



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 PM UTC

PDB ID : 1Y7A / pdb_00001y7a
Title : Structure of D153H/K328W E. coli alkaline phosphatase in presence of cobalt at 1.77 Å resolution
Authors : Wang, J.; Stieglitz, K.; Kantrowitz, E.R.
Deposited on : 2004-12-08
Resolution : 1.77 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

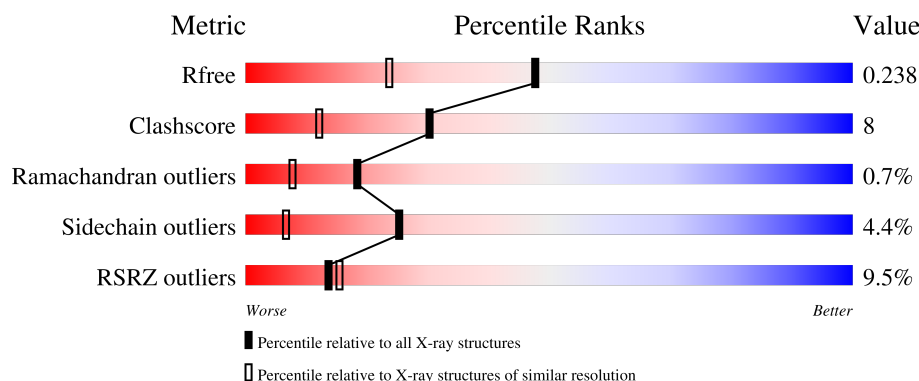
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	
1	B	449	

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
3	PO4	A	1456	-	-	X	-
3	PO4	B	1956	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7317 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
			3311	2049	583	667	12			
1	B	449	Total	C	N	O	S	0	0	0
			3311	2049	583	667	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	HIS	ASP	engineered mutation	UNP P00634
A	328	TRP	LYS	engineered mutation	UNP P00634
B	153	HIS	ASP	engineered mutation	UNP P00634
B	328	TRP	LYS	engineered mutation	UNP P00634

- 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		

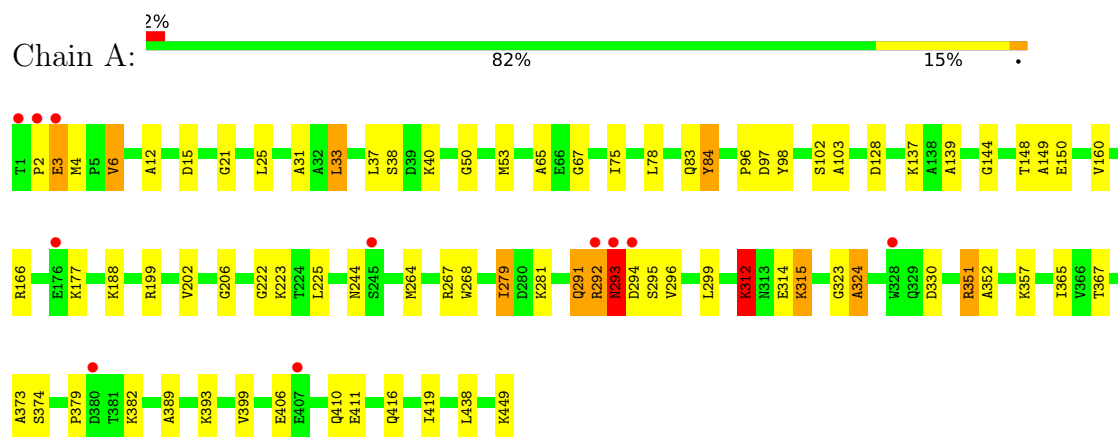
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	391	Total 391	O 391	0	0
5	B	278	Total 278	O 278	0	0

