.49
2:B:436:PHE:O	2:B:438:LEU:N	2.45	0.49
2:A:587:GLU:O	2:A:590:GLY:N	2.46	0.49
2:A:656:CYS:O	2:A:659:ILE:HB	2.12	0.49
2:A:472:ASN:OD1	2:A:472:ASN:N	2.45	0.49
2:A:516:VAL:HG23	2:A:690:LEU:HD23	1.94	0.49
2:B:431:ASP:HB3	2:B:434:LYS:HB3	1.91	0.49
2:A:130:GLY:O	2:A:132:ASN:N	2.46	0.49
2:B:646:VAL:O	2:B:647:TYR:HB3	2.12	0.49
2:A:32:LYS:O	2:A:35:LEU:HB2	2.12	0.49
2:A:336:LEU:O	2:A:339:PHE:N	2.46	0.49
2:A:507:THR:HG22	2:A:508:ARG:N	2.27	0.49
2:A:665:MET:HE2	2:A:665:MET:HA	1.94	0.49
2:B:211:ARG:HG2	2:B:230:LEU:HD11	1.95	0.49
2:B:133:ARG:HH12	2:B:432:PRO:HA	1.77	0.49
2:B:323:LEU:HD12	2:B:327:GLY:HA2	1.95	0.49
2:B:440:ASP:O	2:B:444:ARG:HB2	2.13	0.49
2:B:165:PRO:HG3	2:B:259:LEU:HD11	1.95	0.48
2:B:477:VAL:HG12	2:B:478:LEU:N	2.27	0.48
2:A:529:VAL:O	2:A:530:ARG:CG	2.61	0.48
2:B:613:ILE:HG22	2:B:613:ILE:O	2.13	0.48
2:B:134:LYS:NZ	2:B:167:GLU:HG2	2.28	0.48
1:D:14:G:H2'	1:D:15:C:C6	2.49	0.48
2:A:108:THR:O	2:A:109:LYS:HB2	2.14	0.48
1:C:8:A:C2'	1:C:9:U:O5'	2.62	0.48
2:A:102:ARG:HA	2:A:105:LEU:HD12	1.95	0.48
2:A:476:GLN:HB3	2:A:480:LYS:HE3	1.96	0.48
2:B:374:LYS:HA	2:B:377:ILE:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ASN:HB2	2:B:96:GLU:HG2	1.95	0.48
2:B:543:LEU:HG	2:B:544:THR:N	2.29	0.48
2:A:610:GLU:HG3	2:A:612:PHE:N	2.28	0.48
2:A:616:TYR:O	2:A:627:LEU:HD12	2.13	0.48
2:B:373:LEU:O	2:B:376:LEU:HB2	2.14	0.48
2:A:67:THR:CG2	2:A:68:LEU:N	2.77	0.48
2:A:433:TYR:C	2:A:435:SER:H	2.18	0.48
2:A:680:HIS:CE1	2:A:681:TYR:HD2	2.32	0.48
2:B:6:LEU:HD23	2:B:309:GLU:HB2	1.95	0.48
2:B:468:PHE:CD2	2:B:468:PHE:O	2.66	0.48
2:B:39:ARG:HE	2:B:99:GLU:HG2	1.78	0.47
2:B:565:LYS:HE3	2:B:594:GLU:HG2	1.95	0.47
2:B:381:LYS:O	2:B:383:LYS:N	2.48	0.47
2:A:40:TRP:HE1	2:A:218:THR:HB	1.79	0.47
2:A:101:PHE:CE2	2:A:105:LEU:HD11	2.49	0.47
2:A:108:THR:OG1	2:A:110:VAL:HG22	2.14	0.47
2:A:518:PHE:CE1	2:A:685:ILE:HD12	2.50	0.47
2:A:146:LEU:O	2:A:154:LEU:N	2.47	0.47
2:B:134:LYS:HZ2	2:B:167:GLU:HG2	1.79	0.47
2:B:375:GLU:HB3	2:B:470:LEU:HD11	1.97	0.47
2:A:594:GLU:HG3	2:A:648:GLY:HA3	1.97	0.47
2:A:499:VAL:HG22	2:A:521:ILE:HG12	1.98	0.47
2:A:666:ASN:OD1	2:A:677:ALA:HA	2.14	0.47
2:B:532:TYR:CD1	2:B:532:TYR:N	2.83	0.47
2:A:178:PHE:C	2:A:180:PRO:HD3	2.36	0.46
2:A:615:GLY:HA2	2:A:660:LEU:HD11	1.96	0.46
2:B:319:LYS:HE2	2:B:492:GLU:HG3	1.98	0.46
2:A:266:ASP:HA	2:A:269:ARG:HD2	1.97	0.46
2:B:369:LYS:HE3	2:B:458:ASN:HD21	1.79	0.46
