Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 12:32 PM EDT

PDB ID	:	1URA
Title	:	ALKALINE PHOSPHATASE (D51ZN)
Authors	:	Tibbitts, T.T.; Murphy, J.E.; Kantrowitz, E.R.
Deposited on	:	1996-02-03
Resolution	:	2.04 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:

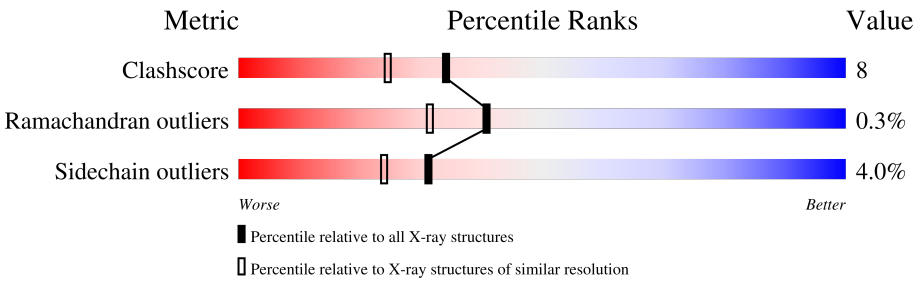
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.04 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	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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	81% 16% •
1	B	446	83% 14% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6916 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	3281	2028	579	662	12	0	0	0
1	B	446	3281	2028	579	662	12	0	0	0

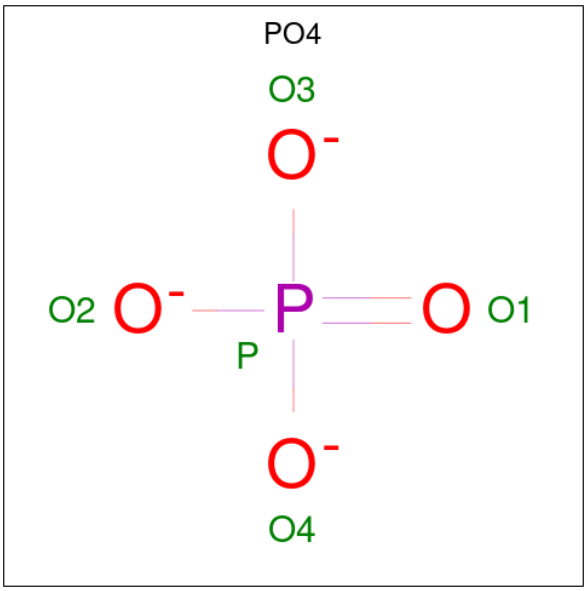
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ASN	ASP	engineered mutation	UNP P00634
B	51	ASN	ASP	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	2	2	2	0	0
2	B	2	2	2	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	204	Total O 204 204	0	0
4	B	126	Total O 126 126	0	0

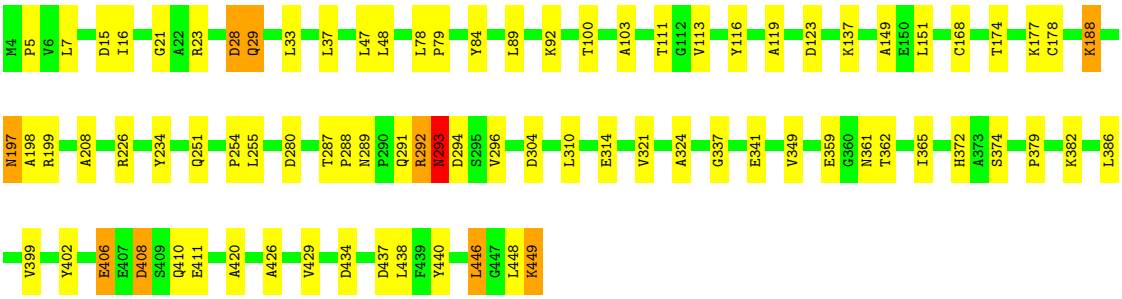
3 Residue-property plots (i)

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.

