Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:19 AM GMT

PDB ID	:	3HVR
Title	:	Crystal structure of T. thermophilus Argonaute complexed with DNA guide strand and 19-nt RNA target strand with two Mg2+ at the cleavage site
Authors	:	Wang, Y.; Li, H.; Sheng, G.; Patel, D.J.
Deposited on	:	2009-06-16
Resolution	:	3.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

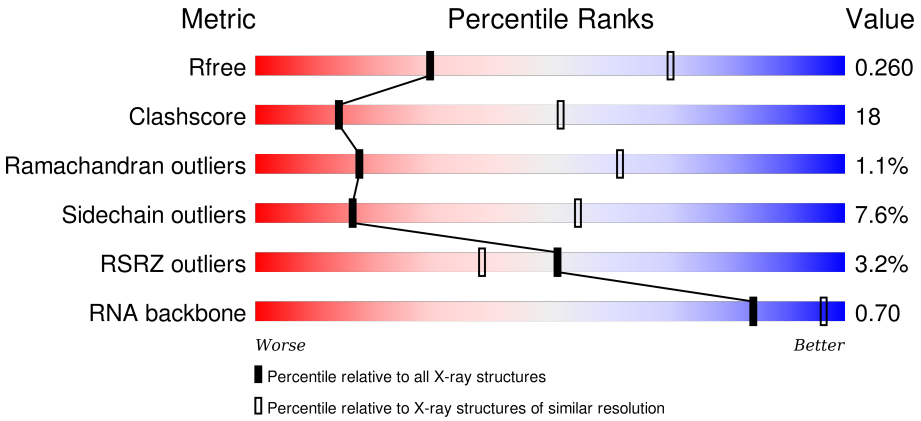
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)
RNA backbone	2183	1004 (3.72-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	685	3%, 62%, 31%
1	B	685	3%, 62%, 31%
2	C	21	29%, 43%, 5%, 24%
2	M	21	29%, 38%, 10%, 24%

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Mol	Chain	Length	Quality of chain
3	D	19	21% 37% 5% 37%
3	N	19	21% 21% 11% 47%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	686	-	-	-	X
4	MG	A	688	-	-	-	X
4	MG	B	686	-	-	-	X
4	MG	B	688	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10637 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	0	0
			4754	3030	889	830	5			
1	B	657	Total	C	N	O	S	0	0	0
			4759	3038	886	830	5			

- Molecule 2 is a DNA chain called 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*TP*GP*AP*TP*AP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	16	Total	C	N	O	P	0	0	0
			338	160	62	100	16			
2	M	16	Total	C	N	O	P	0	0	0
			338	160	62	100	16			

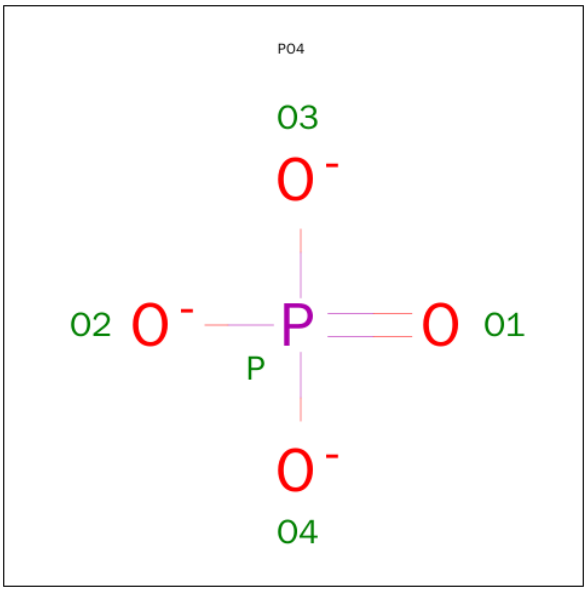
- Molecule 3 is a RNA chain called 5'-R(*UP*AP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP*UP*AP*CP*CP*UP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total	C	N	O	P	0	0	0
			228	101	34	81	12			
3	N	10	Total	C	N	O	P	0	0	0
			204	92	31	71	10			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Mg	0	0
			3	3		
4	A	3	Total	Mg	0	0
			3	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



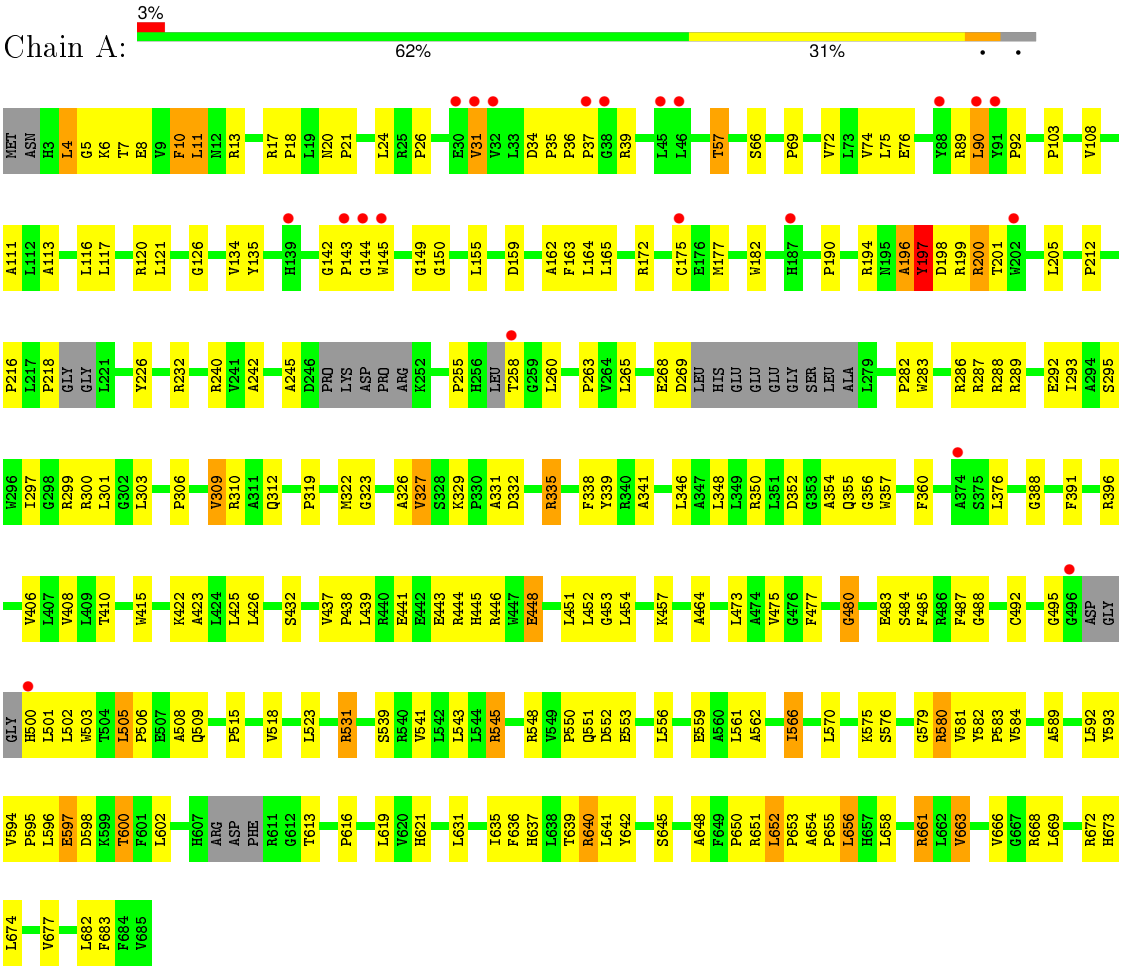
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

