



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:12 PM UTC

PDB ID : 1EW8 / pdb_00001ew8
Title : ALKALINE PHOSPHATASE (E.C. 3.1.3.1) COMPLEX WITH PHOSPHO-
NOACETIC ACID
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Kantrowitz, E.R.
Deposited on : 2000-04-24
Resolution : 2.20 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

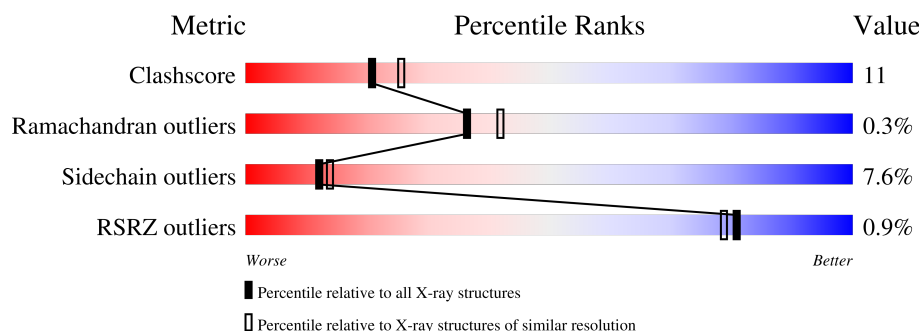
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	% 72% 25% .
1	B	449	% 71% 25% .

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	557[B]	-	-	X	-
3	PO4	B	557[B]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PAE	A	556[A]	-	-	X	-
6	PAE	B	556[A]	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7169 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.

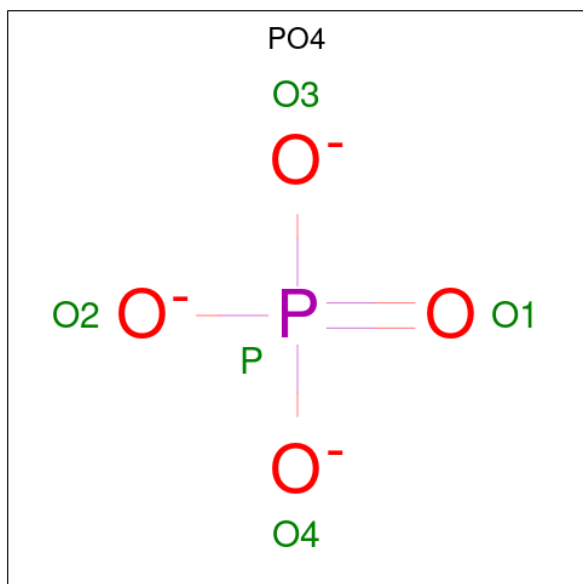
- Molecule 1 is a protein called ALKALINE PHOSPHATASE.

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	3	Total	Zn	0	1
			3	3		
2	B	3	Total	Zn	0	1
			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	1
			5	4	1		
3	B	1	Total	O	P	0	1
			5	4	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

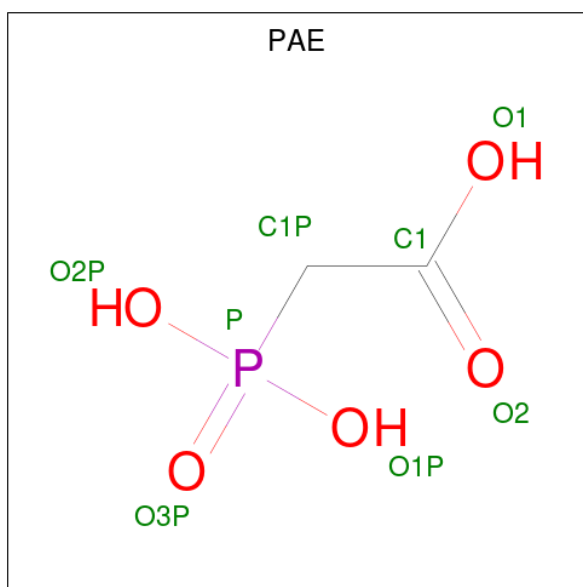


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is PHOSPHONOACETIC ACID (CCD ID: PAE) (formula: C₂H₅O₅P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	1
			8	2	5	1		
6	B	1	Total	C	O	P	0	1
			8	2	5	1		

