Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:14 pm BST

PDB ID	:	1ALK
Title	:	REACTION MECHANISM OF ALKALINE PHOSPHATASE BASED ON CRYSTAL STRUCTURES. TWO METAL ION CATALYSIS
Authors	:	Kim, E.E.; Wyckoff, W.
Deposited on	:	1993-03-03
Resolution	:	2.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

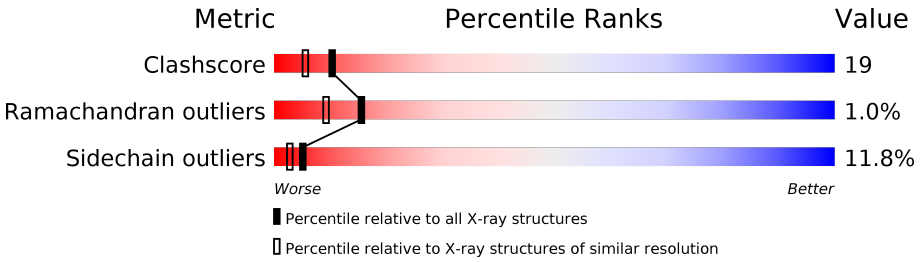
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	71% 23% 6% •
1	B	449	64% 29% 7% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6630 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	582	668	12			
1	B	449	Total	C	N	O	S	0	0	0
			3304	2042	582	668	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASN	ASP	CONFLICT	UNP P00634
A	35	ASN	ASP	CONFLICT	UNP P00634
A	176	GLN	GLU	CONFLICT	UNP P00634
A	228	GLU	GLN	CONFLICT	UNP P00634
A	230	GLU	GLN	CONFLICT	UNP P00634
B	15	ASN	ASP	CONFLICT	UNP P00634
B	35	ASN	ASP	CONFLICT	UNP P00634
B	176	GLN	GLU	CONFLICT	UNP P00634
B	228	GLU	GLN	CONFLICT	UNP P00634
B	230	GLU	GLN	CONFLICT	UNP P00634

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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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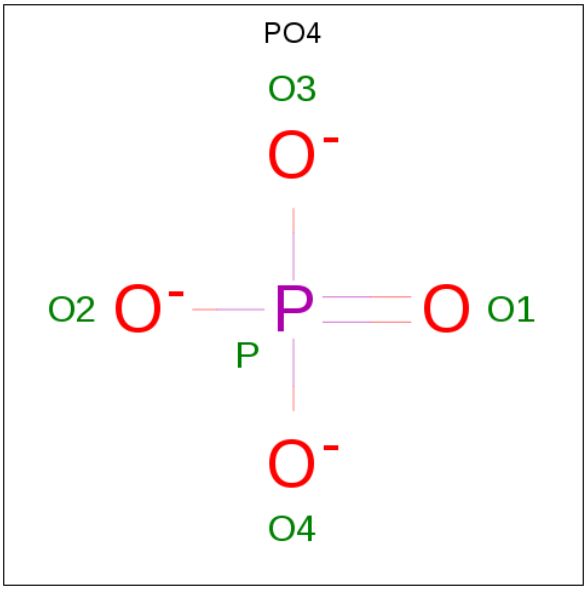
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

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

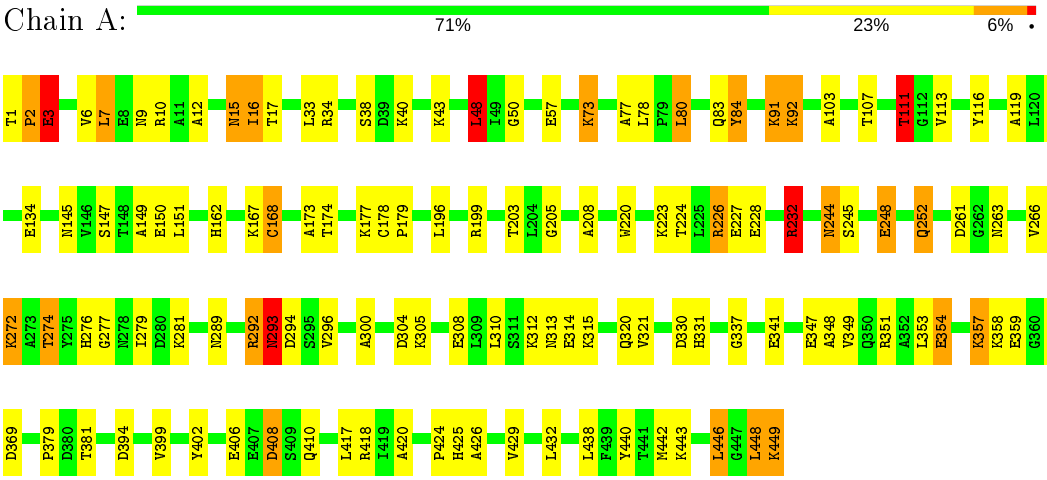
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: ALKALINE PHOSPHATASE

