



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 04:36 PM JST

PDB ID : 5XPG  
Title : Crystal structure of *T. thermophilus* Argonaute protein complexed with a bulge 6'U7' on the target strand  
Authors : Sheng, G.; Gogakos, T.; Wang, J.; Zhao, H.; Serganov, A.; Juranek, S.; Tuschl, T.; Patel, J.D.; Wang, Y.  
Deposited on : 2017-06-02  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

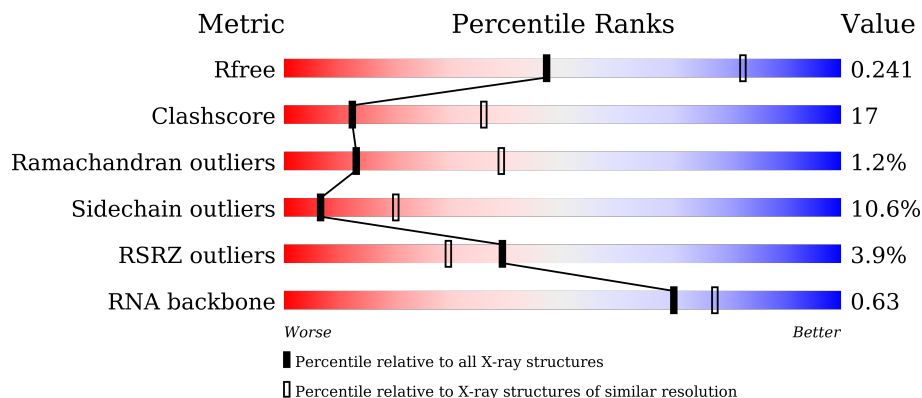
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	 4% 66% 28% 6%
2	C	21	 19% 57% 24%
3	G	20	 5% 40% 25% 10% 10% 15%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6044 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	684	5236	3347	977	906	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	ASN	ASP	engineered mutation	UNP Q746M7

- 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\*A P\*GP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	21	442	210	81	130	21	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	G	17	332	150	57	109	16	1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Mg 1 1	0	0

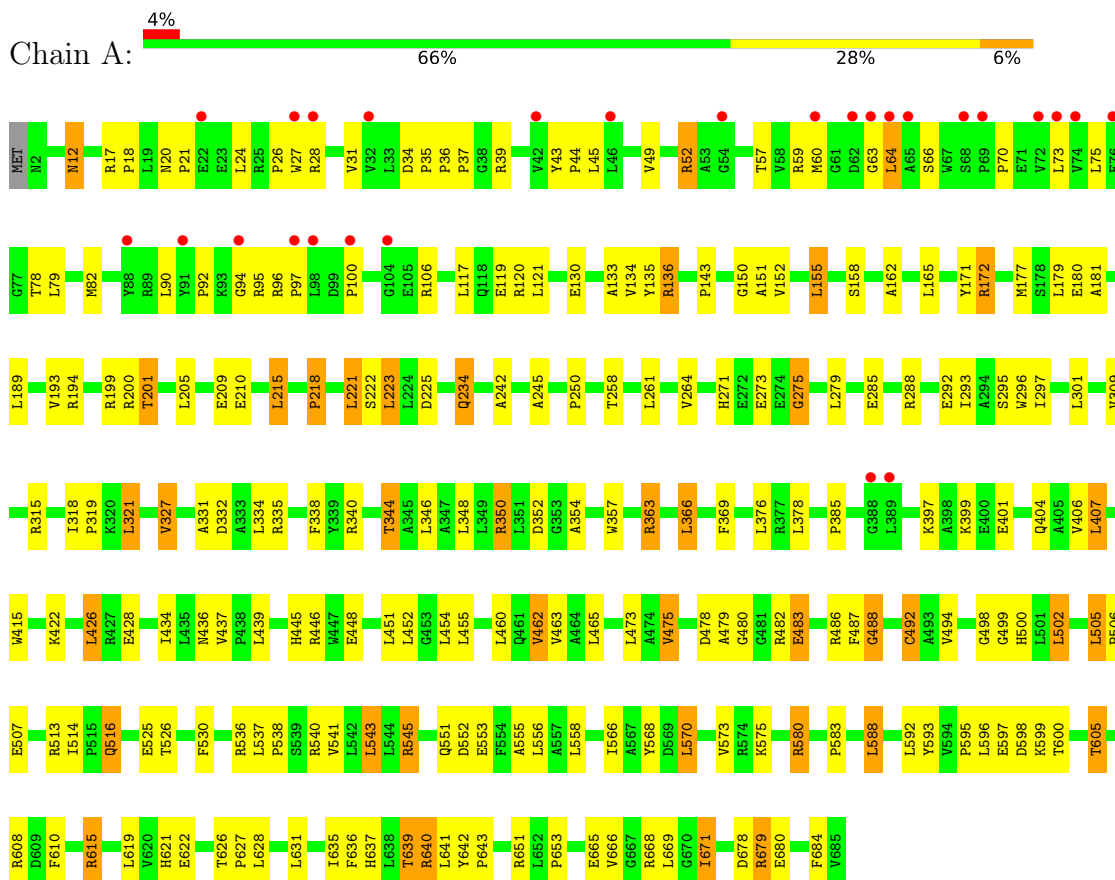
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	22	Total O 22 22	0	0
6	G	1	Total O 1 1	0	0

