



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:09 PM GMT

PDB ID : 1EBH
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

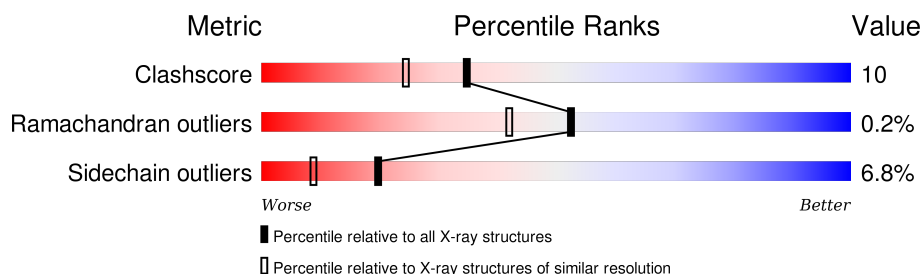
1 Overall quality at a glance

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (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 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 $\leq 5\%$. 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	436	 66% 28% 6%
1	B	436	 70% 26% 5%

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 (three-letter code: CL) (formula: Cl).

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

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

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

- Molecule 4 is water.

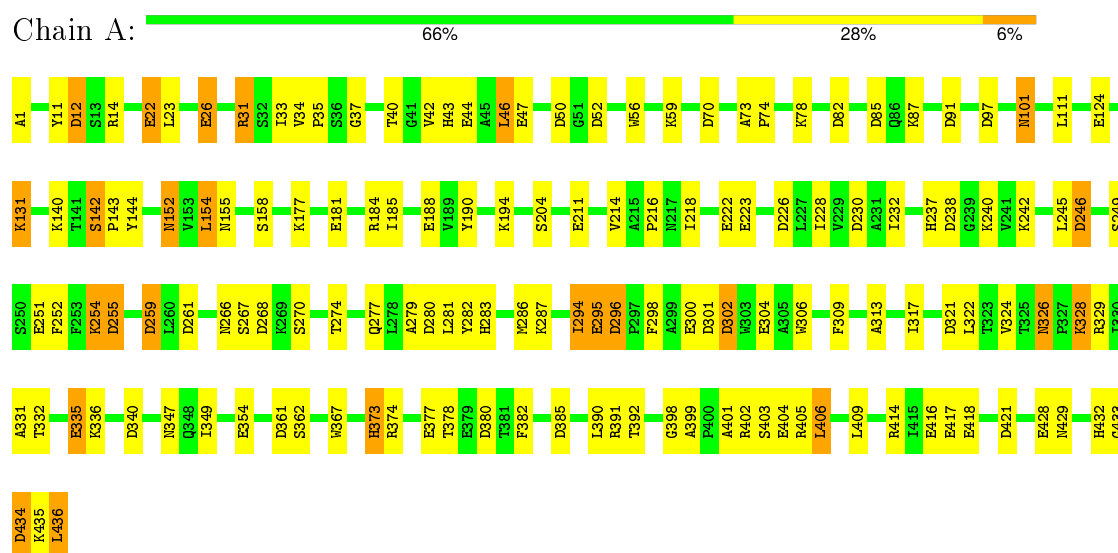
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	280	Total	O	0	0
			280	280		
4	B	227	Total	O	0	0
			227	227		

3 Residue-property plots

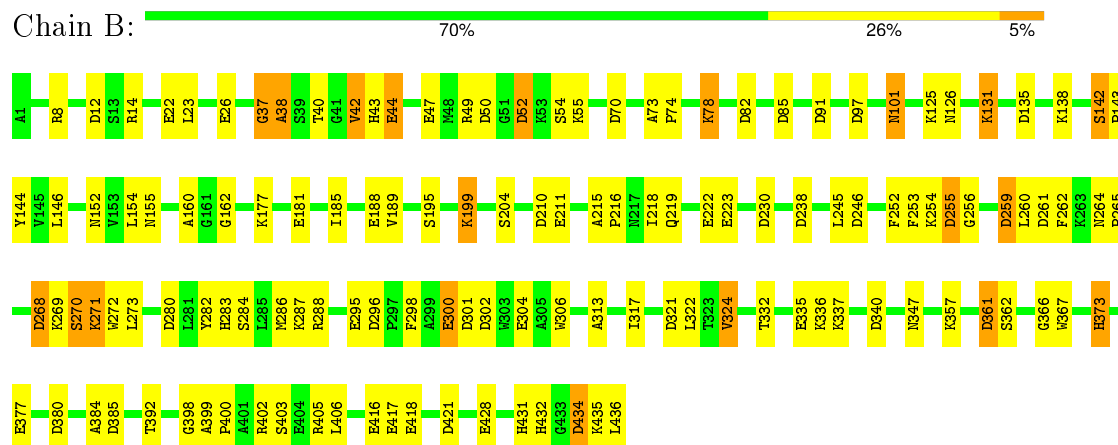
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ENOLASE



