



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:37 PM UTC

PDB ID : 1ANI / pdb_00001ani
Title : ALKALINE PHOSPHATASE (D153H, K328H)
Authors : Murphy, J.E.; Tibbitts, T.T.; Kantrowitz, E.R.
Deposited on : 1995-09-06
Resolution : 2.50 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

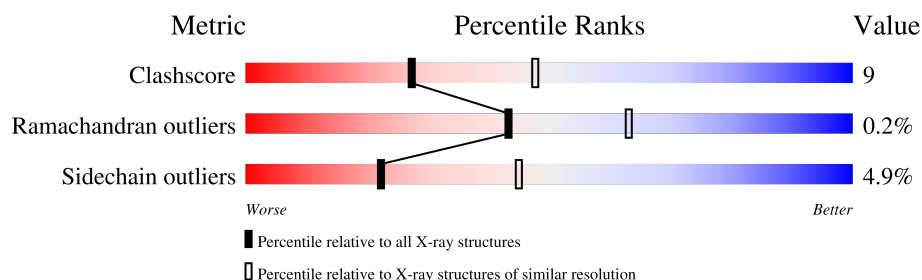
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	
1	B	446	

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	B	453	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6869 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	C	N	O	S	0	0	0
			3284	2030	581	661	12			
1	B	446	Total	C	N	O	S	0	0	0
			3284	2030	581	661	12			

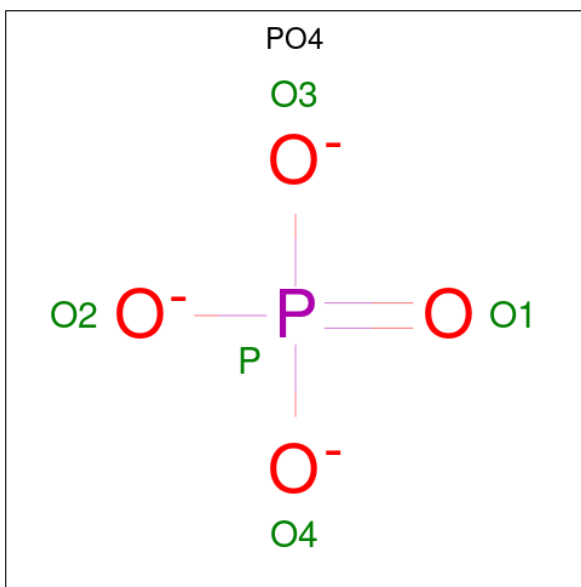
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	HIS	ASP	engineered mutation	UNP P00634
A	328	HIS	LYS	engineered mutation	UNP P00634
B	153	HIS	ASP	engineered mutation	UNP P00634
B	328	HIS	LYS	engineered mutation	UNP P00634

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

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

- Molecule 4 is water.

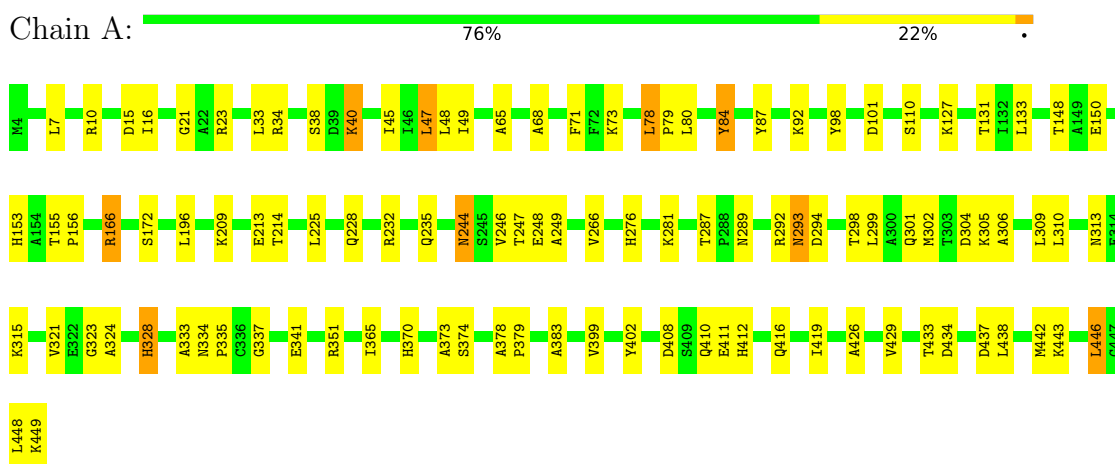
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	137	Total	O	0	0
			137	137		

