Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 02:00 PM EDT

PDB ID	:	3PJR
Title	:	HELICASE SUBSTRATE COMPLEX
Authors	:	Velankar, S.S.; Soultanas, P.; Dillingham, M.S.; Subramanya, H.S.; Wigley, D.B.
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 (i) 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 (1)) were used in the production of this report:

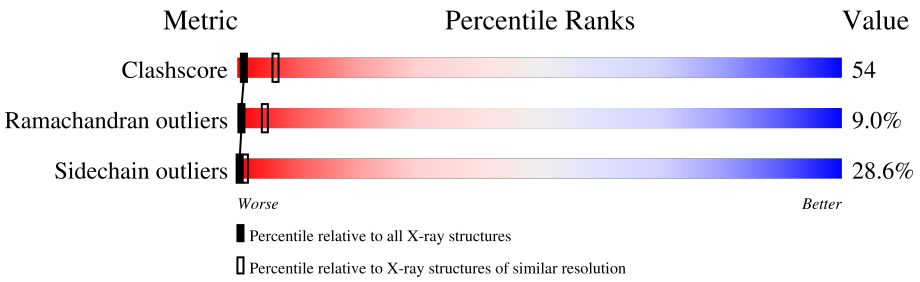
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	Y	15	20% 80%
2	Z	10	100%
3	A	724	23% 40% 21% 6% 11%

2 Entry composition (i)

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
			Total	C	N	O	P			
1	Y	15	303	147	48	94	14	0	0	0

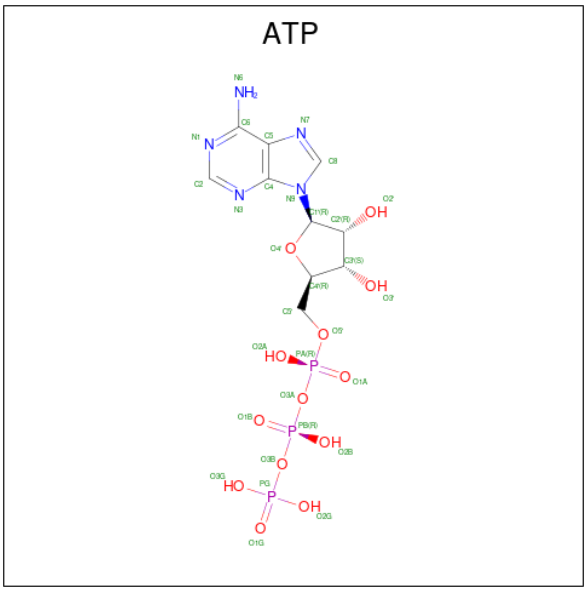
- Molecule 2 is a DNA chain called 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*C)-3'.

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

- Molecule 3 is a protein called HELICASE PCRA.

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	5	13	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: 5'-D(*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*TP*TP*T)-3'

