



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:29 am GMT

PDB ID : 4EME
Title : X-ray crystal structure and specificity of the Plasmodium falciparum malaria aminopeptidase
Authors : McGowan, S.
Deposited on : 2012-04-11
Resolution : 2.60 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

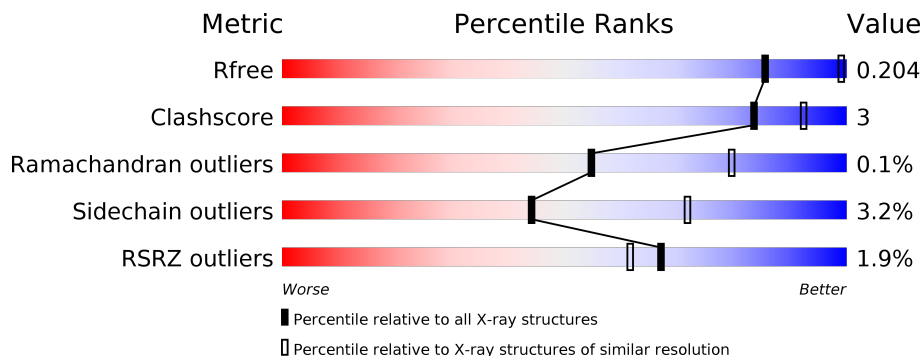
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	571	<div> <div>0.1%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>17%</div> </div> </div>
1	B	571	<div> <div>0.1%</div> <div> <div></div> <div>75%</div> <div>7%</div> <div>17%</div> </div> </div>
1	C	571	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>17%</div> </div> </div>
1	D	571	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>8%</div> <div>18%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15462 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 M18 aspartyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	1	0
			3775	2416	635	703	21			
1	B	473	Total	C	N	O	S	0	2	0
			3779	2419	637	703	20			
1	C	475	Total	C	N	O	S	0	0	0
			3770	2410	635	705	20			
1	D	469	Total	C	N	O	S	0	1	0
			3686	2357	615	694	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	TYR	-	EXPRESSION TAG	UNP Q8I2J3
A	2	VAL	-	EXPRESSION TAG	UNP Q8I2J3
B	1	TYR	-	EXPRESSION TAG	UNP Q8I2J3
B	2	VAL	-	EXPRESSION TAG	UNP Q8I2J3
C	1	TYR	-	EXPRESSION TAG	UNP Q8I2J3
C	2	VAL	-	EXPRESSION TAG	UNP Q8I2J3
D	1	TYR	-	EXPRESSION TAG	UNP Q8I2J3
D	2	VAL	-	EXPRESSION TAG	UNP Q8I2J3

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	141	Total 141	O 141	0	0
3	C	105	Total 105	O 105	0	0
3	D	67	Total 67	O 67	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	200.38Å 200.38Å 200.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.58 – 2.60 55.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (55.58-2.60) 99.9 (55.58-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.159 , 0.196 0.168 , 0.204	Depositor DCC
R_{free} test set	4109 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15462	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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, 0.333 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: ZN

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	0/3856	0.70	0/5213
1	B	0.48	0/3863	0.69	0/5219
1	C	0.48	0/3849	0.68	0/5207
1	D	0.43	0/3765	0.67	0/5101
All	All	0.46	0/15333	0.69	0/20740

