Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:04 PM UTC

PDB ID	:	1ALI / pdb_00001ali
Title	:	ALKALINE PHOSPHATASE MUTANT (H412N)
Authors	:	Ma, L.; Tibbitts, T.T.; Kantrowitz, E.R.
Deposited on	:	1995-06-02
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:

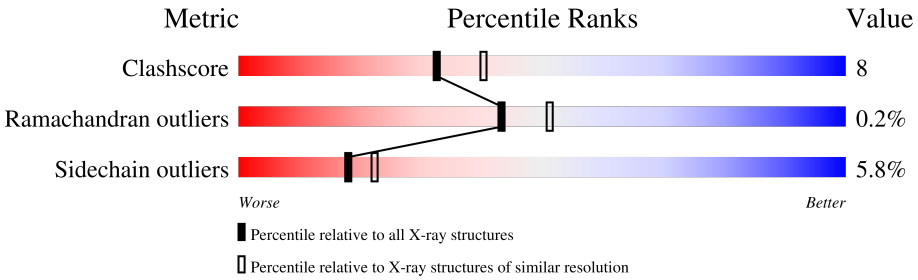
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	76% 22%
1	B	449	74% 22%

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	PO4	A	453	-	X	-	-
4	PO4	B	453	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6813 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	446	Total 3279	C 2026	N 577	O 664	S 12	0	0	0
1	B	446	Total 3279	C 2026	N 577	O 664	S 12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	412	ASN	HIS	engineered mutation	UNP P00634
B	412	ASN	HIS	engineered mutation	UNP P00634

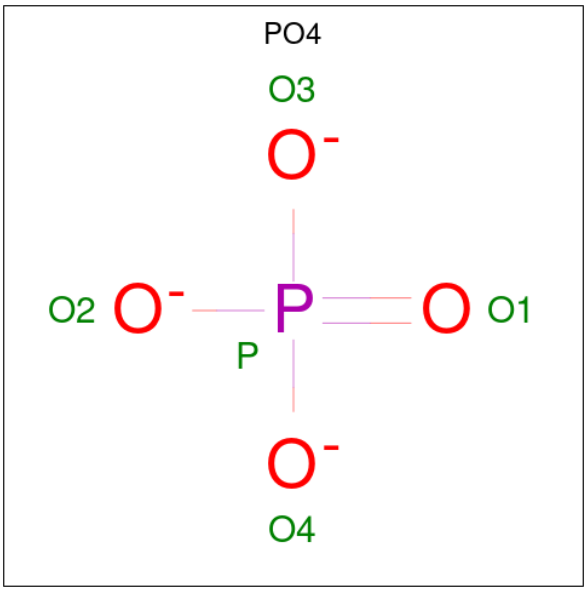
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHATE ION (CCD ID: 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	135	Total O 135 135	0	0
5	B	104	Total O 104 104	0	0

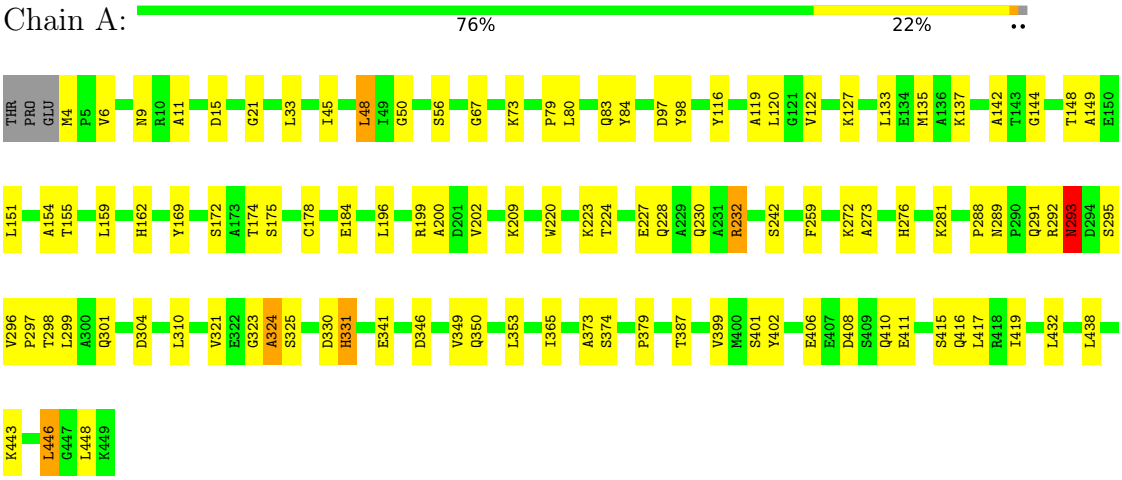
3 Residue-property plots (i)

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. 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.

