Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 01:07 PM EDT

PDB ID	:	4LEW
Title	:	Structure of human cGAS
Authors	:	Li, P.
Deposited on	:	2013-06-26
Resolution	:	2.04 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 (i) 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 (i)) were used in the production of this report:

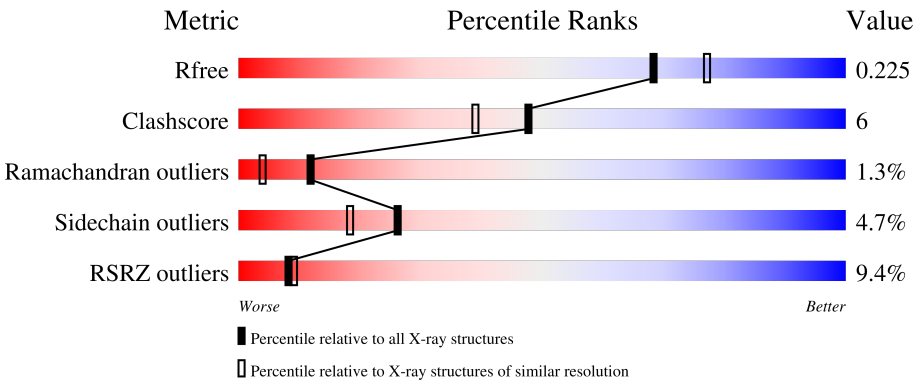
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	366	7% 82% 15% ••
1	B	366	12% 80% 16% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6278 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 Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	B	359	2951	1885	511	540	10	5	0	0	0
1	A	362	2962	1890	514	543	10	5	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	B	1	1	1	0	0
2	A	1	1	1	0	0

- Molecule 3 is water.

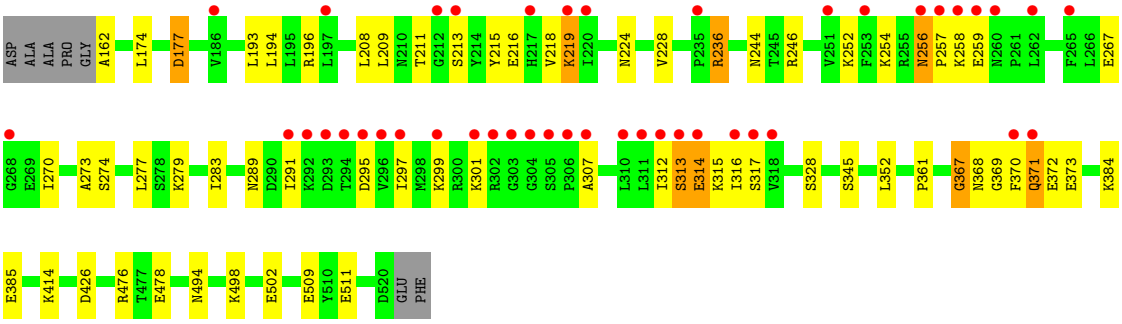
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	131	131	131	0	0
3	A	232	232	232	0	0

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.

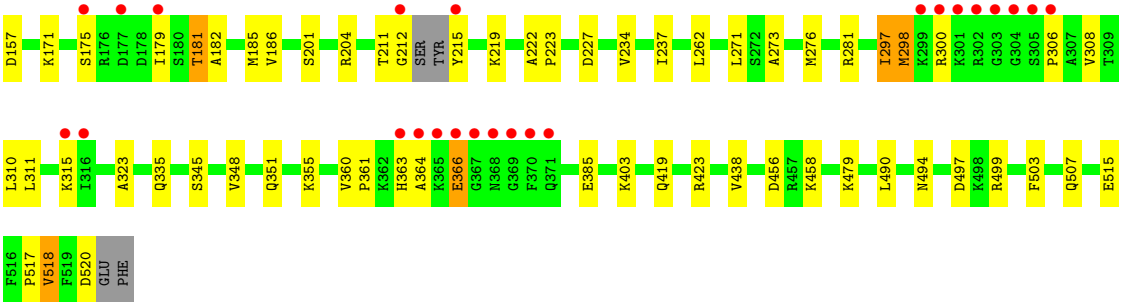
• Molecule 1: Cyclic GMP-AMP synthase

Chain B:



