



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:55 AM UTC

PDB ID : 5WQE / pdb_00005wqe
Title : Crystal structure of Alicyclobacillus acidoterrestris C2c1 in complex with single-guide RNA at 3.1 Angstrom resolution
Authors : Liu, L.; Wang, Y.L.
Deposited on : 2016-11-26
Resolution : 3.13 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

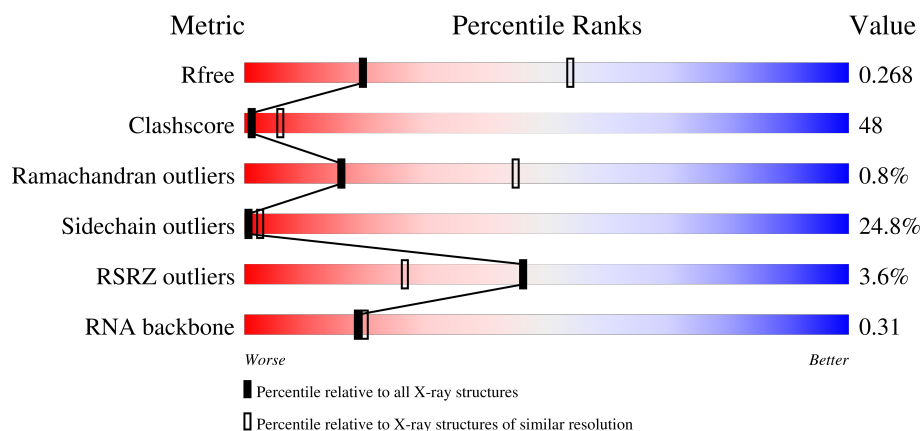
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)
RNA backbone	3983	1017 (3.34-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1137	
2	B	112	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9308 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 CRISPR-associated endonuclease C2c1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	Se	0	0	0
			7988	5033	1476	1452	8	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1130	LEU	-	expression tag	UNP T0D7A2
A	1131	GLU	-	expression tag	UNP T0D7A2
A	1132	HIS	-	expression tag	UNP T0D7A2
A	1133	HIS	-	expression tag	UNP T0D7A2
A	1134	HIS	-	expression tag	UNP T0D7A2
A	1135	HIS	-	expression tag	UNP T0D7A2
A	1136	HIS	-	expression tag	UNP T0D7A2
A	1137	HIS	-	expression tag	UNP T0D7A2

- Molecule 2 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	60	Total	C	N	O	P	0	0	0
			1278	567	241	410	60			

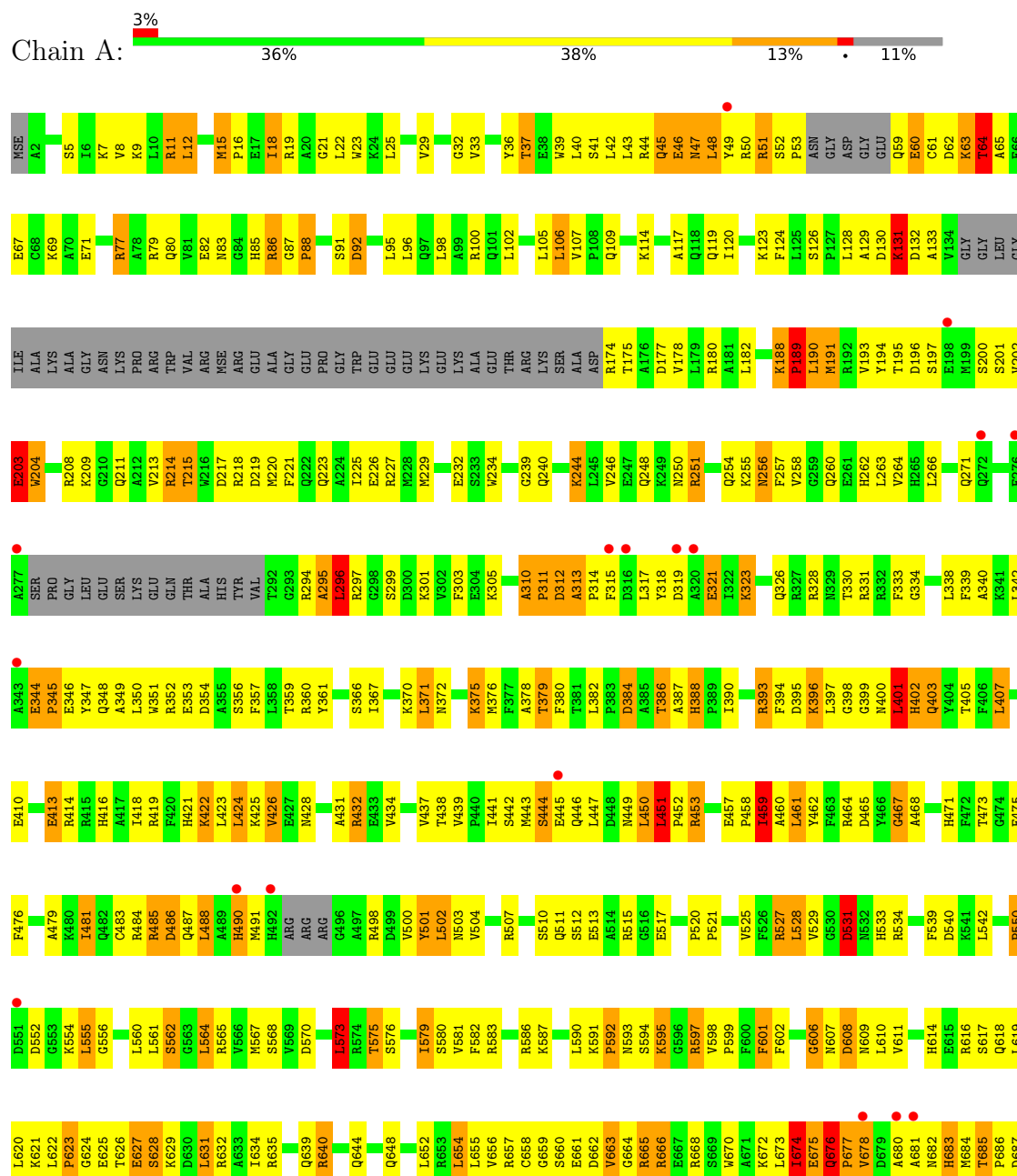
- Molecule 3 is water.

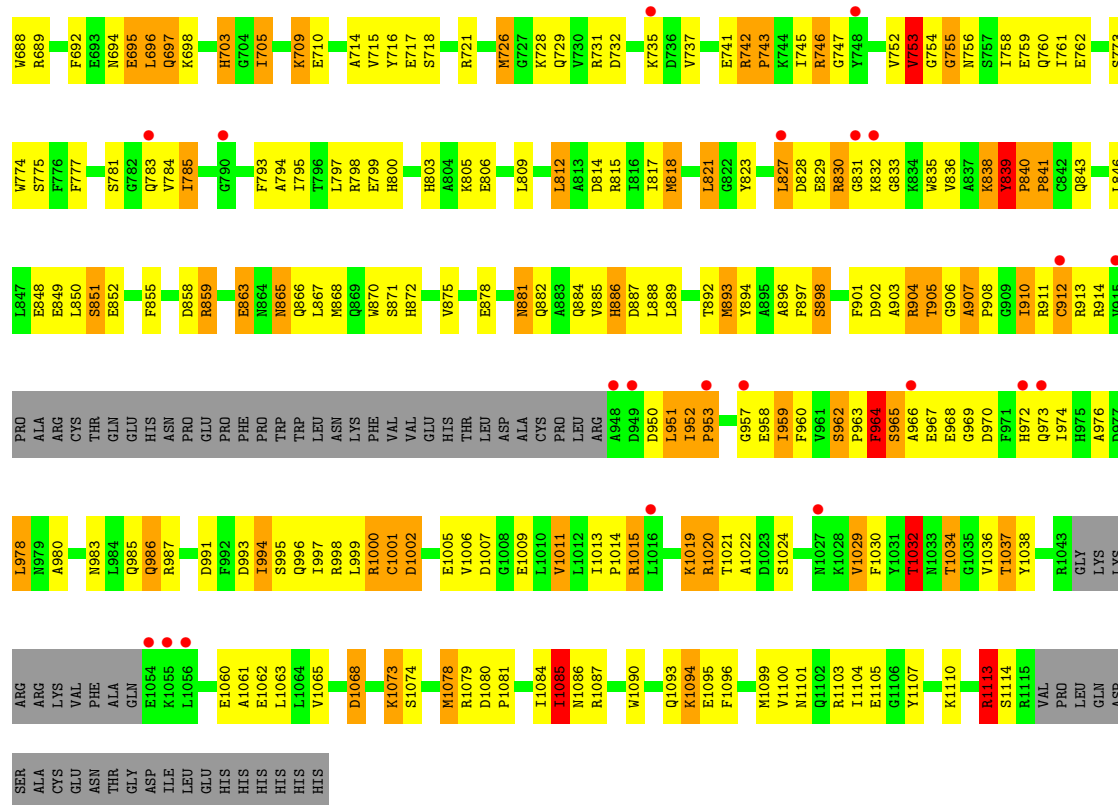
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	3	Total	O	0	0
			3	3		

3 Residue-property plots

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

• Molecule 1: CRISPR-associated endonuclease C2c1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	194.55Å 129.84Å 84.00Å 90.00° 110.00° 90.00°	Depositor
Resolution (Å)	48.64 – 3.13 48.64 – 3.13	Depositor EDS
% Data completeness (in resolution range)	79.3 (48.64-3.13) 79.3 (48.64-3.13)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.238 , 0.268 0.238 , 0.268	Depositor DCC
R_{free} test set	1340 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9308	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.98	25/8134 (0.3%)	1.31	91/10953 (0.8%)
2	B	0.52	0/1427	1.08	12/2217 (0.5%)
All	All	0.92	25/9561 (0.3%)	1.27	103/13170 (0.8%)

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	A	0	5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	MSE	C-N	8.20	1.40	1.33
1	A	841	PRO	N-CD	-6.40	1.38	1.47
1	A	742	ARG	C-N	6.09	1.40	1.33
1	A	839	TYR	C-N	6.06	1.40	1.33
1	A	310	ALA	C-N	6.03	1.40	1.33
1	A	598	VAL	C-N	6.02	1.40	1.33
1	A	907	ALA	C-N	5.95	1.40	1.33
1	A	840	PRO	C-N	5.95	1.40	1.33
1	A	457	GLU	C-N	5.92	1.40	1.33
1	A	313	ALA	C-N	5.55	1.40	1.33
1	A	345	PRO	N-CD	5.47	1.55	1.47
1	A	520	PRO	C-N	5.44	1.40	1.33
1	A	677	PRO	N-CD	5.42	1.55	1.47
1	A	520	PRO	N-CD	5.41	1.55	1.47
1	A	88	PRO	N-CD	5.39	1.55	1.47
1	A	311	PRO	N-CD	5.35	1.55	1.47
1	A	592	PRO	N-CD	5.32	1.55	1.47
1	A	388	HIS	C-N	5.29	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	PRO	N-CD	5.26	1.55	1.47
1	A	107	VAL	C-N	5.22	1.40	1.34
1	A	521	PRO	N-CD	5.19	1.55	1.47
1	A	743	PRO	N-CD	5.18	1.55	1.47
1	A	840	PRO	N-CD	5.09	1.54	1.47
1	A	314	PRO	N-CD	5.08	1.54	1.47
1	A	623	PRO	N-CD	5.02	1.54	1.47

