



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:43 AM UTC

PDB ID : 1Y6V / pdb_00001y6v
Title : Structure of E. coli Alkaline Phosphatase in presence of cobalt at 1.60 Å resolution
Authors : Wang, J.; Stieglitz, K.; Kantrowitz, E.R.
Deposited on : 2004-12-07
Resolution : 1.60 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

<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

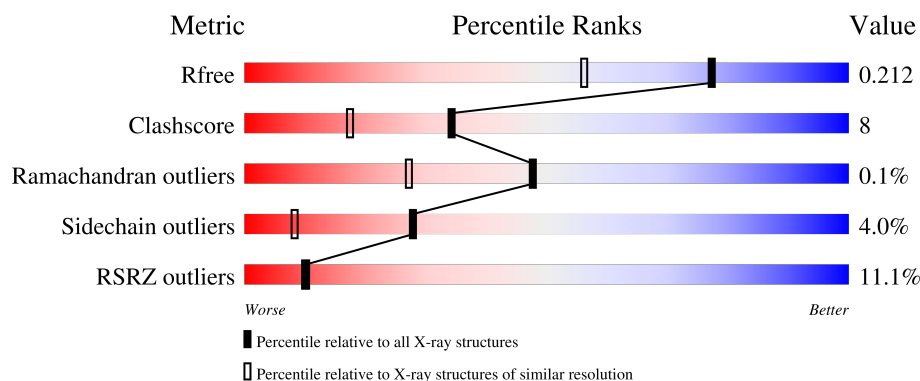
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 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	4% 87% 11% .
1	B	449	18% 80% 16% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	858	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7346 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.

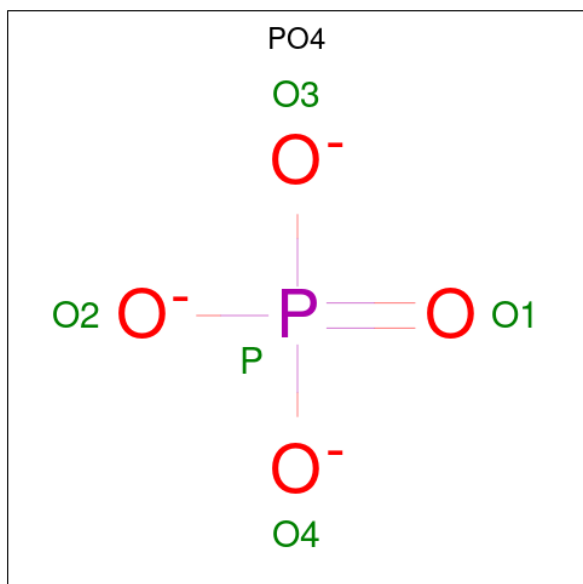
- Molecule 1 is a protein called Alkaline phosphatase.

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 COBALT (II) ION (CCD ID: CO) (formula: Co).

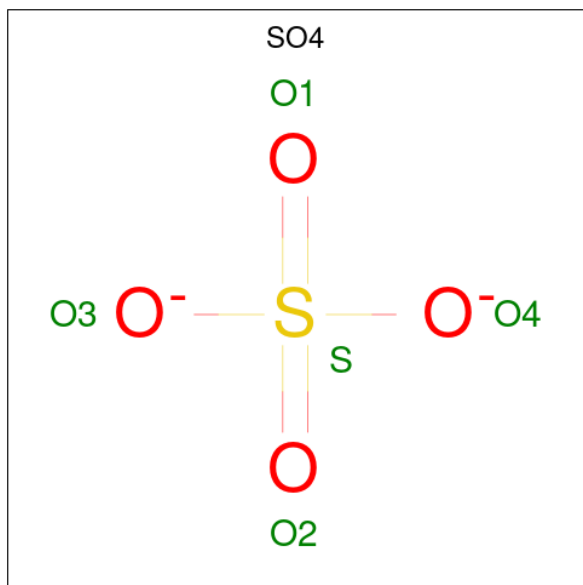
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Co	0	0
			3	3		
2	B	3	Total	Co	0	0
			3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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 (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		

