Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2022 – 03:18 PM EDT

PDB ID	:	7R8I
Title	:	Crystal structure of Pseudooceanicola lipolyticus Argonaute bound to 5' OH guide DNA in the presence of Mg2+
Authors	:	Shin, Y.; Murakami, K.S.
Deposited on	:	2021-06-26
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

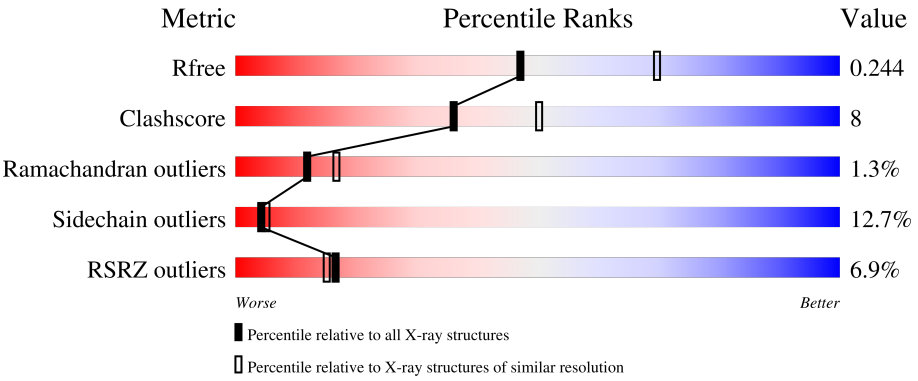
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	789	7% 72% 22%
2	T	18	11% 56% 33% 6% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6465 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	771	Total	C	N	O	S	0	0	0
			6054	3846	1078	1102	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	17	Total	C	N	O	P	0	0	0
			347	166	65	100	16			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

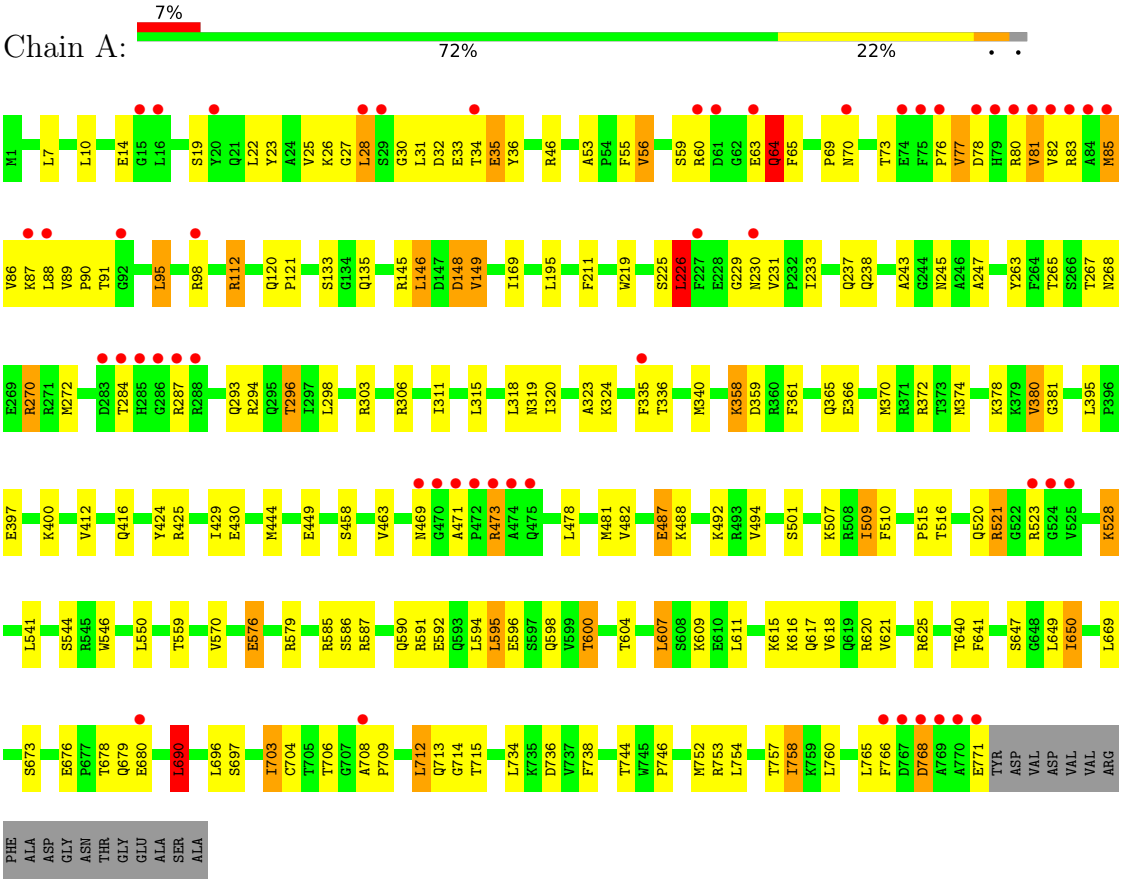
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	T	4	Total	O	0	0
			4	4		