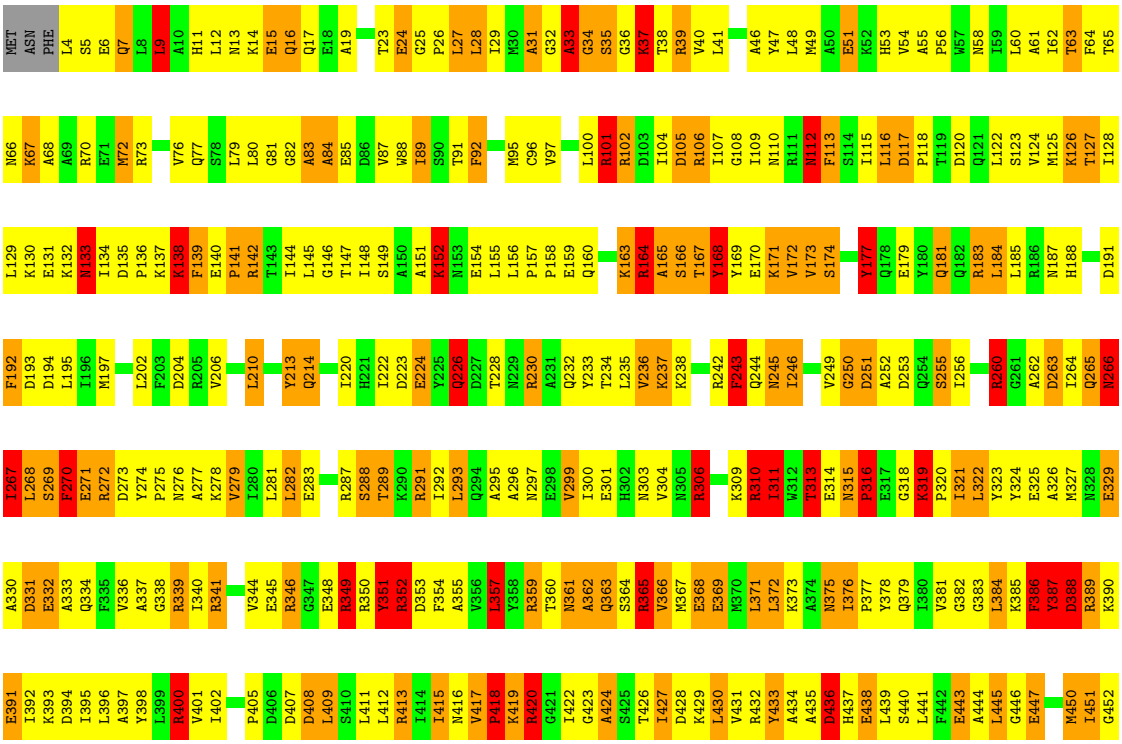
Chain Y: 20% 80%

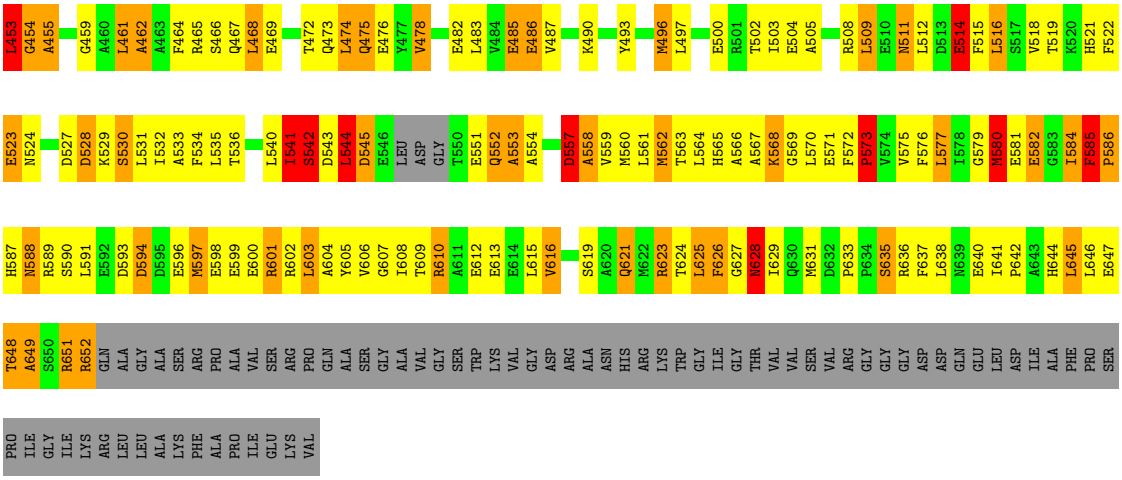
• Molecule 2: 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*C)-3'

Chain Z: 100%

• Molecule 3: HELICASE PCRA

Chain A: 23% 40% 21% 6% 11%




L453 G454 A455 G459 A460 L461 A462 A463 F464 R465 S466 Q467 L468 E469 T472 Q473 L474 Q475 E476 Y477 V478 E482 L483 V484 E485 E486 V487 K490 Y493 M496 L497 E500 R501 T502 I503 E504 A505 R508 L509 E510 N511 L512 D513 E514 F515 L516 S517 V518 T519 K520 H521 F522
E523 N524 D527 D528 K529 S530 L531 I532 A533 F534 L535 T536 L540 I541 S542 D543 L544 D545 E546 LEU ASP GLY T550 E551 Q552 A553 A554 D557 A558 V559 M560 L561 M562 T563 L564 H565 A566 A567 K568 G569 L570 E571 F572 P573 V574 V575 F576 L577 I578 G579 M580 E581 E582 G583 I584 F585 P586
H587 N588 R589 S590 L591 E592 D593 D594 D595 E596 M597 E598 E599 E600 R601 R602 L603 A604 Y605 V606 G607 I608 T609 R610 A611 E612 E613 E614 L615 V616 S619 A620 Q621 M622 R623 T624 L625 F626 G627 N628 I629 Q630 M631 D632 P633 P634 S635 R636 F637 L638 N639 E640 I641 P642 A643 H644 L645 L646 E647
T648 A649 S650 R651 R652 GLN ALA GLY ALA SER ARG PRO ALA VAL SER ARG PRO GLN ALA SER GLY ALA VAL GLY SER TRP LYS VAL GLY ASP ARG ALA ASN HIS ARG LYS TRP GLY ILE GLY THR VAL VAL SER VAL ARG GLY GLY GLY ASP ASP GLN GLU LEU ASP ILE ALA PHE PRO SER
PRO ILE GLY ILE LYS ARG LEU LEU ALA LYS PHE ALA PRO ILE GLU LYS VAL

