



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:32 PM UTC

PDB ID : 3PJR / pdb_00003pjr
Title : HELICASE SUBSTRATE COMPLEX
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Deposited on : 1999-03-12
Resolution : 3.30 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

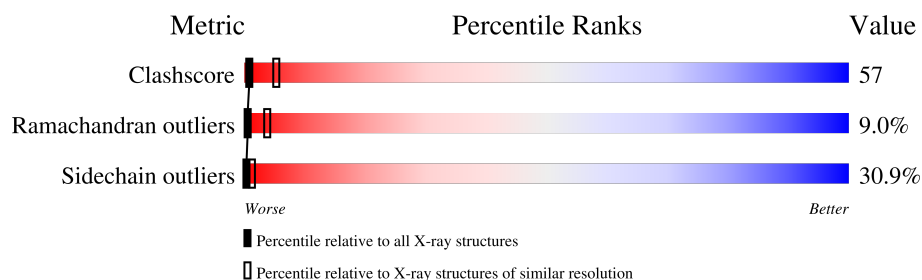
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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	Y	15	7% 53% 40%
2	Z	10	10% 90%
3	A	724	19% 39% 23% 8% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5765 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 DNA chain called 5'-D(*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	15	Total	C	N	O	P	0	0	0
			303	147	48	94	14			

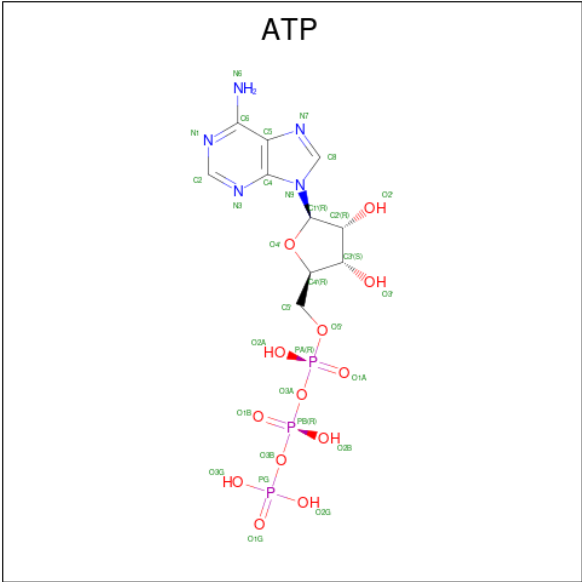
- Molecule 2 is a DNA chain called 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	10	Total	C	N	O	P	0	0	0
			201	96	39	57	9			

- Molecule 3 is a protein called HELICASE PCRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	646	Total	C	N	O	S	0	0	0
			5230	3304	916	991	19			

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



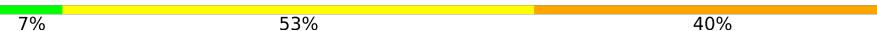
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

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

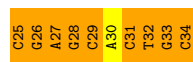
- Molecule 1: 5'-D(*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*TP*TP*T)-3'

Chain Y: 



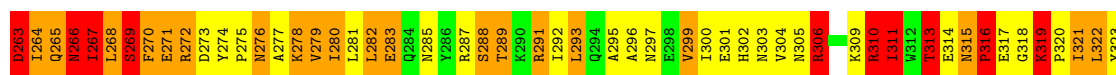
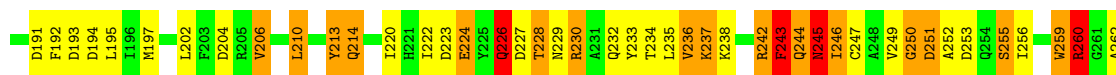
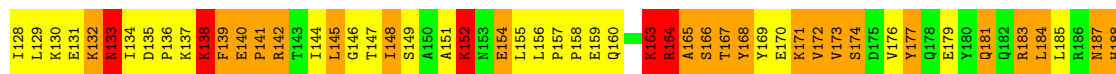
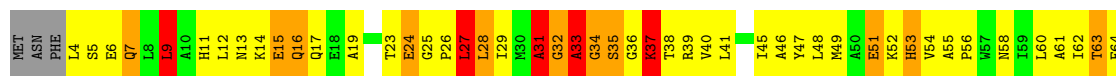
- Molecule 2: 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*C)-3'

Chain Z: 



- Molecule 3: HELICASE PCRA

Chain A: 



GLY	P634	R573	L445
GLY	S635	V574	G446
GLY	R636	V575	E447
ASP	F637	F576	L448
ASP	L638	L577	E449
GLN	M639	I578	M450
GLU	E640	G579	L451
LEU	I641	M580	G452
ASP	P642	E581	L453
ALA	A643	E582	G454
ALA	H644	G583	A455
PHE	L645	I584	K456
PRO	L646	F585	A457
SER	E647	F586	A458
PRO	T648	H587	G459
PRO	A649	N588	A460
ILE	A649	R589	L461
GLY	S650	S590	A462
ILE	R651	L591	S463
LYS	R652	E592	F464
ARG	GLN	D593	R465
LEU	ALA	D594	S466
LEU	GLY	D594	Q467
ALA	ALA	D595	L468
LYS	SER	E596	E469
PHE	ARG	M597	
ALA	PRO	E598	
ALA	ALA	E599	
PRO	VAL	E600	T472
ILE	SER	R601	Q473
GLU	GLY	R602	L474
LYS	ARG	L603	Q475
VAL	PRO	A604	E476
	GLN	Y605	Y477
	ALA	V606	V478
	SER	G607	
	GLY	I608	E482
	ALA	T609	L483
	VAL	R610	V484
	GLY	A611	E485
	SER	E612	E486
	TRP	E613	V487
	LYS	E614	L488
	VAL	L615	D489
	GLY	V616	K490
	ASP		
	ARG		Y493
	ALA	S619	
	ASN	A620	M496
	HIS	Q621	L497
	ARG	M622	
	LYS	R623	E500
	TRP	T624	R501
	GLY	L625	T502
	ILE	F626	I503
	GLY	G627	A504
	THR	N628	A505
	VAL	I629	M506
	VAL	G630	S507
	SER	M631	R508
	VAL	D632	L509
	ARG	P633	E510

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	105.12Å 105.12Å 380.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.30	Depositor
% Data completeness (in resolution range)	92.0 (10.00-3.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5765	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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: 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	Y	0.80	0/337	2.22	17/519 (3.3%)
2	Z	1.08	1/225 (0.4%)	2.85	25/345 (7.2%)
3	A	0.89	8/5319 (0.2%)	2.04	137/7184 (1.9%)
All	All	0.89	9/5881 (0.2%)	2.09	179/8048 (2.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Z	1	0
3	A	0	63
All	All	1	63

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	386	PHE	C-O	8.18	1.34	1.24
3	A	310	ARG	CD-NE	-7.40	1.35	1.46
3	A	383	GLY	N-CA	-6.60	1.37	1.45
3	A	652	ARG	NE-CZ	-6.33	1.26	1.33
3	A	652	ARG	CD-NE	-6.06	1.37	1.46
3	A	310	ARG	NE-CZ	-5.92	1.26	1.33
2	Z	28	DG	C2'-C1'	5.63	1.64	1.52
3	A	570	LEU	N-CA	-5.42	1.39	1.46
3	A	652	ARG	N-CA	-5.25	1.36	1.46