Chain A:



- Molecule 1: ALKALINE PHOSPHATASE

Chain B:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	195.30Å 167.40Å 76.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6630	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.01	2/3359 (0.1%)	1.47	34/4560 (0.7%)
1	B	0.94	0/3359	1.41	27/4560 (0.6%)
All	All	0.98	2/6718 (0.0%)	1.44	61/9120 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	GLN	CD-OE1	6.77	1.38	1.24
1	A	150	GLU	CD-OE2	-6.75	1.18	1.25

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	418	ARG	CD-NE-CZ	22.30	154.82	123.60
1	A	418	ARG	CD-NE-CZ	16.95	147.33	123.60
1	B	418	ARG	NE-CZ-NH2	14.81	127.71	120.30
1	A	232	ARG	NE-CZ-NH1	-14.01	113.29	120.30
1	A	48	LEU	CA-CB-CG	12.53	144.12	115.30
1	B	418	ARG	NH1-CZ-NH2	-10.61	107.73	119.40
1	A	418	ARG	NE-CZ-NH2	9.87	125.23	120.30
1	A	84	TYR	CB-CG-CD1	9.25	126.55	121.00
1	B	48	LEU	CA-CB-CG	9.23	136.54	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	232	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	A	34	ARG	NE-CZ-NH1	-8.54	116.03	120.30
1	A	354	GLU	CA-CB-CG	8.52	132.15	113.40
1	B	418	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	B	34	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	B	3	GLU	C-N-CA	7.74	141.06	121.70
1	B	76	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	166	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	B	369	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	369	ASP	CB-CG-OD2	7.17	124.75	118.30
1	B	351	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	A	84	TYR	CA-CB-CG	7.12	126.93	113.40
1	B	199	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	394	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	34	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	A	292	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	153	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	244	ASN	CB-CA-C	6.15	122.71	110.40
1	A	354	GLU	N-CA-CB	6.15	121.67	110.60
1	A	111	THR	OG1-CB-CG2	6.15	124.14	110.00
1	B	292	ARG	C-N-CA	5.95	136.57	121.70
1	A	111	THR	CA-CB-CG2	5.86	120.61	112.40
1	B	199	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	266	VAL	CA-CB-CG1	5.71	119.46	110.90
1	B	195	LEU	CA-CB-CG	5.70	128.42	115.30
1	A	103	ALA	CB-CA-C	5.66	118.59	110.10
1	A	168	CYS	CA-CB-SG	-5.62	103.89	114.00
1	A	57	GLU	CG-CD-OE1	5.60	129.50	118.30
1	A	418	ARG	CG-CD-NE	5.55	123.45	111.80
1	A	261	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	10	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	B	394	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	330	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	261	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	369	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	A	418	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	A	293	ASN	N-CA-C	5.31	125.34	111.00
1	B	84	TYR	CA-CB-CG	5.28	123.42	113.40
1	A	199	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	226	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	369	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	B	323	GLY	N-CA-C	-5.23	100.02	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	51	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	293	ASN	N-CA-C	5.16	124.94	111.00
1	B	87	TYR	CB-CG-CD1	-5.14	117.91	121.00
1	B	84	TYR	CB-CG-CD1	5.11	124.07	121.00
1	B	166	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	294	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	57	GLU	OE1-CD-OE2	-5.04	117.26	123.30
1	A	50	GLY	N-CA-C	-5.03	100.52	113.10
1	A	348	ALA	CB-CA-C	5.03	117.65	110.10
1	B	51	ASP	CB-CG-OD1	-5.03	113.77	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3304	0	3250	125	0
1	B	3304	0	3249	131	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
All	All	6630	0	6499	245	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 19.