2:B:431:ASP:CB	2:B:434:LYS:CB	2.87	0.46
2:A:102:ARG:O	2:A:105:LEU:HB2	2.14	0.46
2:A:703:MET:HA	2:A:705:TRP:CZ3	2.51	0.46
2:A:505:ARG:HB3	2:A:512:THR:HG23	1.97	0.46
2:A:507:THR:O	2:A:508:ARG:HG3	2.15	0.46
2:B:39:ARG:HH22	2:B:103:ASP:CG	2.18	0.46
1:C:14:G:C2	1:D:12:A:C2	3.04	0.46
2:A:63:VAL:HG12	2:A:64:GLU:N	2.29	0.46
2:B:258:VAL:HG12	2:B:258:VAL:O	2.15	0.46
2:A:98:GLN:HG3	2:A:145:VAL:H	1.80	0.46
2:A:354:VAL:HA	2:A:419:LEU:O	2.14	0.46
2:B:108:THR:HG21	2:B:297:ALA:HB1	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:LYS:O	2:B:410:VAL:HG23	2.16	0.46
2:A:594:GLU:OE1	2:A:650:LEU:N	2.28	0.46
2:B:35:LEU:HD22	2:B:52:ARG:HD2	1.97	0.46
2:B:645:LYS:NZ	2:B:650:LEU:O	2.47	0.46
2:B:691:ARG:HG3	2:B:691:ARG:NH1	2.28	0.46
2:A:219:HIS:HD2	3:A:714:HOH:O	1.99	0.46
2:A:130:GLY:O	2:A:131:LYS:C	2.53	0.46
2:B:13:GLU:OE1	2:B:15:ARG:NH2	2.50	0.45
2:B:367:TRP:CZ3	2:B:368:ARG:CZ	2.99	0.45
2:B:222:SER:O	2:B:226:TRP:HD1	1.99	0.45
2:A:13:GLU:HG3	2:A:304:TYR:HB2	1.99	0.45
2:A:51:PHE:CD2	2:A:100:LEU:HD13	2.51	0.45
2:A:339:PHE:O	2:A:343:CYS:HB2	2.17	0.45
2:B:423:PHE:O	2:B:424:LEU:HD23	2.17	0.45
2:A:209:PHE:C	2:A:209:PHE:CD2	2.90	0.45
2:A:229:LEU:N	2:A:229:LEU:HD23	2.32	0.45
2:A:4:GLU:HG3	2:A:311:ARG:NH1	2.32	0.45
2:A:95:ARG:HD2	2:A:99:GLU:OE2	2.17	0.45
2:A:570:ARG:NH1	2:A:578:GLU:OE1	2.50	0.45
2:B:207:GLU:O	2:B:207:GLU:HG2	2.16	0.45
2:B:322:VAL:HG11	2:B:486:TYR:CG	2.51	0.45
2:B:500:GLY:HA3	2:B:678:THR:O	2.17	0.45
1:D:14:G:C6	1:D:15:C:N4	2.85	0.45
2:A:584:LYS:O	2:A:588:LEU:HG	2.17	0.45
2:B:457:LEU:O	2:B:460:THR:HB	2.16	0.45
2:B:593:LEU:HD23	2:B:647:TYR:OH	2.16	0.45
2:A:433:TYR:O	2:A:435:SER:N	2.49	0.44
2:A:40:TRP:CH2	2:A:44:LEU:HD21	2.53	0.44
2:B:400:ARG:NH1	2:B:436:PHE:O	2.50	0.44
2:B:400:ARG:NH1	2:B:438:LEU:HB2	2.32	0.44
2:B:118:PHE:O	2:B:118:PHE:CD2	2.70	0.44
2:B:264:LEU:HB2	2:B:269:ARG:CG	2.46	0.44
2:B:32:LYS:HA	2:B:35:LEU:CD1	2.48	0.44
2:A:178:PHE:O	2:A:180:PRO:HD3	2.17	0.44
2:A:261:TYR:O	2:A:264:LEU:HB2	2.18	0.44
2:A:322:VAL:HA	2:A:487:LYS:O	2.18	0.44
2:B:177:ASP:O	2:B:179:ASN:ND2	2.51	0.44
1:D:13:U:C2	1:D:14:G:C8	3.06	0.44
2:A:450:MET:HE1	2:A:533:LEU:HD23	2.00	0.44
2:B:381:LYS:C	2:B:383:LYS:H	2.20	0.44
2:A:98:GLN:HG3	2:A:145:VAL:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:232:ASN:HB2	2:A:235:LEU:HD12	2.00	0.44
2:B:613:ILE:HA	2:B:616:TYR:CD1	2.52	0.44
1:C:10:G:C2	1:D:16:A:N3	2.85	0.43
2:A:508:ARG:HD2	2:A:513:VAL:HG21	2.00	0.43