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	652	ARG	CD-NE-CZ	38.37	178.12	124.40
3	A	310	ARG	CD-NE-CZ	36.15	175.00	124.40
3	A	651	ARG	CA-C-N	24.40	165.61	121.70
3	A	651	ARG	C-N-CA	24.40	165.61	121.70
2	Z	28	DG	C8-N9-C1'	-18.09	99.87	127.00
2	Z	28	DG	C4-N9-C1'	17.98	153.97	127.00
3	A	386	PHE	N-CA-C	15.89	144.64	110.80
3	A	386	PHE	O-C-N	-14.05	103.90	122.59
3	A	379	GLN	CA-C-N	13.35	146.00	121.97
3	A	379	GLN	C-N-CA	13.35	146.00	121.97
3	A	315	ASN	CA-CB-CG	13.05	125.65	112.60
3	A	375	ASN	CA-CB-CG	13.04	125.64	112.60
2	Z	28	DG	N9-C1'-C2'	-12.79	94.32	113.50
3	A	365	ARG	CD-NE-CZ	12.51	141.91	124.40
3	A	382	GLY	CA-C-N	12.45	139.97	122.04
3	A	382	GLY	C-N-CA	12.45	139.97	122.04
3	A	388	ASP	CA-C-N	12.13	139.88	122.77
3	A	388	ASP	C-N-CA	12.13	139.88	122.77
1	Y	2	DC	O5'-C5'-C4'	12.09	128.93	110.80
2	Z	27	DA	P-O5'-C5'	11.66	137.49	120.00
3	A	383	GLY	N-CA-C	11.54	133.74	112.27
3	A	545	ASP	N-CA-C	11.53	129.40	109.80
3	A	384	LEU	N-CA-C	11.30	127.28	109.65
3	A	384	LEU	CA-C-N	11.07	138.45	122.40
3	A	384	LEU	C-N-CA	11.07	138.45	122.40
1	Y	5	DT	P-O3'-C3'	10.82	136.43	120.20
1	Y	2	DC	C5'-C4'-C3'	10.28	130.32	114.90
3	A	102	ARG	CD-NE-CZ	9.99	138.39	124.40
3	A	243	PHE	CA-CB-CG	9.54	123.34	113.80
2	Z	26	DG	P-O5'-C5'	-9.50	105.75	120.00
1	Y	11	DT	P-O3'-C3'	9.34	134.21	120.20
3	A	529	LYS	CA-C-N	9.32	139.33	121.54
3	A	529	LYS	C-N-CA	9.32	139.33	121.54
1	Y	10	DG	P-O3'-C3'	9.20	133.99	120.20
2	Z	33	DG	C4'-C3'-O3'	9.15	123.73	110.00
3	A	601	ARG	CD-NE-CZ	9.11	137.16	124.40
3	A	229	ASN	CA-CB-CG	-8.95	103.65	112.60
3	A	66	ASN	CA-C-O	-8.89	111.48	120.82
3	A	112	ASN	CA-CB-CG	8.76	121.36	112.60
2	Z	27	DA	C4'-C3'-O3'	8.76	123.13	110.00
3	A	544	LEU	O-C-N	-8.73	113.03	123.16
3	A	204	ASP	CA-CB-CG	8.70	121.30	112.60
3	A	400	ARG	CD-NE-CZ	-8.65	112.28	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	386	PHE	CA-C-O	-8.59	108.22	120.51
3	A	387	TYR	CA-CB-CG	8.30	128.83	113.90
2	Z	28	DG	O4'-C1'-C2'	-8.15	94.18	106.40
2	Z	27	DA	N9-C1'-C2'	-7.92	101.62	113.50
3	A	188	HIS	CA-CB-CG	-7.77	106.03	113.80
1	Y	5	DT	C2'-C3'-O3'	7.72	123.08	111.50
3	A	227	ASP	CA-C-N	7.70	133.04	122.19
3	A	227	ASP	C-N-CA	7.70	133.04	122.19
2	Z	29	DC	P-O5'-C5'	7.66	131.49	120.00
3	A	112	ASN	CB-CA-C	-7.62	97.29	110.17
3	A	529	LYS	CB-CA-C	7.60	123.56	110.72
3	A	626	PHE	CA-C-N	7.46	128.26	119.98
3	A	626	PHE	C-N-CA	7.46	128.26	119.98
3	A	31	ALA	CA-C-N	-7.44	112.78	119.92
3	A	31	ALA	C-N-CA	-7.44	112.78	119.92
3	A	111	ARG	CA-C-N	7.42	134.00	122.49
3	A	111	ARG	C-N-CA	7.42	134.00	122.49
3	A	92	PHE	CA-CB-CG	-7.33	106.47	113.80
2	Z	25	DC	P-O3'-C3'	7.25	131.08	120.20
1	Y	5	DT	N1-C1'-C2'	7.20	124.30	113.50
3	A	245	ASN	CA-C-O	-7.09	113.55	120.92
2	Z	27	DA	O4'-C1'-N9	7.06	118.98	108.40
3	A	260	ARG	CB-CA-C	6.96	122.32	110.56
3	A	569	GLY	CA-C-N	6.86	134.64	121.54
3	A	569	GLY	C-N-CA	6.86	134.64	121.54
3	A	626	PHE	CA-CB-CG	6.86	120.66	113.80
3	A	544	LEU	CB-CA-C	6.86	120.85	109.53
1	Y	11	DT	P-O5'-C5'	-6.81	109.79	120.00
3	A	585	PHE	N-CA-CB	6.77	122.42	110.37
2	Z	28	DG	C4'-C3'-O3'	6.74	120.11	110.00
3	A	542	SER	CA-C-N	6.69	134.31	121.54
3	A	542	SER	C-N-CA	6.69	134.31	121.54
2	Z	28	DG	N3-C4-C5	-6.62	118.47	128.40
3	A	164	ARG	CA-C-N	6.62	134.19	121.54
3	A	164	ARG	C-N-CA	6.62	134.19	121.54
3	A	37	LYS	CA-CB-CG	6.58	127.26	114.10
2	Z	34	DC	P-O5'-C5'	-6.51	110.23	120.00
3	A	524	ASN	CA-CB-CG	-6.50	106.10	112.60
3	A	32	GLY	N-CA-C	-6.49	103.77	111.36
1	Y	1	DG	P-O3'-C3'	6.46	129.89	120.20
3	A	427	ILE	CA-C-N	6.42	129.17	120.38
3	A	427	ILE	C-N-CA	6.42	129.17	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	29	DC	C2'-C3'-O3'	6.40	121.10	111.50
2	Z	31	DC	N1-C1'-C2'	-6.34	103.99	113.50
3	A	513	ASP	CA-CB-CG	-6.32	106.28	112.60
3	A	260	ARG	CA-C-O	6.30	126.93	119.56
3	A	529	LYS	CA-C-O	6.26	126.98	119.59
3	A	557	ASP	CB-CA-C	6.26	122.88	110.42
3	A	436	ASP	CB-CA-C	6.25	122.38	110.27
3	A	501	ARG	N-CA-C	-6.23	103.80	111.40
2	Z	33	DG	C5'-C4'-O4'	-6.22	100.07	109.40
3	A	317	GLU	N-CA-C	-6.22	102.77	110.41
1	Y	11	DT	C4'-C3'-O3'	6.17	119.25	110.00
2	Z	31	DC	P-O5'-C5'	-6.12	110.81	120.00
3	A	501	ARG	CA-C-N	6.10	133.19	121.54
3	A	501	ARG	C-N-CA	6.10	133.19	121.54
3	A	140	GLU	CB-CG-CD	6.04	122.86	112.60
3	A	529	LYS	N-CA-C	-6.01	105.13	112.88
3	A	527	ASP	N-CA-C	-6.00	100.78	110.32
3	A	408	ASP	CA-CB-CG	-5.99	106.61	112.60
2	Z	26	DG	N9-C1'-C2'	5.91	122.36	113.50
1	Y	9	DC	P-O3'-C3'	5.90	129.05	120.20
3	A	353	ASP	CA-CB-CG	-5.85	106.75	112.60
3	A	311	ILE	CA-C-O	-5.80	113.67	121.32
3	A	339	ARG	CD-NE-CZ	5.77	132.48	124.40
3	A	436	ASP	CA-C-N	5.77	132.56	121.54
3	A	436	ASP	C-N-CA	5.77	132.56	121.54
3	A	251	ASP	CA-C-N	5.71	132.45	121.54
3	A	251	ASP	C-N-CA	5.71	132.45	121.54
2	Z	32	DT	P-O5'-C5'	-5.71	111.44	120.00
3	A	383	GLY	O-C-N	-5.70	117.73	122.92
3	A	163	LYS	CA-C-O	-5.67	114.24	120.70
2	Z	28	DG	N3-C4-N9	5.66	134.49	126.00
3	A	385	LYS	N-CA-CB	5.66	120.90	112.30
3	A	317	GLU	CA-C-O	-5.65	115.55	121.99
3	A	126	LYS	CA-CB-CG	5.64	125.39	114.10
3	A	568	LYS	O-C-N	-5.64	115.09	122.59
3	A	572	PHE	CA-C-N	5.63	126.88	119.84
3	A	572	PHE	C-N-CA	5.63	126.88	119.84
3	A	528	ASP	CA-C-N	-5.58	113.89	122.60
3	A	528	ASP	C-N-CA	-5.58	113.89	122.60
3	A	634	PRO	CA-C-N	5.53	128.57	120.71
3	A	634	PRO	C-N-CA	5.53	128.57	120.71
2	Z	32	DT	C2'-C3'-O3'	5.53	119.80	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	399	LEU	CA-C-N	-5.52	111.50	120.72
3	A	399	LEU	C-N-CA	-5.52	111.50	120.72
3	A	512	LEU	CA-C-N	5.52	127.99	120.54
3	A	512	LEU	C-N-CA	5.52	127.99	120.54
3	A	227	ASP	CB-CA-C	5.51	119.98	111.28
3	A	251	ASP	N-CA-CB	5.49	120.45	110.95
3	A	37	LYS	N-CA-CB	5.49	118.17	109.82
3	A	132	LYS	CA-C-N	5.48	132.00	121.54
3	A	132	LYS	C-N-CA	5.48	132.00	121.54
3	A	541	ILE	O-C-N	-5.47	115.73	122.57
3	A	263	ASP	CA-CB-CG	5.47	118.07	112.60
3	A	247	CYS	CA-C-O	-5.45	114.63	120.46
3	A	285	ASN	CA-CB-CG	5.43	118.03	112.60
3	A	400	ARG	NH1-CZ-NH2	5.42	126.35	119.30
1	Y	2	DC	C2-N1-C1'	5.41	127.82	119.70
2	Z	27	DA	C5'-C4'-C3'	-5.41	106.79	114.90
3	A	27	LEU	O-C-N	-5.39	116.69	123.27
3	A	109	ILE	CA-C-O	-5.39	114.83	120.76
3	A	187	ASN	CA-CB-CG	5.39	117.99	112.60
3	A	386	PHE	N-CA-CB	-5.33	101.49	110.49
3	A	544	LEU	CA-C-O	-5.33	114.80	120.92
3	A	400	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	Y	2	DC	C5'-C4'-O4'	5.29	117.34	109.40
3	A	453	LEU	CA-C-N	-5.28	111.06	121.41
3	A	453	LEU	C-N-CA	-5.28	111.06	121.41
3	A	267	ILE	CB-CA-C	-5.27	102.64	111.29
3	A	259	TRP	CA-C-N	-5.25	114.25	122.65
3	A	259	TRP	C-N-CA	-5.25	114.25	122.65
3	A	538	LEU	N-CA-C	-5.24	105.57	111.28
3	A	598	GLU	CA-C-N	5.23	127.55	120.38
3	A	598	GLU	C-N-CA	5.23	127.55	120.38
3	A	226	GLN	CA-C-N	-5.22	114.28	122.79
3	A	226	GLN	C-N-CA	-5.22	114.28	122.79
3	A	101	ARG	CA-CB-CG	5.19	124.48	114.10
3	A	349	ARG	CA-CB-CG	5.17	124.45	114.10
3	A	454	GLY	N-CA-C	5.14	125.36	113.18
3	A	278	LYS	CA-C-O	-5.13	114.85	120.70
3	A	437	HIS	CA-C-N	5.13	131.33	121.54
3	A	437	HIS	C-N-CA	5.13	131.33	121.54
3	A	475	GLN	CB-CA-C	5.13	120.11	110.63
3	A	33	ALA	CA-C-O	-5.11	113.20	120.51
2	Z	26	DG	O5'-C5'-C4'	-5.09	103.16	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	306	ARG	CD-NE-CZ	5.08	131.51	124.40
1	Y	2	DC	C4'-C3'-O3'	5.06	117.58	110.00
3	A	154	GLU	N-CA-C	-5.05	106.70	112.92
1	Y	1	DG	C8-N9-C1'	5.05	134.58	127.00
1	Y	11	DT	C2-N1-C1'	-5.05	111.78	119.35
3	A	315	ASN	OD1-CG-ND2	-5.02	117.58	122.60
3	A	276	ASN	CA-CB-CG	5.01	117.61	112.60
3	A	280	ILE	CA-C-O	-5.01	116.03	121.19
1	Y	3	DA	C4-N9-C1'	5.00	134.56	127.05
3	A	269	SER	O-C-N	-5.00	116.35	122.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	Z	33	DG	C3'

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	106	ARG	Mainchain
3	A	112	ASN	Mainchain
3	A	117	ASP	Mainchain
3	A	123	SER	Mainchain
3	A	124	VAL	Mainchain
3	A	127	THR	Mainchain
3	A	152	LYS	Mainchain
3	A	159	GLU	Mainchain
3	A	16	GLN	Mainchain
3	A	192	PHE	Mainchain
3	A	210	LEU	Mainchain
3	A	213	TYR	Mainchain
3	A	214	GLN	Mainchain
3	A	226	GLN	Mainchain
3	A	24	GLU	Mainchain
3	A	243	PHE	Mainchain
3	A	245	ASN	Mainchain
3	A	250	GLY	Mainchain
3	A	266	ASN	Mainchain
3	A	268	LEU	Mainchain
3	A	27	LEU	Mainchain
3	A	271	GLU	Mainchain
3	A	275	PRO	Mainchain

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Mol	Chain	Res	Type	Group
3	A	282	LEU	Mainchain
3	A	299	VAL	Mainchain
3	A	304	VAL	Mainchain
3	A	31	ALA	Mainchain
3	A	311	ILE	Mainchain
3	A	313	THR	Mainchain
3	A	316	PRO	Peptide
3	A	322	LEU	Mainchain
3	A	332	GLU	Mainchain
3	A	346	ARG	Mainchain
3	A	362	ALA	Mainchain
3	A	369	GLU	Mainchain
3	A	372	LEU	Mainchain
3	A	38	THR	Mainchain
3	A	418	PRO	Mainchain
3	A	420	ARG	Mainchain
3	A	450	MET	Mainchain
3	A	451	ILE	Mainchain
3	A	454	GLY	Mainchain
3	A	47	TYR	Mainchain
3	A	476	GLU	Mainchain
3	A	487	VAL	Mainchain
3	A	514	GLU	Mainchain
3	A	523	GLU	Mainchain
3	A	541	ILE	Peptide,Mainchain
3	A	544	LEU	Peptide,Mainchain
3	A	554	ALA	Mainchain
3	A	56	PRO	Mainchain
3	A	577	LEU	Mainchain
3	A	580	MET	Mainchain
3	A	586	PRO	Mainchain
3	A	616	VAL	Mainchain
3	A	628	ASN	Mainchain
3	A	63	THR	Mainchain
3	A	633	PRO	Mainchain
3	A	66	ASN	Mainchain
3	A	79	LEU	Mainchain
3	A	9	LEU	Mainchain

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	Y	303	0	174	56	0
2	Z	201	0	113	35	0
3	A	5230	0	5232	568	0
4	A	31	0	12	7	0
All	All	5765	0	5531	644	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 57.