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: Argonaute

Chain A:



• Molecule 2: DNA (5'-D(*TP*TP*AP*CP*TP*GP*CP*AP*CP*AP*GP*GP*TP*GP*AP*CP *GP*A)

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	200.02Å 200.02Å 200.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.73 – 2.40 44.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.73-2.40) 100.0 (44.73-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.213 , 0.248 0.209 , 0.244	Depositor DCC
R_{free} test set	1988 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6465	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.46	0/6189	0.69	3/8371 (0.0%)
2	T	1.24	1/389 (0.3%)	1.16	1/599 (0.2%)
All	All	0.54	1/6578 (0.0%)	0.73	4/8970 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	6	DC	C1'-N1	6.38	1.57	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	226	LEU	CA-CB-CG	6.46	130.15	115.30
2	T	14	DA	O4'-C4'-C3'	-5.88	102.15	104.50
1	A	576	GLU	C-N-CA	-5.61	110.53	122.30
1	A	690	LEU	C-N-CA	-5.08	111.64	122.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	696	LEU	Peptide
1	A	753	ARG	Sidechain

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	6054	0	6087	100	0
2	T	347	0	193	6	0
3	A	1	0	0	0	0
4	A	59	0	0	7	0
4	T	4	0	0	1	0
All	All	6465	0	6280	102	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 8.

