Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 09:10 AM EDT

PDB ID	:	1ANJ
Title	:	ALKALINE PHOSPHATASE (K328H)
Authors	:	Murphy, J.E.; Tibbitts, T.T.; Kantrowitz, E.R.
Deposited on	:	1995-09-06
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

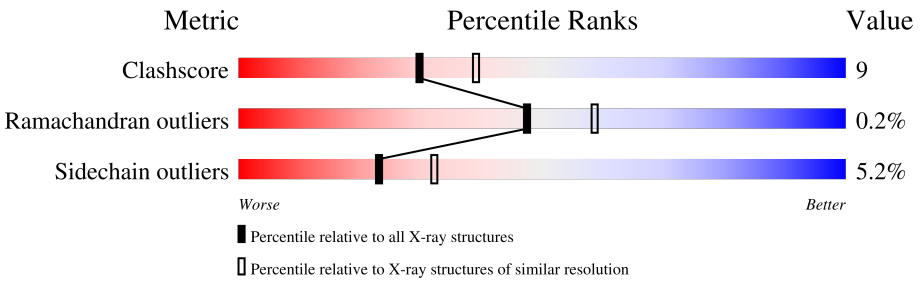
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	446	78% 20% •
1	B	446	78% 20% •

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	457	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6906 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
			Total	C	N	O	S			
1	A	446	3282	2028	579	663	12	0	0	0
1	B	446	3282	2028	579	663	12	0	0	0

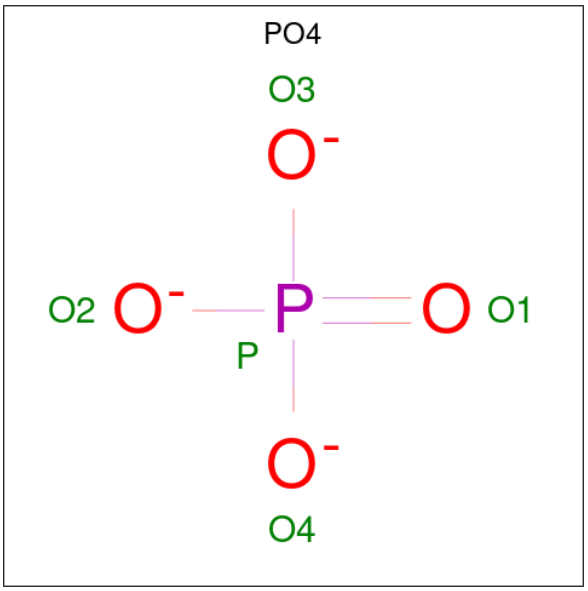
There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	226	Total O 226 226	0	0
4	B	90	Total O 90 90	0	0

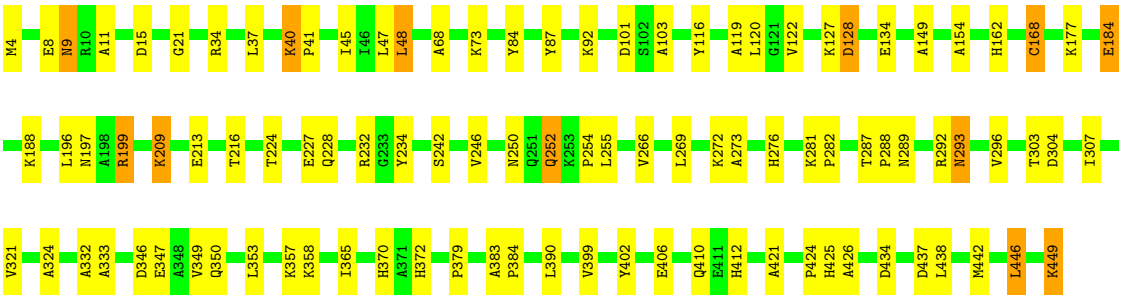
3 Residue-property plots (i)

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.

