



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:15 PM UTC

PDB ID : 1AJB / pdb_00001ajb
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
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

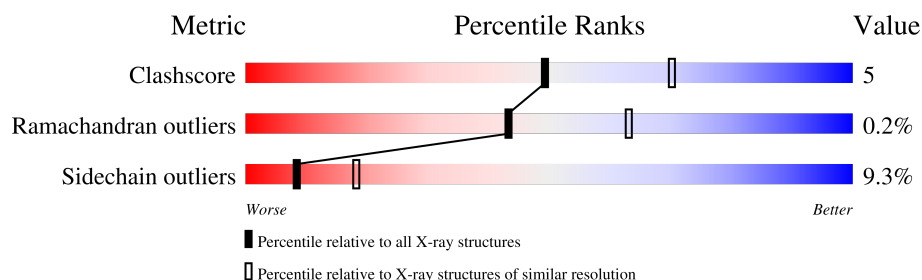
1 Overall quality at a glance

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	449	 75% 21% . .
1	B	449	 76% 20% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6783 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	449	Total	C	N	O	S	0	0	0
			3300	2040	580	668	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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

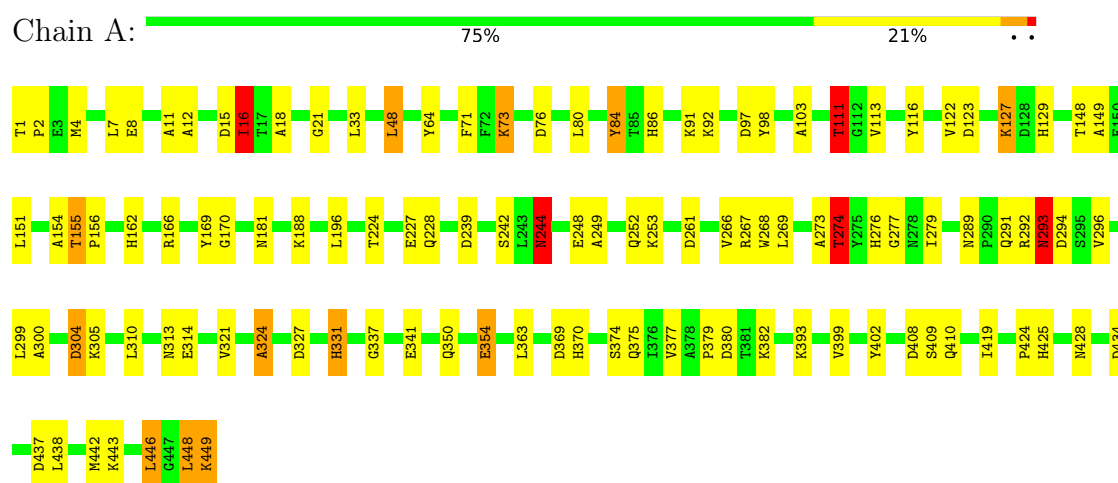
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total	O	8	0
			103	103		
5	B	64	Total	O	0	0
			64	64		