• Molecule 1: Cyclic GMP-AMP synthase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.81Å 111.48Å 76.41Å 90.00° 92.73° 90.00°	Depositor
Resolution (Å)	40.75 – 2.04 43.12 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.75-2.04) 95.7 (43.12-2.04)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.179 , 0.223 0.180 , 0.225	Depositor DCC
R_{free} test set	2011 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6278	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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 (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	0.47	0/3015	0.56	0/4036
1	B	0.41	0/3005	0.52	0/4023
All	All	0.44	0/6020	0.54	0/8059

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	291	ILE	Peptide

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	2962	0	2998	35	0
1	B	2951	0	2989	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	232	0	0	6	0
3	B	131	0	0	6	0
All	All	6278	0	5987	73	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 (73) 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:423:ARG:NH1	3:A:772:HOH:O	2.21	0.73
1:A:479:LYS:NZ	3:A:830:HOH:O	2.26	0.68
1:B:177:ASP:OD1	1:B:177:ASP:N	2.28	0.67
1:B:274:SER:N	1:B:373:GLU:OE1	2.26	0.63
1:A:157:ASP:N	3:A:810:HOH:O	2.32	0.63
1:B:219:LYS:NZ	3:B:757:HOH:O	2.32	0.62
1:B:279:LYS:HE2	1:B:283:ILE:HD11	1.82	0.62
1:A:351:GLN:NE2	3:A:840:HOH:O	2.29	0.61
1:B:209:LEU:O	3:B:756:HOH:O	2.17	0.59
1:B:476:ARG:NH2	1:B:509:GLU:OE2	2.35	0.58
1:B:384:LYS:NZ	3:B:810:HOH:O	2.37	0.57
1:B:213:SER:HB3	1:B:219:LYS:HD2	1.87	0.57
1:A:281:ARG:NH2	1:A:298:MSE:HE3	2.20	0.56
1:A:175:SER:HB3	1:A:223:PRO:HG2	1.86	0.56
1:B:213:SER:OG	1:B:414:LYS:NZ	2.38	0.56
1:A:234:VAL:HG21	1:A:237:ILE:HD11	1.88	0.56
1:A:179:ILE:HA	1:A:182:ALA:HB3	1.88	0.54
1:A:297:ILE:HG23	1:A:311:LEU:HB3	1.90	0.54
1:A:219:LYS:HB3	1:A:222:ALA:HB3	1.89	0.54
1:A:182:ALA:O	1:A:186:VAL:HG22	2.07	0.53
1:A:201:SER:HA	1:A:204:ARG:HE	1.73	0.53
1:B:312:ILE:HB	1:B:316:ILE:HB	1.90	0.53
1:A:311:LEU:HD11	1:A:315:LYS:HA	1.92	0.52
1:A:403:LYS:NZ	3:A:791:HOH:O	2.37	0.52
1:A:211:THR:N	1:A:212:GLY:HA2	2.24	0.52
1:B:224:ASN:O	1:B:317:SER:N	2.39	0.51
1:A:271:LEU:HD21	1:A:276:MSE:HE1	1.93	0.50
1:B:498:LYS:HE3	1:B:502:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:PRO:HA	1:A:520:ASP:OD2	2.13	0.49