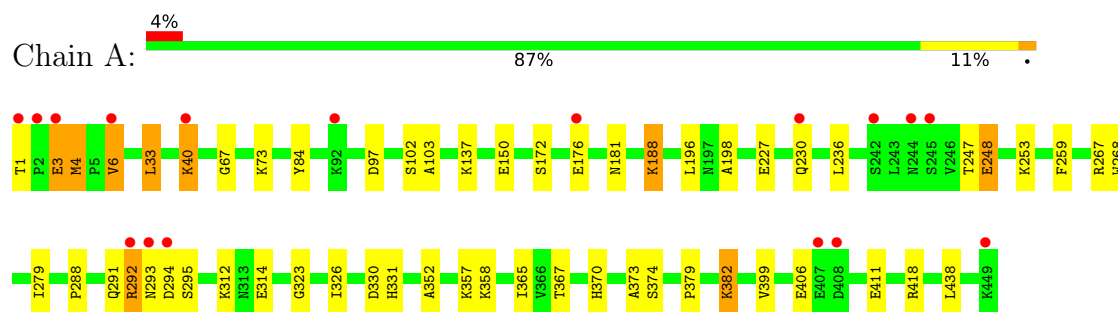
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	408	Total	O	0	0
			408	408		
5	B	304	Total	O	0	0
			304	304		

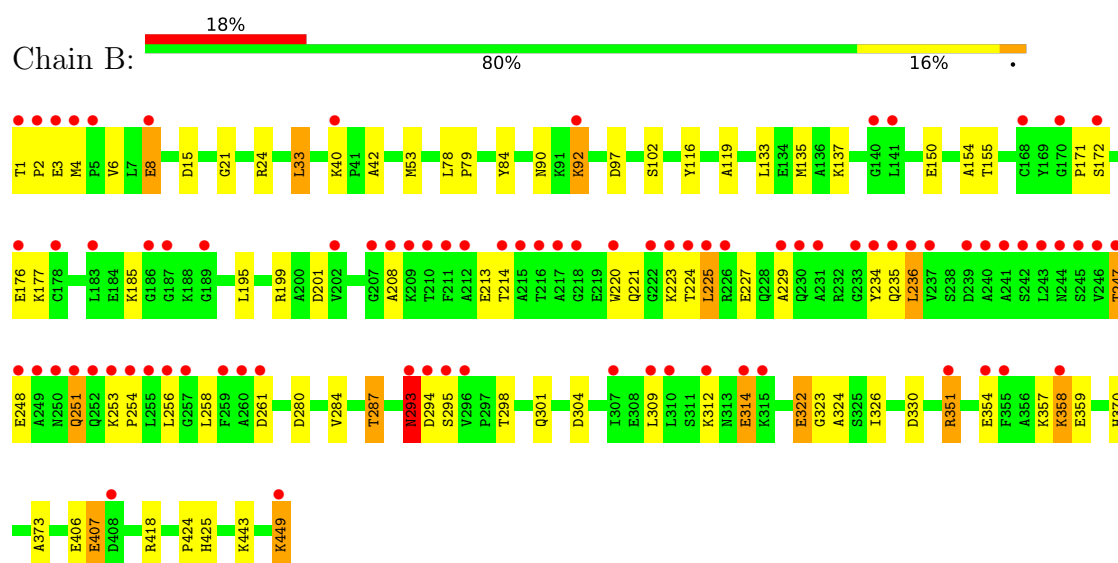
3 Residue-property plots [i](#)

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: 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	76.47Å 164.26Å 192.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.60) 96.3 (30.00-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 1.59Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.212 0.192 , 0.212	Depositor DCC
R_{free} test set	15852 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7346	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: CO, SO4, PO4