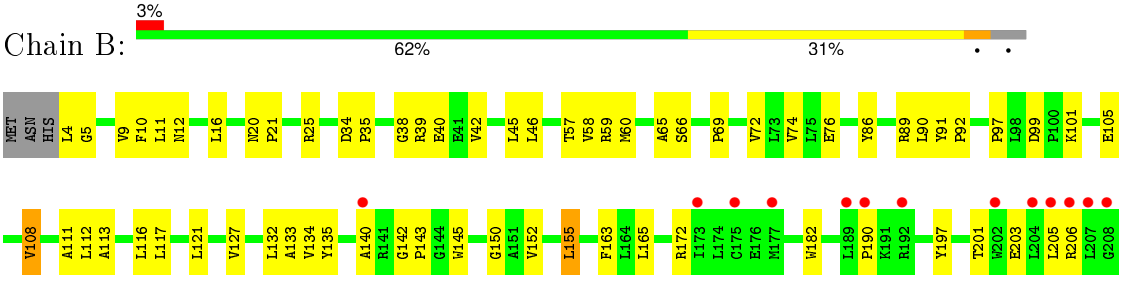
- Molecule 1: Argonaute

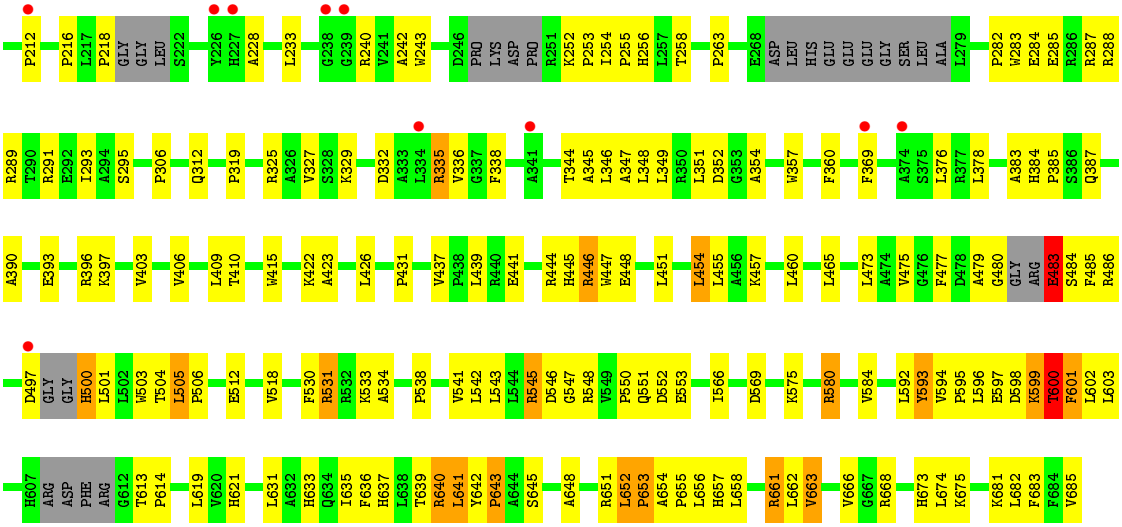
Chain A:



- Molecule 1: Argonaute

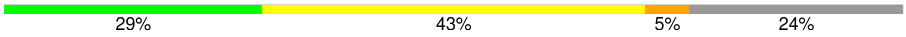
Chain B:





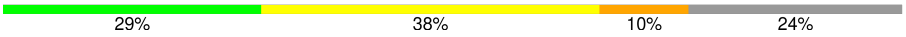
• Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*TP*GP*AP*TP*AP*GP*T)-3'

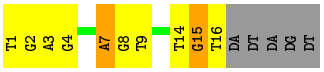
Chain C:



• Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*TP*GP*AP*TP*AP*GP*T)-3'

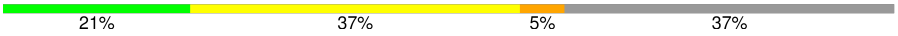
Chain M:

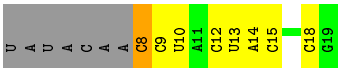




• Molecule 3: 5'-R(*UP*AP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP*UP*AP*CP*CP*UP*CP*G)-3'

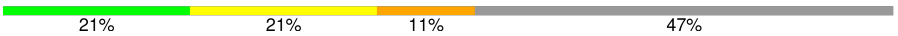
Chain D:

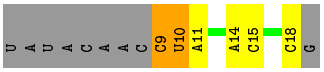




• Molecule 3: 5'-R(*UP*AP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP*UP*AP*CP*CP*UP*CP*G)-3'

Chain N:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.25Å 116.90Å 170.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.68 – 3.21 37.68 – 3.21	Depositor EDS
% Data completeness (in resolution range)	94.4 (37.68-3.21) 94.4 (37.68-3.21)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.226 , 0.273 0.210 , 0.260	Depositor DCC
R_{free} test set	1743 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	100.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 88.0	EDS
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	1 of 34947 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10637	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.33	1/4859 (0.0%)	0.56	14/6624 (0.2%)
1	B	0.39	3/4866 (0.1%)	0.56	11/6635 (0.2%)
2	C	0.88	1/379 (0.3%)	1.21	2/584 (0.3%)
2	M	0.90	2/379 (0.5%)	1.19	2/584 (0.3%)
3	D	0.55	0/251	1.08	1/387 (0.3%)
3	N	0.63	0/225	1.16	2/346 (0.6%)
All	All	0.43	7/10959 (0.1%)	0.67	32/15160 (0.2%)

