



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:45 PM UTC

PDB ID : 1ASZ / pdb_00001asz
Title : THE ACTIVE SITE OF YEAST ASPARTYL-TRNA SYNTHETASE:
STRUCTURAL AND FUNCTIONAL ASPECTS OF THE AMINOACYLA-
TION REACTION
Authors : Cavarelli, J.; Rees, B.; Thierry, J.C.; Moras, D.
Deposited on : 1995-01-19
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

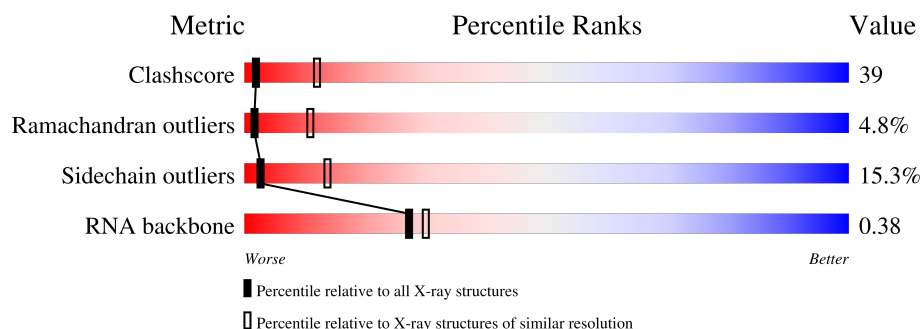
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

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

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11158 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.

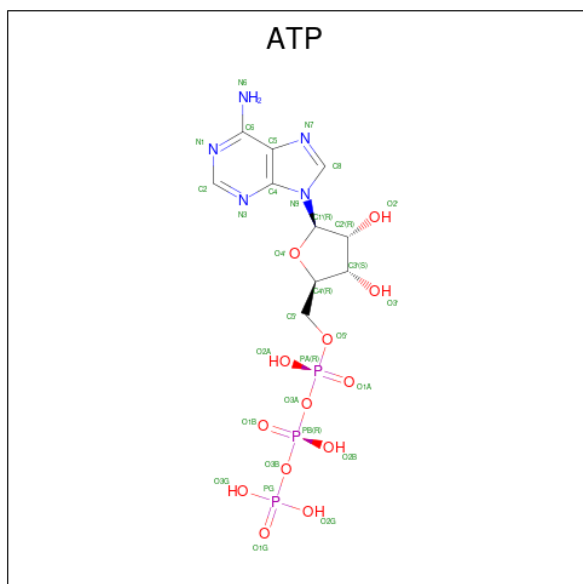
- Molecule 1 is a RNA chain called T-RNA (75-MER).

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			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



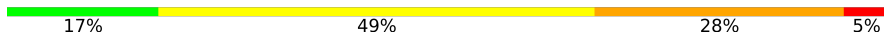
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

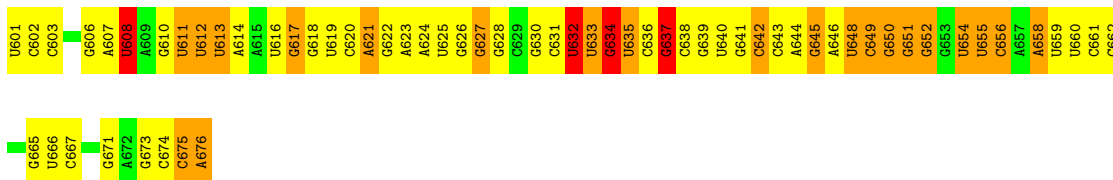
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

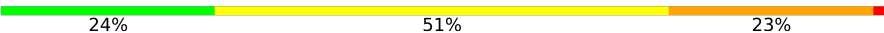
Note EDS was not executed.

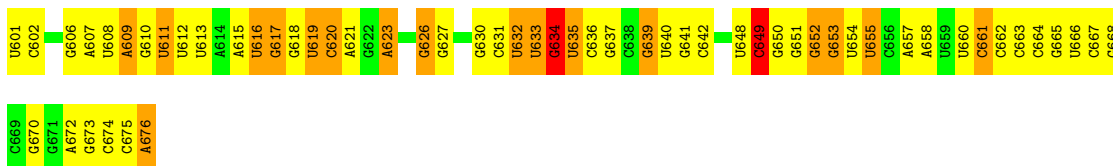
• Molecule 1: T-RNA (75-MER)

Chain R: 



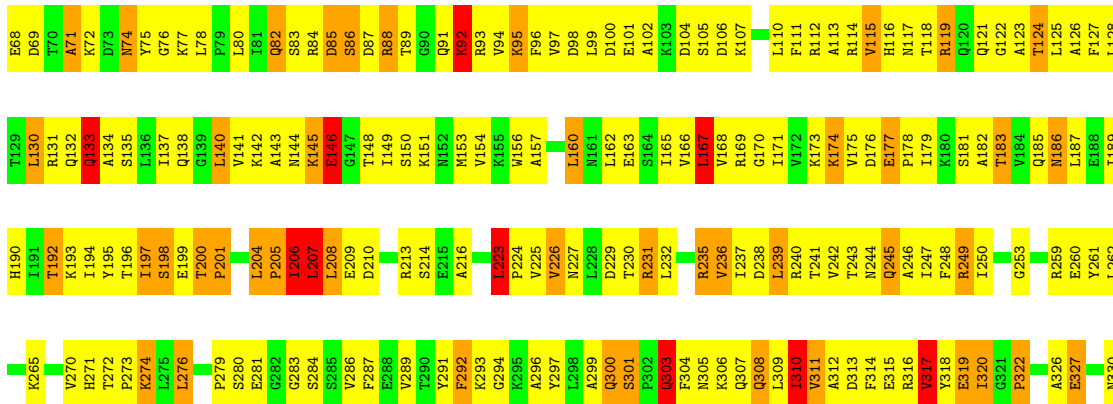
• Molecule 1: T-RNA (75-MER)

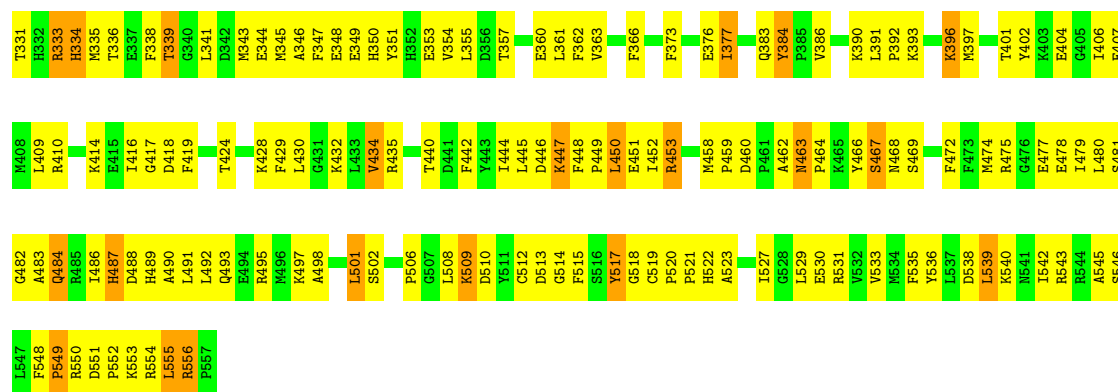
Chain S: 



• Molecule 2: ASPARTYL-tRNA SYNTHETASE

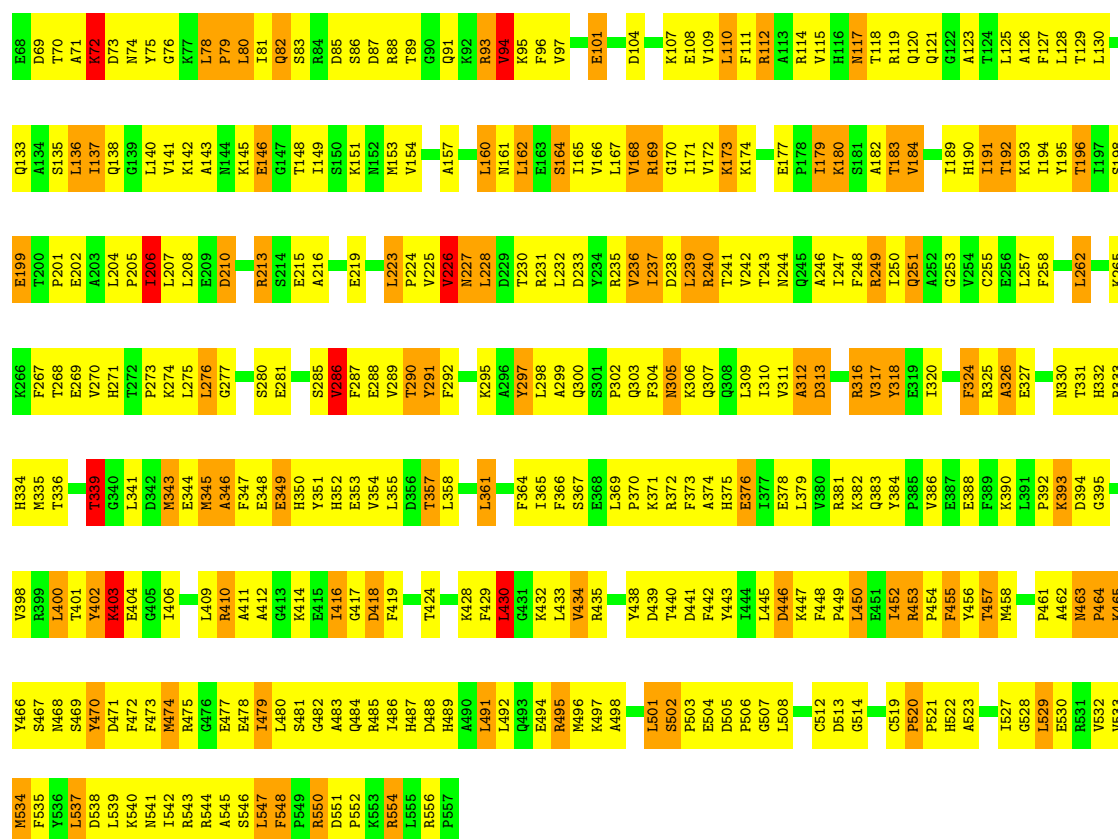
Chain A: 





• Molecule 2: ASPARTYL-tRNA SYNTHETASE

Chain B: 28% 52% 18%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	211.27Å 145.35Å 86.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	80.0 (7.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11158	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 1MG, 5MU, H2U, PSU, ATP

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	0.72	0/1605	1.38	18/2500 (0.7%)
1	S	0.73	0/1605	1.35	13/2500 (0.5%)
2	A	0.72	0/4029	1.21	38/5433 (0.7%)
2	B	0.76	2/4029 (0.0%)	1.24	41/5433 (0.8%)
All	All	0.74	2/11268 (0.0%)	1.27	110/15866 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	339	THR	CA-CB	6.12	1.61	1.53
2	B	534	MET	SD-CE	-5.37	1.66	1.79

