



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2016 – 04:49 PM EDT

PDB ID : 4NCB
Title : Structure of Thermus thermophilus Argonaute bound to guide DNA and 19-mer target DNA with Mg²⁺
Authors : Sheng, G.; Zhao, H.; Wang, J.; Rao, Y.; Wang, Y.
Deposited on : 2013-10-24
Resolution : 2.19 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
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) : rb-20027674

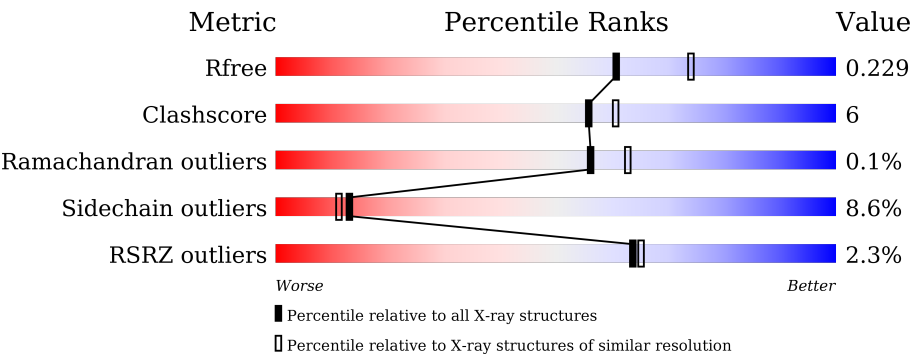
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	685	<div><div>%</div><div><div></div><div>79%</div><div>18%</div><div>..</div></div></div>
1	B	685	<div><div>3%</div><div><div></div><div>79%</div><div>17%</div><div>..</div></div></div>
2	C	21	<div><div></div><div><div></div><div>29%</div><div>43%</div><div>5%</div><div>24%</div></div></div>
2	E	21	<div><div>5%</div><div><div></div><div>48%</div><div>24%</div><div>10%</div><div>19%</div></div></div>
3	H	9	<div><div></div><div><div></div><div>44%</div><div>22%</div><div>33%</div></div></div>
3	P	9	<div><div>11%</div><div><div></div><div>22%</div><div>33%</div><div>44%</div></div></div>

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Mol	Chain	Length	Quality of chain
4	D	19	
5	F	10	

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
7	MG	B	702	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12444 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	676	Total	C	N	O	S	0	0	0
			5275	3371	992	905	7			
1	B	672	Total	C	N	O	S	0	0	0
			5240	3355	983	895	7			

- Molecule 2 is a DNA chain called 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*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	E	17	Total	C	N	O	P	0	0	0
			359	170	67	105	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	5	Total	C	N	O	P	0	5	0
			99	47	19	28	5			
3	H	6	Total	C	N	O	P	0	0	0
			120	57	24	33	6			

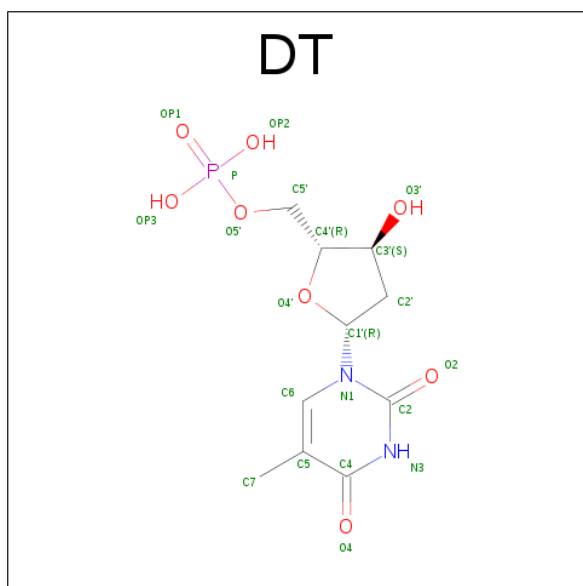
- Molecule 4 is a DNA chain called 5'-D(*TP*AP*TP*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	P	0	6	0
			320	153	54	97	16			