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
1	A	0	4
1	B	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1	DT	OP3-P	-10.62	1.48	1.61
2	C	1	DT	OP3-P	-10.40	1.48	1.61
2	M	15	DG	C1'-N9	-6.48	1.38	1.47
1	A	199	ARG	C-N	6.13	1.48	1.34
1	B	600	THR	C-N	-5.87	1.20	1.34
1	B	599	LYS	C-N	5.39	1.46	1.34
1	B	601	PHE	C-N	-5.12	1.22	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	483	GLU	O-C-N	-10.33	106.17	122.70
3	N	9	C	P-O3'-C3'	9.18	130.72	119.70
1	B	201	THR	O-C-N	8.26	135.92	122.70
2	M	1	DT	OP1-P-OP2	-8.12	107.41	119.60
2	C	1	DT	OP1-P-OP2	-7.75	107.98	119.60
1	A	197	TYR	O-C-N	-7.19	111.19	122.70
1	A	198	ASP	O-C-N	-6.79	111.84	122.70
1	B	201	THR	CA-C-N	-6.46	102.99	117.20
1	A	200	ARG	O-C-N	-6.45	112.39	122.70
1	B	92	PRO	N-CA-CB	6.41	110.99	103.30
1	B	201	THR	C-N-CA	-6.39	105.73	121.70
2	M	7	DA	P-O3'-C3'	-6.34	112.09	119.70
1	A	218	PRO	N-CA-CB	6.12	110.64	103.30
3	N	9	C	C2'-C3'-O3'	6.08	123.43	113.70
1	B	143	PRO	N-CA-CB	6.06	110.58	103.30
1	A	143	PRO	N-CA-CB	5.97	110.46	103.30
1	B	218	PRO	N-CA-CB	5.97	110.46	103.30
1	A	92	PRO	N-CA-CB	5.96	110.45	103.30
1	B	263	PRO	N-CA-CB	5.93	110.42	103.30
1	B	212	PRO	N-CA-CB	5.88	110.36	103.30
1	A	255	PRO	N-CA-CB	5.84	110.31	103.30
1	A	103	PRO	N-CA-CB	5.82	110.29	103.30
1	B	282	PRO	N-CA-CB	5.82	110.29	103.30
1	A	216	PRO	N-CA-CB	5.78	110.23	103.30
1	B	216	PRO	N-CA-CB	5.77	110.22	103.30
1	A	263	PRO	N-CA-CB	5.75	110.20	103.30
1	A	212	PRO	N-CA-CB	5.75	110.20	103.30
2	C	13	DT	N3-C4-O4	5.68	123.31	119.90
1	A	282	PRO	N-CA-CB	5.33	109.69	103.30
1	A	196	ALA	O-C-N	-5.31	114.20	122.70
1	A	198	ASP	CB-CG-OD2	5.27	123.05	118.30
3	D	8	C	C1'-O4'-C4'	-5.12	105.80	109.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	GLY	Peptide
1	A	197	TYR	Mainchain
1	A	200	ARG	Mainchain
1	A	265	LEU	Mainchain
1	B	483	GLU	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	A	4754	0	4408	170	0
1	B	4759	0	4449	177	0
2	C	338	0	183	6	0
2	M	338	0	183	8	0
3	D	228	0	118	8	0
3	N	204	0	108	9	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	5	0	0	1	0
5	B	5	0	0	1	0
All	All	10637	0	9449	366	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 18.

