



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:31 PM UTC

PDB ID : 1ED9 / pdb_00001ed9
Title : STRUCTURE OF E. COLI ALKALINE PHOSPHATASE WITHOUT THE
INORGANIC PHOSPHATE AT 1.75Å RESOLUTION
Authors : Stec, B.; Holtz, K.M.; Kantrowitz, E.R.
Deposited on : 2000-01-27
Resolution : 1.75 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

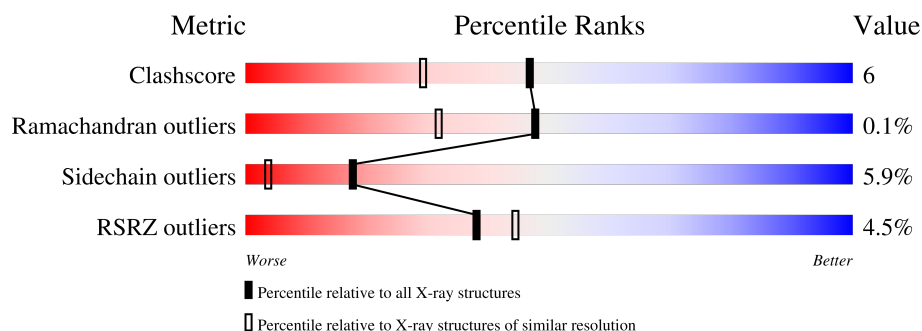
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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 $\leq 5\%$. 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	449	3% 81% 17% .
1	B	449	6% 80% 18% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7240 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 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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is SULFATE ION (CCD ID: 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		

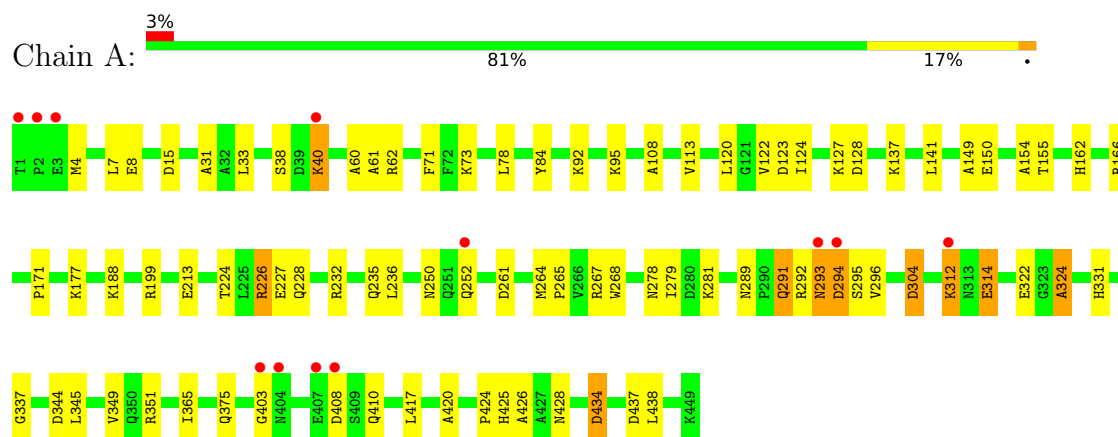
- Molecule 5 is water.

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

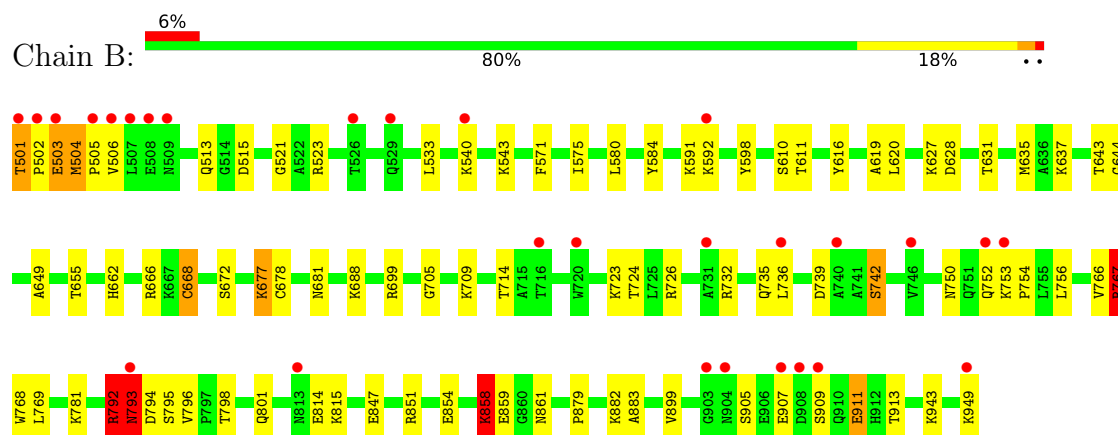
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: ALKALINE PHOSPHATASE



