Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AJD
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 : 1995-08-18
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
http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865
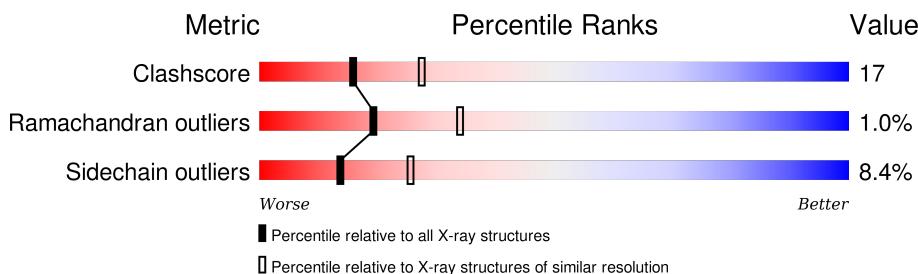
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.
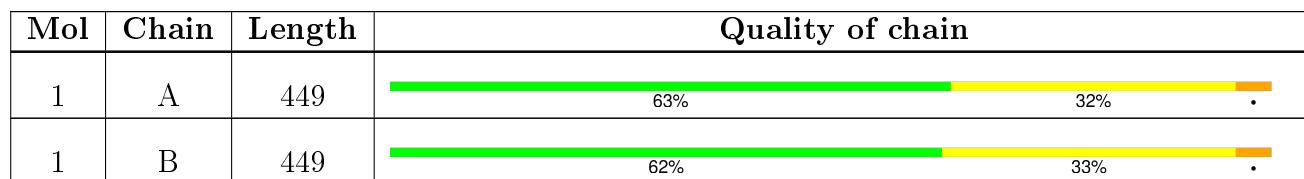
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		17
Ramachandran outliers		1.0%
Sidechain outliers		8.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	63% 32% •
1	B	449	62% 33% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6610 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 INTERMEDIATE II OF HOLO ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total 3300	C 2040	N 580	O 668	S 12	0	0	0
1	B	449	Total 3300	C 2040	N 580	O 668	S 12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	ASP	ENGINEERED	UNP P00634
A	230	GLU	GLN	CONFLICT	UNP P00634
B	153	GLY	ASP	ENGINEERED	UNP P00634
B	230	GLU	GLN	CONFLICT	UNP P00634

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.
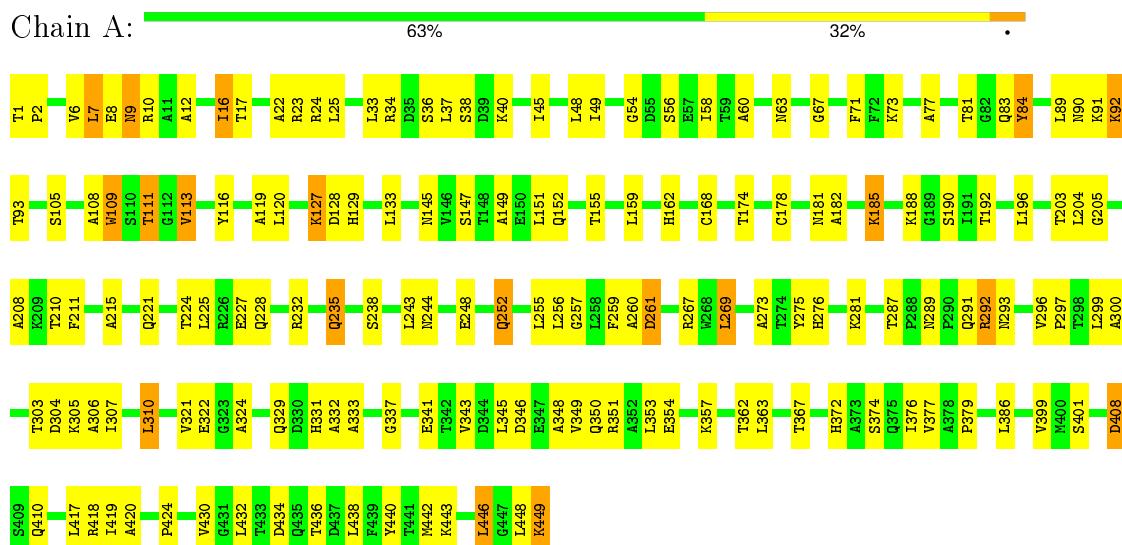
| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	2	Total O 2 2	0	0

3 Residue-property plots ⓘ
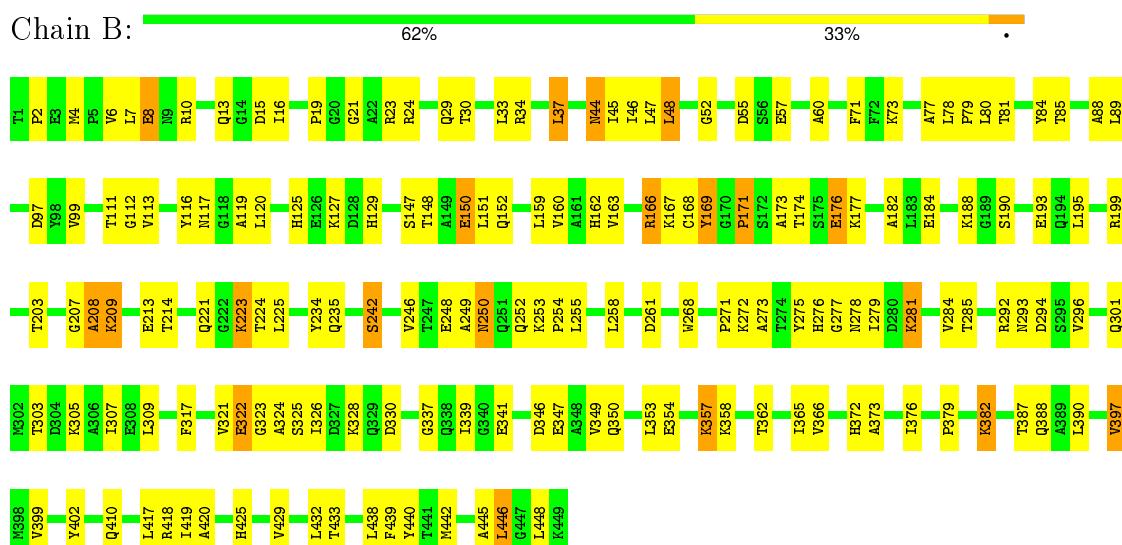
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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 INTERMEDIATE II OF HOLO ENZYME

● Molecule 1: ALKALINE PHOSPHATASE INTERMEDIATE II OF HOLO ENZYME

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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}	0.13	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	6610	wwPDB-VP
Average B, all atoms (Å²)	11.0	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	0.49	0/3355	0.76	1/4554 (0.0%)
1	B	0.46	0/3355	0.73	1/4554 (0.0%)
All	All	0.47	0/6710	0.74	2/9108 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	292	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	B	323	GLY	N-CA-C	-5.22	100.06	113.10

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	123	0
1	B	3300	0	3246	117	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
All	All	6610	0	6492	222	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 17.