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	753	VAL	N-CA-C	32.84	144.12	110.62
1	A	295	ALA	N-CA-C	-20.10	78.36	110.32
1	A	203	GLU	CB-CA-C	-16.59	82.58	109.80
1	A	421	HIS	N-CA-C	-16.29	82.60	109.96
1	A	296	LEU	N-CA-CB	15.89	137.34	110.49
1	A	422	LYS	N-CA-C	11.18	126.83	111.74
1	A	1085	ILE	N-CA-C	10.54	121.37	110.72
1	A	256	ASN	N-CA-C	9.78	122.02	111.36
2	B	3	C	C4'-C3'-O3'	-9.58	98.63	113.00
1	A	204	TRP	N-CA-CB	-9.25	96.54	110.60
1	A	18	ILE	N-CA-C	9.08	119.07	110.53
1	A	753	VAL	CB-CA-C	-9.08	99.88	112.14
2	B	49	G	C2'-C3'-O3'	9.00	127.20	113.70
1	A	953	PRO	CA-N-CD	-8.49	100.11	112.00
1	A	531	ASP	N-CA-C	8.44	122.89	111.24
1	A	625	GLU	N-CA-C	8.25	121.20	111.71
1	A	676	GLN	C-N-CD	8.25	138.74	120.60
1	A	674	ILE	N-CA-C	8.23	118.27	110.53
1	A	562	SER	N-CA-C	7.81	119.80	111.28
1	A	46	GLU	N-CA-C	-7.80	100.47	110.53
2	B	8	G	C4'-C3'-O3'	-7.52	98.13	109.40
1	A	203	GLU	N-CA-C	-7.34	97.28	109.46
2	B	49	G	C3'-C2'-O2'	7.32	121.68	110.70
1	A	598	VAL	CA-C-N	-7.14	113.45	120.52
1	A	598	VAL	C-N-CA	-7.14	113.45	120.52
1	A	457	GLU	CA-C-N	-7.09	113.50	120.52
1	A	457	GLU	C-N-CA	-7.09	113.50	120.52
1	A	573	LEU	N-CA-C	7.08	118.79	111.14
1	A	608	ASP	CB-CA-C	-7.07	95.89	109.95
2	B	4	U	C3'-C2'-O2'	-7.01	104.08	114.60
1	A	310	ALA	CA-C-N	-6.94	113.16	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ALA	C-N-CA	-6.94	113.16	120.03
1	A	1113	ARG	CB-CA-C	-6.87	108.67	116.63
1	A	839	TYR	CA-C-N	-6.80	113.37	120.38
1	A	839	TYR	C-N-CA	-6.80	113.37	120.38
2	B	28	U	C2'-C3'-O3'	6.75	123.83	113.70
1	A	204	TRP	N-CA-C	-6.63	100.40	109.95
1	A	531	ASP	CA-C-N	6.62	133.61	121.70
1	A	531	ASP	C-N-CA	6.62	133.61	121.70
2	B	89	C	C4'-C3'-O3'	-6.58	103.13	113.00
2	B	91	C	C4'-C3'-O3'	-6.50	103.25	113.00
1	A	64	THR	N-CA-C	-6.50	102.42	110.41
1	A	907	ALA	CA-C-N	-6.49	113.61	120.03
1	A	907	ALA	C-N-CA	-6.49	113.61	120.03
1	A	107	VAL	CB-CA-C	-6.47	104.93	111.08
1	A	15	MSE	CA-C-N	-6.47	113.21	121.04
1	A	15	MSE	C-N-CA	-6.47	113.21	121.04
1	A	742	ARG	CA-C-N	-6.46	112.83	120.13
1	A	742	ARG	C-N-CA	-6.46	112.83	120.13
1	A	398	GLY	N-CA-C	-6.29	104.75	112.68
1	A	833	GLY	N-CA-C	-6.29	101.09	110.71
1	A	131	LYS	N-CA-C	-6.25	99.82	109.76
1	A	965	SER	N-CA-C	6.22	120.00	111.54
1	A	388	HIS	CA-C-N	-6.22	113.57	119.85
1	A	388	HIS	C-N-CA	-6.22	113.57	119.85
1	A	313	ALA	CA-C-N	-6.22	113.36	119.76
1	A	313	ALA	C-N-CA	-6.22	113.36	119.76
2	B	86	U	C2'-C3'-O3'	6.13	118.69	109.50
1	A	188	LYS	C-N-CD	6.07	133.96	120.60
1	A	841	PRO	N-CD-CG	5.98	112.17	103.20
1	A	685	THR	CA-C-N	-5.94	112.46	119.05
1	A	685	THR	C-N-CA	-5.94	112.46	119.05
2	B	9	G	C2'-C3'-O3'	-5.92	104.82	113.70
1	A	45	GLN	N-CA-C	-5.83	104.93	111.28
2	B	1	G	C4'-C3'-O3'	-5.81	104.29	113.00
1	A	841	PRO	N-CA-C	5.76	120.06	111.41
1	A	881	ASN	N-CA-C	5.75	117.35	111.14
1	A	107	VAL	CA-C-N	-5.74	113.11	119.19
1	A	107	VAL	C-N-CA	-5.74	113.11	119.19
1	A	755	GLY	N-CA-C	-5.70	104.69	111.36
1	A	703	HIS	N-CA-C	5.65	117.12	111.07
1	A	87	GLY	C-N-CD	5.54	132.80	120.60
1	A	550	PRO	CA-N-CD	-5.48	104.33	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	PRO	CA-C-N	-5.44	114.01	119.56
1	A	520	PRO	C-N-CA	-5.44	114.01	119.56
1	A	886	HIS	N-CA-C	-5.44	100.03	108.90
1	A	453	ARG	N-CA-C	5.43	117.28	111.36
1	A	742	ARG	N-CA-C	-5.41	101.98	108.25
1	A	16	PRO	N-CA-C	-5.40	107.09	114.98
1	A	16	PRO	CA-N-CD	-5.40	104.44	112.00
2	B	5	A	C2'-C3'-O3'	5.39	117.58	109.50
1	A	964	PHE	N-CA-C	5.39	117.17	108.34
1	A	297	ARG	N-CA-C	5.38	117.23	111.36
1	A	840	PRO	CA-C-N	-5.38	114.70	120.03
1	A	840	PRO	C-N-CA	-5.38	114.70	120.03
1	A	962	SER	N-CA-C	5.31	114.41	108.25
1	A	783	GLN	N-CA-C	5.21	116.96	111.28
1	A	606	GLY	N-CA-C	5.20	119.42	112.77
1	A	528	LEU	N-CA-C	-5.18	101.42	109.24
1	A	622	LEU	N-CA-C	-5.16	101.52	109.87
1	A	1032	THR	CB-CA-C	-5.13	98.17	109.56
1	A	1013	ILE	CA-C-N	5.09	126.20	119.84
1	A	1013	ILE	C-N-CA	5.09	126.20	119.84
1	A	451	LEU	CA-C-N	-5.09	113.48	119.84
1	A	451	LEU	C-N-CA	-5.09	113.48	119.84
1	A	384	ASP	N-CA-C	-5.08	101.48	109.50
1	A	601	PHE	N-CA-C	5.07	116.52	108.96
1	A	885	VAL	CB-CA-C	-5.06	105.30	112.14
1	A	676	GLN	CA-C-N	-5.04	114.89	127.00
1	A	676	GLN	C-N-CA	-5.04	114.89	127.00
1	A	180	ARG	N-CA-C	-5.04	105.78	111.28
1	A	387	ALA	N-CA-C	5.02	116.83	111.36
1	A	399	GLY	N-CA-C	-5.00	104.61	112.61

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	467	GLY	Peptide
1	A	531	ASP	Peptide
1	A	64	THR	Peptide
1	A	784	VAL	Peptide
1	A	912	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7988	0	7713	743	0
2	B	1278	0	645	126	0
3	A	39	0	0	3	0
3	B	3	0	0	0	0
All	All	9308	0	8358	841	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 48.