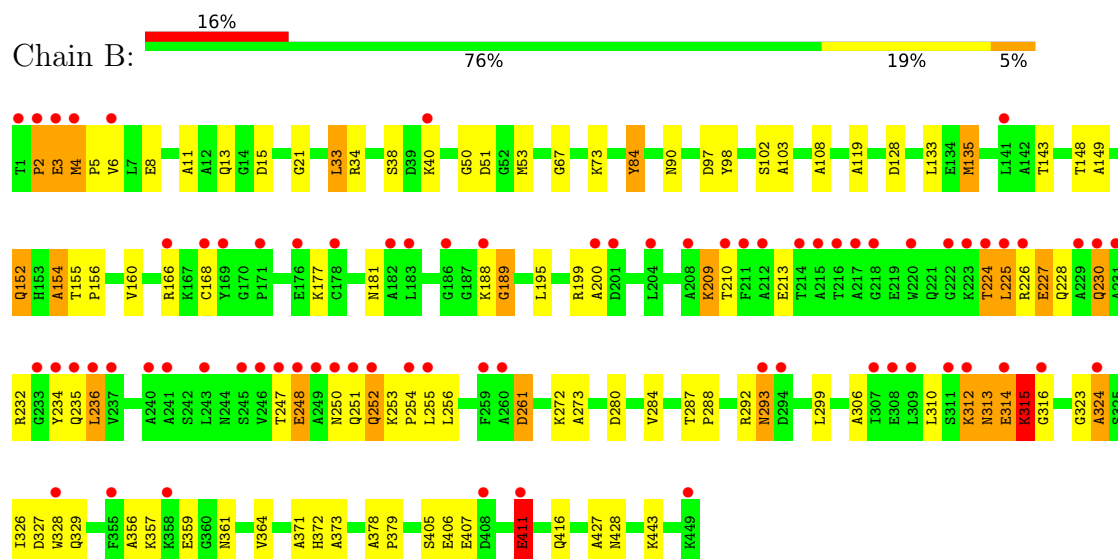
3 Residue-property plots [i](#)

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: 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	76.21Å 164.56Å 192.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.77 30.00 – 1.77	Depositor EDS
% Data completeness (in resolution range)	94.6 (30.00-1.77) 94.7 (30.00-1.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.238 0.205 , 0.238	Depositor DCC
R_{free} test set	11150 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.4	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	0.95	EDS
Total number of atoms	7317	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: CO, 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	1.44	15/3369 (0.4%)	1.35	28/4576 (0.6%)
1	B	1.34	12/3369 (0.4%)	1.38	38/4576 (0.8%)
All	All	1.39	27/6738 (0.4%)	1.36	66/9152 (0.7%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	ASN	N-CA	8.19	1.56	1.46
1	A	373	ALA	CA-CB	7.78	1.66	1.53
1	A	103	ALA	CA-CB	7.03	1.64	1.53
1	A	352	ALA	CA-CB	6.37	1.63	1.53
1	B	156	PRO	CA-C	6.32	1.61	1.52
1	A	264	MET	SD-CE	6.31	1.95	1.79
1	B	284	VAL	CA-CB	5.92	1.62	1.54
1	B	247	THR	CA-CB	5.77	1.62	1.54
1	A	296	VAL	CA-C	5.65	1.57	1.53
1	B	364	VAL	C-O	-5.64	1.18	1.24
1	A	37	LEU	N-CA	5.53	1.52	1.46
1	B	427	ALA	CA-CB	5.47	1.63	1.53
1	B	200	ALA	CA-CB	5.42	1.61	1.53
1	B	135	MET	SD-CE	-5.39	1.66	1.79
1	A	97	ASP	CA-C	5.31	1.59	1.52
1	A	312	LYS	CA-C	5.28	1.59	1.52
1	A	53	MET	SD-CE	5.25	1.92	1.79
1	A	25	LEU	CA-C	5.21	1.59	1.52
1	B	168	CYS	CA-CB	5.21	1.59	1.52
1	A	389	ALA	CA-CB	5.16	1.61	1.53
1	B	371	ALA	CA-CB	5.15	1.60	1.53
1	B	372	HIS	CD2-NE2	5.13	1.43	1.37
1	A	31	ALA	CA-CB	5.08	1.61	1.53
1	A	330	ASP	CA-C	5.07	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	155	THR	CA-CB	5.07	1.59	1.53
1	A	367	THR	CA-CB	5.07	1.60	1.54
1	A	96	PRO	C-O	5.01	1.29	1.23

