



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:27 PM GMT

PDB ID : 1ASY  
Title : CLASS II AMINOACYL TRANSFER RNA SYNTHETASES: CRYSTAL STRUCTURE OF YEAST ASPARTYL-TRNA SYNTHETASE COMPLEXED WITH TRNA ASP  
Authors : Ruff, M.; Cavarelli, J.; Rees, B.; Krishnaswamy, S.; Thierry, J.C.; Moras, D.  
Deposited on : 1995-01-19  
Resolution : 2.90 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](mailto: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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

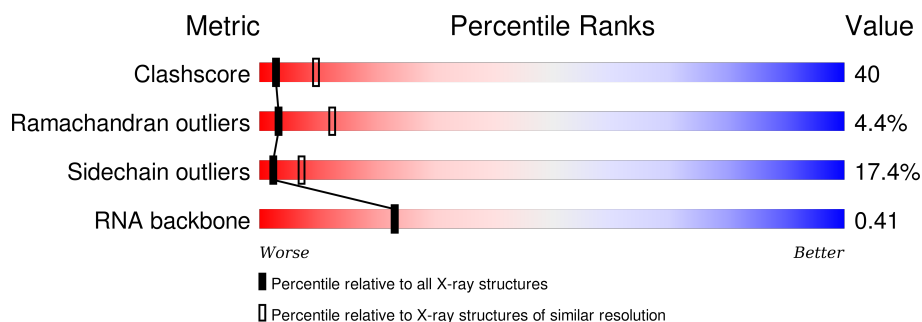
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	R	75	
1	S	75	
2	A	490	
2	B	490	

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
1	H2U	S	619	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11096 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called T-RNA (75-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	75	Total	C	N	O	P	0	0	0
			1602	715	280	532	75			
1	S	75	Total	C	N	O	P	0	0	0
			1602	715	280	532	75			

- Molecule 2 is a protein called ASPARTYL-tRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	490	Total	C	N	O	S	0	0	0
			3946	2513	679	741	13			
2	B	490	Total	C	N	O	S	0	0	0
			3946	2513	679	741	13			

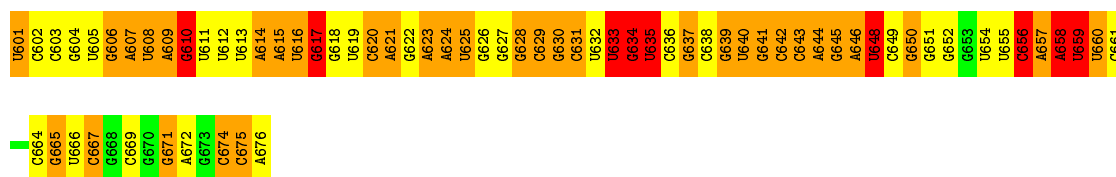
### 3 Residue-property plots

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.

Note EDS was not executed.

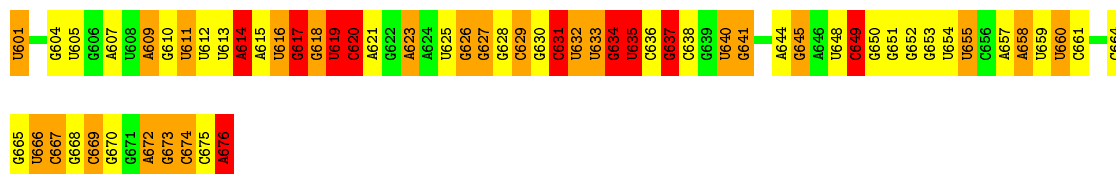
#### • Molecule 1: T-RNA (75-MER)

Chain R: 

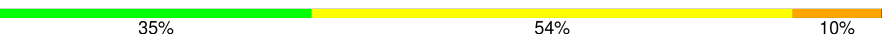


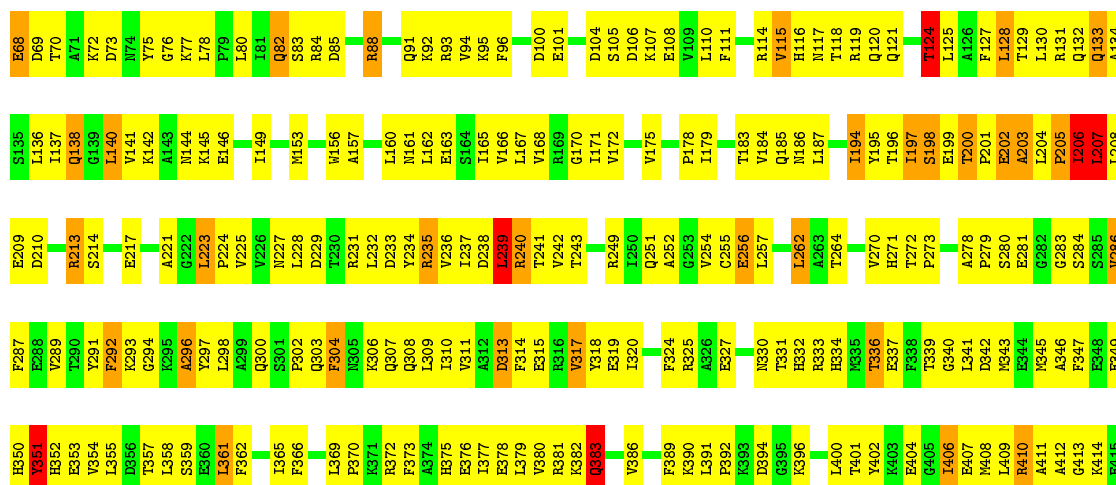
#### • Molecule 1: T-RNA (75-MER)

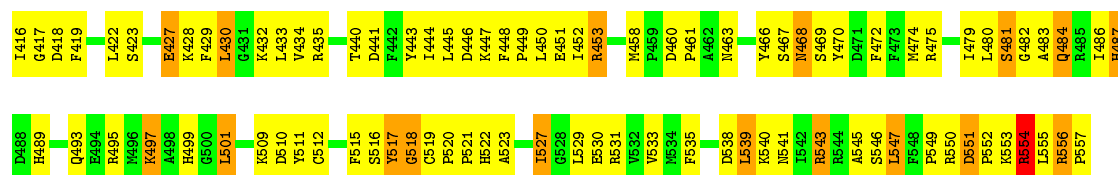
Chain S: 



#### • Molecule 2: ASPARTYL-tRNA SYNTHETASE

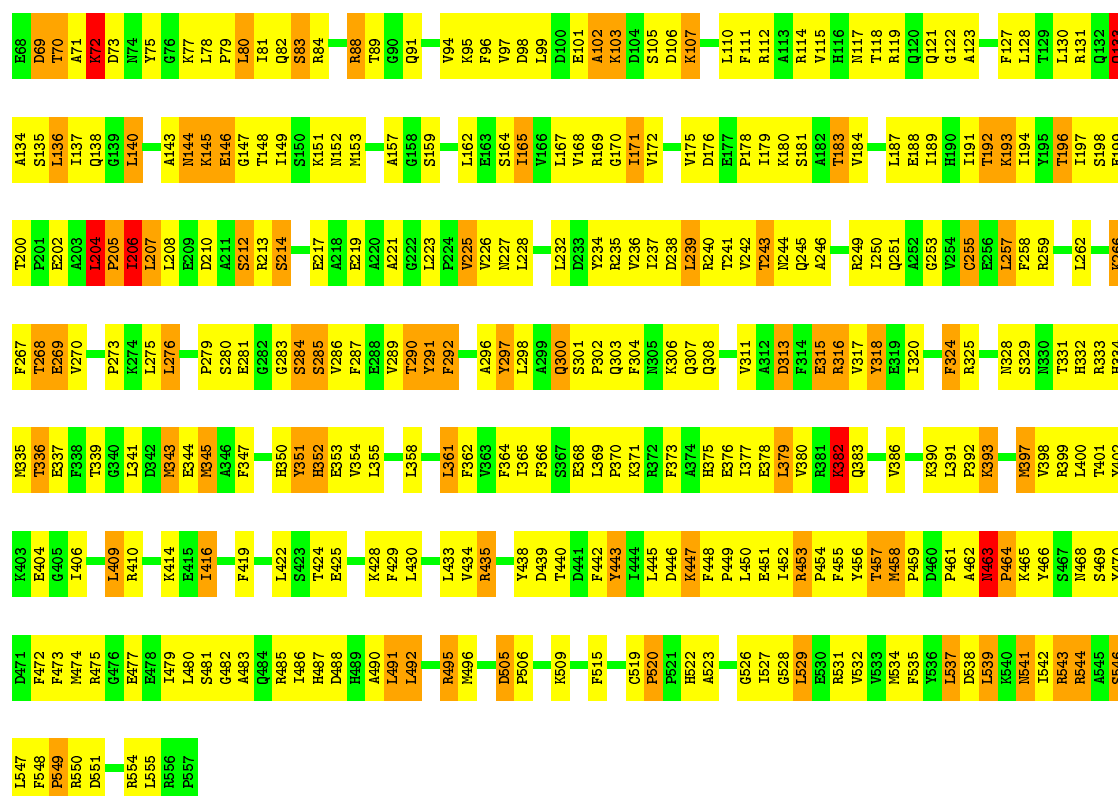
Chain A: 





• Molecule 2: ASPARTYL-tRNA SYNTHETASE

Chain B: 35% 49% 15%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.25Å 146.17Å 86.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.90	Depositor
% Data completeness (in resolution range)	85.0 (7.00-2.90)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.225 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, H2U, 1MG, 5MC, 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	R	1.12	1/1605 (0.1%)	2.05	73/2500 (2.9%)
1	S	1.11	1/1605 (0.1%)	1.89	55/2500 (2.2%)
2	A	0.64	1/4029 (0.0%)	0.89	7/5433 (0.1%)
2	B	0.62	0/4029	0.89	5/5433 (0.1%)
All	All	0.80	3/11268 (0.0%)	1.33	140/15866 (0.9%)

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	A	0	3
2	B	0	4
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	VAL	CB-CG2	-5.58	1.41	1.52
1	R	639	G	C6-N1	-5.30	1.35	1.39
1	S	667	C	N3-C4	5.29	1.37	1.33

