



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:08 PM UTC

PDB ID : 1AJA / pdb_00001aja
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 : 1995-08-19
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

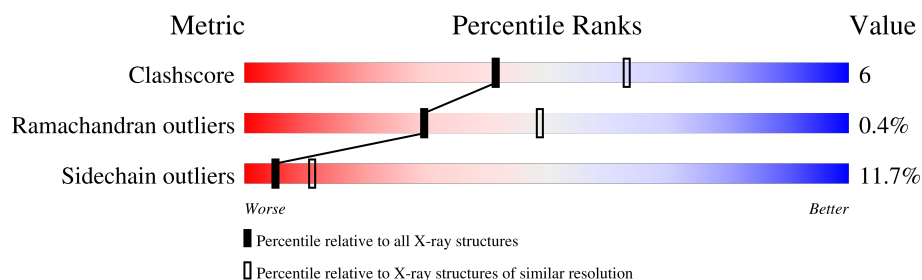
1 Overall quality at a glance

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	
1	B	449	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6352 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	435	Total	C	N	O	S	0	0	0
			3184	1975	560	637	12			
1	B	434	Total	C	N	O	S	0	0	0
			3168	1967	556	633	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

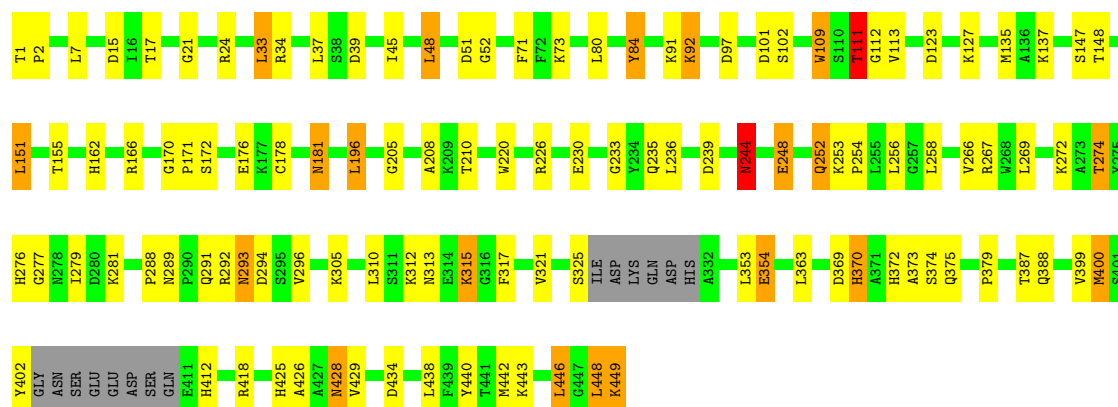
3 Residue-property plots

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.

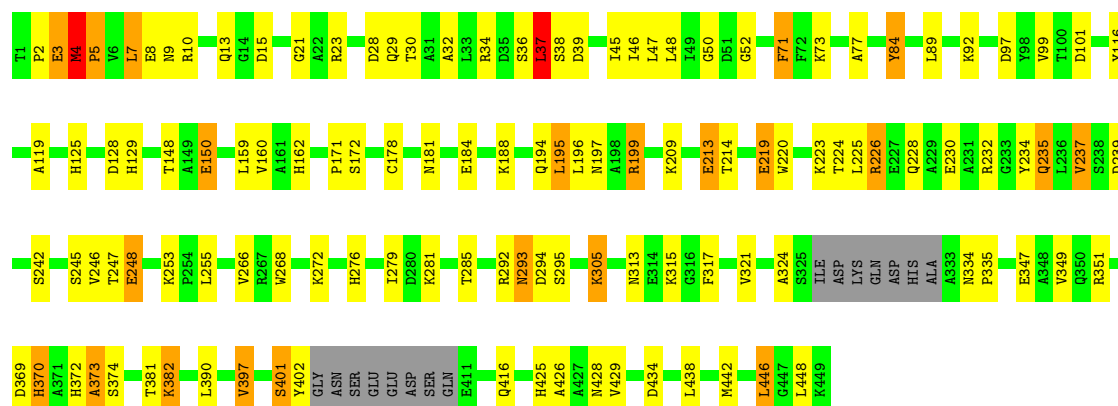
• Molecule 1: ALKALINE PHOSPHATASE

Chain A: 