• Molecule 1: ENOLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.50 Å 73.20 Å 89.10 Å 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	1.21	22/3382 (0.7%)	1.40	58/4576 (1.3%)
1	B	1.25	23/3375 (0.7%)	1.43	54/4565 (1.2%)
All	All	1.23	45/6757 (0.7%)	1.42	112/9141 (1.2%)

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	0	1
1	B	0	1
All	All	0	2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	416	GLU	CD-OE2	10.50	1.37	1.25
1	A	428	GLU	CD-OE1	9.07	1.35	1.25
1	A	416	GLU	CD-OE2	8.61	1.35	1.25
1	B	47	GLU	CD-OE2	8.35	1.34	1.25
1	B	222	GLU	CD-OE2	8.16	1.34	1.25
1	B	223	GLU	CD-OE2	7.83	1.34	1.25
1	B	428	GLU	CD-OE1	7.79	1.34	1.25
1	B	304	GLU	CD-OE2	7.57	1.33	1.25
1	B	335	GLU	CD-OE1	7.50	1.33	1.25
1	A	304	GLU	CD-OE1	7.40	1.33	1.25
1	A	335	GLU	CD-OE1	7.13	1.33	1.25
1	A	181	GLU	CD-OE1	-6.82	1.18	1.25
1	B	188	GLU	CD-OE2	6.76	1.33	1.25
1	A	188	GLU	CD-OE2	6.63	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	GLU	CD-OE2	6.59	1.32	1.25
1	A	404	GLU	CD-OE2	6.44	1.32	1.25
1	B	188	GLU	CD-OE1	-6.44	1.18	1.25
1	A	418	GLU	CD-OE2	-6.38	1.18	1.25
1	A	188	GLU	CD-OE1	-6.25	1.18	1.25
1	B	44	GLU	CD-OE1	6.21	1.32	1.25
1	B	26	GLU	CD-OE2	6.20	1.32	1.25
1	B	22	GLU	CD-OE1	-6.18	1.18	1.25
1	B	295	GLU	CD-OE1	-6.08	1.19	1.25
1	A	211	GLU	CD-OE2	6.06	1.32	1.25
1	B	211	GLU	CD-OE2	6.04	1.32	1.25
1	B	288	ARG	NE-CZ	5.93	1.40	1.33
1	A	251	GLU	CD-OE2	5.91	1.32	1.25
1	B	417	GLU	CD-OE2	5.86	1.32	1.25
1	A	377	GLU	CD-OE2	5.83	1.32	1.25
1	A	44	GLU	CD-OE2	5.78	1.32	1.25
1	A	223	GLU	CD-OE2	5.76	1.31	1.25
1	A	222	GLU	CD-OE1	5.73	1.31	1.25
1	B	22	GLU	CD-OE2	5.42	1.31	1.25
1	B	377	GLU	CD-OE2	5.40	1.31	1.25
1	B	181	GLU	CD-OE1	-5.38	1.19	1.25
1	A	14	ARG	CD-NE	-5.36	1.37	1.46
1	A	124	GLU	CD-OE2	5.28	1.31	1.25
1	A	414	ARG	CZ-NH1	5.21	1.39	1.33
1	B	418	GLU	CD-OE2	5.19	1.31	1.25
1	A	22	GLU	CD-OE2	5.14	1.31	1.25
1	B	384	ALA	CA-CB	5.12	1.63	1.52
1	B	14	ARG	NE-CZ	-5.12	1.26	1.33
1	A	417	GLU	CD-OE2	5.08	1.31	1.25
1	A	295	GLU	CD-OE2	-5.07	1.20	1.25
1	A	56	TRP	CG-CD1	5.01	1.43	1.36