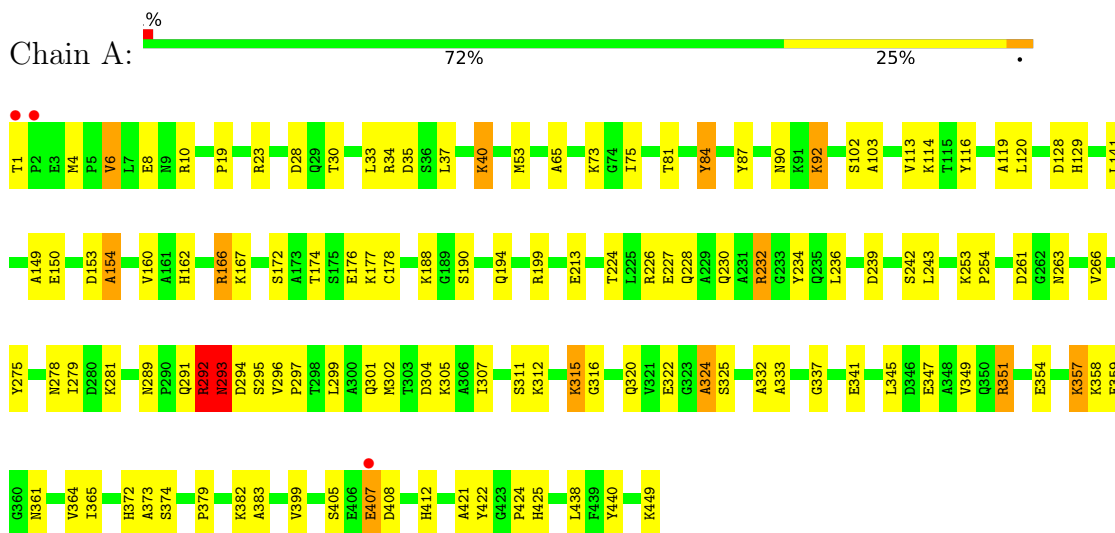
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	307	Total	O	0	6
			307	307		
7	B	210	Total	O	0	6
			210	210		

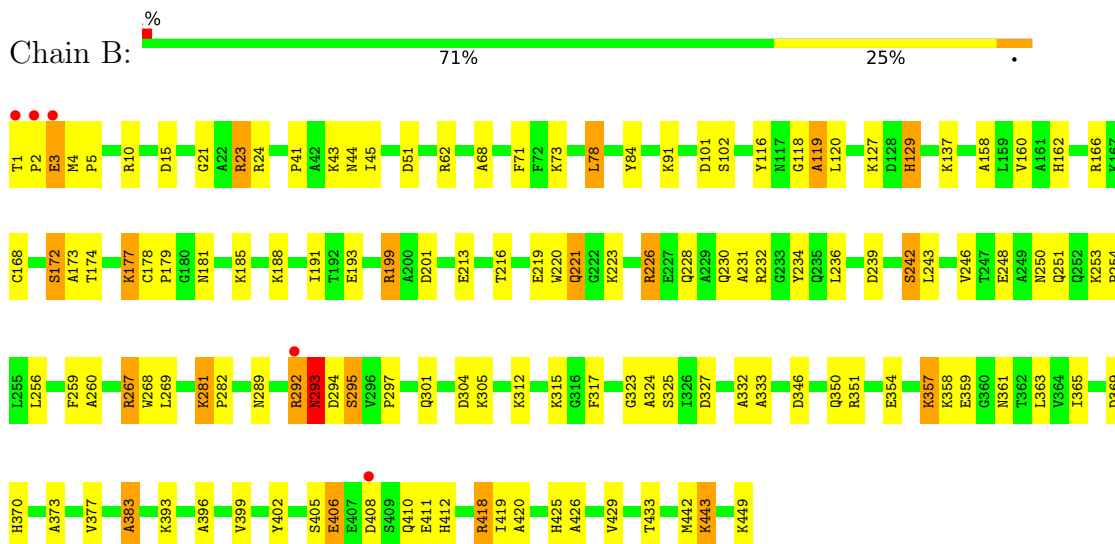
3 Residue-property plots [i](#)