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	ASN	N-CA-C	12.49	137.40	110.80
1	B	97	ASP	N-CA-C	-8.60	92.97	108.02
1	B	326	ILE	N-CA-C	-8.09	102.66	110.42
1	B	292	ARG	CA-C-N	7.80	136.44	121.54
1	B	292	ARG	C-N-CA	7.80	136.44	121.54
1	B	227	GLU	N-CA-C	-7.55	102.74	110.97
1	B	373	ALA	N-CA-C	7.46	120.87	111.69
1	B	4	MET	CA-C-N	7.29	127.05	119.76
1	B	4	MET	C-N-CA	7.29	127.05	119.76
1	B	108	ALA	N-CA-C	7.25	118.83	111.07
1	A	75	ILE	N-CA-C	7.24	117.97	110.36
1	B	315	LYS	N-CA-C	-7.24	102.78	111.69
1	A	406	GLU	N-CA-C	-7.21	103.95	112.89
1	A	324	ALA	N-CA-C	7.19	122.32	112.90
1	B	67	GLY	CA-C-O	-7.10	116.54	122.29
1	A	351	ARG	NE-CZ-NH2	7.09	125.58	119.20
1	B	6	VAL	N-CA-C	-7.03	98.33	108.53
1	B	323	GLY	N-CA-C	-6.91	96.80	113.18
1	A	330	ASP	N-CA-C	-6.83	103.77	111.14
1	A	323	GLY	N-CA-C	-6.60	97.53	113.18
1	A	12	ALA	N-CA-C	-6.57	100.71	110.23
1	A	294	ASP	N-CA-C	-6.51	105.20	113.01
1	A	411	GLU	N-CA-C	6.46	119.70	109.81
1	B	324	ALA	N-CA-C	6.45	120.36	112.23
1	B	292	ARG	N-CA-C	6.26	120.66	112.89
1	B	406	GLU	N-CA-C	-6.19	105.73	113.28
1	B	236	LEU	N-CA-C	6.16	118.75	108.96
1	B	411	GLU	N-CA-C	5.88	119.25	110.14
1	A	351	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	B	280	ASP	N-CA-C	5.81	120.44	113.23
1	A	84	TYR	CA-CB-CG	5.75	124.25	113.90
1	B	160	VAL	N-CA-C	5.72	121.23	109.34
1	B	90	ASN	N-CA-C	-5.68	100.73	109.76
1	A	98	TYR	N-CA-C	5.64	119.26	112.38
1	B	34	ARG	N-CA-C	-5.63	105.14	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	TYR	CA-CB-CG	5.62	124.02	113.90
1	A	177	LYS	N-CA-C	5.62	120.41	113.50
1	A	78	LEU	N-CA-C	-5.59	102.61	109.65
1	B	428	ASN	CA-C-N	-5.58	114.38	122.69
1	B	428	ASN	C-N-CA	-5.58	114.38	122.69
1	A	6	VAL	N-CA-C	-5.55	100.45	108.71
1	B	356	ALA	N-CA-C	5.55	117.33	111.28
1	B	50	GLY	N-CA-C	-5.52	100.10	113.18
1	A	419	ILE	N-CA-C	-5.47	100.30	108.46
1	B	11	ALA	N-CA-C	-5.47	103.47	110.53
1	B	284	VAL	N-CA-C	5.45	116.44	108.53
1	B	98	TYR	N-CA-C	5.38	119.47	113.01
1	A	293	ASN	N-CA-C	5.37	122.25	110.80
1	B	209	LYS	N-CA-C	5.33	117.78	111.33
1	B	189	GLY	N-CA-C	5.32	119.62	112.17
1	A	374	SER	N-CA-C	5.31	117.93	110.23
1	A	279	ILE	CB-CA-C	-5.30	106.21	111.30
1	A	67	GLY	CA-C-O	-5.29	118.01	122.29
1	B	143	THR	N-CA-C	5.27	117.66	108.76
1	A	351	ARG	CG-CD-NE	-5.26	100.42	112.00
1	A	410	GLN	N-CA-C	-5.25	103.10	110.50
1	A	416	GLN	N-CA-C	-5.22	103.59	110.43
1	B	293	ASN	CB-CA-C	-5.20	100.07	110.42
1	A	351	ARG	CD-NE-CZ	5.17	131.64	124.40
1	A	65	ALA	N-CA-C	5.17	118.74	112.23
1	B	416	GLN	N-CA-C	-5.15	103.69	110.43
1	B	53	MET	N-CA-C	5.11	117.52	109.39
1	A	160	VAL	N-CA-C	5.08	118.07	113.20
1	A	97	ASP	N-CA-C	-5.05	99.18	108.02
1	B	154	ALA	N-CA-C	5.03	119.67	111.37
1	A	50	GLY	N-CA-C	-5.03	101.27	113.18