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3775	0	3682	22	0
1	B	3779	0	3702	26	0
1	C	3770	0	3650	26	0
1	D	3686	0	3523	18	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	131	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	141	0	0	1	0
3	C	105	0	0	1	0
3	D	67	0	0	0	0
All	All	15462	0	14557	82	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 3.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:HD2	1:B:388:VAL:HG21	1.58	0.83
1:B:340:LEU:HD13	1:B:557:TYR:HB3	1.69	0.74
1:C:134:LEU:HD21	1:C:141:LEU:HD23	1.73	0.68
1:C:340:LEU:HD13	1:C:557:TYR:HB3	1.76	0.66
1:B:457:HIS:CE1	1:B:542:ALA:HB1	2.33	0.64
1:B:133:VAL:HG11	1:B:289:LEU:HD11	1.80	0.63
1:D:59:CYS:HA	1:D:64:ASN:O	1.99	0.62
1:A:134:LEU:HD11	1:B:475:LEU:HD12	1.81	0.61
1:A:120:HIS:HB3	1:A:174:ILE:HD11	1.83	0.61
1:C:307:GLN:HG3	1:D:307:GLN:HG3	1.85	0.59
1:B:340:LEU:HD13	1:B:557:TYR:CB	2.35	0.57
1:A:323:ARG:NH2	3:A:1169:HOH:O	2.38	0.56
1:A:457:HIS:CE1	1:A:542:ALA:HB1	2.39	0.56
1:C:457:HIS:CE1	1:C:542:ALA:HB1	2.41	0.56
1:C:533:ALA:O	1:C:536:SER:HB3	2.06	0.55
1:B:63:ARG:CD	1:B:388:VAL:HG21	2.34	0.55
1:B:63:ARG:HD3	1:B:378:ASP:OD2	2.07	0.55
1:B:66:CYS:HB2	1:B:375:ILE:HD12	1.89	0.55
1:C:323:ARG:HB3	1:C:327:LEU:HD22	1.89	0.54
1:A:70:VAL:HG11	1:A:406:VAL:HG21	1.91	0.53
1:A:176:TYR:HA	1:A:180:ILE:HD12	1.91	0.52
1:A:63:ARG:O	1:A:378:ASP:HB2	2.08	0.52
1:C:124:ASP:HA	1:C:154:PHE:CZ	2.44	0.52
1:C:170:PHE:N	1:D:176:TYR:HH	2.09	0.51
1:D:457:HIS:CE1	1:D:542:ALA:HB1	2.45	0.51
1:B:134:LEU:HD11	1:C:475:LEU:HD12	1.92	0.51
1:A:53:ASN:HB2	1:A:72:LYS:HG3	1.95	0.49
1:B:393:TYR:CE2	1:B:397:ASN:HB2	2.47	0.49
1:B:63:ARG:O	1:B:88:ILE:HD11	2.13	0.49
1:C:133:VAL:HG11	1:C:289:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:VAL:HG21	1:B:508:CYS:HB2	1.94	0.48
1:A:340:LEU:HD13	1:A:557:TYR:HB3	1.96	0.47
1:C:63:ARG:O	1:C:378:ASP:HB2	2.15	0.47
1:C:114:TYR:OH	1:C:379:HIS:HA	2.14	0.47
1:A:66:CYS:HB2	1:A:375:ILE:HD12	1.97	0.46
1:B:141:LEU:HD11	1:C:482:ARG:HG2	1.97	0.46
1:A:141:LEU:HD21	1:B:482:ARG:HG2	1.98	0.46
1:A:14:LEU:HD22	1:A:309:PRO:HB2	1.97	0.46
1:A:160:ILE:HG12	1:A:165:ARG:HD2	1.99	0.45
1:A:42:LEU:HD23	1:A:58:LEU:HD22	1.97	0.45