- Molecule 5 is a DNA chain called 5'-D(P*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	10	Total	C	N	O	P	0	0	0
			201	96	33	62	10			

- Molecule 6 is THYMIDINE-5'-MONOPHOSPHATE (three-letter code: DT) (formula: $C_{10}H_{15}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 21	C 10	N 2	O 8	P 1	0	0
6	B	1	Total 21	C 10	N 2	O 8	P 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Mg	0	0
			2	2		
7	A	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	E	1	Total	Mg	0	0
			1	1		

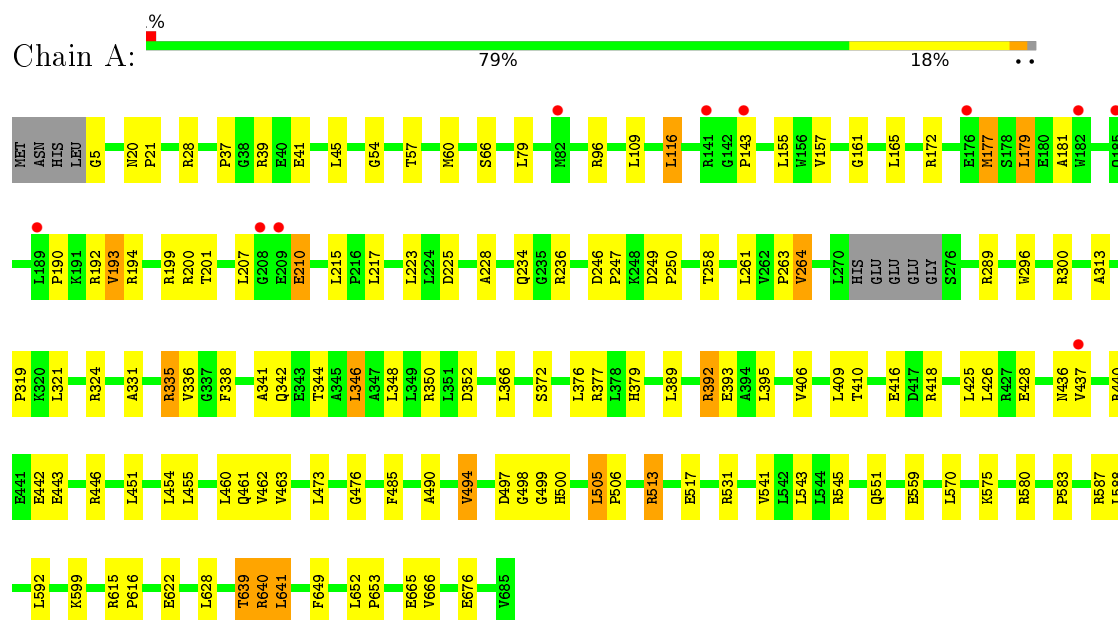
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	171	Total 171	O 171	0	0
8	B	174	Total 174	O 174	0	0
8	C	23	Total 23	O 23	0	0
8	P	2	Total 2	O 2	0	0
8	D	24	Total 24	O 24	0	0
8	E	27	Total 27	O 27	0	0
8	F	18	Total 18	O 18	0	0
8	H	5	Total 5	O 5	0	0