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	194.77Å 167.19Å 76.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.20 12.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (12.00-2.20) 88.8 (12.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.18Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.189 , 0.257 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7169	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 3.43% 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: PO4, ZN, MG, PAE, 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	0.96	1/3359 (0.0%)	1.54	37/4560 (0.8%)
1	B	0.91	1/3359 (0.0%)	1.47	35/4560 (0.8%)
All	All	0.94	2/6718 (0.0%)	1.50	72/9120 (0.8%)

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	8
1	B	0	6
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	325	SER	N-CA	-5.55	1.39	1.46
1	A	293	ASN	N-CA	-5.16	1.39	1.46

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	VAL	CA-C-N	8.89	132.19	120.28
1	A	266	VAL	C-N-CA	8.89	132.19	120.28
1	B	4	MET	CB-CA-C	8.80	120.20	110.08
1	B	281	LYS	CA-C-N	8.11	128.06	120.03
1	B	281	LYS	C-N-CA	8.11	128.06	120.03
1	A	6	VAL	CA-C-O	-7.78	115.53	121.68
1	B	4	MET	CA-C-O	7.71	124.31	119.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ALA	N-CA-C	7.13	119.13	111.36
1	A	292	ARG	CA-C-N	6.82	134.57	121.54
1	A	292	ARG	C-N-CA	6.82	134.57	121.54
1	B	418	ARG	CA-C-N	6.58	132.14	122.99
1	B	418	ARG	C-N-CA	6.58	132.14	122.99
1	A	374	SER	N-CA-CB	6.49	119.19	109.19
1	B	325	SER	N-CA-C	6.34	120.12	112.38
1	A	75	ILE	N-CA-C	6.33	117.83	110.62
1	B	433	THR	CA-C-N	-6.10	112.56	122.81
1	B	433	THR	C-N-CA	-6.10	112.56	122.81
1	B	419	ILE	N-CA-CB	6.08	120.40	111.52
1	A	374	SER	N-CA-C	6.08	119.63	110.64
1	B	324	ALA	CA-C-N	6.07	130.30	120.60
1	B	324	ALA	C-N-CA	6.07	130.30	120.60
1	A	383	ALA	CA-C-N	6.04	125.66	119.56
1	A	383	ALA	C-N-CA	6.04	125.66	119.56
1	B	323	GLY	CA-C-N	6.04	128.29	120.44
1	B	323	GLY	C-N-CA	6.04	128.29	120.44
1	B	2	PRO	N-CA-C	-5.95	106.72	114.03
1	B	293	ASN	N-CA-C	5.94	123.46	110.80
1	A	373	ALA	N-CA-C	5.92	117.53	111.14