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	1.15	7/3359 (0.2%)	1.21	15/4560 (0.3%)
1	B	1.04	2/3359 (0.1%)	1.26	24/4560 (0.5%)
All	All	1.10	9/6718 (0.1%)	1.24	39/9120 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	HIS	CD2-NE2	8.36	1.47	1.37
1	B	370	HIS	CD2-NE2	7.79	1.46	1.37
1	A	331	HIS	CD2-NE2	6.96	1.45	1.37
1	B	322	GLU	CD-OE1	6.80	1.38	1.25
1	A	103	ALA	CA-CB	5.88	1.63	1.53
1	A	352	ALA	CA-CB	5.75	1.62	1.53
1	A	4	MET	SD-CE	-5.42	1.66	1.79
1	A	367	THR	CA-CB	5.40	1.60	1.54
1	A	97	ASP	CA-C	5.27	1.59	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	GLU	N-CA-C	-8.41	102.07	111.07
1	B	326	ILE	N-CA-C	-8.36	102.19	110.30
1	B	293	ASN	N-CA-C	8.26	128.39	110.80
1	B	154	ALA	N-CA-C	7.52	120.13	111.11
1	B	97	ASP	N-CA-C	-7.18	95.45	108.02
1	B	78	LEU	CA-C-N	6.91	126.52	119.19
1	B	78	LEU	C-N-CA	6.91	126.52	119.19
1	B	406	GLU	N-CA-C	-6.90	104.86	113.28
1	A	370	HIS	CE1-NE2-CD2	-6.69	102.31	109.00
1	A	373	ALA	N-CA-C	6.49	119.67	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	GLY	N-CA-C	-6.32	98.20	113.18
1	A	323	GLY	N-CA-C	-6.32	98.21	113.18
1	A	294	ASP	N-CA-C	-6.21	105.67	113.18
1	A	406	GLU	N-CA-C	-6.20	105.71	113.28
1	A	6	VAL	N-CA-C	-6.05	99.69	108.71
1	B	324	ALA	N-CA-C	6.04	119.85	112.23
1	B	373	ALA	N-CA-C	5.94	119.00	111.69
1	B	280	ASP	N-CA-C	5.87	120.44	113.28
1	A	330	ASP	N-CA-C	-5.78	105.06	111.36
1	B	236	LEU	N-CA-C	5.72	118.05	108.96
1	A	418	ARG	N-CA-C	5.66	118.53	110.10
1	B	24	ARG	N-CA-C	-5.46	106.98	113.97
1	A	97	ASP	N-CA-C	-5.46	98.33	107.99
1	B	370	HIS	CE1-NE2-CD2	-5.43	103.56	109.00
1	A	326	ILE	N-CA-C	-5.32	105.31	110.42
1	B	284	VAL	N-CA-C	5.29	116.59	108.71
1	A	259	PHE	N-CA-C	5.28	119.82	113.17
1	B	150	GLU	N-CA-C	-5.25	102.62	110.23
1	B	251	GLN	N-CA-C	5.24	117.73	111.71
1	B	418	ARG	N-CA-C	5.16	117.70	110.23
1	A	411	GLU	N-CA-C	5.11	118.40	110.17
1	B	6	VAL	N-CA-C	-5.11	101.10	108.71
1	A	150	GLU	N-CA-C	-5.06	102.89	110.23
1	B	53	MET	N-CA-C	5.06	117.43	109.39
1	A	374	SER	N-CA-C	5.05	117.55	110.23
1	B	330	ASP	N-CA-C	-5.04	105.87	111.36
1	B	79	PRO	N-CA-C	5.03	120.16	113.57
1	A	67	GLY	CA-C-O	-5.02	117.87	122.24
1	B	42	ALA	N-CA-C	-5.02	101.57	109.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	39	0
1	B	3304	0	3248	59	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
4	A	5	0	0	2	1
4	B	5	0	0	0	0
5	A	408	0	0	12	0
5	B	304	0	0	2	0
All	All	7346	0	6496	100	1

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 8.