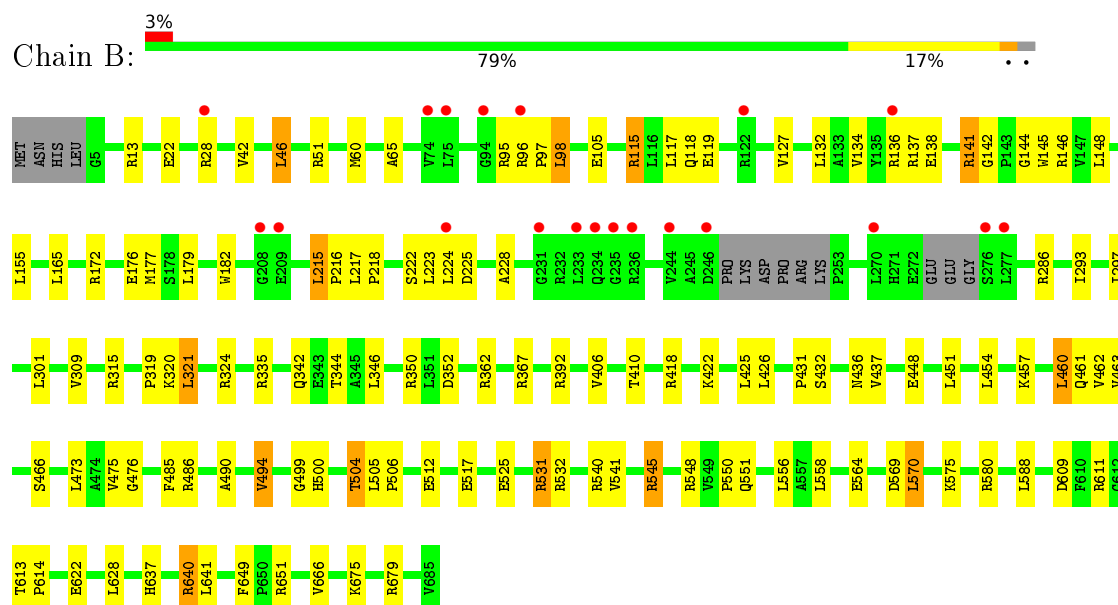
3 Residue-property plots

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

• Molecule 1: Argonaute

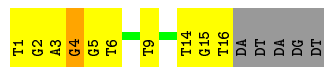


• Molecule 1: Argonaute



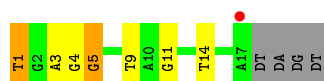
- Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*TP*AP*GP*T)-3'

Chain C: 




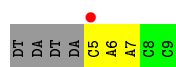
- Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*TP*AP*GP*T)-3'

Chain E: 



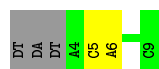
- Molecule 3: 5'-D(*TP*AP*TP*AP*CP*AP*AP*CP*C)-3'

Chain P: 



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

Chain H: 




- Molecule 4: 5'-D(*TP*AP*TP*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3'

Chain D: 



- Molecule 5: 5'-D(P*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3'

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.74Å 105.36Å 92.06Å 90.00° 94.25° 90.00°	Depositor
Resolution (Å)	39.22 – 2.19 39.22 – 2.19	Depositor EDS
% Data completeness (in resolution range)	90.6 (39.22-2.19) 90.5 (39.22-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.175 , 0.230 0.173 , 0.229	Depositor DCC
R_{free} test set	3787 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12444	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: 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	0.30	0/5400	0.52	3/7332 (0.0%)
1	B	0.30	0/5365	0.51	0/7284
2	C	0.78	1/379 (0.3%)	1.23	4/584 (0.7%)
2	E	0.83	1/403 (0.2%)	1.30	4/621 (0.6%)
3	H	0.66	0/134	1.10	0/203
3	P	0.50	0/110	1.07	1/166 (0.6%)
4	D	0.67	0/357	1.27	3/543 (0.6%)
5	F	0.97	1/223 (0.4%)	1.22	0/339
All	All	0.40	3/12371 (0.0%)	0.67	15/17072 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DT	OP3-P	-11.05	1.47	1.61
2	E	1	DT	OP3-P	-10.93	1.48	1.61
5	F	10	DT	OP3-P	-10.63	1.48	1.61