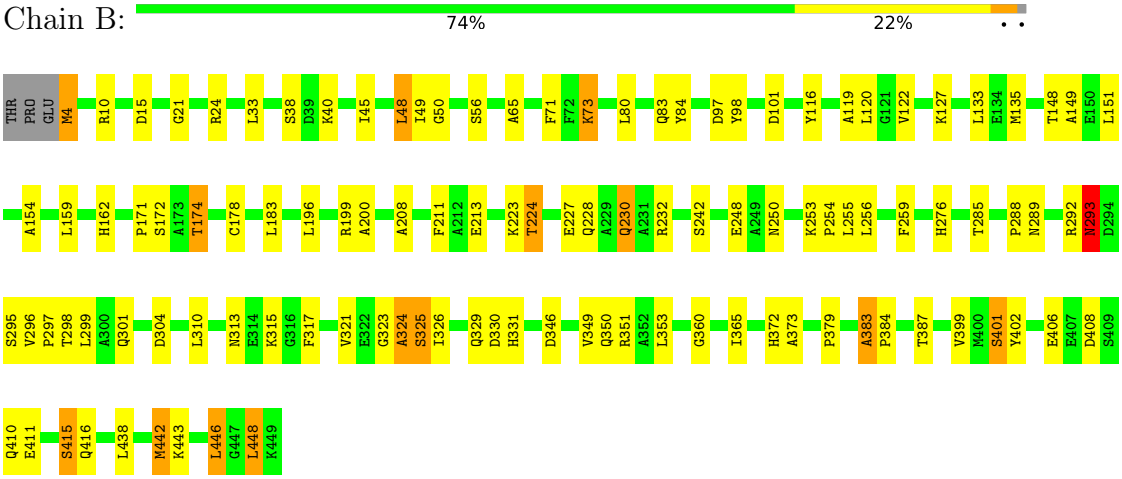
• Molecule 1: ALKALINE PHOSPHATASE

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	194.86Å 167.43Å 76.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6813	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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	1.14	5/3332 (0.2%)	1.26	23/4522 (0.5%)
1	B	1.10	4/3332 (0.1%)	1.28	28/4522 (0.6%)
All	All	1.12	9/6664 (0.1%)	1.27	51/9044 (0.6%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	HIS	CD2-NE2	9.06	1.47	1.37
1	B	331	HIS	CD2-NE2	7.57	1.46	1.37
1	B	331	HIS	ND1-CE1	5.75	1.38	1.32
1	A	11	ALA	CA-CB	-5.52	1.44	1.53
1	A	9	ASN	CA-C	-5.38	1.46	1.52
1	B	401	SER	N-CA	5.29	1.52	1.46
1	B	442	MET	SD-CE	-5.13	1.66	1.79
1	A	155	THR	CA-CB	5.12	1.59	1.53
1	A	331	HIS	ND1-CE1	5.07	1.37	1.32

