



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:12 PM UTC

PDB ID : 1EBG / pdb_00001ebg
Title : CHELATION OF SER 39 TO MG2+ LATCHES A GATE AT THE ACTIVE SITE OF ENOLASE: STRUCTURE OF THE BIS(MG2+) COMPLEX OF YEAST ENOLASE AND THE INTERMEDIATE ANALOG PHOSPHONO ACETOHYDROXAMATE AT 2.1 ANGSTROMS RESOLUTION
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Deposited on : 1994-04-27
Resolution : 2.10 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

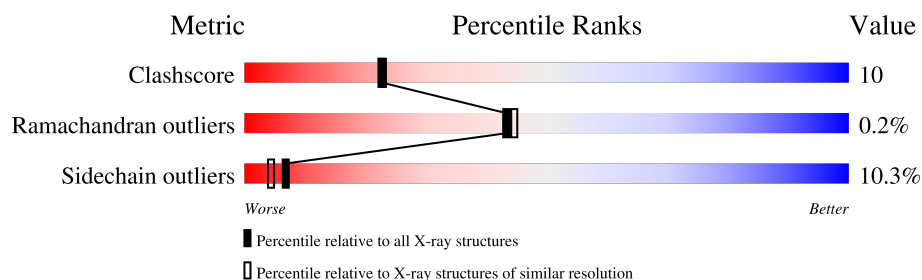
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6960 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.

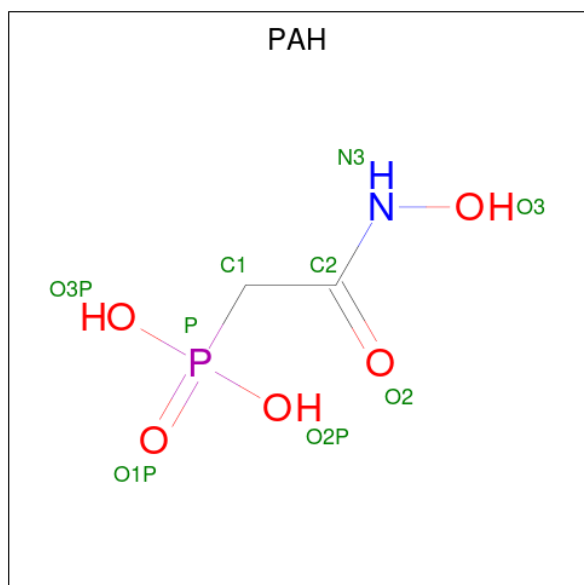
- Molecule 1 is a protein called ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3292	2079	570	637	6			
1	B	436	Total	C	N	O	S	0	0	0
			3292	2079	570	637	6			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHONOACETOHYDROXAMIC ACID (CCD ID: PAH) (formula: C₂H₆NO₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			9	2	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			9	2	1	5	1		

- Molecule 4 is water.

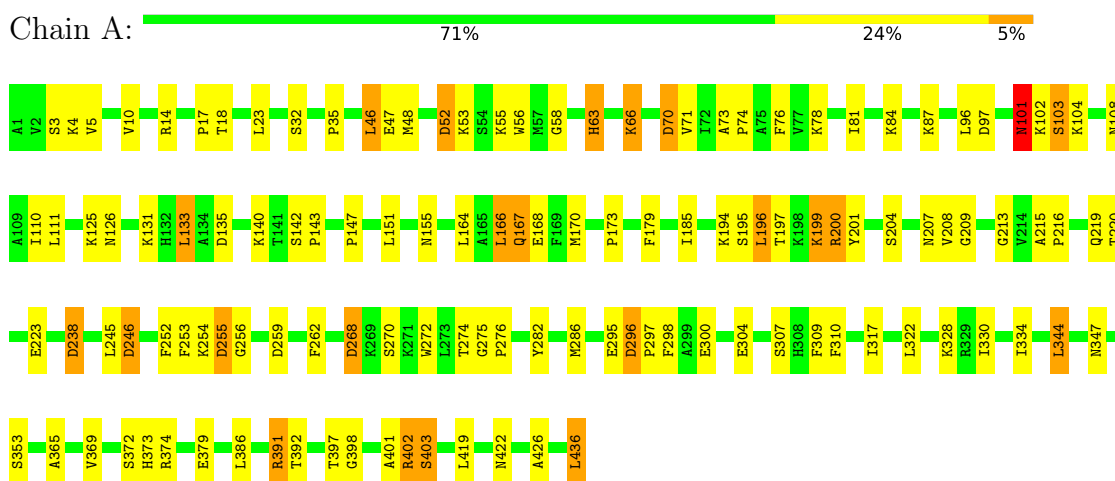
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		
4	B	167	Total	O	0	0
			167	167		