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	249	ARG	N-CA-C	-11.59	98.62	111.14
2	A	204	LEU	N-CA-C	-10.35	96.78	109.72
2	A	353	GLU	N-CA-C	-9.65	100.62	111.82
2	A	183	THR	N-CA-C	-9.56	102.12	113.88
2	B	94	VAL	N-CA-C	8.42	119.72	110.21
1	R	627	G	O3'-P-O5'	-8.34	91.49	104.00
1	S	609	A	OP1-P-O3'	8.21	132.62	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	633	U	P-O3'-C3'	8.19	132.48	120.20
2	B	247	ILE	N-CA-C	-7.70	103.18	110.42
2	B	166	VAL	N-CA-C	7.66	118.83	108.11
2	B	223	LEU	CA-C-N	7.54	129.27	119.84
2	B	223	LEU	C-N-CA	7.54	129.27	119.84
1	S	608	U	O3'-P-O5'	7.50	115.25	104.00
2	A	250	ILE	N-CA-C	-7.47	104.51	111.45
2	B	177	GLU	CA-C-N	7.36	127.41	119.90
2	B	177	GLU	C-N-CA	7.36	127.41	119.90
1	S	611	U	O3'-P-O5'	-7.34	92.99	104.00
2	B	346	ALA	N-CA-C	-7.20	96.51	108.32
2	A	249	ARG	N-CA-C	-7.13	104.39	113.23
1	S	611	U	OP1-P-O3'	7.09	129.27	108.00
2	A	334	HIS	N-CA-C	7.08	120.00	109.59
2	B	79	PRO	N-CA-C	7.08	123.21	113.65
2	A	450	LEU	N-CA-C	-7.03	101.06	110.55
2	A	231	ARG	N-CA-C	-7.03	103.04	111.69
2	B	133	GLN	CB-CA-C	-7.01	107.69	117.23
2	A	320	ILE	CB-CA-C	-6.97	102.92	111.08
1	R	658	A	O3'-P-O5'	6.94	114.40	104.00
2	B	548	PHE	CA-C-N	6.86	126.85	119.78
2	B	548	PHE	C-N-CA	6.86	126.85	119.78
1	R	614	A	C5'-C4'-C3'	-6.85	105.73	116.00
1	S	632	PSU	O3'-P-O5'	6.83	114.24	104.00
2	A	245	GLN	N-CA-C	-6.78	103.89	111.28
2	A	283	GLY	N-CA-C	-6.77	104.30	112.49
1	S	623	A	O3'-P-O5'	-6.72	93.92	104.00
2	A	393	LYS	N-CA-C	6.71	118.59	111.28
1	R	633	U	O3'-P-O5'	6.57	113.85	104.00
2	A	514	GLY	N-CA-C	-6.39	105.81	113.99
2	A	208	LEU	N-CA-C	6.37	117.91	110.97
1	S	673	G	O3'-P-O5'	-6.35	94.47	104.00
2	B	317	VAL	N-CA-CB	-6.27	104.52	112.60
2	B	349	GLU	N-CA-C	6.27	121.01	112.68
2	A	478	GLU	N-CA-C	6.25	119.27	109.96
2	B	168	VAL	N-CA-C	6.21	117.72	108.46
1	R	614	A	OP1-P-O3'	6.15	126.46	108.00
2	B	502	SER	N-CA-C	6.13	118.49	109.42
1	S	627	G	O3'-P-O5'	-6.09	94.86	104.00
2	A	274	LYS	N-CA-C	-6.09	105.97	113.41
2	B	326	ALA	N-CA-C	6.09	120.44	113.19
2	A	317	VAL	N-CA-CB	-6.08	101.48	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	VAL	N-CA-C	6.04	117.39	108.45
2	A	167	LEU	N-CA-C	-6.01	98.94	108.73
1	R	608	U	C5'-C4'-C3'	-6.00	107.00	116.00
2	A	310	ILE	N-CA-C	-6.00	105.00	110.82
2	B	403	LYS	N-CA-C	-5.93	104.45	111.03
1	S	634	G	P-O3'-C3'	5.92	129.08	120.20
2	A	204	LEU	CA-C-N	5.92	127.24	119.84
2	A	204	LEU	C-N-CA	5.92	127.24	119.84
2	A	463	ASN	CA-C-N	5.90	126.85	120.83
2	A	463	ASN	C-N-CA	5.90	126.85	120.83
2	B	430	LEU	N-CA-C	-5.89	104.77	111.07
2	B	418	ASP	N-CA-C	5.85	123.25	110.80
2	B	94	VAL	CB-CA-C	-5.84	104.91	111.45
2	A	151	LYS	N-CA-C	-5.79	106.05	113.23
2	B	213	ARG	N-CA-C	5.79	118.11	109.25
2	B	82	GLN	N-CA-C	-5.76	105.84	112.92
2	B	237	ILE	CB-CA-C	-5.74	104.52	112.04
2	A	418	ASP	N-CA-C	5.70	117.57	111.36
2	B	231	ARG	N-CA-C	-5.69	104.98	111.07
1	R	645	G	OP1-P-O3'	5.65	124.94	108.00
2	A	92	LYS	N-CA-C	5.64	117.28	109.15
2	B	199	GLU	N-CA-C	5.64	117.72	108.52
2	A	447	LYS	N-CA-C	5.62	117.49	110.91
1	R	622	G	OP1-P-O3'	5.62	124.86	108.00
2	B	273	PRO	N-CA-C	5.61	119.49	111.13
1	R	642	C	OP1-P-O3'	5.55	124.64	108.00
1	R	634	G	P-O3'-C3'	5.53	128.49	120.20
2	B	228	LEU	N-CA-C	5.52	118.82	111.75
2	B	290	THR	N-CA-C	-5.47	102.79	110.50
1	R	622	G	C5'-C4'-C3'	-5.41	107.88	116.00
1	S	670	G	O3'-P-O5'	-5.41	95.88	104.00
2	B	446	ASP	N-CA-C	5.41	118.88	110.17
2	A	286	VAL	N-CA-C	5.41	116.27	108.48
1	R	627	G	OP1-P-O3'	5.41	124.22	108.00
1	R	645	G	C5'-C4'-C3'	-5.40	107.90	116.00
1	R	671	G	O3'-P-O5'	-5.36	95.96	104.00
2	B	554	ARG	N-CA-C	5.34	117.52	108.02
1	R	611	U	OP2-P-O3'	5.32	123.97	108.00
2	A	453	ARG	CA-C-N	5.28	125.57	119.92
2	A	453	ARG	C-N-CA	5.28	125.57	119.92
2	A	300	GLN	N-CA-C	5.27	119.47	113.19
1	R	608	U	O3'-P-O5'	5.26	111.89	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	377	ILE	N-CA-C	-5.25	105.28	111.00
2	B	251	GLN	N-CA-C	-5.24	105.46	111.07
1	S	610	G	C5'-C4'-C3'	-5.24	108.14	116.00
2	A	319	GLU	N-CA-C	5.20	116.66	107.61
1	S	639	G	C5'-C4'-C3'	-5.17	108.25	116.00
2	B	286	VAL	N-CA-C	5.14	116.06	108.45
2	B	450	LEU	N-CA-C	5.13	119.03	112.87
2	A	226	VAL	CB-CA-C	-5.12	105.09	111.08
2	B	384	TYR	N-CA-C	-5.12	100.05	108.75
1	R	675	C	C5'-C4'-C3'	-5.09	108.36	116.00
2	B	447	LYS	N-CA-C	5.09	118.84	111.56
2	A	223	LEU	N-CA-C	5.08	121.04	109.81
2	B	465	LYS	N-CA-C	-5.08	106.24	112.90
2	A	384	TYR	N-CA-C	-5.08	97.47	108.74
2	B	85	ASP	N-CA-C	5.06	117.18	111.11
2	B	78	LEU	CA-C-N	5.06	124.84	119.28
2	B	78	LEU	C-N-CA	5.06	124.84	119.28
1	R	626	G	O3'-P-O5'	-5.04	96.44	104.00
2	A	484	GLN	N-CA-C	-5.02	100.10	108.34

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	291	TYR	Sidechain
2	B	297	TYR	Sidechain
2	B	402	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1602	0	815	67	0
1	S	1602	0	814	59	0
2	A	3946	0	3939	341	0
2	B	3946	0	3939	402	0
3	A	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	1	0
All	All	11158	0	9531	806	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 39.