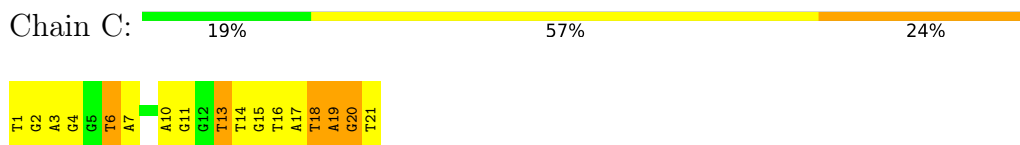
### 3 Residue-property plots [i](#)

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 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.

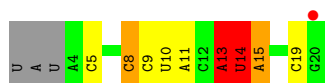
- Molecule 1: Uncharacterized protein



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.35Å 202.35Å 202.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 2.80 49.08 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.08-2.80) 99.6 (49.08-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.81Å)	Xtrriage
Refinement program	PHENIX PHENIX.REFINE	Depositor
R, $R_{free}$	0.203 , 0.246 0.200 , 0.241	Depositor DCC
$R_{free}$ test set	1762 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.6	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, SO4

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	0.38	1/5363 (0.0%)	0.58	2/7300 (0.0%)
2	C	0.85	1/496 (0.2%)	1.53	9/765 (1.2%)
3	G	0.65	0/369	1.29	4/572 (0.7%)
All	All	0.46	2/6228 (0.0%)	0.78	15/8637 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DT	OP3-P	-10.24	1.48	1.61
1	A	492	CYS	CB-SG	-6.64	1.71	1.82

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	11	DG	O4'-C1'-N9	13.76	117.63	108.00
3	G	13	A	P-O3'-C3'	9.73	131.37	119.70
2	C	19	DA	O4'-C4'-C3'	-8.20	101.08	106.00
3	G	8	C	O4'-C1'-N1	7.73	114.38	108.20
2	C	20	DG	O4'-C1'-N9	6.96	112.88	108.00
2	C	1	DT	OP1-P-OP2	-6.57	109.74	119.60
1	A	385	PRO	N-CA-CB	5.79	110.25	103.30
2	C	11	DG	C1'-O4'-C4'	-5.74	104.36	110.10
2	C	13	DT	C6-C5-C7	-5.73	119.46	122.90
2	C	18	DT	O4'-C4'-C3'	-5.67	102.23	104.50
1	A	218	PRO	N-CA-CB	5.54	109.95	103.30
2	C	6	DT	N3-C4-O4	5.42	123.15	119.90
3	G	15	A	C3'-C2'-C1'	5.16	105.63	101.50
2	C	11	DG	O4'-C1'-C2'	-5.06	101.85	105.90
3	G	14	U	P-O3'-C3'	5.02	125.72	119.70



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	5236	0	5193	185	0
2	C	442	0	240	13	0
3	G	332	0	171	6	0
4	A	10	0	0	0	0
5	C	1	0	0	0	0
6	A	22	0	0	0	0
6	G	1	0	0	0	0
All	All	6044	0	5604	198	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 17.

