



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:36 PM UTC

PDB ID : 1AJC / pdb_00001ajc
Title : THREE-DIMENSIONAL STRUCTURE OF THE D153G MUTANT OF E. COLI ALKALINE PHOSPHATASE: A MUTANT WITH WEAKER MAGNESIUM BINDING AND INCREASED CATALYTIC ACTIVITY
Authors : Dealwis, C.G.; Chen, L.; Abad-Zapatero, C.
Deposited on : 1995-07-18
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
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

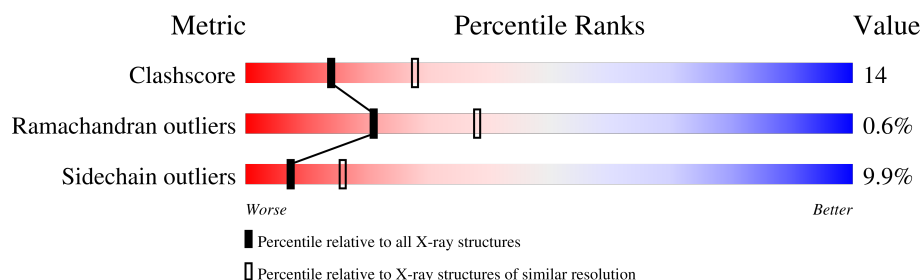
1 Overall quality at a glance

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	449	 68% 26% 6%
1	B	449	 69% 26% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6585 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
			3276	2027	577	660	12			
1	B	449	Total	C	N	O	S	0	0	0
			3300	2040	580	668	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	ASP	engineered mutation	UNP P00634
A	230	GLU	GLN	conflict	UNP P00634
B	153	GLY	ASP	engineered mutation	UNP P00634
B	230	GLU	GLN	conflict	UNP P00634

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

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

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

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

- Molecule 4 is water.

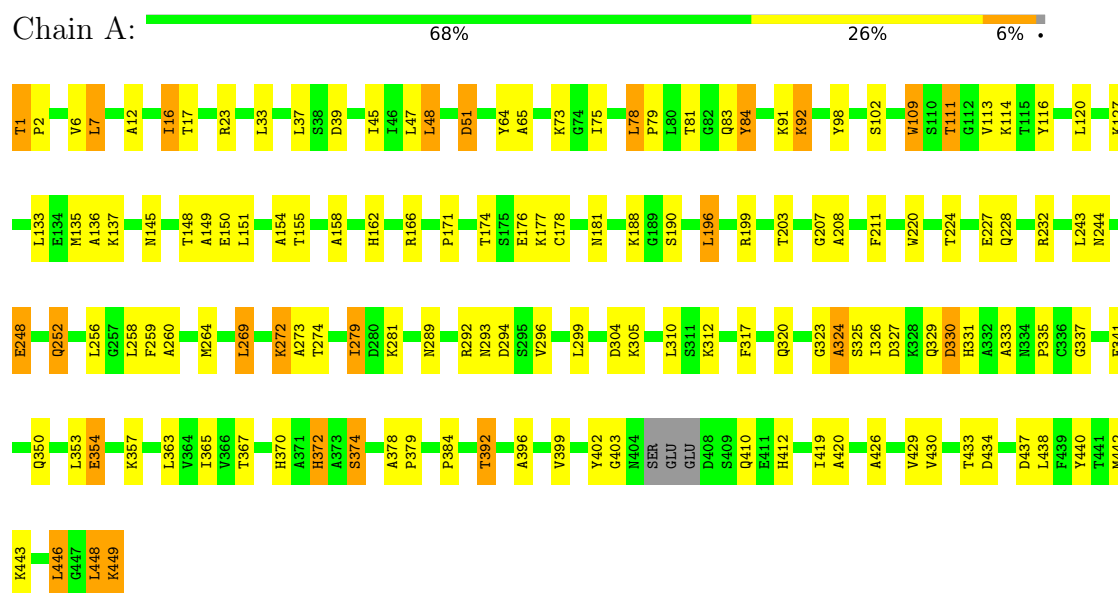
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