1	B	119	ALA	N-CA-C	5.92	118.83	109.96
1	A	65	ALA	N-CA-C	5.91	118.96	111.69
1	B	118	GLY	CA-C-N	5.89	129.20	120.95
1	B	118	GLY	C-N-CA	5.89	129.20	120.95
1	B	4	MET	N-CA-CB	5.82	117.57	110.17
1	A	160	VAL	CB-CA-C	-5.82	104.94	110.70
1	B	71	PHE	CA-CB-CG	5.80	119.60	113.80
1	B	324	ALA	N-CA-C	5.79	117.27	111.07
1	A	154	ALA	N-CA-C	5.79	118.06	111.11
1	A	81	THR	CA-C-N	5.71	129.82	120.51
1	A	81	THR	C-N-CA	5.71	129.82	120.51
1	A	293	ASN	N-CA-C	5.62	122.78	110.80
1	B	129	HIS	CA-CB-CG	5.57	119.36	113.80
1	A	30	THR	N-CA-C	5.56	117.78	111.11
1	A	322	GLU	N-CA-C	5.47	117.33	108.41
1	A	84	TYR	CA-CB-CG	5.41	123.64	113.90
1	B	383	ALA	CA-C-N	5.40	125.02	119.56
1	B	383	ALA	C-N-CA	5.40	125.02	119.56
1	B	317	PHE	N-CA-C	5.37	117.23	109.07
1	A	296	VAL	CA-C-O	5.37	123.12	119.20
1	A	325	SER	N-CA-C	5.37	119.45	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ASN	CA-C-N	-5.34	117.50	123.16
1	A	278	ASN	C-N-CA	-5.34	117.50	123.16
1	A	37	LEU	CA-C-N	5.30	131.26	121.94
1	A	37	LEU	C-N-CA	5.30	131.26	121.94
1	B	325	SER	N-CA-CB	5.20	119.16	110.32
1	B	406	GLU	N-CA-C	-5.19	106.46	112.89
1	A	372	HIS	CA-C-N	5.18	127.49	120.44
1	A	372	HIS	C-N-CA	5.18	127.49	120.44
1	A	296	VAL	N-CA-C	5.17	113.56	107.77
1	A	30	THR	N-CA-CB	5.17	117.64	109.94
1	B	370	HIS	CA-C-O	-5.16	115.91	121.38
1	A	6	VAL	N-CA-C	-5.14	102.36	109.46
1	B	160	VAL	N-CA-C	5.13	118.65	113.47
1	A	40	LYS	CA-C-N	-5.08	115.00	120.03
1	A	40	LYS	C-N-CA	-5.08	115.00	120.03
1	B	396	ALA	CA-C-N	-5.08	116.53	122.93
1	B	396	ALA	C-N-CA	-5.08	116.53	122.93
1	B	295	SER	CA-C-N	-5.08	117.84	123.43
1	B	295	SER	C-N-CA	-5.08	117.84	123.43
1	B	373	ALA	N-CA-C	5.06	118.60	112.23
1	A	320	GLN	CA-C-N	-5.03	116.01	122.99
1	A	320	GLN	C-N-CA	-5.03	116.01	122.99
1	A	153	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ARG	Sidechain
1	A	166	ARG	Sidechain
1	A	226	ARG	Sidechain
1	A	23	ARG	Sidechain
1	A	232	ARG	Sidechain
1	A	292	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	351	ARG	Sidechain
1	B	226	ARG	Sidechain
1	B	23	ARG	Sidechain
1	B	292	ARG	Sidechain
1	B	351	ARG	Sidechain
1	B	418	ARG	Sidechain
1	B	62	ARG	Sidechain