2:A:520:LYS:HE3	2:A:682:SER:OG	2.18	0.43
2:A:665:MET:HA	2:A:665:MET:CE	2.48	0.43
2:B:188:ILE:HD11	2:B:256:LYS:HE3	2.00	0.43
2:A:284:LEU:HB2	2:A:607:PHE:CD2	2.53	0.43
2:B:3:LYS:HE2	2:B:610:GLU:OE1	2.18	0.43
2:B:24:PHE:HB3	2:B:80:LEU:HB3	1.99	0.43
2:B:111:LYS:HD2	2:B:294:TYR:OH	2.18	0.43
2:B:205:LYS:HD3	2:B:209:PHE:CB	2.48	0.43
2:A:449:LYS:HB3	2:A:451:ILE:HD12	2.01	0.43
2:A:48:LEU:HD13	2:A:61:GLY:CA	2.48	0.43
2:B:182:ARG:HG2	2:B:195:ARG:HH11	1.83	0.43
2:B:206:GLY:C	2:B:208:GLU:N	2.70	0.43
2:B:373:LEU:O	2:B:377:ILE:HG13	2.18	0.43
2:B:574:LEU:HD11	2:B:646:VAL:HG21	2.00	0.43
2:A:404:LYS:O	2:A:405:GLU:C	2.56	0.43
2:A:50:THR:HA	2:A:58:TRP:O	2.17	0.43
2:A:529:VAL:O	2:A:530:ARG:HG3	2.19	0.43
2:B:63:VAL:O	2:B:82:ARG:NH1	2.52	0.43
2:A:354:VAL:HG22	2:A:387:LEU:HD22	2.00	0.43
2:A:404:LYS:CD	2:A:436:PHE:CZ	2.99	0.43
2:B:596:LEU:HD13	2:B:643:VAL:HG13	2.00	0.43
2:A:41:ARG:HB3	2:A:70:LEU:HD13	2.01	0.43
2:B:137:LEU:HD22	2:B:272:VAL:HG13	2.00	0.43
2:B:192:PHE:HZ	2:B:246:LYS:HB2	1.84	0.43
2:B:481:THR:HG22	2:B:481:THR:O	2.19	0.43
2:A:46:THR:HG22	2:A:48:LEU:HB2	2.00	0.43
2:A:118:PHE:HE2	2:A:126:ILE:CD1	2.24	0.43
2:A:174:GLU:C	2:A:176:ASN:H	2.22	0.43
1:D:2:G:H2'	1:D:3:A:C8	2.54	0.42
2:A:53:ARG:HE	2:A:92:GLN:CG	2.30	0.42
2:B:701:ASP:OD1	2:B:702:ILE:HD12	2.19	0.42
2:A:25:LYS:HG3	2:A:56:GLU:HG3	1.99	0.42
2:B:19:THR:HG22	2:B:87:GLU:HG2	2.00	0.42
2:B:131:LYS:O	2:B:132:ASN:HB3	2.18	0.42
2:B:145:VAL:HA	2:B:154:LEU:O	2.19	0.42
2:B:180:PRO:O	2:B:196:VAL:CG1	2.66	0.42
2:B:49:PRO:HB2	2:B:100:LEU:HD11	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:THR:N	2:B:263:ASN:HD21	2.17	0.42
2:A:381:LYS:HG2	2:A:386:LYS:HA	2.01	0.42
2:A:476:GLN:HB3	2:A:480:LYS:NZ	2.34	0.42
2:A:611:LYS:O	2:A:631:ASN:HB3	2.19	0.42
1:C:2:G:O2'	1:C:3:A:O5'	2.35	0.42
1:C:5:A:H2'	1:C:6:G:C8	2.54	0.42
2:A:119:TYR:O	2:A:121:LYS:N	2.52	0.42
2:B:679:VAL:O	2:B:682:SER:HB2	2.19	0.42
2:A:131:LYS:HE3	2:A:132:ASN:HD22	1.85	0.42
2:A:507:THR:CG2	2:A:508:ARG:N	2.83	0.42
2:B:140:GLU:OE2	2:B:162:ARG:HD3	2.19	0.42
2:B:434:LYS:HB3	2:B:436:PHE:HD2	1.83	0.42
2:A:407:LEU:O	2:A:411:ILE:HG13	2.19	0.42
2:B:501:ILE:HD11	2:B:551:VAL:HG21	2.02	0.42
2:A:107:LYS:HE2	2:A:107:LYS:HB3	1.86	0.42
2:B:472:ASN:HB2	2:B:670:PHE:CD2	2.54	0.42
1:C:9:U:H3	1:D:16:A:H2	1.66	0.42
2:A:611:LYS:HD3	2:A:612:PHE:CE1	2.46	0.42
2:A:668:SER:HB3	2:A:673:ILE:HD12	2.02	0.42