All (366) 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:B:480:GLY:HA2	1:B:663:VAL:HG13	1.37	1.01
1:A:480:GLY:HA2	1:A:663:VAL:HG13	1.48	0.96
1:B:465:LEU:O	1:B:497:ASP:CB	2.14	0.95
1:A:473:LEU:HB3	1:A:541:VAL:HG12	1.50	0.94
1:B:661:ARG:CG	1:B:661:ARG:HH21	1.81	0.93
1:A:661:ARG:HH21	1:A:661:ARG:HG2	1.35	0.91
1:A:596:LEU:O	1:A:597:GLU:O	1.89	0.90
1:B:465:LEU:HB2	1:B:497:ASP:CB	2.03	0.89
1:B:642:TYR:HD2	1:B:645:SER:HB3	1.38	0.88
1:B:661:ARG:HH21	1:B:661:ARG:HG2	1.40	0.85
1:A:197:TYR:CE1	1:A:232:ARG:NH1	2.46	0.84
1:A:483:GLU:O	1:A:485:PHE:N	2.12	0.82
1:B:473:LEU:HB3	1:B:541:VAL:HG12	1.62	0.81
1:B:598:ASP:O	1:B:599:LYS:HB2	1.80	0.80
1:A:197:TYR:CE1	1:A:232:ARG:CZ	2.65	0.80
1:A:120:ARG:HB3	1:A:301:LEU:HD11	1.62	0.79
1:A:575:LYS:HB3	1:A:651:ARG:HH22	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:HG22	1:A:8:GLU:H	1.45	0.78
1:A:661:ARG:CG	1:A:661:ARG:HH21	1.97	0.78
1:A:453:GLY:O	1:A:457:LYS:HG3	1.86	0.76
1:A:593:TYR:CZ	1:A:595:PRO:HG3	2.20	0.75
1:A:197:TYR:CG	1:A:232:ARG:HD3	2.22	0.75
1:B:465:LEU:H	1:B:497:ASP:CB	2.00	0.75
1:B:117:LEU:HD22	1:B:155:LEU:HB2	1.68	0.74
1:B:242:ALA:HB2	1:B:258:THR:HG22	1.69	0.73
1:B:352:ASP:HB3	1:B:437:VAL:HG21	1.69	0.73
1:A:121:LEU:HD13	1:A:134:VAL:HG21	1.69	0.73
1:A:319:PRO:HA	1:A:637:HIS:CE1	2.24	0.73
1:A:319:PRO:HG2	1:A:640:ARG:HD3	1.70	0.72
1:B:597:GLU:O	1:B:600:THR:HG23	1.89	0.72
3:D:9:C:H2'	3:D:10:U:H6	1.54	0.71
1:B:319:PRO:HG2	1:B:640:ARG:HD3	1.71	0.71
1:B:182:TRP:HZ3	1:B:190:PRO:HD3	1.56	0.70
1:B:287:ARG:O	1:B:291:ARG:HG3	1.92	0.70
1:B:666:VAL:HG22	1:B:674:LEU:HD11	1.72	0.70
1:B:12:ASN:HD22	1:B:580:ARG:HB2	1.57	0.69
1:A:197:TYR:CZ	1:A:232:ARG:NH1	2.60	0.69
1:B:444:ARG:O	1:B:448:GLU:HB2	1.92	0.69
1:B:58:VAL:HG11	1:B:111:ALA:HB1	1.75	0.69
1:B:465:LEU:CB	1:B:497:ASP:CB	2.71	0.69
1:B:58:VAL:HG23	1:B:112:LEU:HD23	1.75	0.69
1:A:113:ALA:HB1	1:A:155:LEU:HD13	1.75	0.68
1:A:654:ALA:HB3	1:A:655:PRO:HD3	1.74	0.68
1:B:635:ILE:HG23	1:B:653:PRO:HG3	1.77	0.67
1:B:423:ALA:HB1	1:B:673:HIS:CE1	2.30	0.67
1:A:289:ARG:O	1:A:293:ILE:HG12	1.95	0.67
1:B:483:GLU:O	1:B:484:SER:C	2.33	0.66
1:B:346:LEU:HD23	1:B:454:LEU:HD13	1.78	0.66
1:A:642:TYR:HD2	1:A:645:SER:HB3	1.61	0.66
1:B:182:TRP:CZ3	1:B:190:PRO:HG3	2.32	0.65
2:M:8:DG:H3'	2:M:9:DT:H71	1.78	0.65
1:A:240:ARG:O	1:A:258:THR:HG23	1.97	0.65
1:B:480:GLY:HA2	1:B:663:VAL:CG1	2.20	0.65
1:B:465:LEU:CA	1:B:497:ASP:CB	2.75	0.64
2:M:15:DG:H2"	2:M:16:DT:H72	1.79	0.64
1:B:422:LYS:O	1:B:426:LEU:HD13	1.97	0.64
1:A:415:TRP:HZ3	1:A:668:ARG:HD2	1.61	0.64
1:B:661:ARG:CG	1:B:661:ARG:NH2	2.51	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LYS:HB3	1:A:651:ARG:NH2	2.12	0.63
1:A:445:HIS:NE2	3:D:18:C:H2'	2.13	0.63
1:A:635:ILE:HG23	1:A:653:PRO:HG3	1.80	0.63
1:A:312:GLN:CD	1:A:312:GLN:H	2.02	0.63
1:B:465:LEU:N	1:B:497:ASP:CB	2.62	0.62
1:B:652:LEU:HB2	1:B:653:PRO:HD2	1.80	0.62
1:B:633:HIS:O	1:B:637:HIS:HD2	1.82	0.62
1:A:197:TYR:CD2	1:A:232:ARG:HD3	2.35	0.62
1:B:360:PHE:CG	1:B:441:GLU:HG2	2.35	0.62
1:A:197:TYR:CD1	1:A:232:ARG:CZ	2.83	0.61
1:A:672:ARG:HA	1:B:505:LEU:HD12	1.82	0.61
1:A:621:HIS:ND1	1:A:631:LEU:HD11	2.15	0.61
1:A:39:ARG:NH1	5:B:689:PO4:O3	2.33	0.61
1:B:38:GLY:C	1:B:40:GLU:H	2.05	0.60
1:B:329:LYS:HG2	1:B:332:ASP:OD2	2.02	0.60
1:A:155:LEU:HD21	1:A:163:PHE:HB3	1.83	0.60
1:B:57:THR:HG22	1:B:66:SER:CB	2.32	0.60
1:A:531:ARG:HD3	1:A:531:ARG:C	2.23	0.59
1:A:350:ARG:HD3	1:A:354:ALA:O	2.02	0.59
1:B:601:PHE:HD2	1:B:602:LEU:O	1.86	0.59
1:A:543:LEU:N	1:A:543:LEU:HD12	2.17	0.59
1:B:445:HIS:NE2	3:N:18:C:H2'	2.17	0.59
1:A:75:LEU:HA	1:A:90:LEU:HD23	1.85	0.58
3:N:9:C:O2'	3:N:10:U:H5'	2.04	0.58
1:A:242:ALA:HB2	1:A:258:THR:HG22	1.86	0.58
1:A:322:MET:HG3	1:A:326:ALA:HA	1.85	0.58
1:B:45:LEU:HD11	1:B:86:TYR:CD2	2.37	0.58
1:A:619:LEU:HD12	1:A:619:LEU:N	2.19	0.57
1:B:542:LEU:C	1:B:543:LEU:HD12	2.24	0.57
1:B:135:TYR:HA	1:B:150:GLY:HA3	1.87	0.57
1:B:500:HIS:NE2	1:B:533:LYS:HG3	2.19	0.57
1:B:12:ASN:ND2	1:B:580:ARG:HB2	2.19	0.57
1:B:596:LEU:O	1:B:597:GLU:C	2.41	0.57
3:D:9:C:O2'	3:D:10:U:H5'	2.05	0.57
1:A:396:ARG:NH1	1:B:531:ARG:HH12	2.03	0.57
1:A:10:PHE:HB3	1:A:310:ARG:HA	1.87	0.56
1:A:13:ARG:HB2	1:A:309:VAL:CG1	2.35	0.56
1:B:661:ARG:HH21	1:B:661:ARG:HG3	1.65	0.56
1:B:661:ARG:HD2	1:B:661:ARG:N	2.19	0.56
1:A:17:ARG:HE	1:A:303:LEU:HD23	1.70	0.56
1:B:360:PHE:H	1:B:360:PHE:HD1	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:MET:HG3	1:A:326:ALA:N	2.20	0.56
1:B:501:LEU:HD21	1:B:641:LEU:HD13	1.87	0.55
1:B:348:LEU:HD11	1:B:409:LEU:HD12	1.88	0.55
1:A:437:VAL:O	1:A:439:LEU:N	2.39	0.55
1:A:661:ARG:CG	1:A:661:ARG:NH2	2.65	0.55
1:A:666:VAL:HG22	1:A:674:LEU:HD11	1.89	0.55
1:A:339:TYR:CE1	1:A:464:ALA:HB3	2.42	0.55
1:B:338:PHE:CZ	1:B:455:LEU:HD13	2.41	0.55
1:A:589:ALA:HB3	1:A:592:LEU:HD11	1.89	0.55
1:A:4:LEU:HD22	1:A:4:LEU:O	2.06	0.55
1:A:598:ASP:O	1:A:600:THR:HG22	2.07	0.55
1:B:415:TRP:HZ3	1:B:668:ARG:HD2	1.71	0.55
1:B:530:PHE:CD2	1:B:538:PRO:HG3	2.42	0.54
2:M:3:DA:H2'	2:M:4:DG:C8	2.42	0.54
2:M:14:DT:C4	2:M:15:DG:C2	2.95	0.54
1:B:89:ARG:HG3	1:B:91:TYR:CE1	2.42	0.54
1:A:18:PRO:HA	1:A:162:ALA:HA	1.89	0.54
1:A:645:SER:HB2	1:A:648:ALA:O	2.07	0.54
1:B:530:PHE:CG	1:B:538:PRO:HG3	2.43	0.54
1:A:487:PHE:CE1	1:A:508:ALA:HB2	2.43	0.54
1:A:422:LYS:O	1:A:426:LEU:HD13	2.07	0.54
1:B:465:LEU:C	1:B:497:ASP:CB	2.76	0.54
1:B:551:GLN:O	1:B:552:ASP:HB2	2.08	0.54