3 Residue-property plots

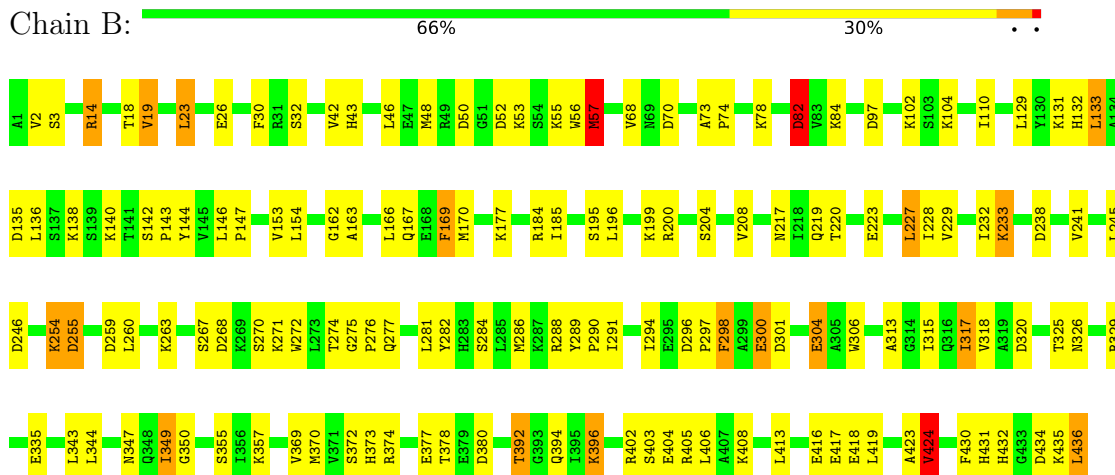
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• Molecule 1: ENOLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.50Å 73.90Å 94.80Å 90.00° 93.30° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6960	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: MG, PAH

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	1.27	4/3352 (0.1%)	1.54	40/4534 (0.9%)
1	B	1.21	6/3352 (0.2%)	1.55	38/4534 (0.8%)
All	All	1.24	10/6704 (0.1%)	1.55	78/9068 (0.9%)

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	1	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	ASP	C-O	-7.54	1.20	1.23
1	B	14	ARG	CD-NE	-6.33	1.37	1.46
1	B	52	ASP	CG-OD2	6.01	1.36	1.25
1	A	135	ASP	CG-OD2	5.95	1.36	1.25
1	B	329	ARG	CZ-NH2	5.55	1.40	1.33
1	B	374	ARG	NE-CZ	5.55	1.39	1.33
1	A	197	THR	CA-CB	5.51	1.62	1.53
1	B	405	ARG	CZ-NH1	5.48	1.40	1.32
1	B	349	ILE	CA-CB	-5.22	1.48	1.54
1	A	185	ILE	CA-CB	-5.04	1.48	1.54