All (222) 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:244:ASN:HA	1:A:305:LYS:HE2	1.48	0.93
1:B:250:ASN:HD21	1:B:253:LYS:HB2	1.36	0.90
1:B:279:ILE:HD11	1:B:382:LYS:HE2	1.58	0.85
1:B:250:ASN:ND2	1:B:253:LYS:HB2	1.96	0.81
1:A:252:GLN:HE21	1:A:252:GLN:N	1.84	0.75
1:B:446:LEU:HB3	1:B:448:LEU:HD13	1.67	0.74
1:A:269:LEU:HD13	1:A:289:ASN:HB2	1.70	0.73
1:B:354:GLU:HG2	1:B:358:LYS:NZ	2.04	0.72
1:A:446:LEU:HB3	1:A:448:LEU:HD13	1.71	0.72
1:B:337:GLY:O	1:B:341:GLU:HG2	1.90	0.72
1:A:45:ILE:HG12	1:A:363:LEU:HB3	1.73	0.70
1:A:224:THR:OG1	1:A:227:GLU:HG3	1.92	0.69
1:B:152:GLN:HB2	1:B:169:TYR:CE2	2.28	0.69
1:B:246:VAL:HG11	1:B:255:LEU:HD22	1.74	0.68
1:B:199:ARG:HA	1:B:234:TYR:OH	1.94	0.68
1:B:301:GLN:O	1:B:305:LYS:HG2	1.94	0.68
1:B:152:GLN:HB2	1:B:169:TYR:CD2	2.29	0.67
1:A:109:TRP:HB2	1:A:438:LEU:HD23	1.77	0.67
1:A:449:LYS:HE3	1:A:449:LYS:N	2.09	0.66
1:A:17:THR:HG22	1:B:89:LEU:HD13	1.75	0.66
1:A:92:LYS:HA	1:A:92:LYS:HE3	1.76	0.65
1:A:182:ALA:HB3	1:A:185:LYS:HB2	1.79	0.65
1:A:289:ASN:O	1:A:292:ARG:HG2	1.97	0.65
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.79	0.64
1:A:7:LEU:HB2	1:A:77:ALA:HA	1.79	0.64
1:B:160:VAL:HG21	1:B:195:LEU:HD22	1.80	0.64
1:A:252:GLN:HE21	1:A:252:GLN:H	1.46	0.63
1:B:48:LEU:HG	1:B:349:VAL:HG22	1.80	0.63
1:B:209:LYS:HB2	1:B:261:ASP:O	1.99	0.63
1:A:178:CYS:HB3	1:A:181:ASN:OD1	1.99	0.63
1:B:390:LEU:O	1:B:397:VAL:HA	1.99	0.63
1:B:438:LEU:O	1:B:442:MET:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.28	0.63
1:A:438:LEU:O	1:A:442:MET:HG3	1.99	0.62
1:A:23:ARG:HD2	1:B:440:TYR:CD2	2.35	0.62
1:A:149:ALA:HB2	1:A:324:ALA:HB1	1.82	0.62
1:A:362:THR:O	1:A:424:PRO:HD2	1.99	0.62
1:A:329:GLN:HA	1:A:332:ALA:HB3	1.82	0.61
1:A:350:GLN:O	1:A:354:GLU:HG2	2.01	0.61
1:B:160:VAL:HG21	1:B:195:LEU:CD2	2.31	0.60
1:A:299:LEU:HD23	1:A:345:LEU:HA	1.84	0.60
1:B:173:ALA:HB1	1:B:177:LYS:HD2	1.84	0.60
1:A:37:LEU:HD21	1:B:33:LEU:HD23	1.84	0.59
1:B:45:ILE:HG13	1:B:446:LEU:HD13	1.84	0.59
1:A:300:ALA:HB1	1:A:351:ARG:HG3	1.84	0.59
1:B:354:GLU:HG2	1:B:358:LYS:HZ1	1.66	0.59
1:A:363:LEU:HD13	1:A:424:PRO:O	2.04	0.58
1:B:214:THR:HA	1:B:224:THR:HA	1.86	0.58
1:B:279:ILE:CD1	1:B:382:LYS:HE2	2.32	0.57
1:B:235:GLN:HG2	1:B:254:PRO:O	2.04	0.57
1:B:248:GLU:HG2	1:B:253:LYS:HZ1	1.70	0.57
1:B:303:THR:O	1:B:307:ILE:HG13	2.04	0.57
