



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:04 PM GMT

PDB ID : 1ED9
Title : STRUCTURE OF E. COLI ALKALINE PHOSPHATASE WITHOUT THE
INORGANIC PHOSPHATE AT 1.75Å RESOLUTION
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Deposited on : 2000-01-27
Resolution : 1.75 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

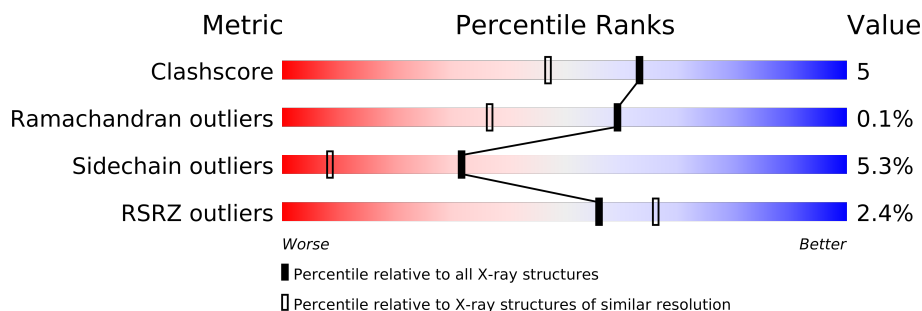
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.75 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))
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	449	
1	B	449	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7240 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ALKALINE PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3304	2042	581	669	12			
1	B	449	Total	C	N	O	S	0	0	0
			3304	2042	581	669	12			

- 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		

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is water.

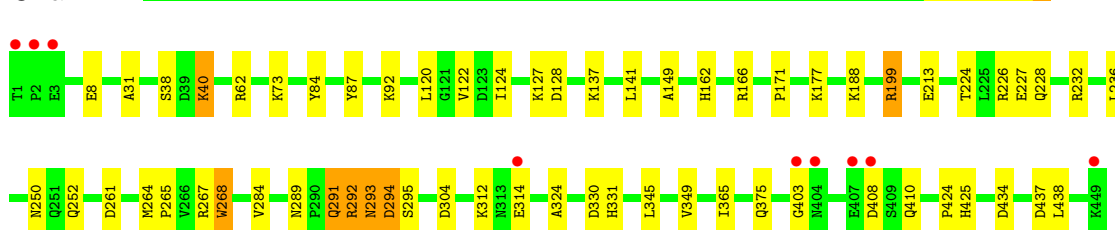
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	359	Total	O	0	0
			359	359		
5	B	257	Total	O	0	0
			257	257		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

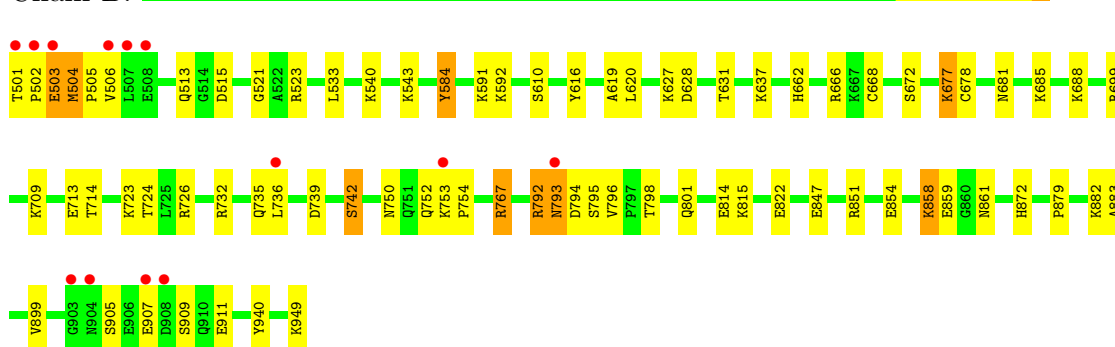
• Molecule 1: ALKALINE PHOSPHATASE

Chain A:



• Molecule 1: ALKALINE PHOSPHATASE

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	194.47Å 167.30Å 76.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.75 126.83 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.0 (15.00-1.75) 91.0 (126.83-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 1.75Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.196 , 0.224 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 116126 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7240	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 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	0.93	0/3359	1.26	9/4560 (0.2%)
1	B	0.85	0/3359	1.22	7/4560 (0.2%)
All	All	0.89	0/6718	1.24	16/9120 (0.2%)

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	1
1	B	1	4
All	All	1	5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	940	TYR	CB-CG-CD1	-9.18	115.49	121.00
1	B	584	TYR	CB-CG-CD1	7.87	125.72	121.00
1	B	732	ARG	NE-CZ-NH1	-7.76	116.42	120.30
1	A	62	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	B	940	TYR	CB-CG-CD2	6.58	124.95	121.00
1	A	62	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	A	292	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	199	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	B	504	MET	CB-CA-C	6.45	123.30	110.40
1	A	293	ASN	N-CA-C	6.06	127.37	111.00
1	A	375	GLN	N-CA-CB	5.62	120.71	110.60
1	B	504	MET	N-CA-CB	5.60	120.67	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	TYR	CB-CG-CD1	5.30	124.18	121.00
1	B	822	GLU	OE1-CD-OE2	-5.23	117.03	123.30
1	A	284	VAL	CG1-CB-CG2	5.12	119.10	110.90
1	A	268	TRP	CB-CG-CD1	5.07	133.59	127.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	504	MET	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	ARG	Sidechain
1	B	726	ARG	Sidechain
1	B	767	ARG	Sidechain
1	B	792	ARG	Sidechain
1	B	851	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3304	0	3178	32	0
1	B	3304	0	3175	39	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	359	0	0	8	0
5	B	257	0	0	9	0
All	All	7240	0	6353	71	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 5.