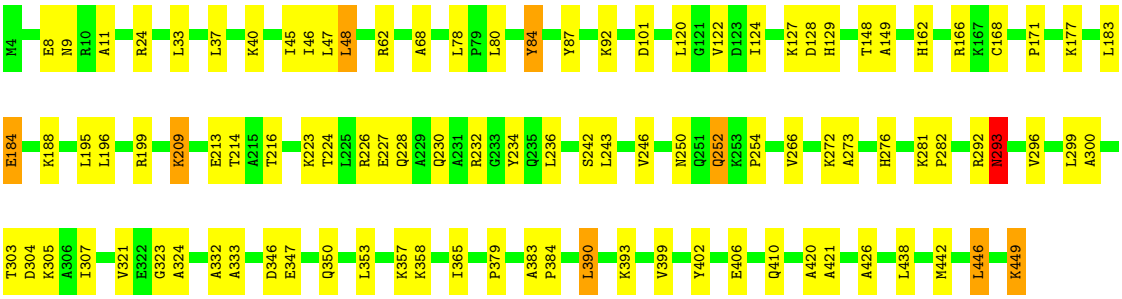
• Molecule 1: ALKALINE PHOSPHATASE

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	195.10Å 167.30Å 76.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	99.0 (8.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1, IMPLOR, POLYVISION, TIBBITTS	Depositor
R, R_{free}	0.194 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6906	wwPDB-VP
Average B, all atoms ($Å^2$)	17.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.89	1/3337 (0.0%)	0.98	5/4530 (0.1%)
1	B	0.87	0/3337	0.95	7/4530 (0.2%)
All	All	0.88	1/6674 (0.0%)	0.97	12/9060 (0.1%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	GLU	CD-OE1	5.24	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	199	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	128	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	101	ASP	CB-CG-OD1	6.11	123.79	118.30
1	A	199	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	B	323	GLY	N-CA-C	-5.69	98.89	113.10
1	B	24	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	293	ASN	N-CA-C	5.58	126.08	111.00
1	B	62	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	101	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	168	CYS	CA-CB-SG	-5.30	104.45	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	48	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	84	TYR	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	3282	0	3219	63	4
1	B	3282	0	3219	65	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	226	0	0	10	4
4	B	90	0	0	1	0
All	All	6906	0	6438	122	4

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 9.