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	324	ALA	N-CA-C	11.92	124.36	111.36
1	A	324	ALA	N-CA-C	9.87	124.67	112.23
1	B	293	ASN	N-CA-C	8.77	129.48	110.80
1	A	293	ASN	N-CA-C	8.07	127.98	110.80
1	A	373	ALA	N-CA-C	7.16	120.50	111.69
1	B	373	ALA	N-CA-C	7.00	120.30	111.69
1	A	416	GLN	N-CA-C	-6.75	101.62	110.53
1	B	360	GLY	N-CA-C	6.68	123.02	115.08
1	B	416	GLN	N-CA-C	-6.63	101.78	110.53
1	B	154	ALA	N-CA-C	6.50	118.91	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	LYS	N-CA-C	6.40	118.83	111.02
1	B	199	ARG	N-CA-C	6.26	120.28	111.52
1	A	97	ASP	N-CA-C	-6.16	97.24	108.02
1	A	98	TYR	N-CA-C	6.15	119.88	112.38
1	A	330	ASP	N-CA-C	-6.10	104.55	111.14
1	B	383	ALA	CA-C-N	6.06	125.61	119.19
1	B	383	ALA	C-N-CA	6.06	125.61	119.19
1	A	142	ALA	N-CA-C	-6.05	102.38	110.55
1	A	50	GLY	N-CA-C	-6.00	99.51	111.34
1	B	323	GLY	N-CA-C	-5.96	99.07	113.18
1	B	317	PHE	N-CA-C	5.95	118.11	109.07
1	A	154	ALA	N-CA-C	5.89	118.18	111.11
1	B	101	ASP	N-CA-C	-5.89	101.47	109.95
1	B	97	ASP	N-CA-C	-5.77	97.92	108.02
1	B	174	THR	N-CA-C	5.77	117.24	111.07
1	A	323	GLY	N-CA-C	-5.74	99.57	113.18
1	A	200	ALA	N-CA-C	-5.73	102.97	110.53
1	B	259	PHE	N-CA-C	5.69	119.85	113.02
1	A	169	TYR	N-CA-C	5.61	117.08	110.97
1	A	6	VAL	N-CA-C	-5.55	100.37	108.97
1	A	79	PRO	N-CA-C	5.46	123.72	112.47
1	B	98	TYR	N-CA-C	5.43	119.01	112.38
1	B	49	ILE	CA-C-N	-5.36	117.52	122.29
1	B	49	ILE	C-N-CA	-5.36	117.52	122.29
1	A	411	GLU	N-CA-C	5.35	118.38	110.46
1	B	326	ILE	N-CA-C	-5.31	105.15	110.30
1	B	411	GLU	N-CA-C	5.29	118.27	110.59
1	B	330	ASP	N-CA-C	-5.29	105.41	111.07
1	B	24	ARG	N-CA-C	-5.27	107.02	113.50
1	B	285	THR	N-CA-C	-5.19	100.43	108.90
1	B	200	ALA	N-CA-C	-5.19	103.30	110.35
1	B	65	ALA	N-CA-C	5.16	118.73	112.23
1	A	419	ILE	N-CA-C	-5.14	100.80	108.46
1	B	50	GLY	N-CA-C	-5.14	101.22	111.34
1	A	281	LYS	CA-C-N	5.12	125.10	120.03
1	A	281	LYS	C-N-CA	5.12	125.10	120.03
1	A	374	SER	N-CA-C	5.10	117.63	110.23
1	B	224	THR	N-CA-C	-5.10	103.66	110.55
1	B	325	SER	N-CA-C	5.05	119.08	113.02
1	A	259	PHE	N-CA-C	5.03	119.11	112.92
1	A	67	GLY	N-CA-C	-5.01	106.42	112.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3279	0	3224	54	0
1	B	3279	0	3224	59	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	1	0
4	B	5	0	0	0	0
5	A	135	0	0	1	0
5	B	104	0	0	0	0
All	All	6813	0	6448	103	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 (103) 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:289:ASN:O	1:A:292:ARG:HG2	1.69	0.91
1:A:56:SER:HA	1:B:415:SER:OG	1.78	0.84
1:A:135:MET:HE1	1:A:443:LYS:HD2	1.65	0.78
1:A:415:SER:OG	1:B:56:SER:HA	1.83	0.77
1:A:45:ILE:HD12	1:A:446:LEU:HD22	1.67	0.76
1:A:227:GLU:HA	1:A:230:GLN:NE2	2.02	0.75
1:B:45:ILE:HD12	1:B:446:LEU:HD22	1.70	0.72
1:A:56:SER:HA	1:B:415:SER:HG	1.50	0.72
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.74	0.69
1:B:227:GLU:HA	1:B:230:GLN:NE2	2.08	0.68
1:A:402:TYR:HB3	1:A:410:GLN:HG3	1.75	0.67
1:B:228:GLN:O	1:B:232:ARG:HG3	1.95	0.66
1:B:135:MET:HE1	1:B:443:LYS:HD2	1.78	0.66
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ASN:O	1:B:292:ARG:HG2	1.96	0.65
1:B:73:LYS:HD2	1:B:73:LYS:N	2.11	0.65
1:A:56:SER:CA	1:B:415:SER:OG	2.45	0.64
1:A:228:GLN:O	1:A:232:ARG:HG2	2.00	0.62
1:A:291:GLN:HG3	5:A:469:HOH:O	1.99	0.62
1:A:415:SER:OG	1:B:56:SER:CA	2.47	0.61
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.82	0.61
1:B:297:PRO:HA	1:B:301:GLN:OE1	2.02	0.59
1:A:224:THR:OG1	1:A:227:GLU:HG3	2.03	0.57
1:A:297:PRO:HA	1:A:301:GLN:OE1	2.04	0.57
1:A:220:TRP:CZ2	1:A:232:ARG:HD2	2.40	0.56
1:A:137:LYS:HE3	1:A:199:ARG:O	2.06	0.56
1:A:73:LYS:HD2	1:A:73:LYS:N	2.22	0.55