• Molecule 1: ALKALINE PHOSPHATASE



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 15.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.0 (15.00-1.75) 90.7 (15.00-1.75)	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.	wwPDB-VP
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 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, 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	1.30	9/3359 (0.3%)	1.68	30/4560 (0.7%)
1	B	1.19	7/3359 (0.2%)	1.64	28/4560 (0.6%)
All	All	1.24	16/6718 (0.2%)	1.66	58/9120 (0.6%)

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	913	THR	N-CA	6.34	1.54	1.45
1	A	78	LEU	CA-C	-6.16	1.46	1.52
1	B	768	TRP	N-CA	-5.78	1.38	1.46
1	A	375	GLN	N-CA	-5.69	1.38	1.45
1	B	756	LEU	N-CA	-5.59	1.40	1.46
1	A	61	ALA	N-CA	-5.55	1.39	1.46
1	A	123	ASP	C-N	5.46	1.40	1.34
1	A	7	LEU	N-CA	5.42	1.52	1.46
1	B	668	CYS	CA-C	-5.41	1.47	1.53
1	A	322	GLU	N-CA	-5.38	1.39	1.46
1	A	293	ASN	N-CA	-5.36	1.39	1.46
1	B	644	GLY	N-CA	-5.23	1.40	1.45
1	A	337	GLY	N-CA	5.22	1.52	1.45
1	A	155	THR	CA-C	-5.20	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	655	THR	CA-C	-5.18	1.46	1.52
1	B	504	MET	CA-CB	-5.13	1.45	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ASN	N-CA-C	7.78	127.37	110.80
1	B	504	MET	CB-CA-C	6.66	123.30	110.17
1	A	322	GLU	N-CA-C	6.47	119.07	108.52
1	A	314	GLU	N-CA-C	6.44	120.40	112.54
1	A	434	ASP	CA-CB-CG	-6.40	106.20	112.60
1	A	337	GLY	N-CA-C	-6.38	104.60	112.77
1	B	793	ASN	N-CA-C	6.35	124.32	110.80
1	B	858	LYS	N-CA-CB	6.14	118.98	110.07
1	A	420	ALA	CA-C-N	-6.12	111.83	121.87
1	A	420	ALA	C-N-CA	-6.12	111.83	121.87
1	B	580	LEU	CA-C-O	6.08	127.01	120.32
1	B	767	ARG	CA-C-N	6.05	132.02	122.94
1	B	767	ARG	C-N-CA	6.05	132.02	122.94
1	B	792	ARG	CA-C-N	6.01	133.02	121.54
1	B	792	ARG	C-N-CA	6.01	133.02	121.54
1	A	324	ALA	N-CA-C	5.95	117.85	111.36
1	B	781	LYS	CA-C-N	5.93	125.91	120.03
1	B	781	LYS	C-N-CA	5.93	125.91	120.03
1	B	649	ALA	O-C-N	5.89	129.85	122.43
1	A	344	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	580	LEU	CA-C-N	-5.85	113.40	122.59
1	B	580	LEU	C-N-CA	-5.85	113.40	122.59
1	A	154	ALA	N-CA-C	5.80	118.07	111.11
1	B	504	MET	N-CA-CB	5.79	120.67	110.37
1	A	278	ASN	CA-C-N	-5.69	117.14	122.66
1	A	278	ASN	C-N-CA	-5.69	117.14	122.66
1	A	150	GLU	O-C-N	5.68	129.85	122.87
1	A	108	ALA	N-CA-C	5.62	117.88	111.02
1	B	911	GLU	N-CA-C	5.54	118.71	110.52
1	B	705	GLY	CA-C-O	-5.50	115.42	120.97
1	A	71	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	426	ALA	CA-C-O	5.42	126.22	120.10
1	A	4	MET	CB-CA-C	5.38	115.99	109.85
1	A	62	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	B	643	THR	CA-C-N	5.33	126.53	121.46
1	B	643	THR	C-N-CA	5.33	126.53	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	598	TYR	CA-C-N	-5.31	115.78	123.11
1	B	598	TYR	C-N-CA	-5.31	115.78	123.11
1	A	296	VAL	CA-C-O	5.31	123.08	119.20
1	A	428	ASN	CA-CB-CG	-5.31	107.29	112.60
1	A	15	ASP	CA-C-O	-5.29	114.62	120.60
1	B	766	VAL	CA-C-N	5.20	127.19	120.44
1	B	766	VAL	C-N-CA	5.20	127.19	120.44
1	B	769	LEU	CA-C-N	5.17	129.99	121.87
1	B	769	LEU	C-N-CA	5.17	129.99	121.87
1	A	293	ASN	CA-C-N	5.17	129.47	120.68
1	A	293	ASN	C-N-CA	5.17	129.47	120.68
1	A	150	GLU	N-CA-C	-5.15	102.77	110.23
1	A	375	GLN	N-CA-CB	5.13	120.71	111.37
1	B	575	ILE	N-CA-C	5.13	115.74	110.36
1	A	226	ARG	CA-C-N	5.11	127.13	120.28
1	A	226	ARG	C-N-CA	5.11	127.13	120.28
1	B	732	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	A	60	ALA	CA-C-N	5.07	127.07	120.28
1	A	60	ALA	C-N-CA	5.07	127.07	120.28
1	A	281	LYS	N-CA-C	5.05	117.25	110.29
1	B	571	PHE	N-CA-CB	-5.04	102.08	110.99
1	B	611	THR	O-C-N	-5.00	116.80	122.10