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	PHE	CA-CB-CG	-10.62	103.18	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	GLN	N-CA-C	8.38	120.19	111.14
1	B	46	LEU	N-CA-C	8.34	121.85	109.59
1	B	372	SER	N-CA-C	7.47	120.53	109.24
1	A	52	ASP	N-CA-CB	-7.45	99.43	110.24
1	A	63	HIS	CA-CB-CG	-7.41	106.39	113.80
1	A	208	VAL	N-CA-C	7.37	120.62	109.20
1	B	208	VAL	N-CA-C	7.24	120.28	108.99
1	A	255	ASP	CB-CA-C	-7.17	101.71	111.89
1	A	167	GLN	N-CA-C	7.14	120.47	111.69
1	B	14	ARG	CB-CA-C	-7.10	98.17	110.17
1	A	207	ASN	CA-CB-CG	-6.87	105.73	112.60
1	B	14	ARG	NE-CZ-NH2	-6.86	113.03	119.20
1	A	48	MET	N-CA-C	6.78	119.63	109.25
1	A	403	SER	N-CA-CB	6.73	120.78	110.14
1	B	255	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	298	PHE	CA-CB-CG	-6.64	107.16	113.80
1	A	216	PRO	CB-CA-C	-6.48	102.60	111.21
1	A	246	ASP	N-CA-CB	6.47	122.79	110.82
1	A	344	LEU	N-CA-C	6.42	118.61	108.67
1	B	424	VAL	CB-CA-C	-6.34	101.05	110.82
1	B	185	ILE	CB-CA-C	-6.33	103.59	112.14
1	B	50	ASP	N-CA-C	6.30	118.23	111.36
1	B	110	ILE	N-CA-C	6.30	116.45	110.53
1	B	19	VAL	N-CA-C	6.26	117.60	108.58
1	A	173	PRO	N-CA-CB	6.23	106.78	102.35
1	A	398	GLY	N-CA-C	6.19	119.63	111.70
1	A	71	VAL	N-CA-CB	-6.16	105.47	111.57
1	A	87	LYS	N-CA-CB	6.14	119.10	109.94
1	B	318	VAL	N-CA-C	6.10	117.08	108.36
1	A	403	SER	N-CA-C	6.07	119.52	111.75
1	A	147	PRO	CB-CA-C	-6.06	101.38	110.17
1	A	101	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	179	PHE	CA-CB-CG	-6.04	107.77	113.80
1	B	68	VAL	CB-CA-C	-6.03	104.12	112.02
1	B	246	ASP	N-CA-CB	6.02	120.62	110.69
1	B	350	GLY	N-CA-C	5.98	121.91	114.37
1	B	57	MET	CB-CA-C	-5.94	102.34	111.66
1	A	46	LEU	N-CA-C	5.90	118.26	109.59
1	B	30	PHE	CA-CB-CG	-5.89	107.91	113.80
1	B	184	ARG	CA-CB-CG	-5.87	102.36	114.10
1	A	254	LYS	CB-CA-C	-5.79	101.78	110.24
1	A	310	PHE	CA-CB-CG	-5.73	108.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ILE	N-CA-C	5.64	115.83	110.53
1	A	70	ASP	CA-C-N	-5.62	117.46	122.97
1	A	70	ASP	C-N-CA	-5.62	117.46	122.97
1	B	396	LYS	CB-CA-C	5.58	119.08	110.14
1	A	426	ALA	N-CA-C	5.58	117.36	111.28
1	B	147	PRO	CB-CA-C	-5.57	102.91	110.60
1	A	391	ARG	CB-CA-C	-5.56	103.68	111.80
1	B	70	ASP	CA-C-N	-5.54	117.54	122.97
1	B	70	ASP	C-N-CA	-5.54	117.54	122.97
1	B	430	PHE	N-CA-C	5.53	117.31	111.28
1	B	288	ARG	N-CA-CB	-5.52	102.30	110.53
1	A	353	SER	N-CA-CB	5.48	118.17	110.12
1	A	215	ALA	N-CA-CB	-5.43	102.40	110.99
1	A	18	THR	N-CA-CB	5.43	120.13	111.56
1	A	10	VAL	N-CA-CB	5.39	118.49	112.45
1	A	254	LYS	N-CA-CB	5.35	119.42	110.59
1	B	48	MET	N-CA-CB	-5.27	101.31	110.17
1	B	169	PHE	CA-CB-CG	-5.27	108.53	113.80
1	B	82	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	372	SER	N-CA-C	5.22	117.12	109.24
1	A	245	LEU	CB-CA-C	-5.21	99.56	109.66
1	A	164	LEU	CB-CA-C	5.18	117.62	110.16
1	B	343	LEU	N-CA-CB	5.18	118.92	110.37
1	A	14	ARG	NE-CZ-NH2	-5.17	114.54	119.20
1	A	268	ASP	N-CA-C	5.17	117.36	107.75
1	B	413	LEU	N-CA-C	-5.14	105.56	111.07
1	B	300	GLU	N-CA-C	5.08	118.25	111.75
1	B	430	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	170	MET	N-CA-C	5.04	117.82	109.85
1	B	326	ASN	CA-C-N	5.04	124.48	119.24
1	B	326	ASN	C-N-CA	5.04	124.48	119.24
1	B	170	MET	N-CA-C	5.03	117.94	109.95
1	B	241	VAL	N-CA-C	5.02	115.14	108.11
1	A	76	PHE	CA-CB-CG	-5.02	108.78	113.80
1	B	403	SER	N-CA-C	5.01	118.85	112.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	403	SER	CA

