Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 02:57 am BST

PDB ID	:	2VTM
Title	:	Identification of N-(4-piperidinyl)-4-(2,6-dichlorobenzoylamino)-1H- pyrazole -3-carboxamide (AT7519), a Novel Cyclin Dependent Kinase Inhibitor Using Fragment-Based X-Ray Crystallography and Structure Based Drug Design.
Authors	:	Wyatt, P.G.; Woodhead, A.J.; Boulstridge, J.A.; Berdini, V.; Carr, M.G.; Cross, D.M.; Danillon, D.; Davis, D.J.; Devine, L.A.; Early, T.R.; Feltell, R.E.; Lewis, E.J.; McMenamin, R.L.; Navarro, E.F.; O'Brien, M.A.; O'Reilly, M.; Reule, M.; Saxty, G.; Seavers, L.C.A.; Smith, D.; Squires, M.S.; Trewartha, G.; Walker, M.T.; Woolford, A.J.
Deposited on	:	2008-05-15
Resolution	:	2.25 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:

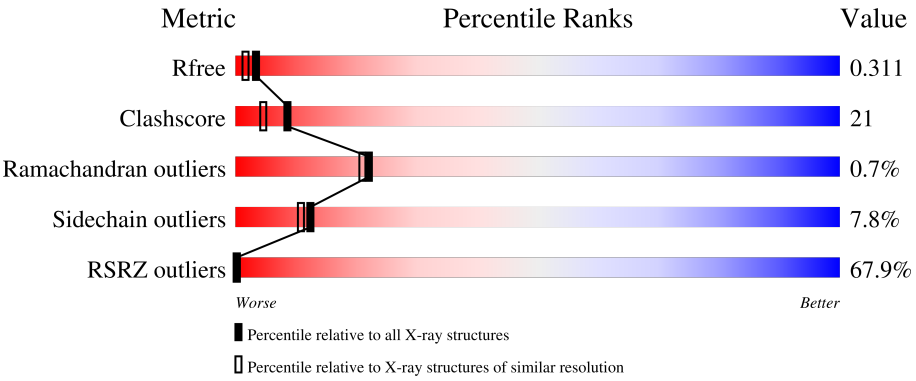
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	298	66% 65% 28%

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

2 Entry composition (i)

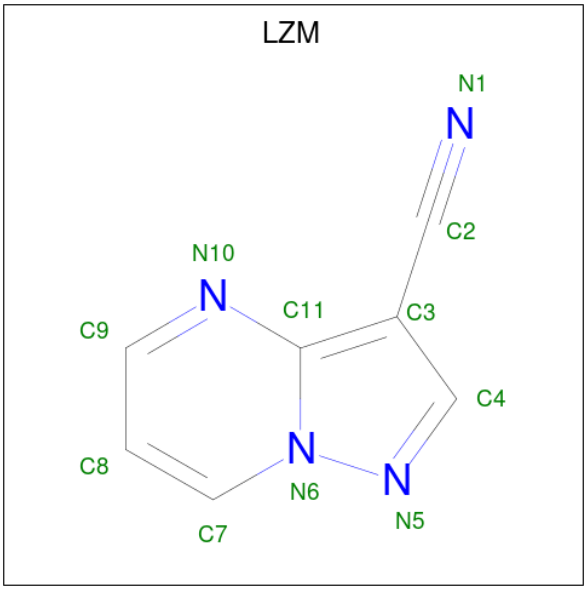
There are 3 unique types of molecules in this entry. The entry contains 2524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2335	1523	397	407	8			

- Molecule 2 is PYRAZOLO[1,5-A]PYRIMIDINE-3-CARBONITRILE (three-letter code: LZM) (formula: $C_7H_4N_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N		0	0
			11	7	4			

- Molecule 3 is water.