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.56	4/337 (1.2%)	3.06	50/519 (9.6%)
2	Z	2.27	6/225 (2.7%)	3.84	39/345 (11.3%)
3	A	0.68	7/5319 (0.1%)	1.60	69/7184 (1.0%)
All	All	0.87	17/5881 (0.3%)	1.88	158/8048 (2.0%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	28	DG	N9-C8	12.27	1.46	1.37
2	Z	28	DG	C2'-C1'	11.86	1.64	1.52
2	Z	28	DG	C8-N7	-11.06	1.24	1.30
1	Y	11	DT	C3'-O3'	-7.58	1.34	1.44
2	Z	27	DA	C2'-C1'	7.16	1.59	1.52
2	Z	33	DG	C4'-O4'	7.05	1.52	1.45
1	Y	5	DT	C3'-O3'	-6.91	1.34	1.44
3	A	310	ARG	CD-NE	-6.21	1.35	1.46
3	A	386	PHE	C-O	5.76	1.34	1.23
2	Z	34	DC	P-O5'	5.69	1.65	1.59
3	A	383	GLY	N-CA	-5.57	1.37	1.46
1	Y	10	DG	C3'-O3'	-5.49	1.36	1.44
3	A	652	ARG	NE-CZ	-5.36	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	652	ARG	CD-NE	-5.11	1.37	1.46
1	Y	3	DA	C8-N7	-5.07	1.28	1.31
3	A	652	ARG	N-CA	-5.04	1.36	1.46
3	A	310	ARG	NE-CZ	-5.01	1.26	1.33