All (198) 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:A:480:GLY:HA3	1:A:486:ARG:HG3	1.45	0.95
1:A:480:GLY:HA2	1:A:487:PHE:H	1.32	0.93
1:A:636:PHE:O	1:A:639:THR:HB	1.71	0.91
1:A:422:LYS:HE2	1:A:434:ILE:HD13	1.52	0.89
1:A:605:THR:HG21	1:A:651:ARG:O	1.75	0.86
1:A:151:ALA:HB2	1:A:293:ILE:HD13	1.61	0.82
1:A:210:GLU:HG3	1:A:215:LEU:HD23	1.62	0.82
1:A:327:VAL:HG22	1:A:332:ASP:HB2	1.61	0.81
1:A:12:ASN:H	1:A:12:ASN:HD22	1.29	0.80
1:A:639:THR:HG22	1:A:640:ARG:HE	1.46	0.79
1:A:52:ARG:HE	1:A:79:LEU:HD13	1.46	0.79
1:A:480:GLY:HA2	1:A:487:PHE:N	1.98	0.78
1:A:422:LYS:HE2	1:A:434:ILE:CD1	2.16	0.76
1:A:473:LEU:HB3	1:A:541:VAL:HG12	1.66	0.76
1:A:480:GLY:CA	1:A:487:PHE:H	1.99	0.76
1:A:27:TRP:HA	1:A:95:ARG:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLN:HG2	1:A:556:LEU:HB2	1.70	0.73
1:A:20:ASN:HB2	1:A:21:PRO:HD2	1.73	0.71
1:A:180:GLU:HG2	1:A:258:THR:OG1	1.91	0.71
1:A:593:TYR:CZ	1:A:595:PRO:HG3	2.26	0.71
1:A:135:TYR:CZ	1:A:172:ARG:HG3	2.26	0.71
1:A:158:SER:HB2	1:A:162:ALA:H	1.56	0.71
2:C:6:DT:H2''	2:C:7:DA:H5''	1.71	0.70
1:A:631:LEU:O	1:A:635:ILE:HG12	1.91	0.70
1:A:318:ILE:HD12	1:A:318:ILE:H	1.56	0.69
1:A:57:THR:HG22	1:A:66:SER:OG	1.91	0.69
1:A:344:THR:HG21	1:A:460:LEU:HD11	1.75	0.68
1:A:446:ARG:HG3	2:C:2:DG:C8	2.29	0.67
1:A:502:LEU:HD23	1:A:680:GLU:HG3	1.78	0.66
1:A:327:VAL:HG22	1:A:332:ASP:CB	2.27	0.64
1:A:344:THR:HG23	1:A:369:PHE:HE2	1.63	0.64
2:C:15:DG:H2''	2:C:16:DT:H5''	1.81	0.62
1:A:319:PRO:HG2	1:A:640:ARG:HD2	1.82	0.62
1:A:134:VAL:CG1	1:A:136:ARG:HH21	2.13	0.61
1:A:537:LEU:HD13	1:A:566:ILE:HD11	1.82	0.61
1:A:478:ASP:O	1:A:488:GLY:HA2	2.01	0.61
1:A:344:THR:HG23	1:A:369:PHE:CE2	2.35	0.60
2:C:13:DT:H2''	2:C:14:DT:C6	2.36	0.60
1:A:556:LEU:HD23	1:A:556:LEU:O	2.01	0.59
1:A:570:LEU:HD13	1:A:622:GLU:HB3	1.84	0.59
1:A:462:VAL:HG22	1:A:463:VAL:HG13	1.85	0.58
1:A:575:LYS:HB3	1:A:651:ARG:HH22	1.67	0.58
1:A:407:LEU:HG	1:A:454:LEU:HD22	1.85	0.58
1:A:516:GLN:HE21	1:A:555:ALA:HB3	1.69	0.58
1:A:319:PRO:HG2	1:A:640:ARG:CD	2.34	0.57
1:A:315:ARG:HH11	1:A:315:ARG:HG3	1.69	0.57
1:A:415:TRP:HZ2	1:A:668:ARG:HD2	1.69	0.57
1:A:350:ARG:HD3	1:A:352:ASP:OD1	2.05	0.56
1:A:545:ARG:HD2	1:A:553:GLU:OE2	2.05	0.56