3 Residue-property plots

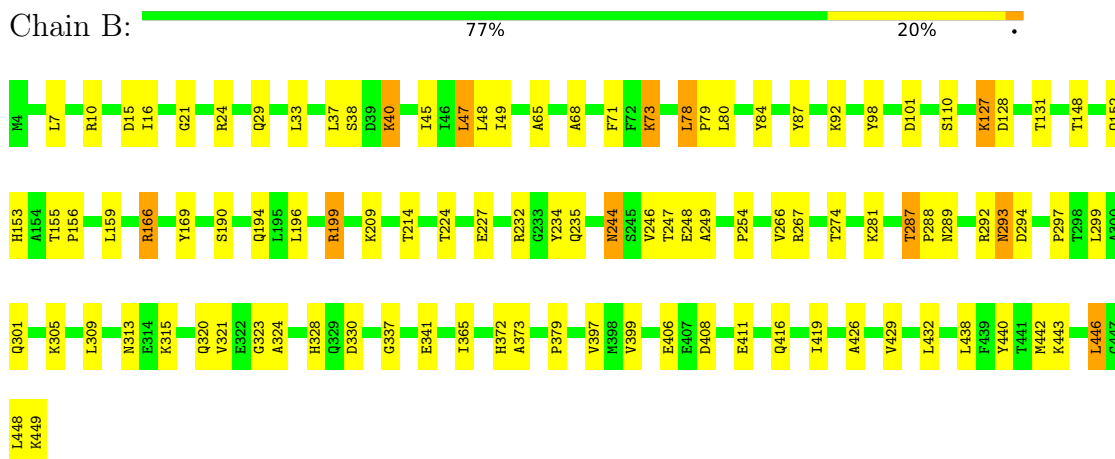
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• Molecule 1: ALKALINE PHOSPHATASE



4 Data and refinement statistics

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	194.60Å 167.30Å 76.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	91.0 (8.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1, IMPLOR, POLYVISION, TIBBITTS	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6869	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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, 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	0.85	5/3340 (0.1%)	1.10	18/4534 (0.4%)
1	B	0.83	5/3340 (0.1%)	1.12	21/4534 (0.5%)
All	All	0.84	10/6680 (0.1%)	1.11	39/9068 (0.4%)