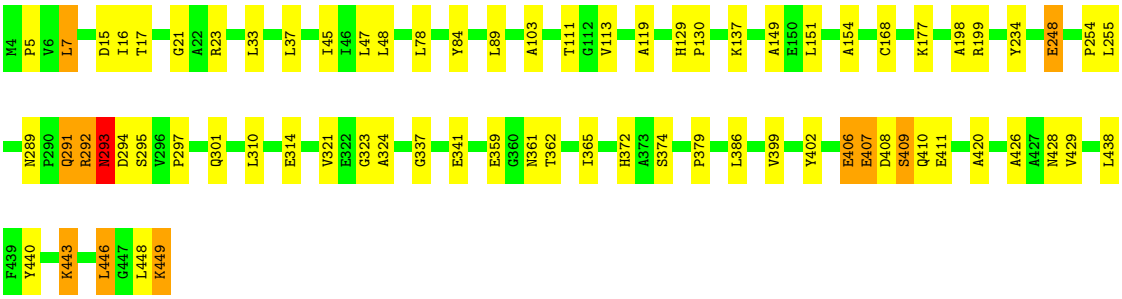
• Molecule 1: ALKALINE PHOSPHATASE

Chain A: 81% 16% •



• Molecule 1: ALKALINE PHOSPHATASE

Chain B: 83% 14% •



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	194.81Å 166.87Å 76.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.04	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.04)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.203 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6916	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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	1.05	11/3335 (0.3%)	1.05	14/4526 (0.3%)
1	B	0.75	11/3335 (0.3%)	0.88	14/4526 (0.3%)
All	All	0.91	22/6670 (0.3%)	0.97	28/9052 (0.3%)

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	2
1	B	0	3
All	All	0	5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLN	N-CA	32.88	2.12	1.46
1	B	406	GLU	C-N	-19.43	0.89	1.34
1	A	406	GLU	C-N	-18.83	0.90	1.34
1	A	197	ASN	CB-CG	17.84	1.92	1.51
1	A	293	ASN	C-N	17.42	1.74	1.34
1	B	293	ASN	C-N	16.30	1.71	1.34
1	A	197	ASN	CG-ND2	-14.73	0.96	1.32
1	B	248	GLU	CD-OE2	13.83	1.40	1.25
1	A	197	ASN	CG-OD1	13.01	1.52	1.24
1	A	188	LYS	CE-NZ	-12.70	1.17	1.49
1	A	28	ASP	C-N	11.95	1.61	1.34
1	A	197	ASN	CA-CB	11.82	1.83	1.53
1	B	443	LYS	CD-CE	10.51	1.77	1.51
1	A	188	LYS	CB-CG	10.30	1.80	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	443	LYS	CG-CD	-9.97	1.18	1.52
1	B	129	HIS	N-CA	-9.23	1.27	1.46
1	B	248	GLU	CD-OE1	8.88	1.35	1.25
1	A	197	ASN	N-CA	-8.62	1.29	1.46
1	B	130	PRO	CG-CD	-6.76	1.28	1.50
1	B	129	HIS	CA-CB	-5.99	1.40	1.53
1	B	129	HIS	CA-C	5.85	1.68	1.52
1	B	443	LYS	CE-NZ	-5.01	1.36	1.49