All (806) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:VAL:HG11	2:B:538:ASP:HB3	1.33	1.02
2:B:453:ARG:HB3	2:B:457:THR:HG21	1.42	0.97
2:A:227:ASN:O	2:A:231:ARG:HG3	1.65	0.97
2:B:424:THR:HG22	2:B:428:LYS:HE3	1.44	0.95
2:A:119:ARG:HH11	2:A:119:ARG:HB3	1.29	0.95
2:A:93:ARG:HG3	2:A:110:LEU:HD12	1.45	0.94
2:B:472:PHE:HB2	2:B:480:LEU:HB3	1.49	0.92
2:A:200:THR:HG22	2:A:201:PRO:HD2	1.51	0.91
2:A:118:THR:HG22	2:A:128:LEU:HD22	1.48	0.91
2:B:170:GLY:HA2	2:B:192:THR:HG23	1.50	0.91
2:A:386:VAL:HG11	2:A:538:ASP:HB3	1.54	0.88
2:A:303:GLN:HE21	2:A:303:GLN:HA	1.38	0.87
2:B:94:VAL:HG23	2:B:111:PHE:HB3	1.56	0.86
2:B:80:LEU:HD12	2:B:82:GLN:HG3	1.60	0.83
2:B:336:THR:HG23	2:B:551:ASP:HA	1.60	0.83
2:B:149:ILE:HG23	2:B:153:MET:HE2	1.60	0.82
2:A:270:VAL:O	2:A:319:GLU:HG3	1.79	0.82
2:B:173:LYS:HG3	2:B:190:HIS:ND1	1.95	0.81
2:A:419:PHE:HE1	2:A:466:TYR:CE1	1.99	0.80
2:A:200:THR:HG21	2:A:204:LEU:HD13	1.64	0.80
2:A:450:LEU:HD12	2:A:467:SER:HB3	1.61	0.80
2:B:239:LEU:HD11	2:B:248:PHE:HE2	1.47	0.79
2:A:308:GLN:HA	2:A:311:VAL:HG13	1.65	0.79
2:A:363:VAL:HG22	2:A:397:MET:HE3	1.65	0.78
2:A:458:MET:HG2	2:A:484:GLN:NE2	1.99	0.77
2:B:253:GLY:O	2:B:257:LEU:HD12	1.85	0.76
2:A:410:ARG:HA	2:A:414:LYS:O	1.85	0.76
1:S:667:C:H2'	1:S:668:G:H8	1.50	0.76
2:B:306:LYS:NZ	2:B:344:GLU:HB2	2.00	0.75
2:B:496:MET:HE3	2:B:508:LEU:HD13	1.67	0.75
2:B:117:ASN:H	2:B:162:LEU:HD22	1.51	0.75
2:A:445:LEU:HD23	2:A:448:PHE:CZ	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:655:PSU:N3	1:R:658:A:OP2	2.15	0.74
2:B:343:MET:HE3	2:B:358:LEU:HD13	1.69	0.74
2:B:141:VAL:O	2:B:154:VAL:HG22	1.87	0.74
2:B:228:LEU:O	2:B:232:LEU:HG	1.86	0.74
2:B:474:MET:HE2	2:B:479:ILE:HG21	1.68	0.74
2:A:419:PHE:HE1	2:A:466:TYR:HE1	1.35	0.74
2:B:450:LEU:HD23	2:B:467:SER:HB3	1.68	0.74
2:A:92:LYS:HD2	2:A:92:LYS:H	1.53	0.74
2:A:450:LEU:CD1	2:A:467:SER:HB3	2.18	0.74
2:A:279:PRO:HD3	2:A:297:TYR:CE1	2.22	0.73
1:S:676:A:H1'	2:B:456:TYR:OH	1.89	0.73
2:A:538:ASP:O	2:A:540:LYS:HD2	1.88	0.73
2:B:226:VAL:HG12	2:B:230:THR:HG23	1.70	0.73
2:A:170:GLY:HA2	2:A:192:THR:HG22	1.70	0.72
2:B:238:ASP:O	2:B:241:THR:HG23	1.90	0.72
2:A:392:PRO:HD3	2:A:440:THR:OG1	1.90	0.72
2:B:169:ARG:HG3	2:B:169:ARG:HH11	1.53	0.72
2:B:534:MET:HE3	2:B:535:PHE:CE1	2.24	0.72
2:A:104:ASP:HA	2:A:107:LYS:HD3	1.72	0.71
2:B:539:LEU:HD23	2:B:544:ARG:HG2	1.70	0.71
2:B:80:LEU:CD1	2:B:82:GLN:HG3	2.20	0.71
2:A:271:HIS:HE1	2:B:255:CYS:SG	2.14	0.71
1:S:655:PSU:N3	1:S:658:A:OP2	2.22	0.71
2:B:239:LEU:HD11	2:B:248:PHE:CE2	2.26	0.70
2:A:119:ARG:HB3	2:A:119:ARG:NH1	2.06	0.70
1:S:676:A:H61	2:B:280:SER:HB2	1.57	0.70
2:A:175:VAL:HG12	2:A:186:ASN:HA	1.74	0.70
2:B:324:PHE:C	2:B:325:ARG:HG2	2.17	0.69
1:S:612:U:H5''	2:B:226:VAL:O	1.93	0.69
2:A:501:LEU:HD23	2:A:508:LEU:HD11	1.75	0.69
2:A:156:TRP:HZ3	2:A:194:ILE:HG23	1.58	0.69
2:B:324:PHE:CD1	2:B:324:PHE:N	2.60	0.69
2:B:453:ARG:HB3	2:B:457:THR:CG2	2.19	0.69
2:B:335:MET:HE2	2:B:542:ILE:HG23	1.74	0.69
2:A:261:TYR:OH	2:A:360:GLU:HB3	1.93	0.69
2:B:226:VAL:O	2:B:227:ASN:HB2	1.91	0.69
2:A:373:PHE:O	2:A:377:ILE:HG12	1.93	0.68
2:B:71:ALA:HB2	2:B:148:THR:O	1.92	0.68
2:B:381:ARG:HH12	2:B:388:GLU:HA	1.58	0.68
2:B:112:ARG:HB3	2:B:112:ARG:HH11	1.58	0.68
2:B:89:THR:OG1	2:B:91:GLN:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:458:MET:HA	2:B:458:MET:HE2	1.76	0.68
2:A:137:ILE:CD1	2:A:189:ILE:HD13	2.23	0.67
2:A:292:PHE:CE2	2:B:552:PRO:HG3	2.27	0.67
1:S:676:A:N1	2:B:280:SER:HB2	2.10	0.67
2:A:480:LEU:HD23	2:A:481:SER:N	2.09	0.67
1:R:666:U:H2'	1:R:667:C:C6	2.28	0.67
2:B:450:LEU:HD11	2:B:495:ARG:NH1	2.10	0.67
2:A:475:ARG:HD2	2:A:535:PHE:O	1.94	0.67
2:A:401:THR:HG23	2:A:404:GLU:OE2	1.94	0.66
2:A:83:SER:HB3	2:B:350:HIS:CD2	2.30	0.66
2:A:135:SER:HA	2:A:183:THR:HG21	1.77	0.66
2:B:311:VAL:HG22	2:B:519:CYS:HB2	1.76	0.66
1:S:676:A:H2'	2:B:300:GLN:OE1	1.96	0.66
2:A:144:ASN:HD22	2:A:146:GLU:HG2	1.60	0.66
2:A:271:HIS:CE1	2:B:255:CYS:SG	2.88	0.66
2:A:204:LEU:HD23	2:A:204:LEU:H	1.61	0.66
2:B:390:LYS:NZ	2:B:435:ARG:HH21	1.93	0.66
2:A:336:THR:HG21	2:B:291:TYR:OH	1.96	0.66
2:A:205:PRO:O	2:A:207:LEU:N	2.29	0.65
2:B:136:LEU:HD13	2:B:182:ALA:HA	1.79	0.65
1:R:644:A:O2'	1:R:645:G:H5'	1.96	0.65
2:A:137:ILE:HD11	2:A:189:ILE:HD13	1.79	0.65
2:A:119:ARG:HG2	2:A:127:PHE:HB2	1.79	0.65
2:A:292:PHE:CZ	2:B:552:PRO:HG3	2.32	0.65
2:A:333:ARG:HH21	2:A:477:GLU:HB3	1.60	0.65
2:B:242:VAL:CG1	2:B:379:LEU:HD23	2.25	0.65
1:S:626:G:H4'	2:B:207:LEU:HD21	1.78	0.65
2:B:343:MET:SD	2:B:343:MET:C	2.80	0.65
2:B:491:LEU:HD12	2:B:491:LEU:O	1.97	0.65
2:B:435:ARG:O	2:B:439:ASP:HA	1.97	0.65
1:R:631:C:H2'	1:R:632:PSU:O4'	1.97	0.64
1:S:620:C:H5''	1:S:621:A:H5'	1.79	0.64
2:B:347:PHE:HB2	2:B:353:GLU:OE1	1.96	0.64
2:B:94:VAL:HG21	2:B:109:VAL:HB	1.80	0.64
2:B:539:LEU:HD23	2:B:544:ARG:CG	2.27	0.64
2:A:472:PHE:HB2	2:A:480:LEU:HB3	1.78	0.64
2:B:118:THR:C	2:B:119:ARG:HD3	2.22	0.64
2:B:496:MET:CE	2:B:508:LEU:HD13	2.28	0.64
2:A:69:ASP:O	2:A:72:LYS:HD2	1.97	0.64
2:B:370:PRO:O	2:B:374:ALA:HB2	1.96	0.64
1:S:640:U:H2'	1:S:641:G:C8	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:95:LYS:HE2	2:A:132:GLN:OE1	1.98	0.64
2:B:306:LYS:HZ3	2:B:344:GLU:HB2	1.61	0.64
2:A:243:THR:HG22	2:A:247:ILE:HD11	1.79	0.64
2:A:249:ARG:HG2	2:A:249:ARG:HH11	1.64	0.63
2:A:276:LEU:HD13	2:A:299:ALA:HB2	1.80	0.63
2:A:486:ILE:HD13	2:A:491:LEU:HG	1.78	0.63
2:B:137:ILE:HG23	2:B:184:VAL:HB	1.80	0.63
2:A:82:GLN:HG3	2:B:458:MET:SD	2.39	0.63
2:B:443:TYR:CE1	2:B:473:PHE:HB2	2.33	0.63
1:R:621:A:H61	1:R:646:A:H2'	1.63	0.63
2:B:454:PRO:O	2:B:457:THR:HG22	1.98	0.63
2:A:82:GLN:O	2:A:83:SER:HB2	1.97	0.63
2:A:483:ALA:O	2:A:523:ALA:HB1	1.99	0.63
2:B:246:ALA:O	2:B:250:ILE:HG13	1.99	0.63
2:A:279:PRO:HD3	2:A:297:TYR:CZ	2.33	0.62
2:B:70:THR:HG23	2:B:71:ALA:H	1.63	0.62
2:B:410:ARG:C	2:B:412:ALA:H	2.06	0.62
2:A:137:ILE:HG12	2:A:138:GLN:N	2.13	0.62
2:A:149:ILE:HG23	2:A:153:MET:HE2	1.81	0.62
2:A:173:LYS:HE2	2:A:173:LYS:HA	1.81	0.62
2:A:236:VAL:HG12	2:B:312:ALA:HB2	1.80	0.62
2:B:136:LEU:O	2:B:182:ALA:HB1	1.99	0.62
2:A:307:GLN:O	2:A:310:ILE:HB	1.98	0.62
1:S:676:A:N6	2:B:280:SER:HB2	2.13	0.62
2:A:87:ASP:O	2:A:89:THR:HG23	1.99	0.62
2:B:335:MET:HE2	2:B:542:ILE:CG2	2.30	0.62
2:A:366:PHE:HB3	2:A:391:LEU:HD11	1.82	0.62
2:A:551:ASP:O	2:A:553:LYS:N	2.33	0.62
2:B:318:TYR:CD1	2:B:318:TYR:C	2.79	0.61
2:B:406:ILE:HG23	2:B:416:ILE:HG12	1.81	0.61
2:A:121:GLN:HG3	2:A:125:LEU:HD23	1.82	0.61
2:B:324:PHE:N	2:B:324:PHE:HD1	1.98	0.61
1:R:651:G:H2'	1:R:652:G:C8	2.36	0.61
2:A:339:THR:HG23	2:A:530:GLU:OE2	2.01	0.61
2:A:237:ILE:O	2:A:240:ARG:HB2	2.01	0.60
2:A:517:TYR:N	2:A:517:TYR:CD1	2.69	0.60
2:B:350:HIS:HD2	2:B:351:TYR:HD1	1.48	0.60
2:A:112:ARG:HD3	2:A:197:ILE:HD11	1.83	0.60
2:B:165:ILE:HG13	2:B:198:SER:HB3	1.82	0.60
1:R:634:G:H4'	1:R:635:U:O4'	2.01	0.60
2:A:137:ILE:HG12	2:A:138:GLN:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:289:VAL:HG22	2:B:289:VAL:HG22	1.84	0.60
2:B:88:ARG:HH11	2:B:88:ARG:HG2	1.66	0.60
2:A:99:LEU:HD12	2:A:99:LEU:O	2.02	0.60
2:B:69:ASP:HA	2:B:72:LYS:HD2	1.83	0.60
2:A:75:TYR:HB3	2:A:153:MET:HG3	1.82	0.60
2:A:292:PHE:O	2:A:293:LYS:HG2	2.02	0.60
2:A:303:GLN:HE21	2:A:303:GLN:CA	2.13	0.60
2:B:325:ARG:NH2	3:B:701:ATP:O2A	2.30	0.60
1:R:640:U:H2'	1:R:641:G:H8	1.67	0.59
2:A:197:ILE:O	2:A:197:ILE:HG13	2.02	0.59
2:A:495:ARG:O	2:A:498:ALA:HB3	2.02	0.59
1:S:649:5MC:H2'	1:S:650:G:H8	1.67	0.59
1:S:661:C:H2'	1:S:662:C:C6	2.37	0.59
2:A:517:TYR:CD2	2:B:237:ILE:HD11	2.36	0.59
2:B:450:LEU:HD13	2:B:450:LEU:O	2.02	0.59
2:B:458:MET:HG2	2:B:484:GLN:NE2	2.17	0.59
2:A:124:THR:O	2:A:142:LYS:HA	2.03	0.59
2:A:493:GLN:O	2:A:497:LYS:HG2	2.02	0.59
2:B:104:ASP:HA	2:B:107:LYS:HD3	1.85	0.59
2:A:100:ASP:H	2:A:104:ASP:HB2	1.67	0.59
2:A:231:ARG:HB3	2:A:238:ASP:OD2	2.03	0.59
2:B:127:PHE:O	2:B:128:LEU:HD23	2.03	0.59
2:A:133:GLN:HA	2:A:133:GLN:HE21	1.68	0.59
2:B:291:TYR:CD1	2:B:292:PHE:HD2	2.21	0.59
2:B:416:ILE:HD13	2:B:416:ILE:H	1.68	0.59
1:S:601:U:H2'	1:S:602:C:C6	2.38	0.59
1:S:640:U:H2'	1:S:641:G:H8	1.66	0.59
2:A:546:SER:O	2:A:549:PRO:HD3	2.02	0.59
2:B:69:ASP:O	2:B:70:THR:HG22	2.02	0.59
2:B:471:ASP:OD1	2:B:481:SER:HA	2.03	0.58
2:A:396:LYS:NZ	2:A:396:LYS:HB3	2.18	0.58
2:B:551:ASP:HB2	2:B:552:PRO:CD	2.34	0.58
2:A:114:ARG:HH12	2:A:240:ARG:NH2	2.01	0.58
2:B:455:PHE:CD1	2:B:455:PHE:C	2.81	0.58
2:B:286:VAL:HG11	2:B:297:TYR:HB3	1.86	0.58
2:A:118:THR:HG22	2:A:128:LEU:CD2	2.29	0.58
2:B:258:PHE:HD2	2:B:320:ILE:HD11	1.69	0.58
1:S:665:G:H2'	1:S:666:U:C6	2.38	0.58
2:A:114:ARG:HH21	2:A:165:ILE:HD11	1.68	0.58
2:B:143:ALA:HA	2:B:149:ILE:HG22	1.83	0.58
2:B:288:GLU:CD	2:B:295:LYS:HD3	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:634:G:H4'	1:R:635:U:C5'	2.34	0.58
2:B:530:GLU:HG2	2:B:546:SER:HB2	1.86	0.58
1:S:607:A:C4	1:S:649:5MC:HM52	2.39	0.57
2:B:180:LYS:HB2	2:B:180:LYS:NZ	2.18	0.57
2:B:398:VAL:HG23	2:B:443:TYR:HB2	1.86	0.57
1:R:607:A:H3'	1:R:608:U:H5'	1.85	0.57
2:B:366:PHE:HZ	2:B:474:MET:SD	2.27	0.57
2:B:303:GLN:HE22	2:B:485:ARG:HE	1.52	0.57
1:S:676:A:C6	2:B:280:SER:HB2	2.40	0.57
2:A:200:THR:CG2	2:A:201:PRO:HD2	2.30	0.57
2:B:136:LEU:HD12	2:B:183:THR:OG1	2.04	0.57
2:B:137:ILE:CG2	2:B:184:VAL:HB	2.35	0.57
1:S:612:U:OP1	2:B:227:ASN:HB2	2.04	0.57
2:A:144:ASN:ND2	2:A:146:GLU:HG2	2.20	0.57
2:B:302:PRO:O	2:B:306:LYS:HD3	2.04	0.57
2:A:115:VAL:HG12	2:A:115:VAL:O	2.05	0.56
2:A:162:LEU:O	2:A:163:GLU:HB2	2.05	0.56
2:B:287:PHE:CZ	2:B:326:ALA:HA	2.40	0.56
2:B:392:PRO:HD3	2:B:440:THR:HB	1.88	0.56
2:A:548:PHE:CE2	2:B:309:LEU:HD21	2.39	0.56
2:B:497:LYS:HG2	2:B:498:ALA:N	2.20	0.56
1:R:659:U:O2'	1:R:660:U:H5'	2.06	0.56
2:B:80:LEU:HD13	2:B:81:ILE:N	2.20	0.56
1:R:648:U:C4	1:R:659:U:N3	2.74	0.56
2:B:378:GLU:O	2:B:382:LYS:HG2	2.06	0.56
2:A:169:ARG:HB3	2:A:193:LYS:HB2	1.88	0.56
2:B:228:LEU:HD13	2:B:544:ARG:HH11	1.71	0.56
2:B:450:LEU:HD23	2:B:467:SER:CB	2.35	0.56
2:B:432:LYS:O	2:B:435:ARG:HB3	2.05	0.56
2:A:320:ILE:HG23	2:A:341:LEU:HD23	1.87	0.56
2:A:366:PHE:CE1	2:A:474:MET:HE3	2.41	0.55
2:B:169:ARG:HH11	2:B:169:ARG:CG	2.19	0.55
2:B:351:TYR:HB2	2:B:523:ALA:HB2	1.87	0.55
2:B:453:ARG:NH1	2:B:469:SER:HB3	2.20	0.55
1:S:668:G:N3	1:S:668:G:H2'	2.20	0.55
2:B:286:VAL:CG1	2:B:297:TYR:HB3	2.37	0.55
2:B:303:GLN:HE22	2:B:485:ARG:NH2	2.05	0.55
1:R:634:G:O2'	1:R:635:U:P	2.64	0.55
2:B:474:MET:HB2	2:B:479:ILE:HG21	1.87	0.55
2:B:502:SER:OG	2:B:505:ASP:HB3	2.06	0.55
2:A:390:LYS:HD2	2:A:435:ARG:HE	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:LYS:HZ3	2:B:435:ARG:HH21	1.54	0.55
2:B:393:LYS:HD3	2:B:394:ASP:N	2.22	0.55
2:A:272:THR:HB	2:A:273:PRO:HD2	1.88	0.55
2:A:350:HIS:CE1	2:B:83:SER:O	2.59	0.55
2:A:520:PRO:HG3	2:B:165:ILE:HD13	1.89	0.55
2:B:303:GLN:HE22	2:B:485:ARG:HH21	1.54	0.55
1:S:635:U:H4'	2:B:121:GLN:NE2	2.22	0.55
2:A:243:THR:HG22	2:A:247:ILE:CD1	2.36	0.55
2:B:289:VAL:HG12	2:B:290:THR:O	2.06	0.55
2:B:417:GLY:O	2:B:419:PHE:N	2.40	0.55
2:B:489:HIS:CE1	2:B:512:CYS:SG	3.00	0.55
2:A:392:PRO:HD3	2:A:440:THR:CB	2.36	0.55
1:S:676:A:N1	2:B:280:SER:CB	2.70	0.54
2:A:111:PHE:CE2	2:A:189:ILE:HG12	2.42	0.54
2:A:363:VAL:CG2	2:A:397:MET:HE3	2.36	0.54
2:B:331:THR:HG22	2:B:332:HIS:N	2.21	0.54
1:S:666:U:H2'	1:S:667:C:C6	2.41	0.54
2:B:119:ARG:HG2	2:B:119:ARG:HH11	1.73	0.54
2:B:463:ASN:OD1	2:B:465:LYS:HB2	2.07	0.54
2:B:303:GLN:HE22	2:B:485:ARG:NE	2.05	0.54
1:R:674:C:H3'	1:R:675:C:C6	2.42	0.54
2:A:112:ARG:HH21	2:B:348:GLU:CD	2.16	0.54
2:A:259:ARG:HH22	2:B:269:GLU:CD	2.16	0.54
2:B:333:ARG:HD3	2:B:477:GLU:OE1	2.06	0.54
2:B:372:ARG:HB2	2:B:373:PHE:CD1	2.43	0.54
1:R:635:U:H4'	1:R:638:C:O2	2.06	0.54
2:B:196:THR:HG21	2:B:199:GLU:OE2	2.08	0.54
2:B:449:PRO:HA	2:B:466:TYR:HD1	1.72	0.54
1:R:674:C:H3'	1:R:675:C:C5	2.43	0.54
2:A:450:LEU:O	2:A:451:GLU:HB2	2.08	0.54