2:A:427:TYR:HA	2:A:428:PRO:HD3	1.84	0.41
2:B:225:ALA:HB2	2:B:254:ILE:HD12	2.01	0.41
2:B:397:ALA:CB	2:B:403:ALA:HB2	2.50	0.41
2:B:322:VAL:CG1	2:B:323:LEU:N	2.83	0.41
2:B:352:LEU:HD21	2:B:481:THR:HG21	2.02	0.41
2:B:604:PRO:HD2	2:B:626:ILE:HD13	2.02	0.41
2:A:244:LEU:HB2	2:A:248:TYR:HB2	2.01	0.41
2:B:627:LEU:HD22	2:B:656:CYS:HB3	2.01	0.41
1:D:18:G:N2	1:D:19:C:C2	2.88	0.41
2:A:291:LEU:HD21	2:A:305:ILE:HG21	2.01	0.41
2:A:225:ALA:HB1	2:A:251:PRO:HG2	2.03	0.41
2:A:440:ASP:O	2:A:441:PHE:C	2.58	0.41
2:A:532:TYR:CE2	2:A:554:LEU:HD13	2.56	0.41
2:A:594:GLU:OE1	2:A:649:GLU:N	2.54	0.41
2:B:163:ILE:HB	2:B:259:LEU:O	2.21	0.41
2:B:604:PRO:HD2	2:B:626:ILE:CD1	2.50	0.41
1:C:10:G:N2	1:D:16:A:C4	2.89	0.41
2:A:150:GLU:CD	2:A:150:GLU:H	2.24	0.41
2:A:337:ARG:O	2:A:341:GLU:HG3	2.21	0.41
2:A:502:ASP:O	2:A:517:ALA:HA	2.21	0.41
2:B:421:ILE:HG23	2:B:456:ILE:HD12	2.02	0.41
2:B:449:LYS:HB2	2:B:451:ILE:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:G:H2'	1:D:11:C:H6	1.85	0.41
2:A:10:TYR:CE2	2:A:309:GLU:HG3	2.56	0.41
2:A:641:ILE:HG22	2:A:643:VAL:HG23	2.03	0.41
2:B:23:VAL:HA	2:B:57:PHE:O	2.20	0.41
2:B:122:PHE:CZ	2:B:275:ILE:CG2	2.67	0.41
2:B:158:ASP:OD1	2:B:283:ARG:NH1	2.51	0.41
2:B:306:SER:HA	2:B:307:PRO:HD3	1.89	0.41
2:B:647:TYR:CD1	2:B:647:TYR:C	2.95	0.41
1:C:10:G:C6	1:C:11:C:C4	3.08	0.41
1:D:6:G:H5'	3:D:28:HOH:O	2.19	0.41
2:A:278:MET:HE1	2:A:286:LEU:HD12	2.03	0.41
2:B:436:PHE:O	2:B:437:LEU:C	2.59	0.41
2:B:481:THR:CG2	2:B:481:THR:O	2.68	0.41
1:D:18:G:C2	1:D:19:C:N3	2.90	0.40
2:A:278:MET:HE2	2:A:278:MET:HB2	1.94	0.40
2:A:489:LYS:C	2:A:490:GLU:HG3	2.40	0.40
2:A:532:TYR:CZ	2:A:554:LEU:HD13	2.56	0.40
2:B:360:SER:HB3	2:B:425:GLU:CG	2.43	0.40
2:B:420:VAL:HG23	2:B:451:ILE:HG21	2.02	0.40
2:A:443:LYS:NZ	2:A:453:SER:O	2.54	0.40
2:A:565:LYS:NZ	2:A:650:LEU:HD21	2.36	0.40
2:B:137:LEU:HD12	2:B:137:LEU:HA	1.85	0.40
2:B:157:LEU:HD23	2:B:287:ILE:HG23	2.01	0.40
2:B:334:THR:HG22	2:B:335:ASN:HD22	1.86	0.40
1:D:14:G:C2	1:D:15:C:N3	2.89	0.40
2:A:46:THR:HB	2:A:48:LEU:H	1.86	0.40
2:A:266:ASP:O	2:A:269:ARG:HB2	2.21	0.40
2:A:310:GLU:HB3	2:A:618:TYR:CE1	2.57	0.40
2:A:381:LYS:C	2:A:383:LYS:N	2.75	0.40
2:A:611:LYS:HB3	2:A:612:PHE:CD1	2.55	0.40
2:B:284:LEU:HD12	2:B:284:LEU:HA	1.84	0.40
1:D:14:G:C6	1:D:15:C:C4	3.10	0.40
2:A:443:LYS:HA	2:A:443:LYS:HD2	1.78	0.40
2:B:179:ASN:HA	2:B:180:PRO:HD3	1.89	0.40
2:B:352:LEU:HD21	2:B:481:THR:CG2	2.51	0.40