All (644) 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)
1:Y:12:DT:C6	1:Y:12:DT:H5''	1.65	1.31
1:Y:12:DT:H6	1:Y:12:DT:C5'	1.47	1.27
1:Y:5:DT:H2'	1:Y:6:DG:C8	1.77	1.19
3:A:31:ALA:HB3	3:A:251:ASP:HB2	1.36	1.08
1:Y:12:DT:C6	1:Y:12:DT:C5'	2.31	1.00
3:A:387:TYR:OH	3:A:518:VAL:HG11	1.62	0.99
3:A:577:LEU:HB3	3:A:580:MET:HE3	1.43	0.99
1:Y:4:DG:H2'	1:Y:5:DT:H6	1.30	0.96
1:Y:4:DG:H2'	1:Y:5:DT:C6	1.99	0.95
2:Z:31:DC:H2'	2:Z:32:DT:H71	1.46	0.93
3:A:163:LYS:O	3:A:164:ARG:HB2	1.68	0.93
3:A:265:GLN:HE21	3:A:265:GLN:N	1.65	0.93
3:A:135:ASP:HB3	3:A:138:LYS:HB2	1.49	0.92
3:A:164:ARG:HG3	3:A:164:ARG:HH11	1.33	0.92
3:A:474:LEU:HD22	3:A:478:VAL:CG2	2.00	0.92
3:A:31:ALA:HB1	3:A:37:LYS:HD3	1.52	0.91
3:A:474:LEU:HD22	3:A:478:VAL:HG21	1.53	0.90
3:A:265:GLN:H	3:A:265:GLN:NE2	1.70	0.89
1:Y:9:DC:H2''	1:Y:10:DG:H5'	1.52	0.89
3:A:116:LEU:HD23	3:A:120:ASP:HB3	1.55	0.88
1:Y:10:DG:N2	2:Z:26:DG:H22	1.71	0.87
3:A:289:THR:HG22	3:A:292:ILE:H	1.37	0.87
3:A:140:GLU:HG2	3:A:141:PRO:HD2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:100:LEU:HD22	3:A:104:ILE:HD12	1.54	0.87
1:Y:2:DC:H2'	1:Y:3:DA:C8	2.09	0.87
3:A:287:ARG:HH12	3:A:610:ARG:NH2	1.73	0.86
3:A:37:LYS:H	3:A:37:LYS:HZ2	1.24	0.86
2:Z:33:DG:H5''	2:Z:33:DG:H8	1.39	0.85
1:Y:10:DG:H22	2:Z:26:DG:H1	1.24	0.83
3:A:601:ARG:HG3	3:A:637:PHE:CE1	2.14	0.83
3:A:386:PHE:CE1	3:A:514:GLU:HB3	2.14	0.83
3:A:117:ASP:HB2	3:A:118:PRO:HD2	1.61	0.82
3:A:265:GLN:HE21	3:A:265:GLN:H	0.85	0.81
1:Y:4:DG:H2''	1:Y:5:DT:H5'	1.59	0.81
3:A:136:PRO:O	3:A:140:GLU:HG3	1.80	0.81
3:A:31:ALA:CB	3:A:37:LYS:HD3	2.09	0.81
3:A:62:ILE:HD12	3:A:222:ILE:HG12	1.62	0.81
3:A:562:MET:HE1	3:A:570:LEU:HD13	1.62	0.81
3:A:222:ILE:HD11	3:A:236:VAL:HG11	1.62	0.80
1:Y:14:DT:OP1	3:A:563:THR:HG21	1.81	0.80
3:A:391:GLU:OE1	3:A:508:ARG:HA	1.81	0.80
1:Y:14:DT:H1'	3:A:260:ARG:HH21	1.47	0.80
3:A:228:THR:HG22	3:A:266:ASN:ND2	1.96	0.80
3:A:37:LYS:H	3:A:37:LYS:NZ	1.79	0.80
2:Z:30:DA:H2''	2:Z:31:DC:H5''	1.63	0.80
3:A:386:PHE:CZ	3:A:514:GLU:HB3	2.18	0.80
3:A:83:ALA:O	3:A:85:GLU:N	2.15	0.79
3:A:144:ILE:HG23	3:A:173:VAL:HG22	1.63	0.79
1:Y:2:DC:H2'	1:Y:3:DA:H8	1.48	0.79
1:Y:12:DT:H6	1:Y:12:DT:H5'	1.43	0.79
3:A:563:THR:HG23	3:A:566:ALA:H	1.47	0.79
3:A:433:TYR:O	3:A:435:ALA:N	2.16	0.79
3:A:562:MET:HG3	3:A:566:ALA:HB3	1.66	0.78
3:A:164:ARG:HH11	3:A:164:ARG:CG	1.97	0.78
3:A:37:LYS:NZ	4:A:725:ATP:PB	2.57	0.77
2:Z:33:DG:H8	2:Z:33:DG:C5'	1.97	0.77
3:A:444:ALA:O	3:A:446:GLY:N	2.17	0.77
3:A:133:ASN:HD22	3:A:133:ASN:H	1.32	0.77
2:Z:33:DG:H5''	2:Z:33:DG:C8	2.19	0.77
3:A:112:ASN:HD22	3:A:532:ILE:HD11	1.48	0.77
3:A:433:TYR:CE1	3:A:436:ASP:HB2	2.20	0.77
3:A:187:ASN:OD1	3:A:408:ASP:OD2	2.03	0.76
3:A:265:GLN:O	3:A:267:ILE:N	2.19	0.76
3:A:230:ARG:HD3	3:A:263:ASP:OD2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:627:GLY:O	3:A:628:ASN:HB2	1.85	0.75
3:A:511:ASN:HD22	3:A:511:ASN:N	1.84	0.74
3:A:562:MET:HE1	3:A:570:LEU:CD1	2.17	0.74
3:A:37:LYS:HZ3	4:A:725:ATP:PB	2.11	0.74
3:A:433:TYR:CE2	3:A:451:ILE:HG13	2.22	0.74
2:Z:33:DG:C5'	2:Z:33:DG:C8	2.70	0.74
3:A:155:LEU:HD23	3:A:197:MET:HG3	1.70	0.74
3:A:133:ASN:HD22	3:A:133:ASN:N	1.86	0.73
3:A:368:GLU:HB3	3:A:378:TYR:CE2	2.22	0.73
3:A:265:GLN:HG2	3:A:266:ASN:N	2.04	0.73
3:A:289:THR:CG2	3:A:292:ILE:H	2.00	0.73
3:A:564:LEU:HB3	3:A:603:LEU:HD21	1.69	0.73
3:A:582:GLU:OE2	3:A:636:ARG:NE	2.18	0.73
3:A:388:ASP:OD1	3:A:393:LYS:HG2	1.89	0.73
3:A:67:LYS:HG2	3:A:68:ALA:H	1.54	0.72
3:A:25:GLY:H	3:A:245:ASN:ND2	1.87	0.72
3:A:413:ARG:HG2	3:A:413:ARG:HH11	1.53	0.72
3:A:606:VAL:HG23	3:A:610:ARG:CD	2.19	0.72
3:A:72:MET:HB3	3:A:89:ILE:HG21	1.71	0.72
3:A:606:VAL:HA	3:A:609:THR:HG22	1.71	0.72
3:A:563:THR:HG22	3:A:566:ALA:HB2	1.71	0.72
1:Y:9:DC:H2''	1:Y:10:DG:C5'	2.19	0.72
3:A:61:ALA:HB1	3:A:72:MET:HE2	1.71	0.72
1:Y:3:DA:H2'	1:Y:4:DG:H8	1.55	0.72
3:A:166:SER:OG	3:A:170:GLU:HB2	1.90	0.71
3:A:242:ARG:O	3:A:242:ARG:HG3	1.89	0.71
3:A:128:ILE:HG23	3:A:179:GLU:OE1	1.90	0.71
3:A:167:THR:O	3:A:168:TYR:C	2.33	0.71
3:A:77:GLN:HG3	3:A:84:ALA:HB3	1.72	0.71
3:A:332:GLU:O	3:A:336:VAL:HG23	1.91	0.71
3:A:67:LYS:HD2	3:A:544:LEU:HD22	1.73	0.70
3:A:344:VAL:HG21	3:A:351:TYR:CE1	2.26	0.70
3:A:397:ALA:O	3:A:401:VAL:HG23	1.90	0.70
1:Y:10:DG:H21	2:Z:26:DG:H22	1.38	0.70
3:A:12:LEU:HD22	3:A:16:GLN:HE21	1.56	0.70
3:A:243:PHE:O	3:A:245:ASN:N	2.25	0.70
3:A:601:ARG:HG3	3:A:637:PHE:HE1	1.56	0.70
3:A:337:ALA:HA	3:A:340:ILE:HD12	1.72	0.70
3:A:67:LYS:CD	3:A:544:LEU:HD22	2.21	0.69
3:A:564:LEU:HB3	3:A:603:LEU:CD2	2.22	0.69
3:A:562:MET:HE2	3:A:567:ALA:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:289:THR:HG22	3:A:292:ILE:N	2.07	0.69
3:A:73:ARG:O	3:A:77:GLN:HB2	1.93	0.69
3:A:349:ARG:NH1	3:A:613:GLU:OE1	2.25	0.69
3:A:412:LEU:O	3:A:413:ARG:C	2.35	0.68
3:A:557:ASP:OD1	3:A:558:ALA:N	2.25	0.68
3:A:586:PRO:HG3	3:A:637:PHE:CE2	2.28	0.68
3:A:31:ALA:HB1	3:A:37:LYS:CD	2.21	0.68
3:A:306:ARG:HH11	3:A:306:ARG:HG3	1.59	0.68
3:A:144:ILE:O	3:A:148:ILE:HG13	1.94	0.68
3:A:497:LEU:HB3	3:A:509:LEU:HD13	1.75	0.68
3:A:336:VAL:O	3:A:340:ILE:HG13	1.94	0.68
3:A:329:GLU:OE2	3:A:624:THR:HB	1.94	0.67
3:A:433:TYR:O	3:A:433:TYR:HD1	1.77	0.67
3:A:117:ASP:HB2	3:A:118:PRO:CD	2.25	0.67
1:Y:13:DT:OP1	3:A:361:ASN:OD1	2.13	0.67
3:A:391:GLU:O	3:A:394:ASP:HB2	1.95	0.67
2:Z:33:DG:H2''	2:Z:34:DC:C6	2.29	0.67
1:Y:3:DA:H2'	1:Y:4:DG:C8	2.29	0.67
2:Z:28:DG:H2''	2:Z:29:DC:O5'	1.95	0.67
3:A:581:GLU:O	3:A:582:GLU:C	2.37	0.67
3:A:116:LEU:HD23	3:A:120:ASP:CB	2.25	0.66
3:A:297:ASN:O	3:A:301:GLU:OE1	2.13	0.66
2:Z:26:DG:H2'	2:Z:27:DA:H5''	1.76	0.66
3:A:300:ILE:HG13	3:A:300:ILE:O	1.96	0.66
3:A:521:HIS:O	3:A:524:ASN:N	2.29	0.66
3:A:388:ASP:HB3	3:A:393:LYS:HZ3	1.61	0.65
3:A:359:ARG:HH12	3:A:600:GLU:CD	2.03	0.65
3:A:417:VAL:O	3:A:419:LYS:N	2.29	0.65
3:A:49:MET:HE1	3:A:83:ALA:HB1	1.77	0.65
3:A:145:LEU:O	3:A:146:GLY:C	2.38	0.65
3:A:567:ALA:HA	3:A:570:LEU:HD12	1.77	0.65
3:A:128:ILE:O	3:A:132:LYS:HB2	1.97	0.65
3:A:606:VAL:HG23	3:A:610:ARG:HD3	1.79	0.64
3:A:259:TRP:CD1	3:A:259:TRP:H	2.13	0.64
1:Y:10:DG:H2''	1:Y:11:DT:O5'	1.98	0.64
3:A:110:ASN:HD21	3:A:112:ASN:CG	2.04	0.64
3:A:139:PHE:CE2	3:A:172:VAL:HG11	2.33	0.64
3:A:371:LEU:HD23	3:A:378:TYR:HB3	1.79	0.63
3:A:416:ASN:O	3:A:419:LYS:HA	1.98	0.63
1:Y:8:DT:H2'	1:Y:9:DC:C6	2.33	0.63
3:A:110:ASN:ND2	3:A:112:ASN:HB2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:2:DC:H2''	1:Y:3:DA:O5'	1.98	0.63
3:A:265:GLN:HG2	3:A:266:ASN:H	1.64	0.63
3:A:585:PHE:HB3	3:A:586:PRO:HD3	1.79	0.63
3:A:326:ALA:HB1	3:A:331:ASP:HB3	1.79	0.63
1:Y:12:DT:H2''	1:Y:13:DT:O5'	1.99	0.62
3:A:12:LEU:CD2	3:A:16:GLN:HE21	2.12	0.62
3:A:163:LYS:O	3:A:164:ARG:CB	2.42	0.62
3:A:67:LYS:HG2	3:A:68:ALA:N	2.12	0.62
3:A:287:ARG:HH12	3:A:610:ARG:HH21	1.44	0.62
3:A:496:MET:HG3	3:A:497:LEU:N	2.14	0.62
3:A:637:PHE:HA	3:A:640:GLU:OE1	1.99	0.62
1:Y:9:DC:H2'	1:Y:10:DG:C8	2.35	0.62
3:A:72:MET:O	3:A:76:VAL:HG23	2.00	0.62
3:A:31:ALA:HB2	3:A:250:GLY:O	2.00	0.61