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	7[A]	DA	O4'-C1'-N9	7.22	113.05	108.00
4	D	16	DC	O4'-C1'-N1	-6.93	103.15	108.00
2	C	1	DT	OP1-P-OP2	-6.26	110.21	119.60
2	E	1	DT	OP1-P-OP2	-6.12	110.42	119.60
3	P	7[B]	DA	O4'-C1'-N9	6.03	112.22	108.00
2	E	9	DT	O4'-C1'-N1	5.96	112.17	108.00
1	A	116	LEU	CA-CB-CG	5.95	128.98	115.30
4	D	11	DA	O4'-C1'-N9	5.94	112.16	108.00
1	A	247	PRO	N-CA-CB	5.86	110.33	103.30
1	A	250	PRO	N-CA-CB	5.72	110.17	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	11	DG	O4'-C1'-N9	5.70	111.99	108.00
2	E	5	DG	O4'-C1'-N9	5.69	111.98	108.00
2	C	9	DT	O4'-C1'-N1	5.42	111.79	108.00
2	C	4	DG	O4'-C4'-C3'	-5.12	102.45	104.50
2	C	6	DT	N3-C4-O4	5.09	122.95	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5275	0	5342	67	0
1	B	5240	0	5324	70	0
2	C	338	0	183	8	0
2	E	359	0	194	5	0
3	H	120	0	66	2	0
3	P	99	0	55	2	0
4	D	320	0	180	5	0
5	F	201	0	114	0	0
6	A	21	0	13	1	0
6	B	21	0	13	4	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	A	171	0	0	5	0
8	B	174	0	0	4	0
8	C	23	0	0	1	0
8	D	24	0	0	2	0
8	E	27	0	0	0	0
8	F	18	0	0	0	0
8	H	5	0	0	0	0
8	P	2	0	0	1	0
All	All	12444	0	11484	145	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 6.

