



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:01 AM GMT

PDB ID : 3KFU
Title : Crystal structure of the transamidosome
Authors : Blaise, M.; Bailly, M.; Frechin, M.; Thirup, S.; Becker, H.D.; Kern, D.
Deposited on : 2009-10-28
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

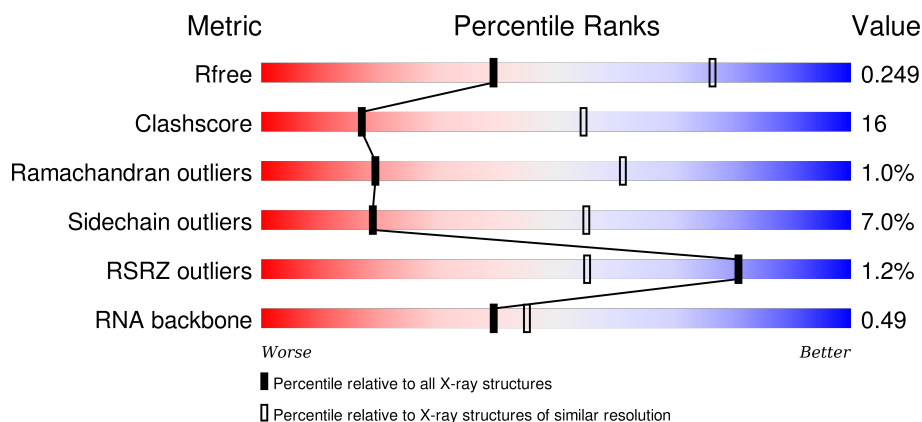
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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 $\leq 5\%$. 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	422	
1	B	422	
1	C	422	
1	D	422	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	471	
2	H	471	
3	F	466	
3	I	466	
4	G	92	
4	J	92	
5	K	76	
5	L	76	
5	M	76	
5	N	76	

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
6	ZN	F	673	-	-	-	X
6	ZN	I	467	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 33436 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 Non-discriminating and archaeal-type aspartyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			3026	1945	525	549	7			
1	B	376	Total	C	N	O	S	0	0	0
			3046	1956	531	552	7			
1	C	377	Total	C	N	O	S	0	0	0
			3053	1961	532	553	7			
1	D	372	Total	C	N	O	S	0	0	0
			3022	1940	528	548	6			

- Molecule 2 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	468	Total	C	N	O	S	0	1	0
			3513	2234	620	652	7			
2	H	467	Total	C	N	O	S	0	1	0
			3505	2228	619	651	7			

- Molecule 3 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	447	Total	C	N	O	S	0	0	0
			3369	2127	612	622	8			
3	I	444	Total	C	N	O	S	0	0	0
			3331	2104	608	612	7			

- Molecule 4 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	86	Total	C	N	O		0	0	0
			675	428	115	132				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	83	Total	C	N	O	0	0	0
			662	421	112	129			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	MET	-	EXPRESSION TAG	UNP Q9LCX4
G	0	PRO	-	EXPRESSION TAG	UNP Q9LCX4
G	1	GLY	-	EXPRESSION TAG	UNP Q9LCX4
J	-1	MET	-	EXPRESSION TAG	UNP Q9LCX4
J	0	PRO	-	EXPRESSION TAG	UNP Q9LCX4
J	1	GLY	-	EXPRESSION TAG	UNP Q9LCX4

- Molecule 5 is a RNA chain called tRNA-Asn.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	74	Total	C	N	O	P	0	0	0
			1587	706	287	520	74			
5	L	74	Total	C	N	O	P	0	0	0
			1587	706	287	520	74			
5	M	71	Total	C	N	O	P	0	0	0
			1525	678	276	500	71			
5	N	71	Total	C	N	O	P	0	0	0
			1525	678	276	500	71			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Zn	0	0
			1	1		
6	F	1	Total	Zn	0	0
			1	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		

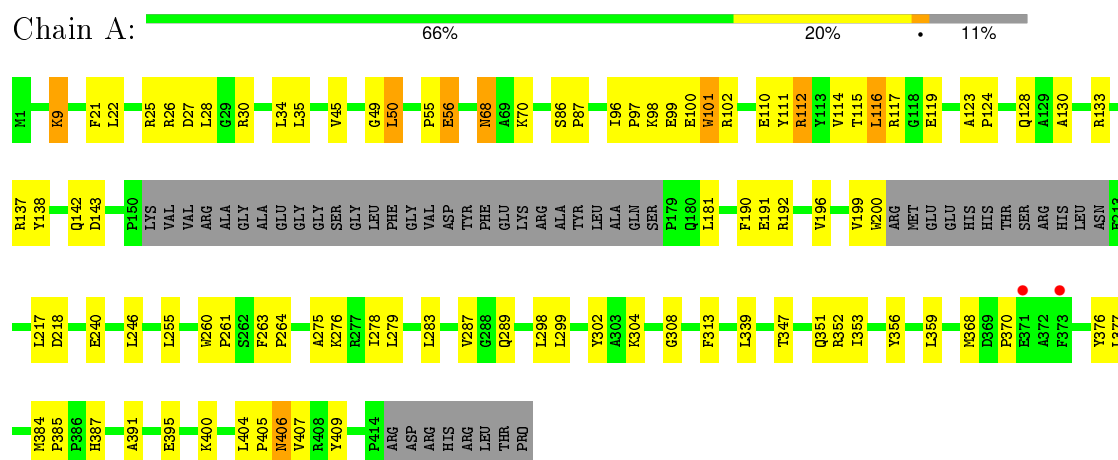
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	3	Total 3	O 3	0	0
8	I	3	Total 3	O 3	0	0

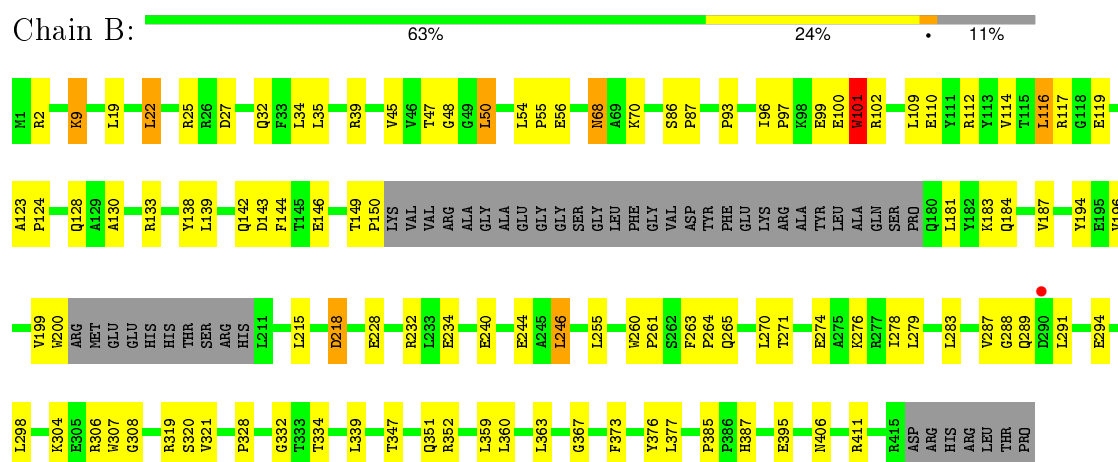
3 Residue-property plots

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.

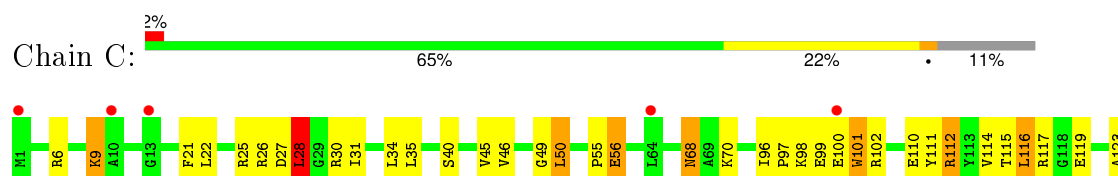
- Molecule 1: Non-discriminating and archaeal-type aspartyl-tRNA synthetase

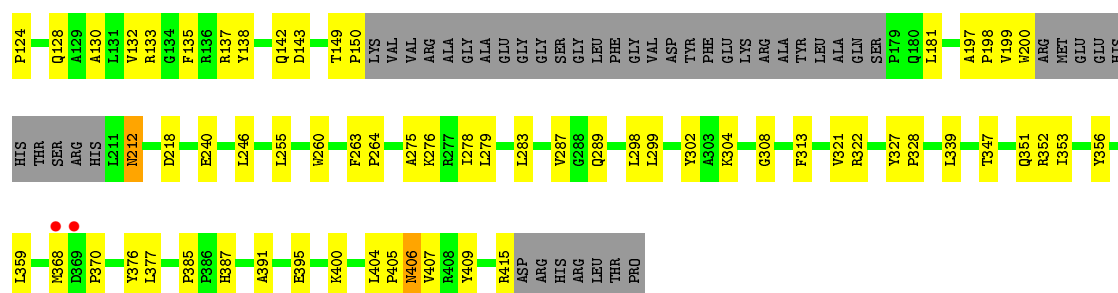


- Molecule 1: Non-discriminating and archaeal-type aspartyl-tRNA synthetase

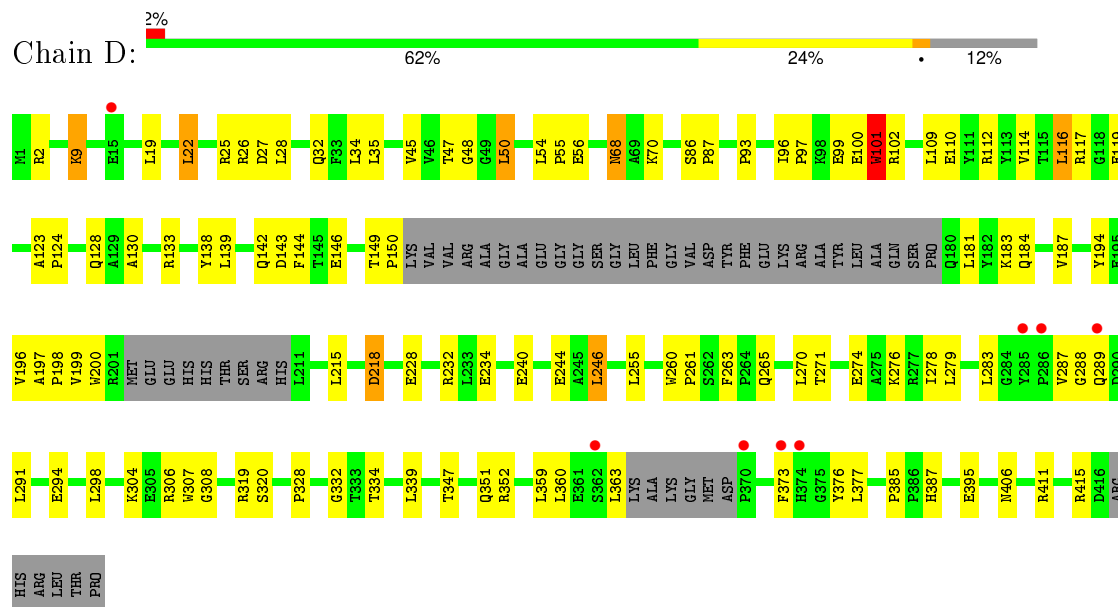


- Molecule 1: Non-discriminating and archaeal-type aspartyl-tRNA synthetase

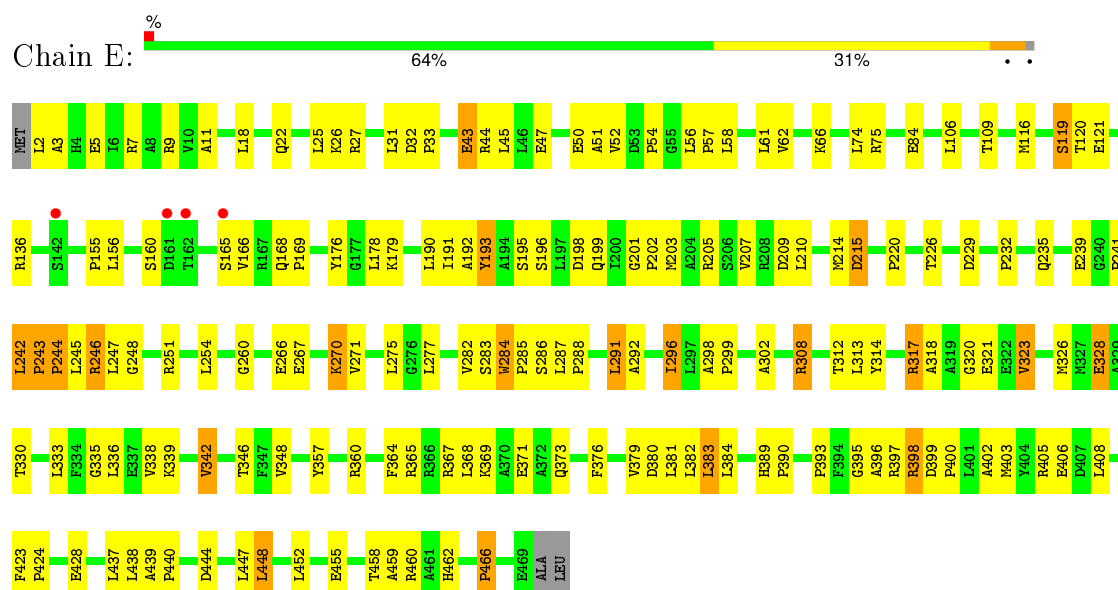




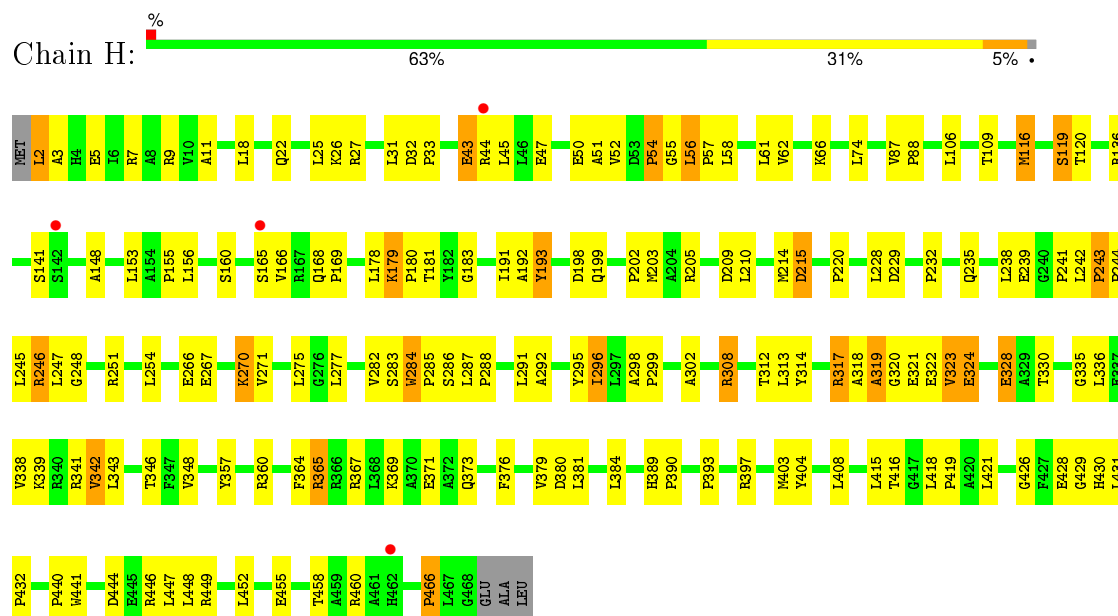
- Molecule 1: Non-discriminating and archaeal-type aspartyl-tRNA synthetase