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	626	G	OP1-P-O3'	11.50	130.50	105.20
1	R	622	G	OP1-P-O3'	10.82	129.01	105.20
1	R	607	A	OP1-P-O3'	10.67	128.67	105.20
1	R	611	U	OP2-P-O3'	10.51	128.32	105.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	641	G	OP1-P-O3'	10.43	128.13	105.20
1	R	642	C	OP1-P-O3'	9.93	127.06	105.20
1	R	634	G	O4'-C1'-N9	9.43	115.74	108.20
1	R	659	U	OP1-P-O3'	9.33	125.73	105.20
1	R	646	A	OP1-P-O3'	9.18	125.40	105.20
1	R	645	G	OP1-P-O3'	9.09	125.20	105.20
1	R	623	A	OP1-P-O3'	8.83	124.64	105.20
1	R	643	C	OP1-P-O3'	8.60	124.12	105.20
1	R	620	C	OP2-P-O3'	8.53	123.96	105.20
1	R	627	G	O3'-P-O5'	-8.46	87.92	104.00
1	R	658	A	OP1-P-O3'	8.44	123.76	105.20
1	S	632	PSU	O3'-P-O5'	8.28	119.72	104.00
1	R	628	G	OP2-P-O3'	8.16	123.16	105.20
1	R	614	A	O4'-C1'-N9	8.15	114.72	108.20
1	S	634	G	P-O3'-C3'	8.05	129.37	119.70
1	R	603	C	O4'-C1'-N1	8.02	114.62	108.20
1	R	625	U	OP1-P-O3'	7.98	122.76	105.20
1	R	610	G	OP1-P-O3'	7.88	122.54	105.20
1	S	635	U	OP2-P-O3'	7.60	121.92	105.20
1	R	624	A	OP1-P-O3'	7.59	121.89	105.20
1	R	626	G	OP1-P-O3'	7.53	121.77	105.20
1	R	608	U	O3'-P-O5'	7.42	118.09	104.00
1	S	653	G	O4'-C1'-N9	7.42	114.13	108.20
1	R	627	G	OP1-P-O3'	7.39	121.45	105.20
1	S	625	U	O4'-C1'-N1	7.32	114.05	108.20
1	R	664	C	O4'-C1'-N1	7.13	113.91	108.20
1	S	623	A	OP1-P-O3'	7.08	120.78	105.20
1	R	634	G	P-O3'-C3'	7.02	128.13	119.70
1	S	631	C	O4'-C1'-N1	6.92	113.74	108.20
1	R	667	C	O4'-C1'-N1	6.91	113.72	108.20
1	S	627	G	O3'-P-O5'	-6.90	90.89	104.00
1	R	633	U	O3'-P-O5'	6.90	117.11	104.00
1	R	631	C	O4'-C1'-N1	6.88	113.71	108.20
1	S	629	C	OP2-P-O3'	6.87	120.31	105.20
1	R	625	U	O4'-C1'-N1	6.85	113.68	108.20
1	S	627	G	OP1-P-O3'	6.80	120.16	105.20
1	S	625	U	O3'-P-O5'	6.77	116.86	104.00
1	S	676	A	O4'-C1'-N9	6.77	113.62	108.20
1	S	611	U	OP1-P-O3'	6.70	119.95	105.20
1	S	609	A	OP1-P-O3'	6.68	119.91	105.20
1	S	633	U	OP2-P-O3'	6.68	119.89	105.20
1	S	664	C	OP2-P-O3'	6.67	119.88	105.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	616	H2U	OP1-P-O3'	6.58	119.68	105.20
1	R	604	G	O4'-C1'-N9	6.53	113.42	108.20
1	R	644	A	OP1-P-O3'	6.52	119.53	105.20
1	R	660	U	OP1-P-O3'	6.49	119.48	105.20
2	B	204	LEU	CA-CB-CG	6.49	130.23	115.30
2	A	400	LEU	CA-CB-CG	6.43	130.09	115.30
1	S	617	G	O4'-C1'-N9	6.41	113.33	108.20
1	S	621	A	O4'-C1'-N9	-6.40	103.08	108.20
1	S	641	G	OP1-P-O3'	6.40	119.28	105.20
1	R	640	U	OP1-P-O3'	6.39	119.25	105.20
1	R	615	A	OP1-P-OP2	-6.27	110.19	119.60
1	R	657	A	OP1-P-O3'	6.26	118.97	105.20
2	B	207	LEU	CA-CB-CG	6.21	129.58	115.30
1	R	633	U	P-O3'-C3'	6.20	127.14	119.70
1	R	660	U	OP1-P-OP2	-6.19	110.32	119.60
1	R	601	U	OP1-P-OP2	-6.12	110.42	119.60
1	S	660	U	OP1-P-OP2	-6.11	110.44	119.60
1	R	629	C	OP1-P-O3'	6.10	118.61	105.20
1	R	648	U	OP1-P-OP2	-6.08	110.48	119.60
1	S	652	G	O4'-C1'-N9	6.03	113.03	108.20
1	S	605	U	O4'-C1'-N1	6.00	113.00	108.20
1	S	666	U	OP1-P-OP2	-5.90	110.75	119.60
1	R	624	A	O3'-P-O5'	-5.89	92.80	104.00
1	S	610	G	OP1-P-OP2	-5.88	110.78	119.60
1	R	646	A	O4'-C1'-N9	5.88	112.90	108.20
1	S	620	C	OP1-P-O3'	5.86	118.10	105.20
1	R	608	U	OP1-P-OP2	-5.86	110.81	119.60
1	S	616	H2U	OP2-P-O3'	5.72	117.79	105.20
1	S	611	U	OP1-P-OP2	-5.70	111.05	119.60
1	R	606	G	O4'-C1'-N9	5.70	112.76	108.20
1	R	617	G	OP1-P-OP2	-5.70	111.05	119.60
1	R	630	G	OP1-P-OP2	-5.68	111.07	119.60
1	R	674	C	OP1-P-OP2	-5.67	111.10	119.60
1	R	646	A	OP2-P-O3'	-5.67	92.73	105.20
1	R	611	U	OP1-P-OP2	-5.63	111.16	119.60
1	S	637	1MG	OP1-P-O3'	5.60	117.53	105.20
1	S	621	A	OP1-P-OP2	-5.59	111.22	119.60
2	A	417	GLY	N-CA-C	5.59	127.07	113.10
1	R	609	A	OP1-P-O3'	5.58	117.48	105.20
1	S	649	5MC	OP1-P-O3'	5.58	117.48	105.20
1	S	623	A	O3'-P-O5'	-5.53	93.49	104.00
1	R	669	C	O4'-C1'-N1	5.52	112.62	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	671	G	N9-C1'-C2'	-5.51	105.94	112.00
2	A	484	GLN	N-CA-C	-5.50	96.16	111.00
2	B	259	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	R	656	C	OP1-P-OP2	-5.49	111.36	119.60
1	S	626	G	OP1-P-OP2	-5.49	111.37	119.60
1	S	645	G	O4'-C1'-N9	5.49	112.59	108.20
1	S	664	C	N1-C1'-C2'	-5.48	105.98	112.00
1	R	635	U	OP1-P-OP2	-5.46	111.40	119.60
1	R	665	G	OP1-P-OP2	-5.46	111.40	119.60
2	A	337	GLU	N-CA-C	-5.46	96.25	111.00
2	A	207	LEU	CA-CB-CG	5.45	127.84	115.30
1	S	626	G	O3'-P-O5'	-5.45	93.65	104.00
1	R	605	U	OP2-P-O3'	5.43	117.14	105.20
1	S	659	U	OP1-P-OP2	-5.42	111.47	119.60
1	S	634	G	O4'-C1'-N9	5.42	112.54	108.20
1	S	674	C	OP1-P-OP2	-5.41	111.48	119.60
1	R	614	A	OP1-P-O3'	5.41	117.10	105.20
1	S	617	G	OP1-P-OP2	-5.40	111.50	119.60
1	R	622	G	C5'-C4'-C3'	-5.39	107.38	116.00
1	R	622	G	OP1-P-OP2	-5.37	111.54	119.60
1	S	605	U	OP2-P-O3'	5.34	116.96	105.20
1	S	672	A	O4'-C1'-N9	5.32	112.46	108.20
1	R	641	G	OP1-P-OP2	-5.30	111.65	119.60
1	S	627	G	OP1-P-OP2	-5.29	111.66	119.60
2	A	223	LEU	CA-CB-CG	-5.29	103.13	115.30
1	S	635	U	OP1-P-OP2	-5.27	111.69	119.60
1	S	673	G	O3'-P-O5'	-5.27	93.99	104.00
1	R	621	A	C5'-C4'-C3'	-5.25	107.60	116.00
1	S	604	G	OP1-P-OP2	-5.25	111.72	119.60
1	R	623	A	OP1-P-OP2	-5.24	111.75	119.60
1	R	614	A	OP1-P-OP2	-5.20	111.80	119.60
1	R	634	G	OP1-P-OP2	-5.20	111.80	119.60
1	R	667	C	N1-C2-O2	5.19	122.01	118.90
1	S	673	G	OP1-P-OP2	-5.17	111.84	119.60
1	S	645	G	OP1-P-O3'	5.17	116.58	105.20
1	S	669	C	O4'-C1'-N1	5.16	112.33	108.20
1	R	641	G	O3'-P-O5'	-5.16	94.20	104.00
1	R	645	G	C5'-C4'-C3'	-5.16	107.75	116.00
1	R	627	G	OP1-P-OP2	-5.15	111.88	119.60
1	S	601	U	OP1-P-OP2	-5.15	111.88	119.60
1	S	641	G	OP1-P-OP2	-5.15	111.88	119.60
1	S	640	U	OP1-P-OP2	-5.14	111.88	119.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	644	A	OP1-P-OP2	-5.13	111.91	119.60
1	R	671	G	OP1-P-OP2	-5.10	111.95	119.60
1	S	614	A	O3'-P-O5'	5.09	113.67	104.00
2	B	313	ASP	N-CA-C	5.06	124.66	111.00
1	S	628	G	OP2-P-O3'	5.05	116.32	105.20
1	R	658	A	O3'-P-O5'	-5.04	94.42	104.00
1	S	619	H2U	O3'-P-O5'	5.04	113.58	104.00
2	B	255	CYS	CA-CB-SG	5.03	123.06	114.00
1	R	640	U	OP1-P-OP2	-5.03	112.06	119.60
2	A	547	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	234	TYR	Sidechain
2	A	351	TYR	Sidechain
2	A	554	ARG	Sidechain
2	B	234	TYR	Sidechain
2	B	291	TYR	Sidechain
2	B	297	TYR	Sidechain
2	B	402	TYR	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	R	1602	0	815	77	0
1	S	1602	0	815	83	0
2	A	3946	0	3939	350	0
2	B	3946	0	3939	380	0
All	All	11096	0	9508	814	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 40.

All (814) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:556:ARG:HD3	2:A:556:ARG:C	1.39	1.28
2:B:539:LEU:HD23	2:B:544:ARG:HB3	1.29	1.13
2:A:556:ARG:C	2:A:556:ARG:CD	2.25	1.01
2:A:196:THR:HG21	2:A:199:GLU:HG3	1.37	1.00
2:A:556:ARG:HD3	2:A:556:ARG:O	1.60	0.99
2:B:170:GLY:HA2	2:B:192:THR:HG23	1.39	0.99
2:B:392:PRO:HD3	2:B:440:THR:HB	1.44	0.97
2:B:165:ILE:HG13	2:B:198:SER:HB3	1.45	0.97
2:A:556:ARG:HD3	2:A:557:PRO:N	1.84	0.92
1:S:618:G:H3'	1:S:619:H2U:H2'	1.47	0.91
2:B:386:VAL:HG11	2:B:538:ASP:HB3	1.53	0.90
2:A:227:ASN:O	2:A:231:ARG:HG3	1.71	0.90
2:A:550:ARG:NH2	2:A:557:PRO:O	2.05	0.90
2:B:307:GLN:HG2	2:B:522:HIS:HE1	1.37	0.88
2:A:92:LYS:H	2:A:92:LYS:HD2	1.37	0.88
2:B:253:GLY:O	2:B:257:LEU:HD12	1.74	0.86
2:B:430:LEU:O	2:B:434:VAL:HG23	1.76	0.85
2:A:200:THR:HG22	2:A:201:PRO:HD2	1.59	0.85
2:A:331:THR:HG22	2:A:333:ARG:H	1.40	0.84
2:B:406:ILE:HG23	2:B:416:ILE:HD13	1.57	0.84
2:A:118:THR:HG22	2:A:128:LEU:HB3	1.60	0.84
2:A:449:PRO:HG2	2:A:452:ILE:HG12	1.60	0.83
2:A:409:LEU:HD21	2:A:430:LEU:HB2	1.58	0.83
2:A:271:HIS:HE1	2:B:255:CYS:SG	2.01	0.83
2:A:137:ILE:HG13	2:A:184:VAL:HB	1.60	0.82
2:A:235:ARG:HD2	2:A:239:LEU:HD22	1.61	0.82
2:B:454:PRO:O	2:B:457:THR:HG22	1.78	0.82
2:B:143:ALA:HA	2:B:149:ILE:HG22	1.61	0.82
2:B:300:GLN:HG3	2:B:325:ARG:HA	1.59	0.82
2:A:156:TRP:HZ3	2:A:194:ILE:HG23	1.45	0.81
2:A:300:GLN:NE2	2:A:325:ARG:HA	1.93	0.81
1:S:676:A:C2	2:B:303:GLN:HB3	2.15	0.81
2:A:541:ASN:OD1	2:A:543:ARG:HD2	1.81	0.81
2:B:307:GLN:HG2	2:B:522:HIS:CE1	2.16	0.81
2:A:200:THR:HG22	2:A:204:LEU:HD21	1.63	0.81
2:A:114:ARG:NH2	2:A:240:ARG:HH21	1.78	0.80
2:A:233:ASP:OD1	2:A:554:ARG:NH1	2.15	0.80
1:S:619:H2U:H3'	1:S:620:C:H5'	1.64	0.79
2:B:463:ASN:ND2	2:B:465:LYS:HB2	1.96	0.79
2:A:270:VAL:O	2:A:319:GLU:HG3	1.82	0.79
2:B:70:THR:HB	2:B:147:GLY:O	1.83	0.78
2:A:392:PRO:HD3	2:A:440:THR:OG1	1.83	0.78

