Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:50 AM GMT

PDB ID	:	2IY5
Title	:	PHENYLALANYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS COMPLEXED WITH TRNA AND A PHENYLALANYL-ADENYLATE ANALOG
Authors	:	Moor, N.; Kotik-Kogan, O.; Tworowski, D.; Sukhanova, M.; Safro, M.
Deposited on	:	2006-07-12
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

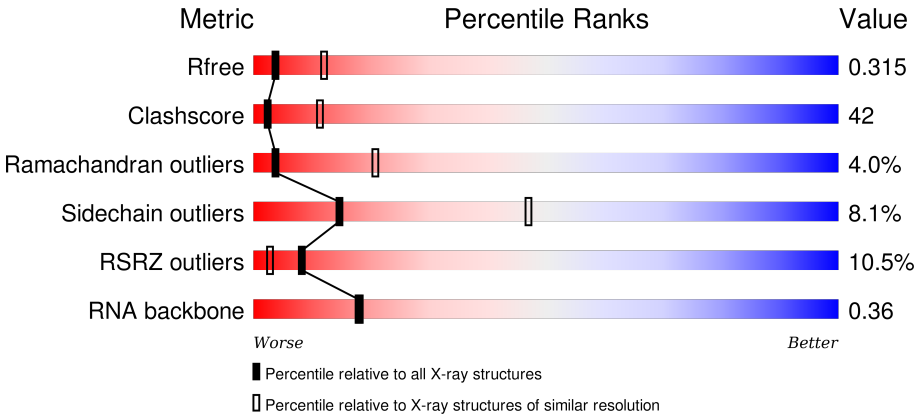
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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

Mol	Chain	Length	Quality of chain
1	A	350	15% 39% 47% 8%
2	B	785	% 41% 51% 7%
3	T	76	88% 16% 39% 33% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	B	1781	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10649 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 PHENYLALANYL-TRNA SYNTHETASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2671	1731	463	469	8			

- Molecule 2 is a protein called PHENYLALANYL-TRNA SYNTHETASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	781	Total	C	N	O	S	0	0	1
			6094	3905	1085	1094	10			

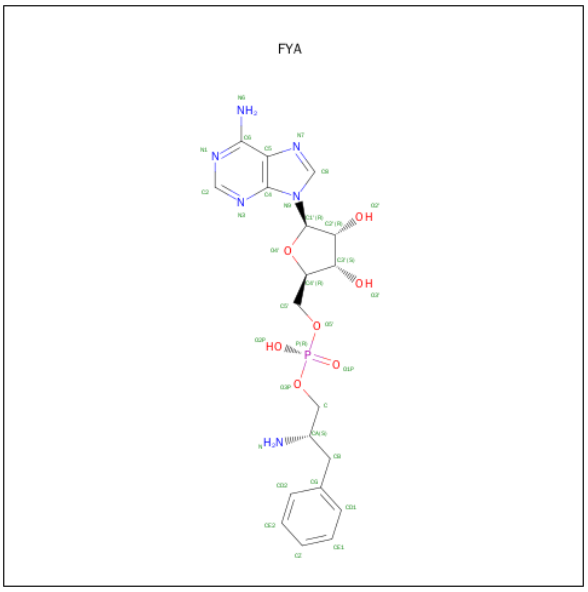
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	467	GLU	GLN	CONFLICT	UNP P27001
B	487	ALA	GLY	CONFLICT	UNP P27001
B	629	GLU	GLN	CONFLICT	UNP P27001

- Molecule 3 is a RNA chain called TRNAPHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	76	Total	C	N	O	P	0	0	0
			1619	723	291	530	75			

- Molecule 4 is ADENOSINE-5'-[PHENYLALANINOL-PHOSPHATE] (three-letter code: FYA) (formula: $C_{19}H_{25}N_6O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			33	19	6	7	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

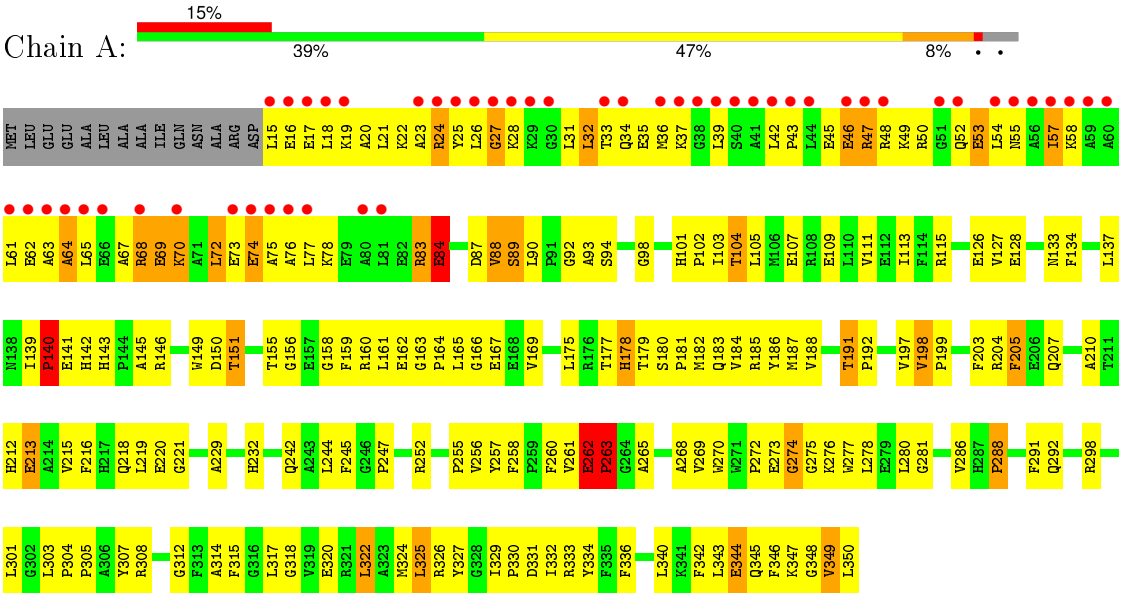
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	50	Total	O	0	0
			50	50		
6	B	149	Total	O	0	0
			149	149		
6	T	32	Total	O	0	0
			32	32		

3 Residue-property plots (i)

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

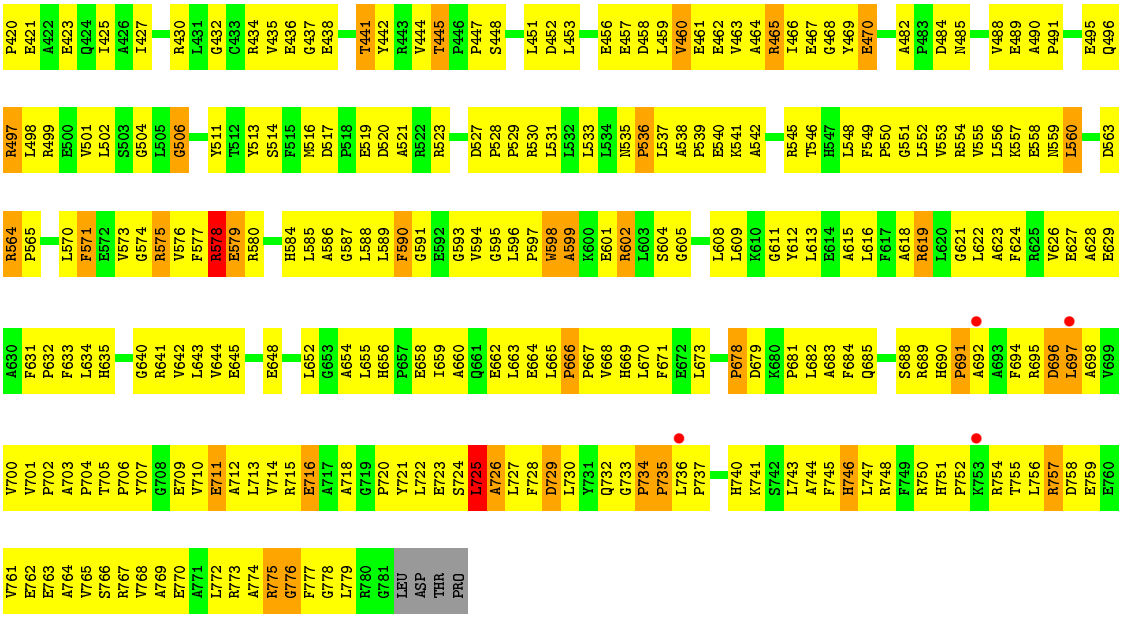
- Molecule 1: PHENYLALANYL-TRNA SYNTHETASE ALPHA CHAIN

Chain A:



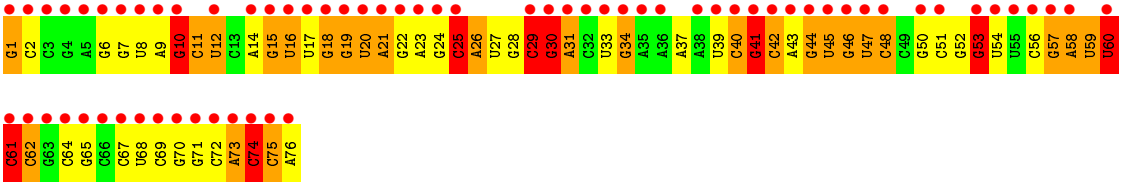
- Molecule 2: PHENYLALANYL-TRNA SYNTHETASE BETA CHAIN

Chain B:



- Molecule 3: TRNAPHE

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.40Å 173.40Å 139.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.99 – 3.10 47.11 – 3.05	Depositor EDS
% Data completeness (in resolution range)	79.8 (9.99-3.10) 85.6 (47.11-3.05)	Depositor EDS
R_{merge}	1.00	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.299 0.260 , 0.315	Depositor DCC
R_{free} test set	1908 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.1	EDS
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 39854 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	10649	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.44	0/2741	0.79	2/3702 (0.1%)
2	B	0.45	1/6246 (0.0%)	0.72	6/8491 (0.1%)
3	T	0.71	0/1809	1.45	28/2819 (1.0%)
All	All	0.50	1/10796 (0.0%)	0.92	36/15012 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	T	19	6
All	All	19	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	243	ASN	CB-CG	-5.49	1.38	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	61	C	O5'-P-OP1	-22.75	83.40	110.70
1	A	262	GLU	C-N-CD	-22.30	71.53	120.60
3	T	60	U	OP1-P-O3'	-17.23	67.30	105.20
3	T	60	U	OP2-P-O3'	-16.26	69.42	105.20
3	T	61	C	O5'-P-OP2	-15.98	91.32	105.70
3	T	25	C	N1-C1'-C2'	14.26	132.54	114.00
1	A	262	GLU	C-N-CA	13.74	179.70	122.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	41	G	N9-C1'-C2'	13.26	131.24	114.00
3	T	61	C	N1-C1'-C2'	12.55	130.31	114.00
3	T	10	G	C5'-C4'-O4'	12.53	124.13	109.10
3	T	29	C	N1-C1'-C2'	11.81	129.35	114.00
3	T	30	G	C5'-C4'-O4'	11.34	122.71	109.10
3	T	30	G	C2'-C3'-O3'	10.62	132.87	109.50
3	T	10	G	N9-C1'-C2'	10.21	127.28	114.00
3	T	74	C	N1-C1'-C2'	9.93	126.90	114.00
3	T	10	G	C5'-C4'-C3'	9.29	130.87	116.00
3	T	10	G	O4'-C1'-N9	-9.26	100.79	108.20
3	T	61	C	C5'-C4'-C3'	8.68	129.88	116.00
3	T	30	G	C5'-C4'-C3'	8.60	129.75	116.00
3	T	30	G	N9-C1'-C2'	8.18	124.63	114.00
3	T	10	G	C1'-O4'-C4'	-7.82	103.65	109.90
2	B	100	GLY	N-CA-C	7.56	132.01	113.10
2	B	133	LEU	CA-CB-CG	7.38	132.26	115.30
3	T	61	C	C2'-C3'-O3'	6.66	124.35	113.70
3	T	1	G	N9-C1'-C2'	6.47	122.42	114.00
3	T	60	U	O3'-P-O5'	6.23	115.84	104.00
2	B	725	LEU	N-CA-C	-6.08	94.59	111.00
3	T	30	G	C1'-O4'-C4'	-5.88	105.19	109.90
3	T	61	C	OP1-P-OP2	5.86	128.39	119.60
3	T	61	C	O4'-C1'-N1	-5.85	103.52	108.20
3	T	10	G	C4'-C3'-C2'	-5.62	96.98	102.60
2	B	38	VAL	N-CA-C	5.60	126.12	111.00
3	T	41	G	C5'-C4'-C3'	5.56	124.90	116.00
2	B	578	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	B	69	GLY	N-CA-C	-5.15	100.22	113.10
3	T	25	C	O4'-C1'-C2'	5.11	112.20	107.60