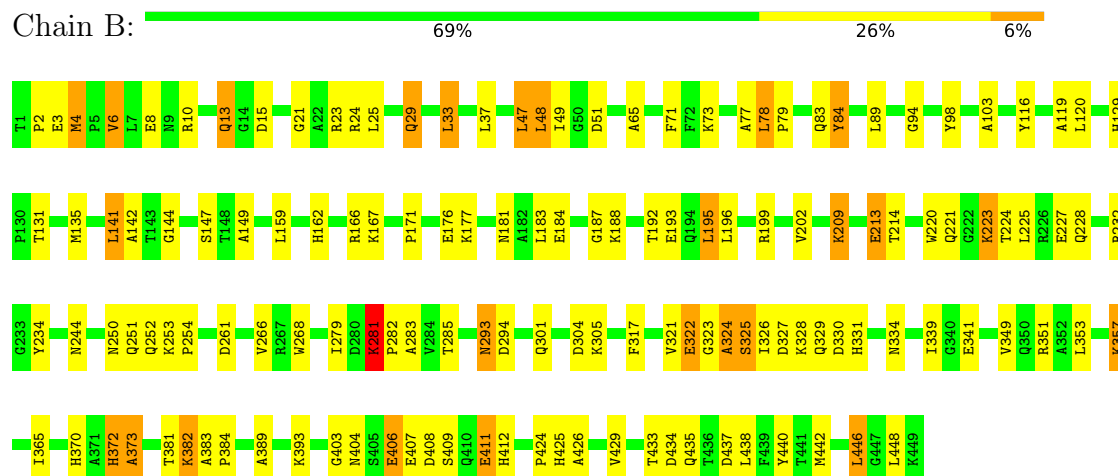
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• 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	195.02Å 166.93Å 76.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6585	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: ZN, MG

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	0.55	0/3330	1.04	16/4519 (0.4%)
1	B	0.52	0/3355	1.06	19/4554 (0.4%)
All	All	0.53	0/6685	1.05	35/9073 (0.4%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	ALA	N-CA-C	10.60	122.58	111.14
1	A	325	SER	N-CA-C	7.60	121.98	112.87
1	B	78	LEU	CA-C-N	7.54	127.42	119.05
1	B	78	LEU	C-N-CA	7.54	127.42	119.05
1	A	294	ASP	N-CA-C	-7.18	104.55	113.38
1	B	325	SER	N-CA-C	7.08	121.01	112.38
1	B	285	THR	N-CA-C	-6.80	97.82	108.90
1	A	293	ASN	N-CA-C	6.78	125.24	110.80
1	B	411	GLU	N-CA-C	6.60	118.53	110.41
1	B	381	THR	N-CA-C	6.49	119.69	109.96
1	A	98	TYR	N-CA-C	6.35	120.59	112.34
1	B	65	ALA	N-CA-C	6.34	119.18	111.82
1	B	323	GLY	N-CA-C	-6.23	98.42	113.18
1	A	378	ALA	CA-C-N	6.22	125.71	119.24
1	A	378	ALA	C-N-CA	6.22	125.71	119.24
1	A	75	ILE	N-CA-C	6.13	117.61	110.62
1	A	330	ASP	N-CA-C	-6.10	104.55	111.14
1	A	154	ALA	N-CA-C	6.04	118.36	111.11
1	B	406	GLU	N-CA-C	-5.91	104.55	113.89
1	B	293	ASN	N-CA-C	5.76	123.07	110.80
1	B	13	GLN	N-CA-C	5.73	117.52	111.28
1	B	251	GLN	N-CA-C	5.69	118.26	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ALA	N-CA-C	5.64	118.62	111.69
1	B	94	GLY	N-CA-C	-5.62	107.88	115.36
1	B	281	LYS	CA-C-N	5.57	125.88	119.92
1	B	281	LYS	C-N-CA	5.57	125.88	119.92
1	B	330	ASP	N-CA-C	-5.36	105.51	111.36
1	A	324	ALA	N-CA-C	5.24	119.58	112.04
1	B	373	ALA	N-CA-C	5.24	119.72	113.23
1	A	323	GLY	N-CA-C	-5.21	100.84	113.18
1	A	136	ALA	N-CA-C	-5.20	105.51	111.07
1	A	78	LEU	CA-C-N	5.17	124.61	119.24
1	A	78	LEU	C-N-CA	5.17	124.61	119.24
1	A	317	PHE	N-CA-C	5.02	115.93	108.60
1	B	195	LEU	N-CA-C	-5.01	105.51	110.97