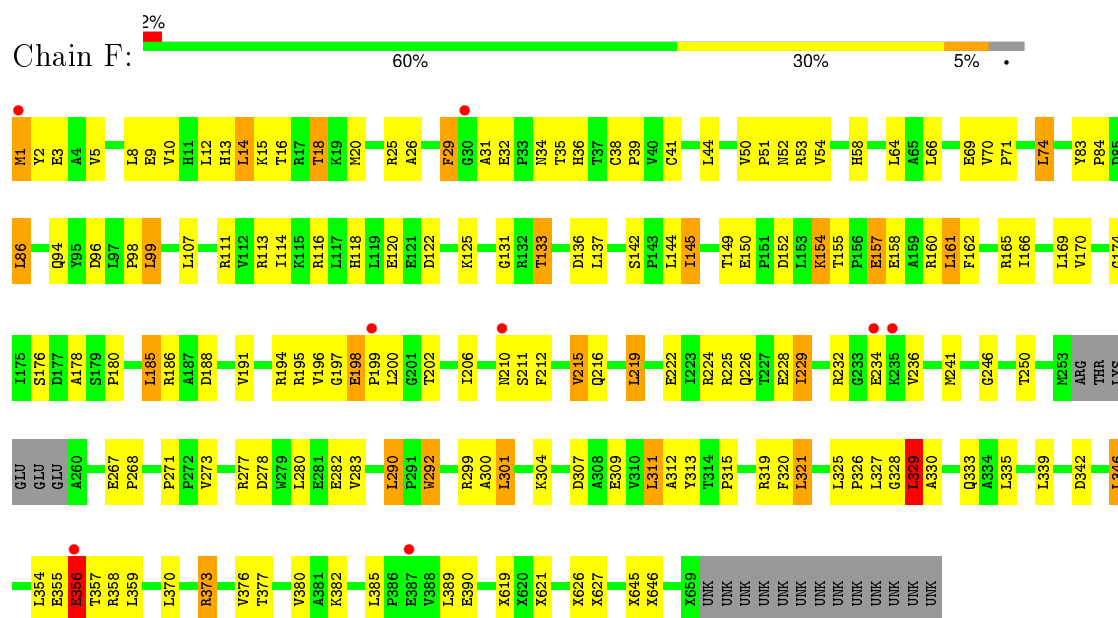
- Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit A



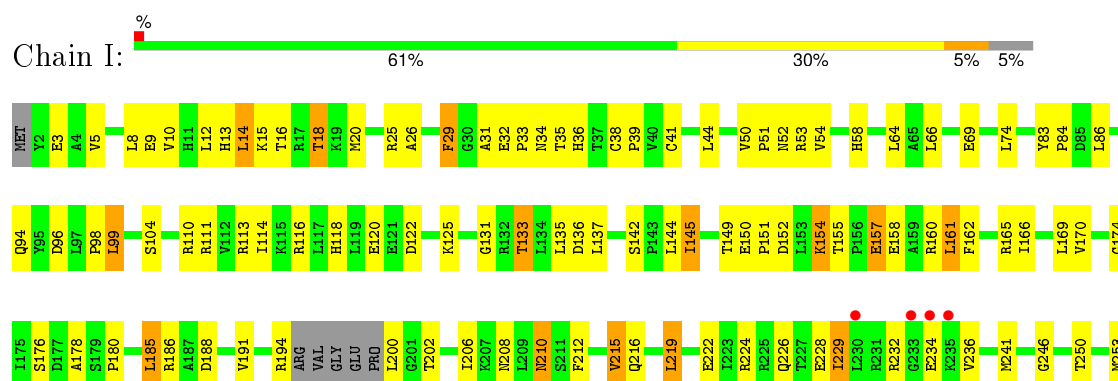
- Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit A

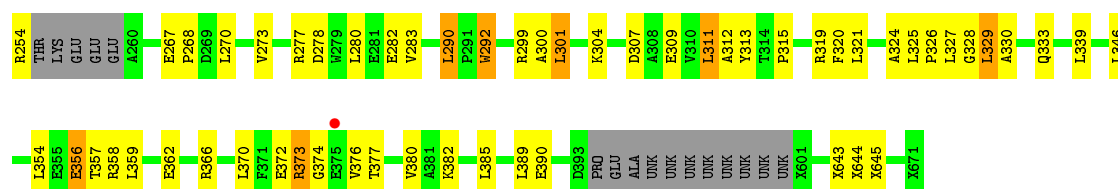


- Molecule 3: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

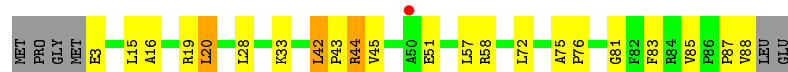


- Molecule 3: Aspartyl / glutamyl-tRNA(Asn/Gln) amidotransferase subunit B





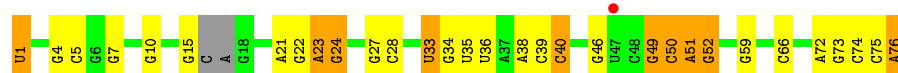
- Molecule 4: Glutamyl-tRNA(Gln) amidotransferase subunit C



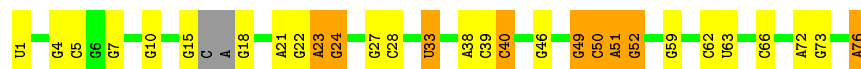
- Molecule 4: Glutamyl-tRNA(Gln) amidotransferase subunit C



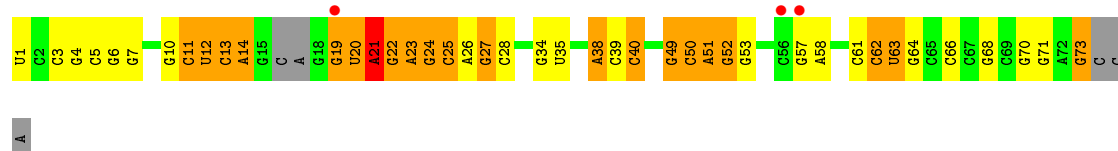
- Molecule 5: tRNA-Asn



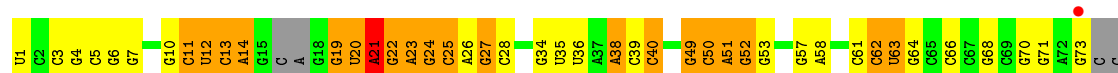
- Molecule 5: tRNA-Asn



- Molecule 5: tRNA-Asn



- Molecule 5: tRNA-Asn



A

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.92Å 214.00Å 127.84Å 90.00° 93.36° 90.00°	Depositor
Resolution (Å)	39.19 – 3.00 39.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.19-3.00) 99.9 (39.19-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.199 , 0.252 0.200 , 0.249	Depositor DCC
R_{free} test set	2487 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 123932 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33436	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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, 0.375 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: 5MU, H2U, ZN, MG, PSU

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	0.26	0/3096	0.40	0/4190
1	B	0.23	0/3115	0.40	0/4215
1	C	0.24	0/3123	0.41	1/4226 (0.0%)
1	D	0.22	0/3090	0.39	0/4181
2	E	0.24	0/3593	0.49	1/4887 (0.0%)
2	H	0.29	0/3585	0.50	1/4876 (0.0%)
3	F	0.25	0/3147	0.48	1/4262 (0.0%)
3	I	0.26	0/3081	0.47	0/4170
4	G	0.22	0/686	0.46	0/930
4	J	0.22	0/672	0.44	0/910
5	K	0.34	1/1705 (0.1%)	0.53	0/2655
5	L	0.38	1/1705 (0.1%)	0.56	0/2655
5	M	0.46	3/1636 (0.2%)	0.52	0/2548
5	N	0.47	3/1636 (0.2%)	0.52	0/2548
All	All	0.29	8/33870 (0.0%)	0.47	4/47253 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	1	U	OP3-P	-10.69	1.48	1.61
5	K	1	U	OP3-P	-10.67	1.48	1.61
5	M	1	U	OP3-P	-10.57	1.48	1.61
5	L	1	U	OP3-P	-10.55	1.48	1.61
5	M	21	A	P-OP2	-8.75	1.34	1.49
5	N	21	A	P-OP1	-8.75	1.34	1.49
5	M	21	A	P-OP1	-8.66	1.34	1.49
5	N	21	A	P-OP2	-8.60	1.34	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	466	PRO	N-CA-CB	5.95	110.43	103.30
2	E	466	PRO	N-CA-CB	5.89	110.37	103.30
1	C	28	LEU	CA-CB-CG	-5.33	103.05	115.30
3	F	329	LEU	CB-CA-C	-5.22	100.28	110.20

There are no chirality outliers.

There are no planarity outliers.

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	3026	0	3036	69	0
1	B	3046	0	3058	80	0
1	C	3053	0	3066	82	0
1	D	3022	0	3028	76	0
2	E	3513	0	3518	149	0
2	H	3505	0	3507	153	0
3	F	3369	0	3206	147	0
3	I	3331	0	3150	140	0
4	G	675	0	687	35	0
4	J	662	0	675	38	0
5	K	1587	0	807	28	0
5	L	1587	0	807	26	0
5	M	1525	0	774	47	0
5	N	1525	0	774	49	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
7	F	1	0	0	0	0
7	I	1	0	0	0	0
8	F	3	0	0	1	0
8	I	3	0	0	1	0
All	All	33436	0	30093	1034	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 16.