1:A:501:LEU:HD13	1:A:658:LEU:HD11	1.90	0.54
1:A:652:LEU:HB2	1:A:653:PRO:HD2	1.90	0.53
1:A:332:ASP:HA	1:A:335:ARG:HD3	1.89	0.53
1:B:319:PRO:HA	1:B:637:HIS:CE1	2.43	0.53
2:C:13:DT:H73	2:C:14:DT:C4	2.43	0.53
1:B:483:GLU:O	1:B:485:PHE:N	2.42	0.53
1:A:503:TRP:HZ2	1:A:677:VAL:HG12	1.73	0.53
1:A:505:LEU:HG	1:B:675:LYS:HB2	1.91	0.53
1:A:268:GLU:O	1:A:269:ASP:CB	2.57	0.53
1:B:34:ASP:HA	1:B:35:PRO:C	2.29	0.53
1:B:295:SER:HA	1:B:306:PRO:HG2	1.90	0.53
1:A:539:SER:O	1:A:566:ILE:HD12	2.09	0.53
1:B:640:ARG:HD2	1:B:640:ARG:N	2.24	0.53
1:A:621:HIS:CE1	1:A:631:LEU:HD11	2.44	0.53
1:B:501:LEU:HD13	1:B:658:LEU:HD11	1.91	0.53
1:A:322:MET:HG3	1:A:326:ALA:CA	2.38	0.53
1:B:446:ARG:HD2	2:M:2:DG:C8	2.44	0.52
1:A:327:VAL:CG2	1:A:332:ASP:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASN:HB2	1:A:21:PRO:HD2	1.89	0.52
1:A:10:PHE:HA	1:A:310:ARG:HA	1.91	0.52
1:B:437:VAL:O	1:B:439:LEU:N	2.41	0.52
1:B:594:VAL:O	1:B:601:PHE:HB2	2.10	0.52
1:B:357:TRP:CZ2	1:B:378:LEU:HD12	2.44	0.52
1:B:657:HIS:O	1:B:661:ARG:HD3	2.09	0.52
1:A:7:THR:HG22	1:A:8:GLU:N	2.20	0.52
1:B:57:THR:HG22	1:B:66:SER:OG	2.10	0.52
1:A:24:LEU:C	1:A:26:PRO:HD3	2.30	0.52
1:A:545:ARG:NH1	1:A:553:GLU:OE1	2.42	0.52
1:B:480:GLY:CA	1:B:663:VAL:HG13	2.26	0.52
1:A:360:PHE:CG	1:A:441:GLU:HG2	2.45	0.51
2:C:15:DG:H2"	2:C:16:DT:OP2	2.10	0.51
1:B:58:VAL:HG12	1:B:59:ARG:H	1.73	0.51
3:D:14:A:H2'	3:D:15:C:C6	2.46	0.51
1:B:390:ALA:O	1:B:393:GLU:HB3	2.10	0.51
1:A:8:GLU:O	1:A:584:VAL:HG23	2.11	0.51
1:A:355:GLN:HG2	1:A:356:GLY:N	2.26	0.51
1:A:360:PHE:CD1	1:A:441:GLU:HG2	2.46	0.51
1:B:140:ALA:HB1	1:B:145:TRP:HZ3	1.75	0.51
1:B:543:LEU:N	1:B:543:LEU:HD12	2.25	0.51
1:A:483:GLU:O	1:A:484:SER:C	2.48	0.51
1:B:69:PRO:O	1:B:72:VAL:HG22	2.11	0.51
2:C:7:DA:H2'	2:C:8:DG:H8	1.75	0.51
1:A:443:GLU:O	1:A:446:ARG:HB2	2.11	0.51
1:A:523:LEU:HD21	1:A:561:LEU:HD11	1.93	0.50
1:A:121:LEU:HD13	1:A:134:VAL:CG2	2.39	0.50
1:B:12:ASN:O	1:B:12:ASN:OD1	2.29	0.50
1:B:16:LEU:HB2	1:B:163:PHE:HB2	1.94	0.50
3:N:9:C:H2'	3:N:10:U:H6	1.77	0.50
1:B:383:ALA:HA	1:B:387:GLN:OE1	2.12	0.50
1:B:12:ASN:C	1:B:12:ASN:OD1	2.49	0.50
1:A:144:GLY:O	1:A:175:CYS:HB2	2.12	0.50
1:A:286:ARG:HD2	1:A:613:THR:HG21	1.93	0.50
1:A:652:LEU:HB2	1:A:653:PRO:CD	2.41	0.49
1:B:58:VAL:HG12	1:B:59:ARG:N	2.27	0.49
1:B:105:GLU:O	1:B:108:VAL:HG13	2.11	0.49
1:A:425:LEU:HD12	1:A:432:SER:HB3	1.94	0.49
1:B:182:TRP:CZ3	1:B:190:PRO:CG	2.95	0.49
1:B:682:LEU:O	1:B:685:VAL:HG22	2.13	0.49
1:B:197:TYR:OH	1:B:256:HIS:CE1	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:TYR:CZ	1:B:595:PRO:HG3	2.48	0.49
1:A:475:VAL:HG23	1:A:477:PHE:CE1	2.48	0.49
1:B:142:GLY:HA3	1:B:145:TRP:CZ2	2.48	0.48
1:A:640:ARG:HD2	1:A:640:ARG:N	2.28	0.48
1:A:113:ALA:HB1	1:A:155:LEU:CD1	2.42	0.48
1:B:285:GLU:HG2	1:B:288:ARG:NH2	2.29	0.48
1:A:556:LEU:O	1:A:556:LEU:HD23	2.13	0.48
1:A:636:PHE:O	1:A:639:THR:HB	2.13	0.48
1:B:642:TYR:CD2	1:B:645:SER:HB3	2.30	0.48
1:B:12:ASN:ND2	1:B:580:ARG:H	2.11	0.48
1:B:172:ARG:HD2	2:M:9:DT:OP1	2.13	0.48
1:B:545:ARG:NH1	1:B:553:GLU:OE1	2.46	0.48
1:A:74:VAL:HG12	1:A:76:GLU:O	2.13	0.48
1:A:339:TYR:CD1	1:A:464:ALA:HB3	2.48	0.48
1:A:327:VAL:HG23	1:A:332:ASP:HB2	1.94	0.48
1:A:135:TYR:CD2	1:A:150:GLY:HA3	2.48	0.48
1:B:25:ARG:HH11	1:B:97:PRO:HG3	1.78	0.48
1:A:4:LEU:O	1:A:6:LYS:N	2.46	0.48
1:B:289:ARG:O	1:B:293:ILE:HG12	2.13	0.48
1:B:99:ASP:OD2	1:B:101:LYS:HG2	2.13	0.48
3:N:10:U:C2	3:N:11:A:C8	3.02	0.48
1:B:661:ARG:NH2	1:B:661:ARG:HG2	2.18	0.47
1:B:57:THR:HG22	1:B:66:SER:HB2	1.97	0.47
1:A:594:VAL:HB	1:A:602:LEU:HB2	1.96	0.47
1:A:480:GLY:CA	1:A:663:VAL:HG13	2.31	0.47
1:B:113:ALA:HB1	1:B:155:LEU:HD13	1.95	0.47
1:B:548:ARG:O	1:B:550:PRO:HD3	2.13	0.47
1:B:203:GLU:O	1:B:205:LEU:HD13	2.14	0.47
1:B:661:ARG:NH2	1:B:661:ARG:HG3	2.25	0.47
1:B:38:GLY:C	1:B:40:GLU:N	2.68	0.47
1:B:134:VAL:O	1:B:150:GLY:HA3	2.14	0.47
1:B:531:ARG:O	1:B:534:ALA:O	2.31	0.47
3:D:12:C:H2'	3:D:13:U:C6	2.49	0.47
1:A:108:VAL:O	1:A:111:ALA:HB3	2.14	0.47
1:A:338:PHE:HB2	1:A:341:ALA:HB2	1.96	0.47
1:A:483:GLU:C	1:A:485:PHE:H	2.17	0.47
1:B:444:ARG:HA	1:B:447:TRP:NE1	2.30	0.47
1:A:76:GLU:HG2	1:A:89:ARG:HD2	1.96	0.47
1:A:299:ARG:HH12	1:A:300:ARG:HH11	1.62	0.47
1:A:331:ALA:HA	1:A:452:LEU:HD11	1.97	0.47
1:A:182:TRP:HZ3	1:A:190:PRO:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:9:C:C2	3:N:10:U:C6	3.03	0.47
1:B:121:LEU:HD13	1:B:134:VAL:HG21	1.96	0.47
2:M:2:DG:H2'	2:M:3:DA:C8	2.50	0.47
1:B:60:MET:SD	1:B:108:VAL:HG21	2.55	0.47
1:A:475:VAL:HG23	1:A:477:PHE:HE1	1.79	0.47
1:A:548:ARG:O	1:A:550:PRO:HD3	2.15	0.46
1:B:133:ALA:HA	1:B:152:VAL:HA	1.96	0.46
1:B:325:ARG:HB2	1:B:336:VAL:CG1	2.45	0.46
1:B:410:THR:N	1:B:437:VAL:HG23	2.30	0.46
1:A:475:VAL:HG12	1:A:492:CYS:HA	1.96	0.46
1:B:327:VAL:CG2	1:B:332:ASP:HB2	2.46	0.46
1:A:35:PRO:HA	1:A:36:PRO:HD3	1.85	0.46
1:B:503:TRP:CZ2	1:B:683:PHE:HE1	2.33	0.46
1:A:295:SER:HA	1:A:306:PRO:HG2	1.98	0.46
1:B:45:LEU:HD11	1:B:86:TYR:CE2	2.50	0.46
1:A:329:LYS:HB3	1:A:329:LYS:HE2	1.79	0.46
1:A:350:ARG:HB3	1:A:352:ASP:OD1	2.16	0.46
1:A:36:PRO:HA	1:A:37:PRO:HD3	1.82	0.45
1:B:654:ALA:HB3	1:B:655:PRO:HD3	1.98	0.45
1:B:545:ARG:C	1:B:545:ARG:HD3	2.37	0.45
1:B:206:ARG:HG3	1:B:243:TRP:HB2	1.98	0.45
1:A:388:GLY:O	1:A:391:PHE:HB3	2.17	0.45
1:A:551:GLN:O	1:A:552:ASP:HB2	2.16	0.45
1:B:415:TRP:CZ3	1:B:668:ARG:HD2	2.49	0.45
1:A:76:GLU:HG2	1:A:89:ARG:CD	2.47	0.45