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	1	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	HIS	CD2-NE2	-9.59	1.27	1.37
1	B	328	HIS	CD2-NE2	-9.52	1.27	1.37
1	B	287	THR	CA-C	-7.42	1.43	1.52
1	A	328	HIS	ND1-CE1	-7.15	1.25	1.32
1	B	328	HIS	ND1-CE1	-6.81	1.25	1.32
1	B	287	THR	CA-CB	-6.74	1.44	1.53
1	A	370	HIS	CD2-NE2	6.28	1.44	1.37
1	A	302	MET	SD-CE	5.46	1.93	1.79
1	A	412	HIS	CG-CD2	5.14	1.41	1.35
1	B	287	THR	CB-OG1	5.04	1.51	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	ALA	N-CA-C	9.58	121.49	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ALA	N-CA-C	9.17	121.21	111.03
1	B	324	ALA	N-CA-C	8.93	120.70	110.97
1	B	287	THR	CA-CB-CG2	8.22	124.47	110.50
1	A	373	ALA	N-CA-C	8.21	120.01	111.14
1	A	294	ASP	N-CA-C	-7.04	104.85	113.50
1	B	294	ASP	N-CA-C	-6.90	105.01	113.50
1	B	98	TYR	N-CA-C	6.32	120.55	112.34
1	A	98	TYR	N-CA-C	6.32	120.55	112.34
1	B	287	THR	OG1-CB-CG2	6.28	121.85	109.30
1	B	199	ARG	N-CA-C	6.07	118.02	110.91
1	B	411	GLU	N-CA-C	5.78	118.97	110.59
1	B	65	ALA	N-CA-C	5.77	119.50	112.23
1	A	411	GLU	N-CA-C	5.76	118.94	110.59
1	A	334	ASN	CA-C-N	5.67	125.14	119.24
1	A	334	ASN	C-N-CA	5.67	125.14	119.24
1	A	323	GLY	N-CA-C	-5.65	99.78	113.18
1	A	78	LEU	CA-C-N	5.65	125.00	118.85
1	A	78	LEU	C-N-CA	5.65	125.00	118.85
1	A	416	GLN	N-CA-C	-5.62	103.11	110.53
1	B	323	GLY	N-CA-C	-5.43	100.31	113.18
1	A	16	ILE	CB-CA-C	-5.41	104.16	112.05
1	A	281	LYS	CA-C-N	5.40	125.37	120.03
1	A	281	LYS	C-N-CA	5.40	125.37	120.03
1	B	372	HIS	N-CA-C	5.36	115.37	108.34
1	B	419	ILE	N-CA-C	-5.35	100.94	108.27
1	B	397	VAL	N-CA-C	5.34	115.99	108.36
1	A	293	ASN	N-CA-C	5.30	122.08	110.80
1	A	419	ILE	N-CA-C	-5.29	100.45	108.17
1	B	293	ASN	N-CA-C	5.28	122.04	110.80
1	B	416	GLN	N-CA-C	-5.28	103.57	110.53
1	B	287	THR	CA-C-N	5.26	125.18	119.76
1	B	287	THR	C-N-CA	5.26	125.18	119.76
1	A	65	ALA	N-CA-C	5.20	118.78	112.23
1	B	78	LEU	CA-C-N	5.17	124.49	118.85
1	B	78	LEU	C-N-CA	5.17	124.49	118.85
1	A	374	SER	N-CA-C	5.10	117.87	110.42
1	B	330	ASP	N-CA-C	-5.07	105.83	111.36
1	B	287	THR	CB-CA-C	-5.01	101.27	108.84

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
1	B	287	THR	CB

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	3284	0	3222	60	0
1	B	3284	0	3223	64	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	15	0	0	1	0
3	B	10	0	0	3	0
4	A	133	0	0	4	0
4	B	137	0	0	5	0
All	All	6869	0	6445	118	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 9.