1:A:492:CYS:HB3	1:A:502:LEU:HD12	1.86	0.56
1:A:134:VAL:O	1:A:150:GLY:HA3	2.05	0.56
1:A:133:ALA:HA	1:A:152:VAL:HA	1.88	0.55
1:A:514:ILE:HD12	1:A:514:ILE:N	2.21	0.55
1:A:552:ASP:HB2	1:A:555:ALA:HB2	1.89	0.55
1:A:64:LEU:HD22	1:A:64:LEU:N	2.21	0.55
1:A:437:VAL:HG22	1:A:437:VAL:O	2.06	0.55
1:A:434:ILE:HD12	1:A:434:ILE:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LYS:HB3	1:A:651:ARG:NH2	2.22	0.55
1:A:285:GLU:HG3	1:A:288:ARG:HH21	1.72	0.55
1:A:437:VAL:O	1:A:439:LEU:N	2.40	0.55
1:A:558:LEU:HD22	1:A:568:TYR:CE2	2.42	0.55
1:A:580:ARG:NH1	1:A:615:ARG:HG3	2.21	0.55
1:A:39:ARG:HG2	2:C:19:DA:H5''	1.89	0.55
1:A:487:PHE:O	1:A:507:GLU:O	2.25	0.55
3:G:13:A:H4'	3:G:14:U:O5'	2.05	0.54
1:A:193:VAL:HG13	1:A:261:LEU:HD22	1.89	0.54
1:A:201:THR:HG21	2:C:10:DA:H5''	1.90	0.54
1:A:64:LEU:HD22	1:A:64:LEU:H	1.73	0.54
1:A:75:LEU:HA	1:A:90:LEU:HD23	1.88	0.54
1:A:24:LEU:O	1:A:26:PRO:HD3	2.08	0.54
1:A:639:THR:CG2	1:A:640:ARG:HE	2.18	0.53
1:A:482:ARG:NH1	1:A:483:GLU:OE1	2.41	0.53
1:A:285:GLU:HG3	1:A:288:ARG:NH2	2.24	0.53
2:C:18:DT:H4'	2:C:19:DA:OP1	2.09	0.53
1:A:605:THR:HG22	1:A:651:ARG:HG3	1.90	0.52
1:A:350:ARG:NH2	1:A:354:ALA:HB3	2.24	0.52
1:A:221:LEU:H	1:A:221:LEU:HD23	1.74	0.52
1:A:242:ALA:HB2	1:A:258:THR:HG22	1.92	0.52
1:A:599:LYS:HD2	1:A:621:HIS:O	2.09	0.52
1:A:516:GLN:HG2	1:A:556:LEU:CB	2.40	0.51
1:A:536:ARG:HD2	1:A:537:LEU:O	2.10	0.51
3:G:9:C:H2'	3:G:10:U:C6	2.45	0.51
1:A:119:GLU:HA	1:A:119:GLU:OE2	2.10	0.51
1:A:516:GLN:NE2	1:A:555:ALA:HB3	2.25	0.51
1:A:588:LEU:C	1:A:588:LEU:HD12	2.30	0.50
1:A:366:LEU:HD13	1:A:376:LEU:HD23	1.93	0.50
1:A:514:ILE:CD1	1:A:545:ARG:NH1	2.74	0.50
1:A:193:VAL:HG22	1:A:261:LEU:HB3	1.94	0.50
1:A:436:ASN:O	1:A:446:ARG:NH2	2.44	0.50
1:A:221:LEU:N	1:A:221:LEU:CD2	2.75	0.50
1:A:12:ASN:HD22	1:A:12:ASN:N	2.03	0.50
1:A:210:GLU:HG3	1:A:215:LEU:CD2	2.38	0.50
1:A:505:LEU:HD22	1:A:506:PRO:HD2	1.94	0.50
1:A:573:VAL:HG22	1:A:619:LEU:HD23	1.93	0.50
1:A:20:ASN:HB2	1:A:21:PRO:CD	2.42	0.49
1:A:121:LEU:HD13	1:A:134:VAL:CG2	2.42	0.49
1:A:288:ARG:O	1:A:292:GLU:HG3	2.11	0.49
1:A:100:PRO:O	1:A:106:ARG:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HH11	1:A:200:ARG:HG3	1.78	0.49