1:B:9:VAL:HA	1:B:584:VAL:HG23	1.99	0.45
1:B:592:LEU:O	1:B:603:LEU:HD12	2.16	0.45
1:A:172:ARG:HD2	2:C:9:DT:OP1	2.15	0.45
1:B:479:ALA:O	1:B:480:GLY:O	2.34	0.45
1:B:38:GLY:O	1:B:40:GLU:N	2.50	0.45
1:A:142:GLY:HA3	1:A:145:TRP:CZ2	2.51	0.45
1:B:410:THR:CA	1:B:437:VAL:HG23	2.47	0.45
1:A:69:PRO:O	1:A:72:VAL:HG22	2.17	0.45
1:A:348:LEU:HB2	1:A:357:TRP:CE2	2.51	0.45
1:A:31:VAL:HG13	1:A:90:LEU:CD1	2.47	0.44
1:B:132:LEU:HD12	1:B:132:LEU:N	2.32	0.44
1:B:116:LEU:HD23	1:B:116:LEU:C	2.37	0.44
1:B:312:GLN:H	1:B:312:GLN:CD	2.21	0.44
1:A:444:ARG:O	1:A:448:GLU:HB2	2.16	0.44
1:B:360:PHE:CD1	1:B:360:PHE:N	2.83	0.44
1:B:140:ALA:HB1	1:B:145:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:14:A:H2'	3:N:15:C:C6	2.52	0.44
1:B:503:TRP:CE2	1:B:683:PHE:HE1	2.35	0.44
1:A:515:PRO:HB2	1:A:518:VAL:CG2	2.47	0.44
1:B:42:VAL:O	1:B:46:LEU:HB3	2.17	0.44
1:A:656:LEU:HA	1:A:656:LEU:HD23	1.54	0.44
1:A:197:TYR:CD1	1:A:232:ARG:NE	2.85	0.44
1:A:593:TYR:O	1:A:595:PRO:HD3	2.17	0.44
1:B:240:ARG:O	1:B:258:THR:HG23	2.18	0.44
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.74	0.44
1:B:345:ALA:C	1:B:346:LEU:HD12	2.37	0.44
1:B:503:TRP:HB2	1:B:662:LEU:HD22	2.00	0.44
1:B:545:ARG:HD3	1:B:546:ASP:N	2.33	0.43
1:B:20:ASN:HB2	1:B:21:PRO:HD2	1.99	0.43
1:B:384:HIS:ND1	1:B:385:PRO:HD2	2.33	0.43
1:A:593:TYR:CE2	1:A:595:PRO:HG3	2.51	0.43
1:B:506:PRO:HG2	1:B:666:VAL:HG21	2.00	0.43
1:A:652:LEU:CB	1:A:653:PRO:CD	2.96	0.43
1:A:589:ALA:O	1:A:592:LEU:HD13	2.18	0.43
1:A:287:ARG:HB3	1:A:582:TYR:CD1	2.53	0.43
1:A:515:PRO:HB2	1:A:518:VAL:HG23	1.99	0.43
1:B:384:HIS:CG	1:B:385:PRO:HD2	2.53	0.43
1:B:652:LEU:CB	1:B:653:PRO:HD2	2.46	0.43
1:A:194:ARG:CB	1:A:201:THR:HG22	2.49	0.43
1:A:196:ALA:HB3	1:A:260:LEU:O	2.19	0.43
1:B:636:PHE:O	1:B:639:THR:HB	2.19	0.43
1:B:349:LEU:HD21	1:B:351:LEU:HD21	2.01	0.43
1:A:117:LEU:HD22	1:A:155:LEU:HB2	2.00	0.43
1:B:329:LYS:HB3	1:B:329:LYS:HE2	1.82	0.43
1:B:645:SER:HB2	1:B:648:ALA:O	2.19	0.43
1:A:652:LEU:HD12	1:A:652:LEU:H	1.84	0.43
1:B:475:VAL:HG23	1:B:477:PHE:HE1	1.84	0.43
1:B:431:PRO:HB2	1:B:457:LYS:HB3	2.00	0.43
1:A:457:LYS:HG2	1:A:682:LEU:O	2.18	0.43
1:A:543:LEU:CD1	1:A:543:LEU:N	2.82	0.43
1:A:226:TYR:C	1:A:226:TYR:CD2	2.92	0.43
1:A:288:ARG:HD2	1:A:289:ARG:HH12	1.84	0.42
1:B:531:ARG:C	1:B:531:ARG:HD3	2.40	0.42
1:B:621:HIS:CE1	1:B:631:LEU:HD11	2.55	0.42
1:B:74:VAL:HG12	1:B:76:GLU:O	2.19	0.42
1:B:347:ALA:HB2	1:B:403:VAL:HG11	2.01	0.42
1:B:332:ASP:HA	1:B:335:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD13	1:A:13:ARG:HG3	2.00	0.42
1:A:205:LEU:HD11	1:A:245:ALA:HB2	2.02	0.42
1:A:116:LEU:C	1:A:116:LEU:HD23	2.40	0.42
1:B:327:VAL:HG23	1:B:332:ASP:HB2	2.01	0.42
2:C:7:DA:H2'	2:C:8:DG:C8	2.53	0.42
1:A:4:LEU:HD12	1:A:4:LEU:H	1.84	0.42
3:D:8:C:O2	3:D:8:C:H2'	2.20	0.42
1:A:408:VAL:HG12	1:A:410:THR:HG22	2.02	0.42
1:A:576:SER:O	3:D:8:C:H5'	2.20	0.42
1:B:344:THR:HG22	1:B:369:PHE:HE2	1.84	0.42
1:B:455:LEU:HD22	1:B:460:LEU:HD22	2.00	0.42
1:B:344:THR:HG22	1:B:369:PHE:CE2	2.54	0.42
1:B:575:LYS:HB3	1:B:651:ARG:HH22	1.83	0.42
1:A:346:LEU:HD23	1:A:454:LEU:HD13	2.01	0.42
1:B:656:LEU:HA	1:B:656:LEU:HD23	1.69	0.42
1:B:546:ASP:OD1	1:B:575:LYS:HE3	2.20	0.42
1:B:619:LEU:N	1:B:619:LEU:HD12	2.35	0.42
1:B:182:TRP:CZ3	1:B:190:PRO:HD3	2.46	0.41
1:A:10:PHE:CB	1:A:310:ARG:HA	2.49	0.41
1:A:580:ARG:O	1:A:581:VAL:HG23	2.19	0.41
1:A:297:ILE:O	1:A:301:LEU:HB2	2.21	0.41
1:A:672:ARG:CZ	1:B:518:VAL:HG22	2.50	0.41
1:A:621:HIS:ND1	1:A:631:LEU:CD1	2.83	0.41
1:B:228:ALA:HA	1:B:233:LEU:CB	2.50	0.41
1:A:10:PHE:HB3	1:A:310:ARG:CA	2.50	0.41
1:B:60:MET:SD	1:B:65:ALA:HB2	2.60	0.41
1:B:205:LEU:HB3	1:B:206:ARG:HG2	2.02	0.41
1:A:488:GLY:HA3	1:A:509:GLN:NE2	2.35	0.41
1:B:252:LYS:HA	1:B:253:PRO:HD3	1.87	0.41
1:A:506:PRO:HG2	1:A:666:VAL:HG21	2.03	0.41
1:B:369:PHE:HE1	1:B:455:LEU:HD21	1.84	0.41
1:A:639:THR:HG23	1:A:650:PRO:O	2.20	0.41
3:D:14:A:H2'	3:D:15:C:H6	1.85	0.41
1:B:197:TYR:OH	1:B:256:HIS:HE1	2.02	0.41
3:N:9:C:C2	3:N:10:U:C5	3.09	0.41
1:A:4:LEU:CD1	1:A:4:LEU:H	2.34	0.41
1:B:486:ARG:NH1	1:B:512:GLU:HB2	2.35	0.41
1:B:642:TYR:HA	1:B:643:PRO:HD3	1.72	0.41
1:A:13:ARG:HB2	1:A:309:VAL:HG11	2.01	0.41
1:B:431:PRO:HG2	1:B:681:LYS:HD3	2.02	0.41
1:B:396:ARG:HH12	1:B:397:LYS:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:PRO:HA	1:A:637:HIS:HE1	1.80	0.41
1:A:288:ARG:O	1:A:292:GLU:HG3	2.20	0.41
2:M:7:DA:C2	3:N:14:A:C2	3.08	0.41
1:A:423:ALA:HB1	1:A:673:HIS:CE1	2.56	0.41
1:B:254:ILE:HA	1:B:255:PRO:HD3	1.77	0.41
1:A:197:TYR:OH	5:A:689:PO4:P	2.79	0.41
1:A:352:ASP:HB3	1:A:437:VAL:HG21	2.03	0.41
1:A:582:TYR:HA	1:A:583:PRO:HD3	1.87	0.40
1:B:613:THR:HA	1:B:614:PRO:HD3	1.87	0.40
1:A:155:LEU:HA	1:A:164:LEU:O	2.21	0.40
1:A:57:THR:HG22	1:A:66:SER:OG	2.21	0.40
1:A:579:GLY:O	1:A:616:PRO:HD2	2.21	0.40
1:B:661:ARG:N	1:B:661:ARG:CD	2.84	0.40
1:A:312:GLN:CD	1:A:312:GLN:N	2.73	0.40
1:A:503:TRP:CZ2	1:A:683:PHE:HE1	2.39	0.40
1:A:34:ASP:HA	1:A:35:PRO:C	2.41	0.40
2:C:3:DA:H2'	2:C:4:DG:C8	2.57	0.40
1:A:319:PRO:HA	1:A:637:HIS:ND1	2.36	0.40
1:B:284:GLU:HA	1:B:287:ARG:HD2	2.03	0.40
1:B:547:GLY:HA2	3:N:9:C:OP1	2.20	0.40
1:A:559:GLU:O	1:A:562:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	646/685 (94%)	567 (88%)	72 (11%)	7 (1%)	17	62
1	B	643/685 (94%)	577 (90%)	59 (9%)	7 (1%)	17	62
All	All	1289/1370 (94%)	1144 (89%)	131 (10%)	14 (1%)	17	62

