



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:15 PM UTC

PDB ID : 1EBH / pdb_00001ebh
Title : OCTAHEDRAL COORDINATION AT THE HIGH AFFINITY METAL SITE IN ENOLASE; CRYSTALLOGRAPHIC ANALYSIS OF THE MG++- ENZYME FROM YEAST AT 1.9 ANGSTROMS RESOLUTION
Authors : Wedekind, J.E.; Reed, G.H.; Rayment, I.
Deposited on : 1994-11-01
Resolution : 1.90 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

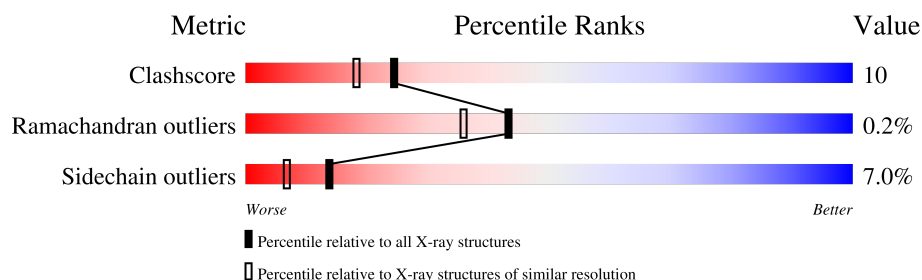
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	436	
1	B	436	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7138 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 ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	5	0
			3317	2094	575	642	6			
1	B	436	Total	C	N	O	S	0	4	0
			3310	2089	574	641	6			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- 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	280	Total	O	0	0
			280	280		
4	B	227	Total	O	0	0
			227	227		

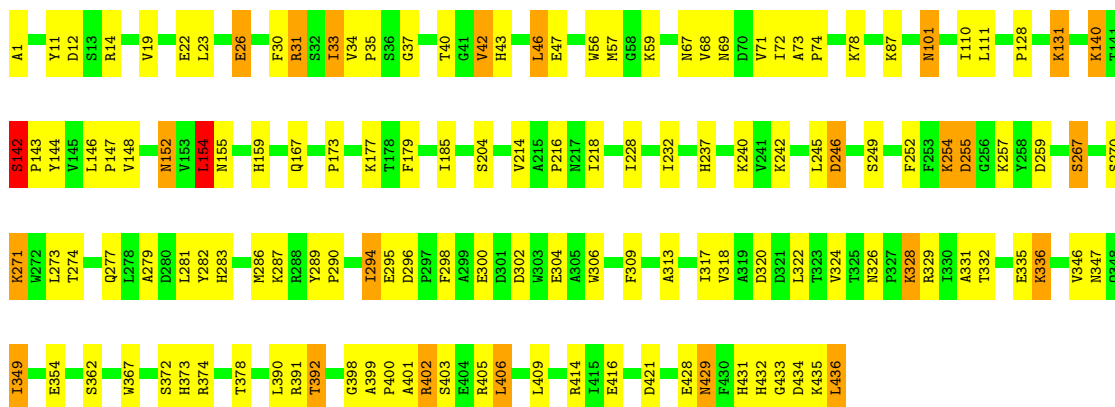
3 Residue-property plots

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.