All (841) 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:B:8:G:H3'	2:B:9:G:C5'	1.71	1.19
1:A:575:THR:CG2	1:A:621:LYS:HE2	1.73	1.18
1:A:758:ILE:HG23	1:A:867:LEU:HD23	1.27	1.14
1:A:1073:LYS:HA	1:A:1073:LYS:HE2	1.15	1.13
2:B:11:C:H2'	2:B:12:A:H5'	1.31	1.11
2:B:8:G:H3'	2:B:9:G:H5'	1.31	1.10
1:A:1062:GLU:HA	1:A:1065:VAL:CG2	1.82	1.08
2:B:47:C:H2'	2:B:48:A:H5''	1.25	1.08
1:A:967:GLU:HA	1:A:1103:ARG:NH2	1.68	1.08
1:A:913:ARG:HB2	1:A:953:PRO:HD2	1.32	1.07
1:A:510:SER:HB2	1:A:513:GLU:HG3	1.33	1.07
2:B:12:A:H2'	2:B:13:G:C8	1.89	1.05
1:A:913:ARG:HB2	1:A:953:PRO:CD	1.87	1.04
1:A:45:GLN:CG	1:A:69:LYS:HD3	1.87	1.04
2:B:11:C:C2'	2:B:12:A:H5'	1.87	1.03
1:A:665:ARG:HH11	1:A:665:ARG:HB3	1.22	1.02
1:A:11:ARG:HH11	1:A:11:ARG:HB3	1.22	1.02
2:B:9:G:C2	2:B:10:A:C5	2.47	1.02
1:A:131:LYS:HE3	1:A:131:LYS:HA	1.38	1.02
1:A:573:LEU:HD12	1:A:573:LEU:H	1.22	1.02
1:A:491:MSE:SE	1:A:498:ARG:CB	2.59	1.00
1:A:607:ASN:HB3	1:A:610:LEU:HB2	1.42	1.00
1:A:575:THR:HG22	1:A:621:LYS:CE	1.91	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:ARG:HG3	1:A:904:ARG:HH11	1.28	0.98
1:A:575:THR:HG22	1:A:621:LYS:HE2	0.99	0.97
1:A:483:CYS:SG	1:A:488:LEU:CD2	2.53	0.97
1:A:303:PHE:CE2	1:A:350:LEU:CB	2.48	0.96
1:A:964:PHE:CE2	1:A:970:ASP:HB3	1.99	0.96
1:A:597:ARG:NH1	1:A:597:ARG:HB3	1.81	0.96
1:A:45:GLN:HG2	1:A:69:LYS:HD3	1.44	0.95
1:A:213:VAL:HG13	1:A:217:ASP:HB2	1.47	0.94
1:A:758:ILE:CG2	1:A:867:LEU:HD23	1.98	0.94
1:A:64:THR:CB	1:A:65:ALA:HB3	1.97	0.94
1:A:758:ILE:HG23	1:A:867:LEU:CD2	1.98	0.93
1:A:1062:GLU:C	1:A:1065:VAL:HG22	1.92	0.93
1:A:726:MSE:HE2	1:A:774:TRP:CZ3	2.04	0.93
1:A:64:THR:HB	1:A:65:ALA:HB3	1.49	0.92
2:B:50:G:H8	2:B:50:G:H5''	1.31	0.92
2:B:8:G:C3'	2:B:9:G:C5'	2.48	0.92
1:A:785:ILE:HD12	1:A:785:ILE:H	1.34	0.92
2:B:47:C:C2'	2:B:48:A:H5''	1.98	0.92
1:A:79:ARG:NH2	1:A:82:GLU:HG2	1.84	0.92
1:A:1062:GLU:CA	1:A:1065:VAL:HG22	1.99	0.91
1:A:1073:LYS:HE2	1:A:1073:LYS:CA	2.01	0.91
1:A:1020:ARG:HG2	1:A:1020:ARG:HH11	1.33	0.91
1:A:674:ILE:HD12	1:A:675:GLU:H	1.36	0.91
1:A:248:GLN:HB3	1:A:1060:GLU:OE2	1.71	0.90
1:A:913:ARG:CB	1:A:953:PRO:HD2	2.00	0.90
1:A:534:ARG:HG3	1:A:534:ARG:HH11	1.36	0.90
1:A:682:ASN:HB3	1:A:683:HIS:ND1	1.86	0.90
1:A:1062:GLU:HA	1:A:1065:VAL:HG22	1.52	0.89
1:A:838:LYS:HB3	1:A:839:TYR:CD1	2.08	0.89
2:B:9:G:C6	2:B:10:A:N6	2.39	0.89
1:A:215:THR:CG2	1:A:422:LYS:NZ	2.36	0.88
1:A:339:PHE:HD1	1:A:342:LEU:HD12	1.36	0.88
1:A:579:ILE:HG21	1:A:620:LEU:HD11	1.55	0.88
1:A:64:THR:CG2	1:A:65:ALA:HB3	2.03	0.88
1:A:897:PHE:CZ	1:A:1078:MSE:HE1	2.09	0.88
1:A:79:ARG:HH22	1:A:82:GLU:HG2	1.40	0.87
1:A:371:LEU:HD12	1:A:372:ASN:N	1.90	0.87
1:A:838:LYS:HB2	1:A:838:LYS:HZ3	1.39	0.87
1:A:967:GLU:HA	1:A:1103:ARG:HH22	1.35	0.87
1:A:510:SER:HB2	1:A:513:GLU:CG	2.06	0.86
2:B:8:G:H3'	2:B:9:G:H5''	1.55	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:GLU:O	1:A:1099:MSE:HG3	1.75	0.85
1:A:527:ARG:O	1:A:528:LEU:HD23	1.75	0.85
1:A:33:VAL:O	1:A:37:THR:OG1	1.95	0.85
1:A:485:ARG:HG2	1:A:485:ARG:HH11	1.40	0.84
1:A:665:ARG:HH11	1:A:665:ARG:CB	1.88	0.84
1:A:215:THR:HG21	1:A:422:LYS:NZ	1.93	0.84
1:A:663:VAL:HG12	1:A:664:GLY:H	1.41	0.84
2:B:9:G:N1	2:B:10:A:C6	2.46	0.84
1:A:677:PRO:O	1:A:678:VAL:CG2	2.26	0.84
1:A:1062:GLU:HA	1:A:1065:VAL:HG21	1.57	0.84
1:A:677:PRO:O	1:A:678:VAL:HG22	1.78	0.83
2:B:9:G:C4	2:B:10:A:N7	2.46	0.83
1:A:755:GLY:N	1:A:760:GLN:HG3	1.94	0.83
2:B:47:C:H2'	2:B:48:A:C5'	2.07	0.83
2:B:11:C:H2'	2:B:12:A:C5'	2.09	0.82
1:A:11:ARG:HH11	1:A:11:ARG:CB	1.92	0.82
2:B:31:G:O2'	2:B:32:C:O5'	1.97	0.82
1:A:43:LEU:HD13	1:A:43:LEU:O	1.79	0.82
1:A:660:SER:HB2	1:A:661:GLU:C	2.04	0.82
1:A:49:TYR:CE1	1:A:380:PHE:CD2	2.68	0.81
1:A:1061:ALA:O	1:A:1065:VAL:HG13	1.80	0.81
1:A:48:LEU:H	1:A:48:LEU:HD23	1.44	0.81
1:A:682:ASN:HB3	1:A:683:HIS:CE1	2.15	0.81
1:A:905:THR:OG1	1:A:906:GLY:HA2	1.79	0.81
1:A:36:TYR:CD1	1:A:191:MSE:HE1	2.16	0.81
1:A:9:LYS:HD3	2:B:29:G:OP1	1.82	0.80
1:A:59:GLN:NE2	1:A:379:THR:HG23	1.95	0.80
1:A:396:LYS:H	1:A:396:LYS:HD3	1.47	0.79
1:A:311:PRO:HD3	1:A:351:TRP:CZ2	2.17	0.79
1:A:958:GLU:O	1:A:976:ALA:HB3	1.83	0.79
2:B:5:A:O2'	2:B:6:G:OP1	2.01	0.79
1:A:951:LEU:HG	1:A:952:ILE:HG13	1.65	0.79
1:A:396:LYS:HD3	1:A:396:LYS:N	1.98	0.79
1:A:958:GLU:O	1:A:976:ALA:CB	2.31	0.78
1:A:1068:ASP:HB3	1:A:1074:SER:HB2	1.65	0.78
2:B:35:A:H4'	2:B:36:U:OP2	1.82	0.78
2:B:9:G:H2'	2:B:10:A:C8	2.18	0.78
1:A:510:SER:CB	1:A:513:GLU:HG3	2.13	0.78
1:A:423:LEU:O	1:A:434:VAL:HG12	1.82	0.78
1:A:674:ILE:HD12	1:A:675:GLU:N	1.97	0.78
2:B:8:G:C3'	2:B:9:G:H5''	2.11	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:G:N3	2:B:10:A:N7	2.31	0.78
1:A:863:GLU:O	1:A:868:MSE:HG3	1.84	0.78
2:B:11:C:C2'	2:B:12:A:C5'	2.63	0.77
2:B:11:C:O2'	2:B:12:A:H5'	1.83	0.77
1:A:827:LEU:HG	1:A:830:ARG:HG2	1.67	0.77
2:B:12:A:H2'	2:B:13:G:H8	1.49	0.77
1:A:754:GLY:HA3	1:A:760:GLN:CG	2.14	0.76
1:A:1085:ILE:HG21	1:A:1096:PHE:CE1	2.21	0.76
1:A:339:PHE:HA	1:A:342:LEU:HD12	1.67	0.76
1:A:904:ARG:HG3	1:A:904:ARG:NH1	1.96	0.76
1:A:12:LEU:HD22	1:A:15:MSE:HG3	1.66	0.76
2:B:9:G:H2'	2:B:10:A:H8	1.50	0.76
1:A:827:LEU:O	1:A:830:ARG:HB3	1.86	0.76
1:A:45:GLN:CG	1:A:69:LYS:CD	2.64	0.75
1:A:131:LYS:HE3	1:A:131:LYS:CA	2.14	0.75
1:A:829:GLU:O	1:A:830:ARG:HG3	1.85	0.75
1:A:1094:LYS:HB2	1:A:1094:LYS:NZ	2.00	0.75
1:A:386:THR:HA	1:A:488:LEU:HD12	1.67	0.75
1:A:64:THR:HG22	1:A:65:ALA:HB3	1.66	0.75
1:A:579:ILE:HD13	1:A:579:ILE:O	1.86	0.75
2:B:7:A:O2'	2:B:8:G:H5'	1.86	0.75
2:B:23:A:H2'	2:B:24:C:H6	1.50	0.75
1:A:617:SER:HB3	1:A:978:LEU:CD1	2.16	0.75
1:A:754:GLY:HA3	1:A:760:GLN:HG3	1.67	0.75
1:A:659:GLY:O	1:A:660:SER:OG	2.04	0.75
1:A:1062:GLU:O	1:A:1065:VAL:HG22	1.86	0.75
1:A:660:SER:HB3	1:A:666:ARG:HB2	1.69	0.74
1:A:967:GLU:CA	1:A:1103:ARG:HH22	2.00	0.74
1:A:215:THR:CG2	1:A:422:LYS:HZ3	1.97	0.74
1:A:555:LEU:N	1:A:555:LEU:HD13	2.01	0.74
1:A:595:LYS:HD3	1:A:595:LYS:C	2.12	0.74
2:B:50:G:H5''	2:B:50:G:C8	2.21	0.74
1:A:453:ARG:HD3	1:A:460:ALA:HB1	1.70	0.74
1:A:485:ARG:HG2	1:A:485:ARG:NH1	1.99	0.74
1:A:1062:GLU:CA	1:A:1065:VAL:CG2	2.59	0.74
1:A:1062:GLU:O	1:A:1065:VAL:CG2	2.34	0.74
1:A:660:SER:OG	1:A:661:GLU:HA	1.86	0.74
1:A:1032:THR:HG23	1:A:1038:TYR:CD2	2.23	0.73
1:A:453:ARG:CG	1:A:460:ALA:HB1	2.17	0.73
1:A:619:LEU:HD12	2:B:10:A:H5'	1.71	0.73
1:A:44:ARG:HG3	1:A:46:GLU:O	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:HD1	1:A:191:MSE:HE1	1.53	0.73
1:A:677:PRO:C	1:A:678:VAL:HG23	2.14	0.73
1:A:695:GLU:HG3	1:A:718:SER:OG	1.89	0.73
1:A:966:ALA:HB1	1:A:1084:ILE:HG12	1.70	0.73
1:A:215:THR:HG21	1:A:422:LYS:HZ3	1.52	0.73
1:A:670:TRP:CH2	1:A:674:ILE:HG21	2.24	0.73
1:A:528:LEU:HA	1:A:534:ARG:O	1.89	0.72
1:A:579:ILE:HD13	1:A:579:ILE:C	2.14	0.72
1:A:573:LEU:HD12	1:A:573:LEU:N	2.01	0.72
2:B:9:G:N3	2:B:10:A:C8	2.57	0.72
1:A:838:LYS:HD2	1:A:839:TYR:CE1	2.25	0.72
1:A:51:ARG:NH2	1:A:52:SER:O	2.23	0.71
1:A:1086:ASN:O	1:A:1087:ARG:HB2	1.88	0.71
1:A:347:TYR:O	1:A:351:TRP:HB2	1.90	0.71
1:A:581:VAL:HG21	1:A:616:ARG:HE	1.56	0.71
1:A:39:TRP:O	1:A:43:LEU:HB2	1.91	0.71
1:A:215:THR:HG23	1:A:422:LYS:NZ	2.04	0.71
1:A:402:HIS:CD2	1:A:402:HIS:H	2.07	0.71
1:A:193:VAL:O	1:A:193:VAL:HG23	1.89	0.71
2:B:93:A:H2'	2:B:94:G:H5'	1.73	0.71
1:A:838:LYS:HB2	1:A:838:LYS:NZ	2.06	0.71
1:A:49:TYR:CD1	1:A:380:PHE:CD2	2.79	0.70
1:A:458:PRO:C	1:A:459:ILE:HG23	2.17	0.70
1:A:394:PHE:HE2	1:A:481:ILE:HD11	1.55	0.70
1:A:1032:THR:HG22	1:A:1037:THR:O	1.90	0.70
1:A:677:PRO:C	1:A:678:VAL:CG2	2.65	0.70
1:A:1020:ARG:HG2	1:A:1020:ARG:NH1	1.99	0.70
1:A:400:ASN:O	1:A:401:LEU:HD13	1.91	0.69
2:B:93:A:C2'	2:B:94:G:H5'	2.22	0.69
1:A:126:SER:O	1:A:130:ASP:HB3	1.92	0.69
1:A:338:LEU:O	1:A:342:LEU:HG	1.91	0.69
1:A:262:HIS:CE1	1:A:263:LEU:HG	2.27	0.69
1:A:213:VAL:HG13	1:A:217:ASP:CB	2.23	0.69
1:A:692:PHE:O	1:A:696:LEU:HB2	1.91	0.69
1:A:131:LYS:CE	1:A:132:ASP:H	2.05	0.69
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.56	0.69
1:A:658:CYS:O	1:A:666:ARG:HG3	1.93	0.69
1:A:753:VAL:HG23	1:A:753:VAL:O	1.92	0.69
1:A:849:GLU:HG3	1:A:894:TYR:HA	1.75	0.69
1:A:1002:ASP:OD1	1:A:1002:ASP:N	2.23	0.69
1:A:1094:LYS:HG3	1:A:1095:GLU:OE1	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HG22	1:A:229:MSE:HE3	1.75	0.68
1:A:597:ARG:HB3	1:A:597:ARG:HH11	1.57	0.68
1:A:555:LEU:HD13	1:A:555:LEU:H	1.59	0.68
1:A:479:ALA:HB2	1:A:504:VAL:HG12	1.76	0.68
1:A:483:CYS:SG	1:A:488:LEU:HD23	2.33	0.68
1:A:838:LYS:HB3	1:A:839:TYR:HD1	1.57	0.68
1:A:86:ARG:HG2	1:A:86:ARG:HH11	1.58	0.68
1:A:450:LEU:HD23	1:A:450:LEU:C	2.19	0.68
1:A:668:ARG:O	1:A:672:LYS:HG2	1.94	0.68
1:A:755:GLY:H	1:A:760:GLN:HG3	1.56	0.68
2:B:1:G:H2'	2:B:2:U:H6	1.58	0.68
1:A:130:ASP:OD2	1:A:132:ASP:HA	1.94	0.68
1:A:326:GLN:O	1:A:330:THR:HB	1.93	0.68
1:A:444:SER:HB2	2:B:29:G:C8	2.29	0.68
1:A:447:LEU:O	1:A:450:LEU:HD22	1.94	0.68
1:A:794:ALA:HB1	1:A:797:LEU:HB3	1.76	0.67
1:A:215:THR:OG1	1:A:402:HIS:HD2	1.77	0.67
1:A:1000:ARG:CZ	1:A:1065:VAL:HB	2.24	0.67
1:A:1085:ILE:CG2	1:A:1096:PHE:CE1	2.77	0.67
1:A:64:THR:HG22	1:A:65:ALA:CB	2.23	0.67
1:A:131:LYS:HD3	1:A:133:ALA:H	1.59	0.67
1:A:964:PHE:HD1	1:A:965:SER:HB3	1.58	0.67
1:A:48:LEU:HD23	1:A:48:LEU:N	2.10	0.67