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	B	12	ASP	CB-CG-OD2	-9.08	110.12	118.30
1	B	12	ASP	CB-CG-OD1	8.92	126.33	118.30
1	B	280	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	A	328	LYS	N-CA-CB	8.53	125.96	110.60
1	A	301	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	A	70	ASP	CB-CG-OD2	-8.15	110.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	ASP	CB-CG-OD1	8.12	125.60	118.30
1	B	434	ASP	CB-CG-OD1	8.06	125.55	118.30
1	A	85	ASP	CB-CG-OD1	8.05	125.55	118.30
1	B	85	ASP	CB-CG-OD1	8.05	125.55	118.30
1	B	259	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	A	82	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	B	434	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	B	14	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	B	246	ASP	CB-CG-OD2	-7.74	111.34	118.30
1	B	85	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	B	91	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	B	97	ASP	CB-CG-OD2	-7.62	111.45	118.30
1	A	31	ARG	N-CA-CB	-7.58	96.96	110.60
1	B	246	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	421	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	70	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	31	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	434	ASP	CB-CG-OD1	7.47	125.02	118.30
1	A	414	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	82	ASP	CB-CG-OD1	7.34	124.91	118.30
1	B	50	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	82	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	52	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	B	8	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	B	321	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	403	SER	N-CA-CB	7.15	121.23	110.50
1	B	261	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	A	50	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	B	91	ASP	CB-CG-OD1	7.06	124.65	118.30
1	B	238	ASP	CB-CG-OD1	-7.04	111.97	118.30
1	B	97	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	49	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	268	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	280	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	A	85	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	A	301	ASP	CB-CG-OD1	6.95	124.55	118.30
1	A	91	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	245	LEU	CB-CA-C	-6.92	97.06	110.20
1	B	50	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	70	ASP	CB-CG-OD1	6.73	124.35	118.30
1	B	82	ASP	CB-CG-OD1	6.71	124.33	118.30
1	B	361	ASP	CB-CG-OD2	-6.70	112.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	261	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	97	ASP	CB-CG-OD1	-6.57	112.39	118.30
1	B	52	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	B	246	ASP	N-CA-CB	6.51	122.33	110.60
1	A	238	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	B	421	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	40	THR	N-CA-CB	6.37	122.41	110.30
1	B	245	LEU	CB-CA-C	-6.33	98.17	110.20
1	B	268	ASP	CB-CG-OD2	-6.29	112.63	118.30
1	B	259	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	91	ASP	CB-CG-OD1	6.25	123.93	118.30
1	A	361	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	254	LYS	CB-CA-C	-6.15	98.10	110.40
1	B	361	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	273	LEU	CB-CA-C	-6.10	98.61	110.20
1	A	12	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	434	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	B	403	SER	N-CA-CB	5.99	119.48	110.50
1	B	261	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	288	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	361	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	50	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	70	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	210	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	280	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	268	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	B	340	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	52	ASP	CB-CG-OD1	5.85	123.57	118.30
1	A	294	ILE	CG1-CB-CG2	-5.84	98.56	111.40
1	B	321	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	385	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	B	301	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	380	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	280	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	321	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	31	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	230	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	302	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	255	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	340	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	321	ASP	CB-CG-OD1	5.51	123.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	296	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	302	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	B	144	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	255	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	184	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	302	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	246	ASP	N-CA-CB	5.44	120.39	110.60
1	A	328	LYS	CA-CB-CG	5.32	125.10	113.40
1	A	230	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	421	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	259	ASP	CB-CG-OD2	-5.22	113.61	118.30
1	B	255	ASP	CB-CG-OD1	-5.22	113.61	118.30
1	A	97	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	226	ASP	CB-CG-OD2	-5.18	113.63	118.30
1	B	255	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	385	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	380	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	230	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	190	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	382	PHE	CB-CG-CD2	-5.04	117.27	120.80

There are no chirality outliers.