All (102) 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:424:TYR:OH	4:A:901:HOH:O	1.89	0.90
1:A:397:GLU:OE1	4:A:902:HOH:O	1.92	0.88
1:A:265:THR:HG22	1:A:267:THR:H	1.41	0.85
1:A:145:ARG:HH12	1:A:148:ASP:H	1.26	0.84
1:A:27:GLY:HA2	1:A:86:VAL:HG12	1.60	0.83
1:A:121:PRO:HG2	1:A:318:LEU:HG	1.61	0.83
1:A:56:VAL:HG22	1:A:112:ARG:HD2	1.61	0.82
1:A:591:ARG:HG2	1:A:592:GLU:HG3	1.67	0.76
1:A:32:ASP:HB2	1:A:35:GLU:HB2	1.68	0.75
1:A:28:LEU:HD13	1:A:30:GLY:H	1.50	0.75
1:A:703:ILE:HG13	1:A:734:LEU:HD22	1.73	0.69
1:A:678:THR:O	1:A:680:GLU:N	2.27	0.68
1:A:618:VAL:HB	1:A:650:ILE:HG13	1.77	0.66
1:A:340:MET:O	4:A:903:HOH:O	2.14	0.66
1:A:754:LEU:HD22	1:A:758:ILE:HD11	1.78	0.65
1:A:604:THR:HG22	1:A:640:THR:HG23	1.79	0.65
1:A:510:PHE:HE1	1:A:515:PRO:HD3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TYR:O	1:A:65:PHE:HA	1.97	0.64
1:A:736:ASP:HB3	4:A:908:HOH:O	1.99	0.61
1:A:293:GLN:O	1:A:296:THR:HG22	2.02	0.59
1:A:311:ILE:HD13	1:A:315:LEU:HD12	1.84	0.59
1:A:145:ARG:NH1	1:A:148:ASP:H	1.98	0.59
1:A:746:PRO:HD2	1:A:752:MET:HE1	1.83	0.59
2:T:15:DC:N3	4:T:101:HOH:O	2.32	0.58
1:A:507:LYS:HG2	1:A:520:GLN:HB3	1.86	0.57
1:A:570:VAL:HG22	1:A:585:ARG:HG2	1.86	0.56
1:A:400:LYS:HE3	1:A:430:GLU:HB3	1.86	0.56
1:A:233:ILE:HD12	1:A:237:GLN:HG2	1.88	0.56
1:A:649:LEU:O	1:A:650:ILE:HD12	2.06	0.55
1:A:510:PHE:CE1	1:A:515:PRO:HD3	2.41	0.55
1:A:120:GLN:NE2	2:T:13:DG:O6	2.39	0.55
1:A:32:ASP:O	1:A:34:THR:N	2.41	0.54
1:A:233:ILE:HG23	1:A:237:GLN:HB3	1.89	0.54
1:A:272:MET:HG3	2:T:16:DG:H21	1.74	0.53
1:A:487:GLU:OE1	1:A:585:ARG:NH2	2.41	0.53
1:A:226:LEU:HD21	1:A:238:GLN:HG3	1.90	0.53
1:A:294:ARG:HH21	1:A:713:GLN:HG3	1.73	0.53
1:A:587:ARG:HD3	1:A:771:GLU:HB3	1.91	0.53
1:A:28:LEU:HD13	1:A:30:GLY:N	2.23	0.52
1:A:600:THR:O	1:A:604:THR:HG23	2.11	0.51
1:A:744:THR:HA	1:A:752:MET:HE1	1.92	0.51
1:A:746:PRO:HD2	1:A:752:MET:CE	2.41	0.50
1:A:673:SER:HB2	4:A:920:HOH:O	2.12	0.50
1:A:46:ARG:HH22	1:A:81:VAL:HB	1.76	0.50
1:A:219:TRP:HB2	1:A:225:SER:HB3	1.94	0.50
1:A:59:SER:HA	1:A:63:GLU:HA	1.93	0.49
1:A:77:VAL:HG13	1:A:88:LEU:O	2.13	0.49
1:A:319:ASN:HA	1:A:323:ALA:O	2.13	0.49
1:A:19:SER:OG	1:A:70:ASN:HB2	2.13	0.49
1:A:473:ARG:HH11	1:A:473:ARG:HA	1.78	0.48
1:A:621:VAL:HG11	1:A:641:PHE:CZ	2.49	0.48
1:A:395:LEU:O	1:A:430:GLU:HA	2.13	0.48
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.96	0.48