1:A:994:ILE:HD12	1:A:994:ILE:H	1.59	0.67
1:A:785:ILE:HD12	1:A:785:ILE:N	2.03	0.67
1:A:865:ASN:HD22	1:A:867:LEU:H	1.43	0.67
1:A:737:VAL:HA	1:A:742:ARG:HH21	1.58	0.66
1:A:597:ARG:HB3	1:A:597:ARG:CZ	2.25	0.66
1:A:45:GLN:HG3	1:A:69:LYS:CD	2.25	0.66
1:A:601:PHE:CD2	1:A:611:VAL:HG21	2.30	0.66
1:A:213:VAL:CG1	1:A:217:ASP:HB2	2.24	0.66
1:A:591:LYS:N	1:A:592:PRO:HD2	2.10	0.66
1:A:731:ARG:HD3	1:A:735:LYS:NZ	2.11	0.66
1:A:453:ARG:CD	1:A:460:ALA:HB1	2.26	0.66
2:B:40:C:H2'	2:B:41:A:H8	1.59	0.66
1:A:339:PHE:CD1	1:A:342:LEU:HD12	2.25	0.66
1:A:1002:ASP:CG	1:A:1015:ARG:NH1	2.53	0.66
1:A:1011:VAL:HG11	1:A:1029:VAL:CG1	2.26	0.66
1:A:579:ILE:HG21	1:A:620:LEU:CD1	2.27	0.65
1:A:967:GLU:HA	1:A:1103:ARG:CZ	2.26	0.65
1:A:1001:CYS:HB3	1:A:1014:PRO:HA	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:CZ	1:A:52:SER:O	2.44	0.65
1:A:564:LEU:HD13	1:A:565:ARG:N	2.11	0.65
1:A:36:TYR:CD1	1:A:191:MSE:CE	2.79	0.65
1:A:131:LYS:HD3	1:A:132:ASP:N	2.11	0.65
2:B:40:C:H2'	2:B:41:A:C8	2.31	0.65
1:A:865:ASN:HD22	1:A:867:LEU:N	1.94	0.65
1:A:967:GLU:CA	1:A:1103:ARG:NH2	2.51	0.65
1:A:1062:GLU:C	1:A:1065:VAL:CG2	2.70	0.65
1:A:467:GLY:N	1:A:468:ALA:O	2.30	0.65
1:A:534:ARG:HG3	1:A:534:ARG:NH1	2.05	0.65
1:A:575:THR:CG2	1:A:621:LYS:CE	2.62	0.64
1:A:594:SER:HB2	1:A:597:ARG:O	1.97	0.64
1:A:968:GLU:HA	1:A:969:GLY:C	2.22	0.64
1:A:213:VAL:HG12	1:A:214:ARG:O	1.96	0.64
1:A:694:ASN:O	1:A:697:GLN:HG3	1.98	0.64
1:A:680:ALA:O	1:A:684:MSE:HE3	1.98	0.64
1:A:726:MSE:HE2	1:A:774:TRP:CE3	2.32	0.64
2:B:36:U:H4'	2:B:37:G:OP2	1.98	0.64
1:A:193:VAL:CG2	1:A:196:ASP:HB3	2.28	0.64
1:A:340:ALA:HB1	1:A:668:ARG:NH2	2.12	0.64
2:B:23:A:H2'	2:B:24:C:C6	2.30	0.64
1:A:215:THR:CG2	1:A:422:LYS:HZ1	2.11	0.64
1:A:339:PHE:HD1	1:A:342:LEU:CD1	2.10	0.63
1:A:670:TRP:NE1	1:A:703:HIS:CE1	2.66	0.63
1:A:407:LEU:CD2	1:A:410:GLU:OE1	2.45	0.63
1:A:902:ASP:HB3	1:A:905:THR:OG1	1.99	0.63
1:A:33:VAL:HG21	1:A:390:ILE:CD1	2.28	0.63
1:A:539:PHE:HB3	1:A:606:GLY:HA3	1.80	0.63
1:A:1101:ASN:O	1:A:1105:GLU:HB2	1.98	0.63
1:A:483:CYS:SG	1:A:488:LEU:HD22	2.36	0.63
1:A:994:ILE:HD12	1:A:994:ILE:N	2.13	0.63
1:A:53:PRO:HG3	1:A:60:GLU:OE2	1.99	0.63
1:A:450:LEU:HD23	1:A:450:LEU:O	1.98	0.63
1:A:458:PRO:O	1:A:459:ILE:HG23	1.99	0.63
1:A:515:ARG:NH2	1:A:517:GLU:OE1	2.30	0.63
1:A:64:THR:OG1	1:A:67:GLU:HG3	1.98	0.62
1:A:746:ARG:NH1	2:B:60:C:OP1	2.31	0.62
1:A:993:ASP:HB2	1:A:1020:ARG:HE	1.64	0.62
1:A:586:ARG:HA	1:A:609:ASN:O	1.99	0.62
1:A:528:LEU:C	1:A:529:VAL:HG23	2.24	0.62
1:A:803:HIS:HB3	2:B:31:G:O2'	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:G:H2'	2:B:32:C:H6	1.65	0.62
2:B:9:G:C2	2:B:10:A:C6	2.87	0.62
1:A:296:LEU:H	1:A:334:GLY:HA3	1.65	0.62
1:A:479:ALA:HB1	1:A:502:LEU:HD22	1.80	0.62
1:A:86:ARG:HH11	1:A:86:ARG:CG	2.12	0.61
2:B:50:G:H8	2:B:50:G:C5'	2.09	0.61
1:A:208:ARG:O	1:A:209:LYS:HB2	2.00	0.61
1:A:330:THR:HA	1:A:331:ARG:C	2.24	0.61
1:A:968:GLU:OE2	1:A:1107:TYR:CD2	2.53	0.61
1:A:418:ILE:HD13	1:A:502:LEU:HD12	1.83	0.61
1:A:486:ASP:OD1	1:A:486:ASP:N	2.33	0.61
1:A:838:LYS:HB3	1:A:839:TYR:CE1	2.35	0.61
1:A:897:PHE:CE2	1:A:1078:MSE:HE1	2.35	0.61
2:B:9:G:C2	2:B:10:A:N7	2.69	0.61
1:A:426:VAL:HG12	1:A:431:ALA:CB	2.31	0.61
1:A:953:PRO:HD2	1:A:953:PRO:O	2.01	0.61
2:B:59:C:H2'	2:B:60:C:H6	1.66	0.61
1:A:912:CYS:O	1:A:959:ILE:HG13	2.01	0.60
2:B:1:G:C4	2:B:2:U:C5	2.89	0.60
1:A:619:LEU:HD21	1:A:978:LEU:HD23	1.82	0.60
2:B:5:A:HO2'	2:B:6:G:P	2.21	0.60
1:A:670:TRP:HE1	1:A:703:HIS:CE1	2.19	0.60
2:B:1:G:H2'	2:B:2:U:C6	2.35	0.60
1:A:624:GLY:HA3	1:A:754:GLY:O	2.02	0.60
1:A:1085:ILE:CG2	1:A:1096:PHE:HE1	2.13	0.60
1:A:43:LEU:HD13	1:A:43:LEU:C	2.26	0.60
1:A:215:THR:OG1	1:A:402:HIS:CD2	2.54	0.60
1:A:568:SER:OG	1:A:580:SER:HB3	2.02	0.59
1:A:396:LYS:H	1:A:396:LYS:CD	2.14	0.59
1:A:865:ASN:HD21	1:A:867:LEU:CB	2.14	0.59
2:B:23:A:O5'	2:B:23:A:H8	1.85	0.59
1:A:838:LYS:CD	1:A:839:TYR:CE1	2.85	0.59
1:A:407:LEU:HD23	1:A:410:GLU:OE1	2.01	0.59
1:A:838:LYS:HD2	1:A:839:TYR:HE1	1.67	0.59
1:A:838:LYS:CG	1:A:839:TYR:CE1	2.85	0.59
1:A:983:ASN:O	1:A:987:ARG:HG3	2.02	0.59
2:B:9:G:N2	2:B:10:A:C4	2.70	0.59
1:A:695:GLU:CG	1:A:718:SER:OG	2.50	0.59
1:A:812:LEU:HD13	1:A:875:VAL:HG21	1.85	0.59
2:B:33:C:OP2	2:B:35:A:O2'	2.18	0.59
2:B:43:U:C2	2:B:50:G:N2	2.69	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PHE:O	1:A:260:GLN:HG2	2.02	0.59
1:A:614:HIS:ND1	2:B:6:G:OP1	2.35	0.59
1:A:991:ASP:O	1:A:1020:ARG:NH2	2.36	0.59
1:A:993:ASP:O	1:A:996:GLN:HG3	2.02	0.59
1:A:1085:ILE:HG22	1:A:1096:PHE:HE1	1.68	0.59
1:A:315:PHE:CE1	1:A:319:ASP:HB2	2.37	0.59
1:A:958:GLU:O	1:A:976:ALA:HB2	2.03	0.59
1:A:371:LEU:HD12	1:A:372:ASN:H	1.65	0.59
1:A:458:PRO:O	1:A:459:ILE:HG12	2.02	0.59
1:A:775:SER:OG	2:B:48:A:H8	1.85	0.59
1:A:901:PHE:CE2	1:A:908:PRO:HG3	2.38	0.59
1:A:258:VAL:HG12	1:A:258:VAL:O	2.01	0.58
2:B:9:G:C2'	2:B:10:A:H8	2.14	0.58
2:B:92:G:H2'	2:B:93:A:O4'	2.02	0.58
2:B:60:C:H2'	2:B:61:C:H6	1.67	0.58
1:A:528:LEU:C	1:A:529:VAL:CG2	2.77	0.58
1:A:11:ARG:HH11	1:A:11:ARG:CG	2.14	0.58
1:A:655:LEU:O	1:A:658:CYS:HB2	2.04	0.58
1:A:994:ILE:H	1:A:994:ILE:CD1	2.16	0.58
1:A:386:THR:HG22	1:A:488:LEU:O	2.04	0.58
1:A:839:TYR:OH	2:B:8:G:OP1	2.12	0.58
1:A:208:ARG:HG2	1:A:209:LYS:N	2.18	0.57
1:A:705:ILE:N	1:A:705:ILE:HD13	2.19	0.57
1:A:648:GLN:OE1	1:A:685:THR:HB	2.05	0.57
1:A:952:ILE:N	1:A:953:PRO:HD3	2.18	0.57
1:A:175:THR:O	1:A:178:VAL:N	2.36	0.57
1:A:1062:GLU:O	1:A:1065:VAL:HG23	2.04	0.57
1:A:215:THR:HG21	1:A:422:LYS:HZ1	1.66	0.57
1:A:305:LYS:HD3	1:A:321:GLU:HG3	1.87	0.57
1:A:743:PRO:HG2	2:B:34:A:C5	2.40	0.57
1:A:865:ASN:HD22	1:A:865:ASN:C	2.12	0.57
2:B:9:G:C2	2:B:10:A:C4	2.93	0.57
1:A:200:SER:OG	1:A:202:VAL:HG12	2.05	0.57
1:A:266:LEU:HD21	1:A:346:GLU:HG3	1.85	0.57
1:A:303:PHE:CD2	1:A:350:LEU:CB	2.88	0.57
1:A:830:ARG:H	1:A:832:LYS:N	2.01	0.57
1:A:85:HIS:HE1	1:A:88:PRO:O	1.88	0.57
1:A:913:ARG:HA	1:A:953:PRO:O	2.04	0.57
1:A:964:PHE:C	1:A:966:ALA:HA	2.29	0.57
1:A:665:ARG:HH11	1:A:665:ARG:CG	2.15	0.57
1:A:775:SER:OG	2:B:48:A:H1'	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:LEU:CG	1:A:952:ILE:HG13	2.33	0.57
1:A:225:ILE:O	1:A:229:MSE:HG3	2.05	0.56
1:A:244:LYS:HG3	1:A:248:GLN:OE1	2.05	0.56
1:A:1019:LYS:HB3	1:A:1022:ALA:HB3	1.86	0.56
2:B:49:G:O2'	2:B:50:G:OP1	2.19	0.56
1:A:117:ALA:CB	1:A:226:GLU:HG3	2.34	0.56
1:A:208:ARG:HG2	1:A:209:LYS:H	1.70	0.56
1:A:587:LYS:N	1:A:609:ASN:O	2.36	0.56
1:A:665:ARG:HB3	1:A:665:ARG:NH1	2.06	0.56
1:A:775:SER:CB	1:A:793:PHE:HZ	2.17	0.56
1:A:775:SER:CB	2:B:48:A:H8	2.19	0.56
1:A:910:ILE:HD11	1:A:1104:ILE:HB	1.86	0.56
1:A:973:GLN:O	2:B:4:U:H5'	2.06	0.56
1:A:203:GLU:HB3	1:A:432:ARG:HA	1.87	0.56
1:A:413:GLU:O	1:A:414:ARG:HB2	2.05	0.56
1:A:660:SER:HB2	1:A:661:GLU:O	2.05	0.56
1:A:965:SER:N	1:A:966:ALA:HA	2.20	0.56
2:B:4:U:HO2'	2:B:5:A:P	2.29	0.56
1:A:539:PHE:HA	1:A:542:LEU:CD1	2.35	0.56
1:A:661:GLU:HG2	1:A:662:ASP:N	2.20	0.56
1:A:754:GLY:CA	1:A:760:GLN:HG3	2.35	0.56
1:A:838:LYS:CB	1:A:839:TYR:CD1	2.87	0.56
1:A:193:VAL:O	1:A:193:VAL:CG2	2.54	0.56
2:B:87:G:O2'	2:B:88:G:OP2	2.19	0.56
1:A:323:LYS:HE3	1:A:672:LYS:HE2	1.86	0.56
1:A:685:THR:HG21	1:A:729:GLN:NE2	2.21	0.56
2:B:11:C:O2'	2:B:12:A:C5'	2.51	0.56
1:A:36:TYR:CE1	1:A:191:MSE:CE	2.89	0.56
1:A:39:TRP:O	1:A:43:LEU:N	2.38	0.55
1:A:402:HIS:CD2	1:A:402:HIS:N	2.75	0.55
1:A:528:LEU:O	1:A:529:VAL:CG2	2.54	0.55
1:A:839:TYR:CD1	1:A:839:TYR:N	2.73	0.55
1:A:893:MSE:O	1:A:894:TYR:C	2.44	0.55
1:A:44:ARG:NH2	1:A:232:GLU:OE2	2.39	0.55
1:A:737:VAL:O	1:A:742:ARG:NH2	2.39	0.55
1:A:131:LYS:HA	1:A:131:LYS:CE	2.25	0.55
1:A:570:ASP:CG	1:A:859:ARG:HH22	2.15	0.55
1:A:1000:ARG:HH11	1:A:1000:ARG:HB3	1.72	0.55
1:A:18:ILE:O	1:A:21:GLY:N	2.40	0.55
1:A:234:TRP:CE3	1:A:378:ALA:HB1	2.42	0.55
1:A:120:ILE:HD12	1:A:229:MSE:CE	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:TYR:O	1:A:351:TRP:N	2.31	0.55
2:B:59:C:H2'	2:B:60:C:C6	2.42	0.55
1:A:219:ASP:O	1:A:223:GLN:HG3	2.06	0.55
1:A:344:GLU:C	1:A:346:GLU:H	2.14	0.55
1:A:602:PHE:CE2	1:A:986:GLN:HB2	2.41	0.55
1:A:45:GLN:HG2	1:A:69:LYS:CD	2.29	0.55
1:A:418:ILE:CD1	1:A:502:LEU:HD12	2.37	0.55
1:A:315:PHE:CD1	1:A:315:PHE:C	2.85	0.54
1:A:775:SER:OG	2:B:48:A:C8	2.59	0.54
1:A:865:ASN:HD21	1:A:867:LEU:HB3	1.73	0.54
1:A:660:SER:CB	1:A:661:GLU:CA	2.85	0.54
1:A:36:TYR:HD1	1:A:191:MSE:CE	2.16	0.54
1:A:49:TYR:CD1	1:A:380:PHE:HD2	2.23	0.54
1:A:105:LEU:HD22	1:A:175:THR:HG22	1.90	0.54
1:A:330:THR:OG1	1:A:331:ARG:HA	2.08	0.54
2:B:31:G:C2'	2:B:32:C:O5'	2.55	0.54
1:A:208:ARG:HG3	1:A:208:ARG:NH1	2.21	0.54
1:A:347:TYR:O	1:A:351:TRP:CB	2.56	0.54
1:A:670:TRP:O	1:A:674:ILE:HG13	2.07	0.54
1:A:754:GLY:HA3	1:A:760:GLN:HG2	1.87	0.54
1:A:63:LYS:HE2	1:A:71:GLU:OE1	2.07	0.54
1:A:904:ARG:HH11	1:A:904:ARG:CG	2.11	0.54
1:A:1006:VAL:HG23	1:A:1007:ASP:N	2.22	0.54
1:A:964:PHE:C	1:A:964:PHE:CD1	2.85	0.54
1:A:1086:ASN:HB2	1:A:1099:MSE:HE1	1.89	0.54
2:B:60:C:H2'	2:B:61:C:C6	2.42	0.54
1:A:260:GLN:HG3	1:A:260:GLN:O	2.08	0.53
1:A:339:PHE:O	1:A:342:LEU:HB2	2.08	0.53
1:A:483:CYS:SG	1:A:488:LEU:HD21	2.48	0.53
1:A:597:ARG:CZ	1:A:597:ARG:CB	2.86	0.53
1:A:670:TRP:CH2	1:A:674:ILE:CG2	2.89	0.53
1:A:1000:ARG:NH2	1:A:1065:VAL:HB	2.23	0.53
