Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 04:21 pm BST

PDB ID	:	1ALH
Title	:	KINETICS AND CRYSTAL STRUCTURE OF A MUTANT E. COLI AL-KALINE PHOSPHATASE (ASP-369–>ASN): A MECHANISM INVOLVING ONE ZINC PER ACTIVE SITE
Authors	:	Tibbitts, T.T.; Xu, X.; Kantrowitz, E.R.
Deposited on	:	1994-08-23
Resolution	:	2.50 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 following versions of software and data (see references (i)) were used in the production of this report:

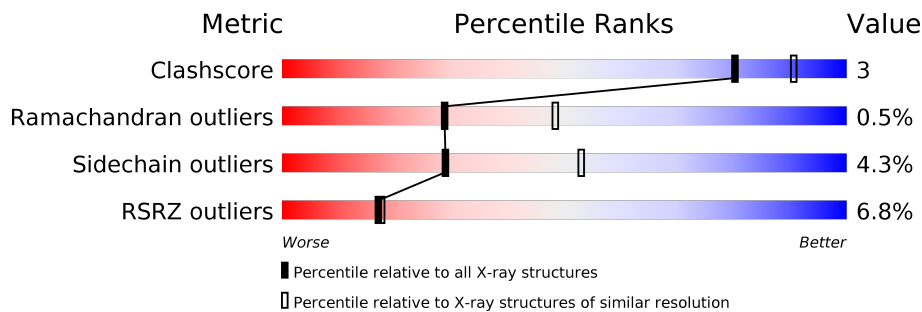|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.5%
Sidechain outliers		4.3%
RSRZ outliers		6.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	446	4% 87% 11% ·
1	B	446	10% 89% 10% ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8978 atoms, of which 2096 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	446	Total 4034	C 2028	H 753	N 578	O 663	S 12	0	0	0
1	B	446	Total 4034	C 2028	H 753	N 578	O 663	S 12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	GLU	GLN	CONFLICT	UNP P00634
A	369	ASN	ASP	CONFLICT	UNP P00634
B	230	GLU	GLN	CONFLICT	UNP P00634
B	369	ASN	ASP	CONFLICT	UNP P00634

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

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

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

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
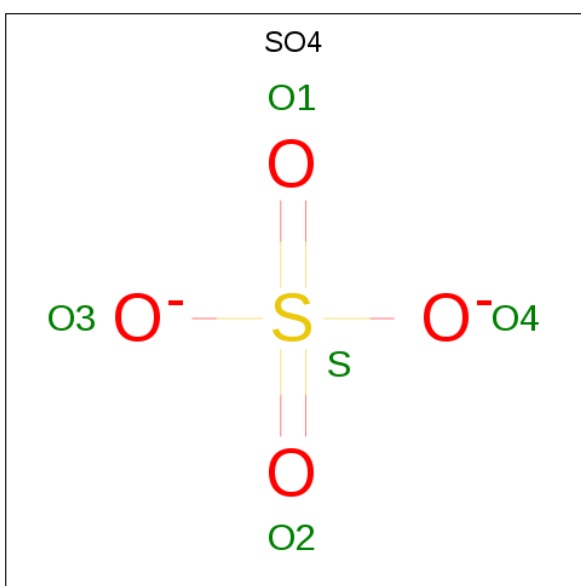
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	175	Total 519	H 344	O 175	0	0
5	B	123	Total 369	H 246	O 123	0	0