All (19) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	T	1	G	C1'
3	T	10	G	C4',C1'
3	T	25	C	C4',C3',C1'
3	T	29	C	C4',C3',C1'
3	T	30	G	C4',C3',C1'
3	T	41	G	C4',C3',C1'
3	T	61	C	C1'
3	T	74	C	C4',C3',C1'

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	243	ASN	Mainchain
3	T	10	G	Sidechain
3	T	25	C	Sidechain
3	T	30	G	Sidechain
3	T	41	G	Sidechain
3	T	53	G	Sidechain
3	T	61	C	Sidechain

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	2671	0	2666	277	0
2	B	6094	0	6146	480	0
3	T	1619	0	823	143	1
4	A	33	0	24	5	0
5	B	1	0	0	0	0
6	A	50	0	0	5	0
6	B	149	0	0	11	0
6	T	32	0	0	6	0
All	All	10649	0	9659	851	1

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 42.

All (851) 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:25:LEU:HD13	2:B:158:LEU:HD11	1.22	1.20
3:T:10:G:H5"	3:T:11:C:C6	1.83	1.13
1:A:35:GLU:HA	1:A:39:LEU:HD21	1.12	1.11
3:T:61:C:H3'	3:T:62:C:C5'	1.82	1.06
3:T:61:C:H3'	3:T:62:C:H5'	1.07	1.03
1:A:140:PRO:O	1:A:143:HIS:HB2	1.60	1.01
2:B:695:ARG:HH21	2:B:761:VAL:HG11	1.25	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:PRO:HG2	2:B:423:GLU:HG3	1.45	0.97
1:A:262:GLU:OE1	2:B:458:ASP:HA	1.65	0.96
2:B:224:ALA:H	2:B:244:ASN:ND2	1.63	0.94
2:B:623:ALA:HB3	2:B:645:GLU:HA	1.49	0.93
1:A:182:MET:HG3	1:A:198:VAL:HG21	1.47	0.92
3:T:74:C:H4'	3:T:75:C:O5'	1.69	0.91
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.54	0.90
1:A:35:GLU:HA	1:A:39:LEU:CD2	2.00	0.90
2:B:283:LEU:HD23	2:B:310:PRO:HB2	1.51	0.90
3:T:52:G:H2'	3:T:53:G:H5"	1.52	0.89
1:A:198:VAL:HG13	1:A:220:GLU:HB2	1.55	0.89
1:A:34:GLN:NE2	3:T:56:C:H1'	1.87	0.89
1:A:54:LEU:HB2	3:T:56:C:H4'	1.55	0.88
2:B:589:LEU:HD21	2:B:608:LEU:HD23	1.56	0.88
2:B:294:HIS:CE1	2:B:296:GLU:HB2	2.09	0.88
2:B:258:GLN:HE22	2:B:369:GLN:HE21	1.22	0.87
1:A:24:ARG:CB	3:T:43:A:H5'	2.05	0.86
2:B:533:LEU:HB2	2:B:536:PRO:HG3	1.56	0.85
2:B:624:PHE:HE1	2:B:642:VAL:HG13	1.42	0.84
1:A:24:ARG:HE	1:A:28:LYS:H	1.24	0.84
1:A:143:HIS:HB3	1:A:146:ARG:HB2	1.57	0.84
1:A:61:LEU:HD12	1:A:62:GLU:N	1.92	0.84
1:A:24:ARG:HB2	3:T:43:A:H5'	1.58	0.84
2:B:564:ARG:H	2:B:564:ARG:NH1	1.74	0.84
2:B:223:VAL:HA	2:B:244:ASN:HD22	1.43	0.84
3:T:33:U:H2'	3:T:34:G:H5"	1.57	0.84
2:B:224:ALA:N	2:B:244:ASN:ND2	2.24	0.84
2:B:762:GLU:HA	2:B:765:VAL:HG22	1.58	0.84
2:B:695:ARG:HG2	2:B:695:ARG:HH11	1.42	0.83
1:A:327:TYR:HB2	1:A:329:ILE:HD11	1.61	0.82
2:B:242:ILE:HG22	2:B:243:ASN:ND2	1.94	0.82
2:B:279:GLU:HB2	2:B:295:PRO:HB3	1.61	0.82
3:T:21:A:O5'	3:T:22:G:H5'	1.79	0.82
2:B:770:GLU:O	2:B:773:ARG:HG2	1.79	0.82
2:B:141:PRO:O	2:B:144:THR:HG23	1.80	0.82
3:T:52:G:C2'	3:T:53:G:H5"	2.09	0.81
2:B:434:ARG:HB3	2:B:445:THR:HG23	1.62	0.81
1:A:165:LEU:HD11	1:A:303:LEU:HD11	1.63	0.80
2:B:353:ARG:O	2:B:353:ARG:HD3	1.82	0.80
1:A:34:GLN:HE22	3:T:56:C:H1'	1.45	0.79
1:A:199:PRO:HG3	1:A:219:LEU:CD1	2.12	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:692:ALA:HB2	2:B:750:ARG:HD2	1.65	0.79
2:B:564:ARG:CZ	2:B:564:ARG:H	1.96	0.79
2:B:695:ARG:NH2	2:B:761:VAL:HG11	1.97	0.79
1:A:50:ARG:HD3	3:T:56:C:C6	2.18	0.79
3:T:19:G:H5'	3:T:20:U:OP1	1.83	0.78
2:B:691:PRO:HG2	3:T:11:C:O2	1.83	0.78
2:B:170:LEU:HD12	2:B:170:LEU:H	1.46	0.78
2:B:578:ARG:HG3	2:B:578:ARG:O	1.82	0.78
3:T:41:G:H4'	3:T:42:C:OP2	1.83	0.78
1:A:331:ASP:HB3	1:A:334:TYR:CE2	2.19	0.77
3:T:45:U:H3'	3:T:46:G:H5"	1.64	0.77
3:T:25:C:H4'	3:T:26:A:OP2	1.85	0.77
1:A:242:GLN:OE1	1:A:247:PRO:HA	1.85	0.77
2:B:41:ILE:HG23	2:B:123:LEU:HD11	1.67	0.77
2:B:258:GLN:HE22	2:B:369:GLN:NE2	1.83	0.76
2:B:101:GLN:OE1	2:B:102:LYS:N	2.18	0.76
1:A:22:LYS:HA	1:A:25:TYR:HB2	1.68	0.76
1:A:165:LEU:HD12	1:A:301:LEU:HD23	1.68	0.76
2:B:224:ALA:H	2:B:244:ASN:HD22	1.31	0.76
2:B:732:GLN:HG3	2:B:740:HIS:O	1.86	0.75
1:A:179:THR:OG1	1:A:220:GLU:HG2	1.87	0.75
2:B:192:LYS:H	2:B:381:GLN:HE22	1.32	0.74
1:A:156:GLY:HA3	2:B:531:LEU:HD23	1.69	0.74
3:T:54:U:H3'	3:T:58:A:N1	2.03	0.74
2:B:564:ARG:N	2:B:564:ARG:NH1	2.35	0.74
3:T:10:G:C5'	3:T:11:C:C6	2.70	0.73
2:B:535:ASN:N	2:B:536:PRO:HD3	2.03	0.73
1:A:39:LEU:HD13	3:T:19:G:C5	2.23	0.73
1:A:336:PHE:HB3	2:B:513:TYR:CE1	2.22	0.73
1:A:16:GLU:HA	1:A:19:LYS:HB2	1.68	0.73
1:A:325:LEU:HD13	1:A:326:ARG:N	2.04	0.73
2:B:407:ARG:HG3	2:B:441:THR:HB	1.68	0.73
3:T:33:U:C2'	3:T:34:G:H5"	2.17	0.73
2:B:191:LEU:HD12	2:B:374:ARG:HD2	1.69	0.73
2:B:264:ASP:OD2	2:B:328:THR:HB	1.87	0.73
3:T:54:U:H3	3:T:61:C:H42	1.37	0.73
2:B:761:VAL:O	2:B:765:VAL:HG13	1.87	0.73
3:T:64:C:H2'	3:T:65:G:C8	2.23	0.73
1:A:327:TYR:HB2	1:A:329:ILE:CD1	2.17	0.73
3:T:50:G:H2'	3:T:51:C:C6	2.23	0.73
1:A:270:TRP:O	1:A:272:PRO:HD3	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:HA	1:A:50:ARG:HG3	1.71	0.73
3:T:29:C:H4'	3:T:30:G:OP2	1.89	0.72
1:A:349:VAL:O	1:A:349:VAL:HG12	1.89	0.72
2:B:80:ASN:HD21	2:B:132:LEU:H	1.38	0.72
1:A:329:ILE:H	1:A:329:ILE:HD12	1.53	0.72
2:B:248:VAL:O	2:B:252:VAL:HG23	1.89	0.71
2:B:25:LEU:HD13	2:B:158:LEU:CD1	2.13	0.71
1:A:98:GLY:H	2:B:506:GLY:HA2	1.54	0.71
1:A:48:ARG:HG2	1:A:48:ARG:HH11	1.54	0.71
3:T:44:G:H8	3:T:44:G:H3'	1.56	0.71
2:B:629:GLU:H	2:B:640:GLY:HA2	1.54	0.71
1:A:191:THR:HG22	2:B:484:ASP:OD1	1.89	0.71
2:B:63:ARG:HD2	2:B:73:GLU:OE1	1.90	0.71
1:A:103:ILE:HD11	1:A:320:GLU:HG3	1.73	0.70
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.73	0.70
1:A:27:GLY:C	1:A:31:LEU:HG	2.12	0.70
2:B:325:ARG:H	2:B:328:THR:CG2	2.04	0.70
2:B:681:PRO:HD3	6:B:2139:HOH:O	1.91	0.70
2:B:32:THR:HG23	6:B:2008:HOH:O	1.90	0.70
1:A:35:GLU:CA	1:A:39:LEU:HD21	2.07	0.70
2:B:624:PHE:CE1	2:B:642:VAL:HG13	2.26	0.70
3:T:58:A:O2'	3:T:59:U:H5"	1.91	0.69
2:B:282:ARG:HH12	2:B:290:GLU:HG3	1.58	0.69
2:B:461:GLU:O	2:B:465:ARG:HG2	1.92	0.69
3:T:10:G:H5'	3:T:11:C:P	2.32	0.69
2:B:535:ASN:H	2:B:536:PRO:HD3	1.56	0.69
1:A:98:GLY:N	2:B:506:GLY:HA2	2.07	0.69
1:A:31:LEU:HD22	1:A:35:GLU:OE1	1.92	0.69
2:B:224:ALA:N	2:B:244:ASN:HD22	1.90	0.69
1:A:109:GLU:O	1:A:113:ILE:HG13	1.93	0.69
2:B:14:GLU:HG2	6:B:2039:HOH:O	1.92	0.68
2:B:495:GLU:O	2:B:498:LEU:HB3	1.92	0.68
2:B:279:GLU:CD	2:B:295:PRO:HG3	2.14	0.68
2:B:604:SER:HA	2:B:608:LEU:HB2	1.76	0.68
2:B:170:LEU:HD12	2:B:254:LEU:O	1.94	0.67
2:B:684:PHE:O	2:B:685:GLN:HG3	1.94	0.67
2:B:710:VAL:HG11	2:B:743:LEU:HD22	1.76	0.67
3:T:50:G:H2'	3:T:51:C:H6	1.59	0.67
3:T:58:A:H5"	6:T:2024:HOH:O	1.94	0.67
2:B:353:ARG:C	2:B:353:ARG:HD3	2.15	0.67
3:T:15:G:H4'	3:T:16:U:OP1	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:67:C:H2'	3:T:68:U:H5'	1.77	0.67
2:B:701:VAL:HG13	2:B:702:PRO:HD2	1.77	0.67
2:B:291:ARG:NH2	2:B:352:LEU:HD21	2.09	0.66
2:B:725:LEU:O	2:B:726:ALA:HB2	1.95	0.66
3:T:44:G:H3'	3:T:44:G:C8	2.29	0.66
2:B:533:LEU:CB	2:B:536:PRO:HG3	2.26	0.66
1:A:182:MET:CG	1:A:198:VAL:HG21	2.23	0.66
1:A:49:LYS:HB2	1:A:50:ARG:NH1	2.11	0.66
3:T:64:C:H2'	3:T:65:G:H8	1.60	0.66
2:B:707:TYR:OH	2:B:711:GLU:HG3	1.96	0.66
1:A:21:LEU:HD22	3:T:43:A:H1'	1.77	0.65
2:B:629:GLU:N	2:B:640:GLY:HA2	2.11	0.65
1:A:159:PHE:N	2:B:530:ARG:HD3	2.11	0.65
1:A:288:PRO:O	1:A:292:GLN:HG3	1.96	0.65
2:B:734:PRO:HB2	2:B:735:PRO:CD	2.26	0.65
2:B:243:ASN:O	2:B:247:ASP:HB2	1.96	0.65
1:A:344:GLU:HG2	1:A:347:LYS:HD2	1.78	0.65
2:B:537:LEU:HB2	2:B:541:LYS:HD2	1.77	0.65
1:A:331:ASP:HB3	1:A:334:TYR:HE2	1.58	0.65
1:A:72:LEU:HA	1:A:75:ALA:HB3	1.77	0.65
2:B:325:ARG:H	2:B:328:THR:HG21	1.61	0.65
3:T:11:C:H42	3:T:25:C:H42	1.44	0.65
3:T:69:C:O2'	3:T:70:G:H5'	1.97	0.65
1:A:325:LEU:HD13	1:A:325:LEU:C	2.17	0.65
1:A:349:VAL:O	1:A:350:LEU:HD23	1.96	0.65
1:A:210:ALA:HA	1:A:331:ASP:OD2	1.96	0.65
2:B:407:ARG:CG	2:B:441:THR:HB	2.26	0.65
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.79	0.65
2:B:434:ARG:HG2	2:B:436:GLU:HG3	1.78	0.64
2:B:609:LEU:HD23	2:B:652:LEU:HD11	1.78	0.64
2:B:695:ARG:HG2	2:B:695:ARG:NH1	2.11	0.64
3:T:45:U:H5'	3:T:46:G:OP2	1.96	0.64
2:B:707:TYR:CE1	2:B:727:LEU:HD12	2.31	0.64
1:A:64:ALA:HA	1:A:68:ARG:NH1	2.13	0.64
2:B:463:VAL:O	2:B:467:GLU:HB2	1.97	0.64
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.78	0.64
2:B:697:LEU:O	2:B:697:LEU:HD12	1.98	0.64
3:T:54:U:H3'	3:T:58:A:C6	2.32	0.64
3:T:28:G:C6	3:T:29:C:N4	2.66	0.63
1:A:325:LEU:O	1:A:325:LEU:HD22	1.98	0.63
2:B:50:VAL:HG11	2:B:82:ARG:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:GLY:HA2	2:B:254:LEU:O	1.99	0.63
1:A:142:HIS:HB3	2:B:344:ARG:HE	1.64	0.63
2:B:571:PHE:HE1	2:B:573:VAL:HG23	1.62	0.63
2:B:696:ASP:HB2	3:T:37:A:C4'	2.27	0.63
1:A:340:LEU:HD21	2:B:570:LEU:HD21	1.79	0.63
2:B:34:ARG:C	2:B:35:ILE:HD12	2.19	0.63
3:T:30:G:O6	3:T:41:G:C6	2.52	0.63
2:B:457:GLU:HA	2:B:460:VAL:CG1	2.28	0.63
2:B:520:ASP:HA	2:B:523:ARG:HB2	1.81	0.63
1:A:39:LEU:HD22	3:T:19:G:C6	2.34	0.63
1:A:261:VAL:O	1:A:261:VAL:HG23	1.99	0.62
2:B:377:LEU:HB3	2:B:388:VAL:HG11	1.81	0.62
1:A:24:ARG:HH21	1:A:27:GLY:HA3	1.64	0.62
2:B:136:PRO:HG2	2:B:227:PRO:HA	1.81	0.62
2:B:761:VAL:HG22	2:B:765:VAL:CG1	2.30	0.62
3:T:21:A:P	3:T:22:G:H5'	2.39	0.62
2:B:409:GLU:OE1	2:B:413:ARG:HD3	2.00	0.62
2:B:258:GLN:NE2	2:B:369:GLN:NE2	2.47	0.62
1:A:70:LYS:HA	1:A:73:GLU:HB2	1.82	0.62
2:B:64:LEU:O	2:B:73:GLU:HA	1.99	0.62
2:B:456:GLU:O	2:B:460:VAL:HG12	2.00	0.62
3:T:61:C:O4'	3:T:62:C:H6	1.83	0.62
2:B:63:ARG:HD3	2:B:111:VAL:HG11	1.81	0.62
2:B:660:ALA:HB1	2:B:665:LEU:O	2.00	0.62
2:B:120:PRO:HB2	2:B:128:TYR:O	1.99	0.62
2:B:694:PHE:HB3	2:B:748:ARG:HG3	1.81	0.61
1:A:27:GLY:O	1:A:31:LEU:HG	2.00	0.61