All (71) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:ASN:O	1:A:292:ARG:HG2	1.94	0.68
1:B:859:GLU:OE2	1:B:861:ASN:N	2.29	0.65
1:A:73:LYS:HE3	5:A:1142:HOH:O	1.95	0.65
1:A:312:LYS:HE2	5:A:1137:HOH:O	1.96	0.65
1:A:137:LYS:HE3	1:A:199:ARG:O	1.98	0.64
1:A:120:LEU:O	1:A:162:HIS:HA	2.00	0.61
1:A:128:ASP:OD1	1:A:188:LYS:HE3	2.01	0.60
1:A:314:GLU:HA	1:A:314:GLU:OE2	2.00	0.60
1:B:620:LEU:O	1:B:662:HIS:HA	2.02	0.59
1:B:793:ASN:OD1	1:B:794:ASP:N	2.36	0.58
1:B:792:ARG:NH1	4:B:958:SO4:O2	2.35	0.57
1:B:907:GLU:HB2	5:B:1547:HOH:O	2.03	0.56
1:B:668:CYS:SG	1:B:677:LYS:HB2	2.45	0.56
1:B:859:GLU:OE1	1:B:861:ASN:HB2	2.05	0.56
1:B:688:LYS:HD2	5:B:1313:HOH:O	2.04	0.56
1:B:739:ASP:OD2	1:B:742:SER:OG	2.18	0.55
1:A:267:ARG:HG2	1:A:268:TRP:CD1	2.43	0.54
1:B:794:ASP:OD1	1:B:794:ASP:O	2.28	0.52
1:A:252:GLN:OE1	1:A:252:GLN:N	2.39	0.52
1:A:122:VAL:HA	1:A:127:LYS:O	2.10	0.52
1:B:793:ASN:HB3	1:B:796:VAL:HG23	1.91	0.52
1:B:515:ASP:O	1:B:521:GLY:HA3	2.10	0.52
1:B:905:SER:O	5:B:1599:HOH:O	2.20	0.50
1:B:506:VAL:HG22	5:B:1446:HOH:O	2.11	0.50
1:B:854:GLU:O	1:B:858:LYS:HG3	2.11	0.49
1:A:224:THR:OG1	1:A:227:GLU:HG3	2.11	0.49
1:B:798:THR:OG1	1:B:801:GLN:HG3	2.12	0.49
1:A:331:HIS:ND1	1:A:410:GLN:O	2.45	0.49
1:B:501:THR:HG23	1:B:502:PRO:HD2	1.95	0.48
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.94	0.48
1:A:228:GLN:O	1:A:232:ARG:HG3	2.15	0.47
1:B:699:ARG:NH2	1:B:754:PRO:HD3	2.29	0.47
1:B:501:THR:O	1:B:503:GLU:N	2.47	0.47
1:B:879:PRO:HA	1:B:899:VAL:HG21	1.96	0.47
1:B:591:LYS:O	5:B:1444:HOH:O	2.21	0.47
1:B:672:SER:HG	1:B:713:GLU:CD	2.18	0.47
1:A:293:ASN:HB3	1:A:295:SER:OG	2.15	0.47
1:B:666:ARG:NH2	5:B:1546:HOH:O	2.47	0.46
1:A:31:ALA:HB1	5:A:1537:HOH:O	2.16	0.45
1:B:699:ARG:HD2	5:B:1245:HOH:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:291:GLN:HG3	5:A:1174:HOH:O	2.17	0.45
1:A:403:GLY:HA2	5:A:1125:HOH:O	2.17	0.45
1:A:188:LYS:HE2	5:A:1149:HOH:O	2.17	0.44
1:B:616:TYR:CZ	1:B:619:ALA:HB2	2.52	0.44
1:B:637:LYS:NZ	1:B:699:ARG:HB3	2.34	0.43
1:B:793:ASN:ND2	1:B:795:SER:OG	2.50	0.43
1:B:859:GLU:OE2	1:B:861:ASN:HB2	2.18	0.43
1:A:264:MET:HB3	1:A:265:PRO:HD2	2.00	0.43
1:A:345:LEU:O	1:A:349:VAL:HG23	2.19	0.43
1:B:513:GLN:HG2	1:B:523:ARG:O	2.19	0.43
1:B:678:CYS:HB3	1:B:681:ASN:OD1	2.19	0.43
1:A:38:SER:OG	1:A:40:LYS:HB2	2.19	0.43
1:A:250:ASN:OD1	1:A:252:GLN:OE1	2.37	0.42
1:B:714:THR:HA	1:B:724:THR:HA	2.00	0.42
1:B:610:SER:O	1:B:631:THR:HA	2.19	0.42
1:A:128:ASP:OD1	1:A:188:LYS:CE	2.65	0.42
1:B:505:PRO:HD2	5:B:1422:HOH:O	2.19	0.41
1:B:750:ASN:OD1	1:B:752:GLN:HB2	2.20	0.41
1:A:250:ASN:CG	1:A:252:GLN:OE1	2.59	0.41
1:A:171:PRO:HD2	1:A:213:GLU:OE1	2.20	0.41
1:B:628:ASP:OD1	1:B:688:LYS:NZ	2.49	0.41
1:B:742:SER:HG	1:B:742:SER:H	1.61	0.41
1:A:294:ASP:HB2	5:A:1571:HOH:O	2.20	0.41
1:B:627:LYS:HG2	1:B:628:ASP:N	2.33	0.41
1:A:166:ARG:NH2	5:A:1544:HOH:O	2.53	0.41
1:B:767:ARG:NH2	1:B:847:GLU:OE2	2.43	0.40
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.51	0.40
1:A:424:PRO:O	1:A:425:HIS:HB2	2.20	0.40
1:B:883:ALA:HB1	5:B:1112:HOH:O	2.20	0.40
1:A:434:ASP:O	1:A:437:ASP:HB2	2.20	0.40
1:A:124:ILE:HD13	1:A:124:ILE:HG21	1.88	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	447/449 (100%)	440 (98%)	7 (2%)	0	100	100
1	B	447/449 (100%)	434 (97%)	12 (3%)	1 (0%)	56	34
All	All	894/898 (100%)	874 (98%)	19 (2%)	1 (0%)	59	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	793	ASN