2:B:414:ILE:H	2:B:414:ILE:HG13	1.52	0.40
1:C:24:U:OP2	1:C:26:U:H5"	2.22	0.40
2:B:465:ASN:HB3	2:B:468:PHE:HB3	2.03	0.40
2:B:551:VAL:HG12	2:B:552:PHE:N	2.36	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	
2	A	702/706 (99%)	605 (86%)	77 (11%)	20 (3%)	5	25
2	B	702/706 (99%)	605 (86%)	78 (11%)	19 (3%)	5	25
All	All	1404/1412 (99%)	1210 (86%)	155 (11%)	39 (3%)	5	25

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	434	LYS
2	A	435	SER
2	B	130	GLY
2	B	132	ASN
2	B	265	GLU
2	B	278	MET
2	B	335	ASN
2	B	577	ASP
2	A	120	LYS
2	A	131	LYS
2	A	206	GLY
2	A	272	VAL
2	A	382	ASN
2	A	436	PHE
2	A	541	GLU
2	A	663	THR
2	B	253	THR
2	B	262	GLU
2	B	382	ASN
2	B	636	GLY
2	A	175	ARG
2	A	269	ARG
2	A	278	MET
2	A	480	LYS
2	B	60	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	207	GLU
2	B	437	LEU
2	B	635	GLU
2	A	65	LYS
2	A	672	PRO
2	B	127	THR
2	B	333	ILE
2	B	553	SER
2	A	263	ASN
2	A	180	PRO
2	B	183	ILE
2	A	428	PRO
2	A	692	GLY
2	B	389	ILE

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
2	A	646/647 (100%)	580 (90%)	66 (10%)	7 27
2	B	646/647 (100%)	550 (85%)	96 (15%)	3 13
All	All	1292/1294 (100%)	1130 (88%)	162 (12%)	4 18

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	17	LYS
2	A	31	GLN
2	A	33	GLU
2	A	53	ARG
2	A	78	VAL
2	A	83	VAL
2	A	87	GLU
2	A	107	LYS
2	A	110	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	113	LYS
2	A	133	ARG
2	A	135	ILE
2	A	156	HIS
2	A	165	PRO
2	A	168	THR
2	A	174	GLU
2	A	201	LYS
2	A	203	LYS
2	A	204	GLU
2	A	213	CYS
2	A	218	THR
2	A	229	LEU
2	A	260	THR
2	A	267	GLU
2	A	271	GLU
2	A	278	MET
2	A	322	VAL
2	A	334	THR
2	A	335	ASN
2	A	348	LYS
2	A	354	VAL
2	A	355	GLU
2	A	375	GLU
2	A	399	THR
2	A	401	GLU
2	A	425	GLU
2	A	430	VAL
2	A	433	TYR
2	A	436	PHE
2	A	440	ASP
2	A	444	ARG
2	A	445	GLU
2	A	470	LEU
2	A	472	ASN
2	A	490	GLU
2	A	501	ILE
2	A	502	ASP
2	A	505	ARG
2	A	509	ASP
2	A	527	GLU
2	A	600	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	601	ARG
2	A	613	ILE
2	A	614	LYS
2	A	621	SER
2	A	623	ASP
2	A	624	SER
2	A	634	TYR
2	A	661	SER
2	A	671	GLN
2	A	675	LEU
2	A	686	THR
2	A	689	MET
2	A	690	LEU
2	A	694	GLU
2	A	702	ILE
2	B	29	GLU
2	B	31	GLN
2	B	39	ARG
2	B	43	PHE
2	B	44	LEU
2	B	45	GLN
2	B	46	THR
2	B	64	GLU
2	B	66	ASP
2	B	67	THR
2	B	71	THR
2	B	86	GLU
2	B	106	THR
2	B	108	THR
2	B	110	VAL
2	B	111	LYS
2	B	117	ASP
2	B	128	VAL
2	B	134	LYS
2	B	143	GLU
2	B	147	LYS
2	B	148	SER
2	B	159	LEU