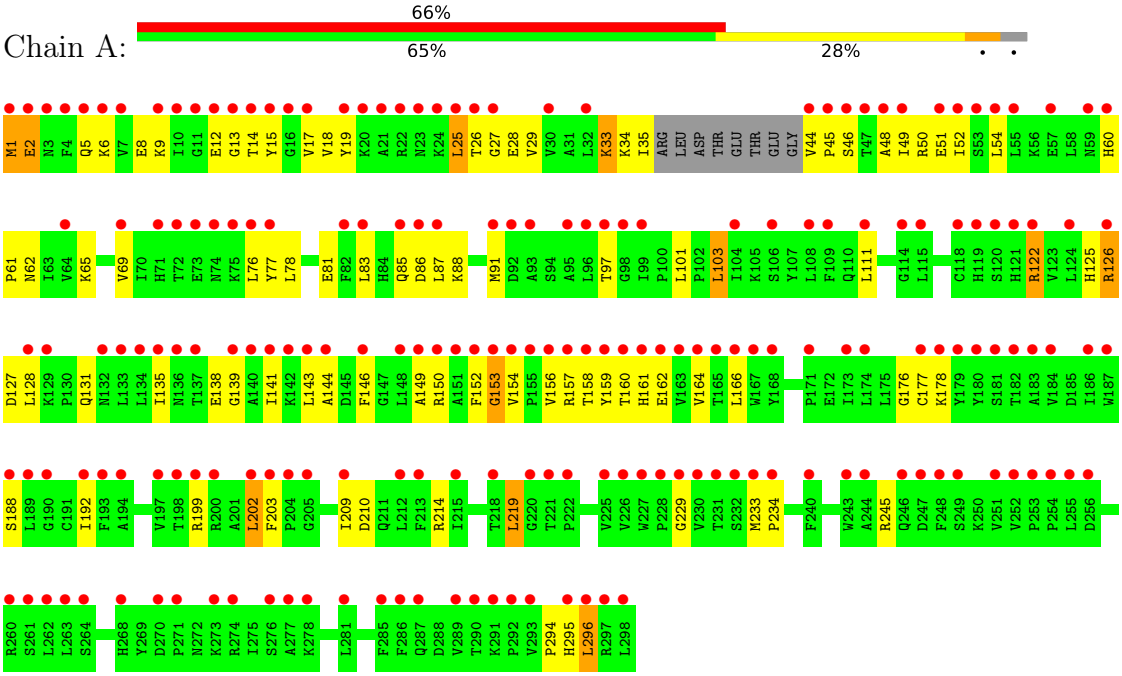
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	0	0
			178	178		

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: CELL DIVISION PROTEIN KINASE 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.52Å 71.70Å 72.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.89 – 2.25 36.90 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.3 (42.89-2.25) 95.5 (36.90-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.41 (at 2.24Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.228 , 0.286 0.242 , 0.311	Depositor DCC
R_{free} test set	651 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 66.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.58$, $< L^2 > = 0.45$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2524	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% 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: LZM

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	0.66	0/2396	0.77	2/3250 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	199	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	296	LEU	CA-CB-CG	5.36	127.62	115.30

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	2335	0	2392	98	0
2	A	11	0	4	3	0
3	A	178	0	0	9	0
All	All	2524	0	2396	98	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 21.