3:A:169:TYR:O	3:A:170:GLU:C	2.41	0.61
3:A:371:LEU:O	3:A:376:ILE:HG12	1.99	0.61
3:A:388:ASP:CG	3:A:393:LYS:HG2	2.25	0.61
3:A:371:LEU:HD12	3:A:376:ILE:HD11	1.82	0.61
3:A:641:ILE:HB	3:A:646:LEU:HD11	1.81	0.61
3:A:580:MET:HE2	3:A:585:PHE:HD2	1.65	0.61
3:A:336:VAL:HB	3:A:367:MET:HE1	1.81	0.61
3:A:299:VAL:HG11	3:A:608:ILE:CD1	2.30	0.61
1:Y:2:DC:C2'	1:Y:3:DA:H8	2.13	0.61
3:A:371:LEU:HD23	3:A:378:TYR:CB	2.30	0.61
3:A:28:LEU:HD23	3:A:279:VAL:HB	1.83	0.60
3:A:626:PHE:HD1	3:A:627:GLY:N	1.99	0.60
3:A:37:LYS:NZ	4:A:725:ATP:O2B	2.34	0.60
3:A:62:ILE:HD12	3:A:222:ILE:CG1	2.32	0.60
3:A:96:CYS:HB3	3:A:195:LEU:O	2.02	0.60
3:A:626:PHE:CD1	3:A:627:GLY:N	2.69	0.60
3:A:371:LEU:HG	3:A:376:ILE:HG13	1.83	0.60
2:Z:33:DG:C2	2:Z:34:DC:N3	2.70	0.60
3:A:306:ARG:HH11	3:A:306:ARG:CG	2.14	0.60
3:A:386:PHE:CD1	3:A:386:PHE:O	2.55	0.60
3:A:580:MET:HE2	3:A:585:PHE:CD2	2.36	0.60
3:A:573:PRO:HA	3:A:612:GLU:HG3	1.83	0.59
1:Y:14:DT:H1'	3:A:260:ARG:NH2	2.16	0.59
3:A:105:ASP:O	3:A:108:GLY:N	2.34	0.59
3:A:154:GLU:HG2	3:A:230:ARG:NH1	2.16	0.59
3:A:417:VAL:HB	3:A:418:PRO:HD3	1.85	0.59
3:A:267:ILE:O	3:A:270:PHE:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:417:VAL:HG12	3:A:418:PRO:CD	2.32	0.59
3:A:606:VAL:HG23	3:A:610:ARG:HD2	1.84	0.59
3:A:60:LEU:HD23	3:A:220:ILE:HG23	1.84	0.59
2:Z:32:DT:H2'	2:Z:33:DG:H5''	1.83	0.59
3:A:26:PRO:HG2	3:A:274:TYR:HB3	1.84	0.59
3:A:293:LEU:HD12	3:A:293:LEU:O	2.03	0.59
3:A:527:ASP:O	3:A:528:ASP:CB	2.51	0.59
3:A:541:ILE:O	3:A:541:ILE:HG23	2.02	0.59
3:A:210:LEU:HD11	3:A:214:GLN:HE21	1.67	0.59
3:A:585:PHE:C	3:A:585:PHE:HD1	2.11	0.59
3:A:625:LEU:O	3:A:626:PHE:C	2.45	0.59
1:Y:4:DG:H2'	1:Y:5:DT:H71	1.84	0.59
3:A:368:GLU:HB3	3:A:378:TYR:CZ	2.38	0.59
3:A:391:GLU:O	3:A:395:ILE:HD12	2.02	0.58
3:A:97:VAL:O	3:A:101:ARG:HB2	2.02	0.58
3:A:606:VAL:O	3:A:610:ARG:HD2	2.02	0.58
3:A:321:ILE:HG22	3:A:615:LEU:O	2.03	0.58
1:Y:12:DT:C6	1:Y:12:DT:C4'	2.86	0.58
3:A:330:ALA:HA	3:A:333:ALA:HB3	1.84	0.58
3:A:395:ILE:HD11	3:A:512:LEU:HD21	1.85	0.58
3:A:36:GLY:O	3:A:37:LYS:C	2.47	0.58
3:A:256:ILE:HD12	3:A:565:HIS:CD2	2.39	0.58
2:Z:25:DC:C2'	2:Z:26:DG:O4'	2.52	0.58
3:A:183:ARG:O	3:A:187:ASN:ND2	2.36	0.58
3:A:413:ARG:HH11	3:A:413:ARG:CG	2.15	0.58
3:A:82:GLY:O	3:A:84:ALA:N	2.37	0.58
3:A:318:GLY:O	3:A:319:LYS:HB2	2.03	0.58
3:A:438:GLU:O	3:A:439:LEU:HD23	2.04	0.58
1:Y:4:DG:O6	2:Z:31:DC:N4	2.34	0.58
3:A:521:HIS:O	3:A:522:PHE:C	2.47	0.58
1:Y:4:DG:C2	1:Y:5:DT:C2	2.92	0.57
3:A:392:ILE:HD11	3:A:511:ASN:HB3	1.85	0.57
3:A:474:LEU:HD22	3:A:478:VAL:HG22	1.84	0.57
3:A:417:VAL:CB	3:A:418:PRO:HD3	2.34	0.57
3:A:475:GLN:HG3	3:A:531:LEU:HD22	1.84	0.57
3:A:48:LEU:HD22	3:A:54:VAL:HG21	1.85	0.57
3:A:191:ASP:O	3:A:194:ASP:HB2	2.04	0.57
3:A:428:ASP:O	3:A:432:ARG:HB2	2.04	0.57
3:A:392:ILE:O	3:A:393:LYS:C	2.45	0.57
3:A:415:ILE:O	3:A:420:ARG:HD2	2.05	0.57
3:A:417:VAL:HG12	3:A:418:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:415:ILE:HG23	3:A:416:ASN:N	2.19	0.57
3:A:41:LEU:HD11	3:A:249:VAL:CG1	2.35	0.57
3:A:97:VAL:HG11	3:A:536:THR:CG2	2.35	0.57
3:A:585:PHE:C	3:A:585:PHE:CD1	2.81	0.57
3:A:45:ILE:CD1	3:A:72:MET:HE3	2.34	0.57
3:A:461:LEU:O	3:A:462:ALA:C	2.48	0.57
3:A:49:MET:HE1	3:A:83:ALA:CB	2.34	0.56
3:A:420:ARG:NH1	3:A:464:PHE:CD1	2.73	0.56
3:A:536:THR:HG22	3:A:536:THR:O	2.05	0.56
3:A:29:ILE:HB	3:A:249:VAL:HG12	1.86	0.56
3:A:110:ASN:ND2	3:A:112:ASN:OD1	2.21	0.56
3:A:291:ARG:HB2	3:A:645:LEU:HD21	1.87	0.56
3:A:265:GLN:HB2	3:A:268:LEU:HB2	1.88	0.56
3:A:446:GLY:HA2	3:A:465:ARG:HH11	1.68	0.56
3:A:466:SER:O	3:A:469:GLU:N	2.38	0.56
3:A:251:ASP:C	3:A:251:ASP:OD1	2.49	0.56
3:A:420:ARG:NH1	3:A:464:PHE:CE1	2.73	0.56
3:A:427:ILE:O	3:A:431:VAL:HG23	2.05	0.56
3:A:113:PHE:HA	3:A:188:HIS:O	2.05	0.56
3:A:417:VAL:CG1	3:A:418:PRO:HD3	2.35	0.56
3:A:140:GLU:CG	3:A:141:PRO:HD2	2.32	0.56
3:A:562:MET:HG3	3:A:566:ALA:CB	2.34	0.56
2:Z:31:DC:H2''	2:Z:32:DT:C6	2.40	0.56
3:A:61:ALA:HB1	3:A:72:MET:CE	2.36	0.56
1:Y:6:DG:N2	2:Z:30:DA:C2	2.73	0.56
3:A:313:THR:HG21	3:A:315:ASN:HB2	1.88	0.55
2:Z:31:DC:H2''	2:Z:32:DT:H6	1.71	0.55
2:Z:33:DG:C8	2:Z:33:DG:H5'	2.41	0.55
3:A:416:ASN:O	3:A:417:VAL:C	2.46	0.55
3:A:32:GLY:O	3:A:34:GLY:N	2.38	0.55
3:A:164:ARG:HG3	3:A:164:ARG:NH1	2.07	0.55
3:A:314:GLU:O	3:A:314:GLU:HG2	2.06	0.55
3:A:505:ALA:O	3:A:508:ARG:HB2	2.06	0.55
3:A:65:THR:O	3:A:68:ALA:HB3	2.07	0.55
3:A:228:THR:CG2	3:A:266:ASN:ND2	2.69	0.55
3:A:367:MET:HG2	3:A:561:LEU:HD21	1.89	0.55
3:A:579:GLY:O	3:A:584:ILE:HG22	2.06	0.55
3:A:127:THR:CG2	3:A:183:ARG:HH12	2.20	0.55
3:A:327:MET:HA	3:A:621:GLN:HG3	1.87	0.55
3:A:642:PRO:HB2	3:A:645:LEU:HB2	1.87	0.55
3:A:289:THR:HG22	3:A:292:ILE:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:37:LYS:HZ1	4:A:725:ATP:PB	2.30	0.54
3:A:283:GLU:O	3:A:311:ILE:HA	2.07	0.54
3:A:336:VAL:HG13	3:A:576:PHE:CD2	2.42	0.54
3:A:416:ASN:O	3:A:417:VAL:O	2.24	0.54
3:A:187:ASN:O	3:A:188:HIS:C	2.48	0.54
3:A:16:GLN:HG3	3:A:282:LEU:HD22	1.88	0.54
3:A:315:ASN:O	3:A:316:PRO:C	2.51	0.54
1:Y:13:DT:H1'	3:A:565:HIS:CE1	2.43	0.54
3:A:351:TYR:CZ	3:A:376:ILE:HG22	2.42	0.54
3:A:386:PHE:CZ	3:A:514:GLU:CB	2.89	0.54
3:A:117:ASP:OD1	3:A:117:ASP:N	2.35	0.54
3:A:303:ASN:ND2	3:A:598:GLU:HG2	2.22	0.54
3:A:467:GLN:OE1	3:A:490:LYS:HE3	2.08	0.54
3:A:530:SER:O	3:A:533:ALA:HB3	2.08	0.54
2:Z:25:DC:H2''	2:Z:26:DG:O4'	2.07	0.54
3:A:14:LYS:HA	3:A:17:GLN:HG3	1.90	0.54
3:A:233:TYR:O	3:A:234:THR:C	2.51	0.54
1:Y:2:DC:C2'	1:Y:3:DA:C8	2.87	0.54
3:A:349:ARG:HE	3:A:349:ARG:HA	1.72	0.54
3:A:577:LEU:CB	3:A:580:MET:HE3	2.29	0.54
1:Y:11:DT:C4	3:A:626:PHE:HB2	2.44	0.53
3:A:152:LYS:HB3	3:A:193:ASP:HB3	1.90	0.53
3:A:451:ILE:HG22	3:A:452:GLY:N	2.22	0.53
3:A:268:LEU:O	3:A:269:SER:C	2.49	0.53
1:Y:4:DG:N2	1:Y:5:DT:C2	2.76	0.53
3:A:125:MET:HG2	3:A:145:LEU:HD21	1.88	0.53
3:A:265:GLN:HA	3:A:268:LEU:HG	1.90	0.53
3:A:417:VAL:HG12	3:A:418:PRO:N	2.24	0.53
3:A:423:GLY:O	3:A:424:ALA:C	2.51	0.53
3:A:37:LYS:HE2	4:A:725:ATP:O2G	2.09	0.53
3:A:223:ASP:O	3:A:224:GLU:C	2.51	0.53
3:A:567:ALA:O	3:A:570:LEU:HB2	2.09	0.53
3:A:585:PHE:O	3:A:586:PRO:C	2.52	0.53
3:A:82:GLY:O	3:A:83:ALA:C	2.52	0.53
3:A:384:LEU:HD23	3:A:384:LEU:H	1.74	0.53
3:A:637:PHE:CD1	3:A:640:GLU:OE1	2.62	0.53
3:A:133:ASN:N	3:A:133:ASN:ND2	2.47	0.53
3:A:407:ASP:O	3:A:408:ASP:C	2.52	0.53
3:A:459:GLY:O	3:A:462:ALA:HB3	2.09	0.53
3:A:117:ASP:OD1	3:A:120:ASP:OD2	2.26	0.52
3:A:357:LEU:HD13	3:A:575:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:444:ALA:C	3:A:446:GLY:H	2.18	0.52
3:A:582:GLU:HG2	3:A:635:SER:HA	1.91	0.52
3:A:45:ILE:HD12	3:A:72:MET:HE3	1.91	0.52
3:A:269:SER:O	3:A:271:GLU:N	2.43	0.52
3:A:637:PHE:HD1	3:A:640:GLU:OE1	1.93	0.52
3:A:31:ALA:CB	3:A:250:GLY:O	2.58	0.52
3:A:222:ILE:CD1	3:A:236:VAL:HG11	2.36	0.52
3:A:407:ASP:OD1	3:A:409:LEU:HD12	2.09	0.52
2:Z:32:DT:C2'	2:Z:33:DG:H5''	2.40	0.52
3:A:33:ALA:HB2	3:A:605:TYR:OH	2.10	0.52
3:A:552:GLN:HG3	3:A:553:ALA:H	1.73	0.52