All (100) 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:293:ASN:ND2	1:B:295:SER:H	1.64	0.93
1:A:279:ILE:HD13	1:A:382:LYS:HE3	1.47	0.93
1:B:293:ASN:HD22	1:B:295:SER:H	0.90	0.90
1:B:293:ASN:HD22	1:B:295:SER:N	1.75	0.80
1:A:292:ARG:O	1:A:293:ASN:HB2	1.83	0.78
1:A:312:LYS:HE2	5:A:1093:HOH:O	1.86	0.74
1:A:267:ARG:HA	1:A:292:ARG:HD2	1.70	0.74
1:A:176:GLU:HB2	5:A:1202:HOH:O	1.87	0.73
1:B:90:ASN:OD1	1:B:92:LYS:HG2	1.88	0.72
1:B:236:LEU:HD23	1:B:256:LEU:HB3	1.69	0.72
1:A:279:ILE:CD1	1:A:382:LYS:HE3	2.19	0.72
1:B:8:GLU:H	1:B:8:GLU:CD	2.01	0.68
1:B:449:LYS:NZ	1:B:449:LYS:HB3	2.09	0.68
1:A:227:GLU:HA	1:A:230:GLN:HE21	1.59	0.66
1:B:176:GLU:HG3	1:B:177:LYS:HG3	1.78	0.65
4:A:858:SO4:O1	5:A:859:HOH:O	2.14	0.64
1:A:230:GLN:HG2	5:A:1098:HOH:O	1.96	0.64
1:B:248:GLU:HA	1:B:312:LYS:NZ	2.14	0.63
1:B:247:THR:O	1:B:248:GLU:HG3	1.99	0.63
1:A:172:SER:O	1:A:176:GLU:HG2	1.99	0.62
1:B:214:THR:HG22	1:B:224:THR:HA	1.82	0.61
1:B:247:THR:C	1:B:248:GLU:HG3	2.26	0.59
1:A:292:ARG:NH1	5:A:902:HOH:O	2.36	0.58
1:A:40:LYS:N	1:A:40:LYS:HD3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:C	1:B:195:LEU:HD23	2.29	0.58
1:B:235:GLN:NE2	1:B:253:LYS:HG2	2.19	0.58
1:A:102:SER:OG	3:A:856:PO4:P	2.61	0.57
1:B:2:PRO:HG2	1:B:357:LYS:HG2	1.85	0.57
1:B:293:ASN:ND2	1:B:295:SER:OG	2.38	0.57
1:A:357:LYS:HE3	5:A:1088:HOH:O	2.05	0.55
1:A:188:LYS:H	1:A:188:LYS:CE	2.19	0.55
1:A:188:LYS:H	1:A:188:LYS:HE2	1.72	0.54
1:B:90:ASN:HD21	1:B:92:LYS:HE3	1.72	0.54
1:B:293:ASN:ND2	1:B:294:ASP:H	2.04	0.54
1:A:1:THR:N	1:A:358:LYS:O	2.41	0.54
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.91	0.53
1:B:201:ASP:OD2	1:B:251:GLN:NE2	2.42	0.53
1:A:314:GLU:HA	1:A:314:GLU:OE2	2.09	0.53
1:A:279:ILE:HD13	1:A:382:LYS:CE	2.30	0.52
1:A:292:ARG:O	1:A:293:ASN:CB	2.56	0.52
1:B:293:ASN:ND2	1:B:295:SER:N	2.47	0.52
1:B:214:THR:HG22	1:B:224:THR:CA	2.39	0.51
1:B:449:LYS:HB3	1:B:449:LYS:HZ2	1.75	0.51
1:B:214:THR:HG22	1:B:224:THR:N	2.26	0.51
1:B:248:GLU:HA	1:B:312:LYS:HZ2	1.76	0.51
1:B:449:LYS:NZ	1:B:449:LYS:CB	2.74	0.50
1:B:195:LEU:HD23	1:B:195:LEU:O	2.11	0.50
1:B:234:TYR:CD1	1:B:254:PRO:HG2	2.47	0.50
1:B:309:LEU:HA	1:B:312:LYS:HE2	1.93	0.49
1:B:358:LYS:HD3	1:B:359:GLU:N	2.27	0.49
1:B:3:GLU:OE2	1:B:3:GLU:HA	2.13	0.49
1:B:229:ALA:O	1:B:234:TYR:HB2	2.13	0.49
1:B:102:SER:OG	3:B:956:PO4:P	2.71	0.49
1:B:449:LYS:HB3	1:B:449:LYS:HZ3	1.78	0.48
1:A:188:LYS:H	1:A:188:LYS:NZ	2.11	0.48
1:B:214:THR:HG22	1:B:223:LYS:C	2.39	0.48
1:A:253:LYS:HE2	5:A:1183:HOH:O	2.14	0.47
1:B:15:ASP:O	1:B:21:GLY:HA3	2.15	0.47
1:A:137:LYS:HE2	1:A:198:ALA:O	2.15	0.46
1:B:304:ASP:OD2	1:B:351:ARG:NH1	2.48	0.46
1:B:155:THR:HB	1:B:322:GLU:CD	2.41	0.46
1:A:188:LYS:HE2	1:A:188:LYS:HB2	1.55	0.45
1:A:1:THR:O	1:A:1:THR:HG23	2.15	0.45
4:A:858:SO4:O2	5:A:902:HOH:O	2.21	0.44
1:B:287:THR:CG2	5:B:1142:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLU:HA	1:B:314:GLU:OE1	2.18	0.44
1:A:267:ARG:HG2	1:A:268:TRP:CD1	2.53	0.44
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.53	0.44
1:B:137:LYS:HE3	1:B:251:GLN:OE1	2.17	0.44
1:A:248:GLU:HB2	5:A:1183:HOH:O	2.18	0.43
1:A:3:GLU:CD	1:A:4:MET:H	2.26	0.43
1:A:247:THR:O	1:A:312:LYS:NZ	2.51	0.43
1:B:135:MET:HE1	1:B:443:LYS:CD	2.49	0.43
1:B:293:ASN:ND2	1:B:294:ASP:N	2.66	0.43
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.90	0.42
1:A:365:ILE:HD13	1:A:438:LEU:HD11	2.00	0.42
1:B:225:LEU:HD12	1:B:225:LEU:HA	1.82	0.42
1:B:424:PRO:O	1:B:425:HIS:HB2	2.19	0.42
1:B:208:ALA:HB2	1:B:258:LEU:HB3	2.00	0.42
1:B:33:LEU:HD12	1:B:33:LEU:HA	1.83	0.42
1:B:298:THR:OG1	1:B:301:GLN:HG3	2.19	0.42
1:A:73:LYS:HD3	5:A:1237:HOH:O	2.20	0.42
1:B:199:ARG:HA	1:B:234:TYR:OH	2.19	0.42
1:B:220:TRP:O	1:B:221:GLN:C	2.63	0.42
1:A:288:PRO:HB3	1:A:292:ARG:NH1	2.35	0.42
1:B:312:LYS:HE3	1:B:312:LYS:HB2	1.76	0.42
1:A:291:GLN:O	1:A:292:ARG:C	2.64	0.41
1:B:407:GLU:H	1:B:407:GLU:HG2	1.70	0.41
1:B:40:LYS:HE3	5:B:1099:HOH:O	2.21	0.41
1:B:155:THR:HB	1:B:322:GLU:OE1	2.20	0.41
1:A:292:ARG:CZ	5:A:902:HOH:O	2.67	0.41
1:A:196:LEU:HD23	1:A:196:LEU:HA	1.90	0.41
1:A:293:ASN:HB3	1:A:295:SER:H	1.85	0.41
1:B:213:GLU:O	1:B:224:THR:HA	2.20	0.41
1:B:351:ARG:HA	1:B:351:ARG:HD2	1.68	0.41
1:A:6:VAL:HG12	5:A:967:HOH:O	2.19	0.41
1:A:181:ASN:HD22	1:A:188:LYS:NZ	2.19	0.41
1:B:8:GLU:CD	1:B:8:GLU:N	2.75	0.41
1:B:133:LEU:HD23	1:B:133:LEU:C	2.46	0.41
1:B:1:THR:OG1	1:B:2:PRO:HD2	2.21	0.40