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	652	ARG	CD-NE-CZ	38.94	178.12	123.60
3	A	310	ARG	CD-NE-CZ	36.72	175.00	123.60
2	Z	28	DG	C4-N9-C1'	21.13	153.97	126.50
2	Z	28	DG	C8-N9-C1'	-20.87	99.87	127.00
2	Z	28	DG	N3-C4-C5	-20.27	118.47	128.60
3	A	651	ARG	C-N-CA	17.57	165.61	121.70
2	Z	27	DA	O4'-C1'-N9	15.69	118.98	108.00
2	Z	28	DG	O4'-C1'-C2'	-14.65	94.18	105.90
2	Z	28	DG	N3-C4-N9	14.15	134.49	126.00
1	Y	5	DT	P-O3'-C3'	13.94	136.43	119.70
3	A	386	PHE	CA-C-N	13.79	147.54	117.20
3	A	365	ARG	CD-NE-CZ	13.08	141.91	123.60
2	Z	33	DG	O4'-C4'-C3'	-12.56	98.47	106.00
3	A	386	PHE	N-CA-C	12.46	144.64	111.00
2	Z	28	DG	C6-C5-N7	-12.28	123.03	130.40
1	Y	11	DT	P-O3'-C3'	12.09	134.21	119.70
2	Z	28	DG	C8-N9-C4	-12.00	101.60	106.40
1	Y	10	DG	P-O3'-C3'	11.91	133.99	119.70
3	A	386	PHE	O-C-N	-11.75	103.90	122.70
2	Z	28	DG	C4-C5-C6	11.60	125.76	118.80
3	A	102	ARG	CD-NE-CZ	10.57	138.39	123.60
2	Z	28	DG	C2-N3-C4	10.39	117.09	111.90
2	Z	27	DA	P-O5'-C5'	10.37	137.49	120.90
3	A	365	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	Y	5	DT	N3-C2-O2	-9.80	116.42	122.30
1	Y	2	DC	N1-C2-O2	9.77	124.76	118.90
3	A	379	GLN	C-N-CA	9.72	146.00	121.70
3	A	601	ARG	CD-NE-CZ	9.69	137.16	123.60
2	Z	28	DG	N9-C1'-C2'	-9.62	94.32	112.60
1	Y	4	DG	O4'-C4'-C3'	-9.60	100.24	106.00
2	Z	25	DC	P-O3'-C3'	9.48	131.08	119.70
2	Z	26	DG	P-O5'-C5'	-9.47	105.75	120.90
1	Y	2	DC	N3-C2-O2	-9.41	115.31	121.90
1	Y	11	DT	O4'-C4'-C3'	-9.31	100.41	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	31	DC	C6-N1-C2	9.03	123.91	120.30
1	Y	2	DC	C5'-C4'-C3'	9.01	130.32	114.10
1	Y	14	DT	O4'-C1'-N1	8.88	114.22	108.00
3	A	387	TYR	CB-CG-CD1	8.81	126.29	121.00
1	Y	1	DG	P-O3'-C3'	8.49	129.89	119.70
3	A	382	GLY	C-N-CA	8.41	139.97	122.30
3	A	383	GLY	N-CA-C	8.26	133.74	113.10
3	A	400	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	Y	2	DC	C2-N1-C1'	8.20	127.82	118.80
3	A	387	TYR	CA-CB-CG	8.12	128.83	113.40
2	Z	28	DG	O4'-C1'-N9	8.11	113.68	108.00
3	A	400	ARG	CD-NE-CZ	-8.08	112.28	123.60
3	A	177	TYR	CB-CG-CD1	8.03	125.82	121.00
1	Y	12	DT	C6-N1-C2	7.95	125.27	121.30
1	Y	12	DT	N3-C2-O2	7.89	127.03	122.30
2	Z	26	DG	O4'-C1'-N9	-7.80	102.54	108.00
1	Y	9	DC	P-O3'-C3'	7.79	129.05	119.70
1	Y	1	DG	O4'-C1'-N9	7.72	113.40	108.00
3	A	39	ARG	NE-CZ-NH1	7.69	124.14	120.30
3	A	601	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	Y	12	DT	C5-C6-N1	-7.53	119.18	123.70
2	Z	28	DG	N7-C8-N9	7.46	116.83	113.10
1	Y	13	DT	O4'-C4'-C3'	-7.40	101.54	104.50
3	A	204	ASP	CB-CG-OD1	7.33	124.89	118.30
1	Y	3	DA	O4'-C1'-N9	-7.27	102.91	108.00
3	A	388	ASP	C-N-CA	7.27	139.88	121.70
1	Y	2	DC	O5'-C5'-C4'	7.17	128.93	111.00
3	A	164	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	Y	8	DT	O4'-C1'-N1	-7.07	103.05	108.00
3	A	529	LYS	C-N-CA	7.05	139.33	121.70
1	Y	11	DT	P-O5'-C5'	-6.95	109.79	120.90
1	Y	13	DT	N3-C2-O2	-6.85	118.19	122.30
3	A	545	ASP	N-CA-C	6.82	129.40	111.00
3	A	101	ARG	NE-CZ-NH1	-6.80	116.90	120.30
3	A	384	LEU	C-N-CA	6.70	138.45	121.70
2	Z	34	DC	P-O5'-C5'	-6.67	110.23	120.90
3	A	359	ARG	NE-CZ-NH1	-6.65	116.98	120.30
2	Z	29	DC	P-O5'-C5'	6.62	131.49	120.90
3	A	529	LYS	CB-CA-C	6.58	123.56	110.40
3	A	585	PHE	N-CA-CB	6.56	122.42	110.60
3	A	112	ASN	CB-CA-C	-6.55	97.29	110.40
2	Z	31	DC	C6-N1-C1'	-6.49	113.01	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	11	DT	O4'-C1'-N1	6.45	112.51	108.00
3	A	177	TYR	CB-CG-CD2	-6.41	117.15	121.00