• Molecule 1: ALKALINE PHOSPHATASE

Chain B: 



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}	0.08	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	6352	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.79	5/3236 (0.2%)	1.61	42/4391 (1.0%)
1	B	0.81	8/3219 (0.2%)	1.62	49/4369 (1.1%)
All	All	0.80	13/6455 (0.2%)	1.62	91/8760 (1.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	425	HIS	CD2-NE2	-7.25	1.29	1.37
1	B	162	HIS	CD2-NE2	-7.21	1.29	1.37
1	A	162	HIS	CD2-NE2	-6.66	1.30	1.37
1	B	370	HIS	CD2-NE2	-6.38	1.30	1.37
1	B	129	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	125	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	370	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	276	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	276	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	372	HIS	CD2-NE2	-5.84	1.31	1.37
1	B	372	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	109	TRP	NE1-CE2	-5.29	1.31	1.37
1	B	129	HIS	CG-ND1	-5.03	1.32	1.38

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	PHE	CA-CB-CG	9.50	123.30	113.80
1	A	244	ASN	CA-CB-CG	-8.70	103.90	112.60
1	A	123	ASP	CA-CB-CG	8.51	121.11	112.60
1	B	381	THR	N-CA-C	8.29	121.93	110.24
1	A	111	THR	N-CA-CB	-8.18	99.71	110.59
1	B	239	ASP	CA-CB-CG	8.12	120.72	112.60
1	A	101	ASP	CA-CB-CG	7.91	120.51	112.60
1	A	369	ASP	CA-CB-CG	7.82	120.42	112.60
1	B	3	GLU	O-C-N	7.55	132.27	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASP	N-CA-C	-7.41	95.05	108.02
1	B	317	PHE	CA-CB-CG	7.37	121.17	113.80
1	B	313	ASN	OD1-CG-ND2	-7.34	115.26	122.60
1	A	425	HIS	CA-CB-CG	-7.22	106.58	113.80
1	B	425	HIS	CB-CG-CD2	-7.17	121.88	131.20
1	B	101	ASP	CA-CB-CG	7.12	119.72	112.60
1	B	162	HIS	CB-CG-CD2	-7.07	122.01	131.20
1	B	228	GLN	OE1-CD-NE2	-6.94	115.66	122.60
1	A	317	PHE	CA-CB-CG	6.80	120.60	113.80
1	A	84	TYR	CA-CB-CG	6.65	125.87	113.90
1	B	334	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	B	293	ASN	N-CA-C	6.63	124.93	110.80
1	A	181	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	B	37	LEU	N-CA-C	6.59	119.02	108.41
1	B	373	ALA	N-CA-C	6.58	121.36	112.88
1	B	39	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	194	GLN	OE1-CD-NE2	-6.46	116.14	122.60
1	A	370	HIS	CA-CB-CG	6.43	120.23	113.80
1	B	370	HIS	CA-CB-CG	6.24	120.04	113.80
1	A	71	PHE	CA-CB-CG	6.19	119.99	113.80
1	B	226	ARG	CB-CG-CD	6.18	125.52	111.30
1	A	39	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	313	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	A	239	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	293	ASN	CB-CA-C	-6.06	98.35	110.42
1	A	354	GLU	CA-CB-CG	5.99	126.08	114.10
1	A	252	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	B	268	TRP	CG-CD2-CE3	5.94	139.84	133.90
1	A	428	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	B	199	ARG	N-CA-C	5.88	119.45	111.17
1	A	162	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	A	388	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	B	285	THR	N-CA-C	-5.74	100.34	109.59
1	A	137	LYS	CG-CD-CE	-5.73	98.11	111.30
1	A	293	ASN	O-C-N	5.72	130.20	122.59
1	B	369	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	111	THR	CB-CA-C	5.67	118.22	109.03
1	A	354	GLU	N-CA-CB	5.66	118.53	110.16
1	B	416	GLN	CG-CD-NE2	5.64	124.87	116.40
1	B	428	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	B	425	HIS	CB-CG-ND1	5.61	131.11	122.70
1	A	325	SER	CA-CB-OG	5.58	122.26	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	CYS	CA-C-N	5.56	125.66	119.32
1	B	178	CYS	C-N-CA	5.56	125.66	119.32
1	B	268	TRP	CE2-CD2-CG	-5.54	100.55	107.20
1	A	294	ASP	N-CA-C	-5.54	106.65	113.41
1	A	291	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	B	220	TRP	CE2-CD2-CG	-5.48	100.63	107.20
1	B	5	PRO	CB-CA-C	-5.48	103.81	110.98
1	A	373	ALA	N-CA-C	5.46	119.64	112.92
1	B	97	ASP	N-CA-C	-5.44	98.33	108.02
1	B	162	HIS	CB-CG-ND1	5.44	130.86	122.70
1	A	354	GLU	CB-CA-C	-5.43	101.62	110.85
1	B	128	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	434	ASP	N-CA-C	-5.33	101.07	109.50
1	B	276	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	A	294	ASP	O-C-N	5.31	129.90	122.36
1	B	84	TYR	CA-CB-CG	5.30	123.44	113.90
1	B	30	THR	N-CA-C	5.29	117.46	111.11
1	A	293	ASN	N-CA-C	5.27	122.02	110.80
1	A	315	LYS	N-CA-C	5.26	119.70	113.28
1	A	418	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	A	220	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	A	24	ARG	N-CA-C	-5.24	106.94	113.38
1	B	181	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	B	46	ILE	N-CA-C	-5.18	100.66	108.12
1	B	99	VAL	N-CA-C	5.18	114.20	106.85
1	B	219	GLU	CA-CB-CG	5.18	124.46	114.10
1	B	324	ALA	CA-C-O	-5.18	114.36	121.98
1	B	7	LEU	CA-C-O	5.18	126.97	121.02
1	B	32	ALA	N-CA-C	-5.13	105.58	111.07
1	A	210	THR	CA-CB-OG1	-5.12	101.91	109.60
1	A	434	ASP	N-CA-C	-5.11	101.77	109.85
1	B	50	GLY	O-C-N	-5.10	119.69	123.61
1	B	129	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	112	GLY	O-C-N	-5.08	115.94	122.39
1	A	267	ARG	N-CA-C	5.08	116.81	111.28
1	A	448	LEU	O-C-N	5.06	129.03	122.81
1	B	416	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	A	170	GLY	CA-C-N	5.01	126.11	119.84
1	A	170	GLY	C-N-CA	5.01	126.11	119.84
1	B	125	HIS	CB-CG-CD2	-5.01	124.69	131.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3184	0	3147	45	0
1	B	3168	0	3133	42	0
All	All	6352	0	6280	81	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 6.