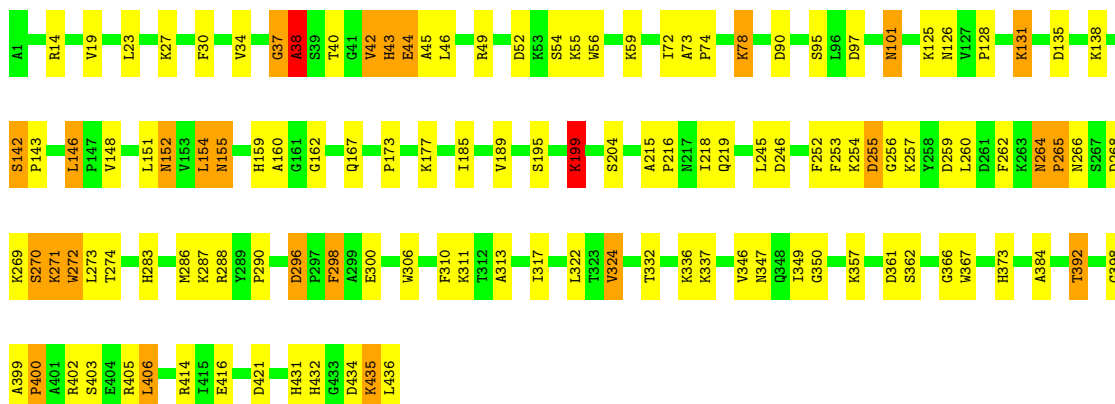
• Molecule 1: ENOLASE

Chain A: 



• Molecule 1: ENOLASE

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.50Å 73.20Å 89.10Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, CHAIN, X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7138	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL

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	1.44	10/3382 (0.3%)	1.56	46/4576 (1.0%)
1	B	1.47	16/3375 (0.5%)	1.58	46/4565 (1.0%)
All	All	1.46	26/6757 (0.4%)	1.57	92/9141 (1.0%)

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	A	2	1
1	B	2	1
All	All	4	2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	ARG	NE-CZ	7.01	1.40	1.33
1	B	274	THR	C-N	-6.91	1.29	1.34
1	B	59	LYS	CA-CB	-6.87	1.43	1.53
1	B	159	HIS	CB-CG	-6.38	1.41	1.50
1	A	14	ARG	CD-NE	-6.37	1.37	1.46
1	B	384	ALA	CA-CB	6.25	1.63	1.53
1	B	416	GLU	CD-OE2	6.24	1.37	1.25
1	B	151	LEU	CA-C	-6.20	1.44	1.52
1	B	14	ARG	NE-CZ	-6.05	1.26	1.33
1	B	43	HIS	CE1-NE2	5.96	1.38	1.32
1	B	43	HIS	CG-ND1	5.86	1.44	1.38
1	A	402	ARG	NE-CZ	5.74	1.39	1.33
1	A	289	TYR	CA-C	-5.65	1.46	1.52
1	B	97	ASP	CG-OD2	5.63	1.36	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	273	LEU	CA-C	-5.59	1.46	1.52
1	A	71	VAL	CA-CB	-5.54	1.50	1.55
1	B	272	TRP	CA-CB	-5.49	1.44	1.53
1	A	428	GLU	CD-OE1	5.41	1.35	1.25
1	A	33	ILE	CA-C	-5.38	1.46	1.52
1	B	14	ARG	CD-NE	-5.31	1.38	1.46
1	A	148	VAL	N-CA	-5.30	1.41	1.46
1	A	246	ASP	CG-OD1	5.29	1.35	1.25
1	B	49	ARG	NE-CZ	5.20	1.38	1.33
1	A	416	GLU	CD-OE2	5.14	1.35	1.25
1	B	296	ASP	C-O	5.10	1.26	1.23
1	A	414	ARG	CZ-NH1	5.05	1.39	1.32