All (118) 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:172:SER:HB2	4:A:502:HOH:O	1.67	0.94
1:B:244:ASN:HA	1:B:305:LYS:NZ	1.93	0.84
1:A:244:ASN:HA	1:A:305:LYS:NZ	1.94	0.81
1:B:47:LEU:HD23	1:B:442:MET:SD	2.25	0.76
1:A:101:ASP:HB2	3:A:453:PO4:O3	1.87	0.75
1:A:47:LEU:HD23	1:A:442:MET:SD	2.30	0.71
1:A:266:VAL:HG23	4:A:548:HOH:O	1.91	0.68
1:B:7:LEU:HD12	4:B:571:HOH:O	1.92	0.68
1:B:38:SER:OG	1:B:40:LYS:HD2	1.98	0.63
1:A:38:SER:OG	1:A:40:LYS:HD2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:HIS:C	1:A:328:HIS:CD2	2.77	0.63
1:A:155:THR:HB	1:A:156:PRO:HD3	1.80	0.62
1:A:228:GLN:O	1:A:232:ARG:HG2	2.00	0.62
1:B:287:THR:HG23	1:B:288:PRO:O	2.00	0.62
1:A:443:LYS:HG3	1:A:448:LEU:HB3	1.82	0.61
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.81	0.60
1:B:155:THR:HB	1:B:156:PRO:HD3	1.84	0.59
1:B:249:ALA:HB2	1:B:309:LEU:HD13	1.85	0.58
1:B:101:ASP:HB2	3:B:453:PO4:O3	2.03	0.58
1:B:244:ASN:HA	1:B:305:LYS:HZ1	1.68	0.57
1:A:249:ALA:HB2	1:A:309:LEU:HD13	1.86	0.57
1:B:443:LYS:HG3	1:B:448:LEU:HB3	1.84	0.57
1:B:10:ARG:HB2	1:B:71:PHE:CE1	2.41	0.56
1:A:426:ALA:O	1:A:429:VAL:HG22	2.06	0.56
1:A:235:GLN:HB2	4:A:558:HOH:O	2.06	0.55
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.88	0.55
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.88	0.55
1:A:10:ARG:HD2	1:B:432:LEU:O	2.07	0.55
1:B:152:GLN:HB2	1:B:169:TYR:CE2	2.42	0.55
1:B:266:VAL:HG23	4:B:569:HOH:O	2.06	0.54
1:B:80:LEU:HD12	1:B:426:ALA:HB3	1.88	0.54
1:B:148:THR:HG23	1:B:299:LEU:HD13	1.90	0.53
1:B:199:ARG:NH2	1:B:232:ARG:O	2.41	0.52
1:A:148:THR:HG23	1:A:299:LEU:HD13	1.91	0.52
1:B:153:HIS:O	1:B:156:PRO:HD2	2.09	0.52
1:B:426:ALA:O	1:B:429:VAL:HG22	2.09	0.52
1:A:244:ASN:HA	1:A:305:LYS:HZ1	1.75	0.51
1:B:249:ALA:HB3	1:B:309:LEU:HB3	1.92	0.51
1:A:45:ILE:HG13	1:A:446:LEU:HD13	1.92	0.51
1:A:80:LEU:HD12	1:A:426:ALA:HB3	1.93	0.50
1:A:328:HIS:C	1:A:328:HIS:HD2	2.17	0.50
1:A:289:ASN:O	1:A:292:ARG:HG2	2.13	0.49
1:A:249:ALA:HB3	1:A:309:LEU:HB3	1.94	0.49
1:B:7:LEU:HD21	1:B:79:PRO:HA	1.94	0.49
1:A:328:HIS:HD2	1:A:328:HIS:O	1.95	0.49
1:B:166:ARG:NH2	3:B:453:PO4:O4	2.46	0.49
1:B:365:ILE:HD13	1:B:438:LEU:HD11	1.94	0.49
1:B:313:ASN:OD1	1:B:315:LYS:HB2	2.13	0.48
1:B:305:LYS:HD2	1:B:305:LYS:HA	1.69	0.48
1:A:10:ARG:HB2	1:A:71:PHE:CE1	2.49	0.47
1:B:159:LEU:HD11	1:B:320:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:GLN:HE22	1:B:246:VAL:HG13	1.79	0.47
1:A:40:LYS:HE2	1:A:40:LYS:HB3	1.69	0.47
1:A:68:ALA:HB1	1:B:87:TYR:CD2	2.49	0.47
1:B:40:LYS:HE2	1:B:40:LYS:HB3	1.68	0.47
1:A:84:TYR:HA	1:A:433:THR:O	2.15	0.47
1:A:438:LEU:O	1:A:442:MET:HG3	2.14	0.47
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.95	0.47
1:A:305:LYS:HA	1:A:305:LYS:HD2	1.66	0.47
1:A:304:ASP:OD2	1:A:351:ARG:HD2	2.14	0.46