All (245) 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:111:THR:CG2	1:A:113:VAL:HG12	1.69	1.23
1:A:1:THR:N	1:A:2:PRO:HD3	1.67	1.09
1:A:111:THR:HG23	1:A:113:VAL:HG12	1.35	1.08
1:A:232:ARG:HH11	1:A:232:ARG:HB3	1.26	0.99
1:B:223:LYS:HG3	1:B:227:GLU:OE1	1.63	0.98
1:B:176:GLN:OE1	1:B:177:LYS:HE2	1.60	0.97
1:A:6:VAL:CG1	1:A:357:LYS:HD3	1.95	0.96
1:A:224:THR:OG1	1:A:227:GLU:HG3	1.66	0.94
1:A:289:ASN:O	1:A:292:ARG:HG2	1.68	0.94
1:A:274:THR:HG21	1:A:281:LYS:HE3	1.49	0.94
1:A:1:THR:H3	1:A:2:PRO:HD3	1.26	0.92
1:A:232:ARG:CB	1:A:232:ARG:HH11	1.82	0.92
1:A:1:THR:N	1:A:2:PRO:CD	2.32	0.90
1:A:2:PRO:O	1:A:3:GLU:HG2	1.71	0.90
1:B:279:ILE:HD11	1:B:382:LYS:HE2	1.53	0.89
1:A:12:ALA:HB1	1:A:16:ILE:HD11	1.53	0.88
1:A:220:TRP:HB3	1:A:223:LYS:HE2	1.56	0.86
1:A:292:ARG:O	1:A:293:ASN:HB2	1.77	0.84
1:A:6:VAL:HG11	1:A:357:LYS:HD3	1.59	0.83
1:A:449:LYS:HE3	1:A:449:LYS:N	1.94	0.82
1:B:6:VAL:HG12	1:B:77:ALA:HB1	1.62	0.81
1:B:228:GLU:O	1:B:232:ARG:HG3	1.80	0.80
1:A:38:SER:OG	1:A:40:LYS:HG2	1.80	0.80
1:A:92:LYS:HA	1:A:92:LYS:HE3	1.64	0.80
1:A:12:ALA:CB	1:A:16:ILE:HD11	2.12	0.79
1:A:6:VAL:HG13	1:A:357:LYS:HD3	1.63	0.79
1:B:137:LYS:NZ	1:B:199:ARG:HB3	1.99	0.77
1:B:236:LEU:HD21	1:B:256:LEU:HD23	1.67	0.76
1:A:111:THR:CG2	1:A:113:VAL:CG1	2.59	0.76
1:A:2:PRO:O	1:A:3:GLU:OE2	2.04	0.76
1:B:279:ILE:HD11	1:B:382:LYS:CE	2.15	0.76
1:B:253:LYS:H	1:B:254:PRO:CD	1.99	0.76
1:B:408:ASP:OD1	1:B:409:SER:N	2.18	0.76
1:A:1:THR:H2	1:A:2:PRO:HD3	1.49	0.75
1:B:199:ARG:NH2	1:B:232:ARG:O	2.20	0.74
1:A:2:PRO:O	1:A:3:GLU:CG	2.35	0.74
1:B:199:ARG:NH1	1:B:251:GLN:O	2.20	0.74
1:A:220:TRP:HD1	1:A:223:LYS:HE3	1.52	0.73
1:B:279:ILE:CD1	1:B:382:LYS:HD3	2.19	0.73
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.24	0.72
1:A:252:GLN:HE21	1:A:252:GLN:H	1.38	0.72
1:A:1:THR:H2	1:A:2:PRO:CD	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLU:HG2	1:B:253:LYS:HZ1	1.53	0.71
1:A:107:THR:O	1:A:111:THR:HB	1.90	0.71
1:B:281:LYS:HB3	1:B:281:LYS:HZ2	1.55	0.71
1:A:6:VAL:HG13	1:A:357:LYS:CD	2.20	0.70
1:B:380:ASP:O	1:B:382:LYS:NZ	2.24	0.70
1:A:111:THR:HG21	1:A:113:VAL:HG12	1.72	0.69
1:B:293:ASN:HB3	1:B:295:SER:H	1.57	0.68
1:A:448:LEU:O	1:A:449:LYS:HB2	1.95	0.67
1:B:226:ARG:O	1:B:230:GLU:HG3	1.95	0.67
1:B:418:ARG:HH11	1:B:420:ALA:CB	2.08	0.67
1:A:220:TRP:HA	1:A:223:LYS:NZ	2.09	0.66
1:A:449:LYS:HE3	1:A:449:LYS:CA	2.25	0.66
1:A:173:ALA:O	1:A:177:LYS:HE2	1.94	0.66
1:B:6:VAL:CG1	1:B:77:ALA:HB1	2.26	0.65
1:A:111:THR:HG22	1:A:113:VAL:H	1.61	0.65
1:A:228:GLU:O	1:A:232:ARG:HG2	1.97	0.65
1:B:199:ARG:HA	1:B:234:TYR:OH	1.97	0.65
1:A:440:TYR:CD2	1:B:23:ARG:HD3	2.32	0.64
1:B:313:ASN:HD21	1:B:315:LYS:HB2	1.62	0.64