2:B:282:ARG:NH1	2:B:290:GLU:HG3	2.15	0.61
2:B:49:ARG:HG3	2:B:137:GLU:HG3	1.83	0.61
1:A:74:GLU:OE1	1:A:74:GLU:HA	2.00	0.61
1:A:88:VAL:HG23	1:A:89:SER:H	1.64	0.61
3:T:10:G:C2	3:T:26:A:H1'	2.36	0.61
3:T:54:U:H3'	3:T:58:A:N6	2.15	0.61
2:B:258:GLN:NE2	2:B:369:GLN:HE21	1.95	0.61
1:A:221:GLY:O	1:A:314:ALA:HA	2.00	0.61
1:A:184:VAL:O	1:A:188:VAL:HG13	2.00	0.61
2:B:554:ARG:O	2:B:558:GLU:HG3	2.01	0.61
2:B:602:ARG:HG3	2:B:602:ARG:HH11	1.66	0.61
3:T:60:U:H3'	3:T:61:C:C5	2.36	0.61
1:A:197:VAL:HA	1:A:220:GLU:O	2.01	0.61
3:T:70:G:H2'	3:T:71:G:O4'	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:ALA:O	2:B:295:PRO:HA	2.00	0.61
3:T:14:A:H2'	3:T:15:G:O4'	2.01	0.61
2:B:758:ASP:HA	2:B:761:VAL:HG12	1.83	0.61
1:A:57:ILE:O	1:A:57:ILE:HD13	2.01	0.61
1:A:58:LYS:O	1:A:62:GLU:HG2	2.01	0.61
2:B:514:SER:HA	2:B:545:ARG:HD3	1.82	0.61
3:T:10:G:N2	3:T:26:A:H1'	2.16	0.60
2:B:192:LYS:N	2:B:381:GLN:HE22	1.98	0.60
1:A:336:PHE:HB3	2:B:513:TYR:HE1	1.63	0.60
1:A:72:LEU:HD22	1:A:75:ALA:HB3	1.82	0.60
2:B:579:GLU:HG2	2:B:580:ARG:HG3	1.82	0.60
1:A:19:LYS:HB3	1:A:68:ARG:HG2	1.83	0.60
2:B:517:ASP:OD2	2:B:519:GLU:HB3	2.02	0.60
1:A:278:LEU:CD1	1:A:325:LEU:HG	2.32	0.60
1:A:87:ASP:O	1:A:89:SER:N	2.35	0.60
1:A:244:LEU:HB3	1:A:245:PHE:CD1	2.37	0.60
2:B:552:LEU:O	2:B:555:VAL:HG22	2.02	0.60
2:B:695:ARG:HH21	2:B:761:VAL:CG1	2.08	0.60
2:B:629:GLU:CD	2:B:641:ARG:HD3	2.22	0.60
1:A:101:HIS:ND1	1:A:102:PRO:HD2	2.17	0.59
2:B:656:HIS:CE1	2:B:658:GLU:HB2	2.37	0.59
2:B:696:ASP:HB2	3:T:37:A:H4'	1.84	0.59
1:A:19:LYS:HA	1:A:22:LYS:HE2	1.84	0.59
3:T:47:U:H5'	3:T:48:C:OP2	2.03	0.59
1:A:199:PRO:HG3	1:A:219:LEU:HD12	1.84	0.59
1:A:348:GLY:C	1:A:350:LEU:H	2.05	0.59
2:B:133:LEU:HB3	2:B:135:PHE:CE2	2.37	0.59
3:T:30:G:H5"	6:T:2012:HOH:O	2.01	0.59
1:A:343:LEU:O	1:A:345:GLN:N	2.36	0.59
2:B:457:GLU:O	2:B:460:VAL:HG13	2.03	0.59
1:A:187:MET:HE1	1:A:291:PHE:HD2	1.68	0.59
3:T:61:C:O4'	3:T:62:C:C6	2.56	0.59
3:T:20:U:O2'	3:T:22:G:H4'	2.02	0.59
1:A:46:GLU:HA	1:A:50:ARG:CG	2.32	0.59
1:A:58:LYS:HE2	1:A:61:LEU:HD11	1.85	0.59
2:B:30:PHE:HA	6:B:2006:HOH:O	2.02	0.59
3:T:26:A:O2'	3:T:27:U:H5'	2.03	0.59
1:A:199:PRO:HG3	1:A:219:LEU:HD11	1.84	0.58
1:A:103:ILE:HB	2:B:511:TYR:CE2	2.38	0.58
2:B:245:VAL:HB	2:B:324:VAL:HG21	1.85	0.58
2:B:588:LEU:HD23	2:B:588:LEU:C	2.24	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:O	1:A:78:LYS:HG3	2.04	0.58
2:B:551:GLY:O	2:B:555:VAL:HG13	2.04	0.58
2:B:775:ARG:HD3	2:B:775:ARG:C	2.24	0.58
1:A:47:ARG:HG3	1:A:47:ARG:HH11	1.67	0.58
2:B:427:ILE:HG23	2:B:466:ILE:HG21	1.86	0.58
1:A:54:LEU:CB	3:T:56:C:H4'	2.30	0.58
3:T:24:G:C6	3:T:25:C:N4	2.71	0.58
2:B:578:ARG:O	2:B:578:ARG:CG	2.51	0.58
2:B:734:PRO:O	2:B:736:LEU:N	2.37	0.58
2:B:35:ILE:HD12	2:B:35:ILE:N	2.19	0.58
3:T:56:C:O2	3:T:56:C:H2'	2.04	0.58
3:T:8:U:H4'	3:T:48:C:H4'	1.85	0.58
1:A:31:LEU:C	1:A:33:THR:H	2.07	0.57
1:A:133:ASN:HA	1:A:181:PRO:HG3	1.84	0.57
2:B:224:ALA:HB1	2:B:225:PRO:HD2	1.86	0.57
2:B:535:ASN:N	2:B:536:PRO:CD	2.66	0.57
1:A:272:PRO:C	1:A:274:GLY:H	2.07	0.57
2:B:578:ARG:C	2:B:580:ARG:H	2.07	0.57
1:A:101:HIS:CE1	1:A:103:ILE:HG12	2.39	0.57
6:A:2009:HOH:O	2:B:496:GLN:HG2	2.03	0.57
1:A:24:ARG:NE	1:A:28:LYS:H	1.97	0.57
2:B:278:ARG:NH2	2:B:308:SER:HB3	2.20	0.57
1:A:149:TRP:HB3	1:A:177:THR:HB	1.85	0.57
2:B:377:LEU:HD22	2:B:388:VAL:HG13	1.87	0.57
2:B:702:PRO:C	2:B:704:PRO:HD2	2.24	0.57
1:A:46:GLU:N	1:A:46:GLU:OE1	2.38	0.57
1:A:58:LYS:HE3	1:A:58:LYS:HA	1.85	0.57
3:T:57:G:H3'	3:T:58:A:C5'	2.34	0.57
2:B:121:ARG:HG3	2:B:127:GLU:O	2.05	0.57
2:B:209:GLY:C	2:B:211:PRO:HD3	2.25	0.57
2:B:274:VAL:HG22	2:B:300:ILE:HD13	1.87	0.57
2:B:141:PRO:HD2	2:B:144:THR:HG21	1.87	0.56
3:T:45:U:C3'	3:T:46:G:H5"	2.35	0.56
2:B:278:ARG:HB2	2:B:281:GLU:HG3	1.88	0.56
2:B:609:LEU:HD23	2:B:652:LEU:CD1	2.35	0.56
2:B:223:VAL:CA	2:B:244:ASN:HD22	2.16	0.56
3:T:61:C:C3'	3:T:62:C:C5'	2.71	0.56
1:A:187:MET:HE1	1:A:291:PHE:CD2	2.40	0.56
2:B:533:LEU:HB3	2:B:536:PRO:HD3	1.87	0.56
2:B:242:ILE:HG22	2:B:243:ASN:HD21	1.68	0.56
1:A:18:LEU:O	1:A:22:LYS:HG3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:OE1	2:B:513:TYR:OH	2.22	0.56
2:B:32:THR:HG22	2:B:158:LEU:CD2	2.35	0.56
1:A:278:LEU:HD13	1:A:325:LEU:HG	1.88	0.56
2:B:222:ARG:HG2	2:B:222:ARG:HH11	1.70	0.56
2:B:564:ARG:HH11	2:B:564:ARG:C	2.09	0.56
1:A:88:VAL:HG23	1:A:89:SER:N	2.20	0.56
1:A:212:HIS:N	1:A:332:ILE:HG21	2.21	0.56
1:A:277:TRP:C	1:A:278:LEU:HD23	2.27	0.56
2:B:557:LYS:HE2	2:B:663:LEU:O	2.05	0.56
2:B:231:GLN:HA	2:B:241:PRO:HG2	1.87	0.56
2:B:728:PHE:O	2:B:729:ASP:HB2	2.06	0.55
2:B:734:PRO:HB2	2:B:735:PRO:HD3	1.87	0.55
1:A:161:LEU:HG	1:A:169:VAL:HG13	1.88	0.55
3:T:58:A:C2'	3:T:59:U:H5"	2.36	0.55
1:A:198:VAL:HG22	1:A:198:VAL:O	2.06	0.55
2:B:631:PHE:O	2:B:633:PHE:N	2.39	0.55
2:B:75:VAL:HG23	2:B:113:SER:HB2	1.87	0.55
2:B:549:PHE:O	2:B:550:PRO:C	2.43	0.55
2:B:725:LEU:O	2:B:726:ALA:CB	2.53	0.55
2:B:369:GLN:O	2:B:372:ALA:HB3	2.06	0.55
2:B:381:GLN:HG3	2:B:386:ALA:O	2.07	0.55
2:B:564:ARG:O	2:B:564:ARG:HD2	2.07	0.55
2:B:178:HIS:HD2	2:B:182:TYR:O	1.90	0.55
3:T:45:U:H5"	3:T:46:G:H5"	1.89	0.55
1:A:65:LEU:O	1:A:69:GLU:HG3	2.06	0.55
2:B:348:ARG:HH11	2:B:348:ARG:HG3	1.72	0.55
2:B:549:PHE:CG	2:B:550:PRO:HD3	2.41	0.55
2:B:666:PRO:HB3	2:B:667:PRO:HD2	1.88	0.55
2:B:682:LEU:HD12	2:B:683:ALA:H	1.71	0.55
2:B:689:ARG:O	3:T:12:U:H5'	2.07	0.55
2:B:615:ALA:O	2:B:618:ALA:HB3	2.06	0.55
3:T:39:U:H2'	3:T:40:C:C6	2.42	0.55
3:T:54:U:C3'	3:T:58:A:N1	2.69	0.55
1:A:16:GLU:HA	1:A:19:LYS:CB	2.36	0.55
2:B:598:TRP:O	2:B:599:ALA:C	2.45	0.55
1:A:35:GLU:O	1:A:39:LEU:HD11	2.07	0.54
1:A:39:LEU:HD22	3:T:19:G:O6	2.07	0.54
2:B:775:ARG:HG3	2:B:775:ARG:HH11	1.71	0.54
2:B:452:ASP:O	2:B:453:LEU:HD23	2.07	0.54
2:B:222:ARG:O	2:B:222:ARG:HG3	2.07	0.54
2:B:530:ARG:HB2	2:B:530:ARG:NH1	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:10:G:H5"	3:T:11:C:H6	1.62	0.54
3:T:10:G:H5'	3:T:11:C:OP2	2.08	0.54
1:A:272:PRO:O	1:A:274:GLY:N	2.40	0.54
2:B:627:GLU:OE1	2:B:641:ARG:NH2	2.41	0.54
1:A:32:LEU:HA	1:A:36:MET:HG3	1.90	0.54
2:B:153:GLU:HG3	2:B:154:VAL:N	2.21	0.54
2:B:32:THR:HG21	2:B:156:LEU:HD23	1.90	0.54
2:B:151:PRO:HG2	2:B:232:ARG:NH2	2.22	0.54
2:B:718:ALA:HA	2:B:768:VAL:HG22	1.89	0.54
1:A:49:LYS:HA	1:A:52:GLN:CD	2.27	0.54
2:B:701:VAL:HG13	2:B:777:PHE:CE1	2.42	0.54
2:B:727:LEU:HD23	2:B:729:ASP:H	1.73	0.54
1:A:24:ARG:HB3	3:T:43:A:H5'	1.87	0.54
1:A:278:LEU:N	1:A:278:LEU:HD23	2.23	0.54
1:A:288:PRO:HG2	2:B:457:GLU:OE1	2.08	0.54
2:B:303:TRP:HB2	2:B:307:GLU:O	2.08	0.54
2:B:629:GLU:HB3	2:B:631:PHE:CE1	2.42	0.54
2:B:763:GLU:O	2:B:767:ARG:HG2	2.08	0.54
1:A:94:SER:O	2:B:594:VAL:HG13	2.07	0.54
3:T:24:G:O6	3:T:25:C:N4	2.41	0.54
2:B:553:VAL:O	2:B:556:LEU:HB3	2.08	0.54
1:A:39:LEU:HB3	3:T:19:G:O6	2.08	0.53
2:B:38:VAL:C	2:B:40:PRO:HD3	2.28	0.53
1:A:140:PRO:HD2	1:A:143:HIS:CD2	2.43	0.53
2:B:590:PHE:CD1	2:B:591:GLY:N	2.77	0.53
2:B:755:THR:HG22	2:B:756:LEU:N	2.22	0.53
1:A:31:LEU:HB3	1:A:35:GLU:OE1	2.07	0.53
2:B:602:ARG:NH1	2:B:602:ARG:HG3	2.20	0.53
1:A:32:LEU:HA	1:A:36:MET:HB2	1.90	0.53
3:T:1:G:O2'	3:T:2:C:H5	1.90	0.53
2:B:408:PRO:HG3	2:B:421:GLU:HG3	1.90	0.53
1:A:146:ARG:HG2	1:A:146:ARG:O	2.09	0.53
1:A:16:GLU:CA	1:A:19:LYS:HB2	2.38	0.53
2:B:516:MET:CE	2:B:546:THR:H	2.22	0.53
2:B:362:ARG:HH11	2:B:362:ARG:HG2	1.73	0.53
2:B:215:LEU:HA	2:B:333:LEU:O	2.08	0.53
3:T:30:G:O4'	3:T:31:A:C8	2.62	0.53
3:T:21:A:N3	3:T:21:A:H2'	2.23	0.53
2:B:621:GLY:O	2:B:622:LEU:HD23	2.09	0.53
2:B:536:PRO:CB	2:B:542:ALA:HA	2.39	0.53
1:A:22:LYS:HA	1:A:25:TYR:CD1	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HB3	1:A:245:PHE:CE1	2.43	0.53
2:B:61:LEU:HD12	2:B:109:GLN:HG3	1.90	0.53
3:T:10:G:H5"	3:T:11:C:C5	2.41	0.53
2:B:176:ASP:OD2	2:B:465:ARG:NH2	2.37	0.53
2:B:163:ASN:O	2:B:164:ARG:HD2	2.09	0.53
2:B:189:ALA:HB2	2:B:375:ARG:HA	1.91	0.53
2:B:140:LEU:HD11	2:B:149:ALA:HB3	1.89	0.53
3:T:23:A:H3'	6:T:2010:HOH:O	2.08	0.53
1:A:139:ILE:N	1:A:140:PRO:HD3	2.23	0.53
2:B:626:VAL:HG13	2:B:641:ARG:O	2.09	0.53
1:A:23:ALA:CB	3:T:44:G:H5"	2.37	0.53
1:A:127:VAL:HG23	2:B:577:PHE:CE2	2.44	0.53
2:B:694:PHE:HB2	2:B:747:LEU:O	2.08	0.53
2:B:682:LEU:HD12	2:B:683:ALA:N	2.24	0.53
1:A:24:ARG:NE	1:A:24:ARG:HA	2.24	0.53
3:T:44:G:C8	3:T:44:G:C3'	2.91	0.53
3:T:54:U:H3'	3:T:58:A:H61	1.73	0.53
2:B:82:ARG:HG2	2:B:82:ARG:HH11	1.74	0.53
2:B:761:VAL:HG13	2:B:762:GLU:N	2.23	0.52
3:T:27:U:H2'	3:T:28:G:H8	1.73	0.52
1:A:33:THR:HA	1:A:37:LYS:HE3	1.92	0.52
1:A:349:VAL:O	1:A:350:LEU:HB2	2.08	0.52
1:A:101:HIS:CE1	1:A:102:PRO:HD2	2.44	0.52
1:A:103:ILE:CD1	1:A:320:GLU:HG3	2.38	0.52
2:B:775:ARG:HD3	2:B:776:GLY:N	2.25	0.52
2:B:694:PHE:HB3	2:B:748:ARG:HA	1.91	0.52
2:B:762:GLU:C	2:B:764:ALA:H	2.12	0.52
3:T:23:A:N6	3:T:24:G:O6	2.42	0.52
1:A:17:GLU:O	1:A:21:LEU:HG	2.09	0.52
3:T:74:C:C4'	3:T:75:C:O5'	2.50	0.52
1:A:63:ALA:HB1	6:A:2004:HOH:O	2.08	0.52
1:A:133:ASN:ND2	1:A:134:PHE:CE2	2.78	0.52
3:T:23:A:C6	3:T:24:G:C6	2.98	0.52
1:A:26:LEU:HD23	1:A:26:LEU:O	2.09	0.52
2:B:633:PHE:CD1	2:B:634:LEU:HG	2.45	0.52
2:B:75:VAL:CG2	2:B:111:VAL:HG23	2.39	0.52
1:A:128:GLU:OE1	1:A:185:ARG:HD2	2.10	0.52
2:B:654:ALA:HB2	2:B:669:HIS:ND1	2.25	0.52
2:B:178:HIS:CD2	2:B:430:ARG:NH2	2.77	0.52
2:B:145:PRO:HB2	2:B:148:GLU:HG3	1.92	0.52