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	340/340 (100%)	327 (96%)	13 (4%)	44	17
1	B	340/340 (100%)	317 (93%)	23 (7%)	22	4
All	All	680/680 (100%)	644 (95%)	36 (5%)	32	8

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	40	LYS
1	A	84	TYR
1	A	92	LYS
1	A	141	LEU
1	A	177	LYS
1	A	236	LEU
1	A	261	ASP
1	A	291	GLN
1	A	294	ASP
1	A	304	ASP
1	A	330	ASP
1	A	408	ASP
1	B	503	GLU
1	B	504	MET
1	B	533	LEU

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Mol	Chain	Res	Type
1	B	540	LYS
1	B	543	LYS
1	B	584	TYR
1	B	592	LYS
1	B	677	LYS
1	B	685	LYS
1	B	709	LYS
1	B	723	LYS
1	B	735	GLN
1	B	736	LEU
1	B	742	SER
1	B	753	LYS
1	B	814	GLU
1	B	815	LYS
1	B	858	LYS
1	B	872	HIS
1	B	882	LYS
1	B	909	SER
1	B	911	GLU
1	B	949	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	752	GLN
1	B	838	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are 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	458	-	4,4,4	1.33	0	6,6,6	0.20	0
4	SO4	B	958	-	4,4,4	1.31	0	6,6,6	0.09	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
4	SO4	A	458	-	-	0/0/0/0	0/0/0/0
4	SO4	B	958	-	-	0/0/0/0	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	449/449 (100%)	-0.04	9 (2%) 62 73	11, 20, 44, 115	0
1	B	449/449 (100%)	0.15	13 (2%) 49 59	13, 26, 58, 134	0
All	All	898/898 (100%)	0.06	22 (2%) 56 66	11, 23, 53, 134	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	THR	17.4
1	A	1	THR	16.1
1	B	502	PRO	8.3
1	A	2	PRO	7.3
1	B	503	GLU	4.8
1	B	904	ASN	4.1
1	A	408	ASP	4.1
1	B	908	ASP	4.1
1	B	508	GLU	3.5
1	B	506	VAL	3.5
1	A	3	GLU	3.3
1	B	507	LEU	3.2
1	B	793	ASN	3.0
1	A	449	LYS	3.0
1	B	907	GLU	2.8
1	A	314	GLU	2.8
1	A	407	GLU	2.7
1	B	753	LYS	2.6
1	A	404	ASN	2.2
1	A	403	GLY	2.1
1	B	736	LEU	2.1
1	B	903	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	B	958	5/5	0.14	0.95	60,75,82,84	5
4	SO4	A	458	5/5	0.14	0.24	34,54,59,62	0
3	MG	A	462	1/1	0.07	-0.48	16,16,16,16	0
3	MG	B	962	1/1	0.07	-1.33	21,21,21,21	0
2	ZN	A	450	1/1	0.04	-3.90	22,22,22,22	0
2	ZN	A	451	1/1	0.03	-4.28	18,18,18,18	0
2	ZN	B	951	1/1	0.03	-4.71	23,23,23,23	0
2	ZN	B	950	1/1	0.04	-4.91	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.