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	3250	68	0
1	B	3304	0	3249	82	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	5	0	0	2	0
3	B	5	0	0	3	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	8	0	2	11	0
6	B	8	0	2	8	0
7	A	307	0	0	10	1
7	B	210	0	0	9	1
All	All	7169	0	6503	146	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 11.

All (146) 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:166:ARG:HH12	6:A:556[A]:PAE:H11	1.10	1.06
1:A:102:SER:HB3	6:A:556[A]:PAE:O3P	1.62	0.97
1:A:166:ARG:HH12	6:A:556[A]:PAE:C1P	1.86	0.88
1:A:289:ASN:O	1:A:292:ARG:HG2	1.73	0.87
1:B:173:ALA:O	1:B:177:LYS:HG2	1.75	0.87
1:A:166:ARG:NH1	6:A:556[A]:PAE:H11	1.91	0.84
1:A:102:SER:HB3	3:A:557[B]:PO4:O3	1.77	0.84
1:B:166:ARG:HH12	6:B:556[A]:PAE:H11	1.41	0.83
1:B:168:CYS:SG	1:B:177:LYS:HB2	2.19	0.82
1:A:102:SER:HB3	6:A:556[A]:PAE:P	2.21	0.79
1:B:102:SER:HB2	7:B:5064:HOH:O	1.84	0.78
1:A:412:HIS:HE1	6:A:556[A]:PAE:H12	1.48	0.78
1:A:102:SER:H	6:A:556[A]:PAE:C1P	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:HB3	3:A:557[B]:PO4:P	2.29	0.72
1:A:90:ASN:OD1	1:A:92:LYS:HG2	1.90	0.71
1:B:43:LYS:HD3	1:B:44:ASN:OD1	1.92	0.69
1:A:228:GLN:O	1:A:232:ARG:HG3	1.93	0.69
1:B:166:ARG:NH1	6:B:556[A]:PAE:H11	2.08	0.68
1:A:405:SER:OG	1:A:407:GLU:HG2	1.94	0.68
1:B:297:PRO:HA	1:B:301:GLN:OE1	1.95	0.66
1:B:289:ASN:O	1:B:292:ARG:HD3	1.97	0.65
1:A:128:ASP:HB2	7:A:5163:HOH:O	1.97	0.64
1:A:297:PRO:HA	1:A:301:GLN:OE1	1.98	0.64
1:B:412:HIS:HE1	6:B:556[A]:PAE:H12	1.63	0.63
1:B:243:LEU:O	1:B:305:LYS:HE2	1.98	0.63
1:A:102:SER:HB2	7:A:5142:HOH:O	1.99	0.62
1:A:102:SER:H	6:A:556[A]:PAE:H11	1.63	0.62
6:A:556[A]:PAE:O1	6:A:556[A]:PAE:O2P	2.13	0.61
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.82	0.61
1:A:19:PRO:O	7:A:5184:HOH:O	2.16	0.61
1:B:346:ASP:O	1:B:350:GLN:HG3	2.01	0.60
1:B:443:LYS:HE2	7:B:5194:HOH:O	2.01	0.60
1:A:102:SER:OG	1:A:154:ALA:HB3	2.02	0.59
1:B:102:SER:HB3	1:B:369:ASP:OD1	2.01	0.59
1:A:224:THR:OG1	1:A:227:GLU:HG3	2.01	0.59
1:A:128:ASP:OD1	1:A:188:LYS:HE3	2.02	0.58
1:B:15:ASP:O	1:B:21:GLY:HA3	2.03	0.58
1:A:440:TYR:CD2	1:B:23:ARG:HD2	2.40	0.57
1:B:10:ARG:O	1:B:24:ARG:HD3	2.05	0.57
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.87	0.57
1:A:291:GLN:HG3	7:A:5120:HOH:O	2.06	0.56
1:A:243:LEU:O	1:A:305:LYS:HE2	2.05	0.55