All (81) 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:293:ASN:HB3	1:A:296:VAL:H	1.53	0.73
1:A:315:LYS:HE2	1:A:315:LYS:HA	1.76	0.68
1:B:45:ILE:HD12	1:B:446:LEU:HD22	1.76	0.66
1:A:111:THR:HG22	1:A:113:VAL:H	1.60	0.66
1:A:293:ASN:HB2	1:A:296:VAL:HG23	1.79	0.65
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.79	0.65
1:A:293:ASN:CB	1:A:296:VAL:HG23	2.26	0.64
1:A:102:SER:HB3	1:A:166:ARG:HH12	1.64	0.62
1:A:248:GLU:HG2	1:A:312:LYS:HE2	1.80	0.62
1:B:426:ALA:O	1:B:429:VAL:HG22	2.01	0.61
1:A:111:THR:CG2	1:A:113:VAL:HG12	2.31	0.61
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.85	0.59
1:B:293:ASN:HB3	1:B:295:SER:H	1.67	0.58
1:B:248:GLU:HG3	1:B:253:LYS:NZ	2.19	0.58
1:A:135:MET:HE3	1:A:449:LYS:HD3	1.85	0.57
1:B:160:VAL:HG21	1:B:195:LEU:HD22	1.85	0.57
1:B:438:LEU:HG	1:B:442:MET:HE2	1.85	0.57
1:B:171:PRO:HD2	1:B:213:GLU:HG2	1.87	0.57
1:B:248:GLU:HG3	1:B:253:LYS:HZ1	1.70	0.56
1:A:289:ASN:O	1:A:292:ARG:HG2	2.05	0.56
1:B:52:GLY:HA2	1:B:370:HIS:O	2.05	0.56
1:A:52:GLY:HA2	1:A:370:HIS:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLU:HG3	1:B:9:ASN:H	1.70	0.56
1:A:293:ASN:HB2	1:A:296:VAL:CG2	2.36	0.56
1:A:17:THR:HG22	1:B:89:LEU:HD13	1.89	0.54
1:B:48:LEU:HG	1:B:349:VAL:HG22	1.90	0.54
1:A:292:ARG:O	1:A:296:VAL:HB	2.09	0.53
1:B:374:SER:HA	1:B:401:SER:O	2.10	0.52
1:A:92:LYS:HE3	1:A:92:LYS:HA	1.91	0.52
1:B:197:ASN:HA	1:B:232:ARG:NH2	2.24	0.52
1:B:10:ARG:HB2	1:B:71:PHE:CD1	2.46	0.51
1:A:426:ALA:O	1:A:429:VAL:HG22	2.11	0.51
1:B:4:MET:HE2	1:B:36:SER:O	2.11	0.51
1:B:197:ASN:HA	1:B:232:ARG:HH22	1.77	0.50
1:B:279:ILE:HD11	1:B:382:LYS:HE2	1.93	0.49
1:A:1:THR:N	1:A:2:PRO:HD3	2.27	0.49
1:A:33:LEU:HD23	1:B:37:LEU:HD11	1.94	0.49
1:B:7:LEU:HB2	1:B:77:ALA:HA	1.95	0.49
1:A:374:SER:HB3	1:A:402:TYR:CE1	2.48	0.48
1:B:235:GLN:HG3	1:B:255:LEU:HA	1.96	0.48
1:B:92:LYS:HD2	1:B:92:LYS:HA	1.62	0.48
1:B:226:ARG:O	1:B:230:GLU:HG3	2.14	0.48
1:B:15:ASP:O	1:B:21:GLY:HA3	2.15	0.47
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.95	0.47
1:A:226:ARG:O	1:A:230:GLU:HG3	2.15	0.47