1:B:298:THR:OG1	1:B:301:GLN:HG3	1.98	0.64
1:A:300:ALA:O	1:A:304:ASP:HB2	1.97	0.64
1:B:293:ASN:HB2	1:B:296:VAL:HG23	1.80	0.63
1:A:381:THR:HG23	1:B:411:GLU:OE1	1.98	0.63
1:B:267:ARG:NH2	1:B:347:GLU:OE2	2.30	0.62
1:A:220:TRP:CB	1:A:223:LYS:HE2	2.29	0.62
1:B:102:SER:OG	4:B:453:PO4:P	2.55	0.62
1:A:305:LYS:NZ	1:A:308:GLU:OE2	2.32	0.62
1:A:274:THR:HG21	1:A:281:LYS:CE	2.29	0.61
1:B:305:LYS:N	1:B:305:LYS:HD3	2.15	0.61
1:A:33:LEU:HD22	1:B:427:ALA:HB1	1.83	0.61
1:B:1:THR:O	1:B:3:GLU:N	2.34	0.61
1:B:171:PRO:HB2	1:B:213:GLU:HG2	1.83	0.60
1:A:406:GLU:OE1	1:B:276:HIS:HE1	1.84	0.60
1:A:252:GLN:HE21	1:A:252:GLN:N	1.99	0.60
1:A:2:PRO:C	1:A:3:GLU:HG2	2.22	0.59
1:A:121:GLY:O	1:A:162:HIS:HD2	1.83	0.59
1:B:151:LEU:HD21	1:B:203:THR:HG22	1.84	0.59
1:B:301:GLN:O	1:B:305:LYS:HG2	2.02	0.59
1:A:276:HIS:HE1	1:B:406:GLU:OE1	1.85	0.59
1:A:1:THR:H3	1:A:2:PRO:CD	2.03	0.58
1:A:248:GLU:OE1	1:A:312:LYS:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLN:HG3	1:B:222:GLY:N	2.17	0.58
1:A:15:ASN:HD21	1:A:17:THR:HB	1.68	0.58
1:A:220:TRP:CD1	1:A:223:LYS:HE3	2.37	0.58
1:A:232:ARG:NH1	1:A:232:ARG:HB3	2.08	0.58
1:B:253:LYS:N	1:B:254:PRO:CD	2.63	0.57
1:A:173:ALA:HB1	1:A:177:LYS:HE3	1.85	0.57
1:B:1:THR:HG23	1:B:2:PRO:HD2	1.85	0.57
1:A:12:ALA:HB1	1:A:16:ILE:CD1	2.30	0.56
1:A:248:GLU:HG2	1:A:312:LYS:HZ3	1.70	0.56
1:A:73:LYS:HB2	1:A:73:LYS:HZ2	1.70	0.56
1:B:313:ASN:ND2	1:B:315:LYS:H	2.04	0.56
1:B:253:LYS:H	1:B:254:PRO:HD3	1.71	0.56
1:B:393:LYS:HG3	1:B:393:LYS:O	2.05	0.56
1:A:6:VAL:CG1	1:A:357:LYS:CD	2.74	0.56
1:A:438:LEU:O	1:A:442:MET:HG3	2.05	0.55
1:B:76:ASP:HA	1:B:418:ARG:HH22	1.71	0.55
1:A:248:GLU:HG2	1:A:312:LYS:NZ	2.22	0.55
1:B:133:LEU:HD23	1:B:133:LEU:C	2.26	0.55
1:A:269:LEU:HD13	1:A:289:ASN:HB2	1.86	0.55
1:B:359:GLU:OE1	1:B:361:ASN:N	2.39	0.55
1:A:15:ASN:ND2	1:A:17:THR:HB	2.23	0.54
1:A:304:ASP:OD2	1:A:351:ARG:HD2	2.08	0.54
1:A:267:ARG:HG2	1:A:292:ARG:NH2	2.22	0.54
1:B:279:ILE:CD1	1:B:382:LYS:CD	2.85	0.54
1:A:224:THR:HG1	1:A:227:GLU:HG3	1.71	0.54
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.88	0.54
1:A:276:HIS:CE1	1:B:406:GLU:OE1	2.61	0.54
1:A:381:THR:CG2	1:B:411:GLU:OE1	2.55	0.54
1:B:137:LYS:HZ1	1:B:199:ARG:HB3	1.72	0.53
1:A:359:GLU:OE1	1:A:361:ASN:N	2.35	0.53
1:B:10:ARG:HB2	1:B:71:PHE:CD1	2.44	0.53
1:A:232:ARG:CG	1:A:232:ARG:HH11	2.14	0.53
1:B:298:THR:H	1:B:301:GLN:HE21	1.56	0.53
1:B:354:GLU:HG2	1:B:358:LYS:HZ1	1.73	0.52
1:B:195:LEU:C	1:B:195:LEU:CD1	2.77	0.52
1:B:45:ILE:CD1	1:B:442:MET:HB3	2.39	0.52
1:B:1:THR:CG2	1:B:2:PRO:HD2	2.38	0.52
1:B:182:ALA:HB1	1:B:184:GLU:OE2	2.09	0.52
1:B:4:MET:HG2	1:B:35:ASN:O	2.10	0.52