All (122) 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:288:PRO:HB3	1:A:292:ARG:HH21	1.37	0.90
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.68	0.76
1:A:293:ASN:HB3	1:A:296:VAL:HG23	1.69	0.74
1:A:288:PRO:HB3	1:A:292:ARG:NH2	2.03	0.72
1:A:73:LYS:HE3	4:A:555:HOH:O	1.89	0.71
1:A:188:LYS:HD2	4:A:648:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ASN:OD1	1:B:252:GLN:HG2	1.91	0.70
1:B:213:GLU:O	1:B:224:THR:HA	1.92	0.70
1:A:224:THR:OG1	1:A:227:GLU:HG3	1.91	0.69
1:B:226:ARG:HH11	1:B:230:GLN:HE21	1.42	0.69
1:B:45:ILE:HD12	1:B:446:LEU:HD22	1.77	0.66
1:A:289:ASN:O	1:A:292:ARG:HG2	1.96	0.66
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.77	0.66
1:B:293:ASN:HB3	1:B:296:VAL:HG23	1.78	0.66
1:B:184:GLU:HG3	1:B:216:THR:OG1	1.95	0.65
1:A:234:TYR:HA	1:A:254:PRO:HG2	1.79	0.64
1:B:224:THR:OG1	1:B:227:GLU:HG3	1.99	0.63
1:B:393:LYS:O	1:B:393:LYS:HG3	1.99	0.62
1:A:213:GLU:O	1:A:224:THR:HA	2.00	0.61
1:A:45:ILE:HD12	1:A:446:LEU:HD22	1.82	0.61
1:B:214:THR:HA	1:B:223:LYS:O	2.03	0.58
1:B:120:LEU:O	1:B:162:HIS:HA	2.04	0.58
1:B:226:ARG:HH11	1:B:230:GLN:NE2	2.01	0.57
1:A:250:ASN:OD1	1:A:252:GLN:HG2	2.06	0.56
1:A:358:LYS:HB2	1:A:358:LYS:NZ	2.21	0.55
1:A:128:ASP:OD2	1:A:188:LYS:HE3	2.06	0.55
1:A:346:ASP:O	1:A:350:GLN:HG3	2.06	0.55
1:B:281:LYS:HB3	1:B:282:PRO:HD2	1.89	0.55
1:B:226:ARG:NH1	1:B:230:GLN:HE21	2.03	0.54
1:B:358:LYS:HB2	1:B:358:LYS:NZ	2.22	0.54
1:A:434:ASP:O	1:A:437:ASP:HB2	2.06	0.54
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.89	0.53
1:A:228:GLN:OE1	1:A:232:ARG:NH1	2.41	0.53
1:A:184:GLU:HG3	1:A:216:THR:OG1	2.09	0.53
1:B:303:THR:O	1:B:307:ILE:HG13	2.10	0.52
1:B:230:GLN:HG3	1:B:236:LEU:HD12	1.93	0.51
1:B:209:LYS:HA	1:B:209:LYS:HE3	1.92	0.51
1:B:272:LYS:HG2	1:B:273:ALA:O	2.11	0.51
1:B:168:CYS:SG	1:B:177:LYS:HB2	2.50	0.51
1:A:303:THR:O	1:A:307:ILE:HG13	2.11	0.51
1:A:168:CYS:SG	1:A:177:LYS:HB2	2.51	0.51
1:B:129:HIS:O	1:B:162:HIS:HE1	1.93	0.51
1:A:199:ARG:HA	1:A:234:TYR:OH	2.11	0.50
1:A:402:TYR:HB3	1:A:410:GLN:HG3	1.93	0.50
1:A:383:ALA:HB1	1:A:384:PRO:HD2	1.93	0.50
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.93	0.49
1:A:68:ALA:HB1	1:B:87:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:HD2	1:B:236:LEU:CD1	2.43	0.49
1:B:226:ARG:HD2	1:B:236:LEU:HD13	1.94	0.49
1:A:370:HIS:NE2	1:A:412:HIS:CE1	2.82	0.48
1:B:199:ARG:HA	1:B:234:TYR:OH	2.14	0.48
1:A:358:LYS:HB2	1:A:358:LYS:HZ2	1.79	0.48
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.44	0.48
1:A:48:LEU:HG	1:A:349:VAL:HG22	1.95	0.48
1:A:424:PRO:O	1:A:425:HIS:HB2	2.13	0.48
1:A:9:ASN:ND2	1:A:11:ALA:H	2.12	0.47
1:B:188:LYS:HD2	4:B:505:HOH:O	2.13	0.47
1:A:287:THR:HG22	4:A:630:HOH:O	2.14	0.47
1:B:383:ALA:HB1	1:B:384:PRO:HD2	1.95	0.47
1:A:87:TYR:CD2	1:B:68:ALA:HB1	2.50	0.47
1:A:272:LYS:HG2	1:A:273:ALA:O	2.14	0.47
1:B:122:VAL:HA	1:B:127:LYS:O	2.15	0.47
1:B:449:LYS:HB2	1:B:449:LYS:NZ	2.29	0.47
1:A:4:MET:N	4:A:518:HOH:O	2.47	0.47
1:B:226:ARG:NH1	1:B:236:LEU:HD13	2.30	0.47
1:B:346:ASP:O	1:B:350:GLN:HG3	2.14	0.47
1:A:40:LYS:HG2	1:A:41:PRO:N	2.30	0.46
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.97	0.46
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.50	0.46
1:A:188:LYS:HG2	4:A:666:HOH:O	2.15	0.46
1:A:281:LYS:HB3	1:A:282:PRO:HD2	1.97	0.46
1:A:421:ALA:HB3	1:A:426:ALA:HB1	1.98	0.45
1:A:120:LEU:O	1:A:162:HIS:HA	2.16	0.45
1:A:276:HIS:HE1	1:B:406:GLU:OE1	1.99	0.45
1:A:293:ASN:ND2	4:A:568:HOH:O	2.49	0.45
1:B:92:LYS:HA	1:B:92:LYS:HE2	1.97	0.45
1:A:15:ASP:O	1:A:21:GLY:HA3	2.16	0.45
1:A:37:LEU:HD21	1:B:33:LEU:HD23	1.97	0.45
1:A:188:LYS:CD	4:A:648:HOH:O	2.59	0.45
1:A:332:ALA:O	1:A:333:ALA:HB3	2.16	0.45
1:A:438:LEU:O	1:A:442:MET:HG3	2.16	0.45
1:B:128:ASP:OD2	1:B:188:LYS:HE3	2.16	0.45
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.97	0.45
1:A:92:LYS:HA	1:A:92:LYS:HE2	1.99	0.45
1:A:269:LEU:HA	4:A:626:HOH:O	2.16	0.45
1:B:379:PRO:HA	1:B:399:VAL:CG2	2.47	0.45
1:B:183:LEU:HD12	1:B:183:LEU:HA	1.80	0.44
1:B:300:ALA:HB2	1:B:347:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ILE:HD13	1:B:438:LEU:HD11	1.99	0.44
1:A:406:GLU:OE1	1:B:276:HIS:HE1	2.01	0.44
1:B:195:LEU:C	1:B:195:LEU:HD23	2.38	0.44
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.48	0.44
1:A:412:HIS:CE1	3:A:453:PO4:P	3.11	0.44
1:B:332:ALA:O	1:B:333:ALA:HB3	2.18	0.44
1:B:421:ALA:HB3	1:B:426:ALA:HB1	2.00	0.44
1:A:122:VAL:HA	1:A:127:LYS:O	2.17	0.44
1:B:390:LEU:CD2	1:B:390:LEU:N	2.82	0.43
1:B:148:THR:HG23	1:B:299:LEU:HD13	2.00	0.43
1:B:390:LEU:N	1:B:390:LEU:HD22	2.34	0.43
1:B:353:LEU:O	1:B:357:LYS:HB2	2.18	0.43
1:B:438:LEU:O	1:B:442:MET:HG3	2.18	0.43
1:B:230:GLN:CG	1:B:236:LEU:HD12	2.48	0.43
1:A:103:ALA:HA	1:A:154:ALA:HB1	2.01	0.43
1:B:149:ALA:HB2	1:B:324:ALA:CB	2.49	0.42
1:A:34:ARG:HG2	1:B:37:LEU:HD12	2.02	0.42
1:B:9:ASN:ND2	1:B:11:ALA:H	2.16	0.42
1:B:124:ILE:HD13	1:B:124:ILE:HG21	1.77	0.42
1:B:46:ILE:HG22	1:B:48:LEU:HD22	2.01	0.42
1:A:353:LEU:O	1:A:357:LYS:HB2	2.20	0.42
1:B:353:LEU:HA	1:B:353:LEU:HD23	1.83	0.42
1:A:209:LYS:HE3	1:A:209:LYS:HA	2.01	0.42
1:B:234:TYR:HA	1:B:254:PRO:HG2	2.01	0.42
1:A:188:LYS:CE	4:A:648:HOH:O	2.67	0.41
1:B:80:LEU:O	1:B:420:ALA:HA	2.20	0.41
1:A:449:LYS:HB2	1:A:449:LYS:NZ	2.35	0.41
1:B:246:VAL:O	1:B:305:LYS:NZ	2.44	0.41
1:B:243:LEU:O	1:B:305:LYS:HE2	2.21	0.41
1:B:129:HIS:O	1:B:162:HIS:CE1	2.72	0.41
1:B:226:ARG:NH1	1:B:230:GLN:NE2	2.65	0.41
1:B:228:GLN:O	1:B:232:ARG:HG3	2.20	0.41
1:A:188:LYS:HD2	4:A:599:HOH:O	2.21	0.40
1:A:246:VAL:HG11	1:A:255:LEU:HD22	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASN:O	4:A:511:HOH:O[3_656]	1.87	0.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASP:CB	4:A:523:HOH:O[3_656]	1.94	0.26
1:A:134:GLU:CA	4:A:471:HOH:O[3_656]	2.19	0.01
1:A:197:ASN:CA	4:A:470:HOH:O[3_656]	2.19	0.01