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	3311	0	3248	38	0
1	B	3311	0	3249	73	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	5	0	0	5	0
3	B	5	0	0	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	391	0	0	3	0
5	B	278	0	0	3	0
All	All	7317	0	6497	111	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 8.

All (111) 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:128:ASP:OD2	1:A:188:LYS:HE3	1.54	1.05
1:B:250:ASN:OD1	1:B:252:GLN:HG2	1.59	1.02
1:B:224:THR:CG2	1:B:227:GLU:H	1.78	0.97
1:B:224:THR:HG22	1:B:227:GLU:HB2	1.48	0.94
1:A:188:LYS:HE2	5:A:1814:HOH:O	1.71	0.91
1:A:166:ARG:NH1	3:A:1456:PO4:O1	2.05	0.90
1:A:102:SER:OG	3:A:1456:PO4:O3	1.94	0.84
1:B:236:LEU:HD23	1:B:256:LEU:HB3	1.60	0.83
1:B:2:PRO:HG2	1:B:357:LYS:HG2	1.63	0.79
1:B:224:THR:HG22	1:B:227:GLU:CB	2.12	0.78
1:B:248:GLU:OE1	1:B:253:LYS:HD2	1.84	0.78
1:B:224:THR:HG22	1:B:227:GLU:H	1.47	0.77
1:B:224:THR:HG23	1:B:227:GLU:H	1.53	0.73
1:B:248:GLU:CD	1:B:253:LYS:HD2	2.16	0.71
1:B:38:SER:OG	1:B:40:LYS:HD3	1.91	0.70
1:A:292:ARG:O	1:A:293:ASN:CB	2.45	0.65
1:B:248:GLU:CG	1:B:253:LYS:HD2	2.26	0.65
1:B:251:GLN:NE2	1:B:251:GLN:H	1.96	0.63
1:A:244:ASN:ND2	5:A:1656:HOH:O	2.30	0.62
1:B:405:SER:HB2	1:B:411:GLU:OE2	1.99	0.61
1:B:312:LYS:HE3	1:B:312:LYS:HA	1.81	0.61
1:A:293:ASN:HB3	1:A:295:SER:H	1.67	0.60
1:B:313:ASN:ND2	1:B:315:LYS:H	1.99	0.60
1:B:234:TYR:CD1	1:B:254:PRO:HG2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:SER:OG	1:A:40:LYS:HG2	2.01	0.59
1:B:152:GLN:NE2	1:B:152:GLN:H	2.00	0.59
1:B:251:GLN:NE2	1:B:251:GLN:N	2.52	0.57
1:B:224:THR:HG22	1:B:227:GLU:N	2.18	0.56
1:A:292:ARG:O	1:A:293:ASN:CG	2.48	0.56
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.87	0.55
1:B:102:SER:OG	3:B:1956:PO4:O2	2.26	0.54
1:B:313:ASN:HD22	1:B:315:LYS:H	1.55	0.54
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.90	0.54
1:B:128:ASP:OD1	1:B:188:LYS:HE3	2.08	0.53
1:A:128:ASP:OD2	1:A:188:LYS:CE	2.43	0.53
1:B:306:ALA:O	1:B:310:LEU:HG	2.09	0.53
1:B:313:ASN:HD21	1:B:315:LYS:HB2	1.73	0.53
1:A:292:ARG:O	1:A:293:ASN:HB2	2.08	0.52
1:B:166:ARG:NH1	3:B:1956:PO4:O1	2.34	0.52
1:A:166:ARG:CZ	3:A:1456:PO4:O1	2.58	0.52
1:A:137:LYS:NZ	1:A:199:ARG:HB3	2.25	0.52
1:B:250:ASN:CG	1:B:252:GLN:HG2	2.34	0.52
1:B:40:LYS:NZ	5:B:2200:HOH:O	2.43	0.51
1:A:6:VAL:H	1:A:357:LYS:HZ2	1.59	0.51
1:A:222:GLY:C	1:A:223:LYS:HE2	2.37	0.50
1:A:291:GLN:O	1:A:292:ARG:O	2.30	0.50
1:B:195:LEU:C	1:B:195:LEU:HD23	2.36	0.49
1:B:313:ASN:HD22	1:B:313:ASN:C	2.21	0.49
1:A:166:ARG:NH2	3:A:1456:PO4:O1	2.46	0.48
1:B:224:THR:HG23	1:B:226:ARG:N	2.28	0.48
1:B:40:LYS:N	1:B:40:LYS:HD2	2.28	0.48
1:A:144:GLY:HA2	1:A:202:VAL:O	2.13	0.48
1:A:4:MET:HE2	1:A:40:LYS:NZ	2.28	0.48
1:B:228:GLN:O	1:B:232:ARG:HG3	2.13	0.48
1:B:252:GLN:CD	1:B:252:GLN:H	2.21	0.48