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.92	0.52
1:B:190:SER:OG	1:B:193:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TYR:CE2	1:A:119:ALA:HB2	2.45	0.51
1:B:121:GLY:O	1:B:162:HIS:HD2	1.93	0.51
1:B:418:ARG:HH11	1:B:420:ALA:HB3	1.74	0.51
1:B:73:LYS:H	1:B:73:LYS:HD2	1.75	0.51
1:B:351:ARG:NH2	1:B:354:GLU:OE1	2.34	0.51
1:B:281:LYS:HB3	1:B:281:LYS:NZ	2.25	0.51
1:B:134:GLU:OE2	1:B:162:HIS:HE1	1.94	0.50
1:B:10:ARG:O	1:B:24:ARG:HD3	2.11	0.50
1:A:92:LYS:HE3	1:A:92:LYS:CA	2.29	0.50
1:B:248:GLU:HG2	1:B:253:LYS:NZ	2.26	0.50
1:B:46:ILE:HG22	1:B:48:LEU:HD22	1.93	0.50
1:B:424:PRO:O	1:B:425:HIS:HB2	2.12	0.50
1:B:131:THR:O	1:B:135:MET:HG3	2.12	0.49
1:B:15:ASN:O	1:B:21:GLY:HA3	2.12	0.49
1:B:149:ALA:HA	1:B:263:ASN:HD22	1.78	0.49
1:A:267:ARG:NH2	1:A:347:GLU:OE2	2.46	0.49
1:A:449:LYS:HE3	1:A:449:LYS:HA	1.95	0.48
1:A:331:HIS:ND1	1:A:410:GLN:O	2.41	0.48
1:B:351:ARG:NE	1:B:351:ARG:HA	2.28	0.48
1:B:380:ASP:O	1:B:382:LYS:CE	2.60	0.48
1:B:426:ALA:O	1:B:429:VAL:HG22	2.12	0.48
1:A:15:ASN:C	1:A:15:ASN:HD22	2.17	0.48
1:A:145:ASN:O	1:A:203:THR:HA	2.14	0.48
1:A:293:ASN:HB3	1:A:296:VAL:H	1.79	0.48
1:B:313:ASN:HD22	1:B:315:LYS:N	2.12	0.48
1:A:149:ALA:HA	1:A:263:ASN:HD22	1.78	0.47
1:B:242:SER:O	1:B:246:VAL:HG23	2.14	0.47
1:B:236:LEU:CD2	1:B:256:LEU:HD23	2.40	0.47
1:B:195:LEU:HD12	1:B:195:LEU:C	2.35	0.47
1:B:369:ASP:CG	1:B:370:HIS:CD2	2.88	0.47
1:A:274:THR:HG22	1:A:277:GLY:CA	2.45	0.47
1:B:176:GLN:OE1	1:B:177:LYS:CE	2.47	0.47
1:A:111:THR:HG21	1:A:113:VAL:CG1	2.39	0.47
1:A:417:LEU:C	1:A:417:LEU:HD12	2.34	0.47
1:B:152:GLN:NE2	1:B:210:THR:HB	2.30	0.47
1:A:33:LEU:HD23	1:B:37:LEU:HD11	1.97	0.47
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.45	0.47
1:A:432:LEU:O	1:B:10:ARG:HD2	2.15	0.47
1:A:293:ASN:HB2	1:A:296:VAL:HB	1.96	0.46
1:B:313:ASN:HD21	1:B:315:LYS:CB	2.26	0.46
1:B:177:LYS:C	1:B:179:PRO:HD3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:CYS:N	1:A:179:PRO:CD	2.78	0.46
1:A:449:LYS:CA	1:A:449:LYS:CE	2.94	0.46
1:B:289:ASN:ND2	1:B:291:GLN:H	2.13	0.46
1:B:354:GLU:O	1:B:358:LYS:NZ	2.41	0.46
1:A:122:VAL:HA	1:A:127:LYS:O	2.16	0.46
1:B:279:ILE:HD13	1:B:382:LYS:HD3	1.97	0.46
1:B:10:ARG:HB2	1:B:71:PHE:CE1	2.51	0.46
1:A:80:LEU:HD23	1:A:426:ALA:HB3	1.97	0.46
1:B:253:LYS:N	1:B:254:PRO:HD2	2.30	0.46
1:B:30:THR:O	1:B:34:ARG:HG3	2.16	0.46
1:B:4:MET:HA	1:B:5:PRO:HD3	1.66	0.46
1:A:80:LEU:HD23	1:A:426:ALA:CB	2.46	0.45
1:B:144:GLY:HA2	1:B:202:VAL:O	2.15	0.45
1:A:315:LYS:HD2	1:A:315:LYS:HA	1.75	0.45
1:A:73:LYS:NZ	1:A:73:LYS:CB	2.79	0.45
1:B:224:THR:OG1	1:B:227:GLU:HG3	2.16	0.45
1:B:48:LEU:HG	1:B:349:VAL:HG22	1.99	0.45
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.84	0.45