2:B:578:ARG:O	2:B:579:GLU:HB3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:LEU:HD21	2:B:590:PHE:CZ	2.45	0.52
2:B:165:PRO:HB2	2:B:363:GLY:O	2.10	0.52
2:B:761:VAL:HG22	2:B:765:VAL:HG13	1.91	0.51
2:B:136:PRO:HD2	2:B:139:ALA:HB2	1.93	0.51
2:B:695:ARG:CG	2:B:695:ARG:NH1	2.73	0.51
2:B:709:GLU:CD	2:B:775:ARG:HH12	2.13	0.51
2:B:425:ILE:HG23	2:B:435:VAL:HG11	1.91	0.51
1:A:33:THR:O	1:A:37:LYS:HD2	2.10	0.51
2:B:533:LEU:HB2	2:B:536:PRO:CG	2.34	0.51
2:B:554:ARG:HG2	2:B:554:ARG:HH11	1.75	0.51
2:B:246:VAL:HG23	2:B:324:VAL:HG22	1.90	0.51
3:T:60:U:H3'	3:T:61:C:H5	1.73	0.51
1:A:34:GLN:OE1	1:A:50:ARG:HA	2.10	0.51
1:A:140:PRO:N	1:A:143:HIS:HD2	2.09	0.51
2:B:99:LEU:O	2:B:101:GLN:N	2.42	0.51
1:A:145:ALA:O	1:A:149:TRP:HZ3	1.92	0.51
2:B:688:SER:HB3	2:B:752:PRO:HA	1.92	0.51
2:B:768:VAL:O	2:B:772:LEU:HB2	2.10	0.51
1:A:48:ARG:NH1	1:A:48:ARG:HG2	2.24	0.51
1:A:274:GLY:O	1:A:276:LYS:HG3	2.11	0.51
2:B:698:ALA:O	2:B:779:LEU:HD12	2.11	0.51
1:A:47:ARG:NH1	1:A:47:ARG:HG3	2.26	0.51
3:T:52:G:C3'	3:T:53:G:H5"	2.39	0.51
1:A:198:VAL:CG1	1:A:220:GLU:HB2	2.36	0.51
2:B:278:ARG:HH22	2:B:308:SER:HB3	1.76	0.51
2:B:309:PHE:CD1	2:B:309:PHE:N	2.79	0.51
2:B:171:LEU:O	2:B:171:LEU:HD13	2.10	0.51
3:T:30:G:O6	3:T:41:G:O6	2.29	0.51
1:A:15:LEU:HD23	1:A:19:LYS:NZ	2.25	0.51
1:A:161:LEU:HG	1:A:169:VAL:CG1	2.41	0.51
2:B:264:ASP:OD1	2:B:266:ARG:HD3	2.11	0.51
2:B:355:GLU:HG2	6:B:2078:HOH:O	2.10	0.51
2:B:692:ALA:HB1	2:B:748:ARG:HG2	1.93	0.50
2:B:300:ILE:HG12	2:B:314:ALA:HB2	1.92	0.50
3:T:6:G:O2'	3:T:7:G:H5'	2.11	0.50
1:A:115:ARG:HD2	6:B:2120:HOH:O	2.10	0.50
2:B:766:SER:O	2:B:769:ALA:N	2.42	0.50
2:B:571:PHE:HA	2:B:586:ALA:O	2.11	0.50
2:B:762:GLU:HA	2:B:765:VAL:CG2	2.35	0.50
3:T:40:C:H5'	3:T:41:G:OP2	2.11	0.50
1:A:331:ASP:HB3	1:A:334:TYR:CD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:PHE:O	1:A:345:GLN:HB2	2.10	0.50
2:B:728:PHE:CZ	2:B:744:ALA:HB1	2.46	0.50
2:B:179:ALA:HA	2:B:430:ARG:HE	1.77	0.50
2:B:709:GLU:CD	2:B:775:ARG:HH22	2.15	0.50
2:B:734:PRO:C	2:B:736:LEU:H	2.14	0.50
2:B:696:ASP:OD2	2:B:746:HIS:NE2	2.44	0.50
2:B:92:PRO:HG3	2:B:114:PHE:CE1	2.46	0.50
2:B:695:ARG:NE	2:B:761:VAL:HG21	2.26	0.50
2:B:718:ALA:HA	2:B:768:VAL:CG2	2.41	0.50
2:B:747:LEU:HD12	2:B:747:LEU:N	2.25	0.50
2:B:764:ALA:O	2:B:768:VAL:HG23	2.11	0.50
2:B:408:PRO:CG	2:B:421:GLU:HG3	2.42	0.50
1:A:218:GLN:HA	1:A:317:LEU:O	2.11	0.50
1:A:39:LEU:HD23	1:A:42:LEU:HD22	1.92	0.50
1:A:288:PRO:HD3	6:A:2032:HOH:O	2.12	0.50
2:B:255:GLU:OE1	2:B:375:ARG:NH1	2.44	0.50
2:B:265:LEU:HD21	2:B:332:ALA:HB2	1.94	0.50
2:B:671:PHE:CD1	2:B:673:LEU:HD12	2.46	0.50
1:A:49:LYS:HB2	1:A:50:ARG:HH12	1.76	0.50
2:B:714:VAL:O	2:B:718:ALA:HB2	2.11	0.49
2:B:758:ASP:O	2:B:761:VAL:HG12	2.12	0.49
3:T:69:C:H2'	3:T:70:G:C8	2.46	0.49
2:B:392:LEU:O	2:B:393:LEU:HD12	2.12	0.49
2:B:671:PHE:C	2:B:671:PHE:CD1	2.85	0.49
1:A:262:GLU:OE1	2:B:458:ASP:CA	2.49	0.49
1:A:57:ILE:HD13	1:A:61:LEU:HD23	1.94	0.49
2:B:28:LEU:HD11	2:B:180:LEU:HD22	1.94	0.49
2:B:219:PHE:CE1	2:B:387:ARG:HB2	2.47	0.49
2:B:576:VAL:HG12	2:B:577:PHE:N	2.26	0.49
3:T:8:U:H1'	3:T:48:C:H1'	1.95	0.49
2:B:147:SER:O	2:B:149:ALA:N	2.45	0.49
2:B:206:ASP:OD2	2:B:276:ARG:NH1	2.29	0.49
2:B:464:ALA:O	2:B:468:GLY:N	2.46	0.49
3:T:45:U:H3'	3:T:46:G:C5'	2.39	0.49
1:A:347:LYS:HA	6:A:2049:HOH:O	2.12	0.49
2:B:516:MET:HE1	2:B:546:THR:H	1.77	0.49
1:A:192:PRO:HD3	1:A:307:TYR:CE2	2.47	0.49
2:B:622:LEU:HA	2:B:645:GLU:OE2	2.13	0.49
2:B:733:GLY:H	2:B:736:LEU:HD12	1.77	0.49
2:B:497:ARG:HD3	2:B:501:VAL:HG23	1.95	0.49
1:A:298:ARG:HB3	1:A:303:LEU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:NH1	1:A:304:PRO:O	2.45	0.49
1:A:213:GLU:H	4:A:1351:FYA:H62	1.60	0.49
1:A:98:GLY:O	1:A:347:LYS:HE3	2.12	0.49
1:A:158:GLY:C	2:B:530:ARG:HD3	2.33	0.49
2:B:775:ARG:HD2	2:B:777:PHE:CE2	2.48	0.49
2:B:497:ARG:NH1	2:B:619:ARG:HH12	2.11	0.49
1:A:207:GLN:HA	1:A:207:GLN:NE2	2.27	0.49
2:B:221:LEU:HB2	2:B:329:GLU:O	2.13	0.49
2:B:709:GLU:OE1	2:B:775:ARG:NH2	2.46	0.49
2:B:707:TYR:CD1	2:B:727:LEU:HD12	2.48	0.48
1:A:256:VAL:HG22	1:A:257:TYR:H	1.78	0.48
2:B:698:ALA:HA	2:B:744:ALA:HA	1.95	0.48
2:B:696:ASP:O	2:B:697:LEU:HB3	2.12	0.48
2:B:596:LEU:O	2:B:598:TRP:N	2.46	0.48
3:T:53:G:H2'	3:T:54:U:O4'	2.13	0.48
1:A:349:VAL:O	1:A:349:VAL:CG1	2.60	0.48
2:B:206:ASP:CG	2:B:276:ARG:HH11	2.12	0.48
3:T:57:G:N2	6:T:2025:HOH:O	2.47	0.48
1:A:54:LEU:HD12	3:T:56:C:H5'	1.95	0.48
2:B:457:GLU:HA	2:B:460:VAL:HG12	1.95	0.48
1:A:162:GLU:O	1:A:185:ARG:NH2	2.47	0.48
2:B:712:ALA:O	2:B:716:GLU:HB2	2.12	0.48
2:B:482:ALA:HB3	2:B:485:ASN:ND2	2.28	0.48
2:B:577:PHE:O	2:B:578:ARG:HB3	2.13	0.48
2:B:536:PRO:CG	2:B:542:ALA:HA	2.44	0.48
1:A:331:ASP:O	1:A:334:TYR:HD2	1.96	0.48
2:B:38:VAL:CG2	2:B:153:GLU:HB3	2.44	0.48
2:B:202:LEU:HD12	2:B:203:LYS:H	1.77	0.48
2:B:695:ARG:HE	2:B:761:VAL:HG11	1.78	0.48
2:B:713:LEU:HD23	2:B:713:LEU:O	2.13	0.48
1:A:186:TYR:HE1	2:B:488:VAL:HG11	1.78	0.48
2:B:723:GLU:OE2	2:B:748:ARG:HD2	2.13	0.48
2:B:39:PHE:O	2:B:41:ILE:HG13	2.14	0.48
2:B:643:LEU:HD13	2:B:648:GLU:HA	1.95	0.48
2:B:722:LEU:HD11	2:B:724:SER:O	2.14	0.48
2:B:294:HIS:O	2:B:296:GLU:N	2.47	0.48
2:B:231:GLN:HG2	2:B:241:PRO:CB	2.44	0.48
1:A:107:GLU:O	1:A:111:VAL:HG23	2.14	0.48
2:B:235:PHE:HA	2:B:239:MET:O	2.13	0.48
1:A:35:GLU:C	1:A:39:LEU:HD11	2.35	0.48
3:T:71:G:C2'	3:T:72:C:H5'	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLY:HA3	4:A:1351:FYA:H1'	1.96	0.48
1:A:87:ASP:O	1:A:88:VAL:C	2.52	0.48
2:B:297:ASP:OD1	2:B:346:THR:HG23	2.14	0.48
2:B:656:HIS:HB3	2:B:659:ILE:HG12	1.96	0.47
1:A:161:LEU:HD12	1:A:162:GLU:H	1.79	0.47
2:B:43:ARG:HH11	2:B:43:ARG:HG3	1.79	0.47
1:A:348:GLY:O	1:A:350:LEU:N	2.42	0.47
2:B:725:LEU:HD13	2:B:745:PHE:HD2	1.77	0.47
1:A:281:GLY:HA2	4:A:1351:FYA:O3'	2.14	0.47
1:A:275:GLY:C	1:A:276:LYS:HG3	2.35	0.47
2:B:709:GLU:OE1	2:B:775:ARG:NH1	2.47	0.47
2:B:564:ARG:N	2:B:564:ARG:HH11	2.13	0.47
2:B:655:LEU:HB3	2:B:668:VAL:CG1	2.44	0.47
2:B:56:ILE:HB	2:B:59:THR:OG1	2.15	0.47
1:A:93:ALA:HA	2:B:595:GLY:O	2.15	0.47
1:A:197:VAL:HG13	1:A:197:VAL:O	2.14	0.47
2:B:641:ARG:NH1	2:B:643:LEU:HD21	2.29	0.47
2:B:231:GLN:NE2	6:B:2050:HOH:O	2.48	0.47
2:B:755:THR:HG22	2:B:756:LEU:H	1.78	0.47
1:A:23:ALA:HB3	3:T:44:G:H5"	1.96	0.47
2:B:294:HIS:ND1	2:B:296:GLU:HB2	2.27	0.47
3:T:45:U:C5'	3:T:46:G:H5"	2.45	0.47
3:T:8:U:H4'	3:T:48:C:C4'	2.44	0.47
2:B:696:ASP:CG	2:B:746:HIS:CD2	2.87	0.47
2:B:754:ARG:NH1	2:B:756:LEU:HD23	2.28	0.47
1:A:48:ARG:CG	1:A:48:ARG:NH1	2.78	0.47
3:T:8:U:C1'	3:T:48:C:H1'	2.45	0.47
2:B:654:ALA:HB2	2:B:669:HIS:CE1	2.49	0.47
1:A:262:GLU:HA	1:A:262:GLU:OE2	2.15	0.47
2:B:191:LEU:CD1	2:B:374:ARG:HD2	2.40	0.47
2:B:348:ARG:HG3	2:B:348:ARG:NH1	2.30	0.47
3:T:67:C:H2'	3:T:68:U:C5'	2.45	0.46
2:B:700:VAL:CG1	2:B:778:GLY:HA3	2.45	0.46
2:B:722:LEU:HD21	2:B:725:LEU:HD23	1.95	0.46
1:A:35:GLU:CA	1:A:39:LEU:HD11	2.45	0.46
3:T:58:A:H3'	3:T:58:A:H8	1.80	0.46
1:A:331:ASP:OD1	1:A:333:ARG:HB2	2.15	0.46
1:A:161:LEU:HD12	1:A:162:GLU:N	2.30	0.46
3:T:58:A:H3'	3:T:58:A:C8	2.50	0.46
2:B:423:GLU:O	2:B:427:ILE:HG13	2.15	0.46
3:T:9:A:H2'	3:T:45:U:O4	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:HA	1:A:19:LYS:CG	2.45	0.46
2:B:713:LEU:HD23	2:B:713:LEU:C	2.36	0.46
2:B:718:ALA:CB	2:B:722:LEU:HD22	2.46	0.46
2:B:623:ALA:HB3	2:B:645:GLU:CA	2.33	0.46
2:B:421:GLU:O	2:B:425:ILE:HG12	2.16	0.46
2:B:147:SER:C	2:B:149:ALA:N	2.69	0.46
1:A:140:PRO:N	1:A:143:HIS:CD2	2.84	0.46
1:A:143:HIS:HB3	1:A:146:ARG:CB	2.37	0.46
1:A:34:GLN:OE1	1:A:53:GLU:HB2	2.15	0.46
2:B:695:ARG:HH12	3:T:26:A:P	2.38	0.46
2:B:470:GLU:HG3	2:B:470:GLU:H	1.50	0.46
1:A:23:ALA:HB3	3:T:44:G:C5'	2.46	0.46
1:A:330:PRO:HG2	1:A:331:ASP:H	1.81	0.46
2:B:75:VAL:HG22	2:B:111:VAL:CG2	2.46	0.46
2:B:523:ARG:HD3	2:B:662:GLU:OE1	2.16	0.46
1:A:26:LEU:C	1:A:26:LEU:HD23	2.36	0.46
2:B:404:ILE:N	2:B:444:VAL:O	2.44	0.46
2:B:285:THR:HB	2:B:317:MET:SD	2.56	0.46
1:A:22:LYS:CA	1:A:25:TYR:HB2	2.42	0.46
1:A:72:LEU:CD1	1:A:76:ALA:HB2	2.45	0.46
1:A:258:PHE:HB2	1:A:261:VAL:HG22	1.98	0.46
2:B:666:PRO:CB	2:B:667:PRO:HD2	2.45	0.46
1:A:265:ALA:HB2	2:B:469:TYR:HE1	1.81	0.46
2:B:96:LEU:HD11	2:B:118:LEU:HD21	1.97	0.45
2:B:38:VAL:O	2:B:40:PRO:HD3	2.16	0.45
2:B:362:ARG:NH1	2:B:362:ARG:HG2	2.30	0.45
3:T:19:G:O2'	3:T:20:U:H5"	2.16	0.45
2:B:578:ARG:O	2:B:580:ARG:N	2.43	0.45
2:B:119:SER:HB2	2:B:131:GLY:O	2.15	0.45
3:T:60:U:H6	3:T:60:U:OP2	1.99	0.45
3:T:46:G:O2'	3:T:47:U:OP1	2.30	0.45
2:B:762:GLU:C	2:B:764:ALA:N	2.69	0.45
2:B:762:GLU:CA	2:B:765:VAL:HG22	2.39	0.45
1:A:50:ARG:HD3	3:T:56:C:H6	1.75	0.45
1:A:204:ARG:NH2	4:A:1351:FYA:O2P	2.42	0.45
2:B:28:LEU:HD11	2:B:180:LEU:CD2	2.47	0.45
1:A:88:VAL:C	1:A:90:LEU:H	2.19	0.45
2:B:38:VAL:HG23	2:B:153:GLU:HB3	1.99	0.45
2:B:715:ARG:NH1	2:B:715:ARG:HB2	2.32	0.45
2:B:502:LEU:C	2:B:504:GLY:N	2.70	0.45
3:T:69:C:H2'	3:T:70:G:H8	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:VAL:HG12	1:A:265:ALA:C	2.37	0.45
2:B:528:PRO:HA	2:B:529:PRO:HD3	1.87	0.45
2:B:710:VAL:O	2:B:714:VAL:HG23	2.16	0.45
2:B:559:ASN:O	2:B:563:ASP:O	2.35	0.45
2:B:720:PRO:C	2:B:722:LEU:H	2.19	0.45
2:B:278:ARG:O	2:B:279:GLU:C	2.55	0.45
1:A:160:ARG:HB3	2:B:580:ARG:NH1	2.32	0.45
2:B:82:ARG:HB2	6:B:2019:HOH:O	2.16	0.45
2:B:358:HIS:HE1	2:B:362:ARG:CZ	2.30	0.45
1:A:229:ALA:N	1:A:232:HIS:ND1	2.47	0.45
3:T:25:C:N1	3:T:26:A:C8	2.85	0.45
2:B:191:LEU:HD21	2:B:388:VAL:CB	2.46	0.45