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:196:THR:CG2	2:A:199:GLU:HG3	2.13	0.78
2:A:311:VAL:HA	2:A:519:CYS:HB3	1.65	0.78
2:A:196:THR:HG21	2:A:199:GLU:CG	2.13	0.78
2:B:303:GLN:HE22	2:B:485:ARG:HE	1.32	0.77
2:B:235:ARG:HG3	2:B:239:LEU:HD22	1.66	0.77
2:B:343:MET:SD	2:B:343:MET:O	2.41	0.77
2:A:493:GLN:O	2:A:497:LYS:HG2	1.85	0.77
2:A:350:HIS:HB2	2:B:88:ARG:HG2	1.65	0.77
2:B:462:ALA:O	2:B:463:ASN:HB2	1.83	0.77
2:A:320:ILE:HG12	2:A:341:LEU:HD22	1.67	0.77
2:B:546:SER:O	2:B:549:PRO:HD3	1.86	0.76
2:B:492:LEU:O	2:B:496:MET:HG3	1.85	0.76
2:A:419:PHE:HE1	2:A:466:TYR:CE1	2.04	0.75
1:R:623:A:H2'	1:R:624:A:H8	1.50	0.75
2:A:92:LYS:N	2:A:92:LYS:HD2	2.02	0.74
2:A:556:ARG:HA	2:A:557:PRO:O	1.87	0.74
2:B:286:VAL:HG23	2:B:300:GLN:HE22	1.53	0.73
1:R:674:C:H2'	1:R:675:C:O4'	1.89	0.72
2:A:83:SER:HB3	2:B:350:HIS:CD2	2.25	0.72
1:S:666:U:H2'	1:S:667:C:C6	2.24	0.72
2:B:118:THR:HG22	2:B:128:LEU:HD22	1.69	0.71
2:B:534:MET:SD	2:B:542:ILE:N	2.63	0.71
2:A:373:PHE:O	2:A:377:ILE:HG13	1.90	0.71
2:A:206:ILE:O	2:A:207:LEU:HB2	1.90	0.71
2:B:544:ARG:HG2	2:B:544:ARG:HH11	1.56	0.71
2:A:390:LYS:HD2	2:A:435:ARG:HH21	1.56	0.71
2:B:89:THR:OG1	2:B:91:GLN:HG3	1.91	0.71
2:B:228:LEU:HD13	2:B:544:ARG:HE	1.56	0.71
2:A:308:GLN:OE1	2:A:511:TYR:HA	1.91	0.71
2:B:486:ILE:HB	2:B:492:LEU:HD12	1.72	0.70
2:A:480:LEU:HD23	2:A:481:SER:N	2.06	0.70
2:B:343:MET:SD	2:B:343:MET:C	2.70	0.70
1:R:623:A:H2'	1:R:624:A:C8	2.25	0.70
2:B:238:ASP:O	2:B:241:THR:HG23	1.92	0.70
2:A:409:LEU:CD2	2:A:430:LEU:HB2	2.21	0.70
2:B:106:ASP:HA	2:B:171:ILE:HD11	1.74	0.69
2:B:136:LEU:HD12	2:B:183:THR:OG1	1.91	0.69
2:A:313:ASP:HB2	2:B:240:ARG:HG3	1.74	0.69
2:A:231:ARG:HB3	2:A:238:ASP:OD2	1.91	0.69
1:S:640:U:H2'	1:S:641:G:H8	1.57	0.69
2:B:480:LEU:HD23	2:B:481:SER:N	2.08	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:95:LYS:HA	2:A:132:GLN:HE22	1.57	0.69
2:B:286:VAL:HG23	2:B:300:GLN:NE2	2.08	0.68
1:R:619:H2U:H1'	1:R:620:C:H5	1.58	0.68
2:B:424:THR:HG22	2:B:428:LYS:HE2	1.73	0.68
2:B:541:ASN:ND2	2:B:543:ARG:H	1.91	0.68
2:B:246:ALA:O	2:B:250:ILE:HG13	1.94	0.68
2:B:350:HIS:HD2	2:B:351:TYR:HD1	1.40	0.68
2:A:390:LYS:HD2	2:A:435:ARG:NH2	2.08	0.68
2:A:131:ARG:NH1	2:A:208:LEU:HD12	2.07	0.68
2:A:235:ARG:HD2	2:A:239:LEU:CD2	2.24	0.68
2:A:300:GLN:HE22	2:A:325:ARG:HA	1.57	0.68
2:A:556:ARG:O	2:A:556:ARG:CD	2.36	0.67
2:B:409:LEU:O	2:B:414:LYS:HB2	1.95	0.67
2:A:82:GLN:NE2	2:B:458:MET:SD	2.67	0.67
2:A:309:LEU:HD21	2:B:547:LEU:HD13	1.74	0.67
2:B:127:PHE:O	2:B:128:LEU:HD23	1.94	0.67
2:A:474:MET:SD	2:A:479:ILE:HD13	2.34	0.67
2:A:381:ARG:HE	2:A:381:ARG:HA	1.60	0.67
2:B:78:LEU:HD11	2:B:167:LEU:HD23	1.77	0.67
1:S:615:A:H2'	1:S:616:H2U:H62	1.76	0.67
1:S:619:H2U:OP2	1:S:620:C:H5'	1.95	0.67
2:A:200:THR:CG2	2:A:204:LEU:HD21	2.26	0.66
2:B:453:ARG:HH11	2:B:469:SER:HB3	1.61	0.66
2:B:286:VAL:HG21	2:B:297:TYR:HB3	1.77	0.66
1:R:638:C:O5'	2:A:119:ARG:HD3	1.95	0.66
2:A:475:ARG:HD2	2:A:535:PHE:O	1.95	0.66
1:R:644:A:O2'	1:R:645:G:H5'	1.95	0.66
1:S:676:A:H1'	2:B:456:TYR:OH	1.95	0.66
2:B:269:GLU:HG2	2:B:318:TYR:CE1	2.31	0.66
2:B:300:GLN:HA	2:B:324:PHE:O	1.95	0.66
2:A:161:ASN:HD22	2:A:202:GLU:N	1.93	0.66
2:B:291:TYR:CD1	2:B:292:PHE:HD2	2.13	0.65
2:B:193:LYS:HB2	2:B:193:LYS:NZ	2.10	0.65
2:A:517:TYR:CD2	2:B:237:ILE:HD11	2.32	0.65
2:A:375:HIS:CE1	2:A:379:LEU:HD21	2.31	0.65
2:B:335:MET:HG2	2:B:550:ARG:O	1.97	0.65
2:B:308:GLN:O	2:B:311:VAL:HB	1.96	0.65
2:B:463:ASN:HD21	2:B:465:LYS:HB2	1.60	0.65
2:B:253:GLY:HA3	2:B:373:PHE:CZ	2.32	0.64
2:B:110:LEU:HD11	2:B:167:LEU:HD11	1.79	0.64
2:A:235:ARG:HE	2:A:239:LEU:HD11	1.62	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:VAL:HG11	2:B:537:LEU:HG	1.78	0.64
2:B:366:PHE:HZ	2:B:474:MET:SD	2.20	0.64
1:S:638:C:H3'	1:S:638:C:H6	1.63	0.64
2:B:137:ILE:HG22	2:B:184:VAL:HB	1.79	0.64
2:A:556:ARG:HA	2:A:557:PRO:C	2.17	0.64
2:A:517:TYR:CD1	2:A:517:TYR:N	2.65	0.64
2:A:205:PRO:O	2:A:207:LEU:N	2.29	0.64
2:B:206:ILE:HG13	2:B:226:VAL:HG21	1.80	0.64
2:A:278:ALA:HB1	2:A:279:PRO:HD2	1.80	0.64
2:A:517:TYR:HD2	2:B:237:ILE:HG13	1.63	0.64
2:A:289:VAL:HG22	2:B:289:VAL:HG22	1.78	0.63
2:B:298:LEU:HD13	2:B:324:PHE:CD2	2.33	0.63
2:B:443:TYR:CE1	2:B:473:PHE:HB2	2.33	0.63
2:B:480:LEU:HG	2:B:526:GLY:O	1.98	0.63
2:A:100:ASP:H	2:A:104:ASP:HB2	1.63	0.63
2:B:140:LEU:HD23	2:B:140:LEU:H	1.64	0.63
2:A:404:GLU:O	2:A:407:GLU:HB2	1.99	0.63
2:B:350:HIS:CD2	2:B:351:TYR:HD1	2.15	0.63
1:S:666:U:H2'	1:S:667:C:H6	1.61	0.62
2:A:309:LEU:O	2:A:314:PHE:HB2	1.98	0.62
2:B:91:GLN:HE22	2:B:169:ARG:NH2	1.96	0.62
1:R:601:U:H2'	1:R:602:C:C6	2.34	0.62
1:S:617:G:H21	1:S:658:A:H5'	1.65	0.62
2:B:453:ARG:HB3	2:B:457:THR:HG21	1.82	0.62
2:B:528:GLY:O	2:B:532:VAL:HG23	2.00	0.62
2:B:175:VAL:HG13	2:B:188:GLU:HG2	1.81	0.62
2:B:69:ASP:H	2:B:72:LYS:HD2	1.65	0.62
2:B:221:ALA:O	2:B:223:LEU:HD22	1.98	0.62
2:A:461:PRO:HG3	2:B:82:GLN:HG2	1.80	0.62
2:A:111:PHE:CE1	2:A:168:VAL:HB	2.35	0.62
2:B:91:GLN:HE22	2:B:169:ARG:HH21	1.48	0.62
2:A:235:ARG:NE	2:A:239:LEU:HD11	2.15	0.62
2:A:381:ARG:NE	2:A:381:ARG:HA	2.14	0.61
2:A:161:ASN:ND2	2:A:202:GLU:N	2.48	0.61
2:A:110:LEU:HD21	2:A:167:LEU:HD11	1.80	0.61
2:B:144:ASN:HD21	2:B:148:THR:H	1.48	0.61
2:B:75:TYR:HA	2:B:194:ILE:O	2.00	0.61
1:S:635:U:C1'	2:B:121:GLN:HE22	2.14	0.61
2:B:331:THR:CG2	2:B:333:ARG:HG2	2.29	0.61
1:S:649:5MC:H2'	1:S:650:G:H8	1.65	0.61
2:B:196:THR:HG21	2:B:199:GLU:OE2	2.00	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:GLN:HB3	2:B:249:ARG:NH2	2.15	0.61
1:S:676:A:N3	2:B:303:GLN:HB3	2.14	0.61
1:R:621:A:H61	1:R:646:A:H2'	1.66	0.61
2:B:410:ARG:HG3	2:B:414:LYS:O	2.00	0.61
2:B:283:GLY:O	2:B:284:SER:HB2	2.00	0.61
2:B:266:LYS:N	2:B:266:LYS:HD2	2.16	0.61
2:A:149:ILE:HG12	2:A:153:MET:HE1	1.83	0.61
2:A:82:GLN:O	2:A:83:SER:HB2	2.00	0.60
2:A:129:THR:HG22	2:A:138:GLN:HB3	1.82	0.60
2:A:406:ILE:HG23	2:A:416:ILE:HG23	1.83	0.60
2:B:527:ILE:HG22	2:B:528:GLY:N	2.16	0.60
1:S:619:H2U:H3'	1:S:619:H2U:OP2	2.01	0.60
2:B:472:PHE:HB2	2:B:480:LEU:HB3	1.82	0.60
2:B:474:MET:CE	2:B:479:ILE:HG21	2.31	0.60
2:B:442:PHE:HA	2:B:473:PHE:O	2.02	0.60
2:A:114:ARG:CZ	2:A:165:ILE:HD11	2.32	0.60
2:A:310:ILE:HG21	2:A:522:HIS:CG	2.37	0.60
1:S:626:G:H4'	2:B:207:LEU:HD21	1.84	0.60
2:B:333:ARG:HG3	2:B:334:HIS:CD2	2.37	0.60
2:B:285:SER:O	2:B:300:GLN:HG2	2.02	0.60
2:B:393:LYS:HE2	2:B:393:LYS:H	1.67	0.60
2:A:359:SER:HB2	2:A:444:ILE:HD11	1.84	0.59
2:A:458:MET:HG2	2:A:484:GLN:OE1	2.02	0.59
1:R:608:U:C4	1:R:613:PSU:C2	2.90	0.59
2:B:392:PRO:HD3	2:B:440:THR:CB	2.27	0.59
2:A:296:ALA:C	2:A:297:TYR:CD1	2.76	0.59
1:R:617:G:H21	1:R:658:A:H5'	1.67	0.59
2:A:124:THR:O	2:A:142:LYS:HA	2.02	0.59
2:B:267:PHE:HD2	2:B:317:VAL:O	1.86	0.59
2:B:80:LEU:HD23	2:B:81:ILE:N	2.18	0.59
1:S:612:U:OP1	2:B:227:ASN:HB2	2.03	0.59
2:A:309:LEU:HD11	2:B:548:PHE:HE1	1.67	0.59
2:A:118:THR:CG2	2:A:128:LEU:HB3	2.30	0.59
2:B:324:PHE:N	2:B:324:PHE:CD1	2.68	0.59
2:B:331:THR:HG22	2:B:333:ARG:H	1.66	0.59
1:S:634:G:H5''	2:B:121:GLN:OE1	2.03	0.59
2:B:378:GLU:O	2:B:382:LYS:HD3	2.03	0.58
2:B:245:GLN:O	2:B:249:ARG:HB2	2.03	0.58
2:B:390:LYS:HD3	2:B:435:ARG:HH21	1.67	0.58
2:B:306:LYS:HG3	2:B:344:GLU:HB2	1.85	0.58
2:A:286:VAL:HG13	2:A:298:LEU:O	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:GLU:HA	2:B:371:LYS:HB3	1.84	0.58
1:S:618:G:H5''	1:S:619:H2U:N3	2.18	0.58
1:R:675:C:O2	2:A:531:ARG:NH2	2.37	0.58
2:A:114:ARG:HG2	2:A:131:ARG:NH2	2.18	0.58
1:S:618:G:H2'	1:S:619:H2U:C4	2.34	0.58
2:A:240:ARG:HG3	2:A:240:ARG:HH11	1.69	0.58
1:R:624:A:H2'	1:R:625:U:C6	2.39	0.58
2:B:505:ASP:HB2	2:B:506:PRO:HD2	1.84	0.58
2:A:251:GLN:NE2	2:A:545:ALA:O	2.37	0.58
2:B:318:TYR:CD1	2:B:318:TYR:C	2.77	0.58
2:A:517:TYR:HD1	2:A:517:TYR:N	2.02	0.58
1:R:643:C:H2'	1:R:644:A:C8	2.39	0.58
2:B:519:CYS:SG	2:B:520:PRO:HD2	2.43	0.58
1:R:654:5MU:H71	1:R:654:5MU:OP2	2.04	0.58
2:B:453:ARG:CB	2:B:457:THR:HG21	2.34	0.57
2:A:107:LYS:H	2:A:172:VAL:HG12	1.68	0.57
2:A:80:LEU:HD21	2:B:491:LEU:HD23	1.86	0.57
2:A:141:VAL:HG21	2:A:157:ALA:CB	2.33	0.57
1:S:637:1MG:OP2	2:B:180:LYS:HE3	2.03	0.57
2:B:541:ASN:HD22	2:B:541:ASN:C	2.07	0.57
2:B:71:ALA:HB2	2:B:148:THR:O	2.04	0.57
1:S:640:U:H2'	1:S:641:G:C8	2.36	0.57
2:B:107:LYS:HE2	2:B:107:LYS:HA	1.86	0.57
2:A:232:LEU:HD23	2:A:235:ARG:NH1	2.20	0.57
2:A:144:ASN:ND2	2:A:146:GLU:HB2	2.19	0.57
2:B:279:PRO:HB3	2:B:286:VAL:HG11	1.86	0.57
2:B:311:VAL:HG22	2:B:519:CYS:HB2	1.86	0.57
2:B:302:PRO:O	2:B:306:LYS:HD3	2.04	0.57
1:S:631:C:H2'	1:S:632:PSU:H6	1.70	0.57
2:A:225:VAL:HG13	2:A:225:VAL:O	2.04	0.57
2:B:258:PHE:CE1	2:B:361:LEU:HD11	2.39	0.56
2:A:166:VAL:HG23	2:A:168:VAL:HG23	1.87	0.56
2:B:249:ARG:HG3	2:B:249:ARG:HH11	1.71	0.56
1:S:649:5MC:H2'	1:S:650:G:C8	2.40	0.56
2:A:486:ILE:CD1	2:A:495:ARG:HG3	2.35	0.56
2:B:204:LEU:O	2:B:204:LEU:HD23	2.05	0.56
1:R:621:A:C5	1:R:648:U:C4	2.93	0.56
2:B:331:THR:HG22	2:B:333:ARG:HG2	1.87	0.56
2:A:409:LEU:O	2:A:414:LYS:HB2	2.06	0.56
2:B:472:PHE:CD1	2:B:480:LEU:HD22	2.40	0.56
2:A:351:TYR:CE2	2:A:468:ASN:HB3	2.39	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:350:HIS:HB2	2:B:88:ARG:CG	2.36	0.56
2:A:419:PHE:HE1	2:A:466:TYR:CZ	2.23	0.56
2:A:347:PHE:HZ	2:A:484:GLN:HE21	1.53	0.56
2:B:455:PHE:CD1	2:B:456:TYR:N	2.74	0.56
2:A:272:THR:HB	2:A:273:PRO:HD2	1.86	0.56
2:A:175:VAL:HG21	2:A:179:ILE:HD11	1.87	0.56
2:A:257:LEU:HD23	2:A:372:ARG:HH21	1.71	0.56
2:B:449:PRO:HA	2:B:466:TYR:HA	1.88	0.56
2:A:136:LEU:H	2:A:183:THR:HB	1.71	0.56
2:A:168:VAL:HG22	2:A:194:ILE:CG1	2.37	0.55
2:B:354:VAL:HG21	2:B:523:ALA:HB3	1.89	0.55
2:B:175:VAL:CG1	2:B:188:GLU:HG2	2.36	0.55
2:A:450:LEU:CD1	2:A:467:SER:HB3	2.37	0.55
2:A:197:ILE:HG13	2:A:197:ILE:O	2.07	0.55
2:B:134:ALA:HA	2:B:242:VAL:HG22	1.88	0.55
2:A:340:GLY:O	2:A:341:LEU:HD23	2.06	0.55
1:R:635:U:C5	1:R:636:C:C5	2.95	0.55
1:R:659:U:O2'	1:R:660:U:H5'	2.05	0.55
1:R:607:A:H4'	1:R:608:U:OP2	2.07	0.55
2:A:106:ASP:H	2:A:172:VAL:HG13	1.71	0.55
2:A:331:THR:CG2	2:A:333:ARG:H	2.16	0.55
2:A:302:PRO:HB2	2:A:306:LYS:HZ3	1.72	0.55
2:A:336:THR:HG21	2:B:291:TYR:OH	2.07	0.55
2:A:419:PHE:CE1	2:A:466:TYR:CE1	2.90	0.55
2:A:386:VAL:HG11	2:A:538:ASP:HB3	1.89	0.55
2:B:541:ASN:HD22	2:B:543:ARG:H	1.52	0.55
1:R:675:C:H2'	1:R:676:A:C8	2.42	0.55
2:A:116:HIS:O	2:A:162:LEU:HD22	2.07	0.55
2:A:354:VAL:HG21	2:A:523:ALA:HB3	1.89	0.55
2:B:286:VAL:HA	2:B:300:GLN:NE2	2.22	0.55
2:A:448:PHE:HB2	2:A:469:SER:OG	2.07	0.54
2:A:287:PHE:HB2	2:A:298:LEU:HD12	1.89	0.54
2:A:145:LYS:HG2	2:A:145:LYS:O	2.07	0.54
2:B:123:ALA:O	2:B:151:LYS:HG3	2.07	0.54
2:B:298:LEU:HD13	2:B:324:PHE:CE2	2.43	0.54
2:B:320:ILE:HG12	2:B:341:LEU:HD22	1.89	0.54
1:R:640:U:O2'	1:R:641:G:H5'	2.07	0.54
2:A:235:ARG:O	2:A:239:LEU:HD22	2.06	0.54
2:B:138:GLN:HE22	2:B:179:ILE:HD12	1.73	0.54
2:B:143:ALA:HA	2:B:149:ILE:CG2	2.37	0.54
2:A:115:VAL:O	2:A:115:VAL:HG12	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:544:ARG:HG2	2:B:544:ARG:NH1	2.21	0.54
1:S:618:G:C3'	1:S:619:H2U:H2'	2.29	0.54
2:A:410:ARG:HA	2:A:414:LYS:O	2.08	0.54
2:A:287:PHE:HB3	2:B:289:VAL:CG1	2.38	0.54
2:A:401:THR:HG23	2:A:404:GLU:OE1	2.08	0.54
2:B:145:LYS:H	2:B:145:LYS:CD	2.19	0.54
2:A:539:LEU:O	2:A:541:ASN:N	2.41	0.54
1:S:667:C:H2'	1:S:668:G:H8	1.71	0.54
2:A:141:VAL:HG21	2:A:157:ALA:HB1	1.89	0.54
1:S:654:5MU:H2'	1:S:655:PSU:O4'	2.06	0.54