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	597	GLU
1	A	5	GLY
1	B	39	ARG
1	B	354	ALA
1	A	480	GLY
1	B	446	ARG
1	A	126	GLY
1	B	5	GLY
1	A	495	GLY
1	B	653	PRO
1	A	323	GLY
1	B	127	VAL
1	A	438	PRO
1	B	643	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/549 (73%)	367 (92%)	33 (8%)	14	49
1	B	407/549 (74%)	379 (93%)	28 (7%)	19	59
All	All	807/1098 (74%)	746 (92%)	61 (8%)	16	55

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	10	PHE
1	A	11	LEU
1	A	31	VAL
1	A	57	THR
1	A	90	LEU
1	A	159	ASP
1	A	165	LEU
1	A	177	MET

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Mol	Chain	Res	Type
1	A	283	TRP
1	A	309	VAL
1	A	327	VAL
1	A	335	ARG
1	A	376	LEU
1	A	406	VAL
1	A	448	GLU
1	A	451	LEU
1	A	500	HIS
1	A	502	LEU
1	A	505	LEU
1	A	531	ARG
1	A	545	ARG
1	A	566	ILE
1	A	570	LEU
1	A	580	ARG
1	A	600	THR
1	A	640	ARG
1	A	641	LEU
1	A	652	LEU
1	A	656	LEU
1	A	661	ARG
1	A	663	VAL
1	A	669	LEU
1	B	4	LEU
1	B	10	PHE
1	B	11	LEU
1	B	90	LEU
1	B	108	VAL
1	B	155	LEU
1	B	165	LEU
1	B	283	TRP
1	B	335	ARG
1	B	376	LEU
1	B	406	VAL
1	B	451	LEU
1	B	454	LEU
1	B	500	HIS
1	B	504	THR
1	B	505	LEU
1	B	531	ARG
1	B	545	ARG