2:B:82:ARG:HH22	2:B:134:GLU:CD	2.19	0.45
2:B:265:LEU:HD23	2:B:268:VAL:HG21	1.98	0.45
1:A:175:LEU:HB3	1:A:203:PHE:CD1	2.52	0.45
2:B:140:LEU:HD11	2:B:149:ALA:CB	2.47	0.45
2:B:730:LEU:HD11	2:B:741:LYS:HD2	1.98	0.45
1:A:104:THR:O	1:A:105:LEU:C	2.56	0.45
1:A:62:GLU:HG3	1:A:63:ALA:N	2.33	0.44
1:A:65:LEU:HD13	1:A:65:LEU:O	2.16	0.44
2:B:725:LEU:HD22	2:B:747:LEU:HG	1.98	0.44
2:B:629:GLU:OE1	2:B:641:ARG:HD3	2.17	0.44
1:A:69:GLU:O	1:A:72:LEU:N	2.49	0.44
1:A:163:GLY:HA2	1:A:185:ARG:NH2	2.33	0.44
2:B:212:HIS:CE1	2:B:394:GLU:OE2	2.70	0.44
2:B:32:THR:HG22	2:B:158:LEU:HD21	1.98	0.44
2:B:221:LEU:HD23	2:B:386:ALA:HB2	1.99	0.44
2:B:432:GLY:O	2:B:447:PRO:HG3	2.17	0.44
1:A:269:VAL:HG13	1:A:280:LEU:HD12	1.99	0.44
3:T:28:G:N1	3:T:29:C:N4	2.65	0.44
1:A:165:LEU:HD11	1:A:303:LEU:CD1	2.39	0.44
2:B:96:LEU:HD12	2:B:99:LEU:HD21	2.00	0.44
1:A:349:VAL:O	1:A:350:LEU:CD2	2.64	0.44
2:B:609:LEU:C	2:B:611:GLY:N	2.66	0.44
3:T:25:C:C2	3:T:26:A:C8	3.06	0.44
2:B:766:SER:O	2:B:770:GLU:HG2	2.17	0.44
2:B:231:GLN:HA	2:B:241:PRO:CG	2.47	0.44
1:A:286:VAL:HG23	1:A:312:GLY:O	2.17	0.44
2:B:221:LEU:CD2	2:B:386:ALA:HB2	2.48	0.44
2:B:325:ARG:O	2:B:328:THR:HG23	2.17	0.44
2:B:37:ARG:NH1	2:B:37:ARG:HG2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:10:G:C6	3:T:26:A:C2	3.06	0.44
1:A:53:GLU:C	1:A:55:ASN:N	2.70	0.44
2:B:325:ARG:H	2:B:328:THR:HG23	1.81	0.44
1:A:203:PHE:CD2	1:A:215:VAL:HG13	2.53	0.44
2:B:34:ARG:NH2	2:B:36:GLU:OE1	2.40	0.44
1:A:163:GLY:N	1:A:169:VAL:HG12	2.33	0.44
3:T:10:G:H5'	3:T:11:C:O5'	2.18	0.44
1:A:141:GLU:C	1:A:143:HIS:N	2.70	0.44
2:B:198:LEU:HD22	2:B:217:TYR:CD2	2.53	0.44
2:B:294:HIS:CD2	2:B:349:ARG:HE	2.36	0.44
1:A:72:LEU:O	1:A:72:LEU:HD13	2.17	0.44
2:B:496:GLN:O	2:B:497:ARG:C	2.55	0.44
2:B:404:ILE:HG12	2:B:444:VAL:O	2.18	0.43
2:B:161:THR:HA	2:B:162:PRO:HD3	1.90	0.43
2:B:530:ARG:CB	2:B:530:ARG:HH11	2.32	0.43
2:B:516:MET:HB2	2:B:545:ARG:HA	2.00	0.43
3:T:72:C:N4	3:T:73:A:N6	2.65	0.43
1:A:73:GLU:O	1:A:77:LEU:HD13	2.17	0.43
3:T:18:G:H2'	3:T:19:G:OP2	2.18	0.43
2:B:167:ALA:C	2:B:169:GLY:H	2.21	0.43
2:B:279:GLU:HG3	2:B:295:PRO:HD3	2.00	0.43
1:A:67:ALA:HB3	1:A:68:ARG:NH2	2.33	0.43
2:B:120:PRO:HG3	2:B:133:LEU:HD13	2.01	0.43
1:A:92:GLY:O	1:A:93:ALA:C	2.56	0.43
1:A:255:PRO:HB2	2:B:29:GLY:HA2	2.01	0.43
2:B:370:VAL:HG22	2:B:392:LEU:CD1	2.49	0.43
1:A:165:LEU:O	1:A:167:GLU:N	2.52	0.43
1:A:261:VAL:HG11	4:A:1351:FYA:HZ	2.00	0.43
1:A:272:PRO:C	1:A:274:GLY:N	2.72	0.43
1:A:102:PRO:HG3	1:A:346:PHE:CD1	2.54	0.43
2:B:612:TYR:O	2:B:615:ALA:HB3	2.18	0.43
2:B:184:LEU:HD23	2:B:185:VAL:N	2.33	0.43
1:A:305:PRO:HG3	1:A:308:ARG:NH2	2.33	0.43
2:B:99:LEU:HD12	2:B:99:LEU:O	2.19	0.43
1:A:332:ILE:O	1:A:332:ILE:HG12	2.19	0.43
2:B:695:ARG:CZ	2:B:761:VAL:HG11	2.48	0.43
2:B:517:ASP:OD1	2:B:540:GLU:HA	2.18	0.43
1:A:145:ALA:O	1:A:149:TRP:CZ3	2.72	0.43
2:B:298:LEU:O	2:B:314:ALA:HB3	2.19	0.43
1:A:334:TYR:HB3	1:A:342:PHE:CZ	2.53	0.43
2:B:701:VAL:HG22	2:B:777:PHE:CD1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:CG	1:A:87:ASP:O	2.57	0.43
2:B:497:ARG:HG2	6:B:2122:HOH:O	2.19	0.43
2:B:165:PRO:HG3	2:B:451:LEU:HD12	1.99	0.43
2:B:270:GLU:OE2	2:B:305:GLY:N	2.46	0.43
2:B:644:VAL:HG11	2:B:678:PRO:HD2	2.01	0.43
1:A:268:ALA:HA	1:A:278:LEU:O	2.18	0.43
1:A:149:TRP:HB3	1:A:177:THR:CB	2.49	0.43
2:B:705:THR:HG23	2:B:706:PRO:HD2	2.00	0.43
2:B:89:LEU:HD22	2:B:90:ALA:N	2.34	0.43
3:T:50:G:O2'	3:T:51:C:H5'	2.18	0.42
2:B:757:ARG:HD3	2:B:758:ASP:H	1.84	0.42
1:A:22:LYS:HA	1:A:25:TYR:CB	2.45	0.42
1:A:32:LEU:HA	1:A:36:MET:CB	2.49	0.42
2:B:198:LEU:HA	2:B:199:PRO:HD3	1.78	0.42
2:B:377:LEU:HB3	2:B:388:VAL:CG1	2.48	0.42
2:B:263:PHE:CZ	2:B:300:ILE:HG21	2.54	0.42
2:B:598:TRP:CD1	2:B:598:TRP:N	2.87	0.42
1:A:137:LEU:O	1:A:260:PHE:HB3	2.19	0.42
2:B:60:ARG:HG2	6:B:2016:HOH:O	2.17	0.42
3:T:41:G:C4'	3:T:42:C:OP2	2.63	0.42
2:B:539:PRO:HG2	2:B:540:GLU:OE2	2.19	0.42
1:A:340:LEU:HD21	2:B:570:LEU:CD2	2.48	0.42
1:A:315:PHE:C	1:A:315:PHE:CD1	2.92	0.42
2:B:299:VAL:CG1	2:B:300:ILE:N	2.82	0.42
2:B:279:GLU:CB	2:B:295:PRO:HB3	2.41	0.42
1:A:221:GLY:HA3	1:A:315:PHE:CZ	2.55	0.42
1:A:115:ARG:NH1	2:B:489:GLU:OE2	2.52	0.42
1:A:203:PHE:CE2	1:A:215:VAL:HG13	2.54	0.42
2:B:200:PHE:HA	2:B:270:GLU:O	2.19	0.42
3:T:61:C:H6	3:T:61:C:P	2.42	0.42
1:A:53:GLU:O	1:A:54:LEU:C	2.58	0.42
2:B:498:LEU:O	2:B:499:ARG:C	2.58	0.42
2:B:696:ASP:HB2	3:T:37:A:O4'	2.20	0.42
2:B:587:GLY:HA3	2:B:671:PHE:CE2	2.55	0.42
1:A:21:LEU:C	1:A:23:ALA:N	2.73	0.42
3:T:67:C:C2'	3:T:68:U:H5'	2.47	0.42
1:A:178:HIS:CD2	1:A:178:HIS:N	2.86	0.42
3:T:24:G:C6	3:T:25:C:C4	3.07	0.42
2:B:633:PHE:HD1	2:B:634:LEU:HG	1.84	0.42
1:A:101:HIS:ND1	1:A:102:PRO:CD	2.82	0.42
2:B:121:ARG:N	2:B:128:TYR:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:668:VAL:HG22	2:B:669:HIS:N	2.35	0.42
2:B:82:ARG:NH1	2:B:82:ARG:HG2	2.34	0.42
1:A:324:MET:SD	1:A:332:ILE:HB	2.60	0.42
2:B:23:GLU:O	2:B:26:ALA:HB3	2.20	0.42
3:T:39:U:H2'	3:T:40:C:C5	2.55	0.42
2:B:578:ARG:C	2:B:580:ARG:N	2.70	0.42
2:B:490:ALA:HB3	2:B:491:PRO:CD	2.47	0.42
2:B:282:ARG:NH1	2:B:290:GLU:CG	2.83	0.42
3:T:1:G:O2'	3:T:2:C:C5	2.71	0.42
2:B:724:SER:HB3	2:B:725:LEU:H	1.68	0.41
1:A:31:LEU:C	1:A:33:THR:N	2.73	0.41
3:T:73:A:N7	3:T:74:C:C4	2.88	0.41
1:A:18:LEU:C	1:A:20:ALA:H	2.23	0.41
1:A:325:LEU:HD22	1:A:325:LEU:C	2.40	0.41
2:B:751:HIS:HB3	2:B:754:ARG:O	2.19	0.41
1:A:141:GLU:C	1:A:143:HIS:H	2.23	0.41
1:A:182:MET:HB3	1:A:198:VAL:HG11	2.01	0.41
1:A:197:VAL:HG23	1:A:220:GLU:O	2.20	0.41
1:A:18:LEU:C	1:A:20:ALA:N	2.73	0.41
1:A:216:PHE:HB2	1:A:320:GLU:OE1	2.20	0.41
1:A:72:LEU:HA	1:A:75:ALA:CB	2.45	0.41
2:B:612:TYR:O	2:B:616:LEU:N	2.45	0.41
2:B:43:ARG:NH1	2:B:43:ARG:HG3	2.35	0.41
2:B:437:GLY:HA3	2:B:442:TYR:CD2	2.54	0.41
2:B:690:HIS:HA	2:B:691:PRO:HD3	1.90	0.41
1:A:34:GLN:HG2	1:A:50:ARG:HH21	1.85	0.41
2:B:703:ALA:N	2:B:704:PRO:HD2	2.34	0.41
3:T:6:G:H2'	3:T:7:G:O4'	2.20	0.41
2:B:37:ARG:HG2	2:B:37:ARG:HH11	1.85	0.41
2:B:539:PRO:HA	2:B:542:ALA:HB2	2.02	0.41
2:B:282:ARG:NH1	2:B:290:GLU:OE2	2.53	0.41
3:T:67:C:C4	3:T:68:U:C5	3.08	0.41
2:B:538:ALA:O	2:B:541:LYS:N	2.48	0.41
2:B:613:LEU:O	2:B:616:LEU:HB3	2.21	0.41
2:B:700:VAL:O	2:B:700:VAL:HG13	2.20	0.41
2:B:365:ASP:OD1	2:B:448:SER:OG	2.34	0.41
2:B:294:HIS:C	2:B:296:GLU:H	2.24	0.41
2:B:519:GLU:C	2:B:521:ALA:N	2.74	0.41
2:B:533:LEU:HD13	2:B:542:ALA:O	2.20	0.41
2:B:564:ARG:O	2:B:565:PRO:C	2.58	0.41
2:B:278:ARG:O	2:B:280:GLY:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLU:HG2	1:A:84:GLU:H	1.54	0.41
3:T:24:G:H4'	6:T:2009:HOH:O	2.19	0.41
1:A:262:GLU:CD	1:A:263:PRO:HD3	2.40	0.41
2:B:549:PHE:HA	2:B:552:LEU:HB2	2.02	0.41
2:B:695:ARG:HE	2:B:761:VAL:CG1	2.33	0.41
3:T:26:A:C2'	3:T:27:U:H5'	2.51	0.41
2:B:773:ARG:CG	2:B:774:ALA:N	2.84	0.41
2:B:28:LEU:HD13	2:B:176:ASP:HB3	2.03	0.41
2:B:631:PHE:C	2:B:633:PHE:H	2.24	0.41
2:B:662:GLU:C	2:B:664:GLU:H	2.24	0.41
2:B:84:GLY:O	2:B:137:GLU:HB2	2.21	0.41
2:B:163:ASN:O	2:B:452:ASP:HB3	2.21	0.41
2:B:108:ILE:HG22	2:B:109:GLN:HG2	2.02	0.41
1:A:175:LEU:HB3	1:A:203:PHE:HD1	1.85	0.41
1:A:180:SER:O	1:A:183:GLN:HB2	2.21	0.41
1:A:21:LEU:C	1:A:23:ALA:H	2.23	0.41
2:B:283:LEU:HD13	2:B:284:LYS:N	2.36	0.41
1:A:48:ARG:O	1:A:52:GLN:HG3	2.21	0.41
1:A:165:LEU:HD12	1:A:301:LEU:CD2	2.45	0.41
1:A:252:ARG:HB2	1:A:277:TRP:CH2	2.56	0.41
2:B:643:LEU:HD13	2:B:648:GLU:CA	2.50	0.41
2:B:634:LEU:O	2:B:635:HIS:C	2.59	0.41
2:B:462:GLU:OE1	2:B:465:ARG:NH1	2.54	0.41
2:B:520:ASP:OD1	2:B:554:ARG:NH2	2.42	0.41
1:A:256:VAL:HG22	1:A:257:TYR:N	2.34	0.41
2:B:297:ASP:OD2	2:B:350:HIS:HE1	2.04	0.41
2:B:212:HIS:HE1	2:B:394:GLU:OE2	2.02	0.41
2:B:527:ASP:OD2	2:B:527:ASP:N	2.54	0.41
3:T:76:A:H3'	6:T:2032:HOH:O	2.20	0.41
2:B:720:PRO:O	2:B:722:LEU:N	2.54	0.41
2:B:761:VAL:CG1	2:B:762:GLU:N	2.84	0.41
1:A:140:PRO:CD	1:A:143:HIS:CD2	3.03	0.41
2:B:178:HIS:CD2	2:B:182:TYR:O	2.70	0.41
2:B:713:LEU:HD22	2:B:772:LEU:HD12	2.03	0.40
3:T:54:U:O5'	3:T:54:U:H6	2.04	0.40
3:T:54:U:H2'	3:T:58:A:C2	2.55	0.40
2:B:535:ASN:N	2:B:535:ASN:OD1	2.54	0.40
1:A:58:LYS:CE	1:A:61:LEU:HD11	2.49	0.40
1:A:327:TYR:CB	1:A:329:ILE:HD11	2.42	0.40
2:B:727:LEU:HD23	2:B:727:LEU:C	2.40	0.40
2:B:573:VAL:HG22	2:B:585:LEU:HD13	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:695:ARG:NE	2:B:761:VAL:HG11	2.35	0.40
3:T:23:A:C6	3:T:24:G:O6	2.75	0.40
1:A:139:ILE:HA	1:A:143:HIS:CD2	2.57	0.40
1:A:49:LYS:O	1:A:52:GLN:HB2	2.19	0.40
2:B:605:GLY:O	2:B:608:LEU:N	2.44	0.40
2:B:50:VAL:HG12	2:B:83:LYS:HA	2.01	0.40
2:B:285:THR:O	2:B:320:ALA:HB2	2.21	0.40
1:A:155:THR:O	1:A:155:THR:HG23	2.22	0.40
1:A:126:GLU:OE2	2:B:575:ARG:HB2	2.21	0.40
1:A:151:THR:HG22	6:A:2013:HOH:O	2.21	0.40
3:T:59:U:H2'	3:T:60:U:O4'	2.22	0.40
2:B:545:ARG:NH2	2:B:574:GLY:HA3	2.36	0.40
2:B:255:GLU:OE2	2:B:375:ARG:HD2	2.21	0.40
2:B:655:LEU:CB	2:B:668:VAL:HG13	2.51	0.40
3:T:58:A:H2'	3:T:59:U:H5"	2.02	0.40
3:T:60:U:H3'	3:T:61:C:C6	2.57	0.40
1:A:322:LEU:O	1:A:326:ARG:HB2	2.20	0.40
2:B:62:LYS:O	2:B:75:VAL:HA	2.20	0.40
2:B:571:PHE:CE1	2:B:573:VAL:HG23	2.48	0.40
2:B:226:SER:HB2	6:B:2046:HOH:O	2.21	0.40
1:A:150:ASP:HB3	1:A:205:PHE:HB3	2.02	0.40
1:A:42:LEU:HB3	1:A:43:PRO:HD3	2.03	0.40
2:B:214:THR:HA	2:B:393:LEU:O	2.21	0.40
1:A:275:GLY:O	1:A:276:LYS:HG3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:53:G:O2'	3:T:53:G:O2'[5_554]	1.74	0.46