1:B:312:LYS:HD3	5:B:2072:HOH:O	2.13	0.48
1:A:291:GLN:C	1:A:292:ARG:O	2.54	0.48
1:B:2:PRO:O	1:B:3:GLU:C	2.57	0.47
1:A:139:ALA:O	1:A:315:LYS:HE2	2.14	0.47
1:B:235:GLN:O	1:B:255:LEU:HD12	2.15	0.47
1:B:251:GLN:H	1:B:251:GLN:HE21	1.63	0.47
1:B:15:ASP:O	1:B:21:GLY:HA3	2.15	0.47
1:B:251:GLN:O	1:B:254:PRO:HD3	2.15	0.47
1:B:152:GLN:H	1:B:152:GLN:HE21	1.63	0.47
1:B:213:GLU:O	1:B:225:LEU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:HG23	1:A:299:LEU:HD13	1.97	0.47
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.79	0.47
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.45	0.46
1:B:224:THR:CG2	1:B:227:GLU:N	2.61	0.46
1:B:199:ARG:HA	1:B:234:TYR:OH	2.15	0.46
1:B:224:THR:HG23	1:B:226:ARG:H	1.81	0.45
1:B:236:LEU:CD2	1:B:256:LEU:HB3	2.38	0.45
1:B:314:GLU:OE2	1:B:314:GLU:HA	2.16	0.45
1:A:312:LYS:O	1:A:312:LYS:HE2	2.17	0.45
1:B:133:LEU:C	1:B:133:LEU:HD23	2.41	0.45
1:B:313:ASN:HD21	1:B:315:LYS:CB	2.30	0.45
1:A:267:ARG:HG2	1:A:268:TRP:CD1	2.52	0.45
1:B:33:LEU:HD12	1:B:33:LEU:HA	1.82	0.45
1:B:4:MET:HE3	5:B:2219:HOH:O	2.18	0.44
1:A:279:ILE:HG13	1:A:382:LYS:HD2	1.99	0.44
1:B:3:GLU:O	1:B:5:PRO:HD3	2.18	0.44
1:B:103:ALA:HB1	1:B:119:ALA:O	2.18	0.44
1:B:209:LYS:HB2	1:B:261:ASP:OD1	2.17	0.44
1:B:225:LEU:HD12	1:B:225:LEU:HA	1.86	0.44
1:B:210:THR:O	1:B:213:GLU:HB2	2.18	0.43
1:B:272:LYS:HG2	1:B:273:ALA:O	2.19	0.43
1:A:222:GLY:O	1:A:223:LYS:HE2	2.18	0.43
1:B:135:MET:HE1	1:B:443:LYS:HD2	2.01	0.43
1:B:313:ASN:HD22	1:B:316:GLY:H	1.66	0.43
1:B:102:SER:HB3	1:B:154:ALA:HB3	1.99	0.43
1:B:148:THR:HG23	1:B:299:LEU:HD13	2.01	0.43
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.89	0.43
1:A:2:PRO:O	1:A:3:GLU:C	2.61	0.42
1:A:15:ASP:O	1:A:21:GLY:HA3	2.19	0.42
1:A:150:GLU:HA	1:A:206:GLY:C	2.44	0.42
1:A:449:LYS:HD2	1:A:449:LYS:HA	1.69	0.42
1:B:378:ALA:HA	1:B:379:PRO:HD3	1.93	0.42
1:B:149:ALA:HB2	1:B:324:ALA:CB	2.50	0.42
1:B:328:TRP:HD1	1:B:329:GLN:OE1	2.02	0.42
1:B:181:ASN:O	1:B:189:GLY:N	2.48	0.42
1:B:195:LEU:HD23	1:B:195:LEU:O	2.19	0.42
1:B:230:GLN:HE21	1:B:230:GLN:HB2	1.66	0.41
1:A:102:SER:OG	3:A:1456:PO4:P	2.79	0.41
1:B:4:MET:HA	1:B:5:PRO:HD2	1.89	0.41
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.50	0.41
1:A:281:LYS:HD3	5:A:1800:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:THR:HA	1:B:288:PRO:HD3	1.80	0.40
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.21	0.40
1:B:252:GLN:CD	1:B:252:GLN:N	2.79	0.40
1:B:51:ASP:OD1	1:B:327:ASP:HB2	2.21	0.40
1:B:359:GLU:OE2	1:B:361:ASN:N	2.39	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%)	436 (98%)	8 (2%)	3 (1%)	18	8
1	B	447/449 (100%)	432 (97%)	12 (3%)	3 (1%)	18	8
All	All	894/898 (100%)	868 (97%)	20 (2%)	6 (1%)	18	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ARG
1	A	293	ASN
1	B	293	ASN
1	A	3	GLU
1	B	2	PRO
1	B	3	GLU