2	B	163	ILE
2	B	166	PHE
2	B	168	THR
2	B	171	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	172	LEU
2	B	207	GLU
2	B	214	MET
2	B	230	LEU
2	B	235	LEU
2	B	237	GLU
2	B	254	ILE
2	B	263	ASN
2	B	264	LEU
2	B	266	ASP
2	B	269	ARG
2	B	311	ARG
2	B	323	LEU
2	B	330	THR
2	B	333	ILE
2	B	335	ASN
2	B	337	ARG
2	B	340	LEU
2	B	349	LYS
2	B	350	ASP
2	B	351	VAL
2	B	353	SER
2	B	355	GLU
2	B	360	SER
2	B	362	TYR
2	B	367	TRP
2	B	368	ARG
2	B	380	LEU
2	B	383	LYS
2	B	393	SER
2	B	394	LEU
2	B	398	GLN
2	B	399	THR
2	B	408	ILE
2	B	431	ASP
2	B	434	LYS
2	B	438	LEU
2	B	464	GLU
2	B	468	PHE
2	B	470	LEU
2	B	480	LYS
2	B	501	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	505	ARG
2	B	507	THR
2	B	508	ARG
2	B	541	GLU
2	B	543	LEU
2	B	554	LEU
2	B	556	GLU
2	B	561	LYS
2	B	564	SER
2	B	574	LEU
2	B	587	GLU
2	B	600	LYS
2	B	601	ARG
2	B	622	GLU
2	B	629	THR
2	B	637	THR
2	B	638	HIS
2	B	647	TYR
2	B	649	GLU
2	B	652	VAL
2	B	668	SER
2	B	674	LYS
2	B	688	LEU
2	B	689	MET
2	B	691	ARG
2	B	693	ILE
2	B	696	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	74	ASN
2	A	98	GLN
2	A	132	ASN
2	A	219	HIS
2	A	263	ASN
2	A	335	ASN
2	A	458	ASN
2	A	569	HIS
2	A	602	ASN
2	B	93	ASN
2	B	179	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	219	HIS
2	B	263	ASN
2	B	335	ASN
2	B	523	ASN
2	B	632	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	25/26 (96%)	6 (24%)	0
1	D	23/26 (88%)	6 (26%)	1 (4%)
All	All	48/52 (92%)	12 (25%)	1 (2%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	3	A
1	C	6	G
1	C	9	U
1	C	10	G
1	C	11	C
1	C	26	U
1	D	2	G
1	D	9	U
1	D	16	A
1	D	17	U
1	D	20	U
1	D	24	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	23	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

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	C	26/26 (100%)	-0.10	0 100 100	31, 58, 79, 82	0
1	D	24/26 (92%)	0.23	0 100 100	26, 59, 89, 91	0
2	A	704/706 (99%)	-0.48	2 (0%) 94 88	27, 54, 82, 96	0
2	B	704/706 (99%)	-0.31	10 (1%) 75 56	30, 55, 78, 93	0
All	All	1458/1464 (99%)	-0.38	12 (0%) 86 72	26, 54, 80, 96	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	132	ASN	3.0
2	A	179	ASN	2.9
2	B	509	ASP	2.8
2	B	435	SER	2.5
2	B	129	GLN	2.5
2	B	198	ASP	2.4
2	B	133	ARG	2.3
2	B	262	GLU	2.2
2	B	635	GLU	2.1
2	A	509	ASP	2.1
2	B	510	GLY	2.0
2	B	436	PHE	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

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.