3 Residue-property plots

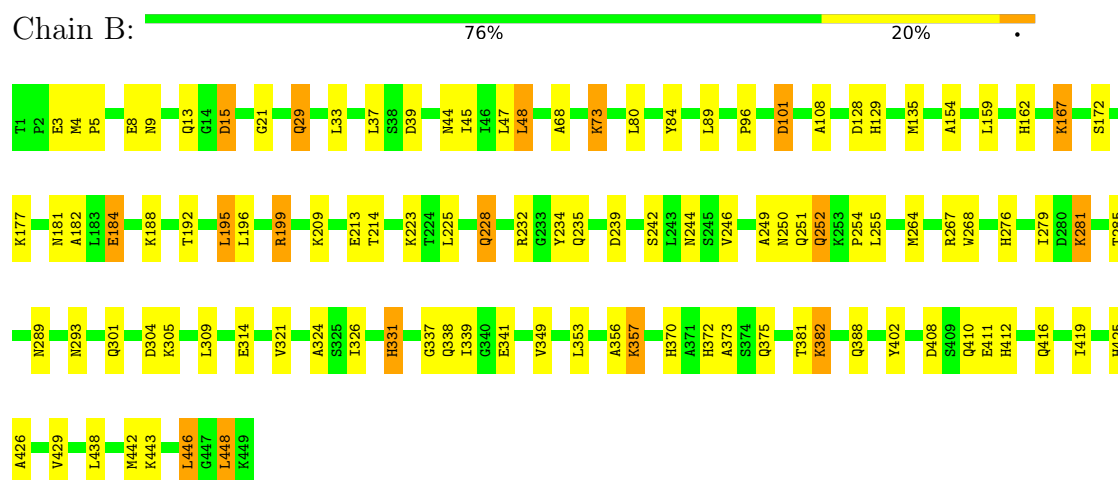
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	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	6783	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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, SO4, 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	0.97	6/3355 (0.2%)	1.66	50/4554 (1.1%)
1	B	0.97	8/3355 (0.2%)	1.68	54/4554 (1.2%)
All	All	0.97	14/6710 (0.2%)	1.67	104/9108 (1.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	HIS	CD2-NE2	-7.49	1.29	1.37
1	B	425	HIS	CD2-NE2	-7.03	1.30	1.37
1	B	162	HIS	CD2-NE2	-6.84	1.30	1.37
1	B	276	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	162	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	331	HIS	CG-ND1	-6.37	1.31	1.38
1	A	129	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	276	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	86	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	276	HIS	CG-ND1	-5.78	1.31	1.38
1	B	293	ASN	N-CA	5.40	1.53	1.46
1	A	331	HIS	CG-ND1	-5.37	1.32	1.38
1	B	419	ILE	CA-CB	5.36	1.61	1.54
1	A	155	THR	N-CA	5.33	1.50	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ASN	CA-CB-CG	-10.79	101.81	112.60
1	B	408	ASP	CA-CB-CG	9.93	122.53	112.60
1	A	111	THR	N-CA-CB	-8.87	99.11	110.90
1	A	71	PHE	CA-CB-CG	8.86	122.66	113.80
1	B	251	GLN	N-CA-C	7.60	120.45	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	372	HIS	CB-CG-CD2	-7.55	121.39	131.20
1	B	408	ASP	N-CA-C	7.25	119.81	111.11
1	B	162	HIS	CB-CG-CD2	-7.01	122.08	131.20
1	A	16	ILE	CA-CB-CG2	6.92	122.27	110.50
1	A	166	ARG	NE-CZ-NH1	6.91	128.41	121.50
1	A	162	HIS	CB-CG-CD2	-6.90	122.23	131.20
1	A	239	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	166	ARG	NE-CZ-NH2	-6.79	113.08	119.20
1	B	324	ALA	N-CA-C	6.74	119.98	111.69
1	B	3	GLU	O-C-N	6.73	131.23	122.68
1	B	5	PRO	CB-CA-C	-6.52	101.31	110.63
1	A	86	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	A	228	GLN	CG-CD-NE2	6.37	125.95	116.40
1	A	84	TYR	CA-CB-CG	6.36	125.35	113.90
1	A	16	ILE	CA-CB-CG1	-6.29	99.70	110.40
1	A	228	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	169	TYR	N-CA-C	6.22	117.75	110.97
1	B	314	GLU	N-CA-C	6.22	118.06	111.28
1	A	324	ALA	N-CA-C	6.19	118.10	111.36
1	B	199	ARG	N-CA-C	6.16	118.72	111.02
1	B	416	GLN	CG-CD-NE2	6.15	125.62	116.40
1	B	101	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	108	ALA	N-CA-C	6.13	117.97	111.28
1	B	228	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	A	16	ILE	N-CA-CB	-6.12	101.14	111.23
1	B	416	GLN	OE1-CD-NE2	-6.09	116.51	122.60
1	B	181	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	B	411	GLU	N-CA-C	5.96	119.23	110.59
1	B	129	HIS	CB-CG-CD2	-5.93	123.49	131.20
1	A	327	ASP	N-CA-C	5.82	117.62	111.28
1	B	293	ASN	CB-CA-C	-5.82	98.85	110.42
1	A	11	ALA	N-CA-C	-5.79	102.74	110.55
1	B	338	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	A	425	HIS	CA-CB-CG	-5.78	108.02	113.80
1	A	274	THR	N-CA-CB	-5.77	101.66	111.69