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	444/446 (100%)	430 (97%)	13 (3%)	1 (0%)	47	58
1	B	444/446 (100%)	425 (96%)	18 (4%)	1 (0%)	47	58
All	All	888/892 (100%)	855 (96%)	31 (4%)	2 (0%)	47	58

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	337/337 (100%)	320 (95%)	17 (5%)	24	34
1	B	337/337 (100%)	319 (95%)	18 (5%)	22	31
All	All	674/674 (100%)	639 (95%)	35 (5%)	23	32

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	ASN
1	A	40	LYS
1	A	47	LEU
1	A	48	LEU
1	A	84	TYR
1	A	184	GLU
1	A	196	LEU
1	A	209	LYS
1	A	242	SER
1	A	252	GLN
1	A	266	VAL
1	A	304	ASP
1	A	372	HIS
1	A	390	LEU
1	A	446	LEU
1	A	449	LYS
1	B	8	GLU
1	B	40	LYS
1	B	47	LEU
1	B	78	LEU
1	B	84	TYR
1	B	166	ARG
1	B	171	PRO
1	B	184	GLU
1	B	196	LEU
1	B	209	LYS
1	B	242	SER
1	B	252	GLN
1	B	266	VAL
1	B	292	ARG
1	B	304	ASP
1	B	390	LEU
1	B	446	LEU
1	B	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	13	GLN

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Mol	Chain	Res	Type
1	A	251	GLN
1	A	276	HIS
1	A	329	GLN
1	A	338	GLN
1	B	9	ASN
1	B	230	GLN
1	B	251	GLN
1	B	276	HIS
1	B	338	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 monosaccharides 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	453	2	4,4,4	1.51	1 (25%)	6,6,6	1.43	1 (16%)
3	PO4	B	457	-	4,4,4	1.62	0	6,6,6	0.79	0
3	PO4	A	457	-	4,4,4	2.60	3 (75%)	6,6,6	1.06	1 (16%)
3	PO4	A	453	2	4,4,4	1.56	2 (50%)	6,6,6	1.06	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	457	PO4	P-O3	-3.04	1.45	1.54
3	A	457	PO4	P-O1	-2.96	1.43	1.50
3	A	457	PO4	P-O4	-2.55	1.46	1.54
3	B	453	PO4	P-O4	-2.41	1.47	1.54
3	A	453	PO4	P-O3	-2.37	1.47	1.54
3	A	453	PO4	P-O4	-2.03	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	453	PO4	O4-P-O1	-2.41	102.08	110.89
3	A	457	PO4	O4-P-O1	-2.28	102.56	110.89

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
3	A	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.