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	3276	0	3228	107	0
1	B	3300	0	3246	95	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	2	0	0	0	0
4	B	1	0	0	1	0
All	All	6585	0	6474	186	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 14.

All (186) 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:51:ASP:OD2	4:B:956:HOH:O	1.77	1.01
1:B:446:LEU:HB3	1:B:448:LEU:HD13	1.52	0.92
1:A:392:THR:HG23	1:A:396:ALA:O	1.71	0.90
1:A:438:LEU:HG	1:A:442:MET:HE2	1.53	0.88
1:A:350:GLN:O	1:A:354:GLU:HG2	1.79	0.82
1:B:301:GLN:O	1:B:305:LYS:HG2	1.79	0.81
1:A:51:ASP:HB3	1:A:327:ASP:HB2	1.70	0.74
1:A:1:THR:N	1:A:2:PRO:HD3	2.08	0.69
1:B:149:ALA:HB2	1:B:324:ALA:HB1	1.76	0.67
1:A:111:THR:HG23	1:A:113:VAL:HG12	1.75	0.67
1:B:51:ASP:HB3	1:B:327:ASP:HB2	1.75	0.66
1:A:16:ILE:CG2	1:B:89:LEU:HD21	2.25	0.66
1:A:403:GLY:O	1:B:384:PRO:HD2	1.97	0.65
1:B:51:ASP:HB3	1:B:327:ASP:CB	2.27	0.65
1:A:83:GLN:HE21	1:B:83:GLN:HE21	1.43	0.64
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.79	0.64
1:B:10:ARG:HB2	1:B:71:PHE:CE1	2.32	0.64
1:A:244:ASN:HA	1:A:305:LYS:HE2	1.81	0.63
1:B:325:SER:HB2	1:B:341:GLU:HG3	1.81	0.62
1:A:449:LYS:N	1:A:449:LYS:HE3	2.15	0.61
1:B:73:LYS:H	1:B:73:LYS:HD2	1.65	0.61
1:A:224:THR:OG1	1:A:227:GLU:HG3	2.01	0.61
1:A:148:THR:HG23	1:A:299:LEU:HD13	1.85	0.59
1:A:228:GLN:O	1:A:232:ARG:HG2	2.03	0.58
1:A:289:ASN:O	1:A:292:ARG:HG2	2.04	0.58
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.85	0.58
1:A:440:TYR:CE2	1:B:23:ARG:HD2	2.39	0.57
1:A:120:LEU:O	1:A:162:HIS:HA	2.03	0.57
1:A:92:LYS:HE3	1:A:92:LYS:HA	1.87	0.57
1:A:434:ASP:O	1:A:437:ASP:HB2	2.07	0.55
1:B:149:ALA:HB2	1:B:324:ALA:CB	2.35	0.55
1:A:23:ARG:HD2	1:B:440:TYR:CD2	2.42	0.55
1:B:6:VAL:HG12	1:B:77:ALA:O	2.07	0.55
1:B:47:LEU:HD22	1:B:49:ILE:HG12	1.87	0.54
1:B:404:ASN:ND2	1:B:411:GLU:HB2	2.22	0.54
1:A:402:TYR:HB3	1:A:410:GLN:HG3	1.90	0.54
1:B:383:ALA:HB1	1:B:384:PRO:HD2	1.89	0.53
1:B:171:PRO:HD2	1:B:213:GLU:HG2	1.90	0.53
1:A:37:LEU:HD21	1:B:33:LEU:HD23	1.91	0.53
1:A:1:THR:H2	1:A:2:PRO:HD3	1.74	0.53
1:B:244:ASN:HD21	1:B:305:LYS:HZ1	1.57	0.52
1:B:426:ALA:O	1:B:429:VAL:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HD22	1:B:193:GLU:OE2	2.09	0.52
1:B:326:ILE:HG13	1:B:341:GLU:HB2	1.92	0.51