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	LYS	N-CA-CB	10.67	125.96	110.16
1	B	255	ASP	CA-CB-CG	9.03	121.63	112.60
1	A	349	ILE	CB-CA-C	9.01	118.99	111.06
1	B	167	GLN	N-CA-C	8.55	120.52	111.03
1	A	31	ARG	N-CA-CB	-8.38	96.96	111.55
1	A	255	ASP	CA-CB-CG	7.79	120.39	112.60
1	A	255	ASP	CB-CA-C	-7.71	100.78	111.73
1	A	30	PHE	CA-CB-CG	-7.50	106.30	113.80
1	B	255	ASP	CB-CA-C	-7.32	102.05	111.86
1	B	349	ILE	CB-CA-C	7.29	118.30	111.30
1	A	392	THR	N-CA-C	7.15	120.11	111.82
1	A	72	ILE	N-CA-C	7.12	117.23	110.53
1	B	246	ASP	N-CA-CB	7.05	122.33	110.69
1	A	40	THR	N-CA-CB	7.05	122.41	110.71
1	B	403	SER	N-CA-C	6.96	120.87	112.38
1	A	254	LYS	CB-CA-C	-6.88	98.10	109.80
1	B	72	ILE	N-CA-C	6.83	116.97	110.42
1	B	148	VAL	N-CA-C	-6.82	102.77	108.63
1	B	350	GLY	N-CA-C	6.66	122.62	114.69
1	A	245	LEU	CB-CA-C	-6.50	97.06	109.66
1	B	155	ASN	CA-CB-CG	6.47	119.07	112.60
1	A	318	VAL	N-CA-C	6.35	117.44	108.36
1	B	30	PHE	CA-CB-CG	-6.33	107.47	113.80
1	A	429	ASN	CB-CA-C	-6.31	101.27	111.06
1	B	159	HIS	CA-CB-CG	-6.30	107.50	113.80
1	A	69	ASN	N-CA-C	6.22	118.06	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	N-CA-C	6.19	119.11	109.52
1	B	273	LEU	CB-CA-C	-6.17	98.61	109.71
1	A	403	SER	N-CA-CB	6.14	121.23	110.18
1	B	298	PHE	CA-CB-CG	-6.13	107.67	113.80
1	A	146	LEU	CB-CA-C	6.13	117.51	108.87
1	A	372	SER	N-CA-C	6.12	119.18	109.50
1	A	110	ILE	N-CA-C	6.06	116.23	110.53
1	B	346	VAL	N-CA-CB	6.02	117.99	110.47
1	B	90	ASP	CA-CB-CG	-6.01	106.59	112.60
1	B	44	GLU	N-CA-C	6.01	118.66	110.55
1	B	406	LEU	N-CA-CB	6.01	119.08	110.06
1	A	173	PRO	N-CA-CB	5.98	106.60	102.35
1	B	45	ALA	N-CA-C	-5.97	102.08	110.50
1	A	179	PHE	CA-CB-CG	-5.91	107.89	113.80
1	A	154	LEU	N-CA-CB	-5.89	100.59	111.13
1	A	294	ILE	N-CA-CB	5.88	120.10	111.52
1	A	246	ASP	N-CA-CB	5.84	120.39	110.87
1	A	271	LYS	CB-CA-C	5.78	119.27	109.55
1	A	128	PRO	N-CA-CB	5.78	108.70	103.33
1	A	167	GLN	N-CA-C	5.77	120.35	112.04
1	A	400	PRO	N-CA-CB	5.75	106.67	102.81
1	B	400	PRO	N-CA-CB	5.75	106.66	102.81
1	A	140	LYS	CB-CA-C	5.74	119.20	109.84
1	B	38[A]	ALA	N-CA-C	5.70	118.76	109.24
1	B	38[B]	ALA	N-CA-C	5.70	118.76	109.24
1	A	273	LEU	N-CA-C	5.68	119.22	110.42
1	A	148	VAL	N-CA-C	-5.67	103.75	108.63
1	B	199	LYS	N-CA-CB	5.67	118.22	110.01
1	A	147	PRO	CB-CA-C	-5.60	102.04	110.17
1	A	142	SER	CB-CA-C	5.59	117.92	110.81
1	B	273	LEU	N-CA-C	5.59	118.81	110.14
1	B	56	TRP	CB-CA-C	-5.59	103.64	111.80
1	A	328	LYS	CA-CB-CG	5.50	125.10	114.10
1	A	431	HIS	CB-CA-C	5.50	120.03	110.68
1	B	152	ASN	CA-CB-CG	-5.46	107.14	112.60
1	A	273	LEU	CB-CA-C	-5.46	100.79	109.80
1	B	19	VAL	N-CA-C	5.45	117.16	108.87
1	A	320	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	95	SER	CB-CA-C	-5.43	101.77	110.79
1	B	392	THR	N-CA-C	5.40	118.08	111.82
1	B	154	LEU	N-CA-CB	-5.39	101.48	111.13
1	B	403	SER	N-CA-CB	5.39	119.48	110.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	LEU	CB-CA-C	-5.36	98.17	109.38
1	A	403	SER	N-CA-C	5.35	119.29	112.34
1	B	264	ASN	CA-CB-CG	-5.35	107.25	112.60
1	B	290	PRO	N-CA-CB	5.26	105.94	102.25
1	A	68	VAL	CB-CA-C	-5.24	105.26	111.97
1	A	346	VAL	N-CA-CB	5.23	117.01	110.47
1	B	34	VAL	N-CA-CB	-5.22	103.90	111.21
1	B	421	ASP	CA-CB-CG	-5.22	107.38	112.60
1	A	19	VAL	N-CA-C	5.21	116.08	108.58
1	A	290	PRO	N-CA-CB	5.20	105.89	102.25
1	B	173	PRO	N-CA-CB	5.18	106.03	102.35
1	B	311	LYS	CB-CA-C	-5.18	102.15	110.74
1	A	159	HIS	N-CA-C	5.17	119.45	113.20
1	B	266	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	421	ASP	CA-CB-CG	-5.13	107.47	112.60
1	B	46	LEU	N-CA-C	5.12	117.96	109.46
1	B	199	LYS	CB-CA-C	5.11	118.90	110.88
1	B	128	PRO	N-CA-CB	5.10	108.73	103.38
1	A	267	SER	N-CA-CB	5.08	117.44	109.97
1	B	414	ARG	N-CA-CB	5.07	117.37	110.01
1	B	146	LEU	CB-CA-C	5.07	116.02	108.87
1	B	310	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	67	ASN	N-CA-CB	5.01	117.49	110.12
1	B	265	PRO	N-CA-C	-5.00	107.60	113.86