1:A:133:VAL:HG11	1:A:289:LEU:HD11	1.98	0.45
1:B:127:LEU:HD13	1:B:303:LEU:HD23	1.99	0.45
1:C:454:LEU:HD21	1:C:500:PHE:HB2	1.98	0.45
1:C:439:CYS:HB2	1:C:530:PRO:HB2	1.99	0.45
1:D:133:VAL:HG11	1:D:289:LEU:HD11	1.99	0.45
1:B:124:ASP:HA	1:B:154:PHE:CZ	2.51	0.44
1:D:407:PHE:HB3	1:D:410:GLU:HB2	1.99	0.44
1:C:79:GLY:HA2	1:C:369:ASN:HD22	1.83	0.43
1:D:24:PHE:HB3	1:D:145:LEU:HD22	2.00	0.43
1:A:124:ASP:HA	1:A:154:PHE:CZ	2.53	0.43
1:C:323:ARG:O	1:C:327:LEU:HB2	2.19	0.43
1:B:99:ASN:HA	1:B:110:ASN:HB2	2.00	0.43
1:D:529:ILE:HG21	1:D:545:ASP:O	2.19	0.43
1:B:506:THR:HG21	3:B:1202:HOH:O	2.19	0.43
1:D:393:TYR:CE2	1:D:397:ASN:HB2	2.54	0.43
1:A:59:CYS:HA	1:A:64:ASN:O	2.19	0.42
1:C:27:CYS:SG	1:C:59:CYS:SG	3.02	0.42
1:B:503:LYS:O	1:B:506:THR:HB	2.20	0.42
1:A:108:GLN:HG2	1:A:183:ILE:HG22	2.01	0.42
1:C:110:ASN:ND2	3:C:1160:HOH:O	2.53	0.42
1:B:114:TYR:OH	1:B:379:HIS:HA	2.19	0.42
1:B:118:LEU:HA	1:B:118:LEU:HD12	1.91	0.42
1:D:326:ASN:OD1	1:D:329:GLY:HA3	2.20	0.42
1:B:134:LEU:HD21	1:C:475:LEU:HG	2.02	0.42
1:A:27[A]:CYS:SG	1:A:59:CYS:SG	3.14	0.41
1:C:63:ARG:O	1:C:88:ILE:HD11	2.20	0.41
1:B:14:LEU:HD21	1:B:319:ILE:HB	2.02	0.41
1:D:124:ASP:HA	1:D:154:PHE:CZ	2.55	0.41
1:C:116:SER:O	1:D:160:ILE:HG21	2.20	0.41
1:D:428:ARG:HA	1:D:564:LEU:HD21	2.03	0.41
1:B:27[B]:CYS:SG	1:B:88:ILE:HG12	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:HG11	1:C:406:VAL:HG21	2.02	0.41
1:D:435:ASP:O	1:D:528:GLY:HA3	2.20	0.41
1:D:482:ARG:HA	1:D:482:ARG:HD3	1.92	0.41
1:A:410:GLU:HA	1:A:414:LYS:HB2	2.03	0.40
1:A:59:CYS:SG	1:A:65:ILE:HD12	2.61	0.40
1:C:540:ILE:HD13	1:D:183:ILE:HD11	2.03	0.40
1:D:127:LEU:HD13	1:D:303:LEU:HD23	2.02	0.40
1:A:482:ARG:HG2	1:C:141:LEU:HD21	2.03	0.40
1:B:24:PHE:HB3	1:B:145:LEU:HD22	2.03	0.40
1:C:14:LEU:HD22	1:C:309:PRO:HB2	2.03	0.40
1:D:126:SER:HB3	1:D:151:SER:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	467/571 (82%)	453 (97%)	14 (3%)	0	100	100
1	B	467/571 (82%)	457 (98%)	10 (2%)	0	100	100
1	C	467/571 (82%)	451 (97%)	16 (3%)	0	100	100
1	D	462/571 (81%)	444 (96%)	17 (4%)	1 (0%)	51	76
All	All	1863/2284 (82%)	1805 (97%)	57 (3%)	1 (0%)	55	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	535	HIS