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 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	3304	0	3248	35	0
1	B	3304	0	3245	40	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	9	0
5	B	257	0	0	9	0
All	All	7240	0	6493	75	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 (75) 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:289:ASN:O	1:A:292:ARG:HG2	1.94	0.68
1:A:73:LYS:HE3	5:A:1142:HOH:O	1.95	0.65
1:B:859:GLU:OE2	1:B:861:ASN:N	2.29	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	0.59
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:688:LYS:HD2	5:B:1313:HOH:O	2.04	0.56
1:B:859:GLU:OE1	1:B:861:ASN:HB2	2.05	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:O	1:B:794:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:293:ASN:HB3	1:A:295:SER:OG	2.15	0.47
1:B:591:LYS:O	5:B:1444:HOH:O	2.21	0.47
1:B:879:PRO:HA	1:B:899:VAL:HG21	1.96	0.47
1:A:250:ASN:CG	1:A:252:GLN:OE1	2.59	0.46
1:A:95:LYS:NZ	5:A:1336:HOH:O	2.48	0.45
1:A:31:ALA:HB1	5:A:1537:HOH:O	2.16	0.45
1:B:635:MET:HE1	1:B:943:LYS:HD2	1.98	0.45
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:B:699:ARG:HD2	5:B:1245:HOH:O	2.17	0.45
1:A:304:ASP:CG	1:A:351:ARG:HH21	2.25	0.44
1:B:666:ARG:NH2	5:B:1546:HOH:O	2.47	0.44
1:A:331:HIS:ND1	1:A:410:GLN:O	2.45	0.44
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:A:264:MET:HB3	1:A:265:PRO:HD2	2.00	0.43
1:B:859:GLU:OE2	1:B:861:ASN:HB2	2.18	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:A:38:SER:OG	1:A:40:LYS:HB2	2.19	0.43
1:B:678:CYS:HB3	1:B:681:ASN:OD1	2.19	0.43
1:A:250:ASN:OD1	1:A:252:GLN:OE1	2.37	0.42
1:B:859:GLU:CD	1:B:861:ASN:HB2	2.43	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:A:417:LEU:HD12	1:A:417:LEU:C	2.44	0.42
1:B:505:PRO:HD2	5:B:1422:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:750:ASN:OD1	1:B:752:GLN:HB2	2.20	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:H	1:B:742:SER:HG	1.61	0.41
1:A:294:ASP:HB2	5:A:1571:HOH:O	2.20	0.41
1:A:166:ARG:NH2	5:A:1544:HOH:O	2.53	0.41
1:B:627:LYS:HG2	1:B:628:ASP:N	2.33	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:A:434:ASP:O	1:A:437:ASP:HB2	2.20	0.40
1:B:883:ALA:HB1	5:B:1112:HOH:O	2.20	0.40
1:A:124:ILE:HG21	1:A:124:ILE:HD13	1.88	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	447/449 (100%)	440 (98%)	7 (2%)	0	100	100
1	B	447/449 (100%)	434 (97%)	12 (3%)	1 (0%)	43	27
All	All	894/898 (100%)	874 (98%)	19 (2%)	1 (0%)	48	32