1:B:273:ALA:H	1:B:373:GLU:HB3	1.77	0.48
1:A:366:GLU:HG3	3:A:760:HOH:O	2.13	0.48
1:A:456:ASP:OD1	1:A:458:LYS:HG2	2.13	0.48
1:A:281:ARG:HG2	1:A:308:VAL:HG22	1.95	0.48
1:B:256:ASN:O	1:B:258:LYS:N	2.47	0.48
1:B:299:LYS:NZ	1:B:301:LYS:HB3	2.28	0.48
1:B:511:GLU:OE2	3:B:779:HOH:O	2.20	0.48
1:B:352:LEU:HD21	1:B:385:GLU:HG2	1.95	0.48
1:A:363:HIS:H	1:A:363:HIS:HD1	1.62	0.48
1:A:262:LEU:HD22	1:A:276:MSE:HE2	1.96	0.47
1:B:244:ASN:N	1:B:244:ASN:OD1	2.49	0.46
1:A:458:LYS:HE2	1:A:458:LYS:HB3	1.81	0.46
1:B:209:LEU:HG	1:B:211:THR:HG23	1.97	0.46
1:B:267:GLU:N	1:B:270:ILE:O	2.44	0.45
1:B:277:LEU:HD21	1:B:361:PRO:HG3	1.99	0.45
1:A:364:ALA:C	1:A:366:GLU:H	2.19	0.45
1:A:366:GLU:HG2	1:A:494:ASN:OD1	2.17	0.45
1:A:348:VAL:HA	1:A:351:GLN:HG2	1.98	0.45
1:B:314:GLU:HB3	1:B:316:ILE:HG12	1.98	0.45
1:B:301:LYS:HD3	1:B:307:ALA:HB3	1.98	0.44
1:B:216:GLU:HG2	1:B:384:LYS:HA	1.99	0.44
1:B:236:ARG:HG3	1:B:254:LYS:HD3	2.00	0.44
1:A:273:ALA:HB1	1:A:361:PRO:HB3	1.99	0.44
1:B:277:LEU:HD11	1:B:361:PRO:HB2	2.00	0.43
1:B:216:GLU:HB2	1:B:218:VAL:HG12	2.00	0.43
1:B:478:GLU:OE2	1:B:498:LYS:NZ	2.31	0.43
1:A:419:GLN:HB3	1:A:518:VAL:HG22	2.01	0.43
1:A:323:ALA:HB2	1:A:360:VAL:HG12	2.02	0.42
1:A:503:PHE:O	1:A:507:GLN:HG2	2.18	0.42
1:B:252:LYS:HE2	1:B:270:ILE:HD11	2.01	0.42
1:B:313:SER:O	1:B:314:GLU:HB2	2.20	0.42
1:A:181:THR:O	1:A:185:MSE:HG3	2.19	0.42
1:B:371:GLN:HE21	1:B:371:GLN:HB2	1.62	0.42
1:A:355:LYS:HE3	1:A:385:GLU:OE1	2.20	0.42
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.77	0.42
1:B:162:ALA:N	3:B:782:HOH:O	2.53	0.41
1:A:281:ARG:NH2	1:A:300:ARG:HG2	2.36	0.41
1:B:236:ARG:NH1	1:B:328:SER:HB3	2.35	0.41
1:A:306:PRO:HG3	1:A:361:PRO:O	2.20	0.41
1:B:215:TYR:HB3	1:B:384:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ASP:N	3:B:827:HOH:O	2.53	0.41
1:B:295:ASP:HB3	1:B:313:SER:HB2	2.03	0.41
1:A:171:LYS:HB3	1:A:171:LYS:HE2	1.93	0.41
1:B:367:GLY:C	1:B:369:GLY:H	2.25	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	358/366 (98%)	338 (94%)	19 (5%)	1 (0%)	41 31
1	B	357/366 (98%)	332 (93%)	17 (5%)	8 (2%)	6 1
All	All	715/732 (98%)	670 (94%)	36 (5%)	9 (1%)	12 4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	ARG
1	B	257	PRO
1	B	314	GLU
1	B	345	SER
1	A	345	SER
1	B	372	GLU
1	B	313	SER
1	B	367	GLY
1	B	256	ASN