1:B:174:THR:HG23	1:B:178:CYS:HB2	1.89	0.55
1:B:346:ASP:O	1:B:350:GLN:HG3	2.08	0.54
1:A:293:ASN:HB3	1:A:296:VAL:HG23	1.89	0.54
1:B:293:ASN:HB3	1:B:296:VAL:HG23	1.89	0.53
1:B:15:ASP:O	1:B:21:GLY:HA3	2.09	0.53
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.91	0.52
1:B:387:THR:HG22	1:B:401:SER:OG	2.10	0.52
1:B:224:THR:OG1	1:B:227:GLU:HG3	2.09	0.52
1:A:144:GLY:HA2	1:A:202:VAL:O	2.10	0.52
1:A:174:THR:HG23	1:A:178:CYS:HB2	1.92	0.51
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.93	0.51
1:A:15:ASP:O	1:A:21:GLY:HA3	2.11	0.50
1:B:383:ALA:HB1	1:B:384:PRO:HD2	1.93	0.50
1:B:446:LEU:HB3	1:B:448:LEU:HD13	1.94	0.50
1:B:288:PRO:HB3	1:B:292:ARG:NH2	2.27	0.49
1:A:272:LYS:HG2	1:A:273:ALA:O	2.12	0.49
1:A:48:LEU:HG	1:A:349:VAL:HG22	1.95	0.49
1:B:379:PRO:HA	1:B:399:VAL:CG2	2.43	0.49
1:A:148:THR:HG23	1:A:299:LEU:HD13	1.94	0.48
1:B:149:ALA:HB2	1:B:324:ALA:HB1	1.95	0.48
1:B:10:ARG:HB2	1:B:71:PHE:CE1	2.49	0.48
1:A:175:SER:OG	1:A:184:GLU:OE2	2.20	0.47
1:B:148:THR:HG23	1:B:299:LEU:HD13	1.96	0.47
1:B:171:PRO:HD2	1:B:213:GLU:OE1	2.15	0.47
1:B:313:ASN:OD1	1:B:315:LYS:HB2	2.15	0.47
1:A:288:PRO:HB3	1:A:292:ARG:NH2	2.30	0.47
1:A:331:HIS:ND1	1:A:410:GLN:O	2.48	0.47
1:A:227:GLU:HA	1:A:230:GLN:HE21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ARG:HB2	1:B:71:PHE:CD1	2.50	0.47
1:A:346:ASP:O	1:A:350:GLN:HG3	2.15	0.46
1:B:250:ASN:OD1	1:B:253:LYS:HG2	2.15	0.46
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.51	0.45
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.51	0.45
1:B:248:GLU:HB2	1:B:253:LYS:HE2	1.98	0.45
1:A:149:ALA:HB2	1:A:324:ALA:HB1	1.98	0.45
1:A:276:HIS:HE1	1:B:406:GLU:OE1	1.99	0.45
1:A:298:THR:OG1	1:A:301:GLN:HG3	2.18	0.44
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.48	0.44
1:A:331:HIS:NE2	4:A:453:PO4:O1	2.44	0.44
1:A:325:SER:HB2	1:A:341:GLU:HG3	1.98	0.44
1:B:250:ASN:O	1:B:254:PRO:N	2.51	0.44
1:B:213:GLU:O	1:B:224:THR:HA	2.18	0.43
1:B:351:ARG:NH1	1:B:351:ARG:HG2	2.32	0.43
1:B:38:SER:OG	1:B:40:LYS:HG2	2.18	0.43
1:B:365:ILE:HD13	1:B:438:LEU:HD11	2.01	0.43
1:A:228:GLN:OE1	1:A:232:ARG:NH1	2.50	0.43
1:A:365:ILE:HD13	1:A:438:LEU:HD11	2.01	0.43
1:A:406:GLU:OE1	1:B:276:HIS:HE1	2.01	0.43
1:A:408:ASP:OD1	1:A:408:ASP:N	2.50	0.43
1:B:438:LEU:HG	1:B:442:MET:HE2	2.00	0.43
1:B:122:VAL:HA	1:B:127:LYS:O	2.19	0.43
1:B:120:LEU:O	1:B:162:HIS:HA	2.19	0.43
1:B:4:MET:HE2	1:B:4:MET:HB2	1.98	0.43
1:A:230:GLN:HE21	1:A:230:GLN:HB2	1.70	0.42
1:B:73:LYS:N	1:B:73:LYS:CD	2.81	0.42
1:B:408:ASP:OD1	1:B:408:ASP:N	2.52	0.42
1:A:175:SER:HG	1:A:184:GLU:CD	2.21	0.42
1:A:122:VAL:HA	1:A:127:LYS:O	2.19	0.42
1:B:230:GLN:HE21	1:B:230:GLN:HB2	1.72	0.42
1:A:133:LEU:HD23	1:A:133:LEU:C	2.45	0.42
1:A:387:THR:HG22	1:A:401:SER:OG	2.19	0.42
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.50	0.42
1:A:120:LEU:O	1:A:162:HIS:HA	2.19	0.42
1:B:133:LEU:C	1:B:133:LEU:HD23	2.45	0.42
1:B:183:LEU:HA	1:B:183:LEU:HD12	1.68	0.42
1:B:208:ALA:O	1:B:211:PHE:HB2	2.20	0.41
1:B:48:LEU:HG	1:B:349:VAL:HG22	2.03	0.41
1:A:432:LEU:O	1:B:10:ARG:HD2	2.21	0.41
1:B:325:SER:O	1:B:329:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ALA:HB2	1:B:324:ALA:CB	2.50	0.41
1:B:255:LEU:HD12	1:B:256:LEU:N	2.36	0.41
1:A:276:HIS:CE1	1:B:406:GLU:OE1	2.74	0.40
1:A:83:GLN:HE21	1:B:83:GLN:HE21	1.69	0.40
1:A:417:LEU:HD12	1:A:417:LEU:C	2.46	0.40
1:B:298:THR:OG1	1:B:301:GLN:HG3	2.21	0.40
1:A:228:GLN:O	1:A:232:ARG:CG	2.68	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	444/449 (99%)	436 (98%)	7 (2%)	1 (0%)	43 51
1	B	444/449 (99%)	435 (98%)	8 (2%)	1 (0%)	43 51
All	All	888/898 (99%)	871 (98%)	15 (2%)	2 (0%)	43 51