1:A:973:GLN:C	1:A:974:ILE:HG13	2.33	0.53
1:A:617:SER:HB3	1:A:978:LEU:HD13	1.89	0.53
2:B:50:G:C8	2:B:50:G:C5'	2.88	0.53
1:A:310:ALA:O	1:A:313:ALA:HB3	2.09	0.53
1:A:353:GLU:HA	1:A:354:ASP:C	2.32	0.53
1:A:681:ALA:HA	1:A:689:ARG:HD2	1.91	0.53
1:A:905:THR:CB	1:A:906:GLY:HA2	2.37	0.53
1:A:951:LEU:CD1	1:A:952:ILE:HG13	2.38	0.53
1:A:809:LEU:HD23	1:A:870:TRP:CH2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:ARG:HG3	1:A:914:ARG:N	2.23	0.53
1:A:1019:LYS:HA	1:A:1022:ALA:H	1.73	0.53
1:A:354:ASP:HB3	1:A:356:SER:OG	2.08	0.53
1:A:533:HIS:O	1:A:892:THR:HG23	2.08	0.53
1:A:534:ARG:HH12	1:A:893:MSE:HE2	1.73	0.53
1:A:339:PHE:HA	1:A:342:LEU:CD1	2.38	0.53
1:A:528:LEU:O	1:A:529:VAL:HG22	2.09	0.53
1:A:52:SER:HB3	1:A:59:GLN:HG2	1.89	0.53
1:A:1011:VAL:HB	1:A:1029:VAL:HG13	1.91	0.53
1:A:221:PHE:CE2	1:A:225:ILE:HD11	2.43	0.52
1:A:344:GLU:CB	1:A:345:PRO:HD2	2.38	0.52
1:A:591:LYS:N	1:A:592:PRO:CD	2.72	0.52
1:A:830:ARG:N	1:A:831:GLY:CA	2.73	0.52
1:A:41:SER:HB2	1:A:49:TYR:CZ	2.44	0.52
1:A:46:GLU:CB	1:A:47:ASN:ND2	2.73	0.52
1:A:131:LYS:HE2	1:A:132:ASP:H	1.74	0.52
1:A:821:LEU:HB3	1:A:823:TYR:CE2	2.43	0.52
1:A:972:HIS:NE2	2:B:4:U:H5'	2.24	0.52
2:B:49:G:C2'	2:B:50:G:OP1	2.57	0.52
1:A:48:LEU:N	1:A:48:LEU:CD2	2.73	0.52
1:A:674:ILE:HG22	1:A:696:LEU:CD1	2.39	0.52
1:A:1005:GLU:O	1:A:1005:GLU:HG3	2.08	0.52
2:B:49:G:H2'	2:B:50:G:O4'	2.09	0.52
1:A:534:ARG:NH1	1:A:534:ARG:CG	2.73	0.52
1:A:851:SER:CB	1:A:852:GLU:HA	2.39	0.52
1:A:262:HIS:HE1	1:A:263:LEU:HG	1.75	0.52
1:A:660:SER:HG	1:A:661:GLU:HA	1.75	0.52
1:A:248:GLN:CB	1:A:1060:GLU:OE2	2.52	0.52
1:A:299:SER:O	1:A:303:PHE:HB2	2.09	0.52
1:A:423:LEU:HB3	1:A:437:VAL:HG21	1.91	0.52
1:A:564:LEU:HD13	1:A:564:LEU:C	2.34	0.52
1:A:682:ASN:CB	1:A:683:HIS:CE1	2.90	0.52
1:A:715:VAL:O	1:A:716:TYR:C	2.53	0.52
1:A:815:ARG:NH2	2:B:8:G:O6	2.43	0.52
1:A:965:SER:O	1:A:965:SER:OG	2.28	0.52
2:B:92:G:H4'	2:B:92:G:OP2	2.10	0.52
1:A:913:ARG:CB	1:A:953:PRO:CD	2.70	0.51
1:A:1107:TYR:CD1	1:A:1107:TYR:C	2.86	0.51
2:B:39:C:H2'	2:B:40:C:C6	2.45	0.51
1:A:555:LEU:HA	1:A:840:PRO:HA	1.92	0.51
1:A:964:PHE:CE2	1:A:970:ASP:CB	2.84	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASP:C	1:A:92:ASP:OD1	2.52	0.51
1:A:405:THR:HA	3:A:1202:HOH:O	2.10	0.51
1:A:623:PRO:HD2	1:A:756:ASN:HD22	1.76	0.51
1:A:660:SER:CB	1:A:661:GLU:HA	2.40	0.51
1:A:829:GLU:HB2	1:A:831:GLY:HA3	1.91	0.51
1:A:1061:ALA:O	1:A:1065:VAL:CG1	2.56	0.51
1:A:993:ASP:HB2	1:A:1020:ARG:NE	2.25	0.51
1:A:1002:ASP:CG	1:A:1015:ARG:HH11	2.19	0.51
1:A:86:ARG:CG	1:A:86:ARG:NH1	2.73	0.51
1:A:665:ARG:CG	1:A:665:ARG:NH1	2.73	0.51
1:A:830:ARG:N	1:A:831:GLY:HA3	2.25	0.51
1:A:964:PHE:CD1	1:A:965:SER:HB3	2.44	0.51
1:A:59:GLN:HE21	1:A:379:THR:HG23	1.71	0.51
1:A:552:ASP:HB2	1:A:562:SER:HB2	1.92	0.51
1:A:674:ILE:HD13	1:A:675:GLU:HB2	1.92	0.51
1:A:654:LEU:O	1:A:657:ARG:HB2	2.11	0.51
1:A:827:LEU:CG	1:A:830:ARG:HG2	2.40	0.51
1:A:896:ALA:H	1:A:987:ARG:HH12	1.57	0.51
2:B:9:G:N1	2:B:10:A:N6	2.55	0.51
1:A:19:ARG:NH1	1:A:498:ARG:O	2.44	0.50
1:A:670:TRP:CZ3	1:A:674:ILE:HG23	2.46	0.50
1:A:858:ASP:CG	1:A:897:PHE:H	2.19	0.50
1:A:174:ARG:NH1	1:A:177:ASP:OD2	2.45	0.50
1:A:394:PHE:CD1	1:A:402:HIS:HB2	2.46	0.50
1:A:818:MSE:HG2	1:A:835:TRP:CZ2	2.47	0.50
1:A:485:ARG:HH11	1:A:485:ARG:CG	2.13	0.50
1:A:830:ARG:HD2	1:A:830:ARG:O	2.11	0.50
1:A:851:SER:HB3	1:A:852:GLU:HA	1.94	0.50
1:A:1020:ARG:HH11	1:A:1020:ARG:CG	2.13	0.50
1:A:515:ARG:HE	1:A:517:GLU:CD	2.19	0.50
1:A:1036:VAL:HG13	1:A:1095:GLU:HG2	1.93	0.50
1:A:25:LEU:O	1:A:29:VAL:HG23	2.11	0.50
1:A:225:ILE:CG2	1:A:229:MSE:HE3	2.41	0.50
1:A:726:MSE:HB3	1:A:774:TRP:CH2	2.47	0.50
1:A:902:ASP:OD1	1:A:903:ALA:N	2.44	0.50
1:A:907:ALA:HB2	1:A:1084:ILE:HD12	1.93	0.50
1:A:912:CYS:O	1:A:959:ILE:N	2.39	0.50
1:A:1034:THR:HB	1:A:1036:VAL:H	1.76	0.50
1:A:190:LEU:HB3	1:A:191:MSE:HG3	1.94	0.50
1:A:348:GLN:HA	1:A:351:TRP:HB3	1.94	0.50
1:A:451:LEU:O	1:A:462:TYR:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:SER:OG	1:A:202:VAL:CG1	2.60	0.50
1:A:384:ASP:HB3	1:A:388:HIS:H	1.76	0.50
1:A:45:GLN:HG3	1:A:96:LEU:HD13	1.93	0.50
1:A:490:HIS:ND1	1:A:490:HIS:O	2.45	0.50
1:A:830:ARG:N	1:A:832:LYS:N	2.60	0.50
1:A:296:LEU:HG	1:A:296:LEU:O	2.11	0.49
1:A:459:ILE:HA	1:A:476:PHE:HD2	1.75	0.49
1:A:656:VAL:HG21	1:A:777:PHE:CE1	2.47	0.49
1:A:836:VAL:O	1:A:836:VAL:HG23	2.11	0.49
1:A:865:ASN:ND2	1:A:867:LEU:CB	2.75	0.49
1:A:453:ARG:HB3	1:A:462:TYR:CE1	2.47	0.49
1:A:911:ARG:C	1:A:912:CYS:SG	2.95	0.49
1:A:1085:ILE:HG23	1:A:1099:MSE:CE	2.42	0.49
1:A:23:TRP:CH2	1:A:491:MSE:HB2	2.47	0.49
1:A:128:LEU:O	1:A:190:LEU:N	2.46	0.49
1:A:564:LEU:C	1:A:564:LEU:CD1	2.85	0.49
1:A:120:ILE:HD12	1:A:229:MSE:HE1	1.94	0.49
1:A:131:LYS:HD3	1:A:131:LYS:C	2.37	0.49
1:A:442:SER:HB3	2:B:29:G:H5''	1.94	0.49
1:A:453:ARG:CG	1:A:460:ALA:CB	2.88	0.49
1:A:662:ASP:O	1:A:665:ARG:HG2	2.12	0.49
1:A:846:LEU:HD22	1:A:893:MSE:HB2	1.94	0.49
1:A:959:ILE:HG13	1:A:959:ILE:O	2.11	0.49
2:B:48:A:N3	2:B:48:A:H5'	2.27	0.49
2:B:92:G:H2'	2:B:93:A:O5'	2.13	0.49
1:A:46:GLU:CB	1:A:47:ASN:CG	2.86	0.49
1:A:131:LYS:CE	1:A:132:ASP:N	2.73	0.49
1:A:555:LEU:C	1:A:555:LEU:CD2	2.85	0.49
1:A:579:ILE:CG2	1:A:620:LEU:CD1	2.90	0.49
1:A:129:ALA:HB1	1:A:193:VAL:HG12	1.95	0.49
1:A:193:VAL:HG23	1:A:196:ASP:HB3	1.94	0.49
1:A:257:PHE:N	1:A:257:PHE:CD1	2.81	0.49
1:A:1113:ARG:NH1	1:A:1113:ARG:HG3	2.27	0.49
1:A:11:ARG:HB3	1:A:11:ARG:NH1	2.07	0.49
1:A:11:ARG:CG	1:A:11:ARG:NH1	2.73	0.49
1:A:315:PHE:O	1:A:318:TYR:HB2	2.13	0.49
1:A:344:GLU:CB	1:A:345:PRO:CD	2.91	0.49
1:A:731:ARG:HD3	1:A:735:LYS:CE	2.42	0.49
2:B:92:G:C2'	2:B:93:A:O5'	2.61	0.49
1:A:326:GLN:O	1:A:330:THR:N	2.46	0.48
1:A:458:PRO:C	1:A:459:ILE:CG2	2.85	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:LYS:HB2	1:A:1094:LYS:HZ1	1.76	0.48
2:B:8:G:C2'	2:B:9:G:H5''	2.43	0.48
1:A:41:SER:HB2	1:A:49:TYR:CE2	2.48	0.48
1:A:601:PHE:HD2	1:A:611:VAL:HG21	1.73	0.48
2:B:39:C:H2'	2:B:40:C:H6	1.77	0.48
1:A:451:LEU:O	1:A:461:LEU:HA	2.13	0.48
1:A:479:ALA:HB1	1:A:502:LEU:CD2	2.43	0.48
1:A:656:VAL:HG21	1:A:777:PHE:HE1	1.78	0.48
1:A:697:GLN:HG3	1:A:698:LYS:N	2.28	0.48
1:A:98:LEU:HD11	1:A:178:VAL:HG13	1.96	0.48
1:A:262:HIS:ND1	1:A:263:LEU:N	2.60	0.48
1:A:830:ARG:CA	1:A:831:GLY:C	2.85	0.48
1:A:747:GLY:HA2	2:B:88:G:O4'	2.13	0.48
1:A:838:LYS:NZ	1:A:838:LYS:CB	2.73	0.48
1:A:194:TYR:O	1:A:197:SER:HB3	2.14	0.48
1:A:531:ASP:HA	1:A:533:HIS:HD2	1.79	0.48
1:A:731:ARG:HD3	1:A:735:LYS:HE3	1.95	0.48
1:A:865:ASN:ND2	1:A:867:LEU:H	2.09	0.48
2:B:31:G:H2'	2:B:32:C:C6	2.46	0.48
1:A:208:ARG:O	1:A:211:GLN:HG2	2.13	0.48
1:A:262:HIS:CG	1:A:263:LEU:N	2.82	0.48
1:A:550:PRO:O	1:A:562:SER:O	2.31	0.48
1:A:673:LEU:HD11	1:A:692:PHE:CE2	2.49	0.48
1:A:677:PRO:O	1:A:678:VAL:HG23	2.04	0.48
1:A:805:LYS:HG2	1:A:870:TRP:CH2	2.49	0.48
1:A:865:ASN:ND2	1:A:867:LEU:N	2.60	0.48
1:A:827:LEU:HD12	1:A:830:ARG:HD3	1.96	0.48
1:A:973:GLN:HB2	2:B:3:C:O2'	2.14	0.48
1:A:1019:LYS:HA	1:A:1020:ARG:C	2.39	0.48
2:B:9:G:N1	2:B:10:A:C5	2.75	0.48
1:A:256:ASN:HD22	1:A:360:ARG:HD2	1.77	0.48
1:A:131:LYS:CD	1:A:132:ASP:N	2.77	0.47
1:A:295:ALA:O	1:A:296:LEU:CD2	2.62	0.47
1:A:617:SER:HB3	1:A:978:LEU:HD11	1.95	0.47
2:B:31:G:O2'	2:B:32:C:P	2.72	0.47
1:A:174:ARG:CZ	1:A:177:ASP:OD2	2.62	0.47
1:A:501:TYR:CD1	1:A:501:TYR:N	2.82	0.47
1:A:827:LEU:HD23	1:A:828:ASP:H	1.80	0.47
1:A:303:PHE:HE2	1:A:350:LEU:CB	2.20	0.47
1:A:211:GLN:O	1:A:211:GLN:HG3	2.14	0.47
1:A:1032:THR:HG23	1:A:1038:TYR:CG	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD21	1:A:346:GLU:CG	2.44	0.47
1:A:564:LEU:HA	1:A:843:GLN:OE1	2.14	0.47
1:A:1061:ALA:O	1:A:1065:VAL:HG22	2.14	0.47
2:B:47:C:C2'	2:B:48:A:C5'	2.80	0.47
1:A:312:ASP:OD1	1:A:312:ASP:N	2.47	0.47
1:A:394:PHE:HD1	1:A:402:HIS:HB2	1.78	0.47
1:A:407:LEU:HD22	1:A:410:GLU:CD	2.39	0.47
1:A:614:HIS:CE1	2:B:6:G:OP1	2.67	0.47
1:A:683:HIS:ND1	1:A:683:HIS:N	2.62	0.47
1:A:898:SER:O	1:A:980:ALA:HA	2.15	0.47
1:A:195:THR:HG22	1:A:204:TRP:CZ2	2.50	0.47
1:A:515:ARG:HB2	1:A:517:GLU:HG3	1.96	0.47
1:A:581:VAL:HG21	1:A:616:ARG:NE	2.27	0.47
1:A:827:LEU:HD23	1:A:828:ASP:N	2.30	0.47
1:A:85:HIS:CE1	1:A:88:PRO:O	2.67	0.47
1:A:818:MSE:HG2	1:A:835:TRP:CH2	2.50	0.47
1:A:953:PRO:CD	1:A:953:PRO:O	2.63	0.47
1:A:12:LEU:CD1	1:A:19:ARG:HA	2.44	0.46
1:A:556:GLY:O	1:A:841:PRO:HD3	2.15	0.46
1:A:579:ILE:CG2	1:A:620:LEU:HG	2.45	0.46
1:A:908:PRO:HG2	1:A:1096:PHE:CZ	2.50	0.46
1:A:1036:VAL:CG1	1:A:1095:GLU:HG2	2.45	0.46
2:B:9:G:C6	2:B:10:A:C6	2.96	0.46
1:A:79:ARG:HA	1:A:79:ARG:HD2	1.66	0.46
1:A:838:LYS:HG2	1:A:839:TYR:CE1	2.51	0.46
2:B:92:G:O2'	2:B:93:A:P	2.73	0.46
1:A:106:LEU:HD13	1:A:106:LEU:HA	1.80	0.46
1:A:257:PHE:N	1:A:257:PHE:HD1	2.14	0.46
1:A:660:SER:CB	1:A:661:GLU:C	2.85	0.46
1:A:851:SER:CB	1:A:852:GLU:CA	2.94	0.46
1:A:855:PHE:CE2	1:A:998:ARG:CZ	2.98	0.46
1:A:426:VAL:HG12	1:A:431:ALA:HA	1.98	0.46
1:A:659:GLY:C	1:A:660:SER:HG	2.16	0.46
1:A:246:VAL:O	1:A:250:ASN:HB2	2.16	0.46
1:A:490:HIS:ND1	1:A:490:HIS:C	2.73	0.46
1:A:674:ILE:CD1	1:A:675:GLU:N	2.73	0.46
1:A:728:LYS:O	1:A:732:ASP:CG	2.59	0.46
1:A:579:ILE:HG23	1:A:620:LEU:HG	1.97	0.46
1:A:587:LYS:HB3	1:A:587:LYS:HE2	1.78	0.46
1:A:775:SER:OG	1:A:793:PHE:HZ	1.99	0.46