1:A:102:SER:H	6:A:556[A]:PAE:H12	1.72	0.55
1:B:243:LEU:HD22	1:B:259:PHE:CZ	2.42	0.55
1:B:166:ARG:HB2	7:B:5082:HOH:O	2.07	0.54
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.43	0.54
1:B:269:LEU:HA	7:B:5103:HOH:O	2.08	0.54
1:B:43:LYS:HD3	1:B:44:ASN:CG	2.33	0.53
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.38	0.53
1:B:137:LYS:HE2	1:B:251:GLN:OE1	2.08	0.53
1:B:179:PRO:O	1:B:185:LYS:HB2	2.09	0.52
1:A:307:ILE:O	1:A:311:SER:HB3	2.09	0.52
1:A:275:TYR:OH	1:B:406:GLU:OE1	2.26	0.52
1:A:53:MET:O	1:A:53:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LYS:HD2	1:B:116:TYR:CD1	2.45	0.52
1:B:188:LYS:HE2	7:B:5214:HOH:O	2.07	0.52
1:B:102:SER:HG	3:B:557[B]:PO4:P	2.33	0.51
1:B:41:PRO:HB3	7:B:5139:HOH:O	2.09	0.51
1:B:236:LEU:HD22	1:B:256:LEU:HD23	1.93	0.51
1:B:359:GLU:OE1	1:B:361:ASN:HB2	2.11	0.51
1:B:120:LEU:HD22	1:B:158:ALA:HB2	1.93	0.50
1:B:102:SER:H	6:B:556[A]:PAE:C1P	2.23	0.50
1:B:177:LYS:C	1:B:179:PRO:HD3	2.35	0.50
1:A:359:GLU:CD	1:A:361:ASN:HD22	2.18	0.50
1:B:236:LEU:CD2	1:B:256:LEU:HD23	2.41	0.49
1:A:239:ASP:OD2	1:A:242:SER:OG	2.25	0.49
1:B:174:THR:HG23	1:B:178:CYS:HB2	1.95	0.48
1:B:168:CYS:O	1:B:191:ILE:HG13	2.13	0.48
1:B:188:LYS:HB2	7:B:5116:HOH:O	2.12	0.48
1:A:199:ARG:HA	1:A:234:TYR:OH	2.13	0.48
1:B:293:ASN:ND2	1:B:295:SER:OG	2.46	0.48
1:B:1:THR:N	1:B:357:LYS:O	2.48	0.47
1:A:299:LEU:N	7:A:5270:HOH:O	2.42	0.47
1:B:102:SER:H	6:B:556[A]:PAE:H11	1.79	0.47
1:A:73:LYS:HE2	7:A:5205:HOH:O	2.13	0.47
1:A:87:TYR:CD2	1:B:68:ALA:HB1	2.49	0.47
1:A:364:VAL:O	1:A:421:ALA:HA	2.15	0.47
1:B:259:PHE:O	1:B:260:ALA:HB2	2.14	0.47
1:A:332:ALA:O	1:A:333:ALA:HB3	2.14	0.47
1:B:172:SER:HB3	1:B:213:GLU:OE1	2.13	0.47
1:B:250:ASN:O	1:B:254:PRO:N	2.48	0.47
1:A:150:GLU:N	1:A:263:ASN:OD1	2.48	0.47
1:B:267:ARG:HG2	1:B:268:TRP:CD1	2.49	0.47
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.50	0.47
1:B:1:THR:CG2	1:B:3:GLU:HB2	2.44	0.47
1:B:354:GLU:O	1:B:358:LYS:HG2	2.15	0.47
1:B:174:THR:O	1:B:178:CYS:N	2.45	0.46
1:A:295:SER:HA	7:A:5217:HOH:O	2.16	0.46
1:B:101:ASP:HB2	6:B:556[A]:PAE:C1P	2.45	0.46
1:B:102:SER:HB3	3:B:557[B]:PO4:O3	2.16	0.46
1:A:359:GLU:OE2	1:A:361:ASN:N	2.41	0.46
1:A:424:PRO:O	1:A:425:HIS:HB2	2.14	0.46
1:B:3:GLU:O	1:B:5:PRO:HD3	2.14	0.46
1:B:78:LEU:HB2	1:B:420:ALA:HB1	1.98	0.46
1:B:219:GLU:HB3	1:B:220:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:HIS:CE1	6:B:556[A]:PAE:H12	2.46	0.46