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	334/350 (95%)	269 (80%)	47 (14%)	18 (5%)	2 14
2	B	779/785 (99%)	662 (85%)	90 (12%)	27 (4%)	4 24
All	All	1113/1135 (98%)	931 (84%)	137 (12%)	45 (4%)	4 21

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ALA
1	A	88	VAL
1	A	263	PRO
1	A	273	GLU
1	A	349	VAL
2	B	100	GLY
2	B	243	ASN
2	B	578	ARG
2	B	632	PRO
2	B	726	ALA
2	B	737	PRO
1	A	27	GLY
1	A	47	ARG
1	A	69	GLU
1	A	84	GLU
1	A	344	GLU
1	A	89	SER
2	B	244	ASN
2	B	279	GLU
2	B	295	PRO
2	B	560	LEU
2	B	599	ALA
2	B	601	GLU
2	B	628	ALA
2	B	735	PRO
2	B	776	GLY
1	A	70	LYS
1	A	83	ARG
1	A	140	PRO
2	B	281	GLU
2	B	697	LEU
2	B	721	TYR
1	A	32	LEU
1	A	166	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	148	GLU
2	B	195	ALA
2	B	691	PRO
2	B	729	ASP
2	B	734	PRO
2	B	597	PRO
1	A	274	GLY
2	B	506	GLY
2	B	666	PRO
1	A	164	PRO
2	B	50	VAL