3:A:265:GLN:CG	3:A:266:ASN:N	2.73	0.52
3:A:577:LEU:HD23	3:A:580:MET:CE	2.40	0.52
3:A:340:ILE:O	3:A:344:VAL:HG23	2.10	0.52
3:A:437:HIS:CG	3:A:439:LEU:HD21	2.45	0.52
3:A:253:ASP:OD2	3:A:306:ARG:NH1	2.43	0.52
3:A:444:ALA:O	3:A:445:LEU:C	2.53	0.52
3:A:295:ALA:O	3:A:299:VAL:HG12	2.10	0.51
1:Y:11:DT:O4	3:A:626:PHE:HB2	2.10	0.51
3:A:112:ASN:O	3:A:113:PHE:C	2.52	0.51
1:Y:4:DG:C4	1:Y:5:DT:C5	2.99	0.51
3:A:303:ASN:HD21	3:A:598:GLU:HA	1.75	0.51
3:A:349:ARG:HE	3:A:349:ARG:CA	2.22	0.51
3:A:408:ASP:O	3:A:409:LEU:C	2.51	0.51
3:A:13:ASN:O	3:A:17:GLN:HG3	2.11	0.51
3:A:61:ALA:CB	3:A:72:MET:HE2	2.40	0.51
3:A:430:LEU:O	3:A:433:TYR:HB2	2.10	0.51
3:A:97:VAL:HG11	3:A:536:THR:HG21	1.92	0.51
3:A:511:ASN:N	3:A:511:ASN:ND2	2.56	0.51
3:A:26:PRO:CG	3:A:274:TYR:HB3	2.41	0.50
3:A:336:VAL:HG13	3:A:576:PHE:CE2	2.45	0.50
3:A:443:GLU:OE1	3:A:443:GLU:HA	2.10	0.50
3:A:597:MET:O	3:A:600:GLU:HB2	2.12	0.50
1:Y:7:DC:H2'	1:Y:8:DT:C6	2.46	0.50
3:A:4:LEU:HA	3:A:7:GLN:CD	2.36	0.50
3:A:100:LEU:C	3:A:102:ARG:H	2.20	0.50
3:A:141:PRO:O	3:A:142:ARG:C	2.54	0.50
3:A:461:LEU:O	3:A:464:PHE:N	2.44	0.50
3:A:541:ILE:O	3:A:541:ILE:CG2	2.59	0.50
3:A:323:TYR:CD1	3:A:324:TYR:N	2.79	0.50
3:A:395:ILE:O	3:A:398:TYR:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:154:GLU:HG2	3:A:230:ARG:HH12	1.75	0.50
3:A:289:THR:HG23	3:A:291:ARG:H	1.77	0.50
3:A:364:SER:O	3:A:365:ARG:C	2.54	0.50
3:A:497:LEU:HD22	3:A:508:ARG:HB2	1.94	0.50
3:A:588:ASN:HA	3:A:591:LEU:HG	1.93	0.50
3:A:408:ASP:CG	3:A:440:SER:HG	2.20	0.49
3:A:433:TYR:HE1	3:A:436:ASP:C	2.20	0.49
3:A:32:GLY:O	3:A:37:LYS:HE3	2.12	0.49
3:A:210:LEU:O	3:A:214:GLN:HB2	2.12	0.49
3:A:610:ARG:NH2	4:A:725:ATP:O1G	2.45	0.49
3:A:41:LEU:CD1	3:A:249:VAL:HG11	2.42	0.49
3:A:395:ILE:CD1	3:A:512:LEU:HD21	2.42	0.49
3:A:55:ALA:HB3	3:A:58:ASN:HD22	1.77	0.49
3:A:132:LYS:O	3:A:134:ILE:N	2.45	0.49
3:A:4:LEU:HA	3:A:7:GLN:OE1	2.12	0.49
3:A:427:ILE:HG22	3:A:428:ASP:N	2.28	0.49
3:A:602:ARG:O	3:A:605:TYR:HB3	2.12	0.49
3:A:6:GLU:O	3:A:9:LEU:HB2	2.12	0.49
3:A:27:LEU:HD12	3:A:278:LYS:O	2.13	0.49
3:A:296:ALA:O	3:A:300:ILE:HG22	2.12	0.49
3:A:349:ARG:HB2	3:A:354:PHE:CZ	2.48	0.49
3:A:365:ARG:HG3	3:A:365:ARG:HH11	1.78	0.49
3:A:454:GLY:O	3:A:455:ALA:C	2.55	0.49
3:A:582:GLU:CD	3:A:636:ARG:HE	2.16	0.49
3:A:28:LEU:HG	3:A:29:ILE:N	2.27	0.49
3:A:289:THR:CG2	3:A:292:ILE:HG13	2.43	0.49
3:A:402:ILE:O	3:A:472:THR:HG23	2.12	0.49
3:A:92:PHE:HE1	3:A:235:LEU:HD23	1.78	0.48
3:A:394:ASP:O	3:A:397:ALA:HB3	2.12	0.48
3:A:402:ILE:HG21	3:A:483:LEU:HD21	1.95	0.48
3:A:433:TYR:CD1	3:A:436:ASP:HB2	2.48	0.48
3:A:135:ASP:OD1	3:A:136:PRO:HD2	2.13	0.48
3:A:226:GLN:CD	3:A:226:GLN:H	2.21	0.48
3:A:246:ILE:O	3:A:246:ILE:HG12	2.13	0.48
3:A:173:VAL:O	3:A:174:SER:C	2.55	0.48
3:A:368:GLU:OE1	3:A:378:TYR:OH	2.17	0.48
3:A:564:LEU:HD13	3:A:603:LEU:HD22	1.94	0.48
3:A:67:LYS:HD3	3:A:544:LEU:HD22	1.96	0.48
3:A:140:GLU:CB	3:A:141:PRO:HD2	2.43	0.48
3:A:177:TYR:CD1	3:A:177:TYR:C	2.91	0.48
3:A:349:ARG:HB2	3:A:354:PHE:HZ	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:269:SER:O	3:A:272:ARG:N	2.47	0.48
3:A:417:VAL:O	3:A:418:PRO:C	2.57	0.48
3:A:582:GLU:OE2	3:A:636:ARG:HB3	2.13	0.48
2:Z:30:DA:C2'	2:Z:31:DC:H5''	2.38	0.48
3:A:105:ASP:C	3:A:108:GLY:H	2.21	0.48
3:A:366:VAL:HA	3:A:369:GLU:HB2	1.96	0.48
3:A:562:MET:HE2	3:A:567:ALA:CA	2.40	0.48
3:A:31:ALA:O	3:A:32:GLY:C	2.54	0.48
3:A:88:TRP:HE1	3:A:95:MET:HG3	1.79	0.48
3:A:475:GLN:HG3	3:A:531:LEU:CD2	2.44	0.48
3:A:360:THR:O	3:A:363:GLN:HB2	2.15	0.47
3:A:367:MET:CG	3:A:561:LEU:HD21	2.44	0.47
3:A:511:ASN:HD22	3:A:511:ASN:H	1.59	0.47
3:A:646:LEU:N	3:A:646:LEU:HD12	2.29	0.47
3:A:125:MET:HE3	3:A:145:LEU:HD23	1.95	0.47
3:A:353:ASP:OD1	3:A:573:PRO:HG2	2.14	0.47
3:A:12:LEU:CD2	3:A:16:GLN:NE2	2.77	0.47
3:A:411:LEU:HD11	3:A:464:PHE:HE2	1.79	0.47
3:A:638:LEU:O	3:A:640:GLU:N	2.46	0.47
3:A:228:THR:O	3:A:262:ALA:HA	2.15	0.47
3:A:289:THR:CG2	3:A:292:ILE:N	2.73	0.47
3:A:478:VAL:HG12	3:A:482:GLU:OE1	2.14	0.47
3:A:497:LEU:HD22	3:A:508:ARG:CB	2.44	0.47
1:Y:4:DG:C2'	1:Y:5:DT:H71	2.44	0.47
1:Y:14:DT:H2'	1:Y:14:DT:O5'	2.14	0.47
3:A:113:PHE:HE1	3:A:115:ILE:HG12	1.79	0.47
3:A:329:GLU:CD	3:A:624:THR:H	2.23	0.47
3:A:344:VAL:HG21	3:A:351:TYR:CD1	2.48	0.47
3:A:415:ILE:CG2	3:A:416:ASN:N	2.77	0.47
3:A:16:GLN:O	3:A:19:ALA:N	2.46	0.47
1:Y:10:DG:N2	2:Z:26:DG:N2	2.52	0.47
2:Z:31:DC:H2''	2:Z:32:DT:O5'	2.14	0.47
2:Z:33:DG:H5'	2:Z:33:DG:H2'	1.65	0.47
3:A:166:SER:OG	3:A:170:GLU:OE1	2.32	0.47
3:A:332:GLU:OE1	3:A:623:ARG:NH1	2.47	0.47
3:A:445:LEU:HD21	3:A:461:LEU:HD22	1.97	0.47
3:A:474:LEU:O	3:A:478:VAL:HG23	2.15	0.47
3:A:585:PHE:HB3	3:A:586:PRO:CD	2.44	0.47
1:Y:8:DT:H2'	1:Y:9:DC:C5	2.49	0.47
3:A:269:SER:O	3:A:272:ARG:HB2	2.15	0.47
3:A:324:TYR:CZ	3:A:326:ALA:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:577:LEU:HD23	3:A:580:MET:HE1	1.97	0.47
3:A:628:ASN:HB3	3:A:629:ILE:H	1.34	0.47
3:A:164:ARG:NH1	3:A:165:ALA:HB3	2.30	0.47
3:A:324:TYR:HB2	3:A:649:ALA:CB	2.45	0.47
3:A:527:ASP:O	3:A:528:ASP:HB2	2.15	0.47
3:A:222:ILE:HD11	3:A:236:VAL:CG1	2.39	0.46
1:Y:12:DT:O2	3:A:359:ARG:NH2	2.45	0.46
3:A:607:GLY:O	3:A:610:ARG:HB2	2.14	0.46
3:A:37:LYS:NZ	3:A:37:LYS:N	2.57	0.46
3:A:154:GLU:O	3:A:155:LEU:HB2	2.14	0.46
3:A:223:ASP:OD1	3:A:224:GLU:N	2.44	0.46
3:A:287:ARG:NH1	3:A:610:ARG:NH2	2.52	0.46
3:A:444:ALA:C	3:A:446:GLY:N	2.73	0.46
3:A:593:ASP:OD1	3:A:594:ASP:N	2.48	0.46
3:A:485:GLU:OE1	3:A:516:LEU:HD21	2.14	0.46
3:A:625:LEU:O	3:A:625:LEU:HD23	2.16	0.46
3:A:647:GLU:O	3:A:648:THR:C	2.59	0.46
1:Y:4:DG:C2'	1:Y:5:DT:H5'	2.37	0.46
3:A:14:LYS:HD2	3:A:17:GLN:OE1	2.14	0.46
3:A:321:ILE:H	3:A:321:ILE:HG12	1.46	0.46
3:A:642:PRO:O	3:A:645:LEU:N	2.40	0.46
1:Y:5:DT:H2''	1:Y:6:DG:O4'	2.16	0.46
3:A:253:ASP:OD1	3:A:300:ILE:HD11	2.15	0.46
3:A:299:VAL:HG11	3:A:608:ILE:HD12	1.98	0.46
3:A:351:TYR:CE1	3:A:376:ILE:HG22	2.50	0.46
3:A:412:LEU:CD2	3:A:441:LEU:HD21	2.46	0.46
3:A:100:LEU:O	3:A:102:ARG:N	2.49	0.46
3:A:140:GLU:O	3:A:144:ILE:HG13	2.16	0.46
3:A:148:ILE:O	3:A:151:ALA:HB3	2.16	0.46
3:A:608:ILE:HG23	3:A:615:LEU:CD2	2.46	0.46
3:A:65:THR:OG1	3:A:68:ALA:HB2	2.16	0.45
3:A:400:ARG:HH11	3:A:400:ARG:HD2	1.38	0.45
3:A:139:PHE:CD1	3:A:139:PHE:N	2.80	0.45
3:A:157:PRO:HD2	3:A:160:GLN:HB2	1.98	0.45
3:A:177:TYR:C	3:A:177:TYR:HD1	2.25	0.45
3:A:426:THR:O	3:A:427:ILE:C	2.58	0.45
3:A:541:ILE:HG13	3:A:542:SER:H	1.81	0.45
3:A:412:LEU:HD21	3:A:441:LEU:HD21	1.97	0.45
3:A:25:GLY:H	3:A:245:ASN:HD22	1.62	0.45
3:A:31:ALA:CB	3:A:251:ASP:HB2	2.26	0.45
3:A:323:TYR:CG	3:A:324:TYR:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:332:GLU:O	3:A:333:ALA:C	2.60	0.45
3:A:433:TYR:CE2	3:A:451:ILE:CG1	2.95	0.45
3:A:563:THR:O	3:A:566:ALA:HB3	2.15	0.45
3:A:585:PHE:O	3:A:587:HIS:N	2.49	0.45
3:A:587:HIS:O	3:A:589:ARG:N	2.49	0.45
1:Y:4:DG:H2''	1:Y:5:DT:C5'	2.40	0.45
1:Y:5:DT:H2'	1:Y:6:DG:N9	2.24	0.45
3:A:372:LEU:O	3:A:373:LYS:C	2.60	0.45
3:A:288:SER:OG	3:A:292:ILE:HG21	2.17	0.45