2:B:9:G:HO2'	2:B:10:A:C5'	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:GLU:CA	1:A:969:GLY:C	2.89	0.46
1:A:1032:THR:HG23	1:A:1038:TYR:CE2	2.51	0.46
1:A:1073:LYS:HA	1:A:1073:LYS:CE	2.09	0.46
1:A:77:ARG:NH1	1:A:80:GLN:OE1	2.49	0.45
1:A:333:PHE:CE1	1:A:339:PHE:CE2	3.03	0.45
1:A:367:ILE:HA	1:A:370:LYS:HE3	1.98	0.45
1:A:952:ILE:O	1:A:952:ILE:HG22	2.17	0.45
2:B:48:A:C2'	2:B:49:G:O5'	2.64	0.45
1:A:193:VAL:HG21	1:A:196:ASP:HB3	1.98	0.45
1:A:251:ARG:O	1:A:254:GLN:N	2.49	0.45
1:A:263:LEU:HD21	1:A:349:ALA:HA	1.98	0.45
1:A:663:VAL:CG1	1:A:664:GLY:H	2.21	0.45
1:A:962:SER:HA	1:A:963:PRO:HD3	1.79	0.45
1:A:1019:LYS:HA	1:A:1021:THR:N	2.30	0.45
2:B:5:A:O2'	2:B:6:G:P	2.71	0.45
1:A:208:ARG:CG	1:A:209:LYS:H	2.30	0.45
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.84	0.45
1:A:473:THR:HG23	3:A:1217:HOH:O	2.16	0.45
1:A:479:ALA:HA	1:A:503:ASN:O	2.16	0.45
1:A:555:LEU:C	1:A:555:LEU:HD22	2.42	0.45
1:A:632:ARG:NH1	1:A:635:ARG:HD2	2.32	0.45
2:B:7:A:O2'	2:B:9:G:H5'	2.16	0.45
2:B:42:C:C2	2:B:43:U:C5	3.05	0.45
1:A:654:LEU:HA	1:A:657:ARG:HG3	1.98	0.45
1:A:957:GLY:HA2	1:A:958:GLU:HA	1.79	0.45
1:A:215:THR:O	1:A:218:ARG:HB2	2.17	0.45
1:A:446:GLN:O	1:A:449:ASN:HB2	2.17	0.45
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.82	0.45
1:A:1011:VAL:HG11	1:A:1029:VAL:HG11	1.96	0.45
1:A:663:VAL:HG12	1:A:664:GLY:N	2.20	0.45
1:A:905:THR:N	1:A:906:GLY:HA2	2.31	0.45
1:A:913:ARG:CG	1:A:914:ARG:N	2.79	0.45
1:A:12:LEU:HD12	1:A:22:LEU:HD12	1.99	0.45
1:A:174:ARG:CZ	1:A:177:ASP:CG	2.89	0.45
1:A:375:LYS:HA	1:A:375:LYS:HD3	1.69	0.45
1:A:504:VAL:HG23	1:A:504:VAL:O	2.17	0.45
1:A:911:ARG:C	1:A:912:CYS:HG	2.25	0.45
1:A:315:PHE:CE1	1:A:319:ASP:OD2	2.70	0.45
1:A:418:ILE:HD13	1:A:502:LEU:CD1	2.45	0.45
1:A:594:SER:HB3	1:A:599:PRO:HD3	1.98	0.45
1:A:964:PHE:CD1	1:A:964:PHE:O	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:NZ	2:B:94:G:OP1	2.50	0.44
1:A:12:LEU:HD22	1:A:15:MSE:CG	2.42	0.44
1:A:459:ILE:O	1:A:459:ILE:HG13	2.17	0.44
1:A:662:ASP:OD1	1:A:663:VAL:O	2.35	0.44
1:A:305:LYS:CD	1:A:321:GLU:HG3	2.47	0.44
1:A:1015:ARG:NH2	1:A:1065:VAL:HG12	2.32	0.44
1:A:1030:PHE:HE2	1:A:1090:TRP:CD1	2.35	0.44
1:A:1113:ARG:HH11	1:A:1113:ARG:CG	2.29	0.44
1:A:422:LYS:HB2	1:A:422:LYS:HE3	1.81	0.44
1:A:424:LEU:C	1:A:424:LEU:HD23	2.42	0.44
1:A:799:GLU:O	1:A:800:HIS:C	2.61	0.44
1:A:960:PHE:CE2	1:A:962:SER:HB3	2.53	0.44
1:A:1002:ASP:OD2	1:A:1015:ARG:NH1	2.51	0.44
2:B:50:G:C5	2:B:51:U:C5	3.05	0.44
1:A:119:GLN:O	1:A:123:LYS:HG2	2.17	0.44
1:A:339:PHE:CD1	1:A:342:LEU:CD1	2.93	0.44
1:A:407:LEU:HD22	1:A:410:GLU:OE1	2.16	0.44
1:A:676:GLN:HA	1:A:677:PRO:HA	1.82	0.44
1:A:326:GLN:O	1:A:330:THR:CB	2.63	0.44
1:A:344:GLU:C	1:A:346:GLU:N	2.76	0.44
1:A:512:SER:HB2	1:A:515:ARG:NH2	2.32	0.44
1:A:619:LEU:HD12	2:B:10:A:C5'	2.44	0.44
1:A:628:SER:HB3	1:A:631:LEU:HB2	1.99	0.44
1:A:972:HIS:CE1	2:B:4:U:C5'	3.01	0.44
1:A:894:TYR:CE2	1:A:896:ALA:HB2	2.52	0.44
1:A:1084:ILE:HG22	1:A:1085:ILE:HD12	1.99	0.44
1:A:419:ARG:HA	1:A:437:VAL:O	2.18	0.44
1:A:451:LEU:O	1:A:461:LEU:HB2	2.18	0.44
1:A:590:LEU:O	1:A:593:ASN:N	2.50	0.44
1:A:1107:TYR:CD1	1:A:1107:TYR:O	2.70	0.44
1:A:5:SER:HB3	2:B:92:G:H1'	1.99	0.44
1:A:256:ASN:C	1:A:257:PHE:HD1	2.26	0.44
1:A:627:GLU:OE1	1:A:628:SER:N	2.51	0.44
1:A:965:SER:N	1:A:966:ALA:CA	2.81	0.44
2:B:43:U:O5'	2:B:43:U:H6	2.01	0.44
1:A:45:GLN:CD	1:A:69:LYS:HD3	2.42	0.44
1:A:994:ILE:N	1:A:994:ILE:CD1	2.77	0.44
2:B:27:G:O2'	2:B:28:U:H5'	2.18	0.44
1:A:515:ARG:NE	1:A:517:GLU:OE1	2.51	0.43
1:A:670:TRP:NE1	1:A:703:HIS:ND1	2.65	0.43
1:A:812:LEU:HD13	1:A:875:VAL:CG2	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:ASN:C	1:A:865:ASN:ND2	2.73	0.43
1:A:731:ARG:HD3	1:A:735:LYS:HZ2	1.80	0.43
1:A:959:ILE:HA	1:A:976:ALA:HB2	2.00	0.43
1:A:15:MSE:H	1:A:15:MSE:HG2	1.57	0.43
1:A:219:ASP:OD1	1:A:393:ARG:NH1	2.51	0.43
1:A:380:PHE:CZ	1:A:382:LEU:CD2	3.01	0.43
1:A:830:ARG:HA	1:A:831:GLY:C	2.43	0.43
1:A:130:ASP:C	1:A:189:PRO:HB3	2.44	0.43
1:A:323:LYS:CE	1:A:672:LYS:HE2	2.48	0.43
1:A:567:MSE:SE	1:A:579:ILE:HG13	2.68	0.43
1:A:587:LYS:CE	1:A:608:ASP:O	2.66	0.43
1:A:838:LYS:CB	1:A:839:TYR:CE1	3.00	0.43
1:A:50:ARG:HA	1:A:61:CYS:HA	1.99	0.43
1:A:203:GLU:OE2	1:A:432:ARG:HD2	2.17	0.43
1:A:400:ASN:O	1:A:401:LEU:HB2	2.18	0.43
1:A:1107:TYR:O	1:A:1107:TYR:HD1	2.00	0.43
1:A:531:ASP:HA	1:A:533:HIS:CD2	2.54	0.43
1:A:972:HIS:HE2	2:B:4:U:H3'	1.84	0.43
1:A:1113:ARG:HB3	1:A:1114:SER:H	1.43	0.43
1:A:814:ASP:O	1:A:818:MSE:HB2	2.19	0.43
1:A:829:GLU:C	1:A:831:GLY:HA3	2.43	0.43
1:A:552:ASP:HB3	1:A:554:LYS:H	1.84	0.43
1:A:805:LYS:HE2	3:A:1215:HOH:O	2.19	0.43
1:A:865:ASN:ND2	1:A:867:LEU:HB2	2.33	0.43
1:A:188:LYS:HA	1:A:189:PRO:HA	1.81	0.42
1:A:239:GLY:HA2	1:A:376:MSE:O	2.19	0.42
1:A:555:LEU:HD22	1:A:556:GLY:N	2.34	0.42
1:A:567:MSE:SE	1:A:579:ILE:CG1	3.17	0.42
1:A:660:SER:HB2	1:A:661:GLU:CA	2.48	0.42
1:A:968:GLU:HA	1:A:968:GLU:OE1	2.19	0.42
2:B:27:G:H2'	2:B:28:U:C6	2.54	0.42
1:A:582:PHE:CE2	1:A:614:HIS:HB2	2.54	0.42
1:A:102:LEU:HG	1:A:106:LEU:HD23	2.00	0.42
1:A:45:GLN:HE21	1:A:69:LYS:CD	2.31	0.42
1:A:672:LYS:HG2	1:A:672:LYS:H	1.66	0.42
1:A:907:ALA:CB	1:A:1084:ILE:HD12	2.48	0.42
1:A:5:SER:H	2:B:92:G:H1'	1.85	0.42
1:A:48:LEU:HD22	1:A:65:ALA:CA	2.49	0.42
1:A:64:THR:HB	1:A:65:ALA:CB	2.34	0.42
1:A:69:LYS:HD2	1:A:96:LEU:HD13	2.02	0.42
1:A:450:LEU:C	1:A:450:LEU:CD2	2.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:GLY:CA	1:A:760:GLN:CG	2.92	0.42
2:B:23:A:C2'	2:B:24:C:O5'	2.67	0.42
1:A:32:GLY:HA3	1:A:220:MSE:SE	2.70	0.42
1:A:109:GLN:N	1:A:109:GLN:OE1	2.53	0.42
1:A:357:PHE:O	1:A:361:TYR:HB2	2.20	0.42
1:A:686:PRO:O	1:A:689:ARG:N	2.53	0.42
1:A:709:LYS:O	1:A:710:GLU:C	2.63	0.42
1:A:754:GLY:C	1:A:760:GLN:HG3	2.43	0.42
1:A:963:PRO:HB2	1:A:1084:ILE:HG21	2.02	0.42
2:B:4:U:O2'	2:B:5:A:O5'	2.35	0.42
1:A:602:PHE:CE2	1:A:986:GLN:CB	3.02	0.42
1:A:731:ARG:HG2	1:A:735:LYS:HE3	2.01	0.42
1:A:45:GLN:NE2	1:A:96:LEU:HD13	2.35	0.42
1:A:694:ASN:O	1:A:697:GLN:CG	2.66	0.42
1:A:395:ASP:O	1:A:403:GLN:HA	2.19	0.42
1:A:817:ILE:O	1:A:821:LEU:HD22	2.20	0.42
1:A:966:ALA:CB	1:A:1084:ILE:HG12	2.46	0.42
2:B:92:G:OP2	2:B:92:G:C4'	2.68	0.42
1:A:48:LEU:HD22	1:A:65:ALA:HB2	2.01	0.41
1:A:794:ALA:N	2:B:50:G:OP2	2.52	0.41
2:B:9:G:C2'	2:B:10:A:C8	2.92	0.41
2:B:36:U:HO2'	2:B:37:G:P	2.42	0.41
1:A:423:LEU:C	1:A:434:VAL:HG12	2.43	0.41
1:A:12:LEU:HD23	1:A:439:VAL:HG13	2.01	0.41
1:A:366:SER:O	1:A:370:LYS:HE3	2.20	0.41
1:A:809:LEU:CD1	1:A:878:GLU:HG3	2.50	0.41
1:A:131:LYS:HD3	1:A:133:ALA:N	2.32	0.41
1:A:670:TRP:CZ3	1:A:674:ILE:CG2	3.03	0.41
1:A:904:ARG:NH1	1:A:904:ARG:CG	2.73	0.41
1:A:968:GLU:OE2	1:A:1107:TYR:CE2	2.73	0.41
1:A:999:LEU:HD23	1:A:999:LEU:HA	1.92	0.41
1:A:41:SER:HA	1:A:49:TYR:OH	2.20	0.41
1:A:717:GLU:O	1:A:721:ARG:HG3	2.20	0.41
1:A:913:ARG:HB2	1:A:953:PRO:HD3	1.89	0.41
2:B:4:U:O2'	2:B:5:A:P	2.78	0.41
1:A:710:GLU:O	1:A:714:ALA:HB2	2.20	0.41
1:A:743:PRO:O	2:B:34:A:C8	2.73	0.41
2:B:40:C:C2	2:B:41:A:N7	2.88	0.41
1:A:416:HIS:CD2	1:A:447:LEU:HD13	2.54	0.41
2:B:90:A:C2'	2:B:91:C:H5'	2.51	0.41
1:A:120:ILE:O	1:A:124:PHE:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:SER:HA	1:A:515:ARG:CZ	2.51	0.41
1:A:640:ARG:O	1:A:644:GLN:HG3	2.21	0.41
1:A:1085:ILE:HG23	1:A:1099:MSE:HE3	2.01	0.41
1:A:1096:PHE:O	1:A:1100:VAL:HG23	2.20	0.41
2:B:9:G:O6	2:B:10:A:N6	2.49	0.41
1:A:12:LEU:CD1	1:A:22:LEU:HD12	2.50	0.41
1:A:674:ILE:HA	1:A:696:LEU:HD11	2.02	0.41
1:A:797:LEU:HD13	2:B:36:U:C6	2.56	0.41
1:A:1068:ASP:HB3	1:A:1074:SER:CB	2.44	0.41
1:A:1113:ARG:NH1	1:A:1113:ARG:CG	2.84	0.41
2:B:9:G:O2'	2:B:10:A:O5'	2.31	0.41
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.86	0.41
1:A:61:CYS:O	1:A:61:CYS:SG	2.79	0.41
1:A:256:ASN:ND2	1:A:360:ARG:HD2	2.36	0.41
1:A:484:ARG:HB2	1:A:487:GLN:HG2	2.03	0.41
1:A:560:LEU:HA	1:A:560:LEU:HD23	1.79	0.41
1:A:628:SER:O	1:A:632:ARG:HB2	2.21	0.41
1:A:234:TRP:CZ3	1:A:378:ALA:HB1	2.56	0.40
1:A:570:ASP:OD1	1:A:859:ARG:NH2	2.54	0.40
1:A:1080:ASP:OD1	1:A:1081:PRO:HD2	2.21	0.40
1:A:36:TYR:O	1:A:39:TRP:HB2	2.21	0.40
1:A:295:ALA:O	1:A:296:LEU:HD22	2.22	0.40
1:A:655:LEU:HD12	1:A:692:PHE:HE1	1.87	0.40
1:A:828:ASP:HA	1:A:829:GLU:C	2.45	0.40
2:B:27:G:H2'	2:B:28:U:H6	1.87	0.40
1:A:340:ALA:CB	1:A:668:ARG:NH2	2.83	0.40
1:A:451:LEU:O	1:A:461:LEU:CA	2.69	0.40
1:A:527:ARG:C	1:A:528:LEU:HD23	2.44	0.40
1:A:570:ASP:OD2	1:A:859:ARG:NH2	2.47	0.40
1:A:758:ILE:O	1:A:762:GLU:HB2	2.20	0.40
1:A:855:PHE:HE2	1:A:998:ARG:CZ	2.34	0.40
2:B:92:G:H8	2:B:92:G:H5''	1.85	0.40
1:A:130:ASP:CG	1:A:131:LYS:O	2.64	0.40
1:A:459:ILE:O	1:A:475:GLU:HA	2.21	0.40
1:A:952:ILE:O	1:A:952:ILE:CG2	2.70	0.40
1:A:400:ASN:O	1:A:401:LEU:CB	2.69	0.40
1:A:865:ASN:ND2	1:A:868:MSE:H	2.19	0.40
1:A:968:GLU:N	1:A:969:GLY:HA3	2.37	0.40
1:A:1037:THR:HB	1:A:1086:ASN:HD21	1.86	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	997/1137 (88%)	965 (97%)	24 (2%)	8 (1%)	16	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	LEU
1	A	401	LEU
1	A	459	ILE
1	A	952	ILE
1	A	344	GLU
1	A	859	ARG
1	A	678	VAL
1	A	452	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	804/955 (84%)	605 (75%)	199 (25%)	1	2