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	ASP	O-C-N	24.56	162.00	122.70
1	A	408	ASP	O-C-N	-24.41	83.65	122.70
1	A	28	ASP	C-N-CA	-19.30	73.46	121.70
1	A	408	ASP	C-N-CA	19.14	169.56	121.70
1	A	28	ASP	CA-C-N	-18.77	75.90	117.20
1	A	408	ASP	CA-C-N	17.59	155.89	117.20
1	B	406	GLU	O-C-N	16.65	149.34	122.70
1	B	406	GLU	CA-C-N	-16.43	81.05	117.20
1	B	406	GLU	C-N-CA	-14.23	86.13	121.70
1	B	248	GLU	OE1-CD-OE2	-13.73	106.83	123.30
1	B	129	HIS	N-CA-CB	13.20	134.35	110.60
1	B	130	PRO	CA-N-CD	-9.15	98.68	111.50
1	B	130	PRO	N-CD-CG	8.87	116.51	103.20
1	A	197	ASN	N-CA-C	8.54	134.06	111.00
1	A	292	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	A	188	LYS	CB-CA-C	-7.19	96.02	110.40
1	A	188	LYS	N-CA-CB	7.00	123.20	110.60
1	A	293	ASN	C-N-CA	-6.85	104.57	121.70
1	A	29	GLN	N-CA-C	6.65	128.94	111.00
1	B	248	GLU	CB-CG-CD	-6.48	96.71	114.20
1	A	188	LYS	CD-CE-NZ	-6.23	97.38	111.70
1	B	291	GLN	C-N-CA	-6.14	106.35	121.70
1	B	129	HIS	C-N-CD	6.05	141.11	128.40
1	A	197	ASN	CA-C-N	-5.96	104.09	117.20
1	B	292	ARG	C-N-CA	5.64	135.79	121.70
1	B	323	GLY	N-CA-C	-5.33	99.76	113.10
1	B	293	ASN	N-CA-C	5.26	125.21	111.00
1	B	291	GLN	O-C-N	5.10	130.87	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	406	GLU	Mainchain
1	A	408	ASP	Peptide
1	B	248	GLU	Sidechain
1	B	406	GLU	Mainchain
1	B	409	SER	Mainchain