1:A:208:ALA:O	1:A:226:ARG:NH2	2.50	0.45
1:B:91:LYS:NZ	1:B:126:GLU:OE2	2.33	0.45
1:A:313:ASN:OD1	1:A:315:LYS:N	2.50	0.45
1:B:281:LYS:NZ	1:B:281:LYS:CB	2.79	0.45
1:A:220:TRP:CD1	1:A:223:LYS:CE	3.00	0.45
1:A:293:ASN:CB	1:A:296:VAL:HB	2.47	0.45
1:B:213:GLU:HB3	1:B:225:LEU:HD22	1.98	0.45
1:B:279:ILE:CD1	1:B:382:LYS:CE	2.90	0.45
1:A:168:CYS:HB3	1:A:174:THR:OG1	2.18	0.44
1:A:406:GLU:OE1	1:B:276:HIS:CE1	2.66	0.44
1:A:220:TRP:HD1	1:A:223:LYS:CE	2.27	0.44
1:B:332:ALA:O	1:B:333:ALA:HB3	2.18	0.44
1:B:178:CYS:HB3	1:B:181:ASN:OD1	2.18	0.44
1:B:382:LYS:HE3	1:B:382:LYS:HB2	1.72	0.44
1:B:354:GLU:HG2	1:B:358:LYS:NZ	2.33	0.43
1:B:40:LYS:HA	1:B:40:LYS:HD2	1.79	0.43
1:B:142:ALA:HA	1:B:201:ASP:OD2	2.18	0.43
1:B:351:ARG:HA	1:B:351:ARG:HE	1.82	0.43
1:B:255:LEU:HD12	1:B:309:LEU:CD1	2.49	0.43
1:B:92:LYS:HD2	1:B:92:LYS:HA	1.33	0.43
1:A:220:TRP:HA	1:A:223:LYS:HZ1	1.79	0.43
1:A:269:LEU:HD13	1:A:289:ASN:CB	2.49	0.43
1:A:2:PRO:O	1:A:3:GLU:CD	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:HG3	1:A:116:TYR:CD1	2.54	0.43
1:B:331:HIS:ND1	1:B:410:GLN:O	2.44	0.43
1:A:272:LYS:HE3	1:A:272:LYS:HB3	1.35	0.43
1:A:33:LEU:HD22	1:B:427:ALA:CB	2.48	0.42
1:B:438:LEU:O	1:B:442:MET:HG3	2.20	0.42
1:B:196:LEU:HA	1:B:196:LEU:HD12	1.87	0.42
1:A:147:SER:O	1:A:205:GLY:HA2	2.20	0.42
1:B:289:ASN:HA	1:B:290:PRO:HD3	1.92	0.42
1:B:45:ILE:HD12	1:B:442:MET:HB3	2.01	0.42
1:A:337:GLY:O	1:A:341:GLU:HG2	2.20	0.42
1:B:148:THR:OG1	1:B:324:ALA:HB3	2.20	0.42
1:B:48:LEU:HD13	1:B:321:VAL:HB	2.01	0.42
1:A:48:LEU:HG	1:A:349:VAL:HG22	2.02	0.42
1:A:7:LEU:HB2	1:A:77:ALA:O	2.19	0.42
1:B:13:GLN:OE1	1:B:23:ARG:O	2.38	0.42
1:B:313:ASN:ND2	1:B:315:LYS:N	2.66	0.42
1:B:379:PRO:HA	1:B:399:VAL:HG21	2.02	0.42
1:A:220:TRP:HA	1:A:223:LYS:CE	2.50	0.41
1:B:313:ASN:HD22	1:B:315:LYS:H	1.68	0.41
1:B:206:GLY:HA3	1:B:262:GLY:O	2.20	0.41
1:B:221:GLN:C	1:B:223:LYS:H	2.23	0.41
1:A:16:ILE:HA	1:A:16:ILE:HD12	1.74	0.41
1:B:214:THR:OG1	1:B:222:GLY:C	2.58	0.41
1:A:402:TYR:HB3	1:A:410:GLN:HG3	2.02	0.41
1:A:48:LEU:HD13	1:A:321:VAL:HB	2.02	0.41
1:B:269:LEU:HD22	1:B:289:ASN:HA	2.02	0.41
1:B:237:VAL:O	1:B:257:GLY:HA2	2.19	0.41
1:A:274:THR:HG22	1:A:277:GLY:HA2	2.01	0.41
1:B:141:LEU:CD1	1:B:315:LYS:HD2	2.51	0.41
1:B:110:SER:O	1:B:132:ILE:N	2.53	0.41
1:B:151:LEU:HD12	1:B:151:LEU:HA	1.90	0.41
1:B:359:GLU:OE2	1:B:361:ASN:HB2	2.20	0.41
1:A:267:ARG:O	1:A:292:ARG:NH2	2.43	0.40
1:A:424:PRO:O	1:A:425:HIS:HB2	2.20	0.40
1:A:78:LEU:HB2	1:A:420:ALA:HB1	2.04	0.40
1:A:73:LYS:HB2	1:A:73:LYS:NZ	2.33	0.40
1:A:134:GLU:OE2	1:A:162:HIS:HE1	2.04	0.40
1:A:449:LYS:HA	1:A:449:LYS:CE	2.51	0.40
1:B:357:LYS:HG3	1:B:357:LYS:HZ3	1.79	0.40