2:B:450:LEU:HD21	2:B:495:ARG:NH1	2.23	0.54
2:A:235:ARG:NE	2:A:239:LEU:CD1	2.71	0.54
2:A:237:ILE:HA	2:A:240:ARG:NH1	2.22	0.54
2:A:556:ARG:CA	2:A:557:PRO:O	2.57	0.53
2:B:324:PHE:HD1	2:B:324:PHE:N	2.05	0.53
2:B:458:MET:CE	2:B:486:ILE:HG12	2.38	0.53
1:S:618:G:H3'	1:S:619:H2U:H61	1.90	0.53
2:A:286:VAL:HG11	2:A:297:TYR:HB3	1.89	0.53
1:S:665:G:H2'	1:S:666:U:C6	2.43	0.53
2:A:430:LEU:O	2:A:434:VAL:HG13	2.07	0.53
2:A:286:VAL:CG1	2:A:297:TYR:HB3	2.38	0.53
2:B:354:VAL:CB	2:B:523:ALA:HB3	2.38	0.53
2:B:425:GLU:CD	2:B:425:GLU:H	2.12	0.53
1:R:659:U:C2'	1:R:660:U:H5'	2.38	0.53
1:R:649:5MC:H2'	1:R:650:G:H8	1.72	0.53
2:B:75:TYR:CD2	2:B:153:MET:HB2	2.44	0.53
2:A:127:PHE:CE2	2:A:140:LEU:HD23	2.44	0.53
2:B:205:PRO:O	2:B:206:ILE:O	2.26	0.53
2:B:228:LEU:HD13	2:B:544:ARG:NE	2.23	0.53
2:B:454:PRO:O	2:B:457:THR:CG2	2.54	0.53
1:S:672:A:H5''	2:B:425:GLU:OE2	2.08	0.53
2:A:76:GLY:O	2:A:195:TYR:HB3	2.08	0.53
2:A:446:ASP:OD1	2:A:447:LYS:N	2.41	0.53
2:B:541:ASN:HD22	2:B:543:ARG:N	2.06	0.53
2:A:238:ASP:O	2:A:241:THR:HG23	2.08	0.53
2:A:351:TYR:C	2:A:351:TYR:CD1	2.82	0.53
2:B:541:ASN:ND2	2:B:543:ARG:HB2	2.24	0.53
2:A:168:VAL:HG22	2:A:194:ILE:HG13	1.91	0.53
2:B:434:VAL:HG13	2:B:438:TYR:HD2	1.74	0.53
2:B:351:TYR:HB2	2:B:523:ALA:HB2	1.91	0.53
1:S:632:PSU:N3	2:B:122:GLY:N	2.57	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:ASP:O	2:B:178:PRO:HD3	2.09	0.53
2:A:175:VAL:HG12	2:A:186:ASN:O	2.08	0.53
2:B:347:PHE:HB2	2:B:353:GLU:OE1	2.08	0.53
1:S:629:C:C4	1:S:630:G:N7	2.77	0.53
1:S:635:U:H1'	2:B:121:GLN:NE2	2.24	0.52
2:A:232:LEU:O	2:A:235:ARG:HB2	2.10	0.52
2:A:115:VAL:HG12	2:A:162:LEU:HA	1.90	0.52
2:B:449:PRO:HG2	2:B:452:ILE:HG12	1.91	0.52
2:A:470:TYR:CE1	2:A:483:ALA:N	2.77	0.52
2:A:202:GLU:O	2:A:203:ALA:HB3	2.08	0.52
1:R:609:A:O4'	1:R:646:A:O4'	2.27	0.52
2:B:228:LEU:O	2:B:232:LEU:HG	2.09	0.52
2:A:88:ARG:HD3	2:B:350:HIS:HB3	1.92	0.52
2:B:354:VAL:HB	2:B:523:ALA:HB3	1.91	0.52
2:B:393:LYS:N	2:B:393:LYS:HE2	2.24	0.52
2:B:375:HIS:CE1	2:B:379:LEU:HD21	2.45	0.52
2:B:335:MET:CE	2:B:542:ILE:HG23	2.39	0.52
2:A:517:TYR:CD2	2:B:237:ILE:HG13	2.44	0.52
2:A:474:MET:HB2	2:A:479:ILE:HG21	1.92	0.52
2:A:146:GLU:N	2:A:146:GLU:CD	2.64	0.52
2:A:84:ARG:HA	2:B:461:PRO:HG3	1.91	0.52
1:S:635:U:C1'	2:B:121:GLN:NE2	2.72	0.52
2:B:370:PRO:HG2	2:B:371:LYS:H	1.75	0.52
2:B:534:MET:SD	2:B:542:ILE:CA	2.98	0.52
1:S:676:A:H62	2:B:280:SER:HB3	1.75	0.52
2:B:541:ASN:HD21	2:B:543:ARG:HE	1.57	0.51
2:B:145:LYS:N	2:B:145:LYS:HD2	2.24	0.51
2:A:359:SER:HB2	2:A:444:ILE:CD1	2.40	0.51
1:S:617:G:N2	1:S:657:A:H2'	2.25	0.51
1:S:618:G:H8	1:S:619:H2U:O4	1.93	0.51
2:B:269:GLU:HG3	2:B:318:TYR:OH	2.10	0.51
2:B:289:VAL:HG12	2:B:290:THR:O	2.10	0.51
2:A:318:TYR:HB2	2:A:342:ASP:O	2.10	0.51
2:A:229:ASP:OD2	2:A:554:ARG:NH2	2.43	0.51
1:R:643:C:H2'	1:R:644:A:H8	1.75	0.51
2:B:275:LEU:HD13	2:B:291:TYR:HE2	1.75	0.51
2:A:271:HIS:CE1	2:B:255:CYS:SG	2.92	0.51
2:B:258:PHE:CD1	2:B:361:LEU:HD11	2.46	0.51
2:A:257:LEU:CD2	2:A:372:ARG:HH21	2.24	0.51
2:A:483:ALA:O	2:A:523:ALA:HB1	2.10	0.51
2:B:291:TYR:CE1	2:B:292:PHE:HD2	2.29	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:533:VAL:CG1	2:A:545:ALA:HB1	2.40	0.51
2:B:355:LEU:CD2	2:B:399:ARG:HE	2.23	0.51
1:R:615:A:C2	1:R:616:H2U:N3	2.78	0.51
2:A:196:THR:HG21	2:A:199:GLU:OE2	2.10	0.51
2:B:410:ARG:HD3	2:B:416:ILE:HD12	1.93	0.51
2:B:145:LYS:CE	2:B:145:LYS:H	2.24	0.51
2:A:75:TYR:HB2	2:A:156:TRP:CZ3	2.46	0.51
1:R:638:C:N4	2:A:120:GLN:O	2.43	0.51
2:B:333:ARG:HG3	2:B:334:HIS:HD2	1.74	0.51
2:B:534:MET:HE2	2:B:535:PHE:CZ	2.46	0.51
2:A:347:PHE:O	2:A:521:PRO:HG2	2.10	0.50
2:A:450:LEU:HD12	2:A:467:SER:HB3	1.94	0.50
2:A:156:TRP:CZ3	2:A:194:ILE:HG23	2.36	0.50
2:A:132:GLN:O	2:A:133:GLN:HB2	2.10	0.50
1:R:634:G:O2'	1:R:635:U:P	2.68	0.50
2:A:392:PRO:HG3	2:A:440:THR:HB	1.93	0.50
2:B:303:GLN:NE2	2:B:485:ARG:HE	2.06	0.50
2:A:450:LEU:O	2:A:451:GLU:HB2	2.11	0.50
2:A:114:ARG:NH2	2:A:240:ARG:NH2	2.56	0.50
2:B:354:VAL:CG2	2:B:523:ALA:HB3	2.41	0.50
2:B:474:MET:HE2	2:B:479:ILE:HG21	1.92	0.50
2:B:336:THR:HG22	2:B:337:GLU:N	2.26	0.50
2:A:200:THR:HG21	2:A:204:LEU:HD11	1.94	0.50
2:B:206:ILE:HG12	2:B:207:LEU:N	2.27	0.50
2:B:333:ARG:NH2	2:B:477:GLU:HG2	2.27	0.50
1:R:675:C:H2'	1:R:675:C:O2	2.11	0.50
2:B:350:HIS:CD2	2:B:351:TYR:CD1	2.98	0.50
2:A:509:LYS:HB2	2:A:509:LYS:NZ	2.26	0.50
2:A:520:PRO:CB	2:B:112:ARG:HH11	2.25	0.50
1:R:634:G:O2'	1:R:635:U:C6	2.64	0.50
2:A:304:PHE:N	2:A:304:PHE:HD1	2.10	0.50
1:R:628:G:C6	1:R:629:C:N4	2.80	0.50
2:B:145:LYS:HE2	2:B:145:LYS:H	1.77	0.49
2:A:289:VAL:HG13	2:B:287:PHE:HB3	1.94	0.49
2:A:308:GLN:HA	2:A:311:VAL:HG13	1.94	0.49
2:A:350:HIS:HA	2:B:83:SER:OG	2.12	0.49
1:S:667:C:O2	1:S:668:G:C8	2.66	0.49
2:A:119:ARG:HB2	2:A:119:ARG:NH1	2.27	0.49
2:A:487:HIS:CD2	2:A:521:PRO:CA	2.94	0.49
2:B:79:PRO:O	2:B:80:LEU:HB2	2.11	0.49
2:A:304:PHE:CD1	2:A:304:PHE:N	2.80	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:GLU:C	2:B:316:ARG:HG2	2.32	0.49
2:B:429:PHE:CE2	2:B:433:LEU:HD11	2.48	0.49
2:A:369:LEU:HB2	2:A:370:PRO:HD3	1.93	0.49
2:B:317:VAL:HG12	2:B:318:TYR:N	2.27	0.49
2:B:463:ASN:HD22	2:B:465:LYS:H	1.58	0.49
2:A:390:LYS:CD	2:A:435:ARG:HH21	2.25	0.49
2:B:245:GLN:HB3	2:B:249:ARG:HH21	1.76	0.49
2:B:361:LEU:O	2:B:365:ILE:HG13	2.12	0.49
2:B:474:MET:HE1	2:B:479:ILE:HG21	1.94	0.49
2:A:175:VAL:HG11	2:A:179:ILE:CD1	2.42	0.49
2:A:107:LYS:O	2:A:171:ILE:HA	2.12	0.49
2:A:499:HIS:O	2:A:501:LEU:HD13	2.12	0.49
2:A:228:LEU:HA	2:A:231:ARG:HD3	1.94	0.49
2:A:160:LEU:HD11	2:A:194:ILE:CD1	2.43	0.49
2:A:474:MET:HB2	2:A:479:ILE:CG2	2.43	0.49
1:S:634:G:O2'	1:S:635:U:P	2.70	0.49
1:S:607:A:C4	1:S:649:5MC:HM52	2.47	0.49
2:B:331:THR:HG21	2:B:333:ARG:HG2	1.95	0.49
2:A:466:TYR:N	2:A:466:TYR:CD1	2.78	0.49
1:R:610:G:H2'	1:R:610:G:N3	2.26	0.49
2:B:144:ASN:HD22	2:B:144:ASN:C	2.16	0.49
2:B:543:ARG:NH1	2:B:551:ASP:OD2	2.46	0.49
2:B:145:LYS:H	2:B:145:LYS:HD2	1.78	0.49
1:R:634:G:H4'	1:R:635:U:H5'	1.94	0.49
1:S:635:U:H4'	1:S:638:C:O2	2.12	0.49
2:B:189:ILE:HG22	2:B:189:ILE:O	2.11	0.48
1:R:636:C:H5'	1:R:638:C:O4'	2.12	0.48
1:S:638:C:C6	1:S:638:C:H3'	2.47	0.48
2:B:331:THR:HG22	2:B:332:HIS:N	2.29	0.48
2:B:307:GLN:NE2	2:B:485:ARG:HB3	2.28	0.48
2:B:237:ILE:O	2:B:240:ARG:HB2	2.14	0.48
2:B:366:PHE:CZ	2:B:474:MET:SD	3.05	0.48
2:B:398:VAL:HG12	2:B:443:TYR:HB2	1.95	0.48
2:A:470:TYR:CD1	2:A:470:TYR:N	2.82	0.48
1:R:630:G:C6	1:R:641:G:C6	3.01	0.48
2:B:75:TYR:CE2	2:B:153:MET:HB2	2.48	0.48
2:A:116:HIS:ND1	2:A:136:LEU:HD11	2.28	0.48
1:S:654:5MU:O2'	1:S:655:PSU:H5''	2.13	0.48
2:A:291:TYR:O	2:A:292:PHE:C	2.51	0.48
2:B:317:VAL:CG1	2:B:318:TYR:N	2.77	0.48
2:B:419:PHE:HE1	2:B:466:TYR:CZ	2.31	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:LEU:HD22	2:B:429:PHE:HD2	1.77	0.48
1:R:633:U:O2'	1:R:634:G:P	2.72	0.48
2:B:214:SER:HB3	2:B:217:GLU:HB2	1.96	0.48
2:B:416:ILE:HD12	2:B:416:ILE:H	1.78	0.47
2:A:350:HIS:O	2:A:353:GLU:HG3	2.14	0.47
1:S:638:C:C3'	1:S:638:C:C6	2.97	0.47
1:R:660:U:OP1	1:R:661:C:N4	2.47	0.47
2:A:468:ASN:HD22	2:A:468:ASN:N	2.12	0.47
1:R:649:5MC:H2'	1:R:650:G:C8	2.48	0.47
2:A:351:TYR:CE1	2:A:352:HIS:ND1	2.82	0.47
2:B:208:LEU:O	2:B:212:SER:OG	2.32	0.47
2:A:430:LEU:HD12	2:A:430:LEU:O	2.14	0.47
2:A:162:LEU:O	2:A:163:GLU:HB2	2.14	0.47
2:A:287:PHE:HB3	2:B:289:VAL:HG13	1.95	0.47
2:A:88:ARG:HD3	2:B:350:HIS:CB	2.44	0.47
2:A:487:HIS:CD2	2:A:521:PRO:HA	2.48	0.47
2:A:345:MET:HG3	2:A:354:VAL:HG22	1.96	0.47
2:B:345:MET:O	2:B:522:HIS:HB2	2.14	0.47
2:B:448:PHE:HB2	2:B:453:ARG:HD2	1.94	0.47
2:A:543:ARG:HH11	2:A:543:ARG:HG2	1.79	0.47
2:A:517:TYR:CD2	2:B:237:ILE:CD1	2.97	0.47
1:S:669:C:H2'	1:S:670:G:H8	1.79	0.47
1:R:635:U:C5	1:R:636:C:H5	2.32	0.47
2:B:296:ALA:C	2:B:297:TYR:CD1	2.88	0.47
2:A:520:PRO:HB3	2:B:112:ARG:HH11	1.80	0.47
1:R:624:A:H2'	1:R:625:U:H6	1.79	0.47
2:A:517:TYR:HD2	2:B:237:ILE:CG1	2.28	0.47
1:R:637:1MG:HM13	2:A:221:ALA:O	2.15	0.47
1:R:621:A:C4	1:R:648:U:C4	3.02	0.47
2:B:115:VAL:HG23	2:B:162:LEU:HA	1.94	0.47
2:A:262:LEU:HA	2:A:262:LEU:HD12	1.44	0.47
2:B:534:MET:SD	2:B:542:ILE:HA	2.54	0.47
2:A:517:TYR:CD2	2:B:237:ILE:CG1	2.98	0.47
1:S:626:G:C4'	2:B:207:LEU:HD21	2.44	0.47
2:B:491:LEU:HD12	2:B:491:LEU:O	2.14	0.47
1:S:654:5MU:C2'	1:S:655:PSU:H5''	2.44	0.47
2:A:68:GLU:O	2:A:69:ASP:HB2	2.13	0.47
2:B:474:MET:HG3	2:B:479:ILE:HD13	1.96	0.47
2:B:377:ILE:O	2:B:380:VAL:HG12	2.15	0.47
2:B:137:ILE:CG2	2:B:184:VAL:HB	2.43	0.47
2:B:531:ARG:HG2	2:B:542:ILE:HD11	1.95	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:306:LYS:HD2	2:A:317:VAL:HG13	1.97	0.47
1:S:669:C:H2'	1:S:670:G:C8	2.50	0.47
2:A:550:ARG:NH1	2:B:273:PRO:HB2	2.31	0.46
2:B:232:LEU:HB3	2:B:554:ARG:HE	1.80	0.46
2:B:238:ASP:O	2:B:244:ASN:ND2	2.48	0.46
1:R:644:A:C2'	1:R:645:G:H5'	2.45	0.46
2:A:358:LEU:O	2:A:361:LEU:N	2.46	0.46
2:A:75:TYR:HA	2:A:194:ILE:O	2.16	0.46
2:A:362:PHE:CE2	2:A:472:PHE:HD2	2.34	0.46
1:R:648:U:C4	1:R:659:U:C2	3.03	0.46
1:R:659:U:C5	1:R:660:U:N3	2.84	0.46
2:A:306:LYS:HD3	2:A:306:LYS:HA	1.46	0.46
2:A:489:HIS:CD2	2:A:512:CYS:SG	3.09	0.46
1:S:674:C:C5	1:S:675:C:C4	3.03	0.46
2:A:411:ALA:C	2:A:413:GLY:H	2.18	0.46
2:B:102:ALA:O	2:B:103:LYS:HG2	2.16	0.46
2:A:416:ILE:CD1	2:A:422:LEU:HD23	2.46	0.46
2:A:289:VAL:CG1	2:B:287:PHE:HB3	2.46	0.46
2:B:235:ARG:O	2:B:239:LEU:HB2	2.15	0.46
2:A:138:GLN:HG2	2:A:179:ILE:HG12	1.97	0.46
2:B:133:GLN:HG3	2:B:249:ARG:NH2	2.30	0.46
2:B:369:LEU:N	2:B:370:PRO:HD2	2.30	0.46
2:A:144:ASN:HD21	2:A:146:GLU:HB2	1.81	0.46
2:A:354:VAL:O	2:A:357:THR:N	2.49	0.46
2:A:280:SER:HB3	2:A:304:PHE:CE2	2.50	0.46
1:S:673:G:H1	2:B:329:SER:HA	1.81	0.46
2:B:458:MET:HE3	2:B:486:ILE:HG12	1.97	0.46
1:S:667:C:C2	1:S:668:G:C8	3.04	0.46
2:B:91:GLN:NE2	2:B:169:ARG:HH21	2.12	0.46
1:S:607:A:C6	1:S:649:5MC:N4	2.83	0.46
2:B:393:LYS:CE	2:B:393:LYS:H	2.29	0.46
1:S:616:H2U:H2'	1:S:660:U:O2	2.15	0.46
2:A:551:ASP:O	2:A:553:LYS:N	2.49	0.46
2:A:249:ARG:HH11	2:A:252:ALA:HB3	1.80	0.46
2:B:101:GLU:HA	2:B:187:LEU:HD21	1.98	0.46
1:S:618:G:H5''	1:S:619:H2U:C4	2.44	0.46
2:B:71:ALA:O	2:B:73:ASP:N	2.49	0.46
2:A:82:GLN:HA	2:A:82:GLN:HE21	1.80	0.46
1:R:650:G:O2'	1:R:651:G:H5'	2.15	0.46
2:A:291:TYR:O	2:A:294:GLY:N	2.48	0.46
1:S:601:U:C2	1:S:673:G:N2	2.84	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:228:LEU:O	2:A:231:ARG:HB2	2.15	0.46
2:A:284:SER:HB3	2:A:300:GLN:CD	2.36	0.46
2:A:125:LEU:HG	2:A:127:PHE:CE1	2.50	0.46
2:B:335:MET:HE2	2:B:542:ILE:CG2	2.46	0.46
2:A:331:THR:CG2	2:A:333:ARG:HG2	2.46	0.46
2:B:362:PHE:CZ	2:B:527:ILE:HD13	2.51	0.46
2:A:350:HIS:HE1	2:B:83:SER:O	1.99	0.45
2:A:487:HIS:HD2	2:A:521:PRO:N	2.13	0.45
2:A:445:LEU:HD23	2:A:448:PHE:CZ	2.52	0.45
2:A:297:TYR:CD1	2:A:297:TYR:N	2.85	0.45
2:B:354:VAL:HG11	2:B:523:ALA:C	2.35	0.45
2:B:291:TYR:CE1	2:B:292:PHE:CD2	3.04	0.45
2:B:358:LEU:HD12	2:B:358:LEU:HA	1.67	0.45
2:B:243:THR:HG21	2:B:383:GLN:NE2	2.32	0.45
2:A:331:THR:HG22	2:A:334:HIS:H	1.80	0.45
2:A:472:PHE:HB2	2:A:480:LEU:HB3	1.98	0.45
2:B:267:PHE:CD2	2:B:317:VAL:O	2.66	0.45
2:B:483:ALA:O	2:B:485:ARG:NH1	2.50	0.45
2:A:347:PHE:HZ	2:A:484:GLN:NE2	2.14	0.45
2:A:243:THR:OG1	2:A:383:GLN:NE2	2.48	0.45
2:B:463:ASN:C	2:B:465:LYS:H	2.20	0.45
2:B:458:MET:HE2	2:B:459:PRO:HD2	1.99	0.45
2:B:225:VAL:O	2:B:225:VAL:HG12	2.16	0.45
2:B:453:ARG:HD3	2:B:469:SER:OG	2.16	0.45