All (98) 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:122:ARG:HH11	1:A:122:ARG:HG2	1.27	0.99
1:A:85:GLN:NE2	1:A:135:ILE:HD11	1.76	0.98
1:A:34:LYS:HG2	1:A:77:TYR:CE1	2.06	0.90
1:A:125:HIS:HD2	1:A:127:ASP:H	1.28	0.81
1:A:85:GLN:HE21	1:A:135:ILE:HD11	1.44	0.81
1:A:122:ARG:N	1:A:122:ARG:HD3	1.95	0.80
1:A:60:HIS:HD2	1:A:62:ASN:H	1.30	0.78
1:A:18:VAL:CG2	1:A:33:LYS:HE3	2.14	0.78
1:A:126:ARG:NH1	1:A:154:VAL:HG11	1.98	0.78
1:A:210:ASP:O	1:A:214:ARG:HG3	1.85	0.77
1:A:178:LYS:HG3	3:A:2099:HOH:O	1.87	0.75
1:A:18:VAL:HG22	1:A:33:LYS:HE3	1.70	0.73
1:A:33:LYS:NZ	2:A:1299:LZM:N1	2.34	0.73
1:A:125:HIS:HE1	1:A:144:ALA:O	1.71	0.72
1:A:111:LEU:HD11	1:A:141:ILE:HD13	1.74	0.70
1:A:34:LYS:HE2	1:A:77:TYR:CE1	2.27	0.69
1:A:60:HIS:CD2	1:A:62:ASN:H	2.09	0.69
1:A:34:LYS:HG2	1:A:77:TYR:CD1	2.27	0.69
1:A:15:TYR:CE1	1:A:152:PHE:HB2	2.28	0.68
1:A:34:LYS:HE2	1:A:77:TYR:HE1	1.58	0.67
1:A:188:SER:O	1:A:192:ILE:HG13	1.95	0.66
1:A:25:LEU:HG	1:A:26:THR:HG23	1.78	0.66
1:A:122:ARG:HG2	1:A:122:ARG:NH1	2.05	0.65
1:A:54:LEU:N	1:A:54:LEU:HD23	2.12	0.64
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.33	0.64
1:A:294:PRO:HG2	1:A:296:LEU:HD13	1.80	0.64
1:A:25:LEU:HD11	1:A:26:THR:HG22	1.80	0.63
1:A:126:ARG:HD3	3:A:2071:HOH:O	2.00	0.62
1:A:177:CYS:HB2	1:A:233:MET:HE1	1.80	0.61
1:A:51:GLU:OE1	1:A:150:ARG:NH1	2.30	0.60
1:A:83:LEU:O	2:A:1299:LZM:H7	2.02	0.60
1:A:126:ARG:CZ	1:A:154:VAL:HG11	2.32	0.60
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.37	0.60
1:A:164:VAL:HB	3:A:2085:HOH:O	2.01	0.59
1:A:1:MET:CE	1:A:2:GLU:H	2.16	0.58
1:A:25:LEU:CD1	1:A:26:THR:HG22	2.34	0.58
1:A:128:LEU:HD21	1:A:143:LEU:CD2	2.34	0.58
1:A:34:LYS:HG2	1:A:77:TYR:HE1	1.66	0.56
1:A:101:LEU:O	1:A:101:LEU:HG	2.06	0.55
1:A:97:THR:HG23	3:A:2057:HOH:O	2.06	0.54
1:A:157:ARG:HB3	1:A:161:HIS:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:NZ	3:A:2036:HOH:O	2.28	0.54
1:A:1:MET:HA	1:A:1:MET:HE2	1.90	0.53
1:A:125:HIS:O	1:A:126:ARG:HB3	2.08	0.53
1:A:9:LYS:HA	1:A:19:TYR:CD1	2.44	0.52
1:A:13:GLY:HA3	3:A:2004:HOH:O	2.10	0.52
1:A:126:ARG:CG	1:A:126:ARG:HH11	2.23	0.51
1:A:159:TYR:CZ	1:A:160:THR:HG23	2.45	0.51
1:A:9:LYS:HG3	1:A:17:VAL:CG1	2.41	0.51
1:A:81:GLU:O	2:A:1299:LZM:H4	2.11	0.51