All (1034) 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:H:56:LEU:N	2:H:56:LEU:HD23	1.49	1.18
3:F:329:LEU:HD11	3:F:373:ARG:HH21	1.13	1.14
3:F:329:LEU:HD11	3:F:373:ARG:NH2	1.64	1.13
2:H:323:VAL:CG1	2:H:324:GLU:N	2.09	1.09
3:F:120:GLU:OE2	8:F:675:HOH:O	1.70	1.09
2:H:323:VAL:HG12	2:H:324:GLU:H	1.17	1.08
2:E:52:VAL:HG12	2:E:52:VAL:O	1.54	1.08
3:I:329:LEU:HD12	3:I:329:LEU:N	1.64	1.07
2:H:323:VAL:CG1	2:H:324:GLU:H	1.68	1.04
3:F:2:TYR:HB2	3:F:195:ARG:HA	1.38	1.04
2:H:323:VAL:HG13	2:H:324:GLU:N	1.69	1.04
2:H:320:GLY:O	2:H:321:GLU:HB3	1.52	1.04
2:H:318:ALA:O	2:H:319:ALA:HB3	1.55	1.01
3:I:325:LEU:N	3:I:326:PRO:HD2	1.76	0.98
2:E:54:PRO:HG2	2:E:56:LEU:HD13	1.44	0.95
1:C:28:LEU:CD1	1:C:28:LEU:N	2.30	0.95
3:I:329:LEU:CD1	3:I:329:LEU:H	1.79	0.95
2:H:56:LEU:CD2	2:H:56:LEU:N	2.30	0.92
3:I:329:LEU:CD1	3:I:329:LEU:N	2.30	0.91
1:C:28:LEU:HD13	1:C:28:LEU:N	1.86	0.90
3:I:39:PRO:HB3	3:I:44:LEU:HD11	1.54	0.88
3:F:39:PRO:HB3	3:F:44:LEU:HD11	1.55	0.86
2:E:54:PRO:HG2	2:E:56:LEU:CD1	2.05	0.86
3:I:120:GLU:OE2	8:I:469:HOH:O	1.93	0.86
2:E:260:GLY:HA3	2:E:428:GLU:HB3	1.57	0.86
4:G:20:LEU:HD12	4:G:20:LEU:H	1.42	0.85
5:M:10:G:O6	5:M:26:A:C6	2.31	0.84
2:H:54:PRO:HG2	2:H:56:LEU:HD21	1.59	0.83
5:N:10:G:O6	5:N:26:A:C6	2.31	0.83
3:I:325:LEU:N	3:I:326:PRO:CD	2.41	0.83
1:B:138:TYR:HB2	1:B:240:GLU:HG2	1.59	0.83
2:H:56:LEU:H	2:H:56:LEU:HD23	1.44	0.83
2:E:192:ALA:HB1	2:E:198:ASP:OD2	1.79	0.82
2:H:318:ALA:O	2:H:319:ALA:CB	2.25	0.82
2:H:192:ALA:HB1	2:H:198:ASP:OD2	1.80	0.82
2:H:397:ARG:HB3	2:H:403:MET:HG2	1.62	0.81
3:F:357:THR:HG22	3:F:358:ARG:H	1.45	0.81
1:D:138:TYR:HB2	1:D:240:GLU:HG2	1.61	0.81
3:I:18:THR:HG21	4:J:58:ARG:HH12	1.46	0.81
1:D:199:VAL:HG12	1:D:200:TRP:H	1.45	0.81
1:B:199:VAL:HG12	1:B:200:TRP:H	1.46	0.80
1:C:279:LEU:HD23	1:C:283:LEU:HD12	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:329:LEU:CD1	3:F:373:ARG:HH21	1.94	0.80
1:C:27:ASP:C	1:C:28:LEU:CD1	2.50	0.80
1:A:279:LEU:HD23	1:A:283:LEU:HD12	1.64	0.80
3:I:324:ALA:C	3:I:326:PRO:HD2	2.03	0.79
3:F:202:THR:HG21	3:F:236:VAL:HB	1.63	0.79
2:E:317:ARG:HH11	4:G:76:PRO:HB2	1.48	0.78
3:I:357:THR:HG22	3:I:358:ARG:H	1.46	0.78
1:C:406:ASN:HD22	1:C:407:VAL:N	1.80	0.78
2:H:242:LEU:HB2	2:H:245:LEU:HG	1.65	0.78
3:I:202:THR:HG21	3:I:236:VAL:HB	1.63	0.78
1:B:96:ILE:HD11	1:B:114:VAL:HG22	1.67	0.77
3:I:149:THR:HG22	3:I:150:GLU:O	1.84	0.77
1:D:96:ILE:HD11	1:D:114:VAL:HG22	1.67	0.77
2:H:320:GLY:O	2:H:321:GLU:CB	2.32	0.76
1:B:70:LYS:HE2	5:N:34:G:O2'	1.86	0.76
5:M:7:G:O2'	5:M:49:G:H5'	1.86	0.76
2:E:318:ALA:HB2	2:E:330:THR:HA	1.67	0.75
3:F:170:VAL:HG11	3:F:176:SER:HB3	1.68	0.75
2:E:54:PRO:CG	2:E:56:LEU:HD13	2.17	0.75
3:I:170:VAL:HG11	3:I:176:SER:HB3	1.67	0.75
3:F:18:THR:HG21	4:G:58:ARG:HH12	1.50	0.75
1:A:406:ASN:HD22	1:A:407:VAL:N	1.82	0.75
3:I:208:ASN:HB3	5:K:75:C:H4'	1.69	0.74
1:C:406:ASN:HD22	1:C:407:VAL:H	1.33	0.74
2:H:318:ALA:HB2	2:H:330:THR:HA	1.68	0.74
3:F:149:THR:HG22	3:F:150:GLU:O	1.86	0.74
3:I:34:ASN:HD22	4:J:72:LEU:HD21	1.53	0.73
5:N:7:G:O2'	5:N:49:G:H5'	1.87	0.73
3:I:327:LEU:CB	3:I:329:LEU:HD13	2.19	0.73
2:E:242:LEU:HB2	2:E:245:LEU:HG	1.69	0.73
5:N:63:U:H2'	5:N:64:G:C8	2.23	0.73
5:M:63:U:H2'	5:M:64:G:C8	2.23	0.73
2:E:52:VAL:CG1	2:E:52:VAL:O	2.30	0.72
2:H:317:ARG:HH11	4:J:76:PRO:HB2	1.54	0.72
1:A:406:ASN:HD22	1:A:407:VAL:H	1.37	0.72
1:C:27:ASP:C	1:C:28:LEU:HD13	2.08	0.72
1:B:34:LEU:HB2	1:B:45:VAL:HB	1.72	0.72
2:E:323:VAL:HG11	4:G:88:VAL:HA	1.71	0.71
2:H:56:LEU:HB3	2:H:57:PRO:HD2	1.70	0.71
3:F:358:ARG:HB2	3:F:390:GLU:HA	1.70	0.71
5:M:63:U:H2'	5:M:64:G:H8	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LEU:HB2	1:D:45:VAL:HB	1.73	0.71
5:N:63:U:H2'	5:N:64:G:H8	1.56	0.70
1:C:34:LEU:HB2	1:C:45:VAL:HB	1.73	0.70
3:I:133:THR:HG23	4:J:85:VAL:HG23	1.71	0.70
1:B:102:ARG:HH21	5:N:25:C:H1'	1.55	0.70
3:I:358:ARG:HB2	3:I:390:GLU:HA	1.71	0.70
2:H:455:GLU:O	2:H:458:THR:O	2.10	0.70
1:C:27:ASP:C	1:C:28:LEU:HD12	2.12	0.70
2:H:18:LEU:HA	2:H:50:GLU:HG2	1.75	0.69
2:E:18:LEU:HA	2:E:50:GLU:HG2	1.75	0.69
3:I:304:LYS:H	3:I:333:GLN:HE22	1.39	0.69
1:A:34:LEU:HB2	1:A:45:VAL:HB	1.75	0.69
4:J:20:LEU:HD23	4:J:20:LEU:H	1.56	0.69
3:I:202:THR:CG2	3:I:236:VAL:HB	2.22	0.68
1:C:199:VAL:HG12	1:C:200:TRP:H	1.58	0.68
3:F:202:THR:CG2	3:F:236:VAL:HB	2.22	0.68
1:A:99:GLU:HB3	1:A:100:GLU:HA	1.76	0.68
2:E:242:LEU:HA	2:E:243:PRO:C	2.14	0.68
1:A:199:VAL:HG12	1:A:200:TRP:H	1.58	0.67
1:C:99:GLU:HB3	1:C:100:GLU:HA	1.76	0.67
2:H:323:VAL:HG12	2:H:324:GLU:N	1.88	0.67
1:A:25:ARG:NH1	1:A:55:PRO:HD3	2.10	0.67
3:I:98:PRO:HG3	3:I:116:ARG:CZ	2.24	0.67
2:H:239:GLU:HB3	2:H:241:PRO:HD3	1.76	0.67
2:H:242:LEU:HA	2:H:243:PRO:C	2.15	0.67
3:F:304:LYS:H	3:F:333:GLN:HE22	1.40	0.67
2:H:322:GLU:O	2:H:323:VAL:HG12	1.95	0.67
2:E:220:PRO:HG3	2:E:229:ASP:HA	1.78	0.67
3:F:376:VAL:HG13	3:F:380:VAL:HB	1.77	0.66
3:I:327:LEU:HB3	3:I:329:LEU:HD13	1.78	0.66
1:C:25:ARG:NH1	1:C:55:PRO:HD3	2.10	0.66
3:I:104:SER:HB3	3:I:111:ARG:HD2	1.78	0.66
2:E:320:GLY:O	2:E:321:GLU:HB3	1.96	0.66
1:C:9:LYS:HD3	1:C:9:LYS:H	1.60	0.66
2:E:239:GLU:HB3	2:E:241:PRO:HD3	1.77	0.66
2:E:242:LEU:HA	2:E:243:PRO:O	1.95	0.66
2:H:242:LEU:HA	2:H:243:PRO:O	1.95	0.66
1:C:199:VAL:HG12	1:C:200:TRP:N	2.11	0.66
2:H:239:GLU:C	2:H:241:PRO:HD3	2.16	0.66
2:E:247:LEU:HD21	2:E:383:LEU:HB2	1.77	0.66
1:C:27:ASP:O	1:C:28:LEU:HD12	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:VAL:HG12	1:A:200:TRP:N	2.11	0.66
3:I:329:LEU:HD12	3:I:329:LEU:H	1.39	0.66
3:F:198:GLU:H	3:F:199:PRO:HD2	1.61	0.66
2:H:220:PRO:HG3	2:H:229:ASP:HA	1.78	0.65
2:E:360:ARG:HB2	4:G:44:ARG:HH12	1.60	0.65
2:H:419:PRO:HB3	2:H:444:ASP:OD1	1.96	0.65
2:H:55:GLY:C	2:H:56:LEU:HD23	2.16	0.65
2:E:239:GLU:C	2:E:241:PRO:HD3	2.17	0.65
1:B:32:GLN:HG2	1:B:48:GLY:HA2	1.79	0.65
4:J:42:LEU:HD23	4:J:43:PRO:HD2	1.78	0.65
3:I:376:VAL:HG13	3:I:380:VAL:HB	1.78	0.65
1:D:32:GLN:HG2	1:D:48:GLY:HA2	1.79	0.65
3:F:98:PRO:HG3	3:F:116:ARG:CZ	2.26	0.65
2:E:395:GLY:C	2:E:398:ARG:HE	2.00	0.65
2:H:287:LEU:N	2:H:288:PRO:HD2	2.12	0.65
1:A:9:LYS:HD3	1:A:9:LYS:H	1.60	0.65
2:E:397:ARG:H	2:E:398:ARG:NH2	1.95	0.64
5:K:15:G:H2'	5:K:59:G:N2	2.12	0.64
1:C:26:ARG:HH21	1:C:35:LEU:HD21	1.62	0.64
2:H:2:LEU:O	2:H:2:LEU:HG	1.98	0.64
3:I:54:VAL:O	3:I:58:HIS:HD2	1.81	0.64
3:I:12:LEU:HB2	3:I:145:ILE:CD1	2.28	0.64
4:G:42:LEU:HD23	4:G:43:PRO:HD2	1.79	0.64
5:L:15:G:H2'	5:L:59:G:N2	2.12	0.64
1:A:25:ARG:HH12	1:A:55:PRO:HD3	1.63	0.64
3:F:370:LEU:O	3:F:373:ARG:O	2.15	0.63
2:H:239:GLU:HG2	2:H:449:ARG:HG3	1.79	0.63
2:H:360:ARG:HB2	4:J:44:ARG:HH12	1.61	0.63
3:F:8:LEU:H	3:F:149:THR:HB	1.63	0.63
1:A:26:ARG:HH21	1:A:35:LEU:HD21	1.62	0.63
2:E:376:PHE:CD2	2:E:440:PRO:HG3	2.33	0.63
3:F:54:VAL:O	3:F:58:HIS:HD2	1.81	0.63
1:D:123:ALA:HB3	1:D:124:PRO:HD3	1.80	0.63
1:D:2:ARG:HD2	1:D:19:LEU:HD12	1.80	0.63
3:F:170:VAL:CG1	3:F:176:SER:HB3	2.29	0.62
1:C:25:ARG:HH12	1:C:55:PRO:HD3	1.63	0.62
3:I:370:LEU:O	3:I:373:ARG:O	2.17	0.62
1:B:2:ARG:HD2	1:B:19:LEU:HD12	1.81	0.62
3:I:9:GLU:HB3	3:I:188:ASP:HB2	1.80	0.62
3:F:320:PHE:CD2	3:F:354:LEU:HD11	2.35	0.62
2:E:287:LEU:N	2:E:288:PRO:HD2	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:170:VAL:CG1	3:I:176:SER:HB3	2.29	0.62
3:I:327:LEU:N	3:I:327:LEU:HD23	2.14	0.62
3:F:12:LEU:HB2	3:F:145:ILE:CD1	2.29	0.62
2:H:312:THR:OG1	2:H:313:LEU:HD12	2.00	0.62
5:N:5:C:H42	5:N:68:G:H1	1.48	0.62
1:A:28:LEU:N	1:A:28:LEU:HD12	2.13	0.62
2:H:2:LEU:HD22	2:H:205:ARG:HH22	1.64	0.62
3:F:330:ALA:HB1	3:F:335:LEU:HG	1.81	0.62
4:J:72:LEU:HD11	4:J:81:GLY:HA2	1.81	0.61
3:F:9:GLU:HB3	3:F:188:ASP:HB2	1.81	0.61
4:G:72:LEU:HD11	4:G:81:GLY:HA2	1.83	0.61
3:F:133:THR:HG22	4:G:87:PRO:HA	1.82	0.61
1:B:123:ALA:HB3	1:B:124:PRO:HD3	1.81	0.61
1:A:138:TYR:HB2	1:A:240:GLU:HG2	1.83	0.61
3:F:307:ASP:O	3:F:311:LEU:HD22	2.01	0.61
1:B:199:VAL:HG12	1:B:200:TRP:N	2.16	0.60
2:E:283:SER:O	2:E:285:PRO:HD3	2.01	0.60
2:E:298:ALA:HB3	2:E:299:PRO:HD3	1.83	0.60
1:C:138:TYR:HB2	1:C:240:GLU:HG2	1.82	0.60
3:F:196:VAL:HG22	3:F:197:GLY:HA2	1.82	0.60
3:I:8:LEU:H	3:I:149:THR:HB	1.66	0.60
1:C:96:ILE:HD11	1:C:114:VAL:HG22	1.84	0.60
5:M:5:C:H42	5:M:68:G:H1	1.48	0.60
1:D:279:LEU:HD23	1:D:283:LEU:HD12	1.84	0.60
2:E:323:VAL:HG22	4:G:87:PRO:O	2.01	0.59
2:E:312:THR:OG1	2:E:313:LEU:HD12	2.02	0.59
2:H:283:SER:O	2:H:285:PRO:HD3	2.02	0.59
1:D:93:PRO:O	5:M:11:C:H5'	2.02	0.59
3:I:307:ASP:O	3:I:311:LEU:HD22	2.03	0.59
1:D:181:LEU:HD22	1:D:376:TYR:HD1	1.68	0.59
2:H:298:ALA:HB3	2:H:299:PRO:HD3	1.84	0.59
2:E:381:LEU:HD13	2:E:437:LEU:HD11	1.84	0.59
2:H:193:TYR:HD2	2:H:302:ALA:HB2	1.68	0.59
3:I:206:ILE:HD12	3:I:241:MET:HB2	1.85	0.59
2:E:7:ARG:NH1	2:E:11:ALA:HB2	2.17	0.59
3:F:53:ARG:HA	4:G:57:LEU:HD23	1.84	0.59
1:B:279:LEU:HD23	1:B:283:LEU:HD12	1.84	0.59
2:H:7:ARG:NH1	2:H:11:ALA:HB2	2.18	0.59
2:H:292:ALA:O	2:H:296:ILE:HG22	2.03	0.59
1:A:96:ILE:HD11	1:A:114:VAL:HG22	1.85	0.59
1:B:22:LEU:HD13	1:B:34:LEU:HD12	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:ARG:NH1	2:H:466:PRO:O	2.35	0.59
3:F:2:TYR:HD2	3:F:195:ARG:HG3	1.67	0.58
4:G:20:LEU:CD1	4:G:20:LEU:H	2.15	0.58
3:F:382:LYS:HE2	5:L:18:G:O6	2.02	0.58
3:I:320:PHE:CD2	3:I:354:LEU:HD11	2.37	0.58
2:E:7:ARG:HH11	2:E:7:ARG:HG3	1.69	0.58
1:B:181:LEU:HD22	1:B:376:TYR:HD1	1.68	0.58
2:E:54:PRO:CG	2:E:56:LEU:CD1	2.80	0.58
3:I:133:THR:HG22	4:J:87:PRO:HA	1.83	0.58
2:E:321:GLU:HG2	2:E:321:GLU:O	2.04	0.58
2:H:360:ARG:HB2	4:J:44:ARG:NH1	2.18	0.58
2:H:296:ILE:HD11	2:H:357:TYR:C	2.24	0.58
2:E:296:ILE:HG13	2:E:348:VAL:HG11	1.84	0.58
1:D:133:ARG:HD2	1:D:244:GLU:OE2	2.04	0.58
1:A:101:TRP:O	1:A:102:ARG:HB3	2.03	0.58
1:B:128:GLN:HE22	1:B:395:GLU:HG3	1.69	0.58
3:F:83:TYR:CD1	5:L:76:A:H2	2.22	0.58
1:B:304:LYS:O	1:B:308:GLY:HA2	2.03	0.58
3:I:191:VAL:HG11	3:I:222:GLU:HG2	1.85	0.58
1:D:304:LYS:O	1:D:308:GLY:HA2	2.03	0.58
1:C:101:TRP:O	1:C:102:ARG:HB3	2.04	0.58
1:B:93:PRO:O	5:N:11:C:H5'	2.04	0.58
1:D:22:LEU:HD13	1:D:34:LEU:HD12	1.86	0.58
4:J:20:LEU:H	4:J:20:LEU:CD2	2.17	0.58
2:H:296:ILE:HG13	2:H:348:VAL:HG11	1.84	0.58
2:E:459:ALA:O	2:E:460:ARG:HG3	2.04	0.58
2:E:390:PRO:HD3	2:E:428:GLU:OE2	2.04	0.57
5:M:10:G:O2'	5:M:11:C:P	2.63	0.57
1:D:199:VAL:HG12	1:D:200:TRP:N	2.15	0.57
1:D:99:GLU:HB3	1:D:100:GLU:HA	1.86	0.57
1:D:128:GLN:HE22	1:D:395:GLU:HG3	1.69	0.57
3:F:34:ASN:HD22	4:G:72:LEU:HD21	1.68	0.57
2:E:292:ALA:O	2:E:296:ILE:HG22	2.05	0.57
2:E:296:ILE:HD11	2:E:357:TYR:C	2.24	0.57
2:H:317:ARG:HH22	4:J:85:VAL:HG12	1.68	0.57
3:I:299:ARG:C	3:I:301:LEU:H	2.08	0.57
1:B:133:ARG:HD2	1:B:244:GLU:OE2	2.05	0.57
3:F:290:LEU:HD23	3:F:292:TRP:CH2	2.39	0.57
2:H:7:ARG:HH11	2:H:7:ARG:HG3	1.69	0.57
1:D:101:TRP:CD1	1:D:102:ARG:N	2.73	0.57
3:I:210:ASN:HB3	5:K:74:C:H1'	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:GLU:HB3	1:B:100:GLU:HA	1.85	0.57
5:N:10:G:O2'	5:N:11:C:P	2.63	0.57
3:F:191:VAL:HG11	3:F:222:GLU:HG2	1.86	0.57
3:F:178:ALA:O	3:F:180:PRO:HD3	2.05	0.56
2:E:193:TYR:HD2	2:E:302:ALA:HB2	1.70	0.56
3:F:206:ILE:HD12	3:F:241:MET:HB2	1.87	0.56
3:F:196:VAL:CG2	3:F:197:GLY:HA2	2.35	0.56
2:H:242:LEU:N	2:H:242:LEU:HD23	2.20	0.56
2:E:207:VAL:HG23	2:E:455:GLU:OE2	2.06	0.56
3:I:290:LEU:HD23	3:I:292:TRP:CH2	2.40	0.56
2:H:447:LEU:HD12	2:H:448:LEU:N	2.20	0.56
1:B:352:ARG:HB2	1:B:387:HIS:CE1	2.40	0.56
2:E:155:PRO:HB2	2:E:156:LEU:HD22	1.87	0.56
3:F:96:ASP:O	3:F:98:PRO:HD3	2.05	0.56
1:D:352:ARG:HB2	1:D:387:HIS:CE1	2.40	0.56
2:H:62:VAL:O	2:H:155:PRO:HD2	2.06	0.56
2:H:308:ARG:HG3	2:H:314:TYR:OH	2.05	0.56
2:E:266:GLU:O	2:E:270:LYS:HD2	2.05	0.56
3:I:229:ILE:O	3:I:234:GLU:HG2	2.05	0.56
5:K:7:G:O2'	5:K:49:G:H5'	2.06	0.56
2:H:247:LEU:HD23	2:H:248:GLY:N	2.21	0.56
2:E:395:GLY:CA	2:E:398:ARG:HE	2.18	0.56
3:F:325:LEU:HB2	3:F:326:PRO:HD3	1.87	0.56
2:E:247:LEU:HD23	2:E:248:GLY:N	2.21	0.55
2:H:426:GLY:HA2	2:H:460:ARG:HD2	1.87	0.55
1:B:101:TRP:CD1	1:B:102:ARG:N	2.75	0.55
2:E:58:LEU:HA	2:E:61:LEU:HD23	1.88	0.55
1:C:30:ARG:HG2	5:K:33:U:OP2	2.07	0.55
2:H:160:SER:O	2:H:165:SER:HB2	2.07	0.55
2:H:27:ARG:HH22	2:H:466:PRO:CB	2.20	0.55
2:E:62:VAL:O	2:E:155:PRO:HD2	2.06	0.55
2:E:308:ARG:HG3	2:E:314:TYR:OH	2.05	0.55
2:H:58:LEU:HA	2:H:61:LEU:HD23	1.89	0.55
2:H:446:ARG:HE	2:H:449:ARG:NH2	2.04	0.55
2:H:266:GLU:O	2:H:270:LYS:HD2	2.07	0.55
1:B:181:LEU:HD13	1:B:376:TYR:CD1	2.42	0.55
2:E:160:SER:O	2:E:165:SER:HB2	2.06	0.55
2:H:376:PHE:CD2	2:H:440:PRO:HG3	2.42	0.55
3:F:133:THR:HG23	4:G:85:VAL:HG23	1.88	0.55
1:D:181:LEU:HD13	1:D:376:TYR:CD1	2.42	0.55
3:F:299:ARG:C	3:F:301:LEU:H	2.08	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:161:LEU:HD12	3:F:162:PHE:N	2.22	0.55
2:E:360:ARG:HB2	4:G:44:ARG:NH1	2.21	0.55
2:E:376:PHE:CG	2:E:440:PRO:HG3	2.42	0.55
2:E:7:ARG:HB2	2:E:61:LEU:HD21	1.88	0.55
1:D:359:LEU:O	1:D:363:LEU:HG	2.07	0.55
3:F:50:VAL:HG12	4:G:58:ARG:HB2	1.87	0.55
5:L:7:G:O2'	5:L:49:G:H5'	2.06	0.54
5:M:70:G:O2'	5:M:71:G:H5'	2.07	0.54
3:F:309:GLU:O	3:F:313:TYR:HD1	1.90	0.54
3:F:1:MET:HB2	3:F:195:ARG:HG3	1.89	0.54
2:E:397:ARG:HD2	2:E:406:GLU:OE2	2.07	0.54
2:E:18:LEU:HD12	2:E:51:ALA:HB2	1.89	0.54
3:I:96:ASP:O	3:I:98:PRO:HD3	2.06	0.54
2:H:155:PRO:HB2	2:H:156:LEU:HD22	1.89	0.54
3:F:229:ILE:O	3:F:234:GLU:HG2	2.05	0.54
1:B:9:LYS:H	1:B:9:LYS:HD3	1.71	0.54
5:N:70:G:O2'	5:N:71:G:H5'	2.07	0.54
1:B:102:ARG:NH2	5:N:25:C:H1'	2.20	0.54
1:B:119:GLU:HB3	1:B:255:LEU:HD21	1.89	0.54
3:I:309:GLU:O	3:I:313:TYR:HD1	1.90	0.54
3:F:215:VAL:O	3:F:219:LEU:HB2	2.08	0.54
1:D:9:LYS:H	1:D:9:LYS:HD3	1.72	0.54
3:I:327:LEU:HB2	3:I:329:LEU:HD13	1.88	0.54
3:I:329:LEU:H	3:I:329:LEU:HD13	1.65	0.54
2:E:308:ARG:HB3	2:E:308:ARG:NH1	2.23	0.54
1:B:319:ARG:HG2	1:B:334:THR:HG23	1.89	0.54
1:D:119:GLU:HB3	1:D:255:LEU:HD21	1.89	0.54
1:B:351:GLN:HG3	1:B:387:HIS:O	2.07	0.54
2:E:367:ARG:HG3	4:G:45:VAL:HG11	1.89	0.54
1:B:359:LEU:O	1:B:363:LEU:HG	2.08	0.54
2:E:338:VAL:O	2:E:342:VAL:HG12	2.07	0.54
2:E:424:PRO:HG2	2:E:462:HIS:HD1	1.73	0.54
2:H:18:LEU:HD12	2:H:51:ALA:HB2	1.89	0.54
1:D:319:ARG:HG2	1:D:334:THR:HG23	1.89	0.54
3:I:178:ALA:O	3:I:180:PRO:HD3	2.07	0.54
1:C:68:ASN:HD22	1:C:70:LYS:H	1.54	0.54
4:J:75:ALA:HB2	4:J:83:PHE:CD1	2.43	0.53
2:H:245:LEU:HB2	2:H:277:LEU:HD22	1.91	0.53
3:F:320:PHE:HD2	3:F:354:LEU:HD11	1.72	0.53
3:I:206:ILE:CD1	3:I:241:MET:HB2	2.39	0.53
2:H:416:THR:O	2:H:441:TRP:CZ2	2.61	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:GLN:HG3	1:D:387:HIS:O	2.08	0.53
3:I:215:VAL:O	3:I:219:LEU:HB2	2.08	0.53
5:K:15:G:H2'	5:K:59:G:H22	1.72	0.53
2:H:296:ILE:HD11	2:H:357:TYR:O	2.09	0.53
1:B:274:GLU:O	1:B:278:ILE:HG13	2.09	0.53
2:E:245:LEU:HB2	2:E:277:LEU:HD22	1.91	0.53
3:F:229:ILE:C	3:F:234:GLU:HG2	2.28	0.53
1:D:319:ARG:HG2	1:D:334:THR:CG2	2.39	0.53
2:H:338:VAL:O	2:H:342:VAL:HG12	2.07	0.53
2:E:202:PRO:HB2	2:E:210:LEU:HD22	1.90	0.53
2:H:367:ARG:CG	4:J:45:VAL:HG11	2.38	0.53
2:E:198:ASP:O	2:E:199:GLN:HG2	2.08	0.53
2:H:446:ARG:HG3	2:H:449:ARG:HH21	1.74	0.53
2:H:421:LEU:HB2	2:H:447:LEU:HD13	1.90	0.53
2:H:248:GLY:N	2:H:379:VAL:HG11	2.24	0.53
2:E:367:ARG:CG	4:G:45:VAL:HG11	2.38	0.53
3:I:161:LEU:HD12	3:I:162:PHE:N	2.23	0.53
3:I:53:ARG:HA	4:J:57:LEU:HD23	1.90	0.53
2:H:198:ASP:O	2:H:199:GLN:HG2	2.08	0.53
3:F:342:ASP:OD2	3:F:382:LYS:HE3	2.09	0.53
2:E:296:ILE:HD11	2:E:357:TYR:O	2.09	0.53
3:I:222:GLU:OE1	3:I:250:THR:HG21	2.09	0.53
2:H:168:GLN:HB3	2:H:169:PRO:HD3	1.91	0.53
1:D:339:LEU:HB3	1:D:347:THR:HB	1.91	0.53
3:I:320:PHE:HD2	3:I:354:LEU:HD11	1.74	0.53
2:E:308:ARG:HH11	2:E:308:ARG:HB3	1.74	0.53
1:B:319:ARG:HG2	1:B:334:THR:CG2	2.39	0.53
2:H:328:GLU:HG2	4:J:19:ARG:HB2	1.90	0.53
3:F:222:GLU:OE1	3:F:250:THR:HG21	2.09	0.53
2:H:308:ARG:HB3	2:H:308:ARG:NH1	2.24	0.53
3:I:25:ARG:O	3:I:26:ALA:HB3	2.09	0.53
2:H:242:LEU:HD12	2:H:245:LEU:HD23	1.91	0.52
2:H:317:ARG:NH2	4:J:85:VAL:HG12	2.23	0.52
3:I:229:ILE:C	3:I:234:GLU:HG2	2.28	0.52
1:D:274:GLU:O	1:D:278:ILE:HG13	2.09	0.52
5:K:76:A:H3'	5:K:76:A:N3	2.24	0.52
2:H:202:PRO:HB2	2:H:210:LEU:HD22	1.91	0.52
2:H:7:ARG:HB2	2:H:61:LEU:HD21	1.89	0.52
2:E:317:ARG:NH1	4:G:76:PRO:HB2	2.20	0.52
2:H:160:SER:C	2:H:166:VAL:HG23	2.30	0.52
2:H:202:PRO:HG2	2:H:214:MET:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:ARG:HG3	2:E:31:LEU:HD12	1.92	0.52
2:E:54:PRO:CB	2:E:56:LEU:HD13	2.38	0.52
2:H:284:TRP:CZ3	2:H:371:GLU:HB2	2.45	0.52
3:F:206:ILE:CD1	3:F:241:MET:HB2	2.40	0.52
5:M:20:H2U:H3'	5:M:21:A:H3'	1.92	0.52
1:C:339:LEU:HB3	1:C:347:THR:HB	1.92	0.52
2:E:239:GLU:HB3	2:E:241:PRO:HG3	1.92	0.52
2:E:284:TRP:CZ3	2:E:371:GLU:HB2	2.44	0.52
3:F:25:ARG:O	3:F:26:ALA:HB3	2.10	0.52
2:E:168:GLN:HB3	2:E:169:PRO:HD3	1.92	0.52
3:I:327:LEU:HB3	3:I:329:LEU:CD1	2.39	0.52
3:I:133:THR:HG23	4:J:85:VAL:CG2	2.37	0.52
3:F:304:LYS:HG2	3:F:333:GLN:NE2	2.25	0.52
1:B:339:LEU:HB3	1:B:347:THR:HB	1.91	0.52
1:A:339:LEU:HB3	1:A:347:THR:HB	1.92	0.52
4:G:75:ALA:HB2	4:G:83:PHE:CD1	2.44	0.52
5:N:10:G:O6	5:N:26:A:N6	2.42	0.52
3:F:155:THR:HG22	3:F:157:GLU:HG2	1.92	0.52
2:E:248:GLY:N	2:E:379:VAL:HG11	2.24	0.52
3:I:12:LEU:HB2	3:I:145:ILE:HD11	1.91	0.52
5:M:13:C:O2'	5:M:14:A:H5'	2.10	0.52
1:A:68:ASN:HD22	1:A:70:LYS:H	1.56	0.52
1:C:212:ASN:HD21	1:C:415:ARG:HH11	1.58	0.51
5:N:10:G:O2'	5:N:11:C:H6	1.94	0.51
2:E:160:SER:C	2:E:166:VAL:HG23	2.31	0.51
5:M:10:G:O2'	5:M:11:C:H6	1.94	0.51
3:I:304:LYS:HG2	3:I:333:GLN:NE2	2.25	0.51
2:E:202:PRO:HG2	2:E:214:MET:HG2	1.92	0.51
2:E:346:THR:HG21	4:G:16:ALA:HB2	1.93	0.51
3:I:155:THR:HG22	3:I:157:GLU:HG2	1.92	0.51
3:I:160:ARG:HH11	3:I:216:GLN:NE2	2.08	0.51
5:M:10:G:O6	5:M:26:A:N6	2.42	0.51
3:F:160:ARG:HH11	3:F:216:GLN:NE2	2.08	0.51
1:C:123:ALA:HB3	1:C:124:PRO:HD3	1.92	0.51
1:D:183:LYS:HE2	1:D:218:ASP:OD2	2.11	0.51
4:G:20:LEU:HD12	4:G:20:LEU:N	2.19	0.51
4:G:3:GLU:N	4:G:33:LYS:HZ3	2.08	0.51
3:F:277:ARG:HD2	3:F:277:ARG:N	2.26	0.51
2:H:239:GLU:HB3	2:H:241:PRO:HG3	1.93	0.51
3:I:12:LEU:HB2	3:I:145:ILE:HD13	1.93	0.51
5:L:76:A:H3'	5:L:76:A:N3	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LYS:HE2	1:B:218:ASP:OD2	2.10	0.51
3:F:12:LEU:HB2	3:F:145:ILE:HD11	1.91	0.51
3:F:304:LYS:HG2	3:F:333:GLN:HE22	1.76	0.51
1:A:27:ASP:C	1:A:28:LEU:HD12	2.31	0.51
3:F:12:LEU:HB2	3:F:145:ILE:HD13	1.93	0.51
1:C:199:VAL:CG1	1:C:200:TRP:H	2.24	0.51
3:F:229:ILE:O	3:F:232:ARG:HG2	2.11	0.51
3:I:229:ILE:O	3:I:232:ARG:HG2	2.11	0.51
1:C:68:ASN:ND2	1:C:70:LYS:H	2.09	0.51
2:H:54:PRO:HG2	2:H:56:LEU:CD2	2.36	0.50
1:B:101:TRP:O	1:B:102:ARG:HB3	2.11	0.50
2:H:179:LYS:HE3	2:H:418:LEU:O	2.11	0.50
2:H:308:ARG:HB3	2:H:308:ARG:HH11	1.76	0.50
3:F:359:LEU:HB3	3:F:389:LEU:HA	1.92	0.50
2:E:328:GLU:HG2	4:G:19:ARG:HB2	1.92	0.50
1:D:50:LEU:H	1:D:50:LEU:HD23	1.75	0.50
1:A:123:ALA:HB3	1:A:124:PRO:HD3	1.93	0.50
3:I:277:ARG:HD2	3:I:277:ARG:N	2.26	0.50
1:D:146:GLU:HB2	1:D:194:TYR:CZ	2.46	0.50
1:C:96:ILE:HB	1:C:97:PRO:HD3	1.92	0.50
3:I:160:ARG:HD2	3:I:216:GLN:HE21	1.77	0.50
2:H:52:VAL:O	2:H:52:VAL:HG12	2.11	0.50
1:B:50:LEU:H	1:B:50:LEU:HD23	1.75	0.50
5:K:38:A:H2'	5:K:39:C:H5'	1.93	0.50
5:N:24:G:O2'	5:N:25:C:P	2.69	0.50
1:B:328:PRO:HA	1:B:334:THR:HG22	1.93	0.50
3:I:29:PHE:O	3:I:29:PHE:CG	2.65	0.50
1:D:56:GLU:HG3	1:D:117:ARG:NH1	2.26	0.50
5:N:13:C:O2'	5:N:14:A:H5'	2.11	0.50
1:C:181:LEU:HD13	1:C:376:TYR:CD1	2.47	0.50
1:D:101:TRP:O	1:D:102:ARG:HB3	2.12	0.50
5:N:20:H2U:H3'	5:N:21:A:H3'	1.92	0.50
1:B:139:LEU:O	1:B:144:PHE:HB2	2.12	0.50
2:E:399:ASP:HB3	2:E:402:ALA:HB3	1.93	0.50
3:I:359:LEU:HB3	3:I:389:LEU:HA	1.92	0.50
5:L:72:A:H2'	5:L:73:G:O4'	2.12	0.50
1:C:28:LEU:HB2	1:C:31:ILE:O	2.12	0.50
1:C:31:ILE:HD11	1:C:46:VAL:CG1	2.42	0.50
3:I:304:LYS:HG2	3:I:333:GLN:HE22	1.77	0.50
2:H:367:ARG:HG3	4:J:45:VAL:HG11	1.93	0.50
1:A:68:ASN:ND2	1:A:70:LYS:H	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:3:GLU:N	4:J:33:LYS:HZ3	2.09	0.50
5:K:72:A:H2'	5:K:73:G:O4'	2.12	0.50
1:A:181:LEU:HD13	1:A:376:TYR:CD1	2.47	0.49
5:N:23:A:O2'	5:N:24:G:P	2.70	0.49
1:A:199:VAL:CG1	1:A:200:TRP:H	2.25	0.49
5:L:15:G:H2'	5:L:59:G:H22	1.73	0.49
3:F:16:THR:HG22	3:F:54:VAL:HG23	1.94	0.49
2:H:27:ARG:HG3	2:H:31:LEU:HD12	1.94	0.49
1:B:271:THR:OG1	1:B:274:GLU:HB2	2.12	0.49
1:A:30:ARG:HG2	5:L:33:U:OP2	2.12	0.49
2:H:178:LEU:HB2	2:H:421:LEU:HD23	1.93	0.49
1:B:56:GLU:HG3	1:B:117:ARG:NH1	2.27	0.49
1:A:22:LEU:HD13	1:A:34:LEU:HD12	1.93	0.49
3:F:377:THR:HG21	3:F:645:UNK:HA	1.94	0.49
1:B:373:PHE:O	1:B:377:LEU:HG	2.12	0.49
3:F:13:HIS:NE2	3:F:142:SER:HB3	2.26	0.49
3:F:29:PHE:CG	3:F:29:PHE:O	2.65	0.49
5:L:38:A:H2'	5:L:39:C:H5'	1.93	0.49
3:I:94:GLN:HB2	3:I:118:HIS:HB2	1.94	0.49
5:N:38:A:O2'	5:N:39:C:H5'	2.12	0.49
1:D:373:PHE:O	1:D:377:LEU:HG	2.12	0.49
3:I:50:VAL:HG12	4:J:58:ARG:HB2	1.93	0.49
5:K:49:G:O6	5:K:66:C:N4	2.45	0.49
1:C:119:GLU:HB3	1:C:255:LEU:HD21	1.94	0.49
5:K:4:G:O2'	5:K:5:C:H5'	2.13	0.49
2:E:226:THR:HG22	3:F:271:PRO:HD3	1.95	0.49
5:M:24:G:O2'	5:M:25:C:P	2.71	0.49
3:I:104:SER:CB	3:I:111:ARG:HD2	2.42	0.49
3:F:180:PRO:HG3	3:F:185:LEU:HB3	1.94	0.49
1:A:304:LYS:O	1:A:308:GLY:HA2	2.13	0.49
2:E:43:GLU:O	2:E:45:LEU:N	2.46	0.49
3:I:13:HIS:NE2	3:I:142:SER:HB3	2.28	0.49
5:M:10:G:O2'	5:M:11:C:O5'	2.26	0.49
3:I:16:THR:HG22	3:I:54:VAL:HG23	1.95	0.49
1:C:101:TRP:CD1	1:C:102:ARG:N	2.81	0.49
5:K:49:G:O2'	5:K:50:C:P	2.70	0.49
1:B:319:ARG:HG3	1:B:332:GLY:O	2.13	0.49
1:D:328:PRO:HA	1:D:334:THR:HG22	1.94	0.49
3:F:160:ARG:HD2	3:F:216:GLN:HE21	1.76	0.49
1:C:356:TYR:HE1	1:C:377:LEU:HB3	1.77	0.49
2:H:43:GLU:O	2:H:45:LEU:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:PRO:HD2	1:A:409:TYR:HD2	1.78	0.49
3:F:619:UNK:C	3:F:621:UNK:N	2.76	0.49
1:C:21:PHE:CE2	1:D:385:PRO:HG3	2.48	0.49
5:M:24:G:HO2'	5:M:25:C:H6	1.60	0.48
5:M:23:A:O2'	5:M:24:G:P	2.71	0.48
2:H:180:PRO:O	2:H:181:THR:C	2.51	0.48
5:M:26:A:HO2'	5:M:27:G:C5'	2.25	0.48
2:E:323:VAL:CG1	4:G:88:VAL:HA	2.40	0.48
1:D:319:ARG:HG3	1:D:332:GLY:O	2.13	0.48
1:D:28:LEU:HA	5:M:38:A:N6	2.28	0.48
1:A:385:PRO:O	1:A:387:HIS:HD2	1.96	0.48
2:H:369:LYS:HE2	2:H:416:THR:O	2.13	0.48
2:H:246:ARG:O	2:H:379:VAL:HG12	2.13	0.48
5:L:49:G:O6	5:L:66:C:N4	2.47	0.48
3:I:137:LEU:HD23	4:J:83:PHE:CD2	2.48	0.48
1:D:271:THR:OG1	1:D:274:GLU:HB2	2.13	0.48
1:C:304:LYS:O	1:C:308:GLY:HA2	2.12	0.48
1:D:320:SER:HB2	3:F:113:ARG:HH12	1.78	0.48
1:D:149:THR:HB	1:D:150:PRO:HD2	1.95	0.48
1:B:146:GLU:HB2	1:B:194:TYR:CZ	2.48	0.48
3:F:99:LEU:HD22	3:F:99:LEU:O	2.14	0.48
2:E:395:GLY:HA2	2:E:398:ARG:HD2	1.96	0.48
3:F:357:THR:HG22	3:F:358:ARG:N	2.23	0.48
2:H:317:ARG:NH1	4:J:76:PRO:HB2	2.26	0.48
1:D:27:ASP:HA	1:D:32:GLN:HB3	1.95	0.48
1:D:181:LEU:HD13	1:D:376:TYR:CE1	2.48	0.48
1:A:101:TRP:CD1	1:A:102:ARG:N	2.82	0.48