1:A:45:ILE:HG12	1:A:363:LEU:HB3	1.92	0.51
1:B:234:TYR:HA	1:B:254:PRO:HG2	1.92	0.51
1:A:333:ALA:O	1:A:335:PRO:HD3	2.10	0.51
1:B:147:SER:OG	1:B:322:GLU:HG2	2.10	0.51
1:B:326:ILE:HG13	1:B:341:GLU:CB	2.40	0.51
1:A:133:LEU:HD23	1:A:133:LEU:C	2.36	0.51
1:A:446:LEU:HB3	1:A:448:LEU:HD13	1.92	0.51
1:B:120:LEU:O	1:B:162:HIS:HA	2.10	0.51
1:B:393:LYS:O	1:B:393:LYS:HG3	2.11	0.50
1:A:51:ASP:O	1:A:327:ASP:HB2	2.12	0.50
1:A:16:ILE:HG23	1:B:89:LEU:HD21	1.94	0.50
1:A:174:THR:HG23	1:A:178:CYS:HB2	1.93	0.50
1:A:174:THR:OG1	1:A:190:SER:HB3	2.11	0.50
1:A:248:GLU:HG2	1:A:312:LYS:NZ	2.27	0.50
1:B:438:LEU:HG	1:B:442:MET:HE2	1.94	0.49
1:A:426:ALA:O	1:A:429:VAL:HG22	2.13	0.49
1:A:392:THR:HG21	1:B:98:TYR:CE2	2.47	0.49
1:B:199:ARG:HA	1:B:234:TYR:OH	2.13	0.49
1:A:430:VAL:HG21	1:B:33:LEU:HD21	1.95	0.49
1:A:269:LEU:HD13	1:A:289:ASN:HB2	1.95	0.49
1:A:292:ARG:O	1:A:296:VAL:HB	2.13	0.49
1:B:181:ASN:C	1:B:187:GLY:HA3	2.37	0.49
1:A:327:ASP:O	1:A:331:HIS:HD2	1.96	0.49
1:B:192:THR:O	1:B:195:LEU:HB3	2.13	0.49
1:B:176:GLU:HG3	1:B:177:LYS:HG3	1.95	0.48
1:B:214:THR:HA	1:B:224:THR:HA	1.96	0.48
1:B:228:GLN:O	1:B:232:ARG:HG3	2.14	0.48
1:A:81:THR:HG22	1:A:420:ALA:HB2	1.96	0.48
1:A:137:LYS:HE3	1:A:199:ARG:O	2.13	0.48
1:B:353:LEU:O	1:B:357:LYS:HB3	2.14	0.48
1:A:326:ILE:O	1:A:330:ASP:HB2	2.13	0.48
1:A:259:PHE:HB2	1:A:264:MET:HE3	1.95	0.47
1:A:208:ALA:HB2	1:A:258:LEU:HB3	1.96	0.47
1:B:10:ARG:HB2	1:B:71:PHE:CD1	2.49	0.47
1:A:150:GLU:HB3	1:A:207:GLY:HA3	1.96	0.47
1:A:135:MET:HE3	1:A:449:LYS:HD3	1.95	0.47
1:A:367:THR:HB	1:A:419:ILE:HG13	1.96	0.47
1:A:384:PRO:HA	1:B:406:GLU:OE2	2.14	0.47
1:A:449:LYS:HE3	1:A:449:LYS:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ALA:HB2	1:B:166:ARG:HD2	1.97	0.47
1:B:327:ASP:OD1	1:B:331:HIS:CD2	2.67	0.47
1:A:113:VAL:HG22	1:A:114:LYS:O	2.15	0.47
1:A:370:HIS:NE2	1:A:412:HIS:CE1	2.83	0.46
1:B:407:GLU:O	1:B:409:SER:N	2.49	0.46
1:A:337:GLY:O	1:A:341:GLU:HG2	2.16	0.46
1:A:45:ILE:HD12	1:A:446:LEU:HD22	1.98	0.46
1:B:48:LEU:HG	1:B:349:VAL:HG22	1.98	0.46
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.46	0.46
1:A:102:SER:HB2	1:A:166:ARG:HH22	1.79	0.46
1:B:15:ASP:O	1:B:21:GLY:HA3	2.16	0.46
1:A:272:LYS:HE3	1:A:272:LYS:HB3	1.57	0.46