2:A:317:VAL:O	2:A:343:MET:HA	2.16	0.45
2:B:527:ILE:CG2	2:B:528:GLY:N	2.78	0.45
2:B:94:VAL:HG23	2:B:111:PHE:HD2	1.80	0.45
2:B:291:TYR:CD1	2:B:292:PHE:CD2	2.99	0.45
1:S:638:C:O2	2:B:121:GLN:NE2	2.50	0.45
2:A:300:GLN:NE2	2:A:324:PHE:O	2.50	0.45
2:B:390:LYS:HD3	2:B:435:ARG:NH2	2.31	0.45
2:A:197:ILE:O	2:A:198:SER:HB2	2.17	0.45
2:A:291:TYR:CZ	2:B:555:LEU:HD21	2.52	0.45
1:S:613:PSU:H2'	1:S:614:A:H5'	1.98	0.45
2:B:541:ASN:HD21	2:B:543:ARG:HB2	1.81	0.45
2:B:69:ASP:HB3	2:B:72:LYS:CE	2.46	0.45
1:R:621:A:C2	1:R:648:U:C2	3.05	0.45
2:A:107:LYS:H	2:A:172:VAL:CG1	2.29	0.45
2:B:391:LEU:HD22	2:B:397:MET:HE1	1.99	0.45
1:S:617:G:N2	1:S:658:A:H5'	2.30	0.44
2:B:257:LEU:HD23	2:B:364:PHE:CE2	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:331:THR:CG2	2:A:332:HIS:N	2.80	0.44
1:R:675:C:C2	2:A:334:HIS:HE1	2.35	0.44
2:A:240:ARG:HG3	2:A:240:ARG:NH1	2.29	0.44
2:B:463:ASN:O	2:B:465:LYS:N	2.51	0.44
1:S:673:G:C6	1:S:674:C:N3	2.85	0.44
1:S:618:G:H2'	1:S:619:H2U:C5	2.48	0.44
2:B:351:TYR:CE1	2:B:352:HIS:ND1	2.85	0.44
1:R:636:C:O3'	1:R:637:1MG:H3'	2.16	0.44
1:S:636:C:O2'	1:S:637:1MG:H5''	2.17	0.44
1:S:637:1MG:HM11	1:S:637:1MG:HN21	1.55	0.44
1:S:674:C:N3	2:B:329:SER:OG	2.45	0.44
2:A:196:THR:HG21	2:A:199:GLU:CD	2.37	0.44
2:B:128:LEU:HD21	2:B:157:ALA:O	2.18	0.44
2:A:140:LEU:H	2:A:140:LEU:HD12	1.82	0.44
2:B:351:TYR:CE2	2:B:468:ASN:HB3	2.52	0.44
1:R:659:U:C5	1:R:660:U:C4	3.06	0.44
2:A:351:TYR:CD2	2:A:468:ASN:HB3	2.53	0.44
2:A:382:LYS:O	2:A:383:GLN:HB2	2.16	0.44
2:B:487:HIS:O	2:B:515:PHE:CD2	2.70	0.44
2:B:145:LYS:HG2	2:B:146:GLU:OE1	2.18	0.44
2:A:270:VAL:CG1	2:A:317:VAL:CG2	2.96	0.44
2:A:270:VAL:CG2	2:A:306:LYS:HE3	2.47	0.44
2:A:460:ASP:HA	2:A:461:PRO:HD3	1.88	0.44
1:S:631:C:H2'	1:S:632:PSU:O4'	2.18	0.44
2:A:280:SER:O	2:A:281:GLU:HB3	2.18	0.44
2:B:225:VAL:O	2:B:225:VAL:CG1	2.65	0.44
2:A:96:PHE:HB3	2:A:184:VAL:HG21	1.99	0.44
2:A:298:LEU:HD22	2:A:324:PHE:CE2	2.53	0.44
2:A:519:CYS:HB2	2:A:520:PRO:HD2	1.99	0.44
2:B:362:PHE:HZ	2:B:527:ILE:HD13	1.82	0.44
2:A:134:ALA:HA	2:A:242:VAL:HG22	2.00	0.44
2:B:95:LYS:HB2	2:B:98:ASP:OD2	2.17	0.44
2:A:118:THR:HG22	2:A:128:LEU:HD23	2.00	0.44
1:R:619:H2U:H1'	1:R:620:C:C5	2.45	0.44
1:R:637:1MG:HM11	1:R:637:1MG:HN21	1.53	0.44
1:R:601:U:H2'	1:R:602:C:H6	1.80	0.44
2:B:145:LYS:N	2:B:145:LYS:CD	2.80	0.44
2:B:148:THR:HG22	2:B:149:ILE:HG13	2.00	0.44
2:A:302:PRO:HB2	2:A:306:LYS:NZ	2.33	0.44
1:S:665:G:C6	1:S:666:U:C4	3.06	0.44
1:R:635:U:O2	2:A:127:PHE:CG	2.71	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:292:PHE:HE2	2:B:328:ASN:HA	1.83	0.44
2:A:429:PHE:O	2:A:432:LYS:N	2.50	0.44
2:B:148:THR:HG22	2:B:149:ILE:N	2.33	0.43
2:A:75:TYR:HB2	2:A:156:TRP:CE3	2.52	0.43
2:B:112:ARG:HG3	2:B:197:ILE:HD12	2.00	0.43
2:A:121:GLN:OE1	2:A:121:GLN:HA	2.18	0.43
1:R:638:C:C5	1:R:639:G:N7	2.86	0.43
1:S:635:U:O2'	2:B:121:GLN:NE2	2.48	0.43
2:A:346:ALA:HA	2:A:521:PRO:O	2.18	0.43
2:A:530:GLU:HG2	2:A:546:SER:HB3	2.00	0.43
2:A:197:ILE:O	2:A:197:ILE:CG1	2.66	0.43
1:R:614:A:C2'	1:R:615:A:O5'	2.66	0.43
1:S:618:G:C8	1:S:619:H2U:O4	2.71	0.43
2:A:409:LEU:HD12	2:A:416:ILE:HG21	2.00	0.43
2:A:378:GLU:O	2:A:381:ARG:HB2	2.18	0.43
2:A:482:GLY:O	2:A:483:ALA:HB2	2.18	0.43
2:B:400:LEU:O	2:B:445:LEU:HD12	2.18	0.43
1:R:631:C:C4	1:R:632:PSU:C2	3.06	0.43
2:A:314:PHE:O	2:A:315:GLU:HB2	2.19	0.43
1:R:636:C:H2'	1:R:636:C:O2	2.17	0.43
2:A:379:LEU:HD23	2:A:379:LEU:N	2.33	0.43
2:B:179:ILE:N	2:B:179:ILE:HD13	2.33	0.43
1:R:619:H2U:H61	1:R:620:C:H41	1.84	0.43
1:R:617:G:N2	1:R:658:A:H5'	2.32	0.43
2:A:533:VAL:HG13	2:A:545:ALA:HB1	2.00	0.43
1:S:601:U:N3	1:S:673:G:N2	2.66	0.43
2:A:334:HIS:CE1	2:A:531:ARG:NH2	2.86	0.43
2:B:453:ARG:NH1	2:B:469:SER:HB3	2.31	0.43
2:A:530:GLU:O	2:A:533:VAL:HG12	2.18	0.43
2:B:331:THR:HG22	2:B:333:ARG:N	2.33	0.43
2:A:449:PRO:HG2	2:A:452:ILE:CG1	2.38	0.43
1:S:636:C:O4'	2:B:119:ARG:NH1	2.51	0.43
2:A:210:ASP:O	2:A:225:VAL:HA	2.18	0.43
2:B:400:LEU:HD12	2:B:400:LEU:O	2.19	0.43
2:B:276:LEU:HD12	2:B:276:LEU:HA	1.74	0.43
2:B:410:ARG:HA	2:B:414:LYS:O	2.18	0.43
2:B:149:ILE:HG12	2:B:153:MET:HE1	2.00	0.43
1:S:631:C:H2'	1:S:632:PSU:C6	2.52	0.43
2:B:114:ARG:HB2	2:B:131:ARG:O	2.19	0.43
2:A:554:ARG:HB2	2:A:554:ARG:HE	1.55	0.43
2:B:331:THR:O	2:B:543:ARG:NH2	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:531:ARG:HD3	2:A:535:PHE:HE2	1.84	0.43
2:A:453:ARG:HH11	2:A:453:ARG:HG3	1.84	0.43
2:B:91:GLN:NE2	2:B:169:ARG:NH2	2.66	0.43
2:A:254:VAL:HG12	2:A:255:CYS:N	2.33	0.43
1:R:675:C:C2	2:A:334:HIS:CE1	3.07	0.43
2:A:307:GLN:NE2	2:A:511:TYR:OH	2.51	0.43
2:B:447:LYS:HG2	2:B:447:LYS:H	1.60	0.43
2:B:470:TYR:CE1	2:B:482:GLY:HA3	2.54	0.43
2:A:94:VAL:HG12	2:A:95:LYS:N	2.34	0.43
1:S:644:A:O2'	1:S:645:G:H5'	2.19	0.43
2:B:94:VAL:CG2	2:B:111:PHE:HD2	2.31	0.43
1:S:676:A:C2	2:B:301:SER:HB3	2.54	0.42
2:A:300:GLN:NE2	2:A:325:ARG:HD3	2.34	0.42
2:A:515:PHE:CD1	2:A:519:CYS:SG	3.11	0.42
1:S:636:C:C1'	2:B:119:ARG:NH1	2.82	0.42
2:A:225:VAL:O	2:A:225:VAL:CG1	2.66	0.42
2:A:292:PHE:CE2	2:B:328:ASN:HA	2.54	0.42
2:B:401:THR:HG23	2:B:404:GLU:OE1	2.19	0.42
2:A:233:ASP:OD1	2:A:556:ARG:NH1	2.52	0.42
2:B:300:GLN:CG	2:B:325:ARG:HA	2.40	0.42
2:B:268:THR:O	2:B:270:VAL:HG13	2.19	0.42
2:B:144:ASN:ND2	2:B:146:GLU:HG2	2.34	0.42
2:B:78:LEU:HD23	2:B:78:LEU:HA	1.78	0.42
2:A:257:LEU:HD13	2:A:365:ILE:HA	2.02	0.42
2:B:355:LEU:HD21	2:B:399:ARG:HE	1.84	0.42
2:B:267:PHE:HZ	2:B:345:MET:HG3	1.85	0.42
2:B:112:ARG:HG3	2:B:197:ILE:CD1	2.49	0.42
2:B:479:ILE:HG13	2:B:480:LEU:N	2.35	0.42
2:B:137:ILE:O	2:B:137:ILE:HD12	2.19	0.42
2:A:460:ASP:HB3	2:A:463:ASN:O	2.19	0.42
1:S:675:C:H6	1:S:675:C:O5'	2.01	0.42
2:A:255:CYS:SG	2:A:255:CYS:O	2.77	0.42
2:A:355:LEU:C	2:A:355:LEU:HD23	2.40	0.42
1:R:636:C:N3	2:A:179:ILE:HA	2.35	0.42
2:A:161:ASN:ND2	2:A:202:GLU:CA	2.82	0.42
2:B:99:LEU:HD22	2:B:172:VAL:HG21	2.01	0.42
2:B:96:PHE:HA	2:B:99:LEU:HD12	2.01	0.42
1:R:666:U:H2'	1:R:667:C:C6	2.54	0.42
2:A:77:LYS:HA	2:A:196:THR:HB	2.02	0.42
2:A:334:HIS:CE1	2:A:531:ARG:HH22	2.37	0.42
2:B:462:ALA:O	2:B:463:ASN:CB	2.59	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:489:HIS:CE1	2:A:493:GLN:OE1	2.73	0.42
2:B:236:VAL:HG23	2:B:237:ILE:N	2.35	0.42
2:A:213:ARG:HH21	2:A:224:PRO:HD2	1.85	0.42
2:B:258:PHE:HE1	2:B:361:LEU:HD11	1.83	0.42
2:B:414:LYS:HD3	2:B:429:PHE:CE2	2.54	0.42
2:B:144:ASN:HD21	2:B:148:THR:N	2.16	0.42
2:A:240:ARG:HD3	2:B:313:ASP:CG	2.40	0.42
1:R:648:U:C4	1:R:659:U:N3	2.87	0.42
2:A:376:GLU:O	2:A:380:VAL:HG23	2.19	0.42
2:B:453:ARG:HD3	2:B:469:SER:CB	2.49	0.42
2:B:110:LEU:HA	2:B:168:VAL:O	2.19	0.42
2:B:133:GLN:CG	2:B:249:ARG:NH2	2.83	0.42
1:R:608:U:O4	1:R:613:PSU:C5	2.72	0.42
2:A:304:PHE:H	2:A:304:PHE:HD1	1.68	0.42
2:A:214:SER:HB3	2:A:383:GLN:HA	2.02	0.42
2:A:223:LEU:HA	2:A:223:LEU:HD23	1.73	0.42
2:B:522:HIS:CD2	2:B:522:HIS:N	2.88	0.42
2:A:286:VAL:HA	2:A:300:GLN:OE1	2.19	0.42
2:B:548:PHE:O	2:B:549:PRO:O	2.37	0.42
2:B:424:THR:HB	2:B:425:GLU:OE2	2.20	0.42
2:B:69:ASP:O	2:B:72:LYS:HB2	2.19	0.42
2:B:251:GLN:HG3	2:B:529:LEU:HD22	2.00	0.42
2:B:333:ARG:CZ	2:B:477:GLU:HG2	2.50	0.42
2:A:114:ARG:HD2	2:A:165:ILE:HG13	2.01	0.42
2:A:82:GLN:HB3	2:B:461:PRO:HB3	2.01	0.42
2:A:202:GLU:O	2:A:203:ALA:CB	2.67	0.42
2:A:117:ASN:HA	2:A:162:LEU:CD2	2.50	0.42
2:B:138:GLN:NE2	2:B:179:ILE:HD12	2.33	0.42
2:A:233:ASP:CG	2:A:556:ARG:HH12	2.23	0.41
2:B:534:MET:HE2	2:B:535:PHE:CE1	2.55	0.41
2:B:286:VAL:HG23	2:B:298:LEU:O	2.19	0.41
2:A:366:PHE:CZ	2:A:474:MET:HE3	2.55	0.41
2:A:284:SER:HB3	2:A:300:GLN:NE2	2.35	0.41
1:S:634:G:HO2'	1:S:635:U:P	2.40	0.41
2:A:149:ILE:HG23	2:A:153:MET:HE2	2.01	0.41
2:A:347:PHE:CZ	2:A:521:PRO:HB2	2.54	0.41
2:A:291:TYR:OH	2:B:336:THR:HG21	2.20	0.41
2:B:115:VAL:HG23	2:B:115:VAL:O	2.20	0.41
2:A:358:LEU:O	2:A:361:LEU:CB	2.68	0.41
2:B:251:GLN:CG	2:B:529:LEU:HD13	2.50	0.41
1:R:656:C:O2	1:R:656:C:H2'	2.19	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:539:LEU:C	2:A:541:ASN:H	2.22	0.41
1:S:636:C:O2	2:B:181:SER:N	2.42	0.41
2:A:249:ARG:HD2	2:A:249:ARG:HA	1.89	0.41
2:B:96:PHE:HE1	2:B:111:PHE:CE2	2.38	0.41
2:B:438:TYR:O	2:B:439:ASP:HB2	2.19	0.41
2:A:341:LEU:HB2	2:A:527:ILE:HG12	2.02	0.41
1:R:648:U:N3	1:R:659:U:O2	2.54	0.41
1:R:612:U:C2'	1:R:613:PSU:O5'	2.69	0.41
1:R:612:U:H1'	2:A:224:PRO:HB3	2.01	0.41
2:A:318:TYR:HA	2:A:342:ASP:O	2.21	0.41
1:R:665:G:H2'	1:R:666:U:C6	2.56	0.41
2:A:516:SER:C	2:A:518:GLY:H	2.24	0.41
2:A:156:TRP:CH2	2:A:194:ILE:HD13	2.56	0.41
2:A:106:ASP:N	2:A:172:VAL:HG13	2.35	0.41
1:S:637:1MG:P	2:B:180:LYS:HE3	2.60	0.41
2:A:389:PHE:O	2:A:441:ASP:OD2	2.37	0.41
2:A:108:GLU:O	2:A:108:GLU:HG2	2.21	0.41
2:A:448:PHE:HD2	2:A:452:ILE:HD11	1.86	0.41
2:B:463:ASN:HA	2:B:464:PRO:HD2	1.85	0.41
2:B:354:VAL:HG11	2:B:523:ALA:O	2.21	0.41
1:R:623:A:C4	1:R:624:A:C8	3.08	0.41
2:B:474:MET:HB2	2:B:474:MET:HE2	1.65	0.41
1:R:621:A:C5	1:R:648:U:C5	3.09	0.41
1:R:648:U:C2	1:R:659:U:O2	2.73	0.41
2:A:355:LEU:O	2:A:355:LEU:HD23	2.20	0.41
2:A:108:GLU:HA	2:A:170:GLY:O	2.20	0.41
2:B:488:ASP:OD1	2:B:490:ALA:N	2.53	0.41
2:B:210:ASP:OD1	2:B:213:ARG:NH2	2.54	0.41
2:B:551:ASP:OD1	2:B:554:ARG:N	2.48	0.41
2:A:433:LEU:HA	2:A:433:LEU:HD23	1.76	0.41
2:B:475:ARG:HH11	2:B:475:ARG:HG2	1.85	0.41
2:B:335:MET:HE2	2:B:542:ILE:HG23	2.02	0.41
2:B:304:PHE:O	2:B:307:GLN:HB2	2.21	0.41
2:A:82:GLN:HG2	2:B:461:PRO:HB3	2.01	0.41
1:S:668:G:C6	1:S:669:C:C4	3.08	0.41
1:R:638:C:C4	2:A:121:GLN:OE1	2.74	0.41
1:S:618:G:C5	1:S:657:A:C2	3.08	0.41
2:A:453:ARG:CZ	2:A:469:SER:HB2	2.51	0.41
2:A:402:TYR:CD2	2:A:449:PRO:HD3	2.55	0.41
2:A:453:ARG:HA	2:A:453:ARG:HD2	1.73	0.41
2:A:408:MET:O	2:A:409:LEU:C	2.59	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:GLN:HG3	2:B:324:PHE:O	2.21	0.41
2:A:515:PHE:CE1	2:A:519:CYS:SG	3.14	0.41
2:A:309:LEU:CD1	2:B:548:PHE:HE1	2.31	0.41
2:B:78:LEU:CD1	2:B:167:LEU:HD23	2.48	0.41
1:S:650:G:H2'	1:S:651:G:H8	1.86	0.41
2:B:77:LYS:HG3	2:B:196:THR:HG22	2.02	0.41
2:A:105:SER:O	2:A:106:ASP:HB2	2.21	0.41
2:B:258:PHE:CE2	2:B:341:LEU:HB3	2.55	0.41
2:B:541:ASN:ND2	2:B:541:ASN:C	2.73	0.41
2:B:455:PHE:CD1	2:B:455:PHE:C	2.94	0.41
1:R:675:C:H2'	1:R:676:A:H8	1.86	0.41
2:A:271:HIS:HB3	2:B:339:THR:HG21	2.02	0.41
1:S:638:C:C2	2:B:121:GLN:NE2	2.89	0.41
2:B:443:TYR:CZ	2:B:473:PHE:CD2	3.09	0.41
2:B:449:PRO:HA	2:B:466:TYR:HD1	1.85	0.41
2:A:423:SER:O	2:A:427:GLU:HB2	2.21	0.41
2:B:534:MET:O	2:B:538:ASP:N	2.53	0.40
2:A:270:VAL:HG11	2:A:317:VAL:CG2	2.51	0.40
1:R:608:U:O4	1:R:613:PSU:C4	2.74	0.40
2:B:269:GLU:CG	2:B:318:TYR:CE1	3.03	0.40
2:B:433:LEU:HA	2:B:433:LEU:HD23	1.79	0.40
2:A:287:PHE:CB	2:A:298:LEU:HD12	2.51	0.40
2:A:307:GLN:HG2	2:A:522:HIS:NE2	2.37	0.40
2:A:350:HIS:CE1	2:B:83:SER:O	2.74	0.40
2:B:130:LEU:O	2:B:136:LEU:HA	2.21	0.40
1:S:635:U:C2'	2:B:121:GLN:HE22	2.34	0.40
1:S:634:G:O2'	1:S:635:U:OP2	2.33	0.40
1:R:617:G:N2	1:R:657:A:H2'	2.36	0.40
1:R:655:PSU:N3	1:R:658:A:OP2	2.21	0.40
2:A:78:LEU:HD12	2:A:197:ILE:HG22	2.02	0.40
2:A:449:PRO:HD2	2:A:452:ILE:HD11	2.04	0.40
2:B:193:LYS:HZ3	2:B:193:LYS:HB2	1.85	0.40
2:B:79:PRO:O	2:B:80:LEU:CB	2.69	0.40
2:A:311:VAL:HA	2:A:519:CYS:CB	2.44	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	488/490 (100%)	400 (82%)	66 (14%)	22 (4%)	3	12
2	B	488/490 (100%)	397 (81%)	70 (14%)	21 (4%)	3	13
All	All	976/980 (100%)	797 (82%)	136 (14%)	43 (4%)	3	12