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	267/277 (96%)	244 (91%)	23 (9%)	13 45
2	B	626/630 (99%)	577 (92%)	49 (8%)	16 49
All	All	893/907 (98%)	821 (92%)	72 (8%)	15 47

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	45	GLU
1	A	46	GLU
1	A	53	GLU
1	A	57	ILE
1	A	68	ARG
1	A	72	LEU
1	A	74	GLU
1	A	83	ARG
1	A	84	GLU
1	A	104	THR
1	A	140	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	151	THR
1	A	178	HIS
1	A	191	THR
1	A	198	VAL
1	A	205	PHE
1	A	213	GLU
1	A	262	GLU
1	A	263	PRO
1	A	288	PRO
1	A	322	LEU
1	A	325	LEU
2	B	22	GLU
2	B	80	ASN
2	B	89	LEU
2	B	101	GLN
2	B	120	PRO
2	B	180	LEU
2	B	184	LEU
2	B	188	GLU
2	B	230	MET
2	B	241	PRO
2	B	276	ARG
2	B	313	LEU
2	B	328	THR
2	B	329	GLU
2	B	333	LEU
2	B	353	ARG
2	B	362	ARG
2	B	375	ARG
2	B	438	GLU
2	B	441	THR
2	B	445	THR
2	B	459	LEU
2	B	460	VAL
2	B	465	ARG
2	B	470	GLU
2	B	497	ARG
2	B	536	PRO
2	B	548	LEU
2	B	564	ARG
2	B	571	PHE
2	B	575	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	578	ARG
2	B	579	GLU
2	B	584	HIS
2	B	590	PHE
2	B	598	TRP
2	B	602	ARG
2	B	619	ARG
2	B	670	LEU
2	B	678	PRO
2	B	679	ASP
2	B	696	ASP
2	B	711	GLU
2	B	716	GLU
2	B	725	LEU
2	B	746	HIS
2	B	757	ARG
2	B	759	GLU
2	B	775	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	207	GLN
1	A	218	GLN
2	B	54	HIS
2	B	80	ASN
2	B	178	HIS
2	B	212	HIS
2	B	231	GLN
2	B	244	ASN
2	B	258	GLN
2	B	350	HIS
2	B	358	HIS
2	B	381	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	T	75/76 (98%)	31 (41%)	11 (14%)