1:A:252:GLN:HE21	1:A:252:GLN:H	1.63	0.46
1:A:327:ASP:OD2	1:A:372:HIS:HE1	1.98	0.46
1:B:325:SER:CB	1:B:341:GLU:HG3	2.45	0.46
1:B:370:HIS:CE1	1:B:412:HIS:CE1	3.04	0.46
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.46	0.45
1:B:209:LYS:HD2	1:B:209:LYS:C	2.41	0.45
1:B:141:LEU:HD21	1:B:446:LEU:HG	1.98	0.45
1:A:111:THR:CG2	1:A:113:VAL:HG12	2.44	0.45
1:A:273:ALA:HB3	1:A:333:ALA:HB1	1.98	0.45
1:A:449:LYS:HE3	1:A:449:LYS:CA	2.47	0.45
1:B:373:ALA:HB2	1:B:404:ASN:ND2	2.31	0.45
1:A:1:THR:H3	1:A:2:PRO:HD3	1.80	0.45
1:A:155:THR:HG22	1:A:320:GLN:NE2	2.31	0.45
1:A:392:THR:HG21	1:B:98:TYR:CZ	2.51	0.45
1:B:78:LEU:HA	1:B:79:PRO:HD2	1.83	0.45
1:B:129:HIS:O	1:B:162:HIS:HE1	2.00	0.45
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.52	0.45
1:A:83:GLN:NE2	1:B:83:GLN:HE21	2.13	0.45
1:B:25:LEU:HD22	1:B:29:GLN:NE2	2.32	0.45
1:A:12:ALA:CB	1:A:16:ILE:HD11	2.47	0.45
1:B:328:LYS:O	1:B:331:HIS:HB2	2.16	0.45
1:A:17:THR:HG22	1:B:89:LEU:HD13	1.99	0.45
1:A:84:TYR:O	1:A:84:TYR:HD1	2.00	0.44
1:A:120:LEU:HD22	1:A:158:ALA:HA	1.98	0.44
1:A:384:PRO:HD2	1:B:403:GLY:O	2.17	0.44
1:A:331:HIS:ND1	1:A:410:GLN:O	2.50	0.44
1:B:84:TYR:CE2	1:B:435:GLN:HG3	2.53	0.44
1:A:23:ARG:HD2	1:B:440:TYR:CE2	2.53	0.44
1:A:64:TYR:CD1	1:A:64:TYR:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ASP:O	1:A:331:HIS:CD2	2.71	0.44
1:B:434:ASP:O	1:B:437:ASP:HB2	2.17	0.44
1:A:6:VAL:CG1	1:A:357:LYS:HD3	2.47	0.43
1:B:220:TRP:CZ2	1:B:232:ARG:HG2	2.53	0.43
1:A:327:ASP:CG	1:A:372:HIS:HE1	2.26	0.43
1:B:84:TYR:CZ	1:B:435:GLN:HG3	2.53	0.43
1:A:220:TRP:CZ2	1:A:232:ARG:HD2	2.54	0.43
1:A:6:VAL:HG11	1:A:357:LYS:HD3	2.01	0.43
1:A:327:ASP:OD1	1:A:331:HIS:CD2	2.72	0.43
1:A:176:GLU:HG2	1:A:177:LYS:HG3	1.99	0.43
1:B:365:ILE:HD13	1:B:438:LEU:HD11	2.01	0.43
1:B:279:ILE:HD11	1:B:382:LYS:HE2	2.01	0.43
1:A:438:LEU:O	1:A:442:MET:HG3	2.18	0.43
1:B:327:ASP:OD2	1:B:372:HIS:HE1	2.01	0.43
1:A:1:THR:N	1:A:2:PRO:CD	2.79	0.43
1:A:211:PHE:CE2	1:A:256:LEU:HD21	2.53	0.43
1:A:329:GLN:HG3	1:A:337:GLY:C	2.44	0.43
1:A:145:ASN:O	1:A:203:THR:HA	2.19	0.42
1:B:51:ASP:HB3	1:B:327:ASP:HB3	1.99	0.42
1:B:268:TRP:CZ3	1:B:339:ILE:HG22	2.54	0.42
1:B:244:ASN:ND2	1:B:305:LYS:NZ	2.67	0.42
1:B:279:ILE:CD1	1:B:382:LYS:HE2	2.49	0.42