All (145) 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)
4:D:10[B]:DT:OP2	8:D:203:HOH:O	1.84	0.95
2:C:3:DA:H2'	2:C:4:DG:C8	2.17	0.79
1:A:344:THR:HG21	1:A:460:LEU:HD11	1.71	0.71
2:E:14:DT:H3	3:H:6:DA:H2	1.38	0.71
1:A:39:ARG:NH1	6:B:701:DT:O2	2.22	0.71
1:B:504:THR:HG21	1:B:525:GLU:HB3	1.72	0.70
1:A:513:ARG:NH2	1:A:551:GLN:O	2.26	0.69
1:A:346:LEU:HG	1:A:454:LEU:HD11	1.74	0.68
1:B:532:ARG:HH12	1:B:679:ARG:HH12	1.39	0.68
1:A:498:GLY:HA3	1:A:641:LEU:HD11	1.74	0.68
1:B:512:GLU:OE2	1:B:545:ARG:NH2	2.26	0.67
1:B:225:ASP:HA	1:B:228:ALA:HB3	1.78	0.66
1:A:494:VAL:HG22	1:A:500:HIS:HB2	1.76	0.66
2:C:14:DT:H3	4:D:6[A]:DA:H2	1.44	0.66
1:A:599:LYS:NZ	8:A:870:HOH:O	2.28	0.65
1:A:473:LEU:HB3	1:A:541:VAL:HG12	1.79	0.65
4:D:16:DC:OP1	8:D:212:HOH:O	2.15	0.64
1:A:236:ARG:NH1	8:A:954:HOH:O	2.29	0.64
1:A:190:PRO:HG3	1:A:263:PRO:HB3	1.80	0.64
1:B:335:ARG:NH2	1:B:448:GLU:OE2	2.30	0.64
1:B:136:ARG:HH12	1:B:293:ILE:HG12	1.63	0.63
1:B:115:ARG:NH2	8:B:915:HOH:O	2.32	0.62
1:A:583:PRO:HD3	1:A:588:LEU:HD13	1.82	0.62
2:E:3:DA:H2'	2:E:4:DG:C8	2.35	0.62
1:B:218:PRO:HD2	6:B:701:DT:H3	1.64	0.61
1:A:392:ARG:NH1	1:B:525:GLU:OE1	2.34	0.61
1:B:609:ASP:O	8:B:885:HOH:O	2.16	0.59
2:C:16:DT:OP2	8:C:206:HOH:O	2.17	0.59
2:C:15:DG:N2	3:P:5[B]:DC:O2	2.27	0.59
1:A:161:GLY:O	8:A:911:HOH:O	2.17	0.58
2:C:15:DG:N2	4:D:5[A]:DC:O2	2.29	0.58
1:A:210:GLU:HG3	1:A:215:LEU:HD23	1.87	0.56
1:A:313:ALA:HB1	1:A:592:LEU:HD12	1.86	0.56
1:A:497:ASP:OD1	1:A:497:ASP:N	2.37	0.56
1:A:440:ARG:HB2	1:A:443:GLU:HG3	1.88	0.56
1:B:177:MET:HE3	1:B:182:TRP:HA	1.87	0.56
1:A:28:ARG:CZ	1:A:96:ARG:HD3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:O	1:A:335:ARG:NH1	2.40	0.55
1:A:506:PRO:HG2	1:A:666:VAL:HG21	1.89	0.54
1:B:136:ARG:NH1	1:B:293:ILE:HG12	2.22	0.54
1:B:506:PRO:HG2	1:B:666:VAL:HG21	1.89	0.54
1:A:665:GLU:HG2	8:A:821:HOH:O	2.06	0.54
1:A:389:LEU:HD12	1:B:564:GLU:HG2	1.90	0.54
2:C:14:DT:H3	3:P:6[B]:DA:H2	1.54	0.53
1:A:392:ARG:NH2	1:A:428:GLU:OE2	2.37	0.53
1:B:98:LEU:HG	1:B:105:GLU:HB3	1.90	0.53
1:B:425:LEU:HD12	1:B:432:SER:HB3	1.90	0.53
1:A:350:ARG:HD2	1:A:352:ASP:OD1	2.09	0.52
1:A:179:LEU:HD13	1:A:258:THR:HG22	1.92	0.51
1:B:215:LEU:HD13	1:B:216:PRO:HD2	1.92	0.51
1:B:218:PRO:HD2	6:B:701:DT:N3	2.26	0.51
1:A:341:ALA:HB2	1:A:372:SER:HB3	1.93	0.51
1:B:342:GLN:O	1:B:344:THR:HG23	2.11	0.50
1:B:640:ARG:HG3	1:B:649:PHE:CE1	2.45	0.50
1:B:146:ARG:NH1	1:B:148:LEU:HD21	2.26	0.50
1:A:377:ARG:HD2	1:A:379:HIS:NE2	2.26	0.50
1:B:144:GLY:HA3	1:B:177:MET:HE1	1.94	0.50
1:A:41:GLU:O	1:A:45:LEU:HB2	2.12	0.50
1:B:494:VAL:HG22	1:B:500:HIS:HB2	1.92	0.50
1:B:461:GLN:HG3	1:B:499:GLY:O	2.10	0.50
1:B:531:ARG:HB3	1:B:531:ARG:HH11	1.77	0.50
1:B:570:LEU:HD13	1:B:622:GLU:HB3	1.94	0.49
1:A:193:VAL:HG11	1:A:261:LEU:HD13	1.95	0.49
1:B:225:ASP:OD1	1:B:225:ASP:N	2.45	0.49
1:A:446:ARG:HG3	2:C:2:DG:C8	2.48	0.49
1:B:319:PRO:CG	1:B:640:ARG:HD2	2.42	0.48
1:B:319:PRO:HB3	1:B:637:HIS:CG	2.48	0.48
1:B:410:THR:O	1:B:436:ASN:HA	2.13	0.48
1:B:575:LYS:O	1:B:651:ARG:NH2	2.42	0.48
1:A:321:LEU:HD22	1:A:463:VAL:HB	1.94	0.48
1:B:28:ARG:HD3	1:B:96:ARG:HB2	1.94	0.48
1:A:60:MET:HE2	1:A:60:MET:HB3	1.54	0.48
1:A:348:LEU:HD11	1:A:409:LEU:HG	1.95	0.48
1:A:192:ARG:HB3	1:A:264:VAL:HG22	1.96	0.47
1:B:418:ARG:O	1:B:422:LYS:HG3	2.14	0.47
1:A:5:GLY:N	8:A:843:HOH:O	2.46	0.47
1:A:575:LYS:HD3	1:A:652:LEU:HD11	1.97	0.47