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	88	ARG
2	A	198	SER
2	A	203	ALA
2	A	256	GLU
2	A	292	PHE
2	A	383	GLN
2	B	72	LYS
2	B	80	LEU
2	B	206	ILE
2	B	446	ASP
2	B	447	LYS
2	B	463	ASN
2	A	206	ILE
2	A	286	VAL
2	A	418	ASP
2	A	518	GLY
2	B	103	LYS
2	B	284	SER
2	B	382	LYS
2	B	509	LYS
2	A	133	GLN
2	A	296	ALA
2	A	540	LYS
2	B	202	GLU
2	B	205	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	539	LEU
2	B	549	PRO
2	A	124	THR
2	A	205	PRO
2	A	549	PRO
2	B	285	SER
2	B	292	PHE
2	A	207	LEU
2	A	239	LEU
2	A	412	ALA
2	B	102	ALA
2	B	133	GLN
2	B	464	PRO
2	A	85	ASP
2	A	283	GLY
2	B	191	ILE
2	B	214	SER
2	A	552	PRO

### 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	
2	A	427/427 (100%)	357 (84%)	70 (16%)	3	8
2	B	427/427 (100%)	348 (82%)	79 (18%)	2	6
All	All	854/854 (100%)	705 (83%)	149 (17%)	2	7