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	337/340 (99%)	319 (95%)	18 (5%)	20 26
1	B	337/340 (99%)	316 (94%)	21 (6%)	16 20
All	All	674/680 (99%)	635 (94%)	39 (6%)	18 22

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	33	LEU
1	A	48	LEU
1	A	80	LEU
1	A	84	TYR
1	A	151	LEU
1	A	159	LEU
1	A	172	SER
1	A	196	LEU
1	A	223	LYS
1	A	232	ARG
1	A	242	SER
1	A	295	SER
1	A	304	ASP
1	A	310	LEU
1	A	353	LEU
1	A	446	LEU
1	A	448	LEU
1	B	4	MET
1	B	33	LEU
1	B	48	LEU
1	B	73	LYS
1	B	80	LEU
1	B	84	TYR
1	B	151	LEU
1	B	159	LEU
1	B	172	SER
1	B	196	LEU
1	B	223	LYS
1	B	230	GLN
1	B	242	SER
1	B	295	SER
1	B	304	ASP
1	B	310	LEU
1	B	353	LEU

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Mol	Chain	Res	Type
1	B	372	HIS
1	B	415	SER
1	B	446	LEU
1	B	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	A	230	GLN
1	A	251	GLN
1	A	252	GLN
1	A	276	HIS
1	A	291	GLN
1	A	338	GLN
1	A	375	GLN
1	A	388	GLN
1	A	410	GLN
1	B	13	GLN
1	B	83	GLN
1	B	125	HIS
1	B	221	GLN
1	B	230	GLN
1	B	252	GLN
1	B	276	HIS
1	B	291	GLN
1	B	388	GLN
1	B	410	GLN
1	B	435	GLN

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 (i)

There are no oligosaccharides 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	2.48	2 (50%)	6,6,6	2.22	3 (50%)
4	PO4	B	453	2	4,4,4	2.58	2 (50%)	6,6,6	2.77	5 (83%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	453	PO4	P-O2	-3.76	1.43	1.54
4	A	453	PO4	P-O3	-3.39	1.44	1.54
4	B	453	PO4	P-O3	-3.16	1.45	1.54
4	A	453	PO4	P-O2	-2.87	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	453	PO4	O3-P-O2	-3.80	96.07	107.91
4	B	453	PO4	O4-P-O1	-3.45	98.76	110.95
4	A	453	PO4	O3-P-O2	-3.42	97.28	107.91
4	B	453	PO4	O4-P-O2	3.32	118.23	107.91
4	A	453	PO4	O4-P-O1	-2.63	101.67	110.95
4	A	453	PO4	O4-P-O2	2.24	114.87	107.91
4	B	453	PO4	O3-P-O1	2.11	118.40	110.95
4	B	453	PO4	O4-P-O3	2.04	114.25	107.91

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	A	453	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

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.