5:L:49:G:O2'	5:L:50:C:P	2.70	0.48
2:E:5:GLU:O	2:E:9:ARG:HG3	2.12	0.48
2:E:439:ALA:N	2:E:447:LEU:HD21	2.27	0.48
1:A:137:ARG:HD2	1:A:240:GLU:OE2	2.13	0.48
1:B:181:LEU:HD13	1:B:376:TYR:CE1	2.48	0.48
3:I:74:LEU:HB3	3:I:273:VAL:HB	1.96	0.48
1:C:275:ALA:HB1	1:C:299:LEU:HD11	1.96	0.48
1:A:119:GLU:HB3	1:A:255:LEU:HD21	1.94	0.48
1:A:356:TYR:HE1	1:A:377:LEU:HB3	1.77	0.48
1:A:98:LYS:O	1:A:102:ARG:HB3	2.14	0.48
1:B:96:ILE:HB	1:B:97:PRO:HD3	1.95	0.48
2:H:287:LEU:N	2:H:288:PRO:CD	2.76	0.48
1:C:137:ARG:HD2	1:C:240:GLU:OE2	2.14	0.48
3:F:94:GLN:HB2	3:F:118:HIS:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:PRO:O	1:C:387:HIS:HD2	1.96	0.48
1:B:109:LEU:O	1:B:109:LEU:HD23	2.14	0.48
3:F:194:ARG:O	3:F:195:ARG:HB3	2.14	0.48
2:E:207:VAL:HG13	2:E:448:LEU:HD13	1.94	0.48
1:D:294:GLU:O	1:D:298:LEU:HD13	2.14	0.48
2:E:242:LEU:H	2:E:242:LEU:HD13	1.78	0.48
1:A:368:MET:O	1:A:370:PRO:HD3	2.14	0.48
2:H:5:GLU:O	2:H:9:ARG:HG3	2.13	0.48
1:D:96:ILE:HB	1:D:97:PRO:HD3	1.95	0.47
3:F:54:VAL:O	3:F:58:HIS:CD2	2.66	0.47
2:H:66:LYS:HZ3	2:H:160:SER:HB3	1.78	0.47
5:M:12:U:O2'	5:M:13:C:P	2.72	0.47
1:B:360:LEU:HD11	1:B:377:LEU:HD13	1.95	0.47
5:L:38:A:C2'	5:L:39:C:H5'	2.44	0.47
1:B:149:THR:HB	1:B:150:PRO:HD2	1.95	0.47
2:E:251:ARG:HA	2:E:254:LEU:HD12	1.96	0.47
1:C:22:LEU:HD13	1:C:34:LEU:HD12	1.95	0.47
1:A:96:ILE:HB	1:A:97:PRO:HD3	1.95	0.47
2:E:3:ALA:HB3	2:E:209:ASP:CG	2.34	0.47
1:B:25:ARG:HH12	1:B:54:LEU:HA	1.78	0.47
3:I:643:UNK:HA	3:I:644:UNK:C	2.45	0.47
1:D:25:ARG:HH12	1:D:54:LEU:HA	1.79	0.47
1:C:22:LEU:HG	1:C:55:PRO:HA	1.95	0.47
4:J:13:GLU:OE2	4:J:20:LEU:HD21	2.13	0.47
2:H:239:GLU:HB3	2:H:241:PRO:CD	2.43	0.47
1:D:360:LEU:HD11	1:D:377:LEU:HD13	1.95	0.47
1:C:405:PRO:HD2	1:C:409:TYR:HD2	1.79	0.47
1:C:368:MET:O	1:C:370:PRO:HD3	2.14	0.47
3:F:327:LEU:O	3:F:329:LEU:N	2.47	0.47
5:K:38:A:C2'	5:K:39:C:H5'	2.44	0.47
5:N:49:G:O2'	5:N:50:C:P	2.72	0.47
3:F:377:THR:OG1	3:F:380:VAL:HG23	2.14	0.47
5:M:38:A:O2'	5:M:39:C:H5'	2.14	0.47
2:E:215:ASP:OD1	2:E:235:GLN:HG3	2.14	0.47
1:C:28:LEU:HD11	5:K:38:A:N7	2.30	0.47
2:E:239:GLU:HB3	2:E:241:PRO:CD	2.44	0.47
3:I:14:LEU:HD11	3:I:145:ILE:HD12	1.96	0.47
2:H:376:PHE:CG	2:H:440:PRO:HG3	2.49	0.47
3:I:180:PRO:HG3	3:I:185:LEU:HB3	1.95	0.47
3:I:125:LYS:HB3	3:I:136:ASP:HB3	1.96	0.47
1:D:287:VAL:HG21	1:D:291:LEU:HD23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:51:A:C4	5:M:52:G:C8	3.02	0.47
1:A:22:LEU:HG	1:A:55:PRO:HA	1.96	0.47
2:E:66:LYS:NZ	2:E:160:SER:HB3	2.30	0.47
3:F:125:LYS:HB3	3:F:136:ASP:HB3	1.95	0.47
1:A:405:PRO:HD2	1:A:409:TYR:CD2	2.50	0.47
3:I:224:ARG:O	3:I:228:GLU:HG3	2.14	0.47
5:M:53:G:C6	5:M:62:C:N4	2.82	0.47
2:H:215:ASP:OD1	2:H:235:GLN:HG3	2.14	0.47
1:B:68:ASN:HD22	1:B:70:LYS:H	1.63	0.47
5:M:49:G:O2'	5:M:50:C:P	2.73	0.47
1:B:27:ASP:HA	1:B:32:GLN:HB3	1.97	0.47
2:H:418:LEU:HD23	2:H:441:TRP:CD1	2.50	0.47
2:H:116:MET:HE2	2:H:341:ARG:HG3	1.96	0.47
2:H:120:THR:O	2:H:120:THR:HG22	2.14	0.47
1:D:196:VAL:HG12	1:D:215:LEU:HD11	1.96	0.47
2:H:251:ARG:HA	2:H:254:LEU:HD12	1.97	0.47
5:L:4:G:O2'	5:L:5:C:H5'	2.15	0.47
1:B:367:GLY:HA2	3:I:110:ARG:HB2	1.96	0.47
1:B:294:GLU:O	1:B:298:LEU:HD13	2.15	0.47
5:K:23:A:O2'	5:K:24:G:H8	1.97	0.47
5:M:49:G:O2'	5:M:50:C:O5'	2.30	0.47
3:F:155:THR:HB	3:F:158:GLU:HG3	1.97	0.47
2:E:399:ASP:OD1	2:E:400:PRO:HD2	2.15	0.47
2:H:346:THR:HG21	4:J:16:ALA:HB2	1.97	0.47
3:I:54:VAL:O	3:I:58:HIS:CD2	2.66	0.47
1:D:68:ASN:HD22	1:D:70:LYS:H	1.63	0.47
1:C:246:LEU:HA	1:C:246:LEU:HD12	1.78	0.47
3:I:99:LEU:HD22	3:I:99:LEU:O	2.15	0.47
2:E:428:GLU:HG3	2:E:428:GLU:O	2.15	0.46
5:N:26:A:HO2'	5:N:27:G:C5'	2.27	0.46
3:I:377:THR:OG1	3:I:380:VAL:HG23	2.14	0.46
3:F:64:LEU:HD11	3:F:280:LEU:HD22	1.97	0.46
5:N:58:A:C8	5:N:61:C:N4	2.82	0.46
1:C:56:GLU:HG3	1:C:117:ARG:HH11	1.80	0.46
5:K:50:C:O2'	5:K:51:A:P	2.74	0.46
5:L:23:A:O2'	5:L:24:G:H8	1.97	0.46
5:N:53:G:C6	5:N:62:C:N4	2.82	0.46
2:H:390:PRO:HD3	2:H:428:GLU:OE1	2.15	0.46
3:I:64:LEU:HD11	3:I:280:LEU:HD22	1.97	0.46
1:C:212:ASN:CG	1:C:415:ARG:HD2	2.35	0.46
1:B:130:ALA:HA	1:B:133:ARG:NH1	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:12:U:O2'	5:N:13:C:P	2.72	0.46
5:M:10:G:O6	5:M:26:A:C5	2.68	0.46
2:E:317:ARG:NH2	4:G:85:VAL:HA	2.29	0.46
2:H:295:TYR:CE2	2:H:404:TYR:HB3	2.51	0.46
2:E:382:LEU:HB2	2:E:438:LEU:CD1	2.45	0.46
2:H:3:ALA:HB3	2:H:209:ASP:CG	2.35	0.46
5:N:51:A:C4	5:N:52:G:C8	3.03	0.46
2:E:284:TRP:HZ3	2:E:371:GLU:HB2	1.80	0.46
3:I:185:LEU:HD13	3:I:186:ARG:N	2.30	0.46
3:I:267:GLU:OE1	3:I:268:PRO:HD2	2.16	0.46
5:M:58:A:C8	5:M:61:C:N4	2.83	0.46
1:B:196:VAL:HG12	1:B:215:LEU:HD11	1.97	0.46
5:N:10:G:O2'	5:N:11:C:O5'	2.27	0.46
3:F:131:GLY:HA2	4:G:87:PRO:HG3	1.96	0.46
2:H:178:LEU:O	2:H:180:PRO:HD3	2.15	0.46
2:H:282:VAL:HG11	2:H:379:VAL:HG21	1.98	0.46
3:F:29:PHE:C	3:F:31:ALA:H	2.18	0.46
3:I:66:LEU:HD13	3:I:114:ILE:HD13	1.98	0.46
5:N:50:C:H1'	5:N:51:A:H5'	1.98	0.46
3:I:131:GLY:HA2	4:J:87:PRO:HG3	1.98	0.46
2:E:287:LEU:N	2:E:288:PRO:CD	2.79	0.46
1:A:353:ILE:CG2	1:A:359:LEU:HD12	2.46	0.46
1:A:275:ALA:HB1	1:A:299:LEU:HD11	1.97	0.46
5:N:10:G:O6	5:N:26:A:C5	2.69	0.46
1:C:405:PRO:HD2	1:C:409:TYR:CD2	2.51	0.46
1:B:287:VAL:HG21	1:B:291:LEU:HD23	1.97	0.46
1:D:109:LEU:O	1:D:109:LEU:HD23	2.16	0.46
3:F:14:LEU:HD11	3:F:145:ILE:HD12	1.98	0.46
2:H:317:ARG:NH2	4:J:85:VAL:HA	2.30	0.46
5:L:23:A:O2'	5:L:24:G:C8	2.69	0.46
3:F:224:ARG:O	3:F:228:GLU:HG3	2.15	0.46
1:A:56:GLU:HG3	1:A:117:ARG:HH11	1.81	0.46
3:I:155:THR:HB	3:I:158:GLU:HG3	1.98	0.46
2:E:242:LEU:CD1	2:E:242:LEU:N	2.79	0.45
1:C:200:TRP:HA	1:C:212:ASN:O	2.16	0.45
3:I:311:LEU:HD23	3:I:312:ALA:N	2.31	0.45
5:L:50:C:O2'	5:L:51:A:P	2.74	0.45
2:H:116:MET:H	2:H:116:MET:HG2	1.59	0.45
2:H:22:GLN:O	2:H:26:LYS:HG3	2.16	0.45
1:C:263:PHE:HA	1:C:264:PRO:HD3	1.76	0.45
3:F:358:ARG:HD2	3:F:390:GLU:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:284:TRP:HZ3	2:H:371:GLU:HB2	1.80	0.45
2:E:7:ARG:HG3	2:E:7:ARG:NH1	2.30	0.45
1:C:98:LYS:O	1:C:102:ARG:HB3	2.16	0.45
3:I:125:LYS:NZ	5:K:73:G:H5''	2.31	0.45
1:A:30:ARG:HG2	5:L:33:U:P	2.56	0.45
2:H:32:ASP:N	2:H:33:PRO:CD	2.79	0.45
3:I:358:ARG:HD2	3:I:390:GLU:HA	1.99	0.45
1:B:320:SER:HB2	3:I:113:ARG:HH22	1.81	0.45
5:N:26:A:O2'	5:N:27:G:O5'	2.32	0.45
2:H:18:LEU:HA	2:H:50:GLU:CG	2.45	0.45
2:H:178:LEU:HD12	2:H:179:LYS:N	2.31	0.45
1:A:21:PHE:CE2	1:B:385:PRO:HG3	2.51	0.45
5:K:23:A:O2'	5:K:24:G:C8	2.69	0.45
2:H:389:HIS:HB2	2:H:390:PRO:HD2	1.98	0.45
2:E:32:ASP:N	2:E:33:PRO:CD	2.79	0.45
2:H:380:ASP:O	2:H:381:LEU:HD23	2.16	0.45
5:N:24:G:HO2'	5:N:25:C:H6	1.61	0.45
2:E:282:VAL:HG11	2:E:379:VAL:HG21	1.98	0.45
3:I:135:LEU:HB2	4:J:83:PHE:HB2	1.99	0.45
2:E:405:ARG:O	2:E:408:LEU:HB2	2.16	0.45
3:F:373:ARG:H	3:F:373:ARG:HG3	1.49	0.45
2:E:317:ARG:HH22	4:G:85:VAL:HG12	1.80	0.45
3:I:150:GLU:HG3	3:I:151:PRO:HD2	1.99	0.45
5:N:49:G:O2'	5:N:50:C:O5'	2.30	0.45
1:A:68:ASN:HD22	1:A:68:ASN:C	2.20	0.45
1:A:356:TYR:CE1	1:A:377:LEU:HB3	2.52	0.45
1:D:139:LEU:O	1:D:144:PHE:HB2	2.16	0.45
3:I:38:CYS:HB2	3:I:39:PRO:HD2	1.99	0.45
5:N:10:G:HO2'	5:N:11:C:P	2.40	0.45
2:H:66:LYS:NZ	2:H:160:SER:HB3	2.31	0.45
3:I:29:PHE:C	3:I:31:ALA:H	2.19	0.45
1:C:356:TYR:CE1	1:C:377:LEU:HB3	2.52	0.45
2:E:382:LEU:HB2	2:E:438:LEU:HD12	1.99	0.45
2:H:320:GLY:O	2:H:322:GLU:HG2	2.17	0.45
3:F:38:CYS:HB2	3:F:39:PRO:HD2	1.98	0.45
5:N:27:G:H2'	5:N:28:C:C6	2.52	0.45
2:E:439:ALA:HB1	2:E:440:PRO:CD	2.47	0.45
3:I:299:ARG:O	3:I:300:ALA:HB3	2.17	0.45
2:E:22:GLN:O	2:E:26:LYS:HG3	2.17	0.45
2:E:389:HIS:HE1	2:E:406:GLU:OE1	2.00	0.45
1:B:70:LYS:HB3	5:N:36:U:O4	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:72:LEU:CD1	4:J:81:GLY:HA2	2.47	0.45
3:I:104:SER:HB3	3:I:111:ARG:CD	2.45	0.45
2:E:246:ARG:O	2:E:379:VAL:HG12	2.17	0.45
5:L:39:C:HO2'	5:L:40:C:P	2.40	0.45
3:I:643:UNK:N	3:I:644:UNK:CB	2.80	0.45
2:H:87:VAL:HA	2:H:88:PRO:HD3	1.75	0.45
5:M:34:G:H4'	5:M:35:U:H5'	1.97	0.45
3:F:194:ARG:HH21	3:F:200:LEU:N	2.15	0.45
5:M:27:G:H2'	5:M:28:C:C6	2.52	0.45
3:I:357:THR:HG22	3:I:358:ARG:N	2.24	0.45
2:H:242:LEU:HD12	2:H:245:LEU:CD2	2.47	0.45
2:E:242:LEU:CD1	2:E:242:LEU:H	2.30	0.45
1:D:130:ALA:HA	1:D:133:ARG:NH1	2.31	0.45
2:H:460:ARG:HG2	2:H:460:ARG:O	2.16	0.45
2:E:32:ASP:N	2:E:33:PRO:HD2	2.32	0.45
2:E:119:SER:O	2:E:120:THR:HB	2.16	0.45
5:N:24:G:C4	5:N:25:C:C5	3.05	0.44
2:E:120:THR:HG22	2:E:120:THR:O	2.16	0.44
3:F:329:LEU:HA	3:F:329:LEU:HD22	1.60	0.44
2:H:242:LEU:CA	2:H:243:PRO:C	2.83	0.44
1:D:385:PRO:O	1:D:387:HIS:HD2	2.00	0.44
3:F:66:LEU:HD13	3:F:114:ILE:HD13	1.98	0.44
1:D:197:ALA:HA	1:D:198:PRO:HD3	1.82	0.44
2:E:121:GLU:OE1	2:E:398:ARG:CZ	2.66	0.44
5:M:24:G:C4	5:M:25:C:C5	3.05	0.44
3:F:304:LYS:HE2	3:F:304:LYS:HA	1.98	0.44
3:F:20:MET:HE3	3:F:52:ASN:H	1.83	0.44
1:A:289:GLN:OE1	1:A:289:GLN:HA	2.17	0.44
1:D:101:TRP:CG	1:D:102:ARG:N	2.85	0.44
3:F:299:ARG:O	3:F:300:ALA:HB3	2.17	0.44
3:I:178:ALA:HB1	3:I:185:LEU:HD23	1.99	0.44
1:D:56:GLU:HG3	1:D:117:ARG:HH11	1.82	0.44
1:C:128:GLN:HE22	1:C:395:GLU:HG3	1.83	0.44
2:H:429:GLY:O	2:H:430:HIS:CG	2.71	0.44
1:C:353:ILE:CG2	1:C:359:LEU:HD12	2.48	0.44
3:I:32:GLU:O	3:I:35:THR:HG22	2.17	0.44
3:F:154:LYS:NZ	3:F:154:LYS:HB3	2.33	0.44
2:H:242:LEU:H	2:H:242:LEU:HD23	1.82	0.44
1:C:212:ASN:ND2	1:C:415:ARG:HD2	2.32	0.44
2:E:284:TRP:HB3	2:E:287:LEU:HB2	1.98	0.44
2:E:380:ASP:O	2:E:381:LEU:HD23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:193:TYR:CD2	2:H:302:ALA:HB2	2.50	0.44
1:D:234:GLU:OE1	1:D:347:THR:HG21	2.17	0.44
2:H:267:GLU:O	2:H:271:VAL:HG23	2.17	0.44
1:C:70:LYS:HE2	5:K:34:G:O2'	2.18	0.44
5:M:19:G:N2	5:M:57:G:H1'	2.33	0.44
5:M:7:G:HO2'	5:M:49:G:H5'	1.81	0.44
1:D:181:LEU:HD22	1:D:376:TYR:CD1	2.50	0.44
5:N:23:A:O2'	5:N:24:G:H8	2.01	0.44
3:I:304:LYS:HA	3:I:304:LYS:HE2	1.98	0.44
2:H:241:PRO:HB3	2:H:449:ARG:HD2	2.00	0.44
2:E:201:GLY:HA2	2:E:202:PRO:HD3	1.85	0.44
2:E:196:SER:OG	3:F:268:PRO:HB3	2.17	0.44
1:A:246:LEU:HD13	1:A:260:TRP:CZ2	2.53	0.44
3:I:194:ARG:HH21	3:I:200:LEU:N	2.15	0.44
2:H:7:ARG:NH1	2:H:7:ARG:HG3	2.31	0.44
5:N:34:G:H4'	5:N:35:U:H5'	1.99	0.44
2:H:27:ARG:CZ	2:H:466:PRO:O	2.66	0.44
3:F:185:LEU:HD13	3:F:186:ARG:N	2.32	0.44
1:A:352:ARG:HB2	1:A:387:HIS:CE1	2.53	0.44
3:F:267:GLU:OE1	3:F:268:PRO:HD2	2.18	0.44
1:A:199:VAL:CG1	1:A:200:TRP:N	2.78	0.43
5:M:38:A:N6	5:M:39:C:N4	2.66	0.43
1:C:246:LEU:HD13	1:C:260:TRP:CZ2	2.53	0.43
1:C:28:LEU:HD12	1:C:28:LEU:HA	1.46	0.43
5:K:39:C:HO2'	5:K:40:C:P	2.41	0.43
2:E:389:HIS:HB2	2:E:390:PRO:HD2	2.00	0.43
2:E:242:LEU:CA	2:E:243:PRO:C	2.84	0.43
4:J:20:LEU:N	4:J:20:LEU:CD2	2.82	0.43
1:C:199:VAL:CG1	1:C:200:TRP:N	2.78	0.43
2:H:32:ASP:N	2:H:33:PRO:HD2	2.32	0.43
3:F:626:UNK:O	3:F:627:UNK:C	2.67	0.43
3:F:32:GLU:O	3:F:35:THR:HG22	2.17	0.43
3:I:330:ALA:HB1	3:I:372:GLU:OE2	2.17	0.43
3:F:2:TYR:HB2	3:F:195:ARG:CA	2.28	0.43
5:M:23:A:O2'	5:M:24:G:H8	2.00	0.43
1:D:102:ARG:HH21	5:M:25:C:H1'	1.83	0.43
2:E:66:LYS:HZ3	2:E:160:SER:HB3	1.83	0.43
3:F:219:LEU:HD12	3:F:219:LEU:HA	1.77	0.43
5:N:19:G:N2	5:N:57:G:H1'	2.33	0.43
1:C:289:GLN:OE1	1:C:289:GLN:HA	2.17	0.43
2:E:423:PHE:HE2	2:E:437:LEU:HB2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:315:PRO:O	3:I:319:ARG:HG3	2.18	0.43
3:F:137:LEU:HD23	4:G:83:PHE:CD2	2.52	0.43
1:B:385:PRO:O	1:B:387:HIS:HD2	2.02	0.43
1:B:270:LEU:HD21	1:B:278:ILE:HD12	2.00	0.43
2:E:3:ALA:HB3	2:E:209:ASP:OD1	2.19	0.43
1:A:112:ARG:O	1:A:116:LEU:HB2	2.19	0.43
1:B:101:TRP:CG	1:B:102:ARG:N	2.86	0.43
5:N:23:A:C6	5:N:24:G:O6	2.72	0.43
5:M:50:C:H1'	5:M:51:A:H5'	1.99	0.43
3:F:311:LEU:HD23	3:F:312:ALA:N	2.33	0.43
5:K:51:A:O2'	5:K:52:G:H5''	2.19	0.43
1:C:68:ASN:HD22	1:C:68:ASN:C	2.22	0.43
3:I:212:PHE:O	3:I:215:VAL:HG22	2.18	0.43
1:C:347:THR:HG23	1:C:391:ALA:O	2.19	0.43
5:N:38:A:N6	5:N:39:C:N4	2.66	0.43
3:I:643:UNK:HA	3:I:645:UNK:N	2.34	0.43
2:H:3:ALA:HB3	2:H:209:ASP:OD1	2.18	0.43
1:A:276:LYS:HG3	1:A:287:VAL:HG13	2.00	0.43
2:H:365:ARG:HD3	2:H:415:LEU:O	2.18	0.43
3:F:198:GLU:HB2	3:F:199:PRO:HD3	2.00	0.43
5:M:25:C:H2'	5:M:26:A:O5'	2.18	0.43
2:E:320:GLY:O	2:E:321:GLU:CB	2.62	0.43
4:J:75:ALA:HB2	4:J:83:PHE:CE1	2.53	0.43
1:D:270:LEU:HD21	1:D:278:ILE:HD12	2.01	0.43
1:D:112:ARG:O	1:D:116:LEU:HB2	2.19	0.43
1:C:130:ALA:HA	1:C:133:ARG:NH1	2.33	0.43
3:I:165:ARG:HA	3:I:165:ARG:HD3	1.79	0.43
3:F:50:VAL:CG1	4:G:58:ARG:HB2	2.48	0.43
2:H:2:LEU:HD22	2:H:205:ARG:NH2	2.32	0.43
2:H:119:SER:O	2:H:120:THR:HB	2.17	0.43
3:F:278:ASP:O	3:F:282:GLU:HG3	2.19	0.43
1:A:128:GLN:HE22	1:A:395:GLU:HG3	1.84	0.43
1:A:86:SER:HA	1:A:87:PRO:HD3	1.86	0.43
2:E:398:ARG:HH12	2:E:403:MET:CE	2.32	0.43
5:L:39:C:O2'	5:L:40:C:P	2.77	0.43
5:N:10:G:C4	5:N:11:C:C5	3.07	0.43
4:G:75:ALA:HB2	4:G:83:PHE:CE1	2.53	0.43
2:E:243:PRO:HA	2:E:244:PRO:HA	1.71	0.43
3:I:219:LEU:HD12	3:I:219:LEU:HA	1.74	0.43
3:I:382:LYS:HZ2	3:I:382:LYS:HB2	1.83	0.43
2:H:323:VAL:O	2:H:324:GLU:C	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:34:ASN:ND2	4:J:72:LEU:HD21	2.28	0.42
1:B:234:GLU:OE1	1:B:347:THR:HG21	2.18	0.42
2:H:136:ARG:HA	2:H:393:PRO:HA	2.00	0.42
1:B:228:GLU:HG3	1:B:232:ARG:NE	2.34	0.42
5:M:26:A:HO2'	5:M:27:G:P	2.42	0.42
5:N:25:C:H2'	5:N:26:A:O5'	2.19	0.42
1:C:406:ASN:ND2	1:C:407:VAL:N	2.58	0.42
3:F:50:VAL:HA	3:F:51:PRO:HD3	1.83	0.42
2:H:284:TRP:HB3	2:H:287:LEU:HB2	2.00	0.42
3:F:178:ALA:HB1	3:F:185:LEU:HD23	2.00	0.42
3:F:232:ARG:HB2	3:I:232:ARG:HB2	2.01	0.42
5:N:39:C:HO2'	5:N:40:C:P	2.42	0.42
1:C:351:GLN:HG3	1:C:387:HIS:O	2.19	0.42
1:C:352:ARG:HB2	1:C:387:HIS:CE1	2.54	0.42
1:C:112:ARG:O	1:C:116:LEU:HB2	2.19	0.42
3:I:278:ASP:O	3:I:282:GLU:HG3	2.19	0.42
1:A:130:ALA:HA	1:A:133:ARG:NH1	2.34	0.42
3:F:197:GLY:HA2	3:F:198:GLU:HA	1.78	0.42
5:M:23:A:C6	5:M:24:G:O6	2.73	0.42
1:A:347:THR:HG23	1:A:391:ALA:O	2.19	0.42
1:C:111:TYR:O	1:C:115:THR:HG23	2.19	0.42
1:D:276:LYS:HE3	1:D:288:GLY:O	2.20	0.42
2:H:56:LEU:CB	2:H:57:PRO:HD2	2.42	0.42
5:M:49:G:O6	5:M:66:C:N4	2.52	0.42
5:N:49:G:O6	5:N:66:C:N4	2.52	0.42
3:I:273:VAL:HG21	4:J:57:LEU:CD1	2.50	0.42
1:D:55:PRO:O	1:D:56:GLU:CB	2.68	0.42
3:F:15:LYS:HE2	3:F:174:GLY:O	2.19	0.42
1:C:327:TYR:HA	1:C:328:PRO:HD3	1.90	0.42
1:B:263:PHE:CD2	1:B:265:GLN:HB2	2.54	0.42
3:F:315:PRO:O	3:F:319:ARG:HG3	2.19	0.42
1:D:263:PHE:CD2	1:D:265:GLN:HB2	2.54	0.42
2:E:267:GLU:O	2:E:271:VAL:HG23	2.19	0.42
2:H:56:LEU:CB	2:H:57:PRO:CD	2.96	0.42
3:F:12:LEU:HD13	3:F:170:VAL:HG21	2.02	0.42
2:E:18:LEU:HA	2:E:50:GLU:CG	2.45	0.42
4:G:3:GLU:O	4:G:3:GLU:HG2	2.20	0.42
3:I:3:GLU:OE1	3:I:194:ARG:HD3	2.20	0.42
3:I:83:TYR:CD2	3:I:84:PRO:HD2	2.55	0.42
3:F:107:LEU:HA	3:F:107:LEU:HD23	1.86	0.42
1:B:112:ARG:O	1:B:116:LEU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:178:LEU:HD12	2:E:179:LYS:N	2.35	0.42
2:E:54:PRO:HB2	2:E:56:LEU:HD13	2.02	0.42
3:F:645:UNK:HA	3:F:646:UNK:HA	1.72	0.42
5:L:51:A:O2'	5:L:52:G:H5''	2.20	0.42
2:E:286:SER:HB2	2:E:364:PHE:CZ	2.53	0.42
1:A:111:TYR:O	1:A:115:THR:HG23	2.20	0.42
4:J:9:LEU:HA	4:J:9:LEU:HD23	1.87	0.42
2:E:260:GLY:HA3	2:E:428:GLU:CB	2.38	0.42
1:B:181:LEU:HD22	1:B:376:TYR:CD1	2.51	0.42
2:E:176:TYR:OH	2:E:462:HIS:CE1	2.72	0.42
1:A:263:PHE:HA	1:A:264:PRO:HD3	1.76	0.42
3:F:165:ARG:HA	3:F:165:ARG:HD3	1.80	0.42
3:I:154:LYS:HB3	3:I:154:LYS:NZ	2.34	0.42
1:B:306:ARG:HD3	1:B:307:TRP:CH2	2.55	0.42
3:F:329:LEU:HD11	3:F:373:ARG:HH22	1.72	0.42
5:K:39:C:O2'	5:K:40:C:P	2.78	0.42
1:C:132:VAL:O	1:C:135:PHE:HB3	2.20	0.42
1:D:228:GLU:HG3	1:D:232:ARG:NE	2.35	0.42
2:E:335:GLY:O	2:E:339:LYS:HG3	2.19	0.42
3:F:194:ARG:HH21	3:F:199:PRO:C	2.22	0.42
3:I:50:VAL:CG1	4:J:58:ARG:HB2	2.49	0.42
4:G:75:ALA:HA	4:G:76:PRO:HD3	1.94	0.42
3:F:83:TYR:CD1	5:L:76:A:C2	3.05	0.42
5:L:27:G:H2'	5:L:28:C:C6	2.55	0.42
1:D:86:SER:HA	1:D:87:PRO:HD3	1.86	0.42
1:D:260:TRP:HA	1:D:261:PRO:HD3	1.82	0.42
1:A:400:LYS:HD3	1:A:400:LYS:HA	1.87	0.42
4:G:72:LEU:CD1	4:G:81:GLY:HA2	2.49	0.42
3:F:83:TYR:CD2	3:F:84:PRO:HD2	2.55	0.42
1:D:385:PRO:O	1:D:387:HIS:CD2	2.72	0.42
5:K:49:G:O2'	5:K:50:C:O5'	2.36	0.42
4:J:3:GLU:HG2	4:J:3:GLU:O	2.19	0.42
2:E:136:ARG:HA	2:E:393:PRO:HA	2.01	0.42
1:C:400:LYS:HD3	1:C:400:LYS:HA	1.87	0.42
2:H:7:ARG:HG2	2:H:57:PRO:O	2.19	0.41
5:M:10:G:C4	5:M:11:C:C5	3.07	0.41
5:M:22:G:O2'	5:M:23:A:P	2.78	0.41
2:E:7:ARG:HG2	2:E:57:PRO:O	2.20	0.41
1:D:35:LEU:N	1:D:35:LEU:HD22	2.35	0.41
3:I:39:PRO:CB	3:I:44:LEU:HD11	2.39	0.41
3:F:226:GLN:HA	3:F:229:ILE:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:359:LEU:HD22	3:F:389:LEU:HD12	2.02	0.41
1:B:56:GLU:HG3	1:B:117:ARG:HH11	1.84	0.41
1:B:55:PRO:O	1:B:56:GLU:CB	2.68	0.41
3:F:74:LEU:HB3	3:F:273:VAL:HB	2.02	0.41
1:B:246:LEU:HA	1:B:246:LEU:HD12	1.76	0.41
1:D:246:LEU:HA	1:D:246:LEU:HD12	1.75	0.41
3:F:5:VAL:CG2	3:F:194:ARG:HD2	2.51	0.41
5:N:24:G:O2'	5:N:25:C:H6	2.03	0.41
3:I:160:ARG:NH2	5:K:1:U:OP2	2.52	0.41
5:N:39:C:O2'	5:N:40:C:P	2.78	0.41
3:I:382:LYS:HB2	3:I:382:LYS:NZ	2.35	0.41
2:H:286:SER:HB2	2:H:364:PHE:CZ	2.54	0.41
1:D:199:VAL:CG1	1:D:200:TRP:H	2.25	0.41
3:F:133:THR:HG23	4:G:85:VAL:CG2	2.51	0.41
5:N:49:G:HO2'	5:N:50:C:P	2.44	0.41
2:E:193:TYR:CD2	2:E:302:ALA:HB2	2.53	0.41
2:E:455:GLU:O	2:E:458:THR:O	2.39	0.41
3:F:212:PHE:O	3:F:215:VAL:HG22	2.20	0.41
1:A:404:LEU:HA	1:A:405:PRO:HD3	1.89	0.41
1:D:320:SER:HB2	3:F:113:ARG:NH1	2.36	0.41
1:A:190:PHE:O	1:A:191:GLU:HB2	2.19	0.41
3:I:10:VAL:HG21	3:I:166:ILE:CD1	2.50	0.41
3:I:15:LYS:HE2	3:I:174:GLY:O	2.20	0.41
1:A:192:ARG:HD2	1:B:39:ARG:NH1	2.34	0.41
2:E:317:ARG:NH2	4:G:85:VAL:HG12	2.35	0.41
3:I:299:ARG:C	3:I:301:LEU:N	2.73	0.41
2:H:369:LYS:O	2:H:373:GLN:HG3	2.21	0.41
5:K:49:G:C6	5:K:66:C:N3	2.89	0.41
3:I:32:GLU:HA	3:I:33:PRO:HD3	1.88	0.41
3:F:10:VAL:HG21	3:F:166:ILE:CD1	2.51	0.41
2:E:369:LYS:O	2:E:373:GLN:HG3	2.21	0.41
1:C:276:LYS:HG3	1:C:287:VAL:HG13	2.01	0.41
3:F:86:LEU:HD23	3:F:86:LEU:HA	1.90	0.41
3:I:18:THR:CG2	4:J:58:ARG:HH12	2.25	0.41
5:M:39:C:O2'	5:M:40:C:P	2.79	0.41
3:F:198:GLU:H	3:F:199:PRO:CD	2.32	0.41
5:M:24:G:O2'	5:M:25:C:H6	2.03	0.41
2:E:190:LEU:O	2:E:192:ALA:N	2.54	0.41
1:A:21:PHE:CZ	1:B:385:PRO:HG3	2.56	0.41
2:E:176:TYR:CZ	2:E:462:HIS:CE1	3.08	0.41
2:E:399:ASP:O	2:E:400:PRO:C	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLN:HG3	1:A:387:HIS:O	2.21	0.41
3:F:64:LEU:HD22	3:F:283:VAL:HG23	2.02	0.41
1:A:278:ILE:HD13	1:A:302:TYR:CE1	2.56	0.41
1:C:149:THR:HB	1:C:150:PRO:CD	2.51	0.41
5:M:3:C:O2'	5:M:4:G:H5'	2.20	0.41
1:B:276:LYS:HE3	1:B:288:GLY:O	2.20	0.41
1:B:184:GLN:O	1:B:187:VAL:HB	2.20	0.41
3:I:362:GLU:HG2	3:I:366:ARG:HE	1.85	0.41
3:F:321:LEU:HD23	3:F:321:LEU:HA	1.88	0.41
1:C:9:LYS:CD	1:C:9:LYS:H	2.31	0.41
2:E:284:TRP:HH2	2:E:368:LEU:O	2.04	0.41
3:F:311:LEU:H	3:F:311:LEU:HD22	1.86	0.41
3:I:359:LEU:HD22	3:I:389:LEU:HD12	2.02	0.41
1:C:278:ILE:HD13	1:C:302:TYR:CE1	2.56	0.41
2:H:335:GLY:O	2:H:339:LYS:HG3	2.20	0.41
2:E:2:LEU:HG	2:E:205:ARG:HH22	1.85	0.41
1:D:306:ARG:HD3	1:D:307:TRP:CH2	2.56	0.41
3:F:122:ASP:CG	3:F:144:LEU:HD11	2.40	0.41
3:I:253:MET:HG3	3:I:254:ARG:N	2.35	0.41
3:I:51:PRO:HD3	3:I:270:LEU:HD22	2.03	0.41
3:F:1:MET:HA	3:F:2:TYR:CG	2.56	0.41
1:B:102:ARG:NH2	5:N:25:C:O2	2.54	0.41
2:H:317:ARG:HH11	4:J:76:PRO:CB	2.29	0.41
2:E:239:GLU:HB3	2:E:241:PRO:CG	2.50	0.41
1:B:47:THR:OG1	1:B:48:GLY:N	2.52	0.41
1:B:385:PRO:O	1:B:387:HIS:CD2	2.74	0.41
3:I:226:GLN:HA	3:I:229:ILE:HG13	2.02	0.41
2:H:160:SER:O	2:H:166:VAL:HG23	2.21	0.41
5:L:50:C:HO2'	5:L:51:A:P	2.44	0.41
3:F:211:SER:O	3:F:215:VAL:HG13	2.21	0.41
3:F:125:LYS:NZ	5:L:73:G:H5''	2.35	0.41
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.77	0.41
3:I:5:VAL:CG2	3:I:194:ARG:HD2	2.51	0.41
3:I:122:ASP:CG	3:I:144:LEU:HD11	2.40	0.41
1:C:197:ALA:HA	1:C:198:PRO:HD3	1.92	0.41
2:E:291:LEU:HD23	2:E:291:LEU:HA	1.83	0.41
1:B:35:LEU:HD22	1:B:35:LEU:N	2.36	0.41
3:I:20:MET:HE3	3:I:52:ASN:H	1.86	0.41
2:E:330:THR:O	2:E:333:LEU:HB2	2.21	0.41
1:A:28:LEU:N	1:A:28:LEU:CD1	2.82	0.41
1:A:384:MET:HA	1:A:385:PRO:HD3	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PHE:HA	1:B:264:PRO:HD3	1.79	0.41
1:A:196:VAL:HG22	1:A:217:LEU:HD22	2.03	0.41
1:B:260:TRP:HA	1:B:261:PRO:HD3	1.83	0.41
2:E:75:ARG:HD2	2:E:84:GLU:O	2.21	0.41
2:H:183:GLY:HA3	2:H:228:LEU:HG	2.03	0.41
1:D:26:ARG:HD3	5:M:38:A:OP2	2.21	0.40
3:I:64:LEU:HD22	3:I:283:VAL:HG23	2.03	0.40
2:E:393:PRO:HD2	2:E:396:ALA:HB2	2.03	0.40
5:K:35:U:C5	5:K:36:U:C4	3.09	0.40
2:H:148:ALA:HA	2:H:153:LEU:HD12	2.03	0.40
5:N:22:G:O2'	5:N:23:A:P	2.79	0.40
1:A:55:PRO:O	1:A:56:GLU:HB2	2.21	0.40
3:F:222:GLU:OE2	3:F:225:ARG:NH1	2.53	0.40
3:F:299:ARG:C	3:F:301:LEU:N	2.73	0.40
3:I:20:MET:HE3	3:I:52:ASN:HB3	2.02	0.40
1:B:86:SER:HA	1:B:87:PRO:HD3	1.87	0.40
5:N:3:C:O2'	5:N:4:G:H5'	2.21	0.40
5:K:27:G:H2'	5:K:28:C:C6	2.56	0.40
3:I:328:GLY:N	3:I:329:LEU:HD12	2.37	0.40
3:F:145:ILE:HG12	3:F:145:ILE:O	2.20	0.40
2:H:239:GLU:HB3	2:H:241:PRO:CG	2.51	0.40
1:D:47:THR:OG1	1:D:48:GLY:N	2.52	0.40
5:K:49:G:C2	5:K:50:C:C4	3.09	0.40
5:L:49:G:C2	5:L:50:C:C4	3.09	0.40
2:E:195:SER:HB2	3:F:268:PRO:HB2	2.03	0.40
2:H:365:ARG:HG3	2:H:415:LEU:HD22	2.03	0.40
3:F:355:GLU:C	3:F:356:GLU:HG3	2.41	0.40
1:C:6:ARG:HB3	1:C:40:SER:HB2	2.04	0.40
2:H:431:LEU:HA	2:H:432:PRO:HD3	1.88	0.40
5:L:62:C:H2'	5:L:63:U:C6	2.56	0.40
5:M:73:G:H5"	5:M:73:G:H8	1.87	0.40
1:C:200:TRP:CD1	1:C:200:TRP:N	2.89	0.40
1:A:200:TRP:CD1	1:A:200:TRP:N	2.89	0.40
2:E:439:ALA:HB1	2:E:440:PRO:HD2	2.03	0.40
5:M:5:C:N4	5:M:68:G:H1	2.16	0.40
1:C:101:TRP:CG	1:C:102:ARG:N	2.90	0.40
1:C:30:ARG:HD2	1:C:30:ARG:HA	1.68	0.40
3:F:70:VAL:HA	3:F:71:PRO:HD3	1.86	0.40
1:D:184:GLN:O	1:D:187:VAL:HB	2.21	0.40
3:F:3:GLU:OE1	3:F:194:ARG:HD3	2.22	0.40
2:E:317:ARG:CZ	2:E:326:MET:HE1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLN:HG3	1:B:47:THR:HG23	2.02	0.40
2:H:141:SER:H	2:H:165:SER:HB3	1.86	0.40
3:I:160:ARG:HH11	3:I:216:GLN:HE22	1.67	0.40
1:C:404:LEU:HA	1:C:405:PRO:HD3	1.90	0.40
1:A:260:TRP:HA	1:A:261:PRO:HD3	1.80	0.40
1:C:321:VAL:O	1:C:322:ARG:HD3	2.21	0.40
3:F:346:LEU:HD22	3:F:346:LEU:HA	1.96	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	368/422 (87%)	343 (93%)	23 (6%)	2 (0%)	34	76
1	B	370/422 (88%)	347 (94%)	22 (6%)	1 (0%)	46	84
1	C	371/422 (88%)	344 (93%)	24 (6%)	3 (1%)	24	66
1	D	364/422 (86%)	342 (94%)	20 (6%)	2 (0%)	34	76
2	E	467/471 (99%)	420 (90%)	39 (8%)	8 (2%)	11	46
2	H	466/471 (99%)	420 (90%)	37 (8%)	9 (2%)	10	43
3	F	386/466 (83%)	354 (92%)	28 (7%)	4 (1%)	19	61
3	I	376/466 (81%)	348 (93%)	25 (7%)	3 (1%)	24	66
4	G	84/92 (91%)	80 (95%)	3 (4%)	1 (1%)	16	56
4	J	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
All	All	3331/3746 (89%)	3075 (92%)	223 (7%)	33 (1%)	19	61