1:A:304:ASP:CG	1:A:351:ARG:HH21	2.24	0.46
1:A:190:SER:O	1:A:194:GLN:HG3	2.16	0.46
1:B:199:ARG:HA	1:B:234:TYR:OH	2.15	0.46
1:A:141:LEU:HD22	1:A:316:GLY:C	2.41	0.45
1:B:281:LYS:HB3	1:B:282:PRO:HD2	1.97	0.45
1:A:149:ALA:HB2	1:A:324:ALA:HB1	1.99	0.45
1:A:6:VAL:HG12	1:A:422:TYR:CE1	2.52	0.44
1:A:234:TYR:HA	1:A:254:PRO:HG2	1.99	0.44
1:B:193:GLU:HG2	7:B:5153:HOH:O	2.16	0.44
1:B:228:GLN:O	1:B:231:ALA:HB3	2.17	0.44
1:B:127:LYS:HE2	1:B:129:HIS:CE1	2.53	0.43
1:A:28:ASP:OD1	1:B:425:HIS:ND1	2.47	0.43
1:A:166:ARG:HH12	6:A:556[A]:PAE:C1	2.31	0.43
1:B:292:ARG:NH1	4:B:568:SO4:O2	2.41	0.43
1:B:393:LYS:HG2	1:B:393:LYS:O	2.18	0.43
1:A:120:LEU:O	1:A:162:HIS:HA	2.18	0.43
1:B:363:LEU:HD21	1:B:365:ILE:HD11	2.01	0.43
1:B:45:ILE:HD13	1:B:442:MET:HG2	2.01	0.43
1:A:141:LEU:HD23	1:A:315:LYS:HB3	2.00	0.42
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.49	0.42
1:B:216:THR:O	1:B:221:GLN:NE2	2.51	0.42
1:B:426:ALA:O	1:B:429:VAL:HG22	2.19	0.42
1:A:213:GLU:O	1:A:224:THR:HA	2.18	0.42
1:A:228:GLN:OE1	1:A:232:ARG:NH2	2.49	0.42
1:A:337:GLY:O	1:A:341:GLU:HG2	2.18	0.42
1:A:291:GLN:HG3	7:A:5158:HOH:O	2.19	0.42
1:B:102:SER:OG	3:B:557[B]:PO4:P	2.78	0.42
1:B:178:CYS:HB3	1:B:181:ASN:OD1	2.20	0.42
1:A:174:THR:HG23	1:A:178:CYS:HB2	2.02	0.42
1:A:347:GLU:OE2	7:A:5227:HOH:O	2.22	0.42
7:A:5079:HOH:O	1:B:383:ALA:HB1	2.19	0.42
1:B:129:HIS:O	1:B:162:HIS:HE1	2.03	0.42
1:B:239:ASP:OD2	1:B:242:SER:OG	2.28	0.41
1:A:149:ALA:HA	1:A:263:ASN:OD1	2.20	0.41
1:A:4:MET:HG2	1:A:35:ASP:O	2.20	0.41
1:B:51:ASP:C	1:B:327:ASP:HB2	2.45	0.41
1:A:354:GLU:HA	1:A:357:LYS:HE3	2.02	0.41
1:A:345:LEU:O	1:A:349:VAL:HG23	2.21	0.41
1:B:23:ARG:NH1	7:B:5178:HOH:O	2.52	0.41
1:A:103:ALA:HA	1:A:154:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:TYR:CE2	1:B:23:ARG:HD2	2.55	0.41
1:B:228:GLN:OE1	1:B:232:ARG:NH1	2.48	0.41
1:B:281:LYS:CB	1:B:282:PRO:HD2	2.51	0.41
1:B:405:SER:HB2	1:B:411:GLU:HG2	2.03	0.41
1:B:1:THR:HB	1:B:3:GLU:HB2	2.03	0.40
1:B:101:ASP:HB2	6:B:556[A]:PAE:H12	2.02	0.40
1:B:377:VAL:CG2	1:B:399:VAL:HG12	2.51	0.40
1:B:332:ALA:O	1:B:333:ALA:HB3	2.21	0.40
1:A:87:TYR:CE1	1:A:114:LYS:HE3	2.56	0.40
1:A:129:HIS:O	1:A:162:HIS:HE1	2.04	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)
7:A:5186:HOH:O	7:B:5089:HOH:O[6_555]	2.19	0.01