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	38[A]	ALA	CA
1	A	38[B]	ALA	CA
1	B	38[A]	ALA	CA
1	B	38[B]	ALA	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37[B]	GLY	Peptide
1	B	37[B]	GLY	Peptide

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	3317	0	3330	67	0
1	B	3310	0	3321	67	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	280	0	0	6	0
4	B	227	0	0	7	0
All	All	7138	0	6651	132	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 10.

All (132) 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:283:HIS:HA	1:B:286:MET:HE3	1.31	1.07
1:B:101:ASN:HD22	1:B:101:ASN:H	1.23	0.86
1:A:283:HIS:O	1:A:287:LYS:HD2	1.79	0.81
1:A:101:ASN:H	1:A:101:ASN:HD22	1.28	0.81
1:A:331:ALA:O	1:A:335:GLU:HG3	1.80	0.81
1:B:283:HIS:O	1:B:287:LYS:HD2	1.80	0.81
1:B:283:HIS:CA	1:B:286:MET:HE3	2.11	0.80
1:B:38[B]:ALA:HB2	4:B:450:HOH:O	1.83	0.78
1:A:242:LYS:HE2	4:A:640:HOH:O	1.84	0.77
1:A:43:HIS:HB2	1:A:324:VAL:HG21	1.67	0.75
1:B:268:ASP:OD1	1:B:270:SER:HB3	1.89	0.72
1:B:216:PRO:HG2	1:B:218:ILE:CD1	2.22	0.70
1:B:216:PRO:HG2	1:B:218:ILE:HD11	1.75	0.68
1:A:140:LYS:HB3	4:A:710:HOH:O	1.94	0.67
1:A:349:ILE:HD13	1:A:354:GLU:HB3	1.76	0.66
1:A:246:ASP:HA	1:A:295:GLU:HB3	1.78	0.65
1:A:254:LYS:NZ	1:A:259:ASP:OD2	2.29	0.64
1:B:126:ASN:HB3	4:B:613:HOH:O	1.97	0.64
1:B:152:ASN:HB2	4:B:532:HOH:O	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLY:HA2	1:A:436:LEU:HD13	1.80	0.64
1:A:274:THR:HG23	1:A:277:GLN:OE1	1.98	0.63
1:A:31:ARG:HD2	4:A:466:HOH:O	1.99	0.62
1:B:101:ASN:H	1:B:101:ASN:ND2	1.97	0.62
1:A:131:LYS:HG2	1:A:144:TYR:OH	1.99	0.61
1:A:349:ILE:CD1	1:A:354:GLU:HB3	2.31	0.61
1:A:1:ALA:N	1:A:26:GLU:OE2	2.32	0.60
1:B:332:THR:O	1:B:336:LYS:HG3	2.02	0.59
1:B:434:ASP:OD2	1:B:435:LYS:HE3	2.03	0.59
1:B:42:VAL:HG23	4:B:595:HOH:O	2.03	0.58
1:B:162:GLY:HA2	1:B:219:GLN:HE22	1.67	0.58
1:B:160:ALA:HB2	1:B:215:ALA:HB1	1.84	0.58
1:B:55:LYS:HG2	4:B:541:HOH:O	2.03	0.58
1:B:283:HIS:ND1	1:B:287:LYS:NZ	2.52	0.57
1:B:357:LYS:HE2	1:B:361:ASP:OD1	2.04	0.57
1:A:434:ASP:OD2	1:A:435:LYS:HE3	2.05	0.56
1:A:249:SER:HA	1:A:252:PHE:CE1	2.40	0.56
1:B:78:LYS:HD3	4:B:605:HOH:O	2.05	0.56
1:A:267:SER:HA	4:A:643:HOH:O	2.05	0.56