1:A:18:VAL:HG21	1:A:33:LYS:HE3	1.92	0.50
1:A:160:THR:OG1	1:A:162:GLU:HG3	2.11	0.49
1:A:8:GLU:OE2	3:A:2003:HOH:O	2.20	0.49
1:A:154:VAL:HG13	3:A:2073:HOH:O	2.12	0.48
1:A:126:ARG:NH1	1:A:126:ARG:HG3	2.28	0.48
1:A:152:PHE:O	1:A:153:GLY:O	2.31	0.48
1:A:85:GLN:HG2	1:A:86:ASP:N	2.28	0.48
1:A:122:ARG:HH11	1:A:122:ARG:CG	2.12	0.48
1:A:17:VAL:HG22	1:A:159:TYR:OH	2.14	0.47
1:A:26:THR:C	1:A:28:GLU:H	2.17	0.47
1:A:158:THR:HG23	1:A:162:GLU:HB2	1.97	0.47
1:A:149:ALA:O	1:A:153:GLY:N	2.48	0.47
1:A:25:LEU:C	1:A:25:LEU:HD12	2.35	0.47
1:A:87:LEU:O	1:A:91:MET:HG3	2.15	0.46
1:A:26:THR:OG1	1:A:28:GLU:HB2	2.16	0.46
1:A:294:PRO:HG2	1:A:296:LEU:CD1	2.44	0.46
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.98	0.46
1:A:125:HIS:CD2	1:A:127:ASP:H	2.19	0.46
1:A:177:CYS:HB2	1:A:233:MET:CE	2.44	0.46
1:A:154:VAL:HG13	1:A:154:VAL:O	2.16	0.46
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.51	0.46
1:A:69:VAL:HG13	1:A:69:VAL:O	2.15	0.46
1:A:35:ILE:HD12	1:A:78:LEU:HG	1.98	0.45
1:A:17:VAL:HG11	1:A:19:TYR:CZ	2.52	0.45
1:A:209:ILE:HD12	1:A:209:ILE:HA	1.85	0.44
1:A:157:ARG:HA	1:A:162:GLU:O	2.17	0.44
1:A:176:GLY:O	1:A:234:PRO:HG2	2.18	0.44
1:A:6:LYS:HE3	1:A:19:TYR:CD2	2.53	0.44
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.84	0.44
1:A:48:ALA:O	1:A:52:ILE:HG12	2.19	0.43
1:A:1:MET:CE	1:A:2:GLU:N	2.81	0.43
1:A:35:ILE:CD1	1:A:78:LEU:HG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD11	1:A:294:PRO:HB3	2.01	0.42
1:A:126:ARG:HG3	1:A:126:ARG:O	2.19	0.42
1:A:219:LEU:O	1:A:245:ARG:HD2	2.19	0.42
1:A:156:VAL:O	1:A:164:VAL:HG12	2.19	0.42
1:A:12:GLU:HB3	1:A:159:TYR:CE1	2.55	0.42
1:A:86:ASP:OD1	1:A:88:LYS:HB3	2.19	0.42
1:A:50:ARG:O	1:A:54:LEU:HG	2.19	0.42
1:A:122:ARG:HD3	1:A:122:ARG:H	1.81	0.42
1:A:158:THR:CG2	1:A:162:GLU:HB2	2.50	0.41
1:A:126:ARG:HH11	1:A:126:ARG:HG3	1.85	0.41
1:A:135:ILE:HG22	1:A:141:ILE:HG13	2.02	0.41
1:A:229:GLY:HA2	3:A:2135:HOH:O	2.20	0.41
1:A:18:VAL:HG22	1:A:33:LYS:CE	2.44	0.41
1:A:158:THR:N	1:A:162:GLU:O	2.53	0.41
1:A:103:LEU:HD22	1:A:103:LEU:O	2.21	0.40
1:A:128:LEU:HD21	1:A:143:LEU:HD22	2.00	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	286/298 (96%)	274 (96%)	10 (4%)	2 (1%)	22 21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	GLY
1	A	27	GLY