2:A:486:ILE:CD1	2:A:495:ARG:HG3	2.38	0.54
2:B:268:THR:HG22	2:B:269:GLU:O	2.07	0.54
2:B:361:LEU:O	2:B:365:ILE:HG13	2.08	0.54
2:A:117:ASN:HA	2:A:162:LEU:HD21	1.90	0.54
2:B:419:PHE:HE1	2:B:466:TYR:CZ	2.26	0.54
1:R:627:G:C2	1:R:644:A:C2	2.95	0.54
2:A:548:PHE:HE2	2:B:309:LEU:HD21	1.73	0.54
2:B:462:ALA:O	2:B:463:ASN:HB2	2.07	0.54
2:B:527:ILE:HG22	2:B:528:GLY:N	2.23	0.54
2:B:354:VAL:CB	2:B:523:ALA:HB3	2.38	0.53
1:R:638:C:H5	1:R:639:G:N7	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:612:U:OP1	2:B:226:VAL:O	2.27	0.53
1:S:649:5MC:H2'	1:S:650:G:C8	2.43	0.53
2:A:419:PHE:CE1	2:A:466:TYR:CE1	2.89	0.53
1:R:650:G:O2'	1:R:651:G:H5'	2.08	0.53
2:B:226:VAL:O	2:B:227:ASN:CB	2.55	0.53
2:B:235:ARG:HG3	2:B:239:LEU:CD2	2.39	0.53
1:R:628:G:N2	1:R:643:C:C2	2.76	0.53
1:R:651:G:H2'	1:R:652:G:H8	1.73	0.53
2:B:110:LEU:HD11	2:B:167:LEU:HD11	1.89	0.53
1:R:608:U:C4	1:R:613:PSU:C2	2.96	0.53
2:A:166:VAL:HG23	2:A:168:VAL:HG23	1.90	0.53
2:A:303:GLN:HA	2:A:303:GLN:NE2	2.17	0.53
2:A:347:PHE:O	2:A:521:PRO:HG2	2.08	0.53
2:A:458:MET:HG2	2:A:484:GLN:HE22	1.70	0.53
2:B:118:THR:HG22	2:B:128:LEU:HD22	1.89	0.53
2:B:480:LEU:HD23	2:B:481:SER:N	2.24	0.53
2:B:551:ASP:HB2	2:B:552:PRO:HD2	1.91	0.53
2:A:354:VAL:HG21	2:A:523:ALA:HB3	1.90	0.53
2:A:460:ASP:HB3	2:A:463:ASN:O	2.10	0.52
2:A:134:ALA:HB1	2:A:242:VAL:HG13	1.91	0.52
2:A:206:ILE:O	2:A:207:LEU:HB3	2.08	0.52
2:B:487:HIS:CE1	2:B:521:PRO:HB3	2.45	0.52
2:B:179:ILE:N	2:B:179:ILE:HD13	2.24	0.52
1:R:649:5MC:H2'	1:R:650:G:H8	1.75	0.52
2:A:93:ARG:HG3	2:A:110:LEU:CD1	2.29	0.52
2:B:386:VAL:HG11	2:B:538:ASP:CB	2.23	0.52
2:B:125:LEU:N	2:B:154:VAL:HG11	2.25	0.52
2:B:238:ASP:O	2:B:244:ASN:ND2	2.43	0.52
2:B:424:THR:CG2	2:B:428:LYS:HE3	2.30	0.52
2:B:534:MET:HE3	2:B:535:PHE:CZ	2.44	0.52
2:A:114:ARG:NH1	2:A:240:ARG:NH2	2.58	0.52
2:A:92:LYS:H	2:A:92:LYS:CD	2.22	0.52
2:A:287:PHE:CD1	2:A:326:ALA:HB2	2.45	0.52
2:B:306:LYS:HZ2	2:B:344:GLU:HB2	1.71	0.52
1:S:663:C:H2'	1:S:664:C:C6	2.45	0.52
2:A:74:ASN:O	2:A:193:LYS:HA	2.10	0.52
2:A:174:LYS:H	2:A:174:LYS:HD2	1.74	0.52
2:A:232:LEU:HB3	2:A:554:ARG:NH1	2.25	0.52
2:A:338:PHE:HB2	2:A:530:GLU:OE1	2.10	0.52
2:A:404:GLU:O	2:A:407:GLU:HB2	2.10	0.52
2:B:69:ASP:HA	2:B:72:LYS:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:PRO:HG2	2:B:452:ILE:HG12	1.92	0.52
2:B:474:MET:HB2	2:B:479:ILE:CG2	2.39	0.52
2:B:534:MET:SD	2:B:542:ILE:HA	2.50	0.52
2:A:170:GLY:C	2:A:171:ILE:HD12	2.35	0.51
2:B:449:PRO:HG2	2:B:452:ILE:HD11	1.92	0.51
2:B:462:ALA:O	2:B:463:ASN:CB	2.58	0.51
1:R:638:C:H42	2:A:121:GLN:HA	1.76	0.51
1:R:638:C:C5	1:R:639:G:C8	2.97	0.51
1:S:620:C:C5'	1:S:621:A:H5'	2.40	0.51
2:B:402:TYR:CD2	2:B:449:PRO:HD3	2.45	0.51
1:R:665:G:H2'	1:R:666:U:C6	2.45	0.51
2:A:197:ILE:O	2:A:198:SER:HB2	2.10	0.51
2:A:533:VAL:CG1	2:A:545:ALA:HB1	2.40	0.51
2:B:104:ASP:O	2:B:107:LYS:HG2	2.10	0.51
2:A:344:GLU:OE1	2:A:344:GLU:HA	2.09	0.51
2:B:210:ASP:OD1	2:B:213:ARG:NH2	2.43	0.51
2:B:402:TYR:O	2:B:406:ILE:HG12	2.10	0.51
2:A:348:GLU:HB3	2:B:93:ARG:CZ	2.40	0.51
2:B:449:PRO:HG2	2:B:452:ILE:CG1	2.40	0.51
2:B:81:ILE:HG22	2:B:81:ILE:O	2.10	0.51
2:B:354:VAL:HB	2:B:523:ALA:HB3	1.93	0.51
2:A:77:LYS:O	2:A:78:LEU:HD23	2.10	0.51
2:A:179:ILE:H	2:A:185:GLN:HB2	1.75	0.51
2:B:146:GLU:H	2:B:146:GLU:CD	2.19	0.51
2:B:149:ILE:HG23	2:B:153:MET:CE	2.38	0.51
2:A:122:GLY:O	2:A:124:THR:N	2.43	0.51
2:A:160:LEU:HD21	2:A:196:THR:CG2	2.41	0.51
2:A:238:ASP:C	2:A:240:ARG:H	2.17	0.51
2:A:116:HIS:O	2:A:162:LEU:HD22	2.10	0.51
2:B:246:ALA:HB1	2:B:376:GLU:CB	2.40	0.51
1:R:636:C:H4'	2:A:119:ARG:NH2	2.26	0.50
2:B:275:LEU:HD13	2:B:291:TYR:HE2	1.77	0.50
1:R:649:5MC:H2'	1:R:650:G:C8	2.46	0.50
2:A:119:ARG:HG2	2:A:119:ARG:O	2.10	0.50
2:B:257:LEU:HD23	2:B:364:PHE:CE2	2.46	0.50
2:A:253:GLY:HA3	2:A:373:PHE:CE2	2.46	0.50
2:A:402:TYR:CD2	2:A:449:PRO:HD3	2.46	0.50
1:R:634:G:O2'	1:R:635:U:OP2	2.28	0.50
2:A:171:ILE:HD12	2:A:171:ILE:N	2.26	0.50
2:A:334:HIS:CD2	2:A:531:ARG:NH2	2.80	0.50
2:A:396:LYS:HB3	2:A:396:LYS:HZ3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:LEU:O	2:B:434:VAL:HG23	2.11	0.50
2:B:480:LEU:HD23	2:B:480:LEU:C	2.36	0.50
2:A:141:VAL:HG12	2:A:154:VAL:HG22	1.94	0.50
2:B:115:VAL:HG23	2:B:164:SER:O	2.12	0.50
2:B:456:TYR:HA	2:B:486:ILE:HD12	1.94	0.50
1:R:666:U:H2'	1:R:667:C:H6	1.72	0.50
1:S:617:G:N2	1:S:657:A:H2'	2.27	0.50
2:A:177:GLU:HB2	2:A:178:PRO:HD2	1.94	0.50
2:A:213:ARG:NH2	2:A:224:PRO:HD2	2.27	0.50
2:B:141:VAL:HG22	2:B:191:ILE:HB	1.93	0.50
1:R:648:U:C4	1:R:659:U:C2	3.00	0.50
2:A:68:GLU:HB2	2:A:72:LYS:NZ	2.27	0.50
2:A:80:LEU:HD23	2:A:80:LEU:O	2.12	0.50
2:A:138:GLN:HG2	2:A:179:ILE:HD13	1.93	0.50
2:B:138:GLN:NE2	2:B:179:ILE:HD12	2.27	0.50
2:A:276:LEU:HD22	2:A:299:ALA:HA	1.93	0.50
1:S:634:G:O2'	1:S:635:U:P	2.70	0.49
2:A:131:ARG:NH2	2:A:240:ARG:HD3	2.26	0.49
2:A:200:THR:CG2	2:A:204:LEU:HD13	2.39	0.49
2:B:96:PHE:HE1	2:B:111:PHE:CE2	2.29	0.49
2:B:227:ASN:O	2:B:230:THR:HG22	2.12	0.49
2:B:429:PHE:CZ	2:B:433:LEU:HD11	2.47	0.49
2:B:463:ASN:C	2:B:465:LYS:H	2.20	0.49
2:A:114:ARG:NH1	2:A:240:ARG:CZ	2.75	0.49
2:A:347:PHE:HZ	2:A:484:GLN:OE1	1.95	0.49
2:A:472:PHE:CD2	2:A:480:LEU:HD13	2.47	0.49
2:B:381:ARG:HH22	2:B:388:GLU:HG2	1.77	0.49
2:B:121:GLN:HA	2:B:121:GLN:OE1	2.12	0.49
1:R:612:U:H5''	2:A:225:VAL:O	2.12	0.49
2:A:236:VAL:CG1	2:B:312:ALA:HB2	2.42	0.49
2:A:351:TYR:CE2	2:A:468:ASN:HB3	2.47	0.49
2:B:331:THR:O	2:B:543:ARG:NH2	2.43	0.49
2:B:453:ARG:HG2	2:B:469:SER:OG	2.13	0.49
2:B:458:MET:HE2	2:B:486:ILE:HG12	1.94	0.49
1:R:640:U:H2'	1:R:641:G:C8	2.46	0.49
2:A:88:ARG:HD3	2:B:350:HIS:HB3	1.94	0.49
2:B:142:LYS:O	2:B:149:ILE:HG21	2.13	0.49
1:R:621:A:C5	1:R:648:U:C4	3.00	0.49
2:A:111:PHE:HE2	2:A:189:ILE:HG12	1.77	0.49
2:B:76:GLY:O	2:B:195:TYR:HB3	2.12	0.49
2:B:485:ARG:HG2	2:B:485:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:667:C:C2	1:S:668:G:C8	3.00	0.49
2:B:96:PHE:HE1	2:B:111:PHE:CD2	2.31	0.49
1:R:641:G:H2'	1:R:642:C:C6	2.48	0.49
1:R:673:G:H2'	1:R:674:C:C6	2.48	0.49
2:B:110:LEU:HA	2:B:168:VAL:O	2.13	0.49
2:B:475:ARG:HG2	2:B:475:ARG:HH11	1.78	0.49
1:R:661:C:H2'	1:R:662:C:H6	1.77	0.49
2:B:398:VAL:HG11	2:B:438:TYR:HB3	1.95	0.49
2:A:345:MET:O	2:A:522:HIS:HA	2.13	0.48
2:A:424:THR:HG22	2:A:428:LYS:HE3	1.94	0.48
2:B:143:ALA:HA	2:B:149:ILE:CG2	2.43	0.48
2:B:449:PRO:CG	2:B:452:ILE:HD11	2.43	0.48
2:A:114:ARG:NH2	2:A:165:ILE:HD11	2.28	0.48
2:A:174:LYS:HA	2:A:187:LEU:HD23	1.95	0.48
2:A:197:ILE:O	2:A:197:ILE:CG1	2.61	0.48
2:A:488:ASP:OD2	2:A:490:ALA:HB3	2.13	0.48
2:B:350:HIS:HD2	2:B:351:TYR:CD1	2.31	0.48
2:B:351:TYR:CZ	2:B:468:ASN:OD1	2.66	0.48
2:A:82:GLN:NE2	2:B:461:PRO:HA	2.28	0.48
2:B:304:PHE:O	2:B:307:GLN:HB2	2.14	0.48
2:A:355:LEU:O	2:A:355:LEU:HD23	2.13	0.48
2:A:489:HIS:CE1	2:A:493:GLN:OE1	2.66	0.48
1:S:619:H2U:H3'	1:S:620:C:H5'	1.95	0.48
2:A:200:THR:HG22	2:A:201:PRO:CD	2.35	0.48
2:B:453:ARG:HH11	2:B:469:SER:HB3	1.78	0.48
2:A:149:ILE:HG23	2:A:153:MET:CE	2.43	0.48
2:B:539:LEU:HB3	2:B:544:ARG:HG2	1.94	0.48
2:A:114:ARG:NH1	2:A:240:ARG:NE	2.62	0.48
2:A:320:ILE:HG23	2:A:341:LEU:CD2	2.44	0.48
2:A:458:MET:HE3	2:B:82:GLN:HA	1.94	0.48
2:B:519:CYS:SG	2:B:520:PRO:HD2	2.54	0.48
1:R:632:PSU:C4	2:A:121:GLN:O	2.66	0.48
2:A:430:LEU:O	2:A:434:VAL:HG13	2.14	0.48
2:B:454:PRO:O	2:B:457:THR:CG2	2.62	0.48
2:B:474:MET:CE	2:B:479:ILE:HG21	2.39	0.48
2:B:453:ARG:CB	2:B:457:THR:HG21	2.30	0.47
1:S:606:G:O2'	1:S:607:A:H5'	2.15	0.47
2:A:112:ARG:HD3	2:A:197:ILE:CD1	2.45	0.47
2:A:318:TYR:HA	2:A:343:MET:HA	1.96	0.47
2:A:355:LEU:HD23	2:A:355:LEU:C	2.40	0.47
2:B:373:PHE:CD1	2:B:373:PHE:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:310:ILE:HG21	2:A:522:HIS:CG	2.49	0.47
2:A:334:HIS:CD2	2:A:334:HIS:N	2.81	0.47
2:B:350:HIS:CD2	2:B:351:TYR:CD1	3.02	0.47
2:B:350:HIS:CD2	2:B:351:TYR:HD1	2.31	0.47
2:A:235:ARG:NE	2:A:239:LEU:HD13	2.29	0.47
2:B:119:ARG:HG2	2:B:119:ARG:NH1	2.28	0.47
2:B:298:LEU:HD13	2:B:324:PHE:CD2	2.50	0.47
2:B:375:HIS:CE1	2:B:379:LEU:HD11	2.49	0.47
2:A:80:LEU:HD11	2:B:491:LEU:HD23	1.96	0.47
2:A:239:LEU:HB3	2:B:312:ALA:HB1	1.97	0.47
2:B:169:ARG:CG	2:B:169:ARG:NH1	2.77	0.47
2:B:267:PHE:CZ	2:B:316:ARG:HD2	2.49	0.47
2:B:270:VAL:O	2:B:271:HIS:HD2	1.97	0.47
2:B:470:TYR:CE2	2:B:482:GLY:C	2.92	0.47
1:S:619:H2U:O5'	1:S:619:H2U:H61	2.14	0.47
1:S:636:C:C4'	2:B:119:ARG:HH12	2.28	0.47
2:A:206:ILE:HG13	2:A:226:VAL:HG11	1.95	0.47
2:A:366:PHE:HE2	2:A:442:PHE:CD2	2.32	0.47
2:A:449:PRO:HD2	2:A:452:ILE:HD11	1.96	0.47
2:A:501:LEU:O	2:A:502:SER:HB3	2.14	0.47
2:B:117:ASN:H	2:B:162:LEU:CD2	2.25	0.47
2:B:265:LYS:HB2	2:B:267:PHE:CD1	2.50	0.47
1:S:675:C:H5'	2:B:327:GLU:OE2	2.14	0.47
2:A:101:GLU:O	2:A:102:ALA:HB3	2.15	0.47
2:A:115:VAL:HG12	2:A:162:LEU:HA	1.96	0.47
2:A:126:ALA:O	2:A:140:LEU:HA	2.14	0.47
2:A:274:LYS:HE3	2:A:322:PRO:HG2	1.97	0.47
2:A:366:PHE:CZ	2:A:474:MET:HE3	2.50	0.47
1:R:634:G:C8	2:A:125:LEU:HD22	2.49	0.47
2:A:137:ILE:HD13	2:A:189:ILE:HD13	1.97	0.47
2:A:517:TYR:HD2	2:B:237:ILE:HG13	1.80	0.47
2:B:487:HIS:ND1	2:B:521:PRO:HA	2.30	0.47
2:A:167:LEU:HB3	2:A:197:ILE:CG2	2.45	0.47
2:A:530:GLU:HB2	2:A:542:ILE:HD11	1.96	0.47
1:R:624:A:H2'	1:R:625:U:C6	2.50	0.46
1:S:660:U:P	1:S:661:C:H41	2.38	0.46
2:B:196:THR:HG22	2:B:196:THR:O	2.15	0.46
2:B:378:GLU:HB3	2:B:382:LYS:NZ	2.30	0.46
2:B:513:ASP:O	2:B:514:GLY:C	2.57	0.46
1:S:639:G:H2'	1:S:640:U:H6	1.80	0.46
2:A:193:LYS:HB3	2:A:195:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:409:LEU:HB3	2:A:414:LYS:HB2	1.97	0.46
2:B:79:PRO:O	2:B:80:LEU:CB	2.63	0.46
2:A:181:SER:O	2:A:182:ALA:HB2	2.15	0.46
2:A:300:GLN:O	2:A:301:SER:HB3	2.15	0.46
2:B:354:VAL:HG21	2:B:523:ALA:HB3	1.96	0.46
2:A:131:ARG:HH21	2:A:240:ARG:HD3	1.80	0.46
2:A:238:ASP:C	2:A:240:ARG:N	2.74	0.46
2:A:390:LYS:HD2	2:A:435:ARG:HH21	1.81	0.46
2:B:502:SER:C	2:B:504:GLU:H	2.23	0.46
2:A:87:ASP:O	2:A:89:THR:N	2.49	0.46
2:A:292:PHE:CD2	2:B:552:PRO:HA	2.51	0.46
2:A:309:LEU:O	2:A:314:PHE:HB2	2.16	0.46
2:A:429:PHE:O	2:A:432:LYS:N	2.48	0.46
2:B:194:ILE:HG23	2:B:194:ILE:O	2.15	0.46
2:A:509:LYS:HZ3	2:A:510:ASP:HA	1.81	0.46
2:A:121:GLN:CA	2:A:121:GLN:OE1	2.64	0.46
2:A:486:ILE:HB	2:A:492:LEU:HD13	1.97	0.46
2:B:369:LEU:N	2:B:370:PRO:CD	2.79	0.46
2:B:470:TYR:CE2	2:B:482:GLY:HA3	2.51	0.46
2:B:534:MET:SD	2:B:542:ILE:CA	3.04	0.46
2:A:238:ASP:O	2:A:241:THR:HG23	2.16	0.46
1:S:658:A:H1'	1:S:660:U:OP2	2.15	0.45
2:A:210:ASP:O	2:A:226:VAL:HG23	2.16	0.45
2:A:489:HIS:NE2	2:A:512:CYS:SG	2.89	0.45
2:B:424:THR:O	2:B:428:LYS:HG3	2.16	0.45
2:A:333:ARG:HB2	2:A:334:HIS:HD2	1.81	0.45
2:B:171:ILE:HD12	2:B:192:THR:HG22	1.98	0.45
2:B:335:MET:CE	2:B:542:ILE:HD13	2.46	0.45
2:B:345:MET:CE	2:B:357:THR:HG21	2.46	0.45
2:B:358:LEU:HD12	2:B:361:LEU:HD13	1.98	0.45
1:S:630:G:C5	1:S:631:C:C5	3.04	0.45
2:B:449:PRO:HG2	2:B:452:ILE:CD1	2.46	0.45
1:S:631:C:H2'	1:S:632:PSU:O4'	2.16	0.45
2:A:141:VAL:O	2:A:154:VAL:HG22	2.16	0.45
2:A:179:ILE:O	2:A:185:GLN:HB3	2.16	0.45
2:A:446:ASP:OD1	2:A:447:LYS:HD2	2.16	0.45
2:B:205:PRO:C	2:B:206:ILE:HG23	2.41	0.45
2:B:233:ASP:CG	2:B:554:ARG:HH22	2.24	0.45
2:A:292:PHE:HZ	2:B:327:GLU:O	2.00	0.45
2:A:111:PHE:CE1	2:A:130:LEU:HD23	2.52	0.45
2:A:144:ASN:CG	2:A:145:LYS:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:335:MET:HE1	2:A:530:GLU:HG2	1.99	0.45
2:B:111:PHE:HE2	2:B:189:ILE:HG13	1.81	0.45
2:B:172:VAL:HG22	2:B:189:ILE:CD1	2.47	0.45
2:B:270:VAL:HG11	2:B:317:VAL:CG2	2.46	0.45
2:B:406:ILE:HG23	2:B:416:ILE:CG1	2.46	0.45
2:B:410:ARG:O	2:B:412:ALA:N	2.49	0.45
2:B:496:MET:HB3	2:B:501:LEU:HD12	1.97	0.45
1:S:635:U:C4'	2:B:121:GLN:NE2	2.80	0.45
2:A:68:GLU:HB2	2:A:72:LYS:CE	2.47	0.45
2:A:94:VAL:HG22	2:A:95:LYS:O	2.17	0.45
2:A:354:VAL:O	2:A:357:THR:N	2.50	0.45
1:S:612:U:C5'	2:B:226:VAL:O	2.62	0.45
2:A:157:ALA:O	2:A:160:LEU:HB2	2.16	0.45