3:A:357:LEU:HD23	3:A:564:LEU:HD23	1.97	0.45
3:A:87:VAL:HG12	3:A:88:TRP:H	1.82	0.45
3:A:303:ASN:HB3	3:A:598:GLU:OE2	2.17	0.45
3:A:329:GLU:OE2	3:A:624:THR:CB	2.62	0.45
3:A:63:THR:HB	3:A:68:ALA:HB1	1.99	0.45
3:A:449:GLU:O	3:A:450:MET:C	2.59	0.45
3:A:475:GLN:CA	3:A:475:GLN:HE21	2.29	0.45
2:Z:26:DG:H2'	2:Z:27:DA:C5'	2.44	0.45
3:A:265:GLN:CG	3:A:266:ASN:H	2.28	0.45
3:A:310:ARG:HG3	3:A:310:ARG:O	2.15	0.45
3:A:389:ARG:HG2	3:A:391:GLU:OE2	2.16	0.45
3:A:433:TYR:O	3:A:433:TYR:CD1	2.65	0.45
3:A:486:GLU:O	3:A:486:GLU:HG3	2.17	0.45
3:A:493:TYR:O	3:A:493:TYR:CD1	2.70	0.45
3:A:41:LEU:HD11	3:A:249:VAL:HG13	1.98	0.44
3:A:84:ALA:HA	3:A:87:VAL:HG23	1.99	0.44
3:A:87:VAL:HG12	3:A:88:TRP:N	2.32	0.44
3:A:158:PRO:HB3	3:A:177:TYR:CD1	2.52	0.44
3:A:507:SER:O	3:A:508:ARG:C	2.59	0.44
3:A:468:LEU:O	3:A:469:GLU:C	2.60	0.44
3:A:5:SER:OG	3:A:51:GLU:HG2	2.18	0.44
3:A:23:THR:OG1	3:A:24:GLU:OE1	2.22	0.44
3:A:71:GLU:O	3:A:72:MET:C	2.60	0.44
3:A:289:THR:HG22	3:A:292:ILE:CG1	2.47	0.44
3:A:635:SER:O	3:A:636:ARG:C	2.61	0.44
1:Y:4:DG:H2'	1:Y:5:DT:C5	2.49	0.44
3:A:9:LEU:CD2	3:A:17:GLN:HE21	2.30	0.44
3:A:139:PHE:HD2	3:A:169:TYR:CD1	2.34	0.44
3:A:626:PHE:HD1	3:A:627:GLY:H	1.52	0.44
2:Z:32:DT:H2'	2:Z:33:DG:C8	2.52	0.44
3:A:127:THR:O	3:A:131:GLU:CB	2.66	0.44
3:A:224:GLU:OE1	3:A:568:LYS:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:124:VAL:O	3:A:125:MET:C	2.61	0.44
3:A:365:ARG:O	3:A:368:GLU:HG3	2.17	0.44
3:A:627:GLY:O	3:A:628:ASN:CB	2.58	0.44
3:A:302:HIS:HD1	3:A:640:GLU:CD	2.26	0.44
3:A:145:LEU:O	3:A:148:ILE:HB	2.18	0.44
3:A:125:MET:HG2	3:A:145:LEU:CD2	2.48	0.44
3:A:145:LEU:O	3:A:148:ILE:N	2.50	0.44
3:A:243:PHE:O	3:A:244:GLN:C	2.61	0.44
3:A:381:VAL:O	3:A:381:VAL:HG12	2.17	0.44
3:A:621:GLN:O	3:A:631:MET:HG3	2.18	0.44
1:Y:12:DT:H2''	1:Y:13:DT:O4'	2.18	0.43
3:A:139:PHE:CD2	3:A:169:TYR:CD1	3.05	0.43
3:A:16:GLN:O	3:A:17:GLN:C	2.61	0.43
3:A:226:GLN:HG2	3:A:251:ASP:C	2.43	0.43
3:A:293:LEU:HD12	3:A:293:LEU:C	2.43	0.43
3:A:210:LEU:O	3:A:210:LEU:HG	2.18	0.43
3:A:467:GLN:HE22	3:A:490:LYS:NZ	2.17	0.43
3:A:489:ASP:O	3:A:490:LYS:C	2.60	0.43
3:A:497:LEU:CB	3:A:509:LEU:HD13	2.47	0.43
3:A:127:THR:HG21	3:A:183:ARG:HH12	1.82	0.43
1:Y:4:DG:C2'	1:Y:5:DT:H6	2.17	0.43
3:A:435:ALA:C	3:A:437:HIS:H	2.26	0.43
3:A:522:PHE:CE2	3:A:534:PHE:HA	2.53	0.43
3:A:15:GLU:H	3:A:15:GLU:HG2	1.41	0.43
3:A:226:GLN:HB2	3:A:255:SER:HB2	2.00	0.43
3:A:6:GLU:O	3:A:9:LEU:N	2.50	0.43
3:A:52:LYS:O	3:A:53:HIS:C	2.62	0.43
3:A:107:ILE:O	3:A:107:ILE:HG13	2.15	0.43
3:A:388:ASP:HB3	3:A:393:LYS:NZ	2.30	0.43
3:A:417:VAL:CB	3:A:418:PRO:CD	2.96	0.43
3:A:512:LEU:O	3:A:515:PHE:HB3	2.18	0.43
3:A:321:ILE:CG2	3:A:615:LEU:HB3	2.49	0.43
3:A:386:PHE:CZ	3:A:514:GLU:CG	3.02	0.43
3:A:392:ILE:O	3:A:394:ASP:N	2.52	0.43
3:A:142:ARG:H	3:A:142:ARG:HG2	1.22	0.42
3:A:213:TYR:O	3:A:214:GLN:C	2.62	0.42
3:A:289:THR:HG22	3:A:292:ILE:CB	2.49	0.42
3:A:395:ILE:HD12	3:A:395:ILE:H	1.83	0.42
3:A:32:GLY:HA3	3:A:311:ILE:HG23	2.00	0.42
3:A:110:ASN:C	3:A:112:ASN:H	2.27	0.42
3:A:369:GLU:O	3:A:373:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:7:DC:H2''	1:Y:8:DT:O4'	2.19	0.42
1:Y:10:DG:H22	2:Z:26:DG:H22	1.59	0.42
3:A:351:TYR:OH	3:A:376:ILE:HG22	2.18	0.42
3:A:418:PRO:O	3:A:420:ARG:HG2	2.20	0.42
3:A:419:LYS:HA	3:A:419:LYS:HD3	1.79	0.42
1:Y:14:DT:O5'	1:Y:14:DT:C2'	2.67	0.42
2:Z:25:DC:H2''	2:Z:26:DG:C4'	2.50	0.42
3:A:354:PHE:HB2	3:A:559:VAL:HG22	2.00	0.42
3:A:417:VAL:O	3:A:419:LYS:HE2	2.19	0.42
1:Y:4:DG:H2''	1:Y:5:DT:O4'	2.19	0.42
3:A:24:GLU:OE1	3:A:24:GLU:N	2.52	0.42
3:A:91:THR:O	3:A:92:PHE:C	2.61	0.42
2:Z:31:DC:H2'	2:Z:32:DT:C7	2.32	0.42
3:A:128:ILE:O	3:A:132:LYS:CB	2.66	0.42
3:A:170:GLU:HG3	3:A:171:LYS:N	2.34	0.42
3:A:320:PRO:HB2	3:A:647:GLU:HB2	2.00	0.42
3:A:416:ASN:O	3:A:419:LYS:HD3	2.20	0.42
3:A:107:ILE:HG21	3:A:202:LEU:HA	2.02	0.42
3:A:303:ASN:ND2	3:A:598:GLU:HA	2.35	0.42
3:A:562:MET:CE	3:A:570:LEU:CD1	2.95	0.42
1:Y:4:DG:H2'	1:Y:5:DT:C7	2.50	0.42
3:A:116:LEU:HD11	3:A:184:LEU:HD11	2.02	0.42
3:A:128:ILE:HG12	3:A:179:GLU:OE1	2.19	0.42
3:A:167:THR:O	3:A:170:GLU:HB3	2.20	0.42
3:A:324:TYR:OH	3:A:326:ALA:HA	2.20	0.42
3:A:352:ARG:HA	3:A:558:ALA:O	2.19	0.42
3:A:435:ALA:C	3:A:437:HIS:N	2.77	0.42
3:A:587:HIS:C	3:A:589:ARG:H	2.27	0.42
3:A:181:GLN:HA	3:A:181:GLN:HE21	1.85	0.42
3:A:264:ILE:HG23	3:A:265:GLN:N	2.34	0.42
3:A:389:ARG:O	3:A:390:LYS:C	2.62	0.42
3:A:451:ILE:CG2	3:A:452:GLY:N	2.82	0.42
3:A:563:THR:CG2	3:A:566:ALA:HB2	2.46	0.42
3:A:597:MET:O	3:A:597:MET:HG3	2.20	0.42
2:Z:28:DG:C2'	2:Z:29:DC:O5'	2.66	0.41
3:A:7:GLN:H	3:A:7:GLN:HG3	1.63	0.41
3:A:37:LYS:HE2	4:A:725:ATP:PG	2.61	0.41
3:A:37:LYS:O	3:A:40:VAL:HB	2.20	0.41
3:A:106:ARG:HD2	3:A:206:VAL:HG11	2.02	0.41
3:A:134:ILE:N	3:A:134:ILE:HD12	2.36	0.41
3:A:228:THR:HG22	3:A:266:ASN:HD21	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:232:GLN:O	3:A:236:VAL:HG22	2.20	0.41
3:A:453:LEU:HD23	3:A:453:LEU:O	2.19	0.41
3:A:127:THR:O	3:A:131:GLU:HB2	2.20	0.41
3:A:321:ILE:HG21	3:A:615:LEU:HD23	2.03	0.41
3:A:368:GLU:O	3:A:369:GLU:C	2.62	0.41
3:A:130:LYS:O	3:A:130:LYS:HG2	2.20	0.41
3:A:411:LEU:O	3:A:412:LEU:C	2.63	0.41
3:A:83:ALA:C	3:A:85:GLU:H	2.28	0.41
3:A:394:ASP:OD1	3:A:413:ARG:NH1	2.52	0.41
2:Z:31:DC:C2'	2:Z:32:DT:C6	3.04	0.41
3:A:46:ALA:HB1	3:A:80:LEU:CD1	2.51	0.41
3:A:233:TYR:OH	3:A:273:ASP:OD2	2.39	0.41
3:A:338:GLY:HA2	3:A:341:ARG:HB3	2.01	0.41
3:A:442:PHE:CD1	3:A:442:PHE:C	2.98	0.41
3:A:571:GLU:O	3:A:571:GLU:HG2	2.20	0.41
3:A:64:PHE:HB2	3:A:224:GLU:HG3	2.03	0.41
3:A:135:ASP:HA	3:A:136:PRO:HD3	1.87	0.41
3:A:136:PRO:O	3:A:140:GLU:HA	2.21	0.41
3:A:243:PHE:C	3:A:245:ASN:N	2.78	0.41
3:A:256:ILE:HD12	3:A:565:HIS:HD2	1.82	0.41
3:A:376:ILE:HA	3:A:377:PRO:HD3	1.97	0.41
3:A:414:ILE:O	3:A:415:ILE:C	2.63	0.41
3:A:457:ALA:O	3:A:458:ALA:C	2.64	0.41
3:A:522:PHE:O	3:A:523:GLU:C	2.64	0.41
3:A:621:GLN:O	3:A:631:MET:HA	2.19	0.41
3:A:269:SER:O	3:A:270:PHE:C	2.63	0.41
3:A:274:TYR:O	3:A:277:ALA:HB2	2.21	0.41
3:A:355:ALA:HA	3:A:560:MET:O	2.21	0.41
3:A:394:ASP:OD2	3:A:493:TYR:CE2	2.74	0.41
3:A:128:ILE:CG2	3:A:179:GLU:OE1	2.64	0.40
3:A:313:THR:HB	3:A:315:ASN:H	1.86	0.40
2:Z:25:DC:C3'	2:Z:25:DC:C6	3.03	0.40
3:A:306:ARG:O	3:A:306:ARG:HG2	2.20	0.40
3:A:585:PHE:CZ	3:A:604:ALA:HA	2.57	0.40
2:Z:27:DA:H4'	2:Z:27:DA:OP1	2.20	0.40
3:A:77:GLN:CG	3:A:84:ALA:HB3	2.47	0.40
3:A:167:THR:HB	3:A:168:TYR:H	1.76	0.40
3:A:12:LEU:HD23	3:A:16:GLN:NE2	2.36	0.40
3:A:164:ARG:CG	3:A:164:ARG:NH1	2.63	0.40
3:A:331:ASP:O	3:A:334:GLN:N	2.54	0.40
3:A:417:VAL:HG11	3:A:493:TYR:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:429:LYS:NZ	3:A:452:GLY:O	2.44	0.40
3:A:444:ALA:O	3:A:447:GLU:N	2.55	0.40
3:A:120:ASP:O	3:A:121:GLN:C	2.64	0.40
3:A:134:ILE:HG23	3:A:139:PHE:CE1	2.57	0.40
3:A:329:GLU:OE1	3:A:623:ARG:HA	2.21	0.40
3:A:411:LEU:HD23	3:A:441:LEU:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	642/724 (89%)	471 (73%)	113 (18%)	58 (9%)	0 4