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	11	ARG
1	A	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	37	THR
1	A	40	LEU
1	A	42	LEU
1	A	47	ASN
1	A	48	LEU
1	A	51	ARG
1	A	60	GLU
1	A	62	ASP
1	A	63	LYS
1	A	64	THR
1	A	77	ARG
1	A	83	ASN
1	A	86	ARG
1	A	91	SER
1	A	92	ASP
1	A	95	LEU
1	A	100	ARG
1	A	106	LEU
1	A	114	LYS
1	A	131	LYS
1	A	182	LEU
1	A	189	PRO
1	A	190	LEU
1	A	191	MSE
1	A	201	SER
1	A	203	GLU
1	A	214	ARG
1	A	215	THR
1	A	227	ARG
1	A	240	GLN
1	A	244	LYS
1	A	251	ARG
1	A	255	LYS
1	A	264	VAL
1	A	271	GLN
1	A	294	ARG
1	A	296	LEU
1	A	301	LYS
1	A	312	ASP
1	A	317	LEU
1	A	321	GLU
1	A	323	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	328	ARG
1	A	352	ARG
1	A	359	THR
1	A	371	LEU
1	A	375	LYS
1	A	379	THR
1	A	386	THR
1	A	393	ARG
1	A	396	LYS
1	A	397	LEU
1	A	401	LEU
1	A	402	HIS
1	A	403	GLN
1	A	407	LEU
1	A	413	GLU
1	A	424	LEU
1	A	425	LYS
1	A	426	VAL
1	A	428	ASN
1	A	432	ARG
1	A	438	THR
1	A	441	ILE
1	A	443	MSE
1	A	444	SER
1	A	445	GLU
1	A	450	LEU
1	A	451	LEU
1	A	459	ILE
1	A	461	LEU
1	A	464	ARG
1	A	465	ASP
1	A	471	HIS
1	A	481	ILE
1	A	485	ARG
1	A	486	ASP
1	A	488	LEU
1	A	490	HIS
1	A	500	VAL
1	A	501	TYR
1	A	502	LEU
1	A	507	ARG
1	A	511	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	525	VAL
1	A	527	ARG
1	A	540	ASP
1	A	555	LEU
1	A	561	LEU
1	A	564	LEU
1	A	573	LEU
1	A	575	THR
1	A	576	SER
1	A	579	ILE
1	A	583	ARG
1	A	595	LYS
1	A	597	ARG
1	A	618	GLN
1	A	626	THR
1	A	627	GLU
1	A	628	SER
1	A	629	LYS
1	A	631	LEU
1	A	634	ILE
1	A	639	GLN
1	A	640	ARG
1	A	652	LEU
1	A	654	LEU
1	A	663	VAL
1	A	665	ARG
1	A	666	ARG
1	A	674	ILE
1	A	675	GLU
1	A	676	GLN
1	A	683	HIS
1	A	687	ASP
1	A	688	TRP
1	A	695	GLU
1	A	696	LEU
1	A	697	GLN
1	A	705	ILE
1	A	709	LYS
1	A	726	MSE
1	A	741	GLU
1	A	745	ILE
1	A	746	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	752	VAL
1	A	753	VAL
1	A	759	GLU
1	A	761	ILE
1	A	773	SER
1	A	781	SER
1	A	785	ILE
1	A	795	ILE
1	A	798	ARG
1	A	806	GLU
1	A	812	LEU
1	A	818	MSE
1	A	821	LEU
1	A	827	LEU
1	A	830	ARG
1	A	838	LYS
1	A	839	TYR
1	A	848	GLU
1	A	850	LEU
1	A	851	SER
1	A	863	GLU
1	A	865	ASN
1	A	866	GLN
1	A	871	SER
1	A	872	HIS
1	A	881	ASN
1	A	882	GLN
1	A	884	GLN
1	A	886	HIS
1	A	887	ASP
1	A	888	LEU
1	A	889	LEU
1	A	893	MSE
1	A	898	SER
1	A	904	ARG
1	A	905	THR
1	A	910	ILE
1	A	950	ASP
1	A	951	LEU
1	A	959	ILE
1	A	964	PHE
1	A	978	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	985	GLN
1	A	986	GLN
1	A	994	ILE
1	A	995	SER
1	A	997	ILE
1	A	1000	ARG
1	A	1001	CYS
1	A	1002	ASP
1	A	1009	GLU
1	A	1011	VAL
1	A	1015	ARG
1	A	1019	LYS
1	A	1020	ARG
1	A	1024	SER
1	A	1029	VAL
1	A	1032	THR
1	A	1034	THR
1	A	1037	THR
1	A	1063	LEU
1	A	1068	ASP
1	A	1073	LYS
1	A	1078	MSE
1	A	1079	ARG
1	A	1085	ILE
1	A	1093	GLN
1	A	1094	LYS
1	A	1110	LYS
1	A	1113	ARG