All (1) 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)
1:B:449:LYS:NZ	4:A:858:SO4:O2[8_466]	1.89	0.31

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%)	437 (98%)	9 (2%)	1 (0%)	43	24
1	B	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
All	All	894/898 (100%)	871 (97%)	22 (2%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ARG

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%)	332 (98%)	8 (2%)	43	19
1	B	340/340 (100%)	321 (94%)	19 (6%)	19	4
All	All	680/680 (100%)	653 (96%)	27 (4%)	28	8

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	33	LEU
1	A	40	LYS
1	A	84	TYR
1	A	188	LYS

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Mol	Chain	Res	Type
1	A	236	LEU
1	A	248	GLU
1	A	382	LYS
1	B	4	MET
1	B	8	GLU
1	B	33	LEU
1	B	84	TYR
1	B	92	LYS
1	B	171	PRO
1	B	172	SER
1	B	185	LYS
1	B	225	LEU
1	B	247	THR
1	B	261	ASP
1	B	287	THR
1	B	293	ASN
1	B	314	GLU
1	B	351	ARG
1	B	354	GLU
1	B	358	LYS
1	B	407	GLU
1	B	449	LYS

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

Mol	Chain	Res	Type
1	A	29	GLN
1	A	230	GLN
1	A	252	GLN
1	A	388	GLN
1	B	83	GLN
1	B	125	HIS
1	B	235	GLN
1	B	293	ASN
1	B	375	GLN
1	B	388	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 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	$\# Z > 2$
4	SO4	B	958	-	4,4,4	0.68	0	6,6,6	0.18	0
4	SO4	A	858	-	4,4,4	0.67	0	6,6,6	0.22	0
3	PO4	B	956	2	4,4,4	0.78	0	6,6,6	0.58	0
3	PO4	A	856	2	4,4,4	1.07	0	6,6,6	1.03	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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	858	SO4	2	1
3	B	956	PO4	1	0
3	A	856	PO4	1	0