1:A:306:ARG:NH2	4:A:911:HOH:O	2.42	0.47
1:A:270:ARG:HH11	1:A:270:ARG:H	1.62	0.47
1:A:81:VAL:HG12	1:A:82:VAL:H	1.80	0.47
1:A:690:LEU:O	1:A:704:CYS:O	2.33	0.46
1:A:80:ARG:HA	1:A:85:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:GLU:O	1:A:600:THR:HG22	2.15	0.46
1:A:145:ARG:O	1:A:149:VAL:O	2.33	0.46
1:A:609:LYS:HB2	1:A:609:LYS:HE2	1.62	0.46
1:A:521:ARG:HE	1:A:521:ARG:HB2	1.55	0.46
1:A:19:SER:HA	1:A:95:LEU:O	2.15	0.45
1:A:488:LYS:HE3	1:A:488:LYS:HB3	1.55	0.45
1:A:487:GLU:HG3	1:A:492:LYS:O	2.17	0.45
1:A:607:LEU:O	1:A:611:LEU:HG	2.17	0.45
1:A:53:ALA:HB1	1:A:69:PRO:HG2	1.99	0.45
1:A:23:TYR:CE2	1:A:90:PRO:HG3	2.51	0.45
1:A:296:THR:HG23	2:T:7:DA:H4'	1.98	0.45
1:A:22:LEU:HG	1:A:95:LEU:HD11	1.98	0.45
1:A:211:PHE:CD1	1:A:263:TYR:HB3	2.51	0.45
1:A:135:GLN:NE2	2:T:11:DG:N7	2.66	0.44
1:A:64:GLN:HB2	1:A:65:PHE:H	1.48	0.44
1:A:358:LYS:H	1:A:358:LYS:HG2	1.66	0.44
1:A:429:ILE:HG22	1:A:430:GLU:H	1.83	0.44
1:A:361:PHE:HE2	1:A:708:ALA:HB1	1.83	0.43
2:T:13:DG:H2"	2:T:14:DA:H5"	2.01	0.43
1:A:478:LEU:O	1:A:482:VAL:HG23	2.18	0.43
1:A:544:SER:HA	1:A:546:TRP:CH2	2.53	0.43
1:A:704:CYS:HB3	1:A:706:THR:O	2.19	0.43
1:A:570:VAL:CG2	1:A:765:LEU:HG	2.48	0.43
1:A:412:VAL:O	1:A:416:GLN:HG3	2.19	0.43
1:A:528:LYS:NZ	1:A:528:LYS:H	2.17	0.42
1:A:594:LEU:HA	1:A:594:LEU:HD23	1.77	0.42
1:A:509:ILE:HD12	1:A:509:ILE:HA	1.62	0.42
1:A:31:LEU:HG	1:A:36:TYR:CD1	2.54	0.42
1:A:55:PHE:O	1:A:112:ARG:NE	2.49	0.41
1:A:595:LEU:HA	1:A:595:LEU:HD22	1.77	0.41
1:A:712:LEU:HD22	1:A:712:LEU:HA	1.91	0.41
1:A:169:ILE:HD13	1:A:169:ILE:HA	1.81	0.41
1:A:294:ARG:HH21	1:A:713:GLN:CG	2.33	0.41
1:A:690:LEU:HD12	1:A:738:PHE:HE1	1.86	0.41
1:A:76:PRO:C	1:A:78:ASP:H	2.23	0.41
1:A:370:MET:HG3	1:A:374:MET:HG3	2.03	0.41
1:A:146:LEU:HD12	1:A:146:LEU:HA	1.85	0.41
1:A:380:VAL:HG22	1:A:381:GLY:N	2.36	0.41
1:A:298:LEU:O	1:A:714:GLY:HA2	2.21	0.41
1:A:559:THR:OG1	1:A:757:THR:HG21	2.21	0.41
1:A:243:ALA:HB1	1:A:247:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLY:O	1:A:231:VAL:N	2.54	0.40
1:A:576:GLU:HB2	1:A:579:ARG:HB2	2.02	0.40
1:A:615:LYS:O	4:A:904:HOH:O	2.22	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	769/789 (98%)	717 (93%)	42 (6%)	10 (1%)	12 17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	679	GLN
1	A	81	VAL
1	A	33	GLU
1	A	64	GLN
1	A	77	VAL
1	A	73	THR
1	A	230	ASN
1	A	245	ASN
1	A	768	ASP
1	A	471	ALA