1	Y	4	DG	C1'-O4'-C4'	-6.35	103.75	110.10
3	A	339	ARG	CD-NE-CZ	6.34	132.48	123.60
3	A	400	ARG	NH1-CZ-NH2	6.32	126.35	119.40
2	Z	31	DC	P-O5'-C5'	-6.30	110.81	120.90
3	A	37	LYS	CA-CB-CG	6.30	127.26	113.40
1	Y	1	DG	N3-C4-N9	-6.27	122.24	126.00
3	A	557	ASP	CB-CA-C	6.24	122.88	110.40
1	Y	1	DG	C8-N9-C4	-6.23	103.91	106.40
1	Y	5	DT	N1-C1'-C2'	6.16	124.30	112.60
2	Z	34	DC	C3'-C2'-C1'	-6.12	95.16	102.50
3	A	544	LEU	O-C-N	-6.04	113.03	122.70
1	Y	11	DT	C4-C5-C6	6.04	121.62	118.00
3	A	384	LEU	N-CA-C	6.03	127.28	111.00
3	A	33	ALA	CA-C-N	6.03	128.26	116.20
3	A	468	LEU	CA-CB-CG	6.00	129.10	115.30
3	A	436	ASP	CB-CA-C	5.99	122.38	110.40
1	Y	5	DT	O4'-C4'-C3'	-5.96	102.11	104.50
2	Z	34	DC	C2-N3-C4	5.96	122.88	119.90
3	A	260	ARG	CB-CA-C	5.96	122.32	110.40
1	Y	3	DA	O4'-C4'-C3'	-5.95	102.12	104.50
2	Z	32	DT	P-O5'-C5'	-5.91	111.44	120.90
1	Y	11	DT	C5-C6-N1	-5.88	120.17	123.70
1	Y	1	DG	C8-N9-C1'	5.83	134.58	127.00
2	Z	27	DA	N9-C1'-C2'	-5.78	101.62	112.60
1	Y	2	DC	C6-N1-C1'	-5.74	113.92	120.80
3	A	351	TYR	CB-CG-CD2	5.72	124.43	121.00
3	A	385	LYS	N-CA-CB	5.72	120.90	110.60
3	A	400	ARG	NE-CZ-NH2	-5.69	117.45	120.30
3	A	386	PHE	CA-C-O	-5.66	108.22	120.10
3	A	306	ARG	CD-NE-CZ	5.65	131.51	123.60
3	A	420	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	Y	13	DT	C5-C6-N1	-5.65	120.31	123.70
3	A	386	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	Y	11	DT	C1'-O4'-C4'	-5.63	104.47	110.10
2	Z	33	DG	C4'-C3'-O3'	5.61	123.73	109.70
3	A	544	LEU	CB-CA-C	5.60	120.85	110.20
1	Y	13	DT	C4-C5-C6	5.59	121.35	118.00
3	A	192	PHE	CB-CG-CD1	-5.59	116.89	120.80
1	Y	3	DA	C4-C5-C6	5.58	119.79	117.00
2	Z	26	DG	P-O3'-C3'	-5.58	113.00	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	315	ASN	CA-CB-CG	5.57	125.65	113.40
2	Z	30	DA	C8-N9-C4	-5.57	103.57	105.80
3	A	375	ASN	CA-CB-CG	5.56	125.64	113.40
2	Z	30	DA	P-O3'-C3'	5.55	126.36	119.70
2	Z	25	DC	C6-N1-C2	5.51	122.50	120.30
3	A	310	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Y	2	DC	C5-C6-N1	5.48	123.74	121.00
1	Y	2	DC	OP1-P-OP2	-5.47	111.39	119.60
3	A	251	ASP	N-CA-CB	5.47	120.45	110.60
3	A	126	LYS	CA-CB-CG	5.45	125.39	113.40
1	Y	4	DG	C8-N9-C4	-5.43	104.23	106.40
1	Y	2	DC	C6-N1-C2	-5.38	118.15	120.30
2	Z	27	DA	C4'-C3'-O3'	5.37	123.13	109.70
1	Y	12	DT	N1-C2-O2	-5.36	118.81	123.10
3	A	453	LEU	C-N-CA	-5.35	111.06	122.30
2	Z	28	DG	C6-N1-C2	-5.32	121.91	125.10
3	A	352	ARG	NE-CZ-NH1	5.27	122.94	120.30
3	A	102	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	Y	12	DT	O4'-C1'-N1	-5.25	104.32	108.00
1	Y	14	DT	N3-C4-O4	5.24	123.04	119.90
1	Y	14	DT	C4-C5-C7	-5.23	115.86	119.00
2	Z	26	DG	C4'-C3'-C2'	5.21	107.79	103.10
3	A	357	LEU	CA-CB-CG	5.21	127.28	115.30
3	A	557	ASP	CA-C-N	5.21	128.66	117.20
3	A	569	GLY	C-N-CA	5.18	134.64	121.70
1	Y	15	DT	C4-C5-C6	5.15	121.09	118.00
1	Y	14	DT	C4-C5-C6	5.14	121.08	118.00
2	Z	26	DG	N9-C1'-C2'	5.14	122.36	112.60
1	Y	1	DG	N9-C4-C5	5.14	107.45	105.40
2	Z	32	DT	C4-C5-C7	-5.14	115.92	119.00
3	A	168	TYR	CB-CG-CD1	-5.09	117.95	121.00
2	Z	29	DC	C4'-C3'-C2'	5.08	107.68	103.10
3	A	350	ARG	CD-NE-CZ	5.08	130.72	123.60
3	A	213	TYR	CB-CG-CD1	-5.08	117.95	121.00
3	A	386	PHE	N-CA-CB	-5.06	101.49	110.60
2	Z	34	DC	O5'-P-OP1	-5.06	101.15	105.70
3	A	542	SER	C-N-CA	5.05	134.31	121.70
3	A	101	ARG	CA-CB-CG	5.04	124.48	113.40
1	Y	6	DG	C4'-C3'-C2'	5.03	107.63	103.10
3	A	349	ARG	CA-CB-CG	5.02	124.45	113.40