1:A:91:LYS:HE2	1:A:116:TYR:CZ	2.55	0.42
1:A:149:ALA:HB2	1:A:324:ALA:HB1	2.00	0.42
1:B:142:ALA:O	1:B:317:PHE:HA	2.19	0.42
1:B:329:GLN:HE21	1:B:334:ASN:HB3	1.85	0.42
1:B:244:ASN:HD21	1:B:305:LYS:NZ	2.16	0.42
1:A:259:PHE:O	1:A:260:ALA:HB2	2.20	0.42
1:A:434:ASP:HB2	1:B:24:ARG:HG3	2.01	0.42
1:A:84:TYR:HA	1:A:433:THR:O	2.20	0.42
1:B:223:LYS:HG3	1:B:227:GLU:OE1	2.19	0.42
1:B:281:LYS:HA	1:B:282:PRO:HD3	1.85	0.42
1:B:424:PRO:O	1:B:425:HIS:HB2	2.19	0.42
1:A:84:TYR:C	1:A:84:TYR:CD1	2.98	0.42
1:B:283:ALA:HA	1:B:389:ALA:O	2.19	0.42
1:A:196:LEU:HA	1:A:196:LEU:HD12	1.81	0.42
1:A:48:LEU:HD22	1:A:48:LEU:N	2.35	0.41
1:B:331:HIS:CD2	1:B:372:HIS:CE1	3.08	0.41
1:A:374:SER:HB3	1:A:402:TYR:CE1	2.55	0.41
1:B:4:MET:H	1:B:4:MET:HG3	1.66	0.41
1:A:78:LEU:HA	1:A:79:PRO:HD2	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:TRP:HB2	1:A:438:LEU:HD23	2.02	0.41
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.84	0.41
1:A:448:LEU:O	1:A:449:LYS:HB2	2.20	0.41
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.88	0.41
1:B:131:THR:O	1:B:135:MET:HG3	2.20	0.41
1:B:446:LEU:HD12	1:B:446:LEU:HA	1.92	0.41
1:A:243:LEU:HD22	1:A:259:PHE:CZ	2.56	0.41
1:A:269:LEU:HD13	1:A:289:ASN:CB	2.50	0.41
1:B:221:GLN:C	1:B:223:LYS:H	2.29	0.41
1:A:188:LYS:HE3	1:A:188:LYS:HB2	1.81	0.40
1:B:84:TYR:HA	1:B:433:THR:O	2.21	0.40
1:A:47:LEU:HD12	1:A:365:ILE:HB	2.01	0.40
1:A:279:ILE:H	1:A:279:ILE:HG12	1.79	0.40
1:A:326:ILE:HG13	1:A:341:GLU:HB2	2.04	0.40
1:A:109:TRP:CD1	1:A:109:TRP:C	2.99	0.40
1:A:178:CYS:HB3	1:A:181:ASN:OD1	2.21	0.40
1:B:209:LYS:HB2	1:B:261:ASP:O	2.21	0.40
1:B:73:LYS:HD2	1:B:73:LYS:N	2.34	0.40
1:B:144:GLY:HA2	1:B:202:VAL:O	2.20	0.40
1:B:404:ASN:HD21	1:B:411:GLU:HB2	1.85	0.40
1:B:438:LEU:O	1:B:442:MET:HG3	2.21	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	442/449 (98%)	411 (93%)	30 (7%)	1 (0%)	43	63
1	B	447/449 (100%)	410 (92%)	33 (7%)	4 (1%)	14	27
All	All	889/898 (99%)	821 (92%)	63 (7%)	5 (1%)	21	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	408	ASP
1	B	4	MET
1	A	7	LEU
1	B	293	ASN
1	B	2	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	336/339 (99%)	302 (90%)	34 (10%)	7	15
1	B	339/339 (100%)	306 (90%)	33 (10%)	8	17
All	All	675/678 (100%)	608 (90%)	67 (10%)	7	16