2:A:284:SER:HA	2:A:327:GLU:OE1	2.16	0.45
2:A:313:ASP:HB2	2:B:240:ARG:HG3	1.99	0.45
2:B:226:VAL:HG12	2:B:230:THR:CG2	2.43	0.45
2:B:372:ARG:HB2	2:B:373:PHE:HD1	1.80	0.45
1:S:619:H2U:OP2	1:S:619:H2U:H2'	2.16	0.45
1:S:666:U:H2'	1:S:667:C:H6	1.80	0.45
2:A:173:LYS:HG3	2:A:190:HIS:CG	2.52	0.45
2:A:486:ILE:HG21	2:A:492:LEU:N	2.32	0.45
2:B:305:ASN:HD22	2:B:305:ASN:HA	1.62	0.45
2:B:483:ALA:O	2:B:485:ARG:NH1	2.50	0.45
2:B:492:LEU:HD23	2:B:496:MET:SD	2.57	0.45
1:S:607:A:C2	1:S:649:5MC:C4	3.04	0.45
1:S:653:G:N2	1:S:662:C:C2	2.85	0.45
2:A:125:LEU:HD21	2:A:127:PHE:CE2	2.52	0.45
2:A:173:LYS:HG3	2:A:190:HIS:ND1	2.32	0.45
2:A:318:TYR:CD1	2:A:318:TYR:C	2.94	0.45
2:A:543:ARG:HG2	2:A:549:PRO:CB	2.47	0.45
2:B:242:VAL:HG12	2:B:379:LEU:HD23	1.96	0.45
2:B:274:LYS:O	2:B:276:LEU:HD13	2.16	0.45
1:R:661:C:H2'	1:R:662:C:C6	2.51	0.44
1:R:610:G:C2	1:R:611:U:C2	3.06	0.44
2:A:446:ASP:OD1	2:A:447:LYS:N	2.51	0.44
2:A:555:LEU:HG	2:B:277:GLY:HA2	1.99	0.44
2:B:112:ARG:HB3	2:B:112:ARG:NH1	2.27	0.44
2:B:403:LYS:C	2:B:403:LYS:HD2	2.42	0.44
2:B:473:PHE:HA	2:B:477:GLU:O	2.17	0.44
1:R:602:C:H2'	1:R:603:C:C6	2.52	0.44
1:R:630:G:C6	1:R:641:G:C6	3.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:453:ARG:CZ	2:A:469:SER:HB2	2.48	0.44
2:B:355:LEU:HD13	2:B:470:TYR:CD1	2.52	0.44
2:B:403:LYS:HG3	2:B:404:GLU:N	2.32	0.44
2:B:410:ARG:HG3	2:B:414:LYS:O	2.18	0.44
2:A:517:TYR:N	2:A:517:TYR:HD1	2.15	0.44
2:A:517:TYR:CD2	2:B:237:ILE:HG13	2.53	0.44
2:B:196:THR:HG21	2:B:199:GLU:CG	2.48	0.44
2:B:303:GLN:HE22	2:B:485:ARG:CZ	2.29	0.44
1:S:667:C:O2	1:S:668:G:C8	2.71	0.44
2:A:453:ARG:NH2	2:A:469:SER:HB2	2.32	0.44
2:B:251:GLN:HA	2:B:533:VAL:HG11	1.99	0.44
2:B:478:GLU:OE2	2:B:481:SER:HB2	2.18	0.44
2:A:93:ARG:HH11	2:A:93:ARG:HG2	1.83	0.44
2:A:280:SER:O	2:A:281:GLU:HB3	2.17	0.44
2:B:75:TYR:CD1	2:B:75:TYR:C	2.96	0.44
2:A:175:VAL:HG22	2:A:176:ASP:H	1.82	0.44
2:B:70:THR:HG23	2:B:71:ALA:N	2.30	0.44
2:B:335:MET:HE2	2:B:542:ILE:HD13	1.99	0.44
2:A:112:ARG:O	2:A:113:ALA:HB2	2.18	0.44
2:B:310:ILE:HD12	2:B:346:ALA:HB2	1.98	0.44
2:A:458:MET:HB3	2:A:484:GLN:HE21	1.83	0.44
2:A:482:GLY:O	2:A:483:ALA:HB2	2.17	0.44
2:A:487:HIS:H	2:A:487:HIS:CD2	2.35	0.44
2:B:403:LYS:HE2	2:B:404:GLU:CG	2.48	0.44
2:B:489:HIS:HE1	2:B:512:CYS:SG	2.41	0.44
1:R:638:C:C5	1:R:639:G:N7	2.84	0.43
2:A:145:LYS:C	2:A:146:GLU:HG3	2.42	0.43
2:A:160:LEU:HD21	2:A:196:THR:HG21	2.00	0.43
2:A:243:THR:HG21	2:A:384:TYR:HE1	1.82	0.43
1:R:611:U:O5'	1:R:611:U:H6	2.01	0.43
2:A:82:GLN:O	2:A:83:SER:CB	2.66	0.43
2:A:96:PHE:C	2:A:98:ASP:H	2.26	0.43
2:A:133:GLN:NE2	2:A:245:GLN:OE1	2.51	0.43
2:A:458:MET:HG2	2:A:484:GLN:HE21	1.77	0.43
2:A:458:MET:CB	2:A:484:GLN:HE21	2.30	0.43
2:B:101:GLU:HG2	2:B:174:LYS:HD3	2.00	0.43
2:B:345:MET:O	2:B:522:HIS:HB2	2.17	0.43
2:B:392:PRO:HD3	2:B:440:THR:CB	2.47	0.43
2:B:409:LEU:HD22	2:B:414:LYS:HG3	1.99	0.43
2:A:214:SER:C	2:A:216:ALA:H	2.27	0.43
2:A:333:ARG:HB2	2:A:334:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:GLY:O	2:B:195:TYR:HA	2.17	0.43
2:B:137:ILE:HG23	2:B:184:VAL:CB	2.47	0.43
2:B:145:LYS:HB2	2:B:146:GLU:OE1	2.17	0.43
2:B:410:ARG:C	2:B:412:ALA:N	2.70	0.43
2:A:105:SER:O	2:A:106:ASP:HB2	2.17	0.43
2:A:341:LEU:HB2	2:A:527:ILE:HB	2.00	0.43
1:R:617:G:C2	1:R:658:A:C4	3.07	0.43
1:R:631:C:C4	1:R:632:PSU:C2	3.07	0.43
2:B:114:ARG:O	2:B:130:LEU:HA	2.19	0.43
2:B:262:LEU:HD12	2:B:262:LEU:HA	1.81	0.43
1:S:634:G:H4'	1:S:635:U:O4'	2.19	0.43
2:A:84:ARG:C	2:A:86:SER:N	2.76	0.43
2:A:273:PRO:HD3	2:B:548:PHE:HB2	1.99	0.43
2:A:304:PHE:CD1	2:A:304:PHE:N	2.87	0.43
2:B:171:ILE:HD12	2:B:192:THR:CG2	2.48	0.43
2:B:270:VAL:HG21	2:B:317:VAL:HG22	2.00	0.43
2:B:276:LEU:HD12	2:B:276:LEU:HA	1.78	0.43
2:B:505:ASP:HB2	2:B:506:PRO:HD2	2.01	0.43
2:A:84:ARG:C	2:A:86:SER:H	2.26	0.43
2:A:100:ASP:O	2:A:104:ASP:N	2.52	0.43
2:A:128:LEU:O	2:A:138:GLN:HA	2.18	0.43
2:A:363:VAL:HG22	2:A:397:MET:CE	2.42	0.43
2:A:486:ILE:O	2:A:486:ILE:HG22	2.18	0.43
2:B:157:ALA:O	2:B:160:LEU:HB2	2.19	0.43
2:B:390:LYS:HZ2	2:B:435:ARG:HH21	1.65	0.43
2:B:448:PHE:HB2	2:B:453:ARG:HD3	2.00	0.43
2:A:131:ARG:NH1	2:A:208:LEU:HD12	2.33	0.43
2:A:317:VAL:O	2:A:343:MET:HA	2.19	0.43
2:A:320:ILE:HG12	2:A:341:LEU:HD22	1.99	0.43
2:B:381:ARG:NH2	2:B:388:GLU:HG2	2.33	0.43
2:B:400:LEU:HD12	2:B:445:LEU:HD12	2.01	0.43
2:B:472:PHE:CD1	2:B:480:LEU:HD22	2.54	0.43
2:B:108:GLU:HG2	2:B:171:ILE:HG13	2.01	0.43
2:B:138:GLN:HE21	2:B:179:ILE:HG13	1.84	0.43
2:B:354:VAL:CG2	2:B:523:ALA:HB3	2.49	0.43
2:B:484:GLN:HA	2:B:523:ALA:HA	2.00	0.43
1:S:641:G:H2'	1:S:642:C:C6	2.54	0.42
2:A:96:PHE:CZ	2:A:137:ILE:HG21	2.54	0.42
2:A:223:LEU:H	2:A:223:LEU:HG	1.64	0.42
2:A:237:ILE:HA	2:A:240:ARG:NH1	2.34	0.42
2:A:335:MET:CE	2:A:530:GLU:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:312:ALA:O	2:A:313:ASP:HB2	2.19	0.42
2:B:88:ARG:HH11	2:B:88:ARG:CG	2.32	0.42
2:B:91:GLN:HE22	2:B:169:ARG:HH22	1.66	0.42
2:B:95:LYS:O	2:B:96:PHE:C	2.61	0.42
2:B:474:MET:CE	2:B:532:VAL:HA	2.48	0.42
2:B:488:ASP:O	2:B:492:LEU:HB2	2.19	0.42
2:B:496:MET:HE1	2:B:503:PRO:HA	2.01	0.42
1:R:621:A:N6	1:R:646:A:H2'	2.32	0.42
1:S:619:H2U:H3'	1:S:620:C:C5'	2.50	0.42
2:A:362:PHE:CZ	2:A:479:ILE:HD12	2.54	0.42
2:B:258:PHE:HE1	2:B:361:LEU:HD11	1.85	0.42
2:B:276:LEU:HD22	2:B:299:ALA:HA	2.00	0.42
2:B:291:TYR:CD1	2:B:292:PHE:CD2	3.05	0.42
2:B:324:PHE:HD1	2:B:324:PHE:H	1.67	0.42
2:B:331:THR:CG2	2:B:332:HIS:N	2.82	0.42
2:B:335:MET:HE3	2:B:335:MET:HB2	1.83	0.42
2:B:339:THR:OG1	2:B:529:LEU:HD12	2.19	0.42
2:B:402:TYR:CE2	2:B:449:PRO:HD3	2.53	0.42
1:S:651:G:H2'	1:S:652:G:O4'	2.19	0.42
2:A:555:LEU:HD12	2:A:555:LEU:O	2.19	0.42
2:B:506:PRO:HG2	2:B:507:GLY:H	1.84	0.42
2:B:248:PHE:CE2	2:B:547:LEU:HD23	2.54	0.42
2:B:414:LYS:HD3	2:B:429:PHE:CE2	2.55	0.42
2:B:474:MET:HE1	2:B:532:VAL:HG13	2.01	0.42
1:R:665:G:C6	1:R:666:U:C4	3.07	0.42
2:A:406:ILE:HD13	2:A:417:GLY:O	2.19	0.42
2:A:517:TYR:CD2	2:B:237:ILE:CG1	3.02	0.42
2:B:223:LEU:HA	2:B:224:PRO:HD3	1.84	0.42
2:B:311:VAL:C	2:B:313:ASP:H	2.28	0.42
2:B:332:HIS:CE1	2:B:477:GLU:OE1	2.72	0.42
2:B:347:PHE:CZ	2:B:521:PRO:HB2	2.55	0.42
1:R:611:U:O2'	1:R:612:U:H5'	2.20	0.42
1:R:624:A:C5	1:R:625:U:C4	3.07	0.42
1:S:639:G:H2'	1:S:640:U:O4'	2.20	0.42
1:S:676:A:H62	2:B:281:GLU:C	2.25	0.42
2:B:201:PRO:O	2:B:202:GLU:C	2.63	0.42
2:B:343:MET:SD	2:B:343:MET:O	2.78	0.42
2:B:443:TYR:CZ	2:B:473:PHE:CD2	3.08	0.42
2:B:527:ILE:CG2	2:B:528:GLY:N	2.82	0.42
2:A:315:GLU:OE2	2:A:346:ALA:HB3	2.19	0.42
2:B:375:HIS:NE2	2:B:379:LEU:HD11	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:612:U:O4'	2:A:224:PRO:HB3	2.19	0.42
2:A:406:ILE:HG23	2:A:416:ILE:HG23	2.01	0.42
2:A:550:ARG:HH21	2:B:276:LEU:HD12	1.84	0.42
2:B:71:ALA:O	2:B:74:ASN:N	2.53	0.42
2:B:243:THR:HG21	2:B:383:GLN:NE2	2.34	0.42
2:B:285:SER:HB2	2:B:327:GLU:OE1	2.19	0.42
2:B:290:THR:HG22	2:B:291:TYR:N	2.33	0.42
2:B:550:ARG:HH11	2:B:550:ARG:CG	2.33	0.42
1:R:654:5MU:C2'	1:R:655:PSU:H5''	2.49	0.42
2:A:69:ASP:OD2	2:A:71:ALA:HB3	2.20	0.42
2:A:89:THR:HB	2:A:91:GLN:HG3	2.01	0.42
2:A:392:PRO:HD3	2:A:440:THR:HB	2.01	0.42
2:A:531:ARG:NH1	3:A:701:ATP:O2G	2.53	0.42
2:B:143:ALA:HA	2:B:149:ILE:O	2.19	0.42
1:R:611:U:C2'	1:R:612:U:H5'	2.50	0.41
1:S:635:U:C4'	2:B:121:GLN:HE21	2.33	0.41
1:S:641:G:C6	1:S:642:C:C4	3.08	0.41
2:A:487:HIS:CD2	2:A:487:HIS:N	2.88	0.41
2:B:228:LEU:HD22	2:B:544:ARG:NH1	2.35	0.41
2:B:239:LEU:HD13	2:B:239:LEU:HA	1.93	0.41
2:B:331:THR:HG22	2:B:333:ARG:H	1.85	0.41
2:B:480:LEU:HD23	2:B:481:SER:C	2.45	0.41
2:B:486:ILE:O	2:B:492:LEU:HD12	2.19	0.41
2:B:542:ILE:C	2:B:544:ARG:N	2.77	0.41
2:A:156:TRP:CZ3	2:A:194:ILE:HG23	2.47	0.41
2:A:173:LYS:HA	2:A:173:LYS:CE	2.49	0.41
2:B:173:LYS:HA	2:B:173:LYS:HZ3	1.85	0.41
2:B:196:THR:CG2	2:B:199:GLU:HG2	2.50	0.41
1:S:615:A:H2'	1:S:616:H2U:H62	2.02	0.41
2:A:75:TYR:CB	2:A:153:MET:HG3	2.49	0.41
2:A:301:SER:C	2:A:303:GLN:H	2.29	0.41
2:A:487:HIS:CE1	2:A:521:PRO:HB3	2.55	0.41
2:A:519:CYS:HA	2:A:520:PRO:HD3	1.85	0.41
2:B:69:ASP:O	2:B:70:THR:CG2	2.67	0.41
2:B:401:THR:HA	2:B:446:ASP:O	2.20	0.41
2:B:539:LEU:O	2:B:541:ASN:N	2.53	0.41
1:R:628:G:C2	1:R:643:C:C2	3.07	0.41
2:A:76:GLY:O	2:A:195:TYR:HA	2.20	0.41
2:A:291:TYR:O	2:A:294:GLY:N	2.54	0.41
2:B:341:LEU:HB2	2:B:527:ILE:HB	2.02	0.41
1:R:623:A:H2'	1:R:624:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:634:G:H4'	1:R:635:U:C4'	2.50	0.41
2:A:229:ASP:O	2:A:232:LEU:N	2.53	0.41
2:A:304:PHE:N	2:A:304:PHE:HD1	2.19	0.41
2:A:331:THR:O	2:A:543:ARG:NH2	2.52	0.41
2:B:472:PHE:HD1	2:B:480:LEU:HD22	1.86	0.41
2:B:494:GLU:HA	2:B:497:LYS:HD3	2.01	0.41
1:R:676:A:N6	2:A:281:GLU:OE1	2.54	0.41
2:A:213:ARG:NE	2:A:224:PRO:O	2.53	0.41
2:A:479:ILE:C	3:A:701:ATP:O3'	2.64	0.41
2:B:333:ARG:NH1	2:B:477:GLU:HB3	2.36	0.41
1:R:621:A:C4	1:R:648:U:C4	3.09	0.41
2:A:143:ALA:HA	2:A:149:ILE:HB	2.03	0.41
2:A:409:LEU:C	2:A:414:LYS:HB2	2.45	0.41
2:B:253:GLY:HA3	2:B:373:PHE:CZ	2.56	0.41
2:B:288:GLU:CG	2:B:295:LYS:HD3	2.51	0.41
2:A:243:THR:O	2:A:246:ALA:HB3	2.21	0.41
2:A:474:MET:SD	2:A:479:ILE:HD13	2.61	0.41
2:B:138:GLN:HE21	2:B:179:ILE:CD1	2.33	0.41
2:B:361:LEU:O	2:B:361:LEU:HD23	2.20	0.41
1:R:601:U:O4	2:A:330:ASN:HB2	2.21	0.41
1:R:630:G:C6	1:R:631:C:C4	3.08	0.41
1:R:631:C:O2'	1:R:632:PSU:H5''	2.20	0.41
1:S:618:G:C4	1:S:657:A:C2	3.09	0.41
1:S:674:C:C5	1:S:675:C:C5	3.09	0.41
2:A:111:PHE:HE1	2:A:130:LEU:HD23	1.86	0.41
2:A:150:SER:O	2:A:154:VAL:HG23	2.21	0.41
2:A:204:LEU:H	2:A:204:LEU:CD2	2.32	0.41
2:A:223:LEU:HA	2:A:224:PRO:HD3	1.89	0.41
2:A:377:ILE:HD12	2:A:536:TYR:HE2	1.86	0.41
2:A:458:MET:HE3	2:B:81:ILE:O	2.21	0.41
2:A:517:TYR:CD2	2:B:237:ILE:CD1	3.03	0.41
2:B:71:ALA:O	2:B:73:ASP:N	2.54	0.41
2:B:196:THR:HG21	2:B:199:GLU:HG2	2.03	0.41
2:B:331:THR:HB	2:B:334:HIS:HB2	2.02	0.41
2:B:346:ALA:HA	2:B:522:HIS:HB3	2.03	0.41
2:B:390:LYS:HB2	2:B:441:ASP:OD2	2.21	0.41
2:B:409:LEU:O	2:B:414:LYS:HG2	2.21	0.41
2:B:442:PHE:CZ	2:B:472:PHE:CD2	3.09	0.41
2:B:485:ARG:HG2	2:B:485:ARG:NH1	2.35	0.41
2:B:550:ARG:NH1	2:B:550:ARG:HG2	2.35	0.41
1:R:638:C:N3	2:A:121:GLN:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:209:GLU:O	2:A:210:ASP:C	2.64	0.41
2:A:244:ASN:O	2:A:248:PHE:HD2	2.03	0.41
2:A:291:TYR:O	2:A:292:PHE:C	2.64	0.41
2:A:305:ASN:O	2:A:309:LEU:HD12	2.22	0.41
2:A:513:ASP:C	2:A:515:PHE:N	2.76	0.41
2:B:320:ILE:HG12	2:B:341:LEU:HD22	2.02	0.41
2:B:463:ASN:HA	2:B:464:PRO:HD2	1.84	0.41
2:A:92:LYS:HD2	2:A:92:LYS:N	2.30	0.40
2:A:458:MET:HA	2:A:459:PRO:HD3	1.92	0.40
2:B:495:ARG:NE	2:B:495:ARG:HA	2.35	0.40
2:B:537:LEU:HB2	2:B:539:LEU:HD13	2.03	0.40
1:R:655:PSU:H2'	1:R:656:C:H5''	2.03	0.40
2:A:306:LYS:HE3	2:A:306:LYS:HB2	1.67	0.40
2:A:551:ASP:C	2:A:553:LYS:H	2.29	0.40
2:B:91:GLN:HE22	2:B:169:ARG:NH2	2.19	0.40
2:B:190:HIS:O	2:B:191:ILE:C	2.63	0.40
2:B:215:GLU:O	2:B:216:ALA:C	2.64	0.40
1:R:620:C:H6	1:R:620:C:P	2.45	0.40
1:R:637:1MG:C4	2:A:223:LEU:HD11	2.56	0.40
1:S:641:G:H2'	1:S:642:C:H6	1.85	0.40
2:A:121:GLN:HA	2:A:121:GLN:OE1	2.21	0.40
2:A:355:LEU:HD21	2:A:444:ILE:HD13	2.04	0.40
2:B:120:GLN:HA	2:B:126:ALA:HA	2.03	0.40
2:A:223:LEU:HA	2:A:223:LEU:HD23	1.72	0.40
2:A:488:ASP:HB3	2:A:491:LEU:HB3	2.02	0.40
2:B:75:TYR:HD2	2:B:153:MET:SD	2.44	0.40
2:B:123:ALA:O	2:B:151:LYS:HG2	2.21	0.40
2:B:236:VAL:CG2	2:B:237:ILE:N	2.84	0.40
2:B:463:ASN:O	2:B:465:LYS:N	2.55	0.40
2:B:554:ARG:HG3	2:B:554:ARG:HH11	1.86	0.40
2:A:68:GLU:HB2	2:A:72:LYS:HE3	2.02	0.40
2:A:297:TYR:CD1	2:A:297:TYR:N	2.89	0.40
2:A:483:ALA:O	2:A:523:ALA:CB	2.69	0.40
2:A:506:PRO:O	2:B:556:ARG:NH2	2.54	0.40
2:A:556:ARG:HD3	2:A:556:ARG:C	2.47	0.40
2:B:267:PHE:CZ	2:B:345:MET:HG2	2.56	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%)	395 (81%)	66 (14%)	27 (6%)	1	8
2	B	488/490 (100%)	412 (84%)	56 (12%)	20 (4%)	2	13
All	All	976/980 (100%)	807 (83%)	122 (12%)	47 (5%)	2	11