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 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
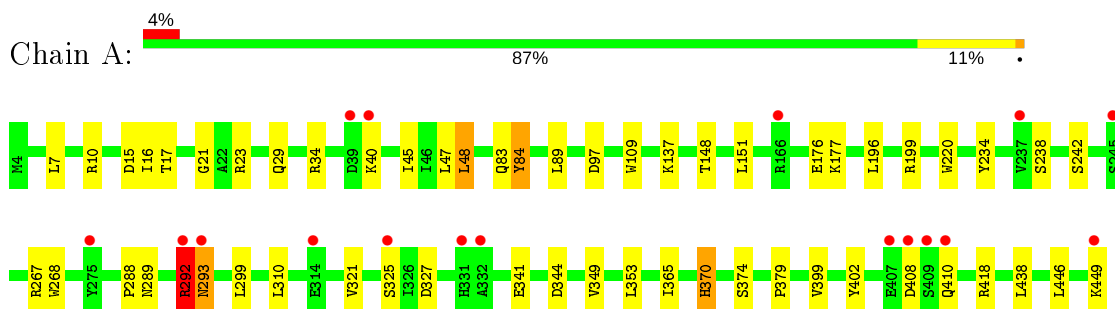
• Molecule 1: ALKALINE PHOSPHATASE
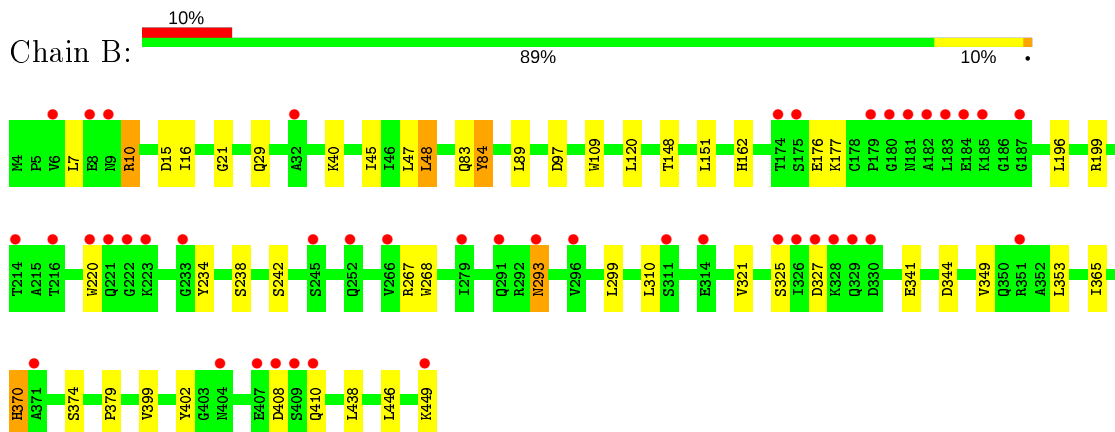
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	194.39Å 167.25Å 76.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 97.20 – 2.48	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 96.6 (97.20-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , (Not available) 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 61.0	EDS
L-test for twinning[1]	$<|L|> = 0.38$, $<L^2> = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8978	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]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, PO4, 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	0.62	0/3335	1.14	21/4526 (0.5%)
1	B	0.62	0/3335	1.13	20/4526 (0.4%)
All	All	0.62	0/6670	1.14	41/9052 (0.5%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	TYR	CB-CG-CD2	-10.81	114.51	121.00
1	B	84	TYR	CB-CG-CD2	-10.41	114.75	121.00
1	B	220	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	A	220	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	B	199	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	84	TYR	CB-CG-CD1	7.98	125.79	121.00
1	B	84	TYR	CB-CG-CD1	7.94	125.76	121.00
1	B	268	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	A	268	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	B	220	TRP	CE2-CD2-CG	-7.32	101.45	107.30
1	A	220	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	B	199	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	268	TRP	CE2-CD2-CG	-6.87	101.80	107.30
1	A	109	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	B	109	TRP	CD1-CG-CD2	6.78	111.72	106.30
1	A	268	TRP	CE2-CD2-CG	-6.77	101.89	107.30
1	B	84	TYR	CA-CB-CG	6.63	126.00	113.40
1	B	109	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	A	109	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	A	84	TYR	CA-CB-CG	6.42	125.60	113.40
1	A	292	ARG	CA-CB-CG	5.90	126.38	113.40
1	A	292	ARG	NE-CZ-NH1	5.87	123.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	B	220	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	B	267	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	199	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	267	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	293	ASN	N-CA-C	5.44	125.69	111.00
1	B	293	ASN	N-CA-C	5.43	125.66	111.00
1	B	234	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	220	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	A	418	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	10	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	97	ASP	N-CA-C	-5.28	96.74	111.00
1	B	268	TRP	CG-CD1-NE1	-5.26	104.83	110.10
1	A	23	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	97	ASP	N-CA-C	-5.20	96.95	111.00
1	B	267	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	48	LEU	CA-CB-CG	5.10	127.02	115.30
1	B	48	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	268	TRP	CG-CD1-NE1	-5.03	105.07	110.10