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.87	0.57
1:A:10:ARG:CZ	1:A:25:LEU:HD21	2.34	0.57
1:A:273:ALA:CB	1:A:386:LEU:HB3	2.35	0.57
1:A:128:ASP:OD1	1:A:162:HIS:HB3	2.05	0.57
1:A:1:THR:N	1:A:2:PRO:HD3	2.20	0.56
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.86	0.56
1:B:234:TYR:HA	1:B:254:PRO:HG2	1.87	0.56
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.86	0.56
1:A:10:ARG:HB2	1:A:71:PHE:CE1	2.41	0.56
1:B:85:THR:HG23	1:B:432:LEU:HD11	1.87	0.55
1:A:83:GLN:HE22	1:B:81:THR:HB	1.71	0.55
1:A:54:GLY:O	1:A:58:ILE:HG13	2.07	0.55
1:B:278:ASN:HD22	1:B:399:VAL:HG11	1.71	0.55
1:A:145:ASN:OD1	1:A:159:LEU:HD12	2.06	0.55
1:A:346:ASP:O	1:A:350:GLN:HG3	2.07	0.55
1:B:365:ILE:HD13	1:B:438:LEU:HD11	1.88	0.54
1:A:289:ASN:HD21	1:A:291:GLN:HB2	1.73	0.54
1:B:271:PRO:HG2	1:B:388:GLN:HE22	1.72	0.54
1:A:84:TYR:O	1:A:84:TYR:HD1	1.90	0.54
1:B:326:ILE:O	1:B:330:ASP:HB2	2.08	0.53
1:B:129:HIS:O	1:B:162:HIS:HE1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ALA:HB3	1:B:261:ASP:HA	1.90	0.53
1:A:108:ALA:HB1	1:A:436:THR:CG2	2.38	0.53
1:A:377:VAL:HA	1:B:99:VAL:HG21	1.90	0.53
1:B:168:CYS:SG	1:B:177:LYS:HB2	2.49	0.53
1:B:151:LEU:HD13	1:B:203:THR:HG22	1.89	0.53
1:A:49:ILE:HG13	1:A:109:TRP:CZ2	2.44	0.53
1:B:45:ILE:HG13	1:B:446:LEU:CD1	2.38	0.53
1:B:10:ARG:HB2	1:B:71:PHE:CD1	2.44	0.52
1:A:90:ASN:OD1	1:A:93:THR:HG23	2.09	0.52
1:B:249:ALA:HB3	1:B:309:LEU:HB3	1.92	0.52
1:B:354:GLU:HG2	1:B:358:LYS:HZ3	1.75	0.52
1:B:46:ILE:HD12	1:B:362:THR:HG21	1.92	0.52
1:A:374:SER:HA	1:A:401:SER:O	2.10	0.52
1:B:88:ALA:HB3	1:B:97:ASP:HB3	1.92	0.52
1:B:268:TRP:CZ3	1:B:339:ILE:HG22	2.46	0.51
1:B:248:GLU:HG2	1:B:253:LYS:NZ	2.25	0.51
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.46	0.51
1:B:15:ASP:O	1:B:21:GLY:HA3	2.10	0.51
1:A:192:THR:OG1	1:A:210:THR:HG21	2.10	0.51
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.93	0.51
1:A:299:LEU:HG	1:A:348:ALA:HB2	1.92	0.51
1:B:242:SER:O	1:B:246:VAL:HG23	2.11	0.50
1:A:133:LEU:HD13	1:A:159:LEU:HB3	1.93	0.50
1:A:24:ARG:HD2	1:B:433:THR:C	2.31	0.50
1:A:303:THR:O	1:A:307:ILE:HG13	2.12	0.50
1:B:353:LEU:O	1:B:357:LYS:HB3	2.11	0.50
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.76	0.50
1:B:148:THR:OG1	1:B:324:ALA:HB3	2.10	0.50
1:A:259:PHE:O	1:A:260:ALA:HB2	2.12	0.50