1	B	381	THR	CA-CB-OG1	-5.76	100.96	109.60
1	B	370	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	B	372	HIS	CB-CG-ND1	5.73	131.30	122.70
1	A	111	THR	CB-CA-C	5.71	118.62	109.02
1	B	425	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	B	29	GLN	CG-CD-NE2	5.70	124.95	116.40
1	A	313	ASN	OD1-CG-ND2	-5.67	116.93	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ILE	N-CA-C	-5.64	105.00	110.42
1	B	96	PRO	O-C-N	5.62	129.83	123.03
1	A	273	ALA	N-CA-C	-5.60	103.14	110.53
1	B	15	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	162	HIS	CB-CG-ND1	5.52	130.98	122.70
1	A	249	ALA	N-CA-C	-5.52	98.92	108.69
1	B	154	ALA	N-CA-C	5.51	118.00	111.33
1	B	29	GLN	OE1-CD-NE2	-5.50	117.09	122.60
1	A	123	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	428	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	408	ASP	N-CA-C	5.50	118.79	111.75
1	A	268	TRP	CG-CD2-CE3	5.49	139.39	133.90
1	B	281	LYS	CA-C-N	5.48	125.79	119.92
1	B	281	LYS	C-N-CA	5.48	125.79	119.92
1	A	296	VAL	N-CA-C	-5.46	101.60	108.05
1	A	375	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	18	ALA	CA-C-N	5.44	126.64	119.84
1	A	18	ALA	C-N-CA	5.44	126.64	119.84
1	A	375	GLN	CG-CD-NE2	5.44	124.56	116.40
1	B	356	ALA	N-CA-C	5.42	117.18	111.28
1	B	388	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	B	39	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	293	ASN	N-CA-C	5.37	122.23	110.80
1	B	267	ARG	N-CA-C	5.36	117.54	111.11
1	A	377	VAL	O-C-N	-5.35	117.35	122.97
1	B	285	THR	N-CA-C	-5.32	100.73	109.40
1	B	239	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	369	ASP	N-CA-C	5.26	118.96	112.54
1	A	380	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	97	ASP	N-CA-C	-5.24	98.85	108.02
1	B	252	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	76	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	267	ARG	N-CA-C	5.21	117.04	111.36
1	A	409	SER	CA-CB-OG	5.19	121.48	111.10
1	A	370	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	B	419	ILE	N-CA-C	-5.16	100.69	108.12
1	B	181	ASN	N-CA-C	-5.16	107.02	113.72
1	B	44	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	8	GLU	CB-CG-CD	5.12	121.31	112.60
1	B	128	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	162	HIS	CB-CG-ND1	5.10	130.36	122.70
1	B	373	ALA	N-CA-C	5.10	119.49	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ILE	N-CA-C	-5.10	100.87	108.46
1	B	289	ASN	CA-C-N	5.08	124.74	119.56
1	B	289	ASN	C-N-CA	5.08	124.74	119.56
1	B	375	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	B	9	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	181	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	A	86	HIS	CB-CG-ND1	5.02	130.23	122.70
1	A	73	LYS	CA-CB-CG	-5.02	104.06	114.10
1	B	264	MET	CA-C-N	5.01	124.94	119.78
1	B	264	MET	C-N-CA	5.01	124.94	119.78
1	B	276	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	B	214	THR	N-CA-CB	-5.01	102.62	110.69
1	A	170	GLY	CA-C-N	5.01	124.45	119.24
1	A	170	GLY	C-N-CA	5.01	124.45	119.24
1	B	244	ASN	CA-CB-CG	-5.00	107.60	112.60