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	33	ALA
3	A	35	SER
3	A	83	ALA
3	A	84	ALA
3	A	113	PHE
3	A	133	ASN
3	A	138	LYS
3	A	165	ALA
3	A	266	ASN
3	A	270	PHE
3	A	365	ARG
3	A	417	VAL
3	A	424	ALA
3	A	434	ALA
3	A	438	GLU

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Mol	Chain	Res	Type
3	A	462	ALA
3	A	541	ILE
3	A	568	LYS
3	A	585	PHE
3	A	588	ASN
3	A	626	PHE
3	A	628	ASN
3	A	166	SER
3	A	168	TYR
3	A	244	GLN
3	A	252	ALA
3	A	386	PHE
3	A	390	LYS
3	A	445	LEU
3	A	455	ALA
3	A	543	ASP
3	A	551	GLU
3	A	553	ALA
3	A	558	ALA
3	A	81	GLY
3	A	224	GLU
3	A	237	LYS
3	A	267	ILE
3	A	316	PRO
3	A	349	ARG
3	A	408	ASP
3	A	453	LEU
3	A	461	LEU
3	A	582	GLU
3	A	649	ALA
3	A	11	HIS
3	A	34	GLY
3	A	141	PRO
3	A	238	LYS
3	A	319	LYS
3	A	362	ALA
3	A	557	ASP
3	A	164	ARG
3	A	418	PRO
3	A	573	PRO
3	A	648	THR
3	A	53	HIS