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	415	ARG
2	E	43	GLU
2	E	243	PRO
2	E	466	PRO
2	H	43	GLU
2	H	54	PRO
2	H	243	PRO
1	B	101	TRP
1	D	101	TRP
3	F	356	GLU
2	H	319	ALA
3	I	356	GLU
2	E	44	ARG
3	F	198	GLU
3	F	328	GLY
4	G	51	GLU
2	H	44	ARG
1	A	50	LEU
1	C	50	LEU
2	E	244	PRO
2	H	244	PRO
1	C	212	ASN
2	E	119	SER
2	H	119	SER
1	A	49	GLY
1	C	49	GLY
2	E	191	ILE
3	F	246	GLY
2	H	191	ILE
3	I	246	GLY
2	E	232	PRO
2	H	232	PRO
3	I	374	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/355 (89%)	302 (96%)	14 (4%)	35	74
1	B	318/355 (90%)	303 (95%)	15 (5%)	32	72
1	C	319/355 (90%)	304 (95%)	15 (5%)	32	72
1	D	316/355 (89%)	302 (96%)	14 (4%)	35	74
2	E	349/354 (99%)	320 (92%)	29 (8%)	14	46
2	H	348/354 (98%)	317 (91%)	31 (9%)	12	42
3	F	328/334 (98%)	294 (90%)	34 (10%)	9	32
3	I	320/334 (96%)	289 (90%)	31 (10%)	10	37
4	G	72/77 (94%)	67 (93%)	5 (7%)	19	56
4	J	72/77 (94%)	68 (94%)	4 (6%)	26	65
All	All	2758/2950 (94%)	2566 (93%)	192 (7%)	19	55