There are no symmetry-related clashes.

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%)	431 (96%)	12 (3%)	4 (1%)	17 11
1	B	447/449 (100%)	424 (95%)	18 (4%)	5 (1%)	14 8
All	All	894/898 (100%)	855 (96%)	30 (3%)	9 (1%)	15 9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	B	253	LYS
1	B	4	MET
1	B	2	PRO
1	B	293	ASN
1	A	2	PRO
1	A	408	ASP
1	A	293	ASN
1	B	171	PRO

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%)	300 (88%)	40 (12%)	5 3
1	B	340/340 (100%)	300 (88%)	40 (12%)	5 3
All	All	680/680 (100%)	600 (88%)	80 (12%)	5 3

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	7	LEU
1	A	9	ASN
1	A	15	ASN
1	A	16	ILE
1	A	43	LYS
1	A	48	LEU
1	A	73	LYS
1	A	80	LEU
1	A	83	GLN
1	A	84	TYR
1	A	91	LYS
1	A	92	LYS
1	A	111	THR
1	A	127	LYS
1	A	151	LEU
1	A	167	LYS
1	A	196	LEU
1	A	232	ARG
1	A	244	ASN
1	A	245	SER
1	A	248	GLU
1	A	252	GLN
1	A	269	LEU
1	A	272	LYS
1	A	274	THR
1	A	279	ILE
1	A	294	ASP
1	A	310	LEU
1	A	314	GLU
1	A	353	LEU
1	A	354	GLU
1	A	357	LYS
1	A	358	LYS
1	A	408	ASP
1	A	429	VAL
1	A	443	LYS
1	A	446	LEU
1	A	448	LEU
1	A	449	LYS
1	B	8	GLU
1	B	37	LEU