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	68	GLU
2	A	70	THR
2	A	72	LYS
2	A	73	ASP
2	A	82	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	91	GLN
2	A	93	ARG
2	A	101	GLU
2	A	115	VAL
2	A	124	THR
2	A	128	LEU
2	A	130	LEU
2	A	138	GLN
2	A	140	LEU
2	A	178	PRO
2	A	185	GLN
2	A	187	LEU
2	A	194	ILE
2	A	197	ILE
2	A	200	THR
2	A	202	GLU
2	A	206	ILE
2	A	209	GLU
2	A	213	ARG
2	A	217	GLU
2	A	235	ARG
2	A	236	VAL
2	A	239	LEU
2	A	240	ARG
2	A	256	GLU
2	A	262	LEU
2	A	264	THR
2	A	293	LYS
2	A	303	GLN
2	A	304	PHE
2	A	313	ASP
2	A	327	GLU
2	A	330	ASN
2	A	336	THR
2	A	339	THR
2	A	349	GLU
2	A	351	TYR
2	A	361	LEU
2	A	383	GLN
2	A	391	LEU
2	A	394	ASP
2	A	396	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	406	ILE
2	A	410	ARG
2	A	427	GLU
2	A	428	LYS
2	A	430	LEU
2	A	443	TYR
2	A	453	ARG
2	A	468	ASN
2	A	481	SER
2	A	487	HIS
2	A	497	LYS
2	A	501	LEU
2	A	510	ASP
2	A	517	TYR
2	A	527	ILE
2	A	529	LEU
2	A	539	LEU
2	A	543	ARG
2	A	547	LEU
2	A	551	ASP
2	A	554	ARG
2	A	555	LEU
2	A	556	ARG
2	B	69	ASP
2	B	70	THR
2	B	72	LYS
2	B	83	SER
2	B	84	ARG
2	B	88	ARG
2	B	97	VAL
2	B	105	SER
2	B	107	LYS
2	B	117	ASN
2	B	133	GLN
2	B	135	SER
2	B	136	LEU
2	B	140	LEU
2	B	144	ASN
2	B	145	LYS
2	B	146	GLU
2	B	152	ASN
2	B	159	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	164	SER
2	B	165	ILE
2	B	171	ILE
2	B	183	THR
2	B	192	THR
2	B	193	LYS
2	B	196	THR
2	B	200	THR
2	B	204	LEU
2	B	206	ILE
2	B	212	SER
2	B	219	GLU
2	B	225	VAL
2	B	239	LEU
2	B	243	THR
2	B	257	LEU
2	B	262	LEU
2	B	266	LYS
2	B	268	THR
2	B	269	GLU
2	B	276	LEU
2	B	281	GLU
2	B	290	THR
2	B	300	GLN
2	B	315	GLU
2	B	316	ARG
2	B	318	TYR
2	B	324	PHE
2	B	336	THR
2	B	343	MET
2	B	345	MET
2	B	351	TYR
2	B	352	HIS
2	B	361	LEU
2	B	376	GLU
2	B	379	LEU
2	B	382	LYS
2	B	393	LYS
2	B	397	MET
2	B	409	LEU
2	B	416	ILE
2	B	422	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	435	ARG
2	B	443	TYR
2	B	451	GLU
2	B	453	ARG
2	B	457	THR
2	B	458	MET
2	B	463	ASN
2	B	491	LEU
2	B	492	LEU
2	B	495	ARG
2	B	505	ASP
2	B	520	PRO
2	B	529	LEU
2	B	537	LEU
2	B	541	ASN
2	B	543	ARG
2	B	544	ARG
2	B	546	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	82	GLN
2	A	91	GLN
2	A	132	GLN
2	A	186	ASN
2	A	251	GLN
2	A	271	HIS
2	A	303	GLN
2	A	307	GLN
2	A	350	HIS
2	A	375	HIS
2	A	383	GLN
2	A	468	ASN
2	A	487	HIS
2	A	499	HIS
2	B	74	ASN
2	B	82	GLN
2	B	91	GLN
2	B	121	GLN
2	B	133	GLN
2	B	144	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	152	ASN
2	B	251	GLN
2	B	305	ASN
2	B	307	GLN
2	B	334	HIS
2	B	350	HIS
2	B	352	HIS
2	B	383	GLN
2	B	463	ASN
2	B	468	ASN
2	B	489	HIS
2	B	522	HIS
2	B	541	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	74/75 (98%)	18 (24%)	2 (2%)
1	S	74/75 (98%)	20 (27%)	1 (1%)
All	All	148/150 (98%)	38 (25%)	3 (2%)