1:A:153:HIS:O	1:A:156:PRO:HD2	2.15	0.46
1:B:33:LEU:HD12	1:B:33:LEU:HA	1.78	0.46
1:A:101:ASP:OD2	1:A:166:ARG:NH1	2.49	0.46
1:A:383:ALA:HB1	4:A:572:HOH:O	2.15	0.46
1:B:235:GLN:NE2	1:B:246:VAL:HG13	2.31	0.46
1:A:298:THR:OG1	1:A:301:GLN:HG3	2.16	0.46
1:A:333:ALA:O	1:A:335:PRO:HD3	2.16	0.46
1:B:29:GLN:HG3	4:B:477:HOH:O	2.16	0.45
1:A:23:ARG:HD2	1:B:440:TYR:CD2	2.52	0.45
1:A:448:LEU:HD12	1:A:448:LEU:HA	1.74	0.45
1:B:289:ASN:O	1:B:292:ARG:HD3	2.16	0.45
1:B:10:ARG:HB2	1:B:71:PHE:CD1	2.52	0.45
1:A:235:GLN:NE2	1:A:246:VAL:HG13	2.31	0.44
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.81	0.44
1:A:78:LEU:HA	1:A:79:PRO:HD2	1.89	0.44
1:B:15:ASP:O	1:B:21:GLY:HA3	2.17	0.44
1:B:110:SER:O	1:B:131:THR:HA	2.16	0.44
1:B:234:TYR:CD1	1:B:254:PRO:HG2	2.53	0.44
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.99	0.44
1:B:10:ARG:O	1:B:24:ARG:HD3	2.18	0.43
1:B:446:LEU:HD12	1:B:446:LEU:HA	1.85	0.43
1:A:213:GLU:O	1:A:225:LEU:HD12	2.18	0.43
1:A:434:ASP:O	1:A:437:ASP:HB2	2.18	0.43
1:B:274:THR:HG21	1:B:281:LYS:HD2	2.00	0.43
1:A:402:TYR:HB3	1:A:410:GLN:HG3	2.01	0.43
1:A:244:ASN:HA	1:A:305:LYS:HZ2	1.78	0.43
1:B:244:ASN:HA	1:B:305:LYS:HZ2	1.79	0.43
1:A:84:TYR:C	1:A:84:TYR:CD1	2.97	0.43
1:B:337:GLY:O	1:B:341:GLU:HG2	2.19	0.43
1:A:313:ASN:OD1	1:A:315:LYS:HB2	2.19	0.42
1:B:127:LYS:HD2	1:B:128:ASP:O	2.19	0.42
1:B:199:ARG:HA	1:B:234:TYR:OH	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:PRO:HA	1:B:301:GLN:OE1	2.20	0.42
1:B:267:ARG:HG3	4:B:524:HOH:O	2.20	0.42
1:A:34:ARG:HG3	1:B:37:LEU:HD23	2.00	0.42
1:A:47:LEU:HD12	1:A:49:ILE:HG12	2.01	0.42
1:A:15:ASP:O	1:A:21:GLY:HA3	2.20	0.42
1:A:110:SER:O	1:A:131:THR:HA	2.20	0.41
1:B:47:LEU:HD12	1:B:49:ILE:HG12	2.01	0.41
1:B:190:SER:O	1:B:194:GLN:HG3	2.20	0.41
1:A:7:LEU:HD21	1:A:79:PRO:HA	2.01	0.41
1:A:276:HIS:HE1	1:B:406:GLU:OE1	2.02	0.41
1:B:16:ILE:HG12	4:B:509:HOH:O	2.20	0.41
1:A:87:TYR:CD1	1:B:68:ALA:HB1	2.56	0.41
1:A:306:ALA:O	1:A:310:LEU:HB2	2.21	0.41
1:B:73:LYS:N	1:B:73:LYS:HD3	2.35	0.41
1:B:224:THR:OG1	1:B:227:GLU:HG3	2.20	0.41
1:B:45:ILE:HG13	1:B:446:LEU:HD13	2.02	0.41
1:B:287:THR:HA	1:B:288:PRO:HD3	1.86	0.41
1:B:33:LEU:O	1:B:37:LEU:HD13	2.20	0.40
1:B:166:ARG:NH2	3:B:453:PO4:P	2.94	0.40
1:A:150:GLU:O	1:A:153:HIS:HB3	2.21	0.40
1:A:133:LEU:HD23	1:A:133:LEU:C	2.46	0.40
1:A:337:GLY:O	1:A:341:GLU:HG2	2.21	0.40
1:A:378:ALA:HA	1:A:379:PRO:HD3	1.97	0.40
1:B:78:LEU:HA	1:B:79:PRO:HD2	1.88	0.40
1:B:78:LEU:HD12	1:B:78:LEU:H	1.86	0.40
1:B:379:PRO:HA	1:B:399:VAL:CG2	2.52	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%)	431 (97%)	12 (3%)	1 (0%)	43	63
1	B	444/446 (100%)	431 (97%)	12 (3%)	1 (0%)	43	63
All	All	888/892 (100%)	862 (97%)	24 (3%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