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	340/340 (100%)	329 (97%)	11 (3%)	34	13
1	B	340/340 (100%)	321 (94%)	19 (6%)	19	4
All	All	680/680 (100%)	650 (96%)	30 (4%)	25	7

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	83	GLN
1	A	84	TYR
1	A	225	LEU
1	A	291	GLN
1	A	293	ASN
1	A	312	LYS
1	A	314	GLU
1	A	315	LYS
1	A	351	ARG
1	A	393	LYS
1	B	8	GLU
1	B	13	GLN
1	B	33	LEU
1	B	73	LYS
1	B	84	TYR
1	B	152	GLN
1	B	177	LYS
1	B	224	THR
1	B	225	LEU
1	B	230	GLN
1	B	248	GLU
1	B	252	GLN
1	B	261	ASP
1	B	312	LYS
1	B	313	ASN
1	B	314	GLU
1	B	315	LYS
1	B	407	GLU
1	B	411	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	A	291	GLN
1	A	293	ASN
1	A	329	GLN
1	A	388	GLN
1	B	13	GLN
1	B	29	GLN
1	B	125	HIS
1	B	145	ASN
1	B	152	GLN
1	B	221	GLN
1	B	230	GLN
1	B	251	GLN
1	B	313	ASN
1	B	329	GLN
1	B	375	GLN
1	B	388	GLN