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	50	LEU
1	A	56	GLU
1	A	68	ASN
1	A	101	TRP
1	A	110	GLU
1	A	112	ARG
1	A	116	LEU
1	A	142	GLN
1	A	143	ASP
1	A	218	ASP
1	A	298	LEU
1	A	313	PHE
1	A	406	ASN
1	B	9	LYS
1	B	22	LEU
1	B	50	LEU
1	B	68	ASN
1	B	101	TRP
1	B	110	GLU
1	B	116	LEU
1	B	142	GLN
1	B	143	ASP
1	B	218	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	246	LEU
1	B	289	GLN
1	B	321	VAL
1	B	406	ASN
1	B	411	ARG
1	C	9	LYS
1	C	28	LEU
1	C	50	LEU
1	C	56	GLU
1	C	68	ASN
1	C	101	TRP
1	C	110	GLU
1	C	112	ARG
1	C	116	LEU
1	C	142	GLN
1	C	143	ASP
1	C	218	ASP
1	C	298	LEU
1	C	313	PHE
1	C	406	ASN
1	D	9	LYS
1	D	22	LEU
1	D	50	LEU
1	D	68	ASN
1	D	101	TRP
1	D	110	GLU
1	D	116	LEU
1	D	142	GLN
1	D	143	ASP
1	D	218	ASP
1	D	246	LEU
1	D	289	GLN
1	D	406	ASN
1	D	411	ARG
2	E	25	LEU
2	E	47	GLU
2	E	74	LEU
2	E	106	LEU
2	E	109	THR
2	E	116	MET
2	E	193	TYR
2	E	203	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	215	ASP
2	E	242	LEU
2	E	246	ARG
2	E	270	LYS
2	E	275	LEU
2	E	284	TRP
2	E	291	LEU
2	E	296	ILE
2	E	308	ARG
2	E	317	ARG
2	E	323	VAL
2	E	328	GLU
2	E	336	LEU
2	E	342	VAL
2	E	365	ARG
2	E	383	LEU
2	E	384	LEU
2	E	398	ARG
2	E	444	ASP
2	E	448	LEU
2	E	452	LEU
3	F	1	MET
3	F	14	LEU
3	F	18	THR
3	F	29	PHE
3	F	36	HIS
3	F	41	CYS
3	F	69	GLU
3	F	74	LEU
3	F	86	LEU
3	F	99	LEU
3	F	111	ARG
3	F	133	THR
3	F	145	ILE
3	F	152	ASP
3	F	154	LYS
3	F	157	GLU
3	F	161	LEU
3	F	169	LEU
3	F	185	LEU
3	F	210	ASN
3	F	215	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	219	LEU
3	F	229	ILE
3	F	290	LEU
3	F	292	TRP
3	F	301	LEU
3	F	311	LEU
3	F	321	LEU
3	F	329	LEU
3	F	339	LEU
3	F	346	LEU
3	F	356	GLU
3	F	373	ARG
3	F	385	LEU
4	G	15	LEU
4	G	20	LEU
4	G	28	LEU
4	G	42	LEU
4	G	44	ARG
2	H	2	LEU
2	H	25	LEU
2	H	47	GLU
2	H	56	LEU
2	H	74	LEU
2	H	106	LEU
2	H	109	THR
2	H	116	MET
2	H	179	LYS
2	H	193	TYR
2	H	203	MET
2	H	215	ASP
2	H	238	LEU
2	H	246	ARG
2	H	270	LYS
2	H	275	LEU
2	H	284	TRP
2	H	291	LEU
2	H	296	ILE
2	H	308	ARG
2	H	317	ARG
2	H	323	VAL
2	H	324	GLU
2	H	328	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	336	LEU
2	H	342	VAL
2	H	343	LEU
2	H	365	ARG
2	H	384	LEU
2	H	408	LEU
2	H	452	LEU
3	I	14	LEU
3	I	18	THR
3	I	29	PHE
3	I	36	HIS
3	I	41	CYS
3	I	69	GLU
3	I	86	LEU
3	I	99	LEU
3	I	133	THR
3	I	145	ILE
3	I	152	ASP
3	I	154	LYS
3	I	157	GLU
3	I	161	LEU
3	I	169	LEU
3	I	185	LEU
3	I	210	ASN
3	I	215	VAL
3	I	219	LEU
3	I	229	ILE
3	I	290	LEU
3	I	292	TRP
3	I	301	LEU
3	I	311	LEU
3	I	321	LEU
3	I	329	LEU
3	I	339	LEU
3	I	346	LEU
3	I	356	GLU
3	I	373	ARG
3	I	385	LEU
4	J	15	LEU
4	J	20	LEU
4	J	42	LEU
4	J	44	ARG