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%)	323 (95%)	17 (5%)	22	5
1	B	340/340 (100%)	317 (93%)	23 (7%)	14	3
All	All	680/680 (100%)	640 (94%)	40 (6%)	18	4

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	33	LEU
1	A	40	LYS
1	A	84	TYR
1	A	92	LYS
1	A	113	VAL
1	A	141	LEU
1	A	177	LYS
1	A	235	GLN
1	A	236	LEU
1	A	261	ASP
1	A	279	ILE
1	A	291	GLN
1	A	294	ASP
1	A	304	ASP
1	A	312	LYS
1	A	408	ASP
1	B	501	THR
1	B	503	GLU
1	B	504	MET
1	B	533	LEU
1	B	540	LYS
1	B	543	LYS
1	B	584	TYR
1	B	592	LYS
1	B	672	SER
1	B	677	LYS

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Mol	Chain	Res	Type
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	882	LYS
1	B	909	SER
1	B	911	GLU
1	B	949	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	145	ASN
1	A	293	ASN
1	A	375	GLN
1	A	410	GLN
1	B	752	GLN
1	B	813	ASN
1	B	875	GLN
1	B	910	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.55	0	6,6,6	0.19	0
4	SO4	B	958	-	4,4,4	0.52	0	6,6,6	0.09	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	958	SO4	1	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, 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%)	0.12	12 (2%) 56 62	11, 20, 44, 115	0
1	B	449/449 (100%)	0.46	28 (6%) 26 30	13, 26, 58, 134	0
All	All	898/898 (100%)	0.29	40 (4%) 38 44	11, 23, 53, 134	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	502	PRO	7.9
1	A	1	THR	6.9
1	A	2	PRO	5.9
1	B	501	THR	5.2
1	B	507	LEU	4.7
1	B	904	ASN	4.1
1	A	293	ASN	3.5
1	B	949	LYS	3.4
1	B	793	ASN	3.3
1	A	408	ASP	3.2
1	B	731	ALA	3.1
1	B	506	VAL	3.0
1	B	508	GLU	3.0
1	B	503	GLU	2.9
1	B	753	LYS	2.8
1	B	509	ASN	2.7
1	B	746	VAL	2.6
1	B	505	PRO	2.6
1	B	909	SER	2.6
1	A	294	ASP	2.5
1	B	526	THR	2.5
1	A	407	GLU	2.5
1	B	720	TRP	2.4
1	B	736	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	903	GLY	2.4
1	A	404	ASN	2.3
1	B	908	ASP	2.3
1	A	3	GLU	2.3
1	B	592	LYS	2.3
1	B	540	LYS	2.3
1	B	740	ALA	2.2
1	A	40	LYS	2.2
1	B	716	THR	2.2
1	A	252	GLN	2.2
1	A	403	GLY	2.2
1	A	312	LYS	2.2
1	B	813	ASN	2.1
1	B	529	GLN	2.1
1	B	752	GLN	2.1
1	B	907	GLU	2.1

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 oligosaccharides 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
4	SO4	B	958	5/5	0.88	0.10	60,75,82,84	5
4	SO4	A	458	5/5	0.90	0.15	34,54,59,62	0
3	MG	A	462	1/1	0.96	0.04	16,16,16,16	0
2	ZN	A	450	1/1	0.99	0.07	22,22,22,22	0
3	MG	B	962	1/1	0.99	0.03	21,21,21,21	0
2	ZN	A	451	1/1	0.99	0.07	18,18,18,18	0
2	ZN	B	951	1/1	0.99	0.07	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	950	1/1	1.00	0.06	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.