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 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
3	PO4	B	1956	2	4,4,4	1.35	1 (25%)	6,6,6	1.42	1 (16%)
4	SO4	B	1958	-	4,4,4	0.68	0	6,6,6	0.23	0
4	SO4	A	1458	-	4,4,4	0.68	0	6,6,6	0.10	0
3	PO4	A	1456	2	4,4,4	1.40	1 (25%)	6,6,6	1.35	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1956	PO4	P-O4	-2.29	1.48	1.54
3	A	1456	PO4	P-O3	2.03	1.60	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1956	PO4	O3-P-O2	2.19	114.72	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1956	PO4	2	0
3	A	1456	PO4	5	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%)	0.10	11 (2%) 59 68	15, 22, 36, 87	0
1	B	449/449 (100%)	0.92	74 (16%) 4 4	16, 28, 52, 93	0
All	All	898/898 (100%)	0.51	85 (9%) 14 15	15, 24, 49, 93	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	PRO	8.2
1	B	1	THR	6.4
1	B	316	GLY	4.9
1	B	328	TRP	4.8
1	B	236	LEU	4.5
1	B	215	ALA	4.4
1	B	249	ALA	4.3
1	B	255	LEU	4.2
1	A	328	TRP	4.2
1	A	2	PRO	4.0
1	B	233	GLY	4.0
1	B	220	TRP	4.0
1	B	243	LEU	3.9
1	A	1	THR	3.9
1	B	223	LYS	3.8
1	B	225	LEU	3.8
1	B	211	PHE	3.7
1	B	293	ASN	3.7
1	B	309	LEU	3.6
1	B	224	THR	3.5
1	B	217	ALA	3.5
1	B	237	VAL	3.5
1	B	212	ALA	3.4
1	B	230	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	186	GLY	3.4
1	B	234	TYR	3.3
1	B	246	VAL	3.3
1	B	247	THR	3.3
1	B	183	LEU	3.2
1	B	231	ALA	3.2
1	B	6	VAL	3.2
1	B	449	LYS	3.1
1	B	169	TYR	3.0
1	B	216	THR	3.0
1	B	358	LYS	2.9
1	B	251	GLN	2.8
1	B	229	ALA	2.8
1	A	294	ASP	2.8
1	B	241	ALA	2.7
1	A	293	ASN	2.7
1	B	254	PRO	2.7
1	A	3	GLU	2.7
1	B	40	LYS	2.7
1	B	210	THR	2.6
1	B	166	ARG	2.6
1	B	259	PHE	2.6
1	B	3	GLU	2.6
1	B	307	ILE	2.6
1	B	178	CYS	2.5
1	B	250	ASN	2.5
1	A	407	GLU	2.5
1	B	248	GLU	2.5
1	B	294	ASP	2.5
1	B	218	GLY	2.5
1	B	308	GLU	2.4
1	B	314	GLU	2.4
1	B	245	SER	2.4
1	B	214	THR	2.4
1	B	208	ALA	2.3
1	B	260	ALA	2.3
1	B	252	GLN	2.3
1	A	245	SER	2.3
1	B	141	LEU	2.2
1	B	204	LEU	2.2
1	B	171	PRO	2.2
1	B	411	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	292	ARG	2.2
1	A	380	ASP	2.1
1	B	201	ASP	2.1
1	B	408	ASP	2.1
1	B	182	ALA	2.1
1	B	222	GLY	2.1
1	B	176	GLU	2.1
1	B	200	ALA	2.1
1	A	176	GLU	2.1
1	B	235	GLN	2.1
1	B	355	PHE	2.1
1	B	324	ALA	2.0
1	B	4	MET	2.0
1	B	226	ARG	2.0
1	B	311	SER	2.0
1	B	168	CYS	2.0
1	B	312	LYS	2.0
1	B	240	ALA	2.0
1	B	188	LYS	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 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
3	PO4	B	1956	5/5	0.61	0.35	71,73,74,75	5
3	PO4	A	1456	5/5	0.66	0.27	65,67,67,69	5
4	SO4	B	1958	5/5	0.87	0.16	46,48,49,49	5
4	SO4	A	1458	5/5	0.95	0.12	40,41,43,43	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CO	B	1950	1/1	0.95	0.07	38,38,38,38	0
2	CO	A	1450	1/1	0.97	0.08	31,31,31,31	0
2	CO	B	1951	1/1	0.98	0.20	46,46,46,46	0
2	CO	A	1452	1/1	0.99	0.13	30,30,30,30	0
2	CO	B	1952	1/1	0.99	0.13	37,37,37,37	0
2	CO	A	1451	1/1	0.99	0.20	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.