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	256/263 (97%)	236 (92%)	20 (8%)	12 11

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	5	GLN
1	A	14	THR
1	A	25	LEU
1	A	29	VAL
1	A	33	LYS
1	A	46	SER
1	A	49	ILE
1	A	76	LEU
1	A	103	LEU
1	A	122	ARG
1	A	126	ARG
1	A	131	GLN
1	A	138	GLU
1	A	146	PHE
1	A	166	LEU
1	A	202	LEU
1	A	219	LEU
1	A	295	HIS

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	3	ASN
1	A	5	GLN
1	A	60	HIS
1	A	85	GLN
1	A	113	GLN

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Mol	Chain	Res	Type
1	A	125	HIS
1	A	161	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LZM	A	1299	-	8,12,12	0.83	0	6,16,16	1.02	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
2	LZM	A	1299	-	-	0/0/2/2	0/2/2/2

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1299	LZM	3	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, 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	290/298 (97%)	2.99	197 (67%)	0	0	18, 31, 73, 93	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	VAL	18.5
1	A	155	PRO	10.8
1	A	160	THR	9.9
1	A	297	ARG	9.6
1	A	159	TYR	9.5
1	A	298	LEU	9.2
1	A	25	LEU	9.2
1	A	161	HIS	8.9
1	A	271	PRO	8.7
1	A	96	LEU	8.0
1	A	75	LYS	7.7
1	A	156	VAL	7.3
1	A	17	VAL	7.2
1	A	14	THR	7.1
1	A	1	MET	6.9
1	A	97	THR	6.6
1	A	49	ILE	6.6
1	A	24	LYS	6.4
1	A	273	LYS	6.3
1	A	44	VAL	6.3
1	A	164	VAL	6.1
1	A	252	VAL	6.1
1	A	22	ARG	6.0
1	A	152	PHE	6.0
1	A	179	TYR	5.9
1	A	74	ASN	5.6
1	A	32	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	296	LEU	5.5
1	A	64	VAL	5.5
1	A	274	ARG	5.4
1	A	21	ALA	5.4
1	A	163	VAL	5.4
1	A	229	GLY	5.3
1	A	150	ARG	5.3
1	A	7	VAL	5.2
1	A	45	PRO	5.2
1	A	10	ILE	5.0
1	A	228	PRO	4.8
1	A	233	MET	4.7
1	A	287	GLN	4.7
1	A	290	THR	4.6
1	A	189	LEU	4.6
1	A	120	SER	4.6
1	A	183	ALA	4.6
1	A	2	GLU	4.6
1	A	73	GLU	4.5
1	A	109	PHE	4.5
1	A	148	LEU	4.4
1	A	246	GLN	4.3
1	A	15	TYR	4.3
1	A	87	LEU	4.3
1	A	153	GLY	4.2
1	A	98	GLY	4.2
1	A	180	TYR	4.2
1	A	135	ILE	4.2
1	A	192	ILE	4.2
1	A	209	ILE	4.1
1	A	251	VAL	4.1
1	A	178	LYS	4.1
1	A	48	ALA	4.1
1	A	93	ALA	4.1
1	A	19	TYR	4.0
1	A	277	ALA	4.0
1	A	11	GLY	3.9
1	A	262	LEU	3.9
1	A	6	LYS	3.8
1	A	134	LEU	3.8
1	A	295	HIS	3.8
1	A	204	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	158	THR	3.7
1	A	76	LEU	3.6
1	A	162	GLU	3.5
1	A	286	PHE	3.5
1	A	118	CYS	3.5
1	A	181	SER	3.5
1	A	20	LYS	3.5
1	A	255	LEU	3.5
1	A	254	PRO	3.4
1	A	166	LEU	3.4
1	A	77	TYR	3.4
1	A	182	THR	3.3
1	A	5	GLN	3.2
1	A	54	LEU	3.2
1	A	293	VAL	3.2
1	A	72	THR	3.2
1	A	122	ARG	3.2
1	A	278	LYS	3.2
1	A	230	VAL	3.2
1	A	186	ILE	3.1
1	A	188	SER	3.1
1	A	248	PHE	3.1
1	A	243	TRP	3.1
1	A	261	SER	3.1
1	A	184	VAL	3.1
1	A	234	PRO	3.1
1	A	23	ASN	3.0
1	A	133	LEU	3.0
1	A	47	THR	3.0
1	A	227	TRP	2.9
1	A	121	HIS	2.9
1	A	213	PHE	2.9
1	A	92	ASP	2.9
1	A	168	TYR	2.9
1	A	55	LEU	2.9
1	A	146	PHE	2.9
1	A	268	HIS	2.8
1	A	52	ILE	2.8
1	A	57	GLU	2.8
1	A	115	LEU	2.8
1	A	4	PHE	2.8
1	A	71	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	85	GLN	2.7
1	A	46	SER	2.7
1	A	289	VAL	2.7
1	A	174	LEU	2.7
1	A	26	THR	2.7
1	A	60	HIS	2.7
1	A	264	SER	2.7
1	A	244	ALA	2.7
1	A	205	GLY	2.7
1	A	82	PHE	2.6
1	A	157	ARG	2.6
1	A	91	MET	2.6
1	A	12	GLU	2.6
1	A	53	SER	2.6
1	A	151	ALA	2.6
1	A	83	LEU	2.6
1	A	141	ILE	2.6
1	A	225	VAL	2.6
1	A	281	LEU	2.6
1	A	119	HIS	2.6
1	A	190	GLY	2.6
1	A	59	ASN	2.6
1	A	129	LYS	2.6
1	A	173	ILE	2.6
1	A	193	PHE	2.6
1	A	149	ALA	2.6
1	A	137	THR	2.5
1	A	218	THR	2.5
1	A	276	SER	2.5
1	A	187	TRP	2.5
1	A	226	VAL	2.5
1	A	203	PHE	2.5
1	A	240	PHE	2.5
1	A	231	THR	2.5
1	A	199	ARG	2.4
1	A	140	ALA	2.4
1	A	171	PRO	2.4
1	A	126	ARG	2.4
1	A	143	LEU	2.4
1	A	202	LEU	2.4
1	A	212	LEU	2.4
1	A	30	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	104	ILE	2.4
1	A	177	CYS	2.4
1	A	167	TRP	2.4
1	A	13	GLY	2.4
1	A	16	GLY	2.4
1	A	220	GLY	2.4
1	A	215	ILE	2.4
1	A	108	LEU	2.4
1	A	128	LEU	2.4
1	A	111	LEU	2.3
1	A	232	SER	2.3
1	A	69	VAL	2.3
1	A	222	PRO	2.3
1	A	114	GLY	2.3
1	A	247	ASP	2.3
1	A	165	THR	2.3
1	A	51	GLU	2.3
1	A	200	ARG	2.3
1	A	124	LEU	2.2
1	A	3	ASN	2.2
1	A	292	PRO	2.2
1	A	27	GLY	2.2
1	A	270	ASP	2.2
1	A	221	THR	2.2
1	A	136	ASN	2.2
1	A	144	ALA	2.2
1	A	198	THR	2.2
1	A	106	SER	2.2
1	A	132	ASN	2.2
1	A	256	ASP	2.1
1	A	285	PHE	2.1
1	A	99	ILE	2.1
1	A	263	LEU	2.1
1	A	9	LYS	2.1
1	A	197	VAL	2.1
1	A	249	SER	2.1
1	A	95	ALA	2.1
1	A	253	PRO	2.1
1	A	142	LYS	2.0
1	A	139	GLY	2.0
1	A	194	ALA	2.0
1	A	260	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	86	ASP	2.0
1	A	291	LYS	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^{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
2	LZM	A	1299	11/11	0.48	0.37	46,51,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.