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	645/659 (98%)	563 (87%)	82 (13%)	4 5

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	10	LEU
1	A	14	GLU
1	A	25	VAL
1	A	26	LYS
1	A	28	LEU
1	A	35	GLU
1	A	56	VAL
1	A	60	ARG
1	A	64	GLN
1	A	83	ARG
1	A	85	MET
1	A	87	LYS
1	A	89	VAL
1	A	91	THR
1	A	95	LEU
1	A	98	ARG
1	A	112	ARG
1	A	133	SER
1	A	146	LEU
1	A	148	ASP
1	A	149	VAL
1	A	195	LEU
1	A	226	LEU
1	A	268	ASN
1	A	270	ARG
1	A	284	THR
1	A	287	ARG
1	A	296	THR
1	A	303	ARG
1	A	320	ILE
1	A	324	LYS
1	A	335	PHE
1	A	336	THR
1	A	358	LYS
1	A	359	ASP

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Mol	Chain	Res	Type
1	A	365	GLN
1	A	366	GLU
1	A	372	ARG
1	A	378	LYS
1	A	380	VAL
1	A	425	ARG
1	A	444	MET
1	A	449	GLU
1	A	458	SER
1	A	463	VAL
1	A	469	ASN
1	A	473	ARG
1	A	481	MET
1	A	487	GLU
1	A	494	VAL
1	A	501	SER
1	A	509	ILE
1	A	516	THR
1	A	521	ARG
1	A	523	ARG
1	A	528	LYS
1	A	541	LEU
1	A	550	LEU
1	A	586	SER
1	A	590	GLN
1	A	595	LEU
1	A	598	GLN
1	A	600	THR
1	A	607	LEU
1	A	616	LYS
1	A	617	GLN
1	A	620	ARG
1	A	625	ARG
1	A	647	SER
1	A	650	ILE
1	A	669	LEU
1	A	676	GLU
1	A	690	LEU
1	A	697	SER
1	A	703	ILE
1	A	712	LEU
1	A	715	THR

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Mol	Chain	Res	Type
1	A	758	ILE
1	A	760	LEU
1	A	766	PHE
1	A	768	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	584	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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^{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	771/789 (97%)	0.31	52 (6%)	17	16	49, 75, 142, 191	0
2	T	17/18 (94%)	0.73	2 (11%)	4	4	69, 84, 168, 200	0
All	All	788/807 (97%)	0.32	54 (6%)	16	15	49, 76, 142, 200	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	PRO	17.9
1	A	471	ALA	13.0
1	A	767	ASP	11.7
1	A	285	HIS	9.2
1	A	770	ALA	8.8
1	A	470	GLY	8.8
1	A	284	THR	8.4
2	T	0	DT	7.7
1	A	473	ARG	7.6
1	A	286	GLY	7.2
1	A	287	ARG	7.1
1	A	288	ARG	6.5
1	A	474	ALA	6.0
1	A	768	ASP	5.9
1	A	523	ARG	5.7
1	A	80	ARG	5.1
1	A	769	ALA	4.7
1	A	81	VAL	4.6
1	A	475	GLN	4.4
1	A	771	GLU	4.1
1	A	60	ARG	4.0
1	A	335	PHE	3.8
1	A	766	PHE	3.4
1	A	708	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	524	GLY	3.4
1	A	63	GLU	3.3
2	T	1	DT	3.2
1	A	88	LEU	3.2
1	A	84	ALA	2.9
1	A	29	SER	2.9
1	A	85	MET	2.7
1	A	78	ASP	2.7
1	A	74	GLU	2.7
1	A	525	VAL	2.6
1	A	79	HIS	2.5
1	A	76	PRO	2.5
1	A	92	GLY	2.5
1	A	83	ARG	2.5
1	A	75	PHE	2.5
1	A	469	ASN	2.4
1	A	82	VAL	2.3
1	A	283	ASP	2.3
1	A	28	LEU	2.3
1	A	87	LYS	2.2
1	A	70	ASN	2.2
1	A	15	GLY	2.2
1	A	34	THR	2.1
1	A	98	ARG	2.1
1	A	680	GLU	2.1
1	A	230	ASN	2.1
1	A	227	PHE	2.1
1	A	16	LEU	2.1
1	A	61	ASP	2.1
1	A	20	TYR	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

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^{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	B-factors(Å^2)	Q<0.9
3	MG	A	801	1/1	0.95	0.75	83,83,83,83	0

6.5 Other polymers

There are no such residues in this entry.