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%)	432 (97%)	14 (3%)	1 (0%)	43	51
1	B	447/449 (100%)	430 (96%)	15 (3%)	2 (0%)	30	34
All	All	894/898 (100%)	862 (96%)	29 (3%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	B	293	ASN
1	B	246	VAL

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%)	312 (92%)	28 (8%)	10	12
1	B	340/340 (100%)	316 (93%)	24 (7%)	13	16
All	All	680/680 (100%)	628 (92%)	52 (8%)	12	14

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
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	167	LYS
1	A	172	SER
1	A	176	GLU
1	A	177	LYS
1	A	230	GLN
1	A	236	LEU
1	A	253	LYS
1	A	261	ASP
1	A	279	ILE
1	A	281	LYS
1	A	293	ASN
1	A	294	ASP
1	A	302	MET
1	A	312	LYS
1	A	315	LYS
1	A	357	LYS
1	A	358	LYS
1	A	382	LYS
1	A	407	GLU
1	A	408	ASP

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Mol	Chain	Res	Type
1	A	449	LYS
1	B	3	GLU
1	B	73	LYS
1	B	78	LEU
1	B	84	TYR
1	B	172	SER
1	B	177	LYS
1	B	199	ARG
1	B	201	ASP
1	B	221	GLN
1	B	223	LYS
1	B	226	ARG
1	B	230	GLN
1	B	242	SER
1	B	248	GLU
1	B	253	LYS
1	B	267	ARG
1	B	294	ASP
1	B	304	ASP
1	B	312	LYS
1	B	315	LYS
1	B	357	LYS
1	B	408	ASP
1	B	443	LYS
1	B	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	GLN
1	A	361	ASN
1	A	388	GLN
1	A	391	ASN
1	A	410	GLN
1	A	425	HIS
1	B	9	ASN
1	B	83	GLN
1	B	125	HIS
1	B	221	GLN
1	B	252	GLN
1	B	293	ASN
1	B	329	GLN

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Mol	Chain	Res	Type
1	B	410	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 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	558	-	4,4,4	0.51	0	6,6,6	0.16	0
6	PAE	A	556[A]	2	7,7,7	2.30	2 (28%)	9,10,10	0.89	0
3	PO4	A	557[B]	2	4,4,4	1.18	0	6,6,6	0.41	0
4	SO4	B	568	-	4,4,4	0.49	0	6,6,6	0.08	0
6	PAE	B	556[A]	2	7,7,7	1.51	1 (14%)	9,10,10	1.25	1 (11%)
3	PO4	B	557[B]	2	4,4,4	1.06	0	6,6,6	0.50	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
6	PAE	B	556[A]	2	-	2/5/5/5	-
6	PAE	A	556[A]	2	-	4/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	556[A]	PAE	C1P-C1	4.82	1.56	1.51
6	A	556[A]	PAE	P-C1P	2.75	1.84	1.79
6	B	556[A]	PAE	P-O3P	-2.65	1.44	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	556[A]	PAE	O2-C1-C1P	-2.15	117.55	122.53

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	556[A]	PAE	O1-C1-C1P-P
6	A	556[A]	PAE	O2-C1-C1P-P
6	B	556[A]	PAE	O1-C1-C1P-P
6	A	556[A]	PAE	C1-C1P-P-O2P
6	A	556[A]	PAE	C1-C1P-P-O3P
6	B	556[A]	PAE	C1-C1P-P-O2P

There are no ring outliers.

5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	556[A]	PAE	11	0
3	A	557[B]	PO4	2	0
4	B	568	SO4	1	0
6	B	556[A]	PAE	8	0
3	B	557[B]	PO4	3	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 [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	449/449 (100%)	-0.32	3 (0%) 84 82	8, 18, 45, 145	0
1	B	449/449 (100%)	-0.11	5 (1%) 78 76	9, 22, 55, 142	0
All	All	898/898 (100%)	-0.22	8 (0%) 81 79	8, 20, 52, 145	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	THR	5.5
1	A	2	PRO	4.9
1	B	2	PRO	3.8
1	B	1	THR	2.7
1	B	408	ASP	2.6
1	A	407	GLU	2.3
1	B	292	ARG	2.2
1	B	3	GLU	2.2

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	568	5/5	0.81	0.15	46,77,86,86	0
2	ZN	A	453[B]	1/1	0.89	0.05	27,27,27,27	1
5	MG	A	452[A]	1/1	0.89	0.05	27,27,27,27	1
6	PAE	B	556[A]	8/8	0.90	0.16	36,37,38,44	8
6	PAE	A	556[A]	8/8	0.92	0.15	22,34,36,36	8
3	PO4	A	557[B]	5/5	0.94	0.12	36,37,38,38	5
5	MG	B	452[A]	1/1	0.94	0.06	34,34,34,34	1
4	SO4	A	558	5/5	0.94	0.08	53,54,60,60	0
2	ZN	B	453[B]	1/1	0.94	0.06	34,34,34,34	1
3	PO4	B	557[B]	5/5	0.95	0.11	38,39,39,39	5
2	ZN	A	451	1/1	0.98	0.04	20,20,20,20	0
2	ZN	A	450	1/1	0.98	0.06	16,16,16,16	0
2	ZN	B	450	1/1	0.98	0.03	25,25,25,25	0
2	ZN	B	451	1/1	0.99	0.03	21,21,21,21	0

6.5 Other polymers

There are no such residues in this entry.