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

Mol	Chain	Res	Type
1	A	45	GLN
1	A	47	ASN
1	A	59	GLN
1	A	85	HIS
1	A	119	GLN
1	A	236	GLN
1	A	256	ASN
1	A	260	GLN
1	A	271	GLN
1	A	400	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	402	HIS
1	A	446	GLN
1	A	503	ASN
1	A	533	HIS
1	A	538	HIS
1	A	607	ASN
1	A	618	GLN
1	A	648	GLN
1	A	697	GLN
1	A	703	HIS
1	A	729	GLN
1	A	756	ASN
1	A	800	HIS
1	A	865	ASN
1	A	877	GLN
1	A	881	ASN
1	A	975	HIS
1	A	1089	ASN
1	A	1093	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	55/112 (49%)	26 (47%)	9 (16%)

All (26) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	4	U
2	B	5	A
2	B	6	G
2	B	7	A
2	B	8	G
2	B	9	G
2	B	12	A
2	B	13	G
2	B	24	C
2	B	29	G
2	B	30	U
2	B	31	G
2	B	32	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	34	A
2	B	35	A
2	B	36	U
2	B	37	G
2	B	48	A
2	B	49	G
2	B	50	G
2	B	51	U
2	B	87	G
2	B	91	C
2	B	92	G
2	B	93	A
2	B	94	G

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	5	A
2	B	8	G
2	B	28	U
2	B	31	G
2	B	36	U
2	B	49	G
2	B	50	G
2	B	86	U
2	B	92	G

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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	992/1137 (87%)	0.16	38 (3%)	44 25	11, 41, 87, 134	6 (0%)
2	B	60/112 (53%)	-0.23	0	100 100	22, 61, 124, 146	0
All	All	1052/1249 (84%)	0.14	38 (3%)	46 26	11, 43, 90, 146	6 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	TYR	7.9
1	A	953	PRO	5.2
1	A	198	GLU	5.1
1	A	790	GLY	4.9
1	A	319	ASP	4.2
1	A	957	GLY	3.8
1	A	1027	ASN	3.7
1	A	1056	LEU	3.7
1	A	972	HIS	3.6
1	A	783	GLN	3.5
1	A	315	PHE	3.4
1	A	277	ALA	3.4
1	A	316	ASP	3.2
1	A	735	LYS	3.2
1	A	551	ASP	3.0
1	A	915	VAL	3.0
1	A	832	LYS	2.9
1	A	912	CYS	2.8
1	A	1055	LYS	2.7
1	A	681	ALA	2.7
1	A	966	ALA	2.6
1	A	948	ALA	2.6
1	A	949	ASP	2.5
1	A	276	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	973	GLN	2.4
1	A	827	LEU	2.4
1	A	445	GLU	2.3
1	A	490	HIS	2.3
1	A	680	ALA	2.3
1	A	831	GLY	2.3
1	A	320	ALA	2.2
1	A	343	ALA	2.2
1	A	1054	GLU	2.2
1	A	748	TYR	2.1
1	A	678	VAL	2.1
1	A	1016	LEU	2.1
1	A	272	GLN	2.1
1	A	492	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.