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	3300	0	3246	43	0
1	B	3300	0	3246	30	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	5	0	0	0	0
4	B	5	0	0	0	0
5	A	103	0	0	0	0
5	B	64	0	0	1	0
All	All	6783	0	6492	71	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 5.

All (71) 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:155:THR:HB	1:A:156:PRO:HD3	1.59	0.82
1:A:111:THR:CG2	1:A:113:VAL:HG12	2.16	0.76
1:A:350:GLN:O	1:A:354:GLU:HG2	1.91	0.69
1:A:111:THR:HG23	1:A:113:VAL:HG12	1.74	0.69
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.75	0.68
1:B:279:ILE:HD11	1:B:382:LYS:HE2	1.76	0.68
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.80	0.64
1:A:155:THR:HB	1:A:156:PRO:CD	2.30	0.60
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.82	0.60
1:A:4:MET:HE1	1:A:424:PRO:HD3	1.84	0.60
1:B:301:GLN:O	1:B:305:LYS:HG2	2.05	0.56
1:A:292:ARG:O	1:A:293:ASN:HB2	2.05	0.55
1:A:363:LEU:HD13	1:A:424:PRO:O	2.07	0.55
1:A:438:LEU:O	1:A:442:MET:HG3	2.07	0.55
1:A:292:ARG:HG3	1:A:293:ASN:H	1.73	0.54
1:B:337:GLY:O	1:B:341:GLU:HG2	2.08	0.54
1:A:149:ALA:HB2	1:A:324:ALA:HB1	1.89	0.54
1:B:246:VAL:HG11	1:B:255:LEU:HD22	1.90	0.53
1:A:16:ILE:HG23	1:B:89:LEU:HD21	1.91	0.53
1:A:12:ALA:HB1	1:A:16:ILE:HD11	1.91	0.53
1:A:292:ARG:HG3	1:A:293:ASN:N	2.25	0.52
1:A:224:THR:OG1	1:A:227:GLU:HG3	2.11	0.51
1:B:192:THR:O	1:B:195:LEU:HB3	2.09	0.51
1:B:438:LEU:O	1:B:442:MET:HG3	2.11	0.50
1:A:274:THR:HG22	1:A:277:GLY:CA	2.41	0.50
1:B:101:ASP:HA	1:B:412:HIS:CE1	2.47	0.50
1:B:101:ASP:HA	1:B:412:HIS:HE1	1.76	0.49
1:A:331:HIS:ND1	1:A:410:GLN:O	2.45	0.49
1:B:234:TYR:CD2	1:B:254:PRO:HG2	2.48	0.49
1:B:446:LEU:HB3	1:B:448:LEU:HD13	1.95	0.48
1:A:300:ALA:O	1:A:304:ASP:HB2	2.15	0.47
1:A:98:TYR:HE1	1:B:68:ALA:HB2	1.79	0.47
1:A:402:TYR:HB3	1:A:410:GLN:HG3	1.97	0.47
1:B:45:ILE:HD12	1:B:446:LEU:HD22	1.97	0.47
1:A:91:LYS:HE2	1:A:116:TYR:CZ	2.50	0.47
1:A:274:THR:HG22	1:A:277:GLY:HA2	1.98	0.46
1:A:48:LEU:HD22	1:A:48:LEU:N	2.30	0.46
1:A:122:VAL:HA	1:A:127:LYS:O	2.15	0.46
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.46	0.46
1:B:199:ARG:NH2	1:B:232:ARG:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ASN:O	1:A:292:ARG:HG2	2.16	0.46
1:B:331:HIS:ND1	1:B:410:GLN:O	2.49	0.45
1:A:188:LYS:HB2	1:A:188:LYS:HE3	1.75	0.44
1:A:446:LEU:HB3	1:A:448:LEU:HD13	1.99	0.44
1:A:448:LEU:O	1:A:449:LYS:HB2	2.17	0.44
1:B:73:LYS:HD2	5:B:986:HOH:O	2.17	0.44
1:A:12:ALA:CB	1:A:16:ILE:HD11	2.46	0.44
1:B:182:ALA:HB1	1:B:184:GLU:OE2	2.18	0.44
1:A:337:GLY:O	1:A:341:GLU:HG2	2.18	0.44
1:A:374:SER:HB3	1:A:402:TYR:CE2	2.53	0.44
1:B:48:LEU:HG	1:B:349:VAL:HG22	2.00	0.44
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.99	0.44
1:B:353:LEU:O	1:B:357:LYS:HB3	2.18	0.44
1:A:64:TYR:O	1:A:393:LYS:HB2	2.19	0.42
1:A:244:ASN:HA	1:A:305:LYS:HE2	2.01	0.42
1:A:1:THR:N	1:A:2:PRO:HD3	2.34	0.42
1:B:135:MET:HE1	1:B:443:LYS:HD2	2.01	0.42
1:B:249:ALA:HB2	1:B:309:LEU:HD13	2.01	0.42
1:A:449:LYS:HE3	1:A:449:LYS:HA	2.01	0.42
1:B:48:LEU:HD22	1:B:48:LEU:N	2.35	0.42
1:B:426:ALA:O	1:B:429:VAL:HG22	2.20	0.42
1:B:268:TRP:CZ3	1:B:339:ILE:HG22	2.55	0.42
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.49	0.41
1:B:167:LYS:HB3	1:B:177:LYS:HD3	2.03	0.41
1:B:15:ASP:O	1:B:21:GLY:HA3	2.21	0.41
1:A:103:ALA:HA	1:A:154:ALA:HB1	2.03	0.41
1:B:228:GLN:O	1:B:232:ARG:HG3	2.20	0.41
1:B:80:LEU:HD12	1:B:426:ALA:HB3	2.02	0.41
1:A:148:THR:HG23	1:A:299:LEU:HD13	2.02	0.41
1:A:15:ASP:O	1:A:21:GLY:HA3	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	447/449 (100%)	439 (98%)	7 (2%)	1 (0%)	43	63
1	B	447/449 (100%)	432 (97%)	14 (3%)	1 (0%)	43	63
All	All	894/898 (100%)	871 (97%)	21 (2%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	MET
1	A	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	339/339 (100%)	306 (90%)	33 (10%)	8	17
1	B	339/339 (100%)	309 (91%)	30 (9%)	9	20
All	All	678/678 (100%)	615 (91%)	63 (9%)	8	18