All (38) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	606	G
1	R	610	G
1	R	617	G
1	R	618	G
1	R	633	U
1	R	634	G
1	R	635	U
1	R	637	1MG
1	R	642	C
1	R	648	U
1	R	650	G
1	R	652	G
1	R	656	C
1	R	658	A
1	R	659	U
1	R	671	G
1	R	672	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	R	675	C
1	S	609	A
1	S	611	U
1	S	614	A
1	S	617	G
1	S	618	G
1	S	619	H2U
1	S	620	C
1	S	623	A
1	S	627	G
1	S	631	C
1	S	633	U
1	S	634	G
1	S	635	U
1	S	637	1MG
1	S	648	U
1	S	649	5MC
1	S	655	PSU
1	S	658	A
1	S	661	C
1	S	676	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	633	U
1	R	634	G
1	S	634	G

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

16 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
1	PSU	R	613	1	13,21,22	1.44	3 (23%)	18,30,33	6.04	5 (27%)
1	H2U	R	616	1	17,21,22	0.64	0	23,30,33	1.45	3 (13%)
1	H2U	R	619	1	17,21,22	0.52	0	23,30,33	1.08	1 (4%)
1	PSU	R	632	1	13,21,22	1.57	2 (15%)	18,30,33	5.70	6 (33%)
1	1MG	R	637	1	16,26,27	0.68	0	19,39,42	1.26	1 (5%)
1	5MC	R	649	1	13,22,23	1.06	1 (7%)	15,32,35	1.01	1 (6%)
1	5MU	R	654	1	12,22,23	1.03	0	14,32,35	4.20	2 (14%)
1	PSU	R	655	1	13,21,22	1.61	3 (23%)	18,30,33	5.89	5 (27%)
1	PSU	S	613	1	13,21,22	1.86	3 (23%)	18,30,33	6.07	5 (27%)
1	H2U	S	616	1	17,21,22	0.55	0	23,30,33	0.92	1 (4%)
1	H2U	S	619	1	17,21,22	0.68	0	23,30,33	1.19	2 (8%)
1	PSU	S	632	1	13,21,22	1.48	2 (15%)	18,30,33	5.48	4 (22%)
1	1MG	S	637	1	16,26,27	0.75	0	19,39,42	1.53	2 (10%)
1	5MC	S	649	1	13,22,23	0.91	1 (7%)	15,32,35	0.97	0
1	5MU	S	654	1	12,22,23	1.35	3 (25%)	14,32,35	4.49	2 (14%)
1	PSU	S	655	1	13,21,22	1.57	3 (23%)	18,30,33	5.84	5 (27%)

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
1	PSU	R	613	1	-	0/7/25/26	0/2/2/2
1	H2U	R	616	1	-	0/7/38/39	0/2/2/2
1	H2U	R	619	1	-	0/7/38/39	0/2/2/2
1	PSU	R	632	1	-	0/7/25/26	0/2/2/2
1	1MG	R	637	1	-	0/3/25/26	0/3/3/3
1	5MC	R	649	1	-	0/3/25/26	0/2/2/2
1	5MU	R	654	1	-	0/3/25/26	0/2/2/2
1	PSU	R	655	1	-	0/7/25/26	0/2/2/2
1	PSU	S	613	1	-	0/7/25/26	0/2/2/2
1	H2U	S	616	1	-	0/7/38/39	0/2/2/2
1	H2U	S	619	1	-	0/7/38/39	0/2/2/2
1	PSU	S	632	1	-	0/7/25/26	0/2/2/2
1	1MG	S	637	1	-	0/3/25/26	0/3/3/3
1	5MC	S	649	1	-	0/3/25/26	0/2/2/2
1	5MU	S	654	1	-	0/3/25/26	0/2/2/2
1	PSU	S	655	1	-	0/7/25/26	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	613	PSU	C5-C1'	-3.95	1.48	1.52
1	R	632	PSU	C6-C5	-3.16	1.34	1.38
1	R	655	PSU	C2'-C1'	-3.15	1.50	1.53
1	S	655	PSU	C2'-C1'	-3.10	1.51	1.53
1	S	632	PSU	C6-C5	-2.80	1.34	1.38
1	R	613	PSU	C6-C5	-2.67	1.34	1.38
1	S	655	PSU	C6-C5	-2.59	1.34	1.38
1	S	613	PSU	O4'-C1'	-2.45	1.40	1.44
1	R	655	PSU	C6-C5	-2.34	1.35	1.38
1	S	649	5MC	C6-C5	-2.32	1.33	1.40
1	R	649	5MC	C6-C5	-2.11	1.34	1.40
1	S	654	5MU	C6-C5	-2.03	1.34	1.40
1	R	613	PSU	C5-C1'	-2.01	1.50	1.52
1	S	654	5MU	C4-N3	2.49	1.37	1.33
1	S	654	5MU	O4'-C1'	2.74	1.44	1.41
1	R	613	PSU	C4-N3	2.93	1.38	1.33
1	R	655	PSU	C4-N3	3.13	1.38	1.33
1	S	632	PSU	C4-N3	3.19	1.39	1.33
1	S	613	PSU	C4-N3	3.20	1.39	1.33
1	S	655	PSU	C4-N3	3.28	1.39	1.33
1	R	632	PSU	C4-N3	3.52	1.39	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	613	PSU	N1-C2-N3	-21.12	114.86	128.33
1	S	613	PSU	N1-C2-N3	-20.54	115.23	128.33
1	S	655	PSU	N1-C2-N3	-20.04	115.55	128.33
1	R	655	PSU	N1-C2-N3	-19.92	115.62	128.33
1	R	632	PSU	N1-C2-N3	-19.15	116.11	128.33
1	S	632	PSU	N1-C2-N3	-18.80	116.34	128.33
1	S	654	5MU	C5-C4-N3	-9.82	114.21	125.14
1	R	654	5MU	C5-C4-N3	-8.88	115.25	125.14
1	R	616	H2U	C5-C4-N3	-5.16	111.84	116.71
1	R	637	1MG	C5-C6-N1	-4.55	112.56	118.33
1	S	637	1MG	C5-C6-N1	-4.52	112.60	118.33
1	S	619	H2U	C5-C4-N3	-3.68	113.25	116.71
1	S	637	1MG	C2'-C1'-N9	-3.61	108.77	114.29
1	S	616	H2U	C5-C4-N3	-3.17	113.72	116.71
1	R	619	H2U	C5-C4-N3	-3.11	113.78	116.71
1	S	613	PSU	C5-C6-N1	-2.43	120.96	124.39
1	R	632	PSU	C5-C6-N1	-2.31	121.14	124.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	613	PSU	C5-C6-N1	-2.15	121.36	124.39
1	R	632	PSU	C5-C1'-C2'	2.01	119.09	115.52
1	R	616	H2U	O4-C4-C5	2.23	127.34	122.34
1	S	619	H2U	C5-C6-N1	2.33	113.22	110.70
1	S	655	PSU	C5-C1'-C2'	2.38	119.75	115.52
1	S	632	PSU	O4'-C1'-C2'	2.45	107.23	104.73
1	R	655	PSU	C5-C1'-C2'	2.55	120.04	115.52
1	R	649	5MC	O4'-C1'-N1	2.57	113.50	108.08
1	R	616	H2U	C5-C6-N1	2.64	113.56	110.70
1	R	613	PSU	O4'-C1'-C2'	3.30	108.09	104.73
1	S	632	PSU	C6-N1-C2	3.86	121.68	115.47
1	R	655	PSU	C6-N1-C2	3.92	121.78	115.47
1	S	613	PSU	O4'-C1'-C2'	4.12	108.93	104.73
1	R	632	PSU	C6-N1-C2	4.18	122.19	115.47
1	S	655	PSU	C6-N1-C2	4.27	122.34	115.47
1	S	613	PSU	C6-N1-C2	4.59	122.85	115.47
1	R	613	PSU	C6-N1-C2	4.77	123.14	115.47
1	S	655	PSU	O4'-C1'-C2'	4.79	109.61	104.73
1	R	655	PSU	O4'-C1'-C2'	4.94	109.77	104.73
1	R	632	PSU	O4'-C1'-C2'	5.07	109.90	104.73
1	S	655	PSU	C4-N3-C2	12.36	125.93	115.25
1	R	632	PSU	C4-N3-C2	12.41	125.98	115.25
1	S	632	PSU	C4-N3-C2	12.46	126.02	115.25
1	R	654	5MU	C4-N3-C2	12.77	126.29	115.25
1	R	613	PSU	C4-N3-C2	12.89	126.39	115.25
1	R	655	PSU	C4-N3-C2	13.10	126.57	115.25
1	S	654	5MU	C4-N3-C2	13.48	126.90	115.25
1	S	613	PSU	C4-N3-C2	13.76	127.15	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	613	PSU	4	0
1	R	616	H2U	1	0
1	R	619	H2U	3	0
1	R	632	PSU	1	0
1	R	637	1MG	3	0
1	R	649	5MC	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	654	5MU	1	0
1	R	655	PSU	1	0
1	S	613	PSU	1	0
1	S	616	H2U	2	0
1	S	619	H2U	12	0
1	S	632	PSU	4	0
1	S	637	1MG	4	0
1	S	649	5MC	4	0
1	S	654	5MU	3	0
1	S	655	PSU	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.