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Mol	Chain	Res	Type
1	B	44	ASN
1	B	47	LEU
1	B	48	LEU
1	B	73	LYS
1	B	84	TYR
1	B	92	LYS
1	B	109	TRP
1	B	151	LEU
1	B	155	THR
1	B	159	LEU
1	B	171	PRO
1	B	172	SER
1	B	176	GLN
1	B	184	GLU
1	B	195	LEU
1	B	196	LEU
1	B	209	LYS
1	B	213	GLU
1	B	221	GLN
1	B	223	LYS
1	B	225	LEU
1	B	235	GLN
1	B	242	SER
1	B	250	ASN
1	B	255	LEU
1	B	269	LEU
1	B	281	LYS
1	B	289	ASN
1	B	294	ASP
1	B	304	ASP
1	B	313	ASN
1	B	345	LEU
1	B	351	ARG
1	B	357	LYS
1	B	382	LYS
1	B	400	MET
1	B	443	LYS
1	B	448	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	35	ASN
1	A	83	GLN
1	A	162	HIS
1	A	194	GLN
1	A	235	GLN
1	A	244	ASN
1	A	252	GLN
1	A	263	ASN
1	A	276	HIS
1	A	301	GLN
1	A	329	GLN
1	A	375	GLN
1	A	388	GLN
1	A	435	GLN
1	B	35	ASN
1	B	83	GLN
1	B	129	HIS
1	B	162	HIS
1	B	194	GLN
1	B	235	GLN
1	B	250	ASN
1	B	263	ASN
1	B	276	HIS
1	B	289	ASN
1	B	301	GLN
1	B	313	ASN
1	B	329	GLN
1	B	388	GLN
1	B	391	ASN

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 (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	A	453	2	4,4,4	0.25	0	6,6,6	0.33	0
4	PO4	B	453	2	4,4,4	1.37	0	6,6,6	0.81	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	453	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.