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	331/331 (100%)	317 (96%)	14 (4%)	30	22
1	B	331/331 (100%)	314 (95%)	17 (5%)	24	15
All	All	662/662 (100%)	631 (95%)	31 (5%)	26	18

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	174	LEU
1	B	177	ASP
1	B	194	LEU
1	B	196	ARG
1	B	208	LEU
1	B	219	LYS
1	B	228	VAL
1	B	246	ARG
1	B	259	GLU
1	B	289	ASN
1	B	297	ILE
1	B	315	LYS
1	B	368	ASN
1	B	370	PHE
1	B	371	GLN
1	B	426	ASP
1	B	494	ASN
1	A	181	THR
1	A	215	TYR
1	A	227	ASP
1	A	297	ILE
1	A	298	MSE
1	A	310	LEU
1	A	335	GLN
1	A	366	GLU
1	A	438	VAL
1	A	490	LEU

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Mol	Chain	Res	Type
1	A	497	ASP
1	A	499	ARG
1	A	515	GLU
1	A	518	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	192	HIS
1	B	238	GLN
1	B	371	GLN
1	B	449	ASN
1	B	494	ASN
1	A	217	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	357/366 (97%)	0.21	24 (6%) 17 19	15, 36, 104, 149	0
1	B	354/366 (96%)	0.54	43 (12%) 4 4	18, 52, 126, 160	0
All	All	711/732 (97%)	0.37	67 (9%) 8 9	15, 42, 122, 160	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	ASP	8.5
1	B	304	GLY	8.2
1	A	303	GLY	8.0
1	B	306	PRO	8.0
1	A	368	ASN	7.8
1	B	292	LYS	7.1
1	A	364	ALA	6.8
1	A	365	LYS	6.6
1	B	317	SER	6.4
1	B	303	GLY	5.8
1	B	305	SER	5.7
1	B	371	GLN	5.4
1	A	366	GLU	5.4
1	B	212	GLY	5.4
1	B	311	LEU	5.1
1	A	363	HIS	4.9
1	A	179	ILE	4.9
1	A	304	GLY	4.8
1	B	307	ALA	4.7
1	B	294	THR	4.7
1	A	300	ARG	4.5
1	A	367	GLY	4.4
1	B	256	ASN	4.2
1	B	301	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	370	PHE	4.1
1	A	370	PHE	3.9
1	B	312	ILE	3.6
1	A	302	ARG	3.6
1	A	371	GLN	3.5
1	A	315	LYS	3.4
1	A	301	LYS	3.4
1	A	175	SER	3.4
1	B	313	SER	3.3
1	A	369	GLY	3.3
1	B	295	ASP	3.2
1	B	259	GLU	3.0
1	B	258	LYS	2.9
1	A	305	SER	2.9
1	A	215	TYR	2.9
1	A	177	ASP	2.9
1	B	220	ILE	2.8
1	B	296	VAL	2.8
1	A	316	ILE	2.7
1	B	197	LEU	2.7
1	A	306	PRO	2.6
1	B	219	LYS	2.6
1	A	212	GLY	2.6
1	B	257	PRO	2.6
1	B	235	PRO	2.6
1	B	253	PHE	2.5
1	A	299	LYS	2.4
1	B	314	GLU	2.4
1	B	297	ILE	2.4
1	B	262	LEU	2.3
1	B	265	PHE	2.3
1	B	316	ILE	2.3
1	B	213	SER	2.3
1	B	268	GLY	2.2
1	B	299	LYS	2.2
1	B	260	ASN	2.2
1	B	251	VAL	2.2
1	B	291	ILE	2.2
1	B	310	LEU	2.2
1	B	318	VAL	2.2
1	B	217	HIS	2.1
1	B	302	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	186	VAL	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, 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	B-factors(Å^2)	Q<0.9
2	ZN	A	601	1/1	0.98	0.12	20,20,20,20	0
2	ZN	B	601	1/1	0.99	0.12	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.