All (31) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	10	G
3	T	11	C
3	T	12	U
3	T	16	U
3	T	17	U
3	T	18	G
3	T	20	U
3	T	21	A
3	T	25	C
3	T	26	A
3	T	29	C
3	T	30	G
3	T	31	A
3	T	34	G
3	T	40	C
3	T	41	G
3	T	42	C
3	T	45	U
3	T	46	G
3	T	47	U
3	T	48	C
3	T	53	G
3	T	57	G
3	T	58	A
3	T	59	U
3	T	60	U
3	T	61	C
3	T	62	C
3	T	73	A
3	T	74	C
3	T	75	C

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	T	10	G
3	T	15	G
3	T	19	G
3	T	25	C
3	T	29	C
3	T	30	G
3	T	41	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	T	44	G
3	T	46	G
3	T	61	C
3	T	74	C

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FYA	A	1351	-	31,36,36	1.56	10 (32%)	30,52,52	1.06	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FYA	A	1351	-	-	0/16/36/36	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1351	FYA	C8-N7	-2.12	1.30	1.34
4	A	1351	FYA	CZ-CE1	2.01	1.43	1.38
4	A	1351	FYA	CE2-CD2	2.15	1.43	1.38
4	A	1351	FYA	CE1-CD1	2.24	1.43	1.38
4	A	1351	FYA	CD2-CG	2.44	1.44	1.38
4	A	1351	FYA	C4-N3	2.49	1.39	1.35
4	A	1351	FYA	C2-N1	2.57	1.38	1.33
4	A	1351	FYA	O4'-C1'	2.58	1.44	1.41
4	A	1351	FYA	CD1-CG	2.68	1.44	1.38
4	A	1351	FYA	C2-N3	2.89	1.37	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1351	FYA	N3-C2-N1	-2.62	126.89	128.89
4	A	1351	FYA	C4'-O4'-C1'	-2.34	107.14	109.72
4	A	1351	FYA	C4-C5-N7	2.57	111.84	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1351	FYA	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	336/350 (96%)	0.45	51 (15%) 3 1	9, 35, 90, 102	0
2	B	781/785 (99%)	-0.14	7 (0%) 85 72	6, 29, 78, 93	0
3	T	76/76 (100%)	3.44	67 (88%) 0 0	65, 67, 73, 75	0
All	All	1193/1211 (98%)	0.26	125 (10%) 8 3	6, 32, 84, 102	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	18	G	7.4
1	A	43	PRO	6.9
1	A	33	THR	6.9
3	T	63	G	6.4
3	T	1	G	5.8
1	A	46	GLU	5.7
3	T	72	C	5.5
3	T	71	G	5.4
1	A	44	LEU	5.3
1	A	62	GLU	5.3
3	T	9	A	5.2
3	T	70	G	5.0
3	T	15	G	4.9
3	T	4	G	4.8
3	T	73	A	4.8
3	T	19	G	4.7
3	T	64	C	4.7
3	T	22	G	4.7
1	A	57	ILE	4.6
1	A	55	ASN	4.6
3	T	3	C	4.5
3	T	24	G	4.4
1	A	64	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	47	ARG	4.3
3	T	58	A	4.3
3	T	67	C	4.3
1	A	15	LEU	4.2
3	T	16	U	4.2
3	T	55	U	4.2
3	T	41	G	4.1
1	A	38	GLY	4.0
3	T	30	G	4.0
3	T	62	C	4.0
3	T	57	G	4.0
1	A	25	TYR	3.9
3	T	61	C	3.9
1	A	36	MET	3.9
3	T	2	C	3.8
3	T	45	U	3.8
3	T	44	G	3.8
3	T	32	C	3.8
1	A	48	ARG	3.7
3	T	7	G	3.7
1	A	63	ALA	3.7
3	T	74	C	3.7
1	A	34	GLN	3.6
1	A	19	LYS	3.6
1	A	51	GLY	3.5
3	T	66	C	3.5
3	T	6	G	3.5
3	T	23	A	3.5
1	A	52	GLN	3.5
3	T	10	G	3.4
3	T	31	A	3.4
3	T	25	C	3.4
3	T	5	A	3.4
3	T	43	A	3.4
3	T	34	G	3.4
1	A	18	LEU	3.4
3	T	42	C	3.3
3	T	35	A	3.3
3	T	20	U	3.3
3	T	47	U	3.3
1	A	24	ARG	3.3
1	A	75	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	73	GLU	3.3
1	A	39	LEU	3.2
3	T	65	G	3.2
3	T	60	U	3.2
1	A	65	LEU	3.2
3	T	68	U	3.1
1	A	30	GLY	3.1
3	T	38	A	3.1
3	T	50	G	3.1
3	T	56	C	3.0
1	A	66	GLU	3.0
3	T	17	U	3.0
3	T	33	U	3.0
3	T	21	A	3.0
1	A	29	LYS	3.0
1	A	42	LEU	3.0
1	A	23	ALA	3.0
3	T	46	G	3.0
3	T	39	U	2.9
1	A	40	SER	2.9
1	A	68	ARG	2.9
3	T	48	C	2.9
3	T	53	G	2.9
3	T	69	C	2.9
2	B	98	GLY	2.9
1	A	37	LYS	2.8
3	T	54	U	2.8
1	A	41	ALA	2.8
1	A	16	GLU	2.8
1	A	59	ALA	2.8
1	A	26	LEU	2.7
1	A	60	ALA	2.7
3	T	40	C	2.7
3	T	29	C	2.6
1	A	56	ALA	2.6
3	T	36	A	2.5
2	B	753	LYS	2.5
3	T	75	C	2.5
3	T	14	A	2.4
2	B	692	ALA	2.4
3	T	51	C	2.4
1	A	76	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	81	LEU	2.3
3	T	8	U	2.3
1	A	61	LEU	2.2
3	T	76	A	2.2
1	A	27	GLY	2.2
1	A	58	LYS	2.2
2	B	736	LEU	2.2
2	B	697	LEU	2.1
2	B	97	PRO	2.1
2	B	99	LEU	2.1
1	A	28	LYS	2.1
1	A	77	LEU	2.1
1	A	74	GLU	2.1
1	A	54	LEU	2.1
1	A	17	GLU	2.1
1	A	70	LYS	2.0
1	A	80	ALA	2.0
3	T	12	U	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	MG	B	1781	1/1	0.88	0.34	2.26	19,19,19,19	0
4	FYA	A	1351	33/33	0.94	0.23	0.12	30,44,52,56	0

6.5 Other polymers (i)

There are no such residues in this entry.