1:A:340:ARG:NH2	1:A:499:GLY:O	2.45	0.49
1:A:505:LEU:HD22	1:A:506:PRO:CD	2.43	0.49
1:A:543:LEU:HB3	1:A:570:LEU:HD23	1.95	0.49
1:A:599:LYS:HA	1:A:621:HIS:HB3	1.95	0.49
1:A:344:THR:CG2	1:A:369:PHE:HE2	2.25	0.49
1:A:94:GLY:O	1:A:95:ARG:HG3	2.13	0.49
1:A:136:ARG:HE	1:A:136:ARG:HB3	1.37	0.48
1:A:194:ARG:HD2	1:A:199:ARG:HE	1.77	0.48
1:A:318:ILE:HD12	1:A:318:ILE:N	2.24	0.48
1:A:57:THR:HG21	1:A:73:LEU:HD21	1.96	0.48
1:A:28:ARG:HG3	1:A:60:MET:HE1	1.95	0.48
1:A:366:LEU:HD12	1:A:366:LEU:HA	1.72	0.48
1:A:199:ARG:O	1:A:201:THR:HG22	2.14	0.47
3:G:9:C:H2'	3:G:10:U:H6	1.79	0.47
1:A:271:HIS:O	1:A:275:GLY:HA2	2.15	0.47
1:A:177:MET:HG2	1:A:181:ALA:HB3	1.95	0.47
1:A:205:LEU:HD11	1:A:245:ALA:HB2	1.97	0.47
1:A:189:LEU:H	1:A:189:LEU:HD12	1.79	0.47
1:A:487:PHE:HE2	1:A:671:ILE:HD12	1.80	0.47
1:A:480:GLY:H	1:A:488:GLY:H	1.63	0.46
2:C:16:DT:H2'	2:C:17:DA:C8	2.51	0.46
1:A:344:THR:HB	1:A:404:GLN:HE22	1.81	0.46
1:A:514:ILE:HD13	1:A:545:ARG:NH1	2.30	0.46
1:A:171:TYR:N	1:A:171:TYR:CD2	2.83	0.46
3:G:5:C:H6	3:G:5:C:O5'	1.99	0.45
1:A:492:CYS:SG	1:A:526:THR:HB	2.56	0.45
1:A:605:THR:CG2	1:A:651:ARG:HA	2.47	0.45
1:A:399:LYS:HD2	1:A:428:GLU:O	2.17	0.45
1:A:479:ALA:HB2	1:A:514:ILE:HD11	1.99	0.45
1:A:492:CYS:CB	1:A:502:LEU:HD12	2.47	0.45
1:A:494:VAL:HB	1:A:500:HIS:HB2	1.98	0.45
1:A:498:GLY:HA3	1:A:641:LEU:HD21	1.99	0.45
1:A:475:VAL:HG13	1:A:543:LEU:HD12	1.99	0.44
1:A:530:PHE:CD2	1:A:538:PRO:HG3	2.51	0.44
1:A:628:LEU:HD12	1:A:628:LEU:HA	1.75	0.44
1:A:201:THR:HG21	2:C:10:DA:H4'	1.99	0.44
1:A:17:ARG:HD3	1:A:18:PRO:O	2.17	0.44
1:A:234:GLN:HE21	1:A:234:GLN:HA	1.82	0.44
1:A:665:GLU:HG3	1:A:684:PHE:HB2	2.00	0.44
1:A:321:LEU:HD22	1:A:463:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HD22	1:A:155:LEU:HB2	2.00	0.44
1:A:12:ASN:H	1:A:12:ASN:ND2	2.08	0.44
1:A:434:ILE:CD1	1:A:434:ILE:N	2.80	0.44
1:A:513:ARG:NH2	1:A:551:GLN:O	2.50	0.44
1:A:583:PRO:CG	1:A:588:LEU:HB3	2.48	0.44
1:A:34:ASP:HA	1:A:35:PRO:C	2.38	0.44
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.88	0.43
1:A:363:ARG:HA	1:A:363:ARG:HD2	1.61	0.43
1:A:436:ASN:HD22	1:A:436:ASN:HA	1.58	0.43
1:A:43:TYR:HB2	1:A:44:PRO:HD3	2.00	0.43
1:A:570:LEU:CD1	1:A:622:GLU:HB3	2.48	0.43