1:A:375:GLN:HE22	1:B:373:ALA:HA	1.80	0.47
1:B:237:VAL:HG22	1:B:242:SER:HB2	1.96	0.46
1:A:440:TYR:CE2	1:B:23:ARG:HD2	2.50	0.46
1:B:199:ARG:HA	1:B:234:TYR:OH	2.15	0.46
1:B:4:MET:HE1	1:B:38:SER:HB3	1.97	0.46
1:A:45:ILE:HD12	1:A:446:LEU:HD22	1.97	0.46
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.45	0.46
1:B:214:THR:HA	1:B:224:THR:HA	1.97	0.45
1:A:438:LEU:HG	1:A:442:MET:HE2	1.99	0.45
1:A:45:ILE:HG12	1:A:363:LEU:HB3	1.98	0.45
1:A:15:ASP:O	1:A:21:GLY:HA3	2.17	0.44
1:A:292:ARG:HG3	1:A:293:ASN:N	2.32	0.44
1:A:387:THR:HA	1:A:400:MET:O	2.17	0.44
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.53	0.44
1:A:111:THR:HG21	1:A:113:VAL:HG12	2.00	0.43
1:A:428:ASN:OD1	1:B:28:ASP:HA	2.19	0.43
1:B:4:MET:HA	1:B:5:PRO:HD2	1.83	0.43
1:A:208:ALA:HB2	1:A:258:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LEU:O	1:B:397:VAL:HA	2.18	0.42
1:A:274:THR:HG22	1:A:277:GLY:CA	2.50	0.42
1:A:37:LEU:HD13	1:B:34:ARG:HG3	2.02	0.41
1:A:244:ASN:HA	1:A:305:LYS:HE2	2.02	0.41
1:B:292:ARG:O	1:B:293:ASN:HB2	2.19	0.41
1:A:48:LEU:CD1	1:A:321:VAL:HB	2.51	0.41
1:A:233:GLY:O	1:A:254:PRO:HD2	2.21	0.41
1:B:150:GLU:H	1:B:150:GLU:HG2	1.62	0.41
1:A:151:LEU:HD12	1:A:151:LEU:HA	1.86	0.41
1:A:147:SER:O	1:A:205:GLY:HA2	2.20	0.41
1:A:178:CYS:HB3	1:A:181:ASN:OD1	2.20	0.41
1:B:347:GLU:O	1:B:351:ARG:HG2	2.21	0.41
1:B:335:PRO:HG3	1:B:402:TYR:CE2	2.56	0.41
1:A:109:TRP:CD1	1:A:109:TRP:C	2.99	0.41
1:A:236:LEU:HA	1:A:256:LEU:O	2.21	0.41
1:B:305:LYS:HD3	1:B:305:LYS:HA	1.90	0.41
1:B:242:SER:O	1:B:246:VAL:HG23	2.21	0.40
1:A:196:LEU:HD12	1:A:196:LEU:HA	1.97	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	429/449 (96%)	415 (97%)	13 (3%)	1 (0%)	43	63
1	B	428/449 (95%)	407 (95%)	19 (4%)	2 (0%)	24	43
All	All	857/898 (95%)	822 (96%)	32 (4%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	MET
1	A	51	ASP
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	325/339 (96%)	286 (88%)	39 (12%)	5	10
1	B	322/339 (95%)	285 (88%)	37 (12%)	5	11
All	All	647/678 (95%)	571 (88%)	76 (12%)	5	11