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Mol	Chain	Res	Type
1	B	566	ILE
1	B	569	ASP
1	B	580	ARG
1	B	593	TYR
1	B	600	THR
1	B	640	ARG
1	B	641	LEU
1	B	652	LEU
1	B	661	ARG
1	B	663	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	382	HIS
1	A	404	GLN
1	A	509	GLN
1	B	256	HIS
1	B	355	GLN
1	B	404	GLN
1	B	637	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	10/19 (52%)	0	0
3	N	9/19 (47%)	1 (11%)	0
All	All	19/38 (50%)	1 (5%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	N	10	U

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PO4	A	689	-	4,4,4	2.03	3 (75%)	6,6,6	0.27	0
5	PO4	B	689	-	4,4,4	2.03	3 (75%)	6,6,6	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	A	689	-	-	0/0/0/0	0/0/0/0
5	PO4	B	689	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	689	PO4	P-O1	2.08	1.61	1.52
5	A	689	PO4	P-O1	2.08	1.61	1.52
5	A	689	PO4	P-O2	2.24	1.61	1.53
5	B	689	PO4	P-O2	2.25	1.61	1.53
5	B	689	PO4	P-O3	2.26	1.61	1.53
5	A	689	PO4	P-O3	2.27	1.61	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	689	PO4	1	0
5	B	689	PO4	1	0

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	660/685 (96%)	0.04	21 (3%) 51 38	54, 93, 143, 187	0
1	B	657/685 (95%)	0.01	23 (3%) 48 34	55, 89, 151, 292	0
2	C	16/21 (76%)	-0.21	0 100 100	76, 101, 134, 140	0
2	M	16/21 (76%)	-0.28	0 100 100	81, 98, 140, 154	0
3	D	12/19 (63%)	-0.47	0 100 100	98, 116, 124, 159	0
3	N	10/19 (52%)	-0.33	0 100 100	105, 113, 117, 118	0
All	All	1371/1450 (94%)	0.01	44 (3%) 51 38	54, 92, 148, 292	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	GLY	8.3
1	B	190	PRO	5.2
1	B	202	TRP	4.6
1	B	207	LEU	4.0
1	A	46	LEU	3.6
1	A	90	LEU	3.5
1	B	341	ALA	3.5
1	A	145	TRP	3.4
1	A	202	TRP	3.4
1	A	258	THR	3.3
1	A	37	PRO	3.2
1	A	374	ALA	3.2
1	B	204	LEU	3.0
1	A	175	CYS	3.0
1	B	206	ARG	2.9
1	A	45	LEU	2.9
1	A	31	VAL	2.7
1	A	143	PRO	2.6
1	B	205	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	239	GLY	2.4
1	A	38	GLY	2.4
1	B	173	ILE	2.3
1	B	227	HIS	2.3
1	B	140	ALA	2.3
1	A	91	TYR	2.3
1	A	144	GLY	2.2
1	A	139	HIS	2.2
1	B	374	ALA	2.2
1	B	212	PRO	2.2
1	A	88	TYR	2.2
1	A	30	GLU	2.1
1	B	226	TYR	2.1
1	B	497	ASP	2.1
1	B	369	PHE	2.1
1	A	32	VAL	2.1
1	B	238	GLY	2.1
1	B	192	ARG	2.1
1	B	177	MET	2.1
1	A	187	HIS	2.0
1	B	175	CYS	2.0
1	A	500	HIS	2.0
1	A	496	GLY	2.0
1	B	189	LEU	2.0
1	B	334	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MG	B	686	1/1	0.90	0.39	5.87	55,55,55,55	0
4	MG	A	686	1/1	0.86	0.34	5.29	66,66,66,66	0
4	MG	B	688	1/1	0.90	0.39	2.54	101,101,101,101	0
4	MG	A	688	1/1	0.92	0.27	2.04	68,68,68,68	0
4	MG	B	687	1/1	0.99	0.20	-0.13	95,95,95,95	0
5	PO4	A	689	5/5	0.90	0.14	-1.34	129,129,129,129	0
4	MG	A	687	1/1	0.99	0.11	-1.93	61,61,61,61	0
5	PO4	B	689	5/5	0.92	0.19	-	140,140,140,140	0

6.5 Other polymers (i)

There are no such residues in this entry.