1:A:376:ILE:HG22	1:B:99:VAL:CG2	2.42	0.50
1:B:48:LEU:HB2	1:B:366:VAL:HG22	1.93	0.49
1:A:440:TYR:CE1	1:B:23:ARG:HD2	2.47	0.49
1:A:120:LEU:O	1:A:162:HIS:HA	2.12	0.49
1:B:52:GLY:O	1:B:57:GLU:HG2	2.13	0.49
1:B:55:ASP:OD1	1:B:418:ARG:HB2	2.11	0.49
1:A:111:THR:HG22	1:A:113:VAL:H	1.77	0.49
1:B:347:GLU:O	1:B:350:GLN:HB2	2.13	0.49
1:B:346:ASP:O	1:B:350:GLN:HG3	2.13	0.48
1:A:417:LEU:HD12	1:A:418:ARG:O	2.14	0.48
1:A:81:THR:HG22	1:A:420:ALA:HB2	1.94	0.48
1:B:379:PRO:HA	1:B:399:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:THR:OG1	1:B:113:VAL:HG12	2.12	0.48
1:A:155:THR:HG21	1:A:322:GLU:HG3	1.94	0.48
1:A:367:THR:HB	1:A:419:ILE:HG13	1.96	0.48
1:B:182:ALA:HB1	1:B:184:GLU:OE2	2.13	0.48
1:B:208:ALA:HB2	1:B:258:LEU:HB3	1.94	0.48
1:B:419:ILE:HG12	1:B:429:VAL:HB	1.96	0.48
1:B:150:GLU:HB2	1:B:152:GLN:OE1	2.14	0.47
1:A:84:TYR:O	1:A:84:TYR:CD1	2.67	0.47
1:B:199:ARG:HG2	1:B:199:ARG:O	2.14	0.47
1:A:273:ALA:HB3	1:A:386:LEU:HB3	1.95	0.47
1:A:292:ARG:O	1:A:296:VAL:HB	2.13	0.47
1:B:281:LYS:HB3	1:B:281:LYS:NZ	2.30	0.47
1:B:166:ARG:HH21	1:B:167:LYS:HD2	1.79	0.47
1:A:345:LEU:O	1:A:349:VAL:HG23	2.15	0.47
1:A:174:THR:OG1	1:A:190:SER:HB3	2.15	0.47
1:A:127:LYS:HD3	1:A:128:ASP:O	2.15	0.47
1:A:24:ARG:HD2	1:B:433:THR:CA	2.45	0.47
1:B:46:ILE:CD1	1:B:362:THR:HG21	2.44	0.46
1:A:91:LYS:HE2	1:A:116:TYR:CZ	2.50	0.46
1:A:12:ALA:CB	1:A:16:ILE:HD11	2.45	0.46
1:A:432:LEU:O	1:B:10:ARG:HD2	2.16	0.46
1:A:63:ASN:O	1:A:67:GLY:HA2	2.16	0.46
1:A:108:ALA:HB1	1:A:436:THR:HG22	1.98	0.46
1:A:113:VAL:HG23	1:B:19:PRO:HA	1.97	0.46
1:B:213:GLU:O	1:B:225:LEU:HD13	2.15	0.46
1:A:449:LYS:H	1:A:449:LYS:HE3	1.78	0.46
1:A:300:ALA:O	1:A:304:ASP:HB2	2.16	0.46
1:B:120:LEU:O	1:B:162:HIS:HA	2.15	0.46
1:A:34:ARG:HG2	1:B:37:LEU:HD23	1.98	0.46
1:A:89:LEU:HD21	1:B:16:ILE:HD12	1.99	0.45
1:A:343:VAL:O	1:A:346:ASP:HB3	2.17	0.45
1:A:168:CYS:SG	1:A:174:THR:HA	2.57	0.45
1:B:166:ARG:NH2	1:B:167:LYS:HD2	2.31	0.45
1:A:12:ALA:HB1	1:A:22:ALA:HA	1.98	0.45
1:B:125:HIS:HB2	1:B:127:LYS:HG2	1.98	0.45
1:B:325:SER:OG	1:B:328:LYS:HD2	2.16	0.45
1:A:60:ALA:HA	1:A:376:ILE:HD11	1.98	0.45
1:B:292:ARG:O	1:B:293:ASN:HB2	2.16	0.45
1:A:33:LEU:O	1:A:36:SER:HB2	2.17	0.45
1:B:60:ALA:HB2	1:B:376:ILE:HD11	1.99	0.45
1:B:373:ALA:CB	1:B:410:GLN:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ALA:HB3	1:A:221:GLN:HA	1.99	0.44