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
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

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Mol	Chain	Res	Type	Group
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 (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	Y	303	0	174	56	0
2	Z	201	0	113	36	0
3	A	5230	0	5230	530	0
4	A	31	0	12	7	0
All	All	5765	0	5529	607	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 54.

All (607) 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
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
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
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
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:37:LYS:NZ	3:A:37:LYS:H	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:37:LYS:H	3:A:37:LYS:HZ2	1.34	0.75
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:37:LYS:HZ1	4:A:725:ATP:PB	2.17	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: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
3:A:167:THR:O	3:A:168:TYR:C	2.33	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:417:VAL:O	3:A:419:LYS:N	2.29	0.65
3:A:567:ALA:HA	3:A:570:LEU:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:128:ILE:O	3:A:132:LYS:HB2	1.97	0.65
3:A:61:ALA:HB1	3:A:72:MET:HE1	1.80	0.64
3:A:606:VAL:HG23	3:A:610:ARG:HD3	1.79	0.64
1:Y:10:DG:H2"	1:Y:11:DT:O5'	1.98	0.64
3:A:139:PHE:CE2	3:A:172:VAL:HG11	2.33	0.64
3:A:412:LEU:O	3:A:413:ARG:C	2.35	0.64
3:A:388:ASP:HB3	3:A:393:LYS:HZ3	1.63	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
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:67:LYS:HG2	3:A:68:ALA:N	2.12	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: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:581:GLU:O	3:A:582:GLU:C	2.37	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:371:LEU:O	3:A:376:ILE:HG12	1.99	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: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:359:ARG:HH12	3:A:600:GLU:CD	2.03	0.60
3:A:562:MET:HE1	3:A:567:ALA:HA	1.82	0.60
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:145:LEU:O	3:A:146:GLY:C	2.38	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:37:LYS:HZ3	4:A:725:ATP:PB	2.23	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: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:110:ASN:HD21	3:A:112:ASN:CG	2.04	0.59
3:A:267:ILE:O	3:A:270:PHE:HB2	2.02	0.59
3:A:417:VAL:HG12	3:A:418:PRO:CD	2.32	0.59
3:A:577:LEU:HB3	3:A:580:MET:HE3	1.85	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
1:Y:4:DG:H2'	1:Y:5:DT:H71	1.84	0.59
2:Z:31:DC:H2'	2:Z:32:DT:C7	2.32	0.59
3:A:368:GLU:HB3	3:A:378:TYR:CZ	2.38	0.59
2:Z:31:DC:H2'	2:Z:32:DT:H72	1.85	0.58
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:169:TYR:O	3:A:170:GLU:C	2.41	0.57
3:A:388:ASP:CG	3:A:393:LYS:HG2	2.25	0.57
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:577:LEU:HD23	3:A:580:MET:HE3	1.87	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
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:16:GLN:HG3	3:A:282:LEU:HD22	1.88	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:585:PHE:C	3:A:585:PHE:HD1	2.11	0.54
3:A:625:LEU:O	3:A:626:PHE:C	2.45	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
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
1:Y:11:DT:C4	3:A:626:PHE:HB2	2.44	0.53
3:A:36:GLY:O	3:A:37:LYS:C	2.47	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
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:416:ASN:O	3:A:417:VAL:C	2.46	0.53
3:A:521:HIS:O	3:A:522:PHE:C	2.47	0.53
3:A:417:VAL:HG12	3:A:418:PRO:N	2.24	0.53
3:A:577:LEU:HB3	3:A:580:MET:CE	2.38	0.53
3:A:37:LYS:HE2	4:A:725:ATP:O2G	2.09	0.53
3:A:567:ALA:O	3:A:570:LEU:HB2	2.09	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:459:GLY:O	3:A:462:ALA:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:585:PHE:C	3:A:585:PHE:CD1	2.81	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
3:A:392:ILE:O	3:A:393:LYS:C	2.45	0.52
3:A:461:LEU:O	3:A:462:ALA:C	2.48	0.52
3:A:582:GLU:HG2	3:A:635:SER:HA	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:49:MET:HE1	3:A:83:ALA:HB1	1.90	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:295:ALA:O	3:A:299:VAL:HG12	2.10	0.51
3:A:443:GLU:OE1	3:A:443:GLU:HA	2.10	0.51
1:Y:11:DT:O4	3:A:626:PHE:HB2	2.10	0.51
3:A:251:ASP:C	3:A:251:ASP:OD1	2.49	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:13:ASN:O	3:A:17:GLN:HG3	2.11	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:187:ASN:O	3:A:188:HIS:C	2.48	0.49
3:A:315:ASN:O	3:A:316:PRO:C	2.51	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:233:TYR:O	3:A:234:THR:C	2.51	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: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:268:LEU:O	3:A:269:SER:C	2.49	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:368:GLU:OE1	3:A:378:TYR:OH	2.17	0.48
3:A:246:ILE:O	3:A:246:ILE:HG12	2.13	0.48
3:A:423:GLY:O	3:A:424:ALA:C	2.51	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:223:ASP:O	3:A:224:GLU:C	2.51	0.48
3:A:349:ARG:HB2	3:A:354:PHE:HZ	1.78	0.48
3:A:585:PHE:O	3:A:586:PRO:C	2.52	0.48
3:A:82:GLY:O	3:A:83:ALA:C	2.52	0.48
3:A:269:SER:O	3:A:272:ARG:N	2.47	0.48
3:A:407:ASP:O	3:A:408:ASP:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:366:VAL:HA	3:A:369:GLU:HB2	1.96	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:444:ALA:C	3:A:446:GLY:H	2.18	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: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: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:444:ALA:O	3:A:445:LEU:C	2.53	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
3:A:112:ASN:O	3:A:113:PHE:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:107:ILE:O	3:A:107:ILE:HG13	2.15	0.46
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:408:ASP:O	3:A:409:LEU:C	2.51	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: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
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:4:LEU:HA	3:A:7:GLN:CD	2.36	0.45
3:A:65:THR:OG1	3:A:68:ALA:HB2	2.16	0.45
3:A:100:LEU:C	3:A:102:ARG:H	2.20	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:541:ILE:HG13	3:A:542:SER:H	1.81	0.45
3:A:141:PRO:O	3:A:142:ARG:C	2.54	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:364:SER:O	3:A:365:ARG:C	2.54	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:429:LYS:NZ	3:A:452:GLY:O	2.44	0.45
3:A:433:TYR:HE1	3:A:436:ASP:C	2.20	0.45
3:A:454:GLY:O	3:A:455:ALA:C	2.55	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:5:SER:OG	3:A:51:GLU:HG2	2.18	0.44
3:A:289:THR:HG22	3:A:292:ILE:CG1	2.47	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
3:A:562:MET:CE	3:A:570:LEU:CD1	2.95	0.44
3:A:582:GLU:CD	3:A:636:ARG:HE	2.16	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:23:THR:OG1	3:A:24:GLU:OE1	2.22	0.44
3:A:145:LEU:O	3:A:148:ILE:HB	2.18	0.44
2:Z:31:DC:C6	2:Z:32:DT:H72	2.53	0.44
3:A:125:MET:HG2	3:A:145:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:145:LEU:O	3:A:148:ILE:N	2.50	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:173:VAL:O	3:A:174:SER:C	2.55	0.43
3:A:31:ALA:O	3:A:32:GLY:C	2.54	0.43
3:A:177:TYR:CD1	3:A:177:TYR:C	2.91	0.43
3:A:210:LEU:O	3:A:210:LEU:HG	2.18	0.43
3:A:417:VAL:O	3:A:418:PRO:C	2.57	0.43
3:A:467:GLN:HE22	3:A:490:LYS:NZ	2.17	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: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:105:ASP:C	3:A:108:GLY:H	2.21	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:388:ASP:HB3	3:A:393:LYS:NZ	2.30	0.43
3:A:49:MET:HE2	3:A:80:LEU:CD2	2.49	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:226:GLN:CD	3:A:226:GLN:H	2.21	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: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:329:GLU:CD	3:A:624:THR:H	2.23	0.42
3:A:369:GLU:O	3:A:373:LYS:HG3	2.19	0.42
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:408:ASP:OD1	3:A:440:SER:OG	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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
3:A:444:ALA:C	3:A:446:GLY:N	2.73	0.41
3:A:580:MET:HE1	3:A:585:PHE:CE2	2.56	0.41
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
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:647:GLU:O	3:A:648:THR:C	2.59	0.41
3:A:130:LYS:O	3:A:130:LYS:HG2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:177:TYR:C	3:A:177:TYR:HD1	2.25	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:426:THR:O	3:A:427:ILE:C	2.58	0.41
3:A:621:GLN:O	3:A:631:MET:HA	2.19	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
3:A:332:GLU:O	3:A:333:ALA:C	2.60	0.40
2:Z:25:DC:C3'	2:Z:25:DC:C6	3.03	0.40
3:A:125:MET:HE3	3:A:145:LEU:HD23	2.02	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:372:LEU:O	3:A:373:LYS:C	2.60	0.40
3:A:12:LEU:HD23	3:A:16:GLN:NE2	2.36	0.40
3:A:37:LYS:HZ3	3:A:37:LYS:N	2.18	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
3:A:444:ALA:O	3:A:447:GLU:N	2.55	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%)	1 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
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