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

Mol	Chain	Res	Type
1	A	68	ASN
1	A	128	GLN
1	A	184	GLN
1	A	354	HIS
1	A	387	HIS
1	A	406	ASN
1	B	11	HIS
1	B	68	ASN
1	B	128	GLN
1	B	184	GLN
1	B	212	ASN
1	B	387	HIS
1	C	68	ASN
1	C	128	GLN
1	C	184	GLN
1	C	212	ASN
1	C	387	HIS
1	C	406	ASN
1	D	11	HIS
1	D	68	ASN
1	D	128	GLN
1	D	184	GLN
1	D	212	ASN
1	D	387	HIS
2	E	389	HIS
3	F	58	HIS
3	F	118	HIS
3	F	210	ASN
3	F	216	GLN
3	F	333	GLN
4	G	68	GLN
2	H	199	GLN
3	I	58	HIS
3	I	118	HIS
3	I	210	ASN
3	I	216	GLN
3	I	333	GLN
4	J	68	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	K	72/76 (94%)	13 (18%)	0
5	L	72/76 (94%)	13 (18%)	0
5	M	69/76 (90%)	22 (31%)	1 (1%)
5	N	69/76 (90%)	22 (31%)	1 (1%)
All	All	282/304 (92%)	70 (24%)	2 (0%)