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	3281	0	3225	71	0
1	B	3281	0	3226	47	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	204	0	0	12	0
4	B	126	0	0	4	0
All	All	6916	0	6451	110	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 (110) 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:B:443:LYS:CD	1:B:443:LYS:CE	1.77	1.59
1:A:188:LYS:CB	1:A:188:LYS:CG	1.80	1.54
1:A:197:ASN:CA	1:A:197:ASN:CB	1.83	1.54
1:B:293:ASN:C	1:B:294:ASP:N	1.71	1.40
1:A:293:ASN:C	1:A:294:ASP:N	1.74	1.38
1:A:197:ASN:CB	1:A:197:ASN:CG	1.92	1.37
1:A:29:GLN:CA	1:A:29:GLN:N	2.12	1.13
1:A:28:ASP:C	1:A:29:GLN:CA	2.27	1.03
1:A:226:ARG:HD2	4:A:575:HOH:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ASP:C	1:A:29:GLN:HA	1.97	0.86
1:A:29:GLN:N	1:B:428:ASN:OD1	2.08	0.85
1:B:443:LYS:CE	1:B:443:LYS:CG	2.52	0.81
1:A:197:ASN:CB	1:A:197:ASN:ND2	2.46	0.76
1:A:293:ASN:C	1:A:294:ASP:CA	2.54	0.76
1:B:446:LEU:HB3	1:B:448:LEU:HD13	1.66	0.75
1:A:5:PRO:HG3	4:A:541:HOH:O	1.85	0.75
1:A:449:LYS:HA	4:A:479:HOH:O	1.87	0.75
1:A:92:LYS:HE3	4:A:572:HOH:O	1.86	0.74
1:A:446:LEU:HB3	1:A:448:LEU:HD13	1.70	0.73
1:A:292:ARG:O	1:A:293:ASN:HB2	1.88	0.72
1:B:408:ASP:OD1	1:B:409:SER:N	2.23	0.72
1:A:188:LYS:CB	1:A:188:LYS:CD	2.66	0.71
1:A:382:LYS:HD2	1:B:407:GLU:OE2	1.90	0.71
1:B:293:ASN:C	1:B:294:ASP:CA	2.60	0.70
1:A:188:LYS:CG	1:A:188:LYS:CA	2.71	0.68
1:A:23:ARG:HD3	1:B:440:TYR:CD1	2.28	0.67
1:B:293:ASN:HB3	1:B:295:SER:H	1.60	0.67
1:A:197:ASN:CB	1:A:197:ASN:C	2.61	0.67
1:B:443:LYS:CD	1:B:443:LYS:NZ	2.54	0.66
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.79	0.64
1:B:365:ILE:HD13	1:B:438:LEU:HD11	1.82	0.62
1:A:288:PRO:HB3	1:A:292:ARG:NH2	2.17	0.60
1:B:359:GLU:HG3	1:B:361:ASN:H	1.67	0.60
1:A:293:ASN:HB3	1:A:296:VAL:H	1.67	0.59
1:A:359:GLU:HG3	1:A:361:ASN:H	1.67	0.59
1:A:23:ARG:HD2	4:B:523:HOH:O	2.03	0.59
1:B:293:ASN:CA	1:B:294:ASP:N	2.65	0.58
1:B:154:ALA:HB3	4:B:473:HOH:O	2.04	0.58
1:A:16:ILE:HG22	1:B:89:LEU:HD21	1.87	0.57
1:A:291:GLN:HG2	4:A:659:HOH:O	2.04	0.57
1:B:15:ASP:O	1:B:21:GLY:HA3	2.06	0.55
1:A:89:LEU:HD21	1:B:16:ILE:HG22	1.89	0.55
1:A:289:ASN:O	1:A:292:ARG:HG2	2.07	0.54
1:A:28:ASP:O	1:A:29:GLN:HA	2.08	0.53
1:A:168:CYS:SG	1:A:177:LYS:HB2	2.49	0.53
1:A:287:THR:HG22	4:A:462:HOH:O	2.09	0.52
1:B:168:CYS:SG	1:B:177:LYS:HB2	2.50	0.52
1:B:359:GLU:HG2	1:B:362:THR:OG1	2.11	0.51
1:B:5:PRO:HB3	4:B:484:HOH:O	2.11	0.51
1:A:199:ARG:HA	1:A:234:TYR:OH	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASN:CB	1:A:197:ASN:N	2.60	0.50
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.93	0.49
1:B:199:ARG:HA	1:B:234:TYR:OH	2.11	0.49
1:A:293:ASN:CA	1:A:294:ASP:N	2.72	0.49
1:B:149:ALA:HB2	1:B:324:ALA:CB	2.42	0.49
1:A:440:TYR:CD2	1:B:23:ARG:HD3	2.47	0.49
4:A:645:HOH:O	1:B:17:THR:HG21	2.12	0.49
1:A:15:ASP:O	1:A:21:GLY:HA3	2.13	0.49
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.43	0.49
1:A:359:GLU:HG2	1:A:362:THR:OG1	2.13	0.48
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.95	0.48
1:B:103:ALA:HB1	1:B:119:ALA:O	2.13	0.48
1:B:7:LEU:HD12	4:B:487:HOH:O	2.13	0.48
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.94	0.48
1:A:449:LYS:CA	4:A:479:HOH:O	2.55	0.48
1:B:78:LEU:HB2	1:B:420:ALA:HB1	1.96	0.48
1:A:234:TYR:HA	1:A:254:PRO:HG2	1.96	0.48
1:A:23:ARG:HD3	1:B:440:TYR:CG	2.49	0.47
1:A:123:ASP:HB2	4:A:493:HOH:O	2.15	0.47
1:A:174:THR:HG23	1:A:178:CYS:HB2	1.97	0.46
1:A:48:LEU:HG	1:A:349:VAL:HG22	1.98	0.46
1:B:289:ASN:O	1:B:292:ARG:HG2	2.14	0.46
1:B:137:LYS:HE3	1:B:198:ALA:O	2.16	0.46
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.98	0.46
1:A:78:LEU:HB2	1:A:420:ALA:HB1	1.98	0.46
1:B:291:GLN:O	1:B:293:ASN:ND2	2.48	0.46
1:B:111:THR:OG1	1:B:113:VAL:HG12	2.16	0.46
1:B:449:LYS:H	1:B:449:LYS:HD3	1.80	0.46
1:B:407:GLU:HB3	1:B:408:ASP:H	1.55	0.45
1:B:426:ALA:O	1:B:429:VAL:HG22	2.16	0.45
1:B:234:TYR:HA	1:B:254:PRO:HG2	1.97	0.45
1:B:379:PRO:HA	1:B:399:VAL:CG2	2.47	0.45
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.47	0.45
1:A:426:ALA:O	1:A:429:VAL:HG22	2.17	0.44
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.98	0.44
1:A:280:ASP:HA	4:A:647:HOH:O	2.17	0.44
1:A:16:ILE:CG2	1:B:89:LEU:HD21	2.47	0.43
1:A:337:GLY:O	1:A:341:GLU:HG2	2.18	0.43
1:B:33:LEU:HD23	1:B:33:LEU:HA	1.89	0.43
1:A:292:ARG:HG3	1:A:293:ASN:H	1.84	0.43
1:A:402:TYR:HB3	1:A:410:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HE2	1:A:251:GLN:OE1	2.19	0.43
1:B:374:SER:HB3	1:B:402:TYR:CE2	2.53	0.43
1:A:103:ALA:HB1	1:A:119:ALA:O	2.19	0.43
1:A:208:ALA:HB1	1:A:226:ARG:HH12	1.84	0.43
1:A:291:GLN:NE2	4:A:505:HOH:O	2.52	0.42
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.55	0.42
1:A:137:LYS:HE3	1:A:198:ALA:O	2.19	0.42
1:A:78:LEU:HA	1:A:79:PRO:HD2	1.95	0.42
1:B:45:ILE:HD12	1:B:446:LEU:HD22	2.00	0.41
1:A:374:SER:HB3	1:A:402:TYR:CE2	2.55	0.41
1:A:292:ARG:HG3	1:A:293:ASN:N	2.34	0.41
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.87	0.41
1:A:111:THR:OG1	1:A:113:VAL:HG12	2.20	0.41
1:A:292:ARG:NH2	3:A:457:PO4:O1	2.54	0.41
1:A:100:THR:HG22	4:A:652:HOH:O	2.20	0.41
1:A:449:LYS:H	1:A:449:LYS:HD3	1.86	0.41
1:B:297:PRO:HA	1:B:301:GLN:OE1	2.21	0.41
1:B:337:GLY:O	1:B:341:GLU:HG2	2.21	0.40
1:A:434:ASP:O	1:A:437:ASP:HB2	2.21	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	444/446 (100%)	428 (96%)	15 (3%)	1 (0%)	47 39
1	B	444/446 (100%)	430 (97%)	12 (3%)	2 (0%)	29 18
All	All	888/892 (100%)	858 (97%)	27 (3%)	3 (0%)	41 31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	ASN
1	B	407	GLU
1	A	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%)	323 (96%)	14 (4%)	30	22
1	B	337/337 (100%)	324 (96%)	13 (4%)	32	25
All	All	674/674 (100%)	647 (96%)	27 (4%)	31	24