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	7	LEU
1	A	16	ILE
1	A	33	LEU
1	A	39	ASP
1	A	48	LEU
1	A	51	ASP
1	A	73	LYS
1	A	84	TYR
1	A	92	LYS
1	A	109	TRP
1	A	111	THR
1	A	127	LYS
1	A	151	LEU
1	A	171	PRO
1	A	196	LEU
1	A	248	GLU
1	A	252	GLN

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	272	LYS
1	A	274	THR
1	A	279	ILE
1	A	281	LYS
1	A	304	ASP
1	A	310	LEU
1	A	353	LEU
1	A	354	GLU
1	A	372	HIS
1	A	374	SER
1	A	392	THR
1	A	443	LYS
1	A	446	LEU
1	A	448	LEU
1	A	449	LYS
1	B	3	GLU
1	B	6	VAL
1	B	8	GLU
1	B	13	GLN
1	B	29	GLN
1	B	33	LEU
1	B	37	LEU
1	B	47	LEU
1	B	48	LEU
1	B	84	TYR
1	B	141	LEU
1	B	159	LEU
1	B	167	LYS
1	B	184	GLU
1	B	188	LYS
1	B	196	LEU
1	B	209	LYS
1	B	213	GLU
1	B	223	LYS
1	B	225	LEU
1	B	250	ASN
1	B	252	GLN
1	B	253	LYS
1	B	266	VAL
1	B	281	LYS
1	B	294	ASP

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Mol	Chain	Res	Type
1	B	304	ASP
1	B	322	GLU
1	B	351	ARG
1	B	357	LYS
1	B	372	HIS
1	B	382	LYS
1	B	446	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	GLN
1	A	338	GLN
1	A	391	ASN
1	A	410	GLN
1	B	13	GLN
1	B	29	GLN
1	B	83	GLN
1	B	235	GLN
1	B	244	ASN
1	B	250	ASN
1	B	276	HIS
1	B	320	GLN
1	B	329	GLN
1	B	338	GLN
1	B	372	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.