1:A:395:LEU:HD11	1:A:425:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD22	1:A:376:LEU:HD11	1.96	0.47
1:B:46:LEU:HA	1:B:46:LEU:HD12	1.80	0.47
1:B:422:LYS:NZ	2:E:1:DT:OP1	2.48	0.47
1:B:117:LEU:HD23	1:B:132:LEU:HD22	1.96	0.47
1:B:28:ARG:HH11	1:B:96:ARG:HB2	1.79	0.46
1:A:461:GLN:HG3	1:A:499:GLY:O	2.15	0.46
1:B:611:ARG:HD3	2:E:5:DG:C1'	2.46	0.46
1:A:350:ARG:HD3	1:A:409:LEU:HD12	1.98	0.45
1:B:115:ARG:NH1	1:B:119:GLU:OE2	2.50	0.45
1:A:410:THR:O	1:A:436:ASN:HA	2.16	0.45
1:B:22:GLU:OE1	1:B:95:ARG:NH1	2.45	0.45
1:A:57:THR:HG22	1:A:66:SER:OG	2.17	0.45
1:A:505:LEU:HD12	1:B:675:LYS:HB2	1.99	0.45
1:B:141:ARG:HG3	1:B:142:GLY:N	2.32	0.45
1:A:194:ARG:HB2	1:A:201:THR:HG22	1.98	0.44
1:B:350:ARG:HD2	1:B:352:ASP:OD1	2.17	0.44
1:A:393:GLU:OE1	1:B:531:ARG:NE	2.50	0.44
1:A:615:ARG:HA	1:A:616:PRO:HD2	1.85	0.44
1:B:344:THR:HG21	1:B:460:LEU:HD11	1.99	0.44
1:B:362:ARG:HD2	8:B:906:HOH:O	2.16	0.44
2:C:4:DG:H2'	2:C:5:DG:C8	2.52	0.44
1:A:392:ARG:HD3	1:A:428:GLU:HG2	2.00	0.44
1:B:569:ASP:OD2	8:B:924:HOH:O	2.21	0.44
1:B:142:GLY:HA3	1:B:145:TRP:CE2	2.53	0.44
1:B:611:ARG:HD3	2:E:5:DG:H1'	2.00	0.43
1:A:246:ASP:HB3	1:A:249:ASP:O	2.18	0.43
1:B:286:ARG:HD2	1:B:613:THR:HG21	2.01	0.43
8:P:101:HOH:O	4:D:8[A]:DC:H1'	2.17	0.43
1:B:548:ARG:O	1:B:550:PRO:HD3	2.18	0.43
1:A:207:LEU:HA	1:A:207:LEU:HD23	1.87	0.43
1:A:342:GLN:O	1:A:344:THR:HG23	2.19	0.43
1:A:37:PRO:HB3	1:A:45:LEU:HD23	2.01	0.43
1:A:319:PRO:CG	1:A:640:ARG:HD2	2.48	0.43
1:B:588:LEU:HD21	1:B:614:PRO:HG2	2.00	0.43
1:A:640:ARG:HG3	1:A:649:PHE:CD1	2.54	0.42
1:B:217:LEU:HD22	6:B:701:DT:C2	2.54	0.42
1:A:476:GLY:O	1:A:490:ALA:HA	2.19	0.42
1:B:60:MET:HE2	1:B:65:ALA:HB2	2.01	0.42
1:A:177:MET:HG3	1:A:181:ALA:HB3	2.01	0.42
1:B:476:GLY:O	1:B:490:ALA:HA	2.19	0.42
1:B:222:SER:HB2	1:B:225:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:O	1:B:309:VAL:HG13	2.20	0.42
1:B:431:PRO:HB2	1:B:457:LYS:HB3	2.01	0.42
1:A:338:PHE:CZ	1:A:455:LEU:HD13	2.54	0.42
1:B:319:PRO:HG2	1:B:640:ARG:HD2	2.01	0.42
1:A:639:THR:CG2	1:A:640:ARG:HH21	2.33	0.41
1:B:177:MET:HE2	1:B:182:TRP:HE3	1.86	0.41
1:B:321:LEU:HD22	1:B:463:VAL:HB	2.03	0.41
1:A:20:ASN:HB2	1:A:21:PRO:HD2	2.02	0.41
1:B:517:GLU:CD	1:B:517:GLU:H	2.23	0.41
1:B:473:LEU:HB3	1:B:541:VAL:HG12	2.03	0.41
1:A:225:ASP:HA	1:A:228:ALA:HB3	2.03	0.41
1:B:127:VAL:CG1	1:B:134:VAL:HG13	2.51	0.41
1:A:300:ARG:HA	1:A:300:ARG:HD3	1.85	0.41
1:A:366:LEU:HD22	1:A:376:LEU:HD23	2.03	0.41
1:A:109:LEU:HB3	1:A:157:VAL:HG21	2.03	0.41
1:B:95:ARG:O	1:B:97:PRO:HD3	2.20	0.41
1:A:639:THR:HA	1:A:653:PRO:HA	2.02	0.41
1:A:200:ARG:NH2	6:A:701:DT:OP3	2.46	0.41
1:B:138:GLU:OE1	1:B:141:ARG:HB2	2.21	0.41
1:A:416:GLU:H	1:A:416:GLU:CD	2.23	0.40
1:B:320:LYS:HB2	1:B:466:SER:HB3	2.02	0.40
1:A:485:PHE:HB3	1:B:485:PHE:HB3	2.04	0.40
3:H:5:DC:H2"	3:H:6:DA:C8	2.56	0.40
1:B:505:LEU:HD23	1:B:505:LEU:HA	1.96	0.40
1:A:54:GLY:O	1:A:57:THR:HG23	2.21	0.40
1:B:51:ARG:NH2	1:B:118:GLN:OE1	2.54	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	672/685 (98%)	648 (96%)	23 (3%)	1 (0%)	56	63
1	B	666/685 (97%)	650 (98%)	16 (2%)	0	100	100
All	All	1338/1370 (98%)	1298 (97%)	39 (3%)	1 (0%)	56	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	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	521/549 (95%)	476 (91%)	45 (9%)	13	11
1	B	518/549 (94%)	474 (92%)	44 (8%)	13	11
All	All	1039/1098 (95%)	950 (91%)	89 (9%)	13	11