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	88	ARG
2	A	124	THR
2	B	80	LEU
2	B	162	LEU
2	B	206	ILE
2	B	226	VAL
2	B	227	ASN
2	B	418	ASP
2	B	463	ASN
2	B	540	LYS
2	A	123	ALA
2	A	186	ASN
2	A	198	SER
2	A	205	PRO
2	A	223	LEU
2	A	292	PHE
2	A	303	GLN
2	A	462	ALA
2	A	501	LEU
2	A	539	LEU
2	B	72	LYS
2	B	87	ASP
2	B	191	ILE
2	B	395	GLY
2	A	201	PRO

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Mol	Chain	Res	Type
2	A	549	PRO
2	A	552	PRO
2	B	97	VAL
2	B	545	ALA
2	A	71	ALA
2	A	85	ASP
2	A	206	ILE
2	A	296	ALA
2	B	117	ASN
2	B	547	LEU
2	A	133	GLN
2	A	146	GLU
2	A	207	LEU
2	A	235	ARG
2	B	312	ALA
2	B	411	ALA
2	A	97	VAL
2	A	301	SER
2	B	225	VAL
2	B	464	PRO
2	A	518	GLY
2	A	322	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%)	372 (87%)	55 (13%)	4	19
2	B	427/427 (100%)	351 (82%)	76 (18%)	2	10
All	All	854/854 (100%)	723 (85%)	131 (15%)	3	14