1:A:8:GLU:O	1:A:9:ASN:HB2	2.16	0.44
1:B:6:VAL:HG12	1:B:77:ALA:HB1	1.98	0.44
1:B:425:HIS:CD2	1:B:445:ALA:HA	2.53	0.44
1:A:152:GLN:NE2	1:A:210:THR:HB	2.33	0.44
1:B:272:LYS:HG2	1:B:273:ALA:N	2.33	0.44
1:A:145:ASN:O	1:A:203:THR:HA	2.17	0.44
1:A:243:LEU:HD23	1:A:297:PRO:HB3	2.00	0.44
1:A:83:GLN:O	1:A:432:LEU:HA	2.18	0.44
1:A:430:VAL:HG21	1:B:33:LEU:HD21	2.00	0.43
1:A:24:ARG:NH1	1:A:24:ARG:HG2	2.33	0.43
1:B:293:ASN:HB2	1:B:296:VAL:HG23	1.99	0.43
1:A:16:ILE:CG2	1:B:89:LEU:HD21	2.48	0.43
1:A:228:GLN:O	1:A:232:ARG:HG2	2.17	0.43
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.53	0.43
1:A:6:VAL:HG11	1:A:357:LYS:HD3	2.00	0.43
1:B:221:GLN:C	1:B:223:LYS:H	2.21	0.43
1:B:277:GLY:HA3	1:B:387:THR:O	2.18	0.43
1:B:190:SER:N	1:B:193:GLU:HB2	2.34	0.43
1:B:30:THR:HG22	1:B:34:ARG:NH1	2.33	0.43
1:A:235:GLN:HB2	1:A:255:LEU:HD12	2.01	0.43
1:A:331:HIS:ND1	1:A:410:GLN:O	2.52	0.43
1:A:438:LEU:HG	1:A:442:MET:CE	2.49	0.42
1:B:252:GLN:O	1:B:253:LYS:HG3	2.19	0.42
1:A:211:PHE:CE2	1:A:256:LEU:HD21	2.54	0.42
1:B:275:TYR:CZ	1:B:276:HIS:CE1	3.07	0.42
1:B:438:LEU:HG	1:B:442:MET:CE	2.49	0.42
1:A:333:ALA:CB	1:A:386:LEU:HD12	2.48	0.42
1:A:127:LYS:HD2	1:A:129:HIS:NE2	2.35	0.42
1:A:225:LEU:O	1:A:228:GLN:HB3	2.19	0.42
1:A:188:LYS:HB2	1:A:188:LYS:HE3	1.74	0.42
1:B:44:ASN:HA	1:B:317:PHE:O	2.20	0.42
1:A:267:ARG:HG2	1:A:292:ARG:NH2	2.34	0.42
1:B:78:LEU:CB	1:B:420:ALA:HB1	2.50	0.42
1:A:292:ARG:HG3	1:A:293:ASN:H	1.85	0.42
1:A:40:LYS:NZ	1:A:424:PRO:HG3	2.34	0.42
1:B:207:GLY:O	1:B:209:LYS:N	2.53	0.42
1:B:176:GLU:HG2	1:B:177:LYS:HG3	2.01	0.42
1:A:306:ALA:O	1:A:310:LEU:HB2	2.20	0.42
1:A:208:ALA:HB3	1:A:261:ASP:HA	2.01	0.42
1:A:448:LEU:O	1:A:449:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:CYS:SG	1:B:174:THR:HA	2.60	0.42
1:B:6:VAL:O	1:B:8:GLU:N	2.52	0.42
1:A:331:HIS:CD2	1:A:372:HIS:HE2	2.38	0.41
1:A:147:SER:O	1:A:205:GLY:HA2	2.20	0.41
1:A:38:SER:O	1:A:424:PRO:HA	2.20	0.41
1:A:127:LYS:O	1:A:129:HIS:CD2	2.72	0.41
1:A:24:ARG:HD2	1:B:433:THR:HA	2.03	0.41
1:A:275:TYR:O	1:A:276:HIS:HB2	2.20	0.41
1:A:267:ARG:HG2	1:A:292:ARG:HH21	1.85	0.41
1:A:337:GLY:O	1:A:341:GLU:HG2	2.21	0.41
1:A:293:ASN:CB	1:A:296:VAL:HG23	2.50	0.41
1:A:292:ARG:HG3	1:A:293:ASN:N	2.36	0.41
1:B:418:ARG:HG2	1:B:419:ILE:N	2.35	0.41