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	116	LEU
1	A	155	LEU
1	A	165	LEU
1	A	172	ARG
1	A	177	MET
1	A	179	LEU
1	A	193	VAL
1	A	199	ARG
1	A	210	GLU
1	A	217	LEU
1	A	223	LEU
1	A	234	GLN
1	A	264	VAL
1	A	289	ARG

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Mol	Chain	Res	Type
1	A	296	TRP
1	A	324	ARG
1	A	335	ARG
1	A	336	VAL
1	A	346	LEU
1	A	392	ARG
1	A	406	VAL
1	A	418	ARG
1	A	426	LEU
1	A	437	VAL
1	A	442	GLU
1	A	451	LEU
1	A	462	VAL
1	A	494	VAL
1	A	505	LEU
1	A	513	ARG
1	A	517	GLU
1	A	531	ARG
1	A	543	LEU
1	A	545	ARG
1	A	559	GLU
1	A	570	LEU
1	A	580	ARG
1	A	587	ARG
1	A	622	GLU
1	A	628	LEU
1	A	639	THR
1	A	640	ARG
1	A	641	LEU
1	A	676	GLU
1	B	42	VAL
1	B	46	LEU
1	B	98	LEU
1	B	115	ARG
1	B	137	ARG
1	B	141	ARG
1	B	155	LEU
1	B	165	LEU
1	B	172	ARG
1	B	176	GLU
1	B	179	LEU
1	B	215	LEU

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Mol	Chain	Res	Type
1	B	223	LEU
1	B	224	LEU
1	B	297	ILE
1	B	301	LEU
1	B	315	ARG
1	B	321	LEU
1	B	324	ARG
1	B	346	LEU
1	B	367	ARG
1	B	392	ARG
1	B	406	VAL
1	B	426	LEU
1	B	437	VAL
1	B	451	LEU
1	B	454	LEU
1	B	460	LEU
1	B	462	VAL
1	B	475	VAL
1	B	486	ARG
1	B	494	VAL
1	B	504	THR
1	B	531	ARG
1	B	540	ARG
1	B	545	ARG
1	B	551	GLN
1	B	556	LEU
1	B	558	LEU
1	B	570	LEU
1	B	580	ARG
1	B	628	LEU
1	B	640	ARG
1	B	641	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 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	$\# Z > 2$
6	DT	A	701	-	17,22,22	1.22	2 (11%)	22,33,33	4.07	5 (22%)
6	DT	B	701	-	17,22,22	1.20	2 (11%)	22,33,33	3.98	3 (13%)