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	74	ASN

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Mol	Chain	Res	Type
2	A	82	GLN
2	A	85	ASP
2	A	86	SER
2	A	92	LYS
2	A	95	LYS
2	A	115	VAL
2	A	119	ARG
2	A	130	LEU
2	A	133	GLN
2	A	140	LEU
2	A	145	LYS
2	A	146	GLU
2	A	148	THR
2	A	160	LEU
2	A	167	LEU
2	A	174	LYS
2	A	177	GLU
2	A	192	THR
2	A	197	ILE
2	A	199	GLU
2	A	200	THR
2	A	206	ILE
2	A	207	LEU
2	A	230	THR
2	A	236	VAL
2	A	239	LEU
2	A	260	GLU
2	A	262	LEU
2	A	265	LYS
2	A	276	LEU
2	A	303	GLN
2	A	308	GLN
2	A	310	ILE
2	A	311	VAL
2	A	316	ARG
2	A	317	VAL
2	A	327	GLU
2	A	333	ARG
2	A	339	THR
2	A	349	GLU
2	A	361	LEU
2	A	376	GLU

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Mol	Chain	Res	Type
2	A	383	GLN
2	A	396	LYS
2	A	434	VAL
2	A	464	PRO
2	A	467	SER
2	A	487	HIS
2	A	509	LYS
2	A	517	TYR
2	A	529	LEU
2	A	539	LEU
2	A	555	LEU
2	A	556	ARG
2	B	72	LYS
2	B	78	LEU
2	B	86	SER
2	B	93	ARG
2	B	94	VAL
2	B	101	GLU
2	B	110	LEU
2	B	112	ARG
2	B	129	THR
2	B	135	SER
2	B	136	LEU
2	B	137	ILE
2	B	140	LEU
2	B	146	GLU
2	B	160	LEU
2	B	161	ASN
2	B	164	SER
2	B	169	ARG
2	B	173	LYS
2	B	179	ILE
2	B	180	LYS
2	B	183	THR
2	B	184	VAL
2	B	192	THR
2	B	193	LYS
2	B	196	THR
2	B	204	LEU
2	B	206	ILE
2	B	208	LEU
2	B	210	ASP

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Mol	Chain	Res	Type
2	B	219	GLU
2	B	226	VAL
2	B	236	VAL
2	B	239	LEU
2	B	240	ARG
2	B	249	ARG
2	B	262	LEU
2	B	276	LEU
2	B	286	VAL
2	B	305	ASN
2	B	313	ASP
2	B	316	ARG
2	B	318	TYR
2	B	324	PHE
2	B	330	ASN
2	B	339	THR
2	B	343	MET
2	B	345	MET
2	B	349	GLU
2	B	352	HIS
2	B	357	THR
2	B	361	LEU
2	B	367	SER
2	B	371	LYS
2	B	376	GLU
2	B	393	LYS
2	B	400	LEU
2	B	403	LYS
2	B	410	ARG
2	B	416	ILE
2	B	430	LEU
2	B	434	VAL
2	B	452	ILE
2	B	453	ARG
2	B	455	PHE
2	B	457	THR
2	B	470	TYR
2	B	474	MET
2	B	479	ILE
2	B	491	LEU
2	B	495	ARG
2	B	501	LEU

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Mol	Chain	Res	Type
2	B	520	PRO
2	B	529	LEU
2	B	537	LEU
2	B	550	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	82	GLN
2	A	117	ASN
2	A	120	GLN
2	A	133	GLN
2	A	185	GLN
2	A	244	ASN
2	A	251	GLN
2	A	271	HIS
2	A	303	GLN
2	A	305	ASN
2	A	332	HIS
2	A	334	HIS
2	A	350	HIS
2	A	352	HIS
2	A	383	GLN
2	A	426	ASN
2	A	468	ASN
2	A	484	GLN
2	B	82	GLN
2	B	91	GLN
2	B	121	GLN
2	B	303	GLN
2	B	305	ASN
2	B	308	GLN
2	B	350	HIS
2	B	352	HIS
2	B	383	GLN
2	B	489	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	74/75 (98%)	17 (22%)	1 (1%)
1	S	74/75 (98%)	17 (22%)	2 (2%)
All	All	148/150 (98%)	34 (22%)	3 (2%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	606	G
1	R	608	U
1	R	612	U
1	R	617	G
1	R	618	G
1	R	621	A
1	R	632	PSU
1	R	633	U
1	R	634	G
1	R	635	U
1	R	637	1MG
1	R	648	U
1	R	650	G
1	R	651	G
1	R	652	G
1	R	656	C
1	R	676	A
1	S	609	A
1	S	611	U
1	S	617	G
1	S	619	H2U
1	S	620	C
1	S	623	A
1	S	626	G
1	S	633	U
1	S	634	G
1	S	635	U
1	S	648	U
1	S	649	5MC
1	S	652	G
1	S	653	G
1	S	661	C
1	S	672	A
1	S	676	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	634	G
1	S	633	U
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	5MC	R	649	1	19,22,23	0.71	1 (5%)	26,32,35	0.90	1 (3%)
1	1MG	R	637	1	23,26,27	0.47	0	33,39,42	1.03	3 (9%)
1	PSU	R	655	1	18,21,22	0.64	0	21,30,33	1.31	3 (14%)
1	H2U	S	619	1	18,21,22	0.52	0	19,30,33	0.72	0
1	PSU	S	655	1	18,21,22	0.90	1 (5%)	21,30,33	1.19	2 (9%)
1	H2U	R	616	1	18,21,22	0.52	0	19,30,33	1.15	2 (10%)
1	PSU	R	632	1	18,21,22	0.60	0	21,30,33	1.13	2 (9%)
1	PSU	S	613	1	18,21,22	0.62	0	21,30,33	1.22	3 (14%)
1	PSU	S	632	1	18,21,22	0.51	0	21,30,33	0.77	0
1	5MU	R	654	1	19,22,23	0.58	0	27,32,35	0.95	2 (7%)
1	H2U	R	619	1	18,21,22	0.63	0	19,30,33	0.87	1 (5%)
1	5MU	S	654	1	19,22,23	0.45	0	27,32,35	1.14	3 (11%)
1	PSU	R	613	1	18,21,22	0.62	0	21,30,33	1.17	2 (9%)
1	5MC	S	649	1	19,22,23	0.71	0	26,32,35	0.94	1 (3%)
1	H2U	S	616	1	18,21,22	0.44	0	19,30,33	0.76	1 (5%)
1	1MG	S	637	1	23,26,27	0.55	0	33,39,42	1.19	3 (9%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	655	PSU	O4'-C1'	-2.44	1.40	1.43
1	R	649	5MC	C5-C4	-2.12	1.42	1.44