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	65	0
1	B	3310	0	3321	69	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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:101:ASN:H	1:B:101:ASN:HD22	1.23	0.86
1:B:283:HIS:HA	1:B:286:MET:HE3	1.58	0.85
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: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:283:HIS:HA	1:B:286:MET:CE	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
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:B:283:HIS:CA	1:B:286:MET:HE3	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLY:HA2	1:B:219:GLN:HE22	1.67	0.58
1:B:42:VAL:HG23	4:B:595:HOH:O	2.03	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: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:254:LYS:NZ	1:B:259:ASP:OD2	2.39	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:CE1	2.99	0.51
1:B:431:HIS:CD2	1:B:432:HIS:NE2	2.78	0.51
1:B:216:PRO:HG2	1:B:218:ILE:HD12	1.93	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:H	1:B:373:HIS:CD2	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
1:B:282:TYR:C	1:B:286:MET:HE3	2.34	0.48
1:B:300:GLU:O	1:B:322:LEU:HD12	2.13	0.48
1:A:281:LEU:O	1:A:281:LEU:HD12	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:HD23	1:B:260:LEU:HA	1.76	0.47
1:B:272:TRP:CD1	1:B:272:TRP:N	2.81	0.47
1:B:399:ALA:HB1	1:B:400:PRO:HD2	1.96	0.47
1:A:429:ASN:CB	1:A:436:LEU:HD11	2.45	0.47
1:A:300:GLU:O	1:A:322:LEU:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ASN:N	1:B:101:ASN:HD22	1.93	0.47
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:A:73:ALA:N	1:A:74:PRO:HD2	2.31	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:431:HIS:HD2	1:B:432:HIS:NE2	2.14	0.46
1:B:313:ALA:HB3	1:B:317:ILE:HD11	1.98	0.46
1:B:199:LYS:HB3	1:B:199:LYS:HE3	1.45	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:B:38[A]:ALA:HB3	1:B:44:GLU:HG3	1.97	0.45
1:A:185:ILE:HG12	1:A:237:HIS:CE1	2.52	0.45
1:A:142:SER:HA	1:A:143:PRO:HA	1.49	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:B:282:TYR:O	1:B:286:MET:HE3	2.18	0.44
1:B:431:HIS:HD2	1:B:432:HIS:CD2	2.36	0.44
1:A:432:HIS:HD2	4:A:664:HOH:O	1.99	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:CD2	1:A:373:HIS:H	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: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
1:B:252:PHE:HB3	1:B:262:PHE:CD1	2.55	0.42
1:A:373:HIS:CD2	1:A:373:HIS:N	2.86	0.42
1:B:298:PHE:HB2	1:B:306:TRP:CD1	2.55	0.42
1:A:401:ALA:O	1:A:402:ARG:HB2	2.19	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:HD23	1:A:390:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:101:ASN:ND2	2.64	0.41
1:A:152:ASN:O	1:A:399:ALA:HB2	2.19	0.41
1:A:252:PHE:HB2	1:A:259:ASP:O	2.21	0.41
1:A:22:GLU:CG	1:A:31:ARG:HG3	2.50	0.41
1:A:296:ASP:HA	1:A:306:TRP:CH2	2.55	0.41
1:A:279:ALA:HB1	1:A:309:PHE:HD1	1.83	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:154:LEU:HD22	1:A:214:VAL:HG23	2.03	0.41
1:B:366:GLY:O	1:B:432:HIS:HE1	2.04	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:A:242:LYS:HD3	1:A:242:LYS:HA	1.76	0.40
1:B:252:PHE:HB2	1:B:259:ASP:O	2.21	0.40
1:A:282:TYR:O	1:A:286:MET:HG3	2.22	0.40
1:A:33:ILE:CG2	1:A:378:THR:HG21	2.51	0.40
1:B:324:VAL:HG23	1:B:324:VAL:O	2.20	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	439/436 (101%)	425 (97%)	14 (3%)	0	100	100
1	B	438/436 (100%)	422 (96%)	13 (3%)	3 (1%)	26	14
All	All	877/872 (101%)	847 (97%)	27 (3%)	3 (0%)	52	35

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%)	18	7
1	B	346/344 (101%)	324 (94%)	22 (6%)	22	10
All	All	693/688 (101%)	646 (93%)	47 (7%)	20	9

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	26	GLU
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
1	A	142	SER
1	A	152	ASN
1	A	154	LEU
1	A	158	SER
1	A	194	LYS
1	A	204	SER
1	A	240	LYS
1	A	266	ASN
1	A	270	SER
1	A	294	ILE
1	A	326	ASN
1	A	328	LYS

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Mol	Chain	Res	Type
1	A	373	HIS
1	A	392	THR
1	A	406	LEU
1	A	436	LEU
1	B	23	LEU
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	269	LYS
1	B	270	SER
1	B	271	LYS
1	B	284	SER
1	B	324	VAL
1	B	337	LYS
1	B	373	HIS
1	B	392	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	101	ASN
1	A	126	ASN
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	101	ASN
1	B	207	ASN
1	B	217	ASN

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Mol	Chain	Res	Type
1	B	219	GLN
1	B	348	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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 [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.