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.81	0.43
1:A:598:ASP:O	1:A:600:THR:HG22	2.18	0.43
1:A:70:PRO:HA	1:A:73:LEU:HD12	2.01	0.43
1:A:445:HIS:NE2	3:G:19:C:H2'	2.34	0.43
1:A:592:LEU:HA	1:A:592:LEU:HD12	1.68	0.43
1:A:189:LEU:HD12	1:A:189:LEU:N	2.34	0.43
1:A:215:LEU:HB3	1:A:223:LEU:HB2	1.99	0.43
1:A:296:TRP:HE3	1:A:297:ILE:HG13	1.84	0.43
1:A:452:LEU:HD23	1:A:452:LEU:HA	1.88	0.43
1:A:502:LEU:HB3	1:A:679:ARG:O	2.18	0.43
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.67	0.43
2:C:20:DG:C8	2:C:21:DT:C4	3.07	0.42
1:A:31:VAL:HG23	1:A:63:GLY:HA2	2.02	0.42
1:A:366:LEU:CD1	1:A:376:LEU:HD23	2.49	0.42
1:A:597:GLU:HB2	1:A:600:THR:CG2	2.49	0.42
1:A:635:ILE:CG2	1:A:653:PRO:HG3	2.49	0.42
1:A:335:ARG:NH2	1:A:448:GLU:OE2	2.52	0.42
1:A:96:ARG:HA	1:A:97:PRO:HD3	1.79	0.42
1:A:462:VAL:CG2	1:A:463:VAL:HG13	2.48	0.42
1:A:27:TRP:CD1	1:A:70:PRO:HD3	2.54	0.42
1:A:36:PRO:HA	1:A:37:PRO:HD3	1.84	0.42
1:A:17:ARG:HG2	1:A:18:PRO:HD2	2.02	0.42
1:A:348:LEU:HB2	1:A:357:TRP:CE2	2.55	0.42
2:C:19:DA:C8	2:C:19:DA:H5'	2.55	0.42
1:A:397:LYS:O	1:A:401:GLU:HG3	2.20	0.42
1:A:318:ILE:H	1:A:318:ILE:CD1	2.28	0.41
1:A:120:ARG:HA	1:A:120:ARG:HD3	1.75	0.41
1:A:319:PRO:HG3	1:A:637:HIS:CD2	2.56	0.41
1:A:331:ALA:O	1:A:334:LEU:HB2	2.21	0.41
1:A:338:PHE:CZ	1:A:455:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:TRP:NE1	1:A:70:PRO:HD3	2.36	0.41
1:A:52:ARG:NE	1:A:79:LEU:HD13	2.24	0.41
1:A:201:THR:HG21	2:C:10:DA:C4'	2.50	0.41
1:A:17:ARG:HG2	1:A:18:PRO:N	2.36	0.41
1:A:193:VAL:CG2	1:A:261:LEU:HB3	2.51	0.41
1:A:556:LEU:HD23	1:A:556:LEU:C	2.42	0.41
3:G:10:U:H2'	3:G:11:A:C8	2.56	0.41
1:A:465:LEU:HG	1:A:641:LEU:HD13	2.03	0.40
1:A:315:ARG:HG3	1:A:315:ARG:NH1	2.36	0.40
1:A:642:TYR:HA	1:A:643:PRO:HD3	1.83	0.40
1:A:130:GLU:OE2	1:A:172:ARG:NH1	2.53	0.40
1:A:626:THR:HG23	1:A:627:PRO:HD2	2.03	0.40
1:A:45:LEU:O	1:A:49:VAL:HG23	2.22	0.40
1:A:75:LEU:HD22	1:A:90:LEU:HB2	2.02	0.40
1:A:426:LEU:HD12	1:A:426:LEU:HA	1.80	0.40
2:C:3:DA:H2''	2:C:4:DG:C8	2.57	0.40
1:A:143:PRO:HD2	1:A:273:GLU:OE1	2.22	0.40
1:A:222:SER:HB2	1:A:225:ASP:HB2	2.03	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	682/685 (100%)	636 (93%)	38 (6%)	8 (1%)	<b>13</b> <b>39</b>