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	33	LEU
1	A	34	ARG
1	A	48	LEU
1	A	73	LYS
1	A	80	LEU
1	A	84	TYR
1	A	91	LYS
1	A	92	LYS
1	A	111	THR
1	A	127	LYS
1	A	148	THR
1	A	151	LEU
1	A	155	THR
1	A	171	PRO
1	A	172	SER
1	A	176	GLU
1	A	196	LEU
1	A	235	GLN
1	A	244	ASN
1	A	248	GLU

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Mol	Chain	Res	Type
1	A	252	GLN
1	A	253	LYS
1	A	266	VAL
1	A	269	LEU
1	A	272	LYS
1	A	274	THR
1	A	279	ILE
1	A	281	LYS
1	A	288	PRO
1	A	310	LEU
1	A	353	LEU
1	A	354	GLU
1	A	400	MET
1	A	412	HIS
1	A	443	LYS
1	A	446	LEU
1	A	448	LEU
1	A	449	LYS
1	B	3	GLU
1	B	4	MET
1	B	13	GLN
1	B	29	GLN
1	B	37	LEU
1	B	47	LEU
1	B	73	LYS
1	B	84	TYR
1	B	148	THR
1	B	150	GLU
1	B	159	LEU
1	B	172	SER
1	B	184	GLU
1	B	188	LYS
1	B	195	LEU
1	B	196	LEU
1	B	209	LYS
1	B	213	GLU
1	B	219	GLU
1	B	223	LYS
1	B	225	LEU
1	B	235	GLN
1	B	237	VAL
1	B	245	SER

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Mol	Chain	Res	Type
1	B	247	THR
1	B	248	GLU
1	B	266	VAL
1	B	272	LYS
1	B	281	LYS
1	B	294	ASP
1	B	305	LYS
1	B	315	LYS
1	B	382	LYS
1	B	397	VAL
1	B	401	SER
1	B	446	LEU
1	B	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	GLN
1	A	338	GLN
1	A	375	GLN
1	B	29	GLN
1	B	235	GLN
1	B	276	HIS
1	B	289	ASN
1	B	338	GLN
1	B	370	HIS
1	B	388	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.