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
6	DT	A	701	-	-	0/6/22/22	0/2/2/2
6	DT	B	701	-	-	0/6/22/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	701	DT	C6-C5	-2.50	1.33	1.40
6	A	701	DT	C6-C5	-2.38	1.33	1.40
6	B	701	DT	C4-N3	2.68	1.37	1.33
6	A	701	DT	C4-N3	2.88	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	A	701	DT	C5-C4-N3	-12.18	115.13	125.35
6	B	701	DT	C5-C4-N3	-11.99	115.29	125.35
6	A	701	DT	C7-C5-C4	-2.28	117.43	119.97
6	A	701	DT	C7-C5-C6	2.05	122.78	118.63
6	A	701	DT	OP2-P-OP1	2.70	119.44	110.63
6	B	701	DT	OP2-P-OP3	2.89	118.06	107.44
6	B	701	DT	C4-N3-C2	13.56	126.47	115.16
6	A	701	DT	C4-N3-C2	13.71	126.60	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	701	DT	1	0
6	B	701	DT	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	676/685 (98%)	-0.15	10 (1%) 76 77	14, 30, 63, 151	0
1	B	672/685 (98%)	-0.15	20 (2%) 54 56	12, 30, 72, 131	0
2	C	16/21 (76%)	-0.17	0 100 100	18, 25, 75, 84	0
2	E	17/21 (80%)	-0.50	1 (5%) 26 28	15, 20, 67, 133	0
3	H	6/9 (66%)	-0.51	0 100 100	36, 50, 66, 71	0
3	P	5/9 (55%)	0.42	1 (20%) 1 1	42, 51, 106, 194	5 (100%)
4	D	15/19 (78%)	-0.33	1 (6%) 21 22	23, 29, 68, 148	5 (33%)
5	F	10/10 (100%)	-0.87	0 100 100	22, 24, 27, 29	0
All	All	1417/1459 (97%)	-0.16	33 (2%) 64 65	12, 30, 67, 194	10 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	GLU	7.8
1	A	208	GLY	3.8
1	B	209	GLU	3.6
1	B	234	GLN	3.5
1	B	246	ASP	3.2
1	A	143	PRO	3.0
1	B	231	GLY	2.9
1	A	82	MET	2.8
1	B	74	VAL	2.8
1	B	236	ARG	2.8
4	D	5[A]	DC	2.7
3	P	5[B]	DC	2.7
1	A	437	VAL	2.6
1	B	94	GLY	2.5
1	B	277	LEU	2.5
1	B	224	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	75	LEU	2.4
1	B	122	ARG	2.4
1	B	276	SER	2.4
1	B	28	ARG	2.4
1	B	235	GLY	2.4
1	B	270	LEU	2.3
2	E	17	DA	2.3
1	B	244	VAL	2.3
1	B	96	ARG	2.3
1	A	189	LEU	2.3
1	B	136	ARG	2.3
1	A	185	GLN	2.3
1	A	176	GLU	2.2
1	B	233	LEU	2.1
1	B	208	GLY	2.1
1	A	141	ARG	2.1
1	A	182	TRP	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, 95th 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
7	MG	B	702	1/1	0.97	0.15	2.58	24,24,24,24	0
7	MG	E	101	1/1	0.91	0.16	1.68	24,24,24,24	0
7	MG	A	702	1/1	0.88	0.13	0.78	27,27,27,27	0
6	DT	A	701	21/21	0.97	0.13	-0.01	43,45,58,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MG	C	101	1/1	0.98	0.12	-0.09	20,20,20,20	0
6	DT	B	701	21/21	0.97	0.14	-0.11	37,47,63,71	0
7	MG	D	101	1/1	0.96	0.11	-0.19	24,24,24,24	0
7	MG	B	703	1/1	0.96	0.07	-1.80	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.