1:B:254:LYS:NZ	1:B:259:ASP:OD2	2.39	0.56
1:B:254:LYS:O	1:B:255:ASP:HB2	2.06	0.56
1:A:34[B]:VAL:HG23	1:A:35[B]:PRO:HD2	1.88	0.55
1:B:37[A]:GLY:CA	1:B:347:ASN:HD21	2.20	0.55
1:B:43:HIS:HB2	1:B:324:VAL:HG21	1.87	0.55
1:B:131:LYS:HE2	1:B:135:ASP:OD1	2.07	0.54
1:A:326:ASN:HD22	1:A:329:ARG:H	1.56	0.53
1:A:429:ASN:HB2	1:A:436:LEU:HD11	1.90	0.52
1:B:268:ASP:HB3	1:B:271:LYS:HG3	1.90	0.52
1:A:101:ASN:H	1:A:101:ASN:ND2	2.02	0.51
1:B:253:PHE:CZ	1:B:256:GLY:HA2	2.46	0.51
1:B:431:HIS:CD2	1:B:432:HIS:NE2	2.78	0.51
1:B:431:HIS:CD2	1:B:432:HIS:CE1	2.99	0.51
1:B:216:PRO:HG2	1:B:218:ILE:HD12	1.93	0.50
1:B:283:HIS:HA	1:B:286:MET:CE	2.22	0.50
1:B:37[A]:GLY:HA3	1:B:347:ASN:HD21	1.77	0.50
1:A:254:LYS:O	1:A:255:ASP:HB2	2.11	0.50
1:B:296:ASP:HA	1:B:306:TRP:CH2	2.46	0.50
1:B:373:HIS:CD2	1:B:373:HIS:H	2.29	0.49
1:B:162:GLY:HA2	1:B:219:GLN:NE2	2.26	0.49
1:A:216:PRO:HG2	1:A:218:ILE:CD1	2.43	0.49
1:A:313:ALA:HB3	1:A:317:ILE:HD11	1.93	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLU:O	1:B:322:LEU:HD12	2.13	0.48
1:A:281:LEU:HD12	1:A:281:LEU:O	2.13	0.47
1:A:154:LEU:HD13	1:A:155:ASN:N	2.29	0.47
1:B:125:LYS:O	1:B:126:ASN:HB2	2.15	0.47
1:B:260:LEU:HA	1:B:260:LEU:HD23	1.76	0.47
1:B:272:TRP:CD1	1:B:272:TRP:N	2.81	0.47
1:A:300:GLU:O	1:A:322:LEU:HD12	2.14	0.47
1:A:429:ASN:CB	1:A:436:LEU:HD11	2.45	0.47
1:B:399:ALA:HB1	1:B:400:PRO:HD2	1.96	0.47
1:B:101:ASN:HD22	1:B:101:ASN:N	1.93	0.47
1:A:73:ALA:N	1:A:74:PRO:HD2	2.31	0.46
1:B:37[A]:GLY:HA3	1:B:347:ASN:ND2	2.30	0.46
1:B:43:HIS:HB2	1:B:324:VAL:CG2	2.45	0.46
1:B:152:ASN:O	1:B:399:ALA:HB2	2.15	0.46
1:A:140:LYS:O	1:A:391:ARG:HD2	2.14	0.46
1:B:199:LYS:HB3	1:B:199:LYS:HE3	1.45	0.46
1:B:313:ALA:HB3	1:B:317:ILE:HD11	1.98	0.46
1:B:431:HIS:HD2	1:B:432:HIS:NE2	2.14	0.46
1:B:362:SER:O	1:B:367:TRP:HB2	2.16	0.46
1:A:313:ALA:CB	1:A:317:ILE:HD11	2.45	0.45
1:A:142:SER:HA	1:A:143:PRO:HA	1.49	0.45
1:A:185:ILE:HG12	1:A:237:HIS:CE1	2.52	0.45
1:B:38[A]:ALA:HB3	1:B:44:GLU:HG3	1.97	0.45
1:B:38[A]:ALA:HB1	4:B:450:HOH:O	2.16	0.45
1:A:298:PHE:HB2	1:A:306:TRP:CD1	2.52	0.45
1:A:31:ARG:CD	4:A:466:HOH:O	2.61	0.44
1:B:264:ASN:OD1	1:B:265:PRO:HD2	2.17	0.44