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.90	0.41
1:B:249:ALA:HB2	1:B:309:LEU:HD13	2.03	0.41
1:A:273:ALA:N	1:A:333:ALA:O	2.49	0.41
1:B:80:LEU:O	1:B:420:ALA:HA	2.21	0.41
1:B:112:GLY:HA3	1:B:439:PHE:CD2	2.56	0.41
1:A:434:ASP:HB2	1:B:24:ARG:HG3	2.03	0.41
1:B:446:LEU:HB3	1:B:448:LEU:CD1	2.42	0.40
1:B:147:SER:OG	1:B:322:GLU:HG2	2.21	0.40
1:A:34:ARG:CG	1:B:37:LEU:HD23	2.52	0.40
1:B:77:ALA:O	1:B:79:PRO:HD3	2.21	0.40
1:A:204:LEU:HD23	1:A:257:GLY:HA3	2.03	0.40
1:B:284:VAL:HG12	1:B:285:THR:N	2.36	0.40
1:A:108:ALA:HB1	1:A:436:THR:HG23	2.02	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	447/449 (100%)	408 (91%)	37 (8%)	2 (0%)	39	61
1	B	447/449 (100%)	403 (90%)	37 (8%)	7 (2%)	12	21
All	All	894/898 (100%)	811 (91%)	74 (8%)	9 (1%)	19	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	ASP
1	B	7	LEU
1	B	208	ALA
1	B	171	PRO
1	A	9	ASN
1	B	117	ASN
1	B	4	MET
1	B	169	TYR
1	B	2	PRO

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	339/339 (100%)	311 (92%)	28 (8%)	14	26
1	B	339/339 (100%)	310 (91%)	29 (9%)	13	24
All	All	678/678 (100%)	621 (92%)	57 (8%)	14	25

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	16	ILE
1	A	56	SER
1	A	73	LYS
1	A	84	TYR
1	A	92	LYS
1	A	105	SER

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Mol	Chain	Res	Type
1	A	109	TRP
1	A	111	THR
1	A	113	VAL
1	A	127	LYS
1	A	151	LEU
1	A	185	LYS
1	A	196	LEU
1	A	235	GLN
1	A	238	SER
1	A	248	GLU
1	A	252	GLN
1	A	261	ASP
1	A	269	LEU
1	A	281	LYS
1	A	287	THR
1	A	310	LEU
1	A	353	LEU
1	A	408	ASP
1	A	443	LYS
1	A	446	LEU
1	A	449	LYS
1	B	8	GLU
1	B	13	GLN
1	B	29	GLN
1	B	37	LEU
1	B	44	ASN
1	B	47	LEU
1	B	48	LEU
1	B	73	LYS
1	B	84	TYR
1	B	150	GLU
1	B	159	LEU
1	B	163	VAL
1	B	166	ARG
1	B	171	PRO
1	B	176	GLU
1	B	188	LYS
1	B	209	LYS
1	B	223	LYS
1	B	242	SER
1	B	250	ASN
1	B	281	LYS

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Mol	Chain	Res	Type
1	B	294	ASP
1	B	322	GLU
1	B	357	LYS
1	B	372	HIS
1	B	382	LYS
1	B	397	VAL
1	B	417	LEU
1	B	446	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	83	GLN
1	A	244	ASN
1	A	252	GLN
1	A	338	GLN
1	A	391	ASN
1	B	244	ASN
1	B	250	ASN
1	B	276	HIS
1	B	293	ASN
1	B	338	GLN
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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.