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

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	337/337 (100%)	320 (95%)	17 (5%)	22	44
1	B	337/337 (100%)	321 (95%)	16 (5%)	23	47
All	All	674/674 (100%)	641 (95%)	33 (5%)	22	45

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	47	LEU
1	A	73	LYS
1	A	84	TYR
1	A	92	LYS
1	A	127	LYS
1	A	166	ARG
1	A	196	LEU
1	A	209	LYS
1	A	214	THR
1	A	244	ASN
1	A	247	THR
1	A	248	GLU
1	A	287	THR

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Mol	Chain	Res	Type
1	A	408	ASP
1	A	446	LEU
1	A	449	LYS
1	B	40	LYS
1	B	47	LEU
1	B	73	LYS
1	B	84	TYR
1	B	92	LYS
1	B	127	LYS
1	B	166	ARG
1	B	196	LEU
1	B	209	LYS
1	B	214	THR
1	B	244	ASN
1	B	247	THR
1	B	248	GLU
1	B	408	ASP
1	B	446	LEU
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	13	GLN
1	A	276	HIS
1	A	291	GLN
1	A	328	HIS
1	A	329	GLN
1	A	388	GLN
1	A	391	ASN
1	B	13	GLN
1	B	235	GLN
1	B	251	GLN
1	B	276	HIS
1	B	329	GLN
1	B	375	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 [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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	457	-	4,4,4	2.05	2 (50%)	6,6,6	0.58	0
3	PO4	A	458	-	4,4,4	1.72	1 (25%)	6,6,6	1.31	1 (16%)
3	PO4	B	453	2	4,4,4	1.97	2 (50%)	6,6,6	1.11	0
3	PO4	A	457	-	4,4,4	1.72	1 (25%)	6,6,6	0.81	0
3	PO4	A	453	-	4,4,4	2.67	3 (75%)	6,6,6	1.06	0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	453	PO4	P-O3	-3.76	1.43	1.54
3	B	457	PO4	P-O1	-2.74	1.44	1.50
3	A	453	PO4	P-O2	-2.67	1.46	1.54
3	B	457	PO4	P-O2	-2.66	1.46	1.54
3	A	458	PO4	P-O4	-2.50	1.47	1.54
3	A	453	PO4	P-O4	-2.49	1.47	1.54
3	B	453	PO4	P-O4	-2.41	1.47	1.54
3	A	457	PO4	P-O2	-2.21	1.48	1.54
3	B	453	PO4	P-O3	-2.20	1.48	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	458	PO4	O4-P-O3	-2.06	101.49	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	453	PO4	3	0
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

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.