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	3281	753	3227	22	0
1	B	3281	753	3227	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	175	344	0	0	2
5	B	123	246	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6882	2096	6454	35	2

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 (35) 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:16:ILE:HG22	1:B:89:LEU:HD21	1.67	0.77
1:A:402:TYR:HB3	1:A:410:GLN:HG3	1.74	0.68
1:A:89:LEU:HD21	1:B:16:ILE:HG22	1.73	0.68
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.75	0.68
1:A:48:LEU:HG	1:A:349:VAL:HG22	1.82	0.62
1:B:48:LEU:HG	1:B:349:VAL:HG22	1.81	0.61
1:A:288:PRO:HB3	1:A:292:ARG:HH21	1.66	0.59
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.85	0.58
1:A:10:ARG:HH21	1:A:29:GLN:NE2	2.02	0.58
1:B:45:ILE:HD12	1:B:446:LEU:HD22	1.85	0.58
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.85	0.57
1:A:45:ILE:HD12	1:A:446:LEU:HD22	1.86	0.57
1:A:16:ILE:CG2	1:B:89:LEU:HD21	2.37	0.53
1:A:325:SER:HB2	1:A:341:GLU:HG3	1.91	0.52
1:B:325:SER:HB2	1:B:341:GLU:HG3	1.92	0.51
1:A:288:PRO:HB3	1:A:292:ARG:NH2	2.26	0.51
1:B:176:GLU:HG3	1:B:177:LYS:HG3	1.95	0.49
1:A:176:GLU:HG3	1:A:177:LYS:HG3	1.95	0.49
1:A:17:THR:HG22	1:B:89:LEU:HD13	1.95	0.49
1:B:15:ASP:O	1:B:21:GLY:HA3	2.13	0.48
1:A:15:ASP:O	1:A:21:GLY:HA3	2.13	0.48
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.97	0.45
1:A:34:ARG:HD3	5:B:557:HOH:O	2.15	0.45
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.98	0.45
1:A:289:ASN:O	1:A:292:ARG:HG3	2.17	0.44
1:A:137:LYS:HB3	1:A:137:LYS:HE2	1.84	0.43
1:A:148:THR:HG23	1:A:299:LEU:HD13	2.00	0.43
1:B:365:ILE:HD13	1:B:438:LEU:HD11	2.01	0.43
1:B:148:THR:HG23	1:B:299:LEU:HD13	2.01	0.42
1:B:10:ARG:HH21	1:B:29:GLN:NE2	2.17	0.42
1:A:327:ASP:OD1	1:A:370:HIS:HE1	2.02	0.42
1:A:365:ILE:HD13	1:A:438:LEU:HD11	2.00	0.42
1:A:83:GLN:HE21	1:B:83:GLN:HE21	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:O	1:B:162:HIS:HA	2.20	0.41
1:B:327:ASP:OD1	1:B:370:HIS:HE1	2.04	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:587:HOH:O	5:A:587:HOH:O[3_656]	0.59	1.61
5:A:574:HOH:O	5:A:574:HOH:O[3_656]	1.39	0.81

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	444/446 (100%)	433 (98%)	9 (2%)	2 (0%)	29	48
1	B	444/446 (100%)	434 (98%)	8 (2%)	2 (0%)	29	48
All	All	888/892 (100%)	867 (98%)	17 (2%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	408	ASP
1	B	293	ASN
1	B	408	ASP

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	337/337 (100%)	322 (96%)	15 (4%)	27	51
1	B	337/337 (100%)	323 (96%)	14 (4%)	30	54
All	All	674/674 (100%)	645 (96%)	29 (4%)	29	53