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	37	LEU
1	A	47	LEU
1	A	84	TYR
1	A	151	LEU
1	A	255	LEU
1	A	304	ASP
1	A	310	LEU
1	A	314	GLU
1	A	372	HIS
1	A	386	LEU
1	A	411	GLU
1	A	446	LEU
1	A	449	LYS
1	B	7	LEU
1	B	37	LEU
1	B	47	LEU
1	B	84	TYR
1	B	151	LEU
1	B	255	LEU
1	B	310	LEU

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Mol	Chain	Res	Type
1	B	314	GLU
1	B	372	HIS
1	B	386	LEU
1	B	411	GLU
1	B	446	LEU
1	B	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	GLN
1	B	291	GLN
1	B	425	HIS

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 8 ligands modelled in this entry, 4 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	A	457	-	4,4,4	1.26	0	6,6,6	0.42	0
3	PO4	B	453	2	4,4,4	1.17	0	6,6,6	0.62	0
3	PO4	B	457	-	4,4,4	1.25	0	6,6,6	0.37	0
3	PO4	A	453	2	4,4,4	1.27	0	6,6,6	0.72	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
3	A	457	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	293:ASN	C	294:ASP	N	1.74
1	B	293:ASN	C	294:ASP	N	1.71
1	A	28:ASP	C	29:GLN	N	1.61
1	A	406:GLU	C	407:GLU	N	0.90
1	B	406:GLU	C	407:GLU	N	0.89

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.