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	417/527 (79%)	406 (97%)	11 (3%)	51	78
1	B	418/527 (79%)	404 (97%)	14 (3%)	43	70
1	C	414/527 (79%)	400 (97%)	14 (3%)	42	69
1	D	399/527 (76%)	385 (96%)	14 (4%)	41	68
All	All	1648/2108 (78%)	1595 (97%)	53 (3%)	44	72

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

Mol	Chain	Res	Type
1	A	2	VAL
1	A	65	ILE
1	A	109	ILE
1	A	118	LEU
1	A	191	GLN
1	A	195	CYS
1	A	369	ASN
1	A	440	SER
1	A	478	SER
1	A	482	ARG
1	A	526	ASP
1	B	2	VAL
1	B	18	GLN
1	B	118	LEU
1	B	141	LEU
1	B	146	ILE
1	B	173	LYS
1	B	181	LYS
1	B	191	GLN
1	B	193	ASN
1	B	340	LEU
1	B	409	LYS
1	B	468	LYS
1	B	478	SER

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Mol	Chain	Res	Type
1	B	482	ARG
1	C	3	ASP
1	C	84	SER
1	C	161	HIS
1	C	181	LYS
1	C	191	GLN
1	C	290	ASN
1	C	340	LEU
1	C	350	ASN
1	C	369	ASN
1	C	482	ARG
1	C	526	ASP
1	C	531	GLN
1	C	536	SER
1	C	569	HIS
1	D	3	ASP
1	D	18	GLN
1	D	27[A]	CYS
1	D	27[C]	CYS
1	D	75	ASN
1	D	141	LEU
1	D	181	LYS
1	D	191	GLN
1	D	340	LEU
1	D	458	GLU
1	D	478	SER
1	D	482	ARG
1	D	526	ASP
1	D	531	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	191	GLN
1	A	412	HIS
1	A	561	ASN
1	B	18	GLN
1	C	37	ASN
1	C	369	ASN
1	C	412	HIS
1	C	561	ASN

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Mol	Chain	Res	Type
1	D	368	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are 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, 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	474/571 (83%)	-0.71	4 (0%) 86 83	22, 34, 64, 103	0
1	B	473/571 (82%)	-0.56	6 (1%) 77 73	21, 34, 62, 99	0
1	C	475/571 (83%)	-0.40	12 (2%) 58 50	26, 40, 68, 114	0
1	D	469/571 (82%)	-0.24	13 (2%) 53 46	34, 53, 79, 117	0
All	All	1891/2284 (82%)	-0.48	35 (1%) 67 61	21, 40, 73, 117	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	349	SER	5.8
1	C	350	ASN	5.6
1	A	195	CYS	5.3
1	C	348	THR	5.1
1	C	351	GLU	4.8
1	C	349	SER	4.4
1	C	352	ASN	4.4
1	D	348	THR	4.3
1	B	346	ASN	4.2
1	C	172	VAL	3.8
1	C	195	CYS	3.8
1	B	170	PHE	3.7
1	B	2	VAL	3.7
1	D	347	HIS	3.5
1	C	347	HIS	3.4
1	C	170	PHE	3.2
1	D	344	ILE	3.2
1	D	3	ASP	3.0
1	D	346	ASN	2.9
1	D	367	ILE	2.6
1	B	347	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	3	ASP	2.5
1	D	392	SER	2.4
1	D	413	GLU	2.3
1	C	192	LEU	2.3
1	A	347	HIS	2.2
1	D	511	THR	2.2
1	D	391	ARG	2.2
1	D	72	LYS	2.2
1	A	2	VAL	2.2
1	C	346	ASN	2.1
1	C	413	GLU	2.1
1	D	172	VAL	2.1
1	A	165	ARG	2.0
1	B	273	ILE	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
2	ZN	A	1002	1/1	0.99	0.13	0.81	40,40,40,40	0
2	ZN	A	1001	1/1	0.98	0.12	0.42	42,42,42,42	0
2	ZN	D	1002	1/1	0.97	0.13	0.26	54,54,54,54	0
2	ZN	B	1002	1/1	0.98	0.15	0.20	41,41,41,41	0
2	ZN	B	1001	1/1	0.99	0.13	-0.46	36,36,36,36	0
2	ZN	C	1001	1/1	0.99	0.14	-0.49	44,44,44,44	0
2	ZN	C	1002	1/1	0.98	0.13	-0.59	47,47,47,47	0
2	ZN	D	1001	1/1	0.99	0.12	-0.71	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.