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Mol	Chain	Res	Type
3	A	415	ILE

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
3	A	560/618 (91%)	387 (69%)	173 (31%)	0 1

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	7	GLN
3	A	9	LEU
3	A	15	GLU
3	A	28	LEU
3	A	35	SER
3	A	37	LYS
3	A	39	ARG
3	A	51	GLU
3	A	67	LYS
3	A	70	ARG
3	A	72	MET
3	A	89	ILE
3	A	91	THR
3	A	101	ARG
3	A	105	ASP
3	A	109	ILE
3	A	116	LEU
3	A	122	LEU
3	A	124	VAL
3	A	126	LYS
3	A	129	LEU
3	A	133	ASN
3	A	137	LYS
3	A	138	LYS
3	A	139	PHE

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Mol	Chain	Res	Type
3	A	142	ARG
3	A	145	LEU
3	A	147	THR
3	A	148	ILE
3	A	149	SER
3	A	152	LYS
3	A	156	LEU
3	A	163	LYS
3	A	164	ARG
3	A	167	THR
3	A	171	LYS
3	A	172	VAL
3	A	173	VAL
3	A	174	SER
3	A	176	VAL
3	A	177	TYR
3	A	181	GLN
3	A	183	ARG
3	A	184	LEU
3	A	185	LEU
3	A	206	VAL
3	A	226	GLN
3	A	228	THR
3	A	230	ARG
3	A	236	VAL
3	A	237	LYS
3	A	242	ARG
3	A	243	PHE
3	A	246	ILE
3	A	255	SER
3	A	260	ARG
3	A	263	ASP
3	A	264	ILE
3	A	265	GLN
3	A	267	ILE
3	A	269	SER
3	A	272	ARG
3	A	276	ASN
3	A	279	VAL
3	A	280	ILE
3	A	281	LEU
3	A	283	GLU

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Mol	Chain	Res	Type
3	A	288	SER
3	A	289	THR
3	A	291	ARG
3	A	293	LEU
3	A	305	ASN
3	A	306	ARG
3	A	309	LYS
3	A	310	ARG
3	A	311	ILE
3	A	313	THR
3	A	319	LYS
3	A	321	ILE
3	A	322	LEU
3	A	325	GLU
3	A	329	GLU
3	A	331	ASP
3	A	336	VAL
3	A	339	ARG
3	A	342	GLU
3	A	346	ARG
3	A	348	GLU
3	A	349	ARG
3	A	352	ARG
3	A	357	LEU
3	A	361	ASN
3	A	363	GLN
3	A	365	ARG
3	A	366	VAL
3	A	368	GLU
3	A	371	LEU
3	A	372	LEU
3	A	375	ASN
3	A	376	ILE
3	A	386	PHE
3	A	387	TYR
3	A	388	ASP
3	A	389	ARG
3	A	391	GLU
3	A	396	LEU
3	A	400	ARG
3	A	405	PRO
3	A	409	LEU

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Mol	Chain	Res	Type
3	A	413	ARG
3	A	419	LYS
3	A	420	ARG
3	A	422	ILE
3	A	427	ILE
3	A	429	LYS
3	A	430	LEU
3	A	443	GLU
3	A	447	GLU
3	A	450	MET
3	A	453	LEU
3	A	468	LEU
3	A	474	LEU
3	A	475	GLN
3	A	478	VAL
3	A	485	GLU
3	A	486	GLU
3	A	496	MET
3	A	500	GLU
3	A	502	THR
3	A	503	ILE
3	A	504	GLU
3	A	509	LEU
3	A	510	GLU
3	A	511	ASN
3	A	514	GLU
3	A	516	LEU
3	A	519	THR
3	A	523	GLU
3	A	524	ASN
3	A	530	SER
3	A	532	ILE
3	A	535	LEU
3	A	540	LEU
3	A	542	SER
3	A	545	ASP
3	A	546	GLU
3	A	552	GLN
3	A	557	ASP
3	A	559	VAL
3	A	562	MET
3	A	564	LEU

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Mol	Chain	Res	Type
3	A	568	LYS
3	A	571	GLU
3	A	572	PHE
3	A	573	PRO
3	A	580	MET
3	A	581	GLU
3	A	584	ILE
3	A	590	SER
3	A	594	ASP
3	A	596	GLU
3	A	597	MET
3	A	599	GLU
3	A	603	LEU
3	A	606	VAL
3	A	610	ARG
3	A	616	VAL
3	A	619	SER
3	A	621	GLN
3	A	625	LEU
3	A	635	SER
3	A	644	HIS
3	A	645	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	16	GLN
3	A	17	GLN
3	A	58	ASN
3	A	110	ASN
3	A	112	ASN
3	A	121	GLN
3	A	133	ASN
3	A	160	GLN
3	A	178	GLN
3	A	182	GLN
3	A	214	GLN
3	A	232	GLN
3	A	245	ASN
3	A	265	GLN
3	A	303	ASN
3	A	315	ASN

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Mol	Chain	Res	Type
3	A	375	ASN
3	A	467	GLN
3	A	475	GLN
3	A	511	ASN
3	A	524	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
4	ATP	A	725	-	32,33,33	1.65	5 (15%)	48,52,52	1.52	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	725	-	-	12/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	725	ATP	PA-O3A	4.25	1.64	1.59
4	A	725	ATP	C5-N7	-4.04	1.31	1.39
4	A	725	ATP	C2-N1	2.41	1.38	1.33
4	A	725	ATP	PG-O2G	-2.35	1.46	1.54
4	A	725	ATP	PB-O2B	-2.09	1.45	1.55

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	725	ATP	C4-N9-C8	-4.06	101.48	105.74
4	A	725	ATP	O4'-C1'-N9	3.36	114.55	108.09
4	A	725	ATP	O2B-PB-O3B	3.00	115.38	107.27
4	A	725	ATP	C6-C5-N7	-2.97	126.36	132.09
4	A	725	ATP	N9-C8-N7	2.82	117.94	113.94
4	A	725	ATP	O2B-PB-O3A	2.77	114.76	107.27
4	A	725	ATP	C4-C5-N7	2.39	113.31	110.58
4	A	725	ATP	C6-C5-C4	2.30	120.32	117.18
4	A	725	ATP	O2'-C2'-C3'	-2.27	104.54	111.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

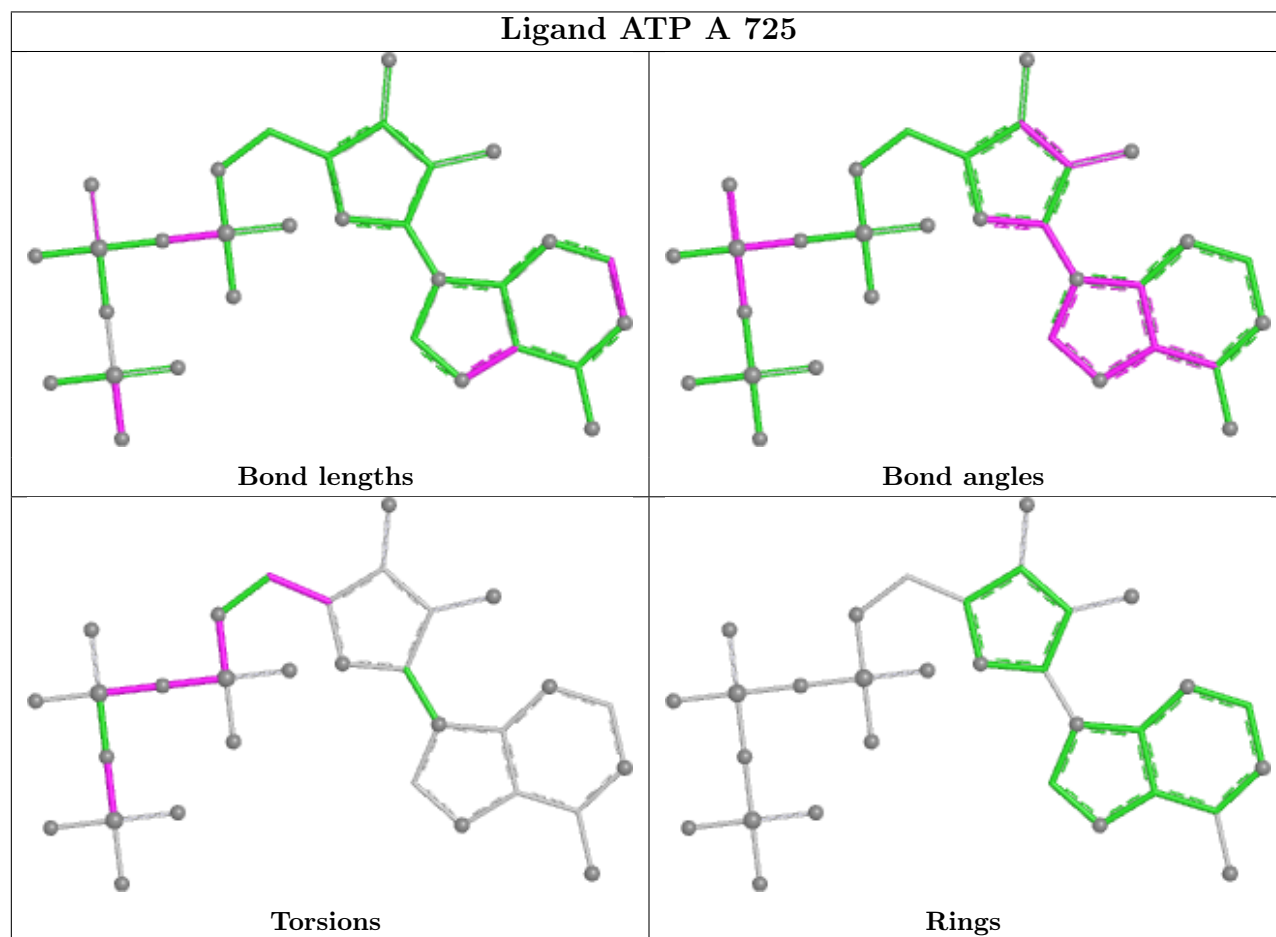
Mol	Chain	Res	Type	Atoms
4	A	725	ATP	PB-O3B-PG-O3G
4	A	725	ATP	C5'-O5'-PA-O1A
4	A	725	ATP	C5'-O5'-PA-O2A
4	A	725	ATP	C5'-O5'-PA-O3A
4	A	725	ATP	O4'-C4'-C5'-O5'
4	A	725	ATP	C3'-C4'-C5'-O5'
4	A	725	ATP	PA-O3A-PB-O1B
4	A	725	ATP	PB-O3B-PG-O1G
4	A	725	ATP	PB-O3B-PG-O2G
4	A	725	ATP	PB-O3A-PA-O1A
4	A	725	ATP	PB-O3A-PA-O2A
4	A	725	ATP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	725	ATP	7	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.