1:A:432:HIS:HD2	4:A:664:HOH:O	1.99	0.44
1:B:431:HIS:HD2	1:B:432:HIS:CD2	2.36	0.44
1:B:52:ASP:OD1	1:B:54:SER:HB2	2.17	0.44
1:A:332:THR:O	1:A:336:LYS:HG3	2.18	0.44
1:B:142:SER:HA	1:B:143:PRO:HA	1.57	0.44
1:B:398:GLY:HA3	1:B:405:ARG:HD2	2.00	0.44
1:A:373:HIS:H	1:A:373:HIS:CD2	2.35	0.43
1:A:228:ILE:O	1:A:232:ILE:HG13	2.17	0.43
1:A:177:LYS:HD3	1:A:177:LYS:HA	1.60	0.43
1:A:281:LEU:HD12	1:A:281:LEU:C	2.44	0.43
1:A:12:ASP:O	1:B:406:LEU:HD13	2.19	0.42
1:A:347:ASN:OD1	1:A:374:ARG:NH1	2.43	0.42
1:A:11:TYR:HB2	1:B:406:LEU:HD22	2.00	0.42
1:A:111:LEU:HD22	1:A:347:ASN:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:HIS:CD2	1:A:373:HIS:N	2.86	0.42
1:B:252:PHE:HB3	1:B:262:PHE:CD1	2.55	0.42
1:A:401:ALA:O	1:A:402:ARG:HB2	2.19	0.42
1:B:298:PHE:HB2	1:B:306:TRP:CD1	2.55	0.42
1:B:436:LEU:HD23	1:B:436:LEU:HA	1.80	0.42
1:A:302:ASP:O	1:A:306:TRP:HD1	2.02	0.42
1:A:390:LEU:HA	1:A:390:LEU:HD23	1.81	0.42
1:B:74:PRO:O	1:B:78:LYS:HB2	2.20	0.42
1:A:42:VAL:HG13	1:A:43:HIS:CD2	2.54	0.42
1:A:362:SER:O	1:A:367:TRP:HB2	2.20	0.41
1:B:138:LYS:HA	1:B:138:LYS:HD3	1.74	0.41
1:A:101:ASN:ND2	1:A:101:ASN:N	2.64	0.41
1:A:152:ASN:O	1:A:399:ALA:HB2	2.19	0.41
1:A:22:GLU:CG	1:A:31:ARG:HG3	2.50	0.41
1:A:252:PHE:HB2	1:A:259:ASP:O	2.21	0.41
1:A:279:ALA:HB1	1:A:309:PHE:HD1	1.83	0.41
1:A:296:ASP:HA	1:A:306:TRP:CH2	2.55	0.41
1:A:406:LEU:HD13	1:A:409:LEU:HD12	2.02	0.41
1:A:398:GLY:HA3	1:A:405:ARG:HD2	2.02	0.41
1:B:73:ALA:N	1:B:74:PRO:HD2	2.35	0.41
1:A:56:TRP:C	1:A:57:MET:HG2	2.45	0.41
1:A:154:LEU:HD22	1:A:214:VAL:HG23	2.03	0.41
1:A:216:PRO:HG2	1:A:218:ILE:HD11	2.03	0.41
1:B:185:ILE:O	1:B:189:VAL:HG23	2.21	0.41
1:B:366:GLY:O	1:B:432:HIS:HE1	2.04	0.41
1:A:242:LYS:HD3	1:A:242:LYS:HA	1.76	0.40
1:A:282:TYR:O	1:A:286:MET:HG3	2.22	0.40
1:B:252:PHE:HB2	1:B:259:ASP:O	2.21	0.40
1:A:33:ILE:CG2	1:A:378:THR:HG21	2.51	0.40
1:B:324:VAL:O	1:B:324:VAL:HG23	2.20	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	439/436 (101%)	425 (97%)	14 (3%)	0	100	100
1	B	438/436 (100%)	422 (96%)	13 (3%)	3 (1%)	18	10
All	All	877/872 (101%)	847 (97%)	27 (3%)	3 (0%)	43	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	402	ARG
1	B	38[A]	ALA
1	B	38[B]	ALA