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	637	1MG	C2-N1-C6	4.33	124.60	120.99
1	S	655	PSU	C6-C5-C4	3.49	120.53	118.17
1	R	637	1MG	N2-C2-N1	-3.41	116.05	118.79
1	S	654	5MU	C6-C5-C4	3.38	120.81	118.02
1	R	613	PSU	C6-C5-C4	3.23	120.35	118.17
1	R	632	PSU	O4'-C1'-C2'	3.21	109.59	105.15
1	S	613	PSU	O4'-C1'-C2'	3.21	109.59	105.15
1	R	637	1MG	C2-N1-C6	3.15	123.61	120.99
1	R	655	PSU	O4'-C1'-C2'	3.02	109.33	105.15
1	R	655	PSU	C6-C5-C4	2.97	120.18	118.17
1	S	655	PSU	O4'-C1'-C2'	2.79	109.00	105.15
1	S	654	5MU	C5M-C5-C6	-2.76	119.11	122.85
1	R	616	H2U	C5-C4-N3	-2.75	113.76	116.69
1	R	649	5MC	C5-C6-N1	-2.74	120.34	123.31
1	S	637	1MG	CM1-N1-C2	-2.69	117.92	120.70
1	R	654	5MU	C6-C5-C4	2.62	120.18	118.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	616	H2U	O4'-C1'-N1	2.55	112.77	109.30
1	R	632	PSU	C6-C5-C4	2.46	119.83	118.17
1	R	613	PSU	O4'-C1'-C2'	2.44	108.52	105.15
1	S	649	5MC	C5-C6-N1	-2.35	120.77	123.31
1	R	655	PSU	C6-N1-C2	-2.24	120.62	122.69
1	S	613	PSU	C3'-C2'-C1'	-2.22	99.06	101.69
1	S	613	PSU	C6-C5-C4	2.17	119.64	118.17
1	R	654	5MU	C5M-C5-C6	-2.16	119.93	122.85
1	S	616	H2U	C5-C4-N3	-2.12	114.43	116.69
1	R	619	H2U	C5-C4-N3	-2.08	114.47	116.69
1	S	654	5MU	C5-C6-N1	-2.04	121.09	123.31
1	R	637	1MG	CM1-N1-C2	-2.03	118.60	120.70
1	S	637	1MG	C2'-C1'-N9	-2.01	107.66	113.25

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	R	619	H2U	O4'-C1'-N1-C2
1	R	619	H2U	O4'-C1'-N1-C6
1	S	613	PSU	C2'-C1'-C5-C4
1	S	619	H2U	O4'-C4'-C5'-O5'
1	S	649	5MC	O4'-C4'-C5'-O5'
1	S	616	H2U	O4'-C4'-C5'-O5'
1	R	649	5MC	C3'-C4'-C5'-O5'
1	R	632	PSU	O4'-C1'-C5-C4
1	R	655	PSU	O4'-C1'-C5-C4
1	S	655	PSU	O4'-C1'-C5-C4
1	S	619	H2U	C4'-C5'-O5'-P
1	S	619	H2U	C3'-C4'-C5'-O5'
1	S	649	5MC	C3'-C4'-C5'-O5'
1	R	649	5MC	O4'-C4'-C5'-O5'
1	S	613	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	649	5MC	2	0
1	R	637	1MG	1	0
1	R	655	PSU	3	0

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
3	ATP	B	701	-	32,33,33	0.98	3 (9%)	48,52,52	0.74	0
3	ATP	A	701	-	32,33,33	1.20	3 (9%)	48,52,52	0.81	2 (4%)

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
3	ATP	B	701	-	-	4/22/38/38	0/3/3/3
3	ATP	A	701	-	-	10/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ATP	PB-O3A	4.46	1.64	1.59
3	A	701	ATP	PB-O3B	3.54	1.63	1.59
3	B	701	ATP	PB-O3B	3.07	1.62	1.59
3	B	701	ATP	PB-O3A	2.66	1.62	1.59
3	B	701	ATP	PA-O3A	2.27	1.61	1.59
3	A	701	ATP	PA-O3A	2.09	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ATP	C2'-C1'-N9	-2.52	107.04	113.30
3	A	701	ATP	O4'-C1'-N9	2.42	112.75	108.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	ATP	PG-O3B-PB-O1B
3	A	701	ATP	O4'-C4'-C5'-O5'
3	A	701	ATP	PB-O3B-PG-O1G
3	B	701	ATP	PB-O3A-PA-O2A
3	A	701	ATP	PA-O3A-PB-O2B
3	A	701	ATP	PB-O3A-PA-O2A
3	B	701	ATP	PA-O3A-PB-O2B
3	A	701	ATP	PG-O3B-PB-O2B
3	A	701	ATP	PB-O3B-PG-O2G
3	A	701	ATP	PB-O3B-PG-O3G
3	A	701	ATP	PA-O3A-PB-O1B
3	A	701	ATP	PB-O3A-PA-O1A
3	B	701	ATP	PB-O3A-PA-O1A
3	B	701	ATP	PA-O3A-PB-O1B

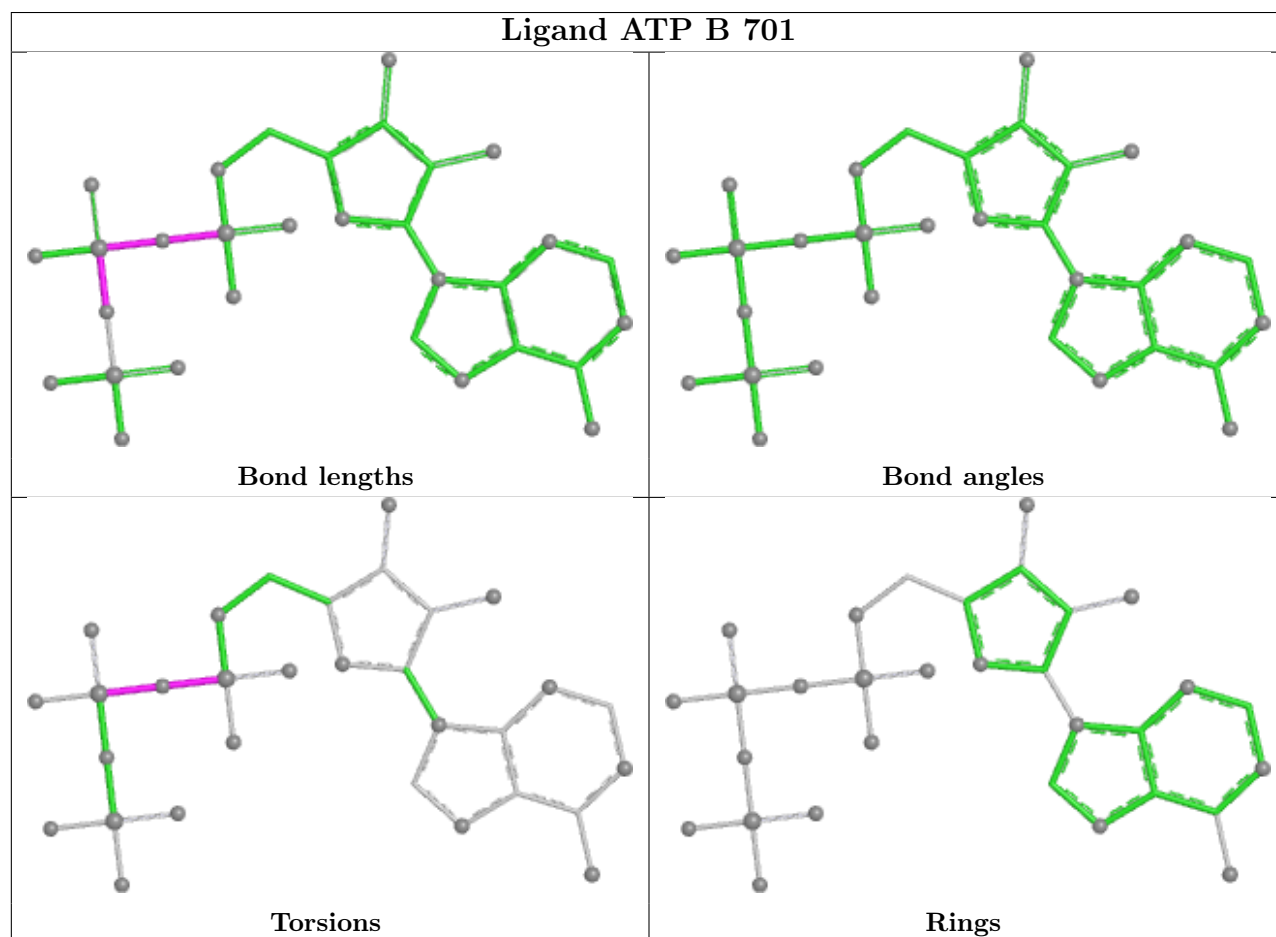
There are no ring outliers.

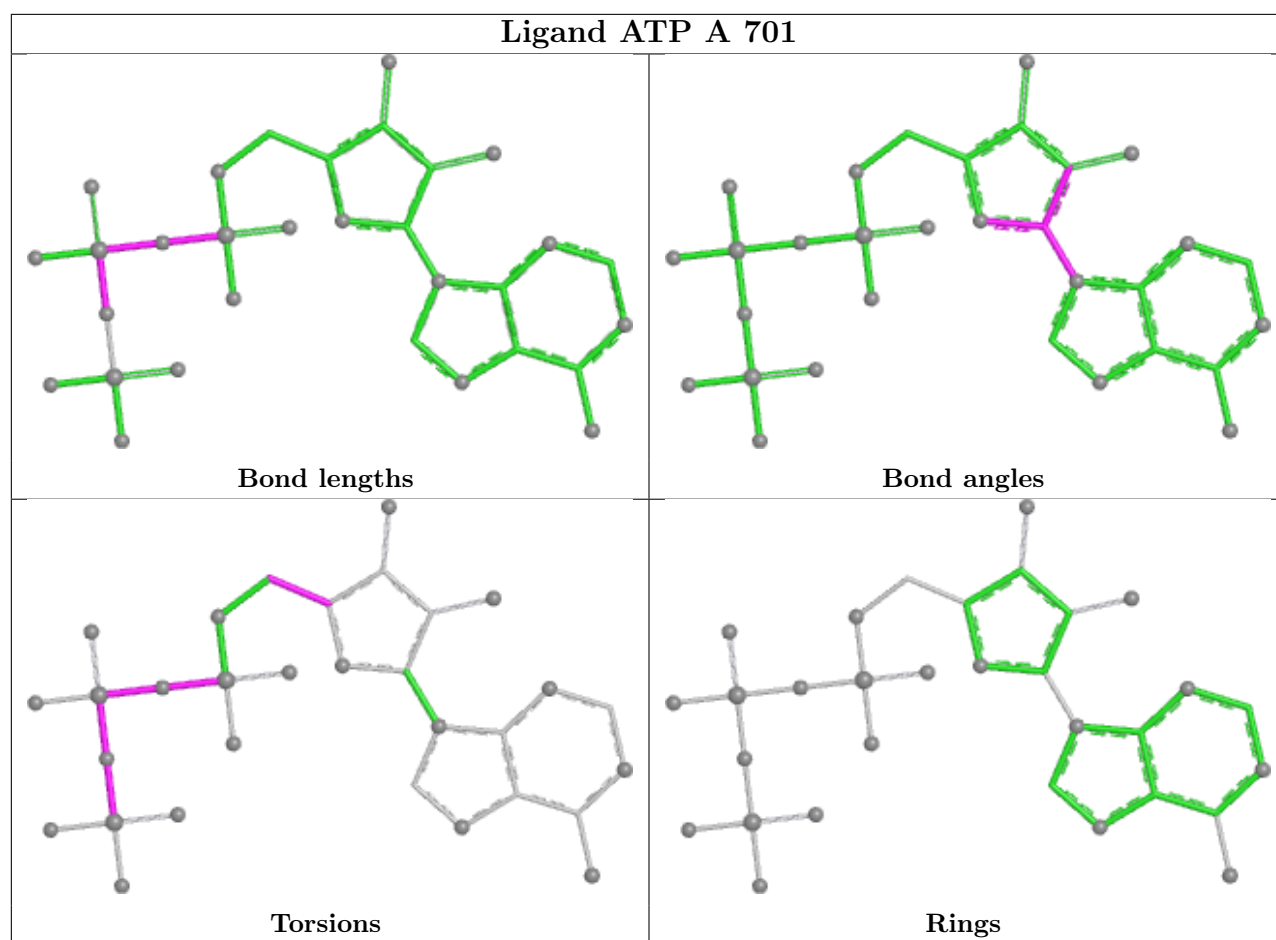
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	ATP	1	0
3	A	701	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.