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Mol	Chain	Res	Type
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
3	A	415	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	560/618 (91%)	400 (71%)	160 (29%)	0 1

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	7	GLN
3	A	9	LEU

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Mol	Chain	Res	Type
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	92	PHE
3	A	101	ARG
3	A	105	ASP
3	A	109	ILE
3	A	116	LEU
3	A	122	LEU
3	A	126	LYS
3	A	129	LEU
3	A	133	ASN
3	A	137	LYS
3	A	138	LYS
3	A	139	PHE
3	A	142	ARG
3	A	147	THR
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	177	TYR
3	A	181	GLN
3	A	183	ARG
3	A	184	LEU
3	A	185	LEU
3	A	226	GLN
3	A	230	ARG

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Mol	Chain	Res	Type
3	A	236	VAL
3	A	237	LYS
3	A	243	PHE
3	A	246	ILE
3	A	255	SER
3	A	260	ARG
3	A	263	ASP
3	A	265	GLN
3	A	267	ILE
3	A	269	SER
3	A	270	PHE
3	A	272	ARG
3	A	276	ASN
3	A	279	VAL
3	A	281	LEU
3	A	288	SER
3	A	289	THR
3	A	291	ARG
3	A	293	LEU
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	339	ARG
3	A	341	ARG
3	A	345	GLU
3	A	346	ARG
3	A	348	GLU
3	A	349	ARG
3	A	351	TYR
3	A	352	ARG
3	A	357	LEU
3	A	361	ASN
3	A	363	GLN
3	A	365	ARG

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Mol	Chain	Res	Type
3	A	366	VAL
3	A	368	GLU
3	A	371	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
3	A	413	ARG
3	A	419	LYS
3	A	420	ARG
3	A	422	ILE
3	A	427	ILE
3	A	430	LEU
3	A	433	TYR
3	A	436	ASP
3	A	443	GLU
3	A	447	GLU
3	A	450	MET
3	A	468	LEU
3	A	473	GLN
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	511	ASN
3	A	514	GLU
3	A	516	LEU
3	A	519	THR

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Mol	Chain	Res	Type
3	A	523	GLU
3	A	528	ASP
3	A	530	SER
3	A	535	LEU
3	A	540	LEU
3	A	542	SER
3	A	545	ASP
3	A	552	GLN
3	A	557	ASP
3	A	562	MET
3	A	572	PHE
3	A	573	PRO
3	A	580	MET
3	A	584	ILE
3	A	585	PHE
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	610	ARG
3	A	616	VAL
3	A	619	SER
3	A	621	GLN
3	A	623	ARG
3	A	625	LEU
3	A	635	SER
3	A	644	HIS
3	A	645	LEU
3	A	651	ARG
3	A	652	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) 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	133	ASN

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Mol	Chain	Res	Type
3	A	160	GLN
3	A	178	GLN
3	A	181	GLN
3	A	182	GLN
3	A	187	ASN
3	A	214	GLN
3	A	232	GLN
3	A	245	ASN
3	A	265	GLN
3	A	266	ASN
3	A	284	GLN
3	A	303	ASN
3	A	315	ASN
3	A	375	ASN
3	A	467	GLN
3	A	475	GLN
3	A	511	ASN
3	A	565	HIS