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	16	ILE
1	A	33	LEU
1	A	48	LEU
1	A	73	LYS
1	A	80	LEU
1	A	84	TYR
1	A	92	LYS
1	A	111	THR
1	A	127	LYS
1	A	151	LEU

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Mol	Chain	Res	Type
1	A	196	LEU
1	A	242	SER
1	A	244	ASN
1	A	248	GLU
1	A	252	GLN
1	A	253	LYS
1	A	261	ASP
1	A	266	VAL
1	A	269	LEU
1	A	274	THR
1	A	279	ILE
1	A	291	GLN
1	A	294	ASP
1	A	304	ASP
1	A	310	LEU
1	A	314	GLU
1	A	354	GLU
1	A	382	LYS
1	A	443	LYS
1	A	446	LEU
1	A	448	LEU
1	A	449	LYS
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	73	LYS
1	B	84	TYR
1	B	159	LEU
1	B	167	LYS
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	223	LYS
1	B	225	LEU

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Mol	Chain	Res	Type
1	B	235	GLN
1	B	242	SER
1	B	250	ASN
1	B	252	GLN
1	B	281	LYS
1	B	304	ASP
1	B	357	LYS
1	B	382	LYS
1	B	446	LEU
1	B	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	251	GLN
1	A	388	GLN
1	B	244	ASN
1	B	293	ASN
1	B	338	GLN
1	B	388	GLN
1	B	410	GLN
1	B	435	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 [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z > 2$
4	SO4	A	457	-	4,4,4	0.56	0	6,6,6	0.79	0
4	SO4	B	957	-	4,4,4	0.45	0	6,6,6	0.81	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.

No monomer is involved in short contacts.

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.