All (70) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	K	10	G
5	K	21	A
5	K	22	G
5	K	23	A
5	K	24	G
5	K	33	U
5	K	40	C
5	K	46	G
5	K	49	G
5	K	50	C
5	K	51	A
5	K	52	G
5	K	76	A
5	L	10	G
5	L	21	A
5	L	22	G
5	L	23	A
5	L	24	G
5	L	33	U
5	L	40	C
5	L	46	G
5	L	49	G
5	L	50	C
5	L	51	A
5	L	52	G
5	L	76	A
5	M	6	G
5	M	11	C
5	M	12	U
5	M	13	C
5	M	14	A
5	M	19	G
5	M	20	H2U
5	M	21	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	22	G
5	M	23	A
5	M	24	G
5	M	25	C
5	M	27	G
5	M	38	A
5	M	40	C
5	M	49	G
5	M	50	C
5	M	51	A
5	M	52	G
5	M	62	C
5	M	63	U
5	M	73	G
5	N	6	G
5	N	11	C
5	N	12	U
5	N	13	C
5	N	14	A
5	N	19	G
5	N	20	H2U
5	N	21	A
5	N	22	G
5	N	23	A
5	N	24	G
5	N	25	C
5	N	27	G
5	N	38	A
5	N	40	C
5	N	49	G
5	N	50	C
5	N	51	A
5	N	52	G
5	N	62	C
5	N	63	U
5	N	73	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	M	20	H2U
5	N	20	H2U

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	H2U	K	20	5	17,21,22	3.94	7 (41%)	23,30,33	4.89	9 (39%)
5	5MU	K	54	5	12,22,23	1.87	2 (16%)	14,32,35	2.19	2 (14%)
5	PSU	K	55	5	13,21,22	1.12	1 (7%)	18,30,33	3.53	6 (33%)
5	H2U	L	20	5	17,21,22	3.92	7 (41%)	23,30,33	4.90	9 (39%)
5	5MU	L	54	5	12,22,23	1.85	2 (16%)	14,32,35	2.18	2 (14%)
5	PSU	L	55	5	13,21,22	1.06	1 (7%)	18,30,33	3.65	6 (33%)
5	H2U	M	20	5	17,21,22	3.97	7 (41%)	23,30,33	5.03	9 (39%)
5	5MU	M	54	5	12,22,23	1.88	2 (16%)	14,32,35	2.18	2 (14%)
5	PSU	M	55	5	13,21,22	1.08	1 (7%)	18,30,33	3.62	6 (33%)
5	H2U	N	20	5	17,21,22	3.95	7 (41%)	23,30,33	5.02	9 (39%)
5	5MU	N	54	5	12,22,23	1.88	2 (16%)	14,32,35	2.16	2 (14%)
5	PSU	N	55	5	13,21,22	1.06	1 (7%)	18,30,33	3.66	6 (33%)

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
5	H2U	K	20	5	-	0/7/38/39	0/2/2/2
5	5MU	K	54	5	-	0/3/25/26	0/2/2/2
5	PSU	K	55	5	-	0/7/25/26	0/2/2/2
5	H2U	L	20	5	-	0/7/38/39	0/2/2/2
5	5MU	L	54	5	-	0/3/25/26	0/2/2/2
5	PSU	L	55	5	-	0/7/25/26	0/2/2/2
5	H2U	M	20	5	-	0/7/38/39	0/2/2/2
5	5MU	M	54	5	-	0/3/25/26	0/2/2/2
5	PSU	M	55	5	-	0/7/25/26	0/2/2/2
5	H2U	N	20	5	-	0/7/38/39	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5MU	N	54	5	-	0/3/25/26	0/2/2/2
5	PSU	N	55	5	-	0/7/25/26	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	20	H2U	C6-N1	-2.44	1.44	1.47
5	N	20	H2U	C6-N1	-2.40	1.44	1.47
5	M	20	H2U	C5-C4	-2.39	1.45	1.50
5	N	20	H2U	C5-C4	-2.38	1.45	1.50
5	L	20	H2U	C5-C4	-2.36	1.45	1.50
5	L	20	H2U	C6-N1	-2.32	1.44	1.47
5	K	20	H2U	C6-N1	-2.31	1.44	1.47
5	K	20	H2U	C5-C4	-2.30	1.45	1.50
5	L	55	PSU	C4-N3	2.72	1.38	1.33
5	N	55	PSU	C4-N3	2.78	1.38	1.33
5	M	55	PSU	C4-N3	2.85	1.38	1.33
5	L	54	5MU	C4-N3	2.86	1.38	1.33
5	K	55	PSU	C4-N3	2.87	1.38	1.33
5	K	54	5MU	C4-N3	2.95	1.38	1.33
5	M	54	5MU	C4-N3	3.02	1.38	1.33
5	N	54	5MU	C4-N3	3.09	1.38	1.33
5	K	20	H2U	C4-N3	3.86	1.43	1.37
5	N	20	H2U	C4-N3	3.90	1.43	1.37
5	L	20	H2U	C4-N3	3.92	1.43	1.37
5	M	20	H2U	C4-N3	3.93	1.43	1.37
5	L	54	5MU	O4-C4	5.27	1.37	1.24
5	N	54	5MU	O4-C4	5.30	1.37	1.24
5	K	54	5MU	O4-C4	5.34	1.37	1.24
5	M	54	5MU	O4-C4	5.34	1.37	1.24
5	L	20	H2U	C2-N1	6.09	1.45	1.35
5	K	20	H2U	C2-N1	6.16	1.45	1.35
5	N	20	H2U	C2-N1	6.29	1.45	1.35
5	M	20	H2U	C2-N1	6.30	1.45	1.35
5	N	20	H2U	C2-N3	6.70	1.50	1.38
5	M	20	H2U	C2-N3	6.74	1.50	1.38
5	K	20	H2U	C2-N3	6.74	1.50	1.38
5	L	20	H2U	C2-N3	6.80	1.50	1.38
5	L	20	H2U	O2-C2	8.51	1.39	1.23
5	M	20	H2U	O2-C2	8.59	1.39	1.23
5	N	20	H2U	O2-C2	8.60	1.39	1.23
5	K	20	H2U	O2-C2	8.61	1.39	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	20	H2U	O4-C4	8.66	1.41	1.23
5	N	20	H2U	O4-C4	8.71	1.41	1.23
5	K	20	H2U	O4-C4	8.76	1.41	1.23
5	M	20	H2U	O4-C4	8.81	1.41	1.23

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	20	H2U	C4-N3-C2	-15.19	113.26	125.79
5	M	20	H2U	C4-N3-C2	-15.09	113.34	125.79
5	K	20	H2U	C4-N3-C2	-14.97	113.44	125.79
5	L	20	H2U	C4-N3-C2	-14.89	113.50	125.79
5	N	55	PSU	N1-C2-N3	-13.14	119.95	128.33
5	L	55	PSU	N1-C2-N3	-12.94	120.07	128.33
5	M	55	PSU	N1-C2-N3	-12.94	120.08	128.33
5	K	55	PSU	N1-C2-N3	-12.52	120.34	128.33
5	L	20	H2U	O2-C2-N1	-10.37	109.73	123.30
5	K	20	H2U	O2-C2-N1	-10.18	109.98	123.30
5	M	20	H2U	O2-C2-N1	-9.99	110.23	123.30
5	N	20	H2U	O2-C2-N1	-9.96	110.27	123.30
5	M	20	H2U	C6-N1-C2	-7.67	110.64	122.23
5	N	20	H2U	C6-N1-C2	-7.61	110.73	122.23
5	K	20	H2U	O4-C4-N3	-7.51	108.73	120.45
5	M	20	H2U	O4-C4-N3	-7.37	108.96	120.45
5	N	20	H2U	O4-C4-N3	-7.36	108.98	120.45
5	L	20	H2U	O4-C4-N3	-7.32	109.03	120.45
5	L	20	H2U	O4-C4-C5	-6.40	107.99	122.34
5	L	20	H2U	C6-N1-C2	-6.39	112.58	122.23
5	N	20	H2U	O4-C4-C5	-6.25	108.32	122.34
5	K	20	H2U	C6-N1-C2	-6.25	112.79	122.23
5	M	20	H2U	O4-C4-C5	-6.21	108.42	122.34
5	K	20	H2U	O4-C4-C5	-6.19	108.45	122.34
5	K	20	H2U	O2-C2-N3	-5.94	109.88	121.48
5	L	20	H2U	O2-C2-N3	-5.84	110.07	121.48
5	M	20	H2U	O2-C2-N3	-5.69	110.36	121.48
5	N	20	H2U	O2-C2-N3	-5.66	110.41	121.48
5	M	20	H2U	C1'-N1-C2	-5.41	110.79	118.27
5	N	20	H2U	C1'-N1-C2	-5.33	110.90	118.27
5	M	20	H2U	C5-C4-N3	-5.21	111.80	116.71
5	N	20	H2U	C5-C4-N3	-5.09	111.91	116.71
5	L	20	H2U	C5-C4-N3	-4.76	112.22	116.71
5	K	54	5MU	C5-C4-N3	-4.72	119.89	125.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	54	5MU	C5-C4-N3	-4.66	119.94	125.14
5	K	20	H2U	C5-C4-N3	-4.60	112.38	116.71
5	N	54	5MU	C5-C4-N3	-4.59	120.02	125.14
5	L	54	5MU	C5-C4-N3	-4.55	120.08	125.14
5	K	20	H2U	C1'-N1-C2	-3.83	112.97	118.27
5	L	20	H2U	C1'-N1-C2	-3.81	113.00	118.27
5	L	55	PSU	C5-C1'-C2'	-3.45	109.40	115.52
5	K	20	H2U	N3-C2-N1	-3.32	113.28	116.60
5	L	20	H2U	N3-C2-N1	-3.30	113.30	116.60
5	K	55	PSU	C5-C1'-C2'	-3.12	109.97	115.52
5	L	55	PSU	C5-C6-N1	-3.09	120.04	124.39
5	M	55	PSU	C5-C1'-C2'	-3.07	110.07	115.52
5	N	55	PSU	C5-C6-N1	-3.06	120.07	124.39
5	N	55	PSU	C5-C1'-C2'	-3.04	110.13	115.52
5	M	55	PSU	C5-C6-N1	-2.97	120.19	124.39
5	K	55	PSU	C5-C6-N1	-2.89	120.31	124.39
5	N	20	H2U	N3-C2-N1	-2.68	113.92	116.60
5	M	20	H2U	N3-C2-N1	-2.64	113.97	116.60
5	K	55	PSU	O4'-C1'-C2'	2.77	107.56	104.73
5	N	55	PSU	O4'-C1'-C2'	2.78	107.57	104.73
5	M	55	PSU	O4'-C1'-C2'	2.81	107.59	104.73
5	L	55	PSU	O4'-C1'-C2'	2.88	107.67	104.73
5	K	55	PSU	C6-N1-C2	3.06	120.39	115.47
5	M	55	PSU	C6-N1-C2	3.22	120.65	115.47
5	L	55	PSU	C6-N1-C2	3.32	120.80	115.47
5	N	55	PSU	C6-N1-C2	3.34	120.85	115.47
5	N	55	PSU	C4-N3-C2	5.07	119.62	115.25
5	M	55	PSU	C4-N3-C2	5.13	119.68	115.25
5	L	55	PSU	C4-N3-C2	5.14	119.69	115.25
5	K	55	PSU	C4-N3-C2	5.24	119.77	115.25
5	N	54	5MU	C4-N3-C2	6.47	120.84	115.25
5	M	54	5MU	C4-N3-C2	6.51	120.87	115.25
5	K	54	5MU	C4-N3-C2	6.51	120.88	115.25
5	L	54	5MU	C4-N3-C2	6.61	120.96	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	20	H2U	1	0
5	N	20	H2U	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	374/422 (88%)	-0.47	2 (0%) 91 76	23, 54, 101, 153	0
1	B	376/422 (89%)	-0.41	1 (0%) 94 84	27, 62, 136, 209	0
1	C	377/422 (89%)	-0.33	7 (1%) 70 41	30, 71, 129, 187	0
1	D	372/422 (88%)	-0.23	8 (2%) 65 35	29, 74, 141, 224	0
2	E	468/471 (99%)	-0.25	4 (0%) 85 64	27, 65, 120, 211	0
2	H	467/471 (99%)	-0.35	4 (0%) 85 64	24, 56, 104, 209	0
3	F	390/466 (83%)	-0.20	8 (2%) 67 36	18, 67, 137, 233	0
3	I	382/466 (81%)	-0.26	5 (1%) 79 53	18, 67, 127, 247	0
4	G	86/92 (93%)	-0.39	1 (1%) 81 55	41, 79, 132, 200	0
4	J	83/92 (90%)	-0.33	0 100 100	36, 64, 113, 147	0
5	K	71/76 (93%)	-0.08	1 (1%) 78 51	48, 82, 120, 161	0
5	L	71/76 (93%)	-0.26	0 100 100	40, 62, 84, 111	0
5	M	68/76 (89%)	0.57	3 (4%) 38 16	69, 101, 175, 190	0
5	N	68/76 (89%)	0.23	1 (1%) 76 49	57, 85, 156, 277	0
All	All	3653/4050 (90%)	-0.28	45 (1%) 81 55	18, 65, 128, 277	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	235	LYS	5.5
1	D	370	PRO	4.0
2	H	44	ARG	3.9
2	E	165	SER	3.9
3	I	233	GLY	3.7
1	C	369	ASP	3.6
3	F	235	LYS	3.4
3	I	234	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	285	TYR	3.3
2	H	165	SER	3.3
3	F	1	MET	3.2
5	K	47	U	3.1
4	G	50	ALA	3.0
5	M	56	C	3.0
3	F	234	GLU	2.9
1	D	374	HIS	2.9
3	F	387	GLU	2.8
3	F	30	GLY	2.8
2	E	162	THR	2.8
1	C	64	LEU	2.7
5	M	57	G	2.7
1	D	373	PHE	2.7
5	M	19	G	2.7
5	N	73	G	2.6
1	D	362	SER	2.6
1	D	15	GLU	2.5
2	H	462	HIS	2.4
2	E	161	ASP	2.4
2	H	142	SER	2.4
1	B	290	ASP	2.3
3	F	210	ASN	2.3
2	E	142	SER	2.3
3	I	230	LEU	2.3
3	F	199	PRO	2.3
1	C	1	MET	2.3
1	D	289	GLN	2.3
1	C	368	MET	2.2
1	C	100	GLU	2.1
1	A	371	GLU	2.1
1	D	286	PRO	2.1
1	C	10	ALA	2.1
1	C	13	GLY	2.1
3	F	356	GLU	2.1
3	I	375	GLU	2.0
1	A	373	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	5MU	M	54	21/22	0.74	0.32	-	183,194,249,494	0
5	PSU	L	55	20/21	0.97	0.16	-	63,67,68,165	0
5	5MU	K	54	21/22	0.96	0.15	-	78,82,86,195	0
5	PSU	K	55	20/21	0.95	0.13	-	75,81,88,201	0
5	PSU	N	55	20/21	0.84	0.23	-	100,133,138,254	0
5	H2U	M	20	20/21	0.74	0.50	-	189,193,344,404	0
5	PSU	M	55	20/21	0.67	0.35	-	197,203,217,454	0
5	5MU	L	54	21/22	0.97	0.15	-	55,61,65,151	0
5	5MU	N	54	21/22	0.89	0.28	-	86,110,113,235	0
5	H2U	K	20	20/21	0.93	0.17	-	102,107,110,242	0
5	H2U	L	20	20/21	0.96	0.18	-	61,63,66,162	0
5	H2U	N	20	20/21	0.80	0.32	-	141,145,197,259	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	ZN	F	673	1/1	0.97	0.22	5.39	100,100,100,100	0
6	ZN	I	467	1/1	0.95	0.20	4.33	133,133,133,133	0
7	MG	I	468	1/1	0.96	0.07	-4.60	46,46,46,46	0
7	MG	F	674	1/1	0.85	0.11	-	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.