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 monosaccharides 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	-	28,33,33	1.79	8 (28%)	34,52,52	1.66	7 (20%)

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	-	-	12/18/38/38	0/3/3/3

All (8) 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	C8-N7	-3.42	1.28	1.34
4	A	725	ATP	C1'-N9	-2.80	1.43	1.49
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	O4'-C1'	-2.27	1.37	1.40
4	A	725	ATP	C5-N7	-2.26	1.31	1.39
4	A	725	ATP	PB-O2B	-2.09	1.45	1.55

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	725	ATP	O4'-C1'-N9	4.38	114.55	108.75
4	A	725	ATP	C4-C5-N7	3.76	113.31	109.34
4	A	725	ATP	O2B-PB-O3B	3.00	115.38	107.27
4	A	725	ATP	O2B-PB-O3A	2.77	114.76	107.27
4	A	725	ATP	O2'-C2'-C3'	-2.27	104.54	111.82
4	A	725	ATP	C5-C6-N1	-2.23	114.92	120.23
4	A	725	ATP	C1'-N9-C4	2.09	130.31	126.64

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

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Mol	Chain	Res	Type	Atoms
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

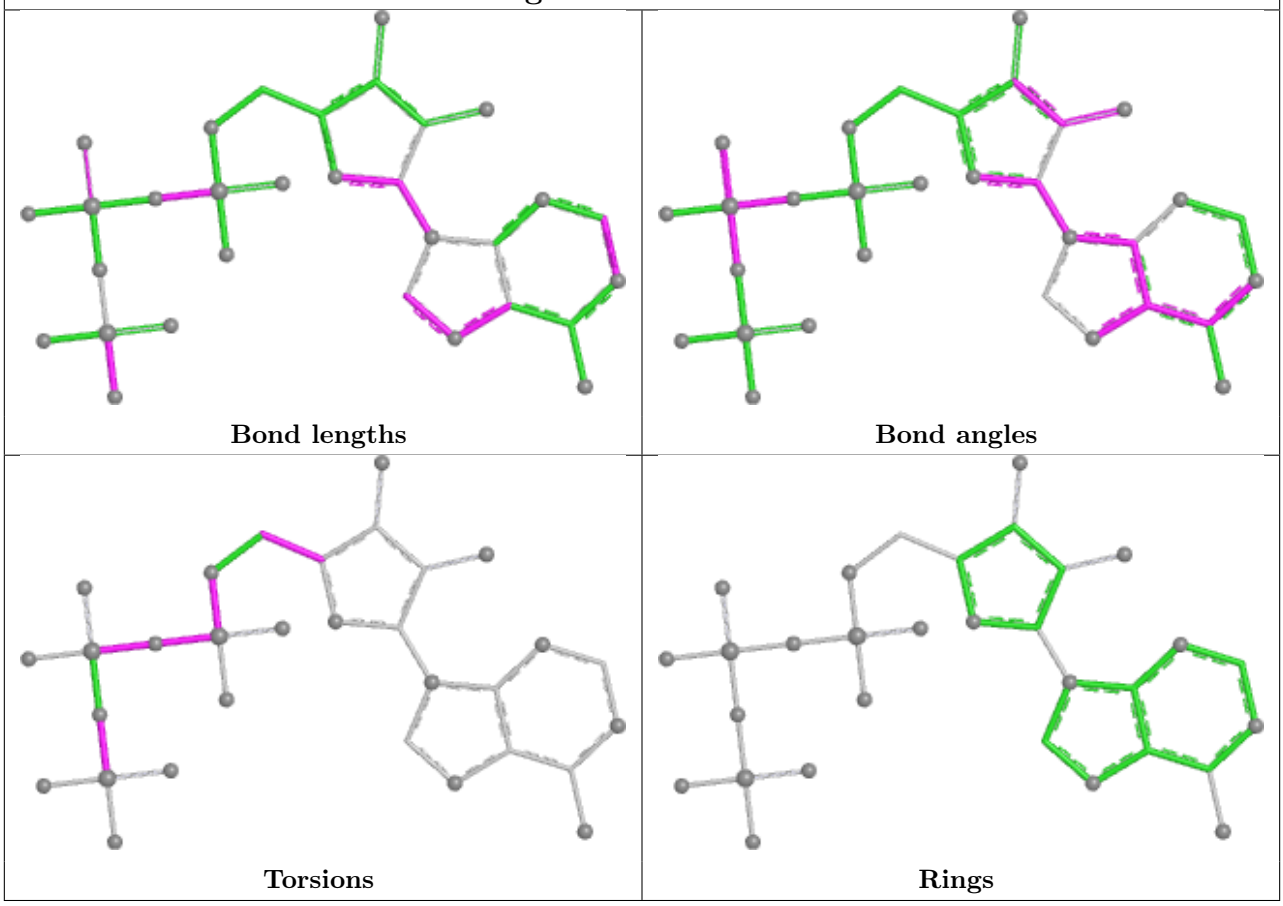
There are no ring outliers.

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 then 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.

Ligand ATP A 725



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.