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	347/344 (101%)	322 (93%)	25 (7%)	13	6
1	B	346/344 (101%)	323 (93%)	23 (7%)	15	8
All	All	693/688 (101%)	645 (93%)	48 (7%)	14	7

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	26	GLU
1	A	42	VAL
1	A	46	LEU
1	A	47	GLU
1	A	59	LYS
1	A	78	LYS
1	A	87	LYS
1	A	101	ASN
1	A	131	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	142	SER
1	A	152	ASN
1	A	154	LEU
1	A	204	SER
1	A	240	LYS
1	A	257	LYS
1	A	270	SER
1	A	271	LYS
1	A	294	ILE
1	A	304	GLU
1	A	328	LYS
1	A	336	LYS
1	A	392	THR
1	A	406	LEU
1	A	436	LEU
1	B	23	LEU
1	B	27	LYS
1	B	40	THR
1	B	42	VAL
1	B	78	LYS
1	B	101	ASN
1	B	131	LYS
1	B	142	SER
1	B	146	LEU
1	B	154	LEU
1	B	155	ASN
1	B	177	LYS
1	B	195	SER
1	B	199	LYS
1	B	204	SER
1	B	257	LYS
1	B	269	LYS
1	B	270	SER
1	B	271	LYS
1	B	324	VAL
1	B	337	LYS
1	B	392	THR
1	B	435	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	63	HIS
1	A	101	ASN
1	A	126	ASN
1	A	159	HIS
1	A	191	HIS
1	A	217	ASN
1	A	266	ASN
1	A	326	ASN
1	A	348	GLN
1	A	432	HIS
1	B	16	ASN
1	B	101	ASN
1	B	159	HIS
1	B	191	HIS
1	B	217	ASN
1	B	219	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 4 ligands modelled in this entry, 4 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

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.