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	40	LYS
1	A	47	LEU
1	A	84	TYR
1	A	151	LEU
1	A	196	LEU
1	A	238	SER
1	A	242	SER
1	A	292	ARG
1	A	310	LEU
1	A	344	ASP
1	A	353	LEU
1	A	370	HIS
1	A	374	SER
1	A	449	LYS
1	B	7	LEU
1	B	40	LYS
1	B	47	LEU
1	B	84	TYR
1	B	151	LEU
1	B	196	LEU
1	B	238	SER
1	B	242	SER
1	B	310	LEU
1	B	344	ASP
1	B	353	LEU
1	B	370	HIS
1	B	374	SER
1	B	449	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	125	HIS
1	A	338	GLN
1	A	370	HIS
1	B	29	GLN
1	B	83	GLN
1	B	338	GLN
1	B	370	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 carbohydrates in this entry.

5.6   Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#|Z| > 2$
3	PO4	A	453	2	4,4,4	1.25	0	6,6,6	0.41	0
4	SO4	A	454	-	4,4,4	0.51	0	6,6,6	0.08	0
3	PO4	B	453	2	4,4,4	1.29	0	6,6,6	0.41	0
4	SO4	B	454	-	4,4,4	0.53	0	6,6,6	0.06	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.

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	446/446 (100%)	0.20	17 (3%)	40	43	3, 14, 43, 82	0
1	B	446/446 (100%)	0.44	44 (9%)	7	7	2, 16, 45, 83	0
All	All	892/892 (100%)	0.32	61 (6%)	17	17	2, 14, 44, 83	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	ALA	5.0
1	B	187	GLY	4.7
1	B	223	LYS	4.7
1	A	449	LYS	4.5
1	B	179	PRO	4.1
1	B	325	SER	4.0
1	B	222	GLY	3.8
1	A	408	ASP	3.7
1	B	326	ILE	3.7
1	B	449	LYS	3.6
1	B	174	THR	3.6
1	B	408	ASP	3.6
1	B	252	GLN	3.5
1	B	407	GLU	3.5
1	B	329	GLN	3.4
1	B	8	GLU	3.3
1	B	220	TRP	3.3
1	B	351	ARG	3.1
1	B	216	THR	3.1
1	B	328	LYS	3.1
1	A	39	ASP	3.1
1	A	237	VAL	2.9
1	B	184	GLU	2.9
1	A	292	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	275	TYR	2.9
1	B	32	ALA	2.8
1	B	266	VAL	2.8
1	B	221	GLN	2.7
1	B	410	GLN	2.7
1	A	331	HIS	2.7
1	B	180	GLY	2.6
1	B	245	SER	2.6
1	B	214	THR	2.6
1	A	407	GLU	2.5
1	B	327	ASP	2.5
1	B	279	ILE	2.5
1	B	291	GLN	2.5
1	A	293	ASN	2.4
1	B	181	ASN	2.4
1	B	233	GLY	2.4
1	B	185	LYS	2.4
1	B	296	VAL	2.4
1	A	40	LYS	2.3
1	A	409	SER	2.3
1	B	183	LEU	2.3
1	B	314	GLU	2.3
1	A	325	SER	2.2
1	A	245	SER	2.2
1	A	410	GLN	2.2
1	B	330	ASP	2.2
1	A	166	ARG	2.2
1	B	9	ASN	2.1
1	B	404	ASN	2.1
1	B	311	SER	2.1
1	A	314	GLU	2.1
1	B	371	ALA	2.1
1	B	175	SER	2.1
1	B	409	SER	2.1
1	A	332	ALA	2.0
1	B	6	VAL	2.0
1	B	293	ASN	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. 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	454	5/5	0.87	0.28	66,67,68,68	0
3	PO4	B	453	5/5	0.88	0.24	65,68,72,73	0
3	PO4	A	453	5/5	0.94	0.27	67,74,74,76	0
4	SO4	A	454	5/5	0.94	0.25	66,66,67,70	0
2	ZN	A	450	1/1	0.94	0.08	27,27,27,27	0
2	ZN	B	450	1/1	0.95	0.09	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.