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	MET
1	A	218	PRO
1	A	488	GLY

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Mol	Chain	Res	Type
1	A	610	PHE
1	A	92	PRO
1	A	608	ARG
1	A	275	GLY
1	A	250	PRO

### 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
1	A	501/549 (91%)	448 (89%)	53 (11%)	<b>6</b> <b>20</b>

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	52	ARG
1	A	59	ARG
1	A	64	LEU
1	A	78	THR
1	A	136	ARG
1	A	155	LEU
1	A	165	LEU
1	A	172	ARG
1	A	179	LEU
1	A	201	THR
1	A	209	GLU
1	A	215	LEU
1	A	221	LEU
1	A	223	LEU
1	A	234	GLN
1	A	264	VAL
1	A	295	SER
1	A	309	VAL
1	A	321	LEU
1	A	327	VAL

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Mol	Chain	Res	Type
1	A	344	THR
1	A	346	LEU
1	A	350	ARG
1	A	363	ARG
1	A	366	LEU
1	A	378	LEU
1	A	406	VAL
1	A	407	LEU
1	A	426	LEU
1	A	451	LEU
1	A	462	VAL
1	A	475	VAL
1	A	483	GLU
1	A	502	LEU
1	A	505	LEU
1	A	516	GLN
1	A	525	GLU
1	A	540	ARG
1	A	543	LEU
1	A	545	ARG
1	A	570	LEU
1	A	580	ARG
1	A	588	LEU
1	A	605	THR
1	A	615	ARG
1	A	639	THR
1	A	640	ARG
1	A	666	VAL
1	A	669	LEU
1	A	671	ILE
1	A	678	ASP
1	A	679	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	234	GLN
1	A	312	GLN
1	A	404	GLN
1	A	461	GLN
1	A	509	GLN

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Mol	Chain	Res	Type
1	A	621	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	15/20 (75%)	3 (20%)	2 (13%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	G	8	C
3	G	13	A
3	G	14	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	G	13	A
3	G	15	A

## 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](#)

Of 3 ligands modelled in this entry, 1 is 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
4	SO4	A	702	-	4,4,4	0.16	0	6,6,6	0.25	0
4	SO4	A	701	-	4,4,4	0.17	0	6,6,6	0.20	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	684/685 (99%)	-0.06	27 (3%) 39 29	31, 52, 102, 125	0
2	C	21/21 (100%)	-0.15	0 100 100	31, 44, 95, 103	0
3	G	17/20 (85%)	-0.20	1 (5%) 22 14	39, 44, 108, 121	1 (5%)
All	All	722/726 (99%)	-0.06	28 (3%) 39 29	31, 51, 102, 125	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	GLU	4.0
1	A	91	TYR	3.9
1	A	73	LEU	3.6
1	A	94	GLY	3.6
1	A	65	ALA	3.4
1	A	63	GLY	3.2
1	A	72	VAL	3.2
1	A	64	LEU	3.1
1	A	98	LEU	3.1
1	A	32	VAL	2.9
1	A	388	GLY	2.5
1	A	54	GLY	2.5
1	A	42	VAL	2.4
1	A	69	PRO	2.4
1	A	97	PRO	2.4
1	A	389	LEU	2.4
1	A	104	GLY	2.4
1	A	74	VAL	2.3
3	G	20	G	2.3
1	A	100	PRO	2.3
1	A	46	LEU	2.2
1	A	62	ASP	2.2
1	A	76	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	27	TRP	2.1
1	A	68	SER	2.1
1	A	88	TYR	2.1
1	A	28	ARG	2.1
1	A	60	MET	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 monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	A	701	5/5	0.96	0.25	62,73,82,94	0
4	SO4	A	702	5/5	0.98	0.13	46,47,57,58	0
5	MG	C	101	1/1	0.98	0.25	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.