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%)	-0.15	17 (3%)	44 46	11, 18, 35, 118	0
1	B	449/449 (100%)	0.71	83 (18%)	3 3	13, 25, 51, 144	0
All	All	898/898 (100%)	0.28	100 (11%)	10 10	11, 21, 48, 144	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	THR	8.3
1	B	2	PRO	7.8
1	B	1	THR	7.5
1	A	2	PRO	7.4
1	B	244	ASN	6.5
1	B	245	SER	5.7
1	A	244	ASN	5.2
1	A	292	ARG	5.0
1	B	293	ASN	4.9
1	B	449	LYS	4.8
1	B	92	LYS	4.6
1	B	231	ALA	4.6
1	A	3	GLU	4.3
1	B	236	LEU	4.2
1	B	246	VAL	4.1
1	B	212	ALA	4.0
1	B	217	ALA	4.0
1	B	312	LYS	3.9
1	B	243	LEU	3.7
1	A	40	LYS	3.7
1	B	216	THR	3.7
1	B	234	TYR	3.7
1	B	215	ALA	3.6
1	B	309	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	407	GLU	3.5
1	B	255	LEU	3.5
1	A	293	ASN	3.5
1	B	249	ALA	3.3
1	B	247	THR	3.3
1	A	176	GLU	3.3
1	B	253	LYS	3.3
1	B	186	GLY	3.2
1	A	6	VAL	3.2
1	B	208	ALA	3.2
1	B	176	GLU	3.2
1	A	449	LYS	3.2
1	B	248	GLU	3.1
1	A	294	ASP	3.1
1	B	354	GLU	3.0
1	B	218	GLY	3.0
1	B	229	ALA	3.0
1	B	241	ALA	3.0
1	B	225	LEU	3.0
1	B	3	GLU	3.0
1	B	237	VAL	2.9
1	B	294	ASP	2.9
1	B	40	LYS	2.9
1	B	314	GLU	2.8
1	A	92	LYS	2.8
1	B	210	THR	2.8
1	A	408	ASP	2.8
1	B	223	LYS	2.8
1	B	220	TRP	2.8
1	B	214	THR	2.8
1	B	189	GLY	2.8
1	B	256	LEU	2.7
1	B	261	ASP	2.7
1	B	187	GLY	2.7
1	B	260	ALA	2.7
1	B	224	THR	2.7
1	B	408	ASP	2.7
1	B	178	CYS	2.7
1	B	251	GLN	2.6
1	B	8	GLU	2.6
1	B	233	GLY	2.6
1	B	4	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	240	ALA	2.6
1	B	5	PRO	2.6
1	B	222	GLY	2.5
1	B	211	PHE	2.5
1	B	183	LEU	2.5
1	B	310	LEU	2.5
1	B	239	ASP	2.5
1	B	252	GLN	2.5
1	B	295	SER	2.5
1	B	207	GLY	2.5
1	B	168	CYS	2.4
1	B	202	VAL	2.4
1	A	242	SER	2.4
1	B	230	GLN	2.3
1	B	296	VAL	2.3
1	B	254	PRO	2.3
1	B	358	LYS	2.3
1	A	230	GLN	2.3
1	B	257	GLY	2.3
1	B	140	GLY	2.3
1	A	245	SER	2.2
1	B	235	GLN	2.2
1	B	242	SER	2.2
1	B	226	ARG	2.2
1	B	170	GLY	2.2
1	B	250	ASN	2.1
1	B	209	LYS	2.1
1	B	172	SER	2.1
1	B	351	ARG	2.1
1	B	259	PHE	2.1
1	B	315	LYS	2.1
1	B	355	PHE	2.1
1	B	141	LEU	2.0
1	B	307	ILE	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 [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($\text{\AA}^2$)	Q<0.9
4	SO4	B	958	5/5	0.85	0.13	26,27,27,28	5
4	SO4	A	858	5/5	0.88	0.13	26,27,29,30	5
3	PO4	B	956	5/5	0.90	0.13	27,28,31,31	0
3	PO4	A	856	5/5	0.92	0.10	17,18,20,24	0
2	CO	B	952	1/1	0.97	0.05	19,19,19,19	0
2	CO	B	951	1/1	0.99	0.05	19,19,19,19	0
2	CO	B	950	1/1	0.99	0.03	19,19,19,19	0
2	CO	A	851	1/1	1.00	0.07	12,12,12,12	0
2	CO	A	852	1/1	1.00	0.02	14,14,14,14	0
2	CO	A	850	1/1	1.00	0.09	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.