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	3292	0	3301	63	0
1	B	3292	0	3300	75	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	3	0	0
3	B	9	0	3	0	0
4	A	187	0	0	3	0
4	B	167	0	0	5	0
All	All	6960	0	6607	138	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 (138) 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:101:ASN:N	1:A:101:ASN:HD22	1.55	0.99
1:A:101:ASN:ND2	1:A:101:ASN:H	1.54	0.90
1:A:101:ASN:HD22	1:A:101:ASN:H	0.92	0.88
1:A:238:ASP:HB2	4:A:614:HOH:O	1.77	0.82
1:B:304:GLU:H	1:B:304:GLU:CD	1.90	0.79
1:B:313:ALA:HB3	4:B:492:HOH:O	1.83	0.77
1:B:232:ILE:HB	1:B:233:LYS:HE3	1.67	0.76
1:A:4:LYS:HG2	1:A:5:VAL:N	2.03	0.72
1:B:286:MET:HE2	1:B:315:ILE:HD11	1.74	0.70
1:A:74:PRO:O	1:A:78:LYS:HG3	1.92	0.70
1:B:254:LYS:NZ	1:B:259:ASP:OD2	2.25	0.67
1:B:219:GLN:HB2	4:B:538:HOH:O	1.96	0.66
1:A:101:ASN:ND2	1:A:103:SER:OG	2.28	0.66
1:A:101:ASN:N	1:A:101:ASN:ND2	2.22	0.66
1:B:73:ALA:HB3	1:B:74:PRO:HD3	1.79	0.63
1:B:245:LEU:HD12	1:B:294:ILE:CD1	2.29	0.62
1:A:246:ASP:HA	1:A:295:GLU:HB3	1.81	0.62
1:B:286:MET:CE	1:B:315:ILE:HD11	2.30	0.61
1:B:313:ALA:HB1	1:B:317:ILE:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLY:O	1:B:263:LYS:HE2	1.99	0.61
1:B:233:LYS:HG3	1:B:238:ASP:HB2	1.83	0.61
1:A:330:ILE:O	1:A:334:ILE:HG13	2.01	0.60
1:B:53:LYS:HD3	1:B:53:LYS:H	1.66	0.60
1:B:380:ASP:O	1:B:408:LYS:HE3	2.02	0.60
1:B:282:TYR:O	1:B:286:MET:HG3	2.02	0.59
1:A:252:PHE:HB3	1:A:262:PHE:CD2	2.37	0.59
1:B:220:THR:HG23	1:B:223:GLU:OE1	2.03	0.59
1:B:297:PRO:HD2	1:B:306:TRP:CH2	2.39	0.58
1:B:2:VAL:HG13	1:B:23:LEU:CD2	2.34	0.58
1:A:286:MET:HE1	1:A:309:PHE:CZ	2.39	0.57
1:A:286:MET:HE1	1:A:309:PHE:HZ	1.71	0.56
1:B:56:TRP:C	1:B:57:MET:HG2	2.29	0.56
1:B:313:ALA:HB1	1:B:317:ILE:HD11	1.88	0.56
1:A:97:ASP:OD1	1:A:104:LYS:HB3	2.06	0.56
1:B:104:LYS:HD2	4:B:580:HOH:O	2.06	0.56
1:B:267:SER:HA	4:B:547:HOH:O	2.06	0.56
1:B:154:LEU:HB3	1:B:169:PHE:HB2	1.88	0.55
1:B:132:HIS:O	1:B:135:ASP:HB2	2.06	0.55
1:B:143:PRO:HB2	1:B:423:ALA:HA	1.88	0.55
1:B:325:THR:HG22	1:B:325:THR:O	2.07	0.55
1:A:272:TRP:N	1:A:272:TRP:CD1	2.72	0.55
1:A:334:ILE:HD13	1:A:365:ALA:HB2	1.88	0.55
1:B:431:HIS:HD2	1:B:432:HIS:CD2	2.27	0.53
1:B:268:ASP:HB3	1:B:271:LYS:HD2	1.91	0.52
1:A:300:GLU:O	1:A:322:LEU:HD12	2.09	0.52
1:B:272:TRP:CD1	1:B:272:TRP:N	2.75	0.52
1:B:431:HIS:CD2	1:B:432:HIS:NE2	2.78	0.52
1:B:78:LYS:HG3	1:B:78:LYS:O	2.09	0.51
1:B:43:HIS:HE1	1:B:301:ASP:OD2	1.93	0.51
1:B:370:MET:HA	1:B:394:GLN:HG3	1.92	0.51
1:A:282:TYR:HB3	1:A:286:MET:CE	2.41	0.51
1:A:275:GLY:N	1:A:276:PRO:CD	2.74	0.50
1:A:391:ARG:HG3	4:A:591:HOH:O	2.11	0.50
1:A:97:ASP:OD2	1:A:102:LYS:HA	2.11	0.50
1:A:373:HIS:H	1:A:373:HIS:CD2	2.29	0.50
1:B:431:HIS:CD2	1:B:432:HIS:CD2	2.99	0.50
1:B:82:ASP:OD1	1:B:84:LYS:HB2	2.11	0.50
1:B:315:ILE:O	1:B:317:ILE:HD12	2.12	0.49
1:A:166:LEU:N	1:A:166:LEU:CD1	2.76	0.48
1:A:268:ASP:OD2	1:A:270:SER:OG	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ILE:O	1:B:232:ILE:HG13	2.12	0.48
1:B:431:HIS:HD2	1:B:432:HIS:NE2	2.11	0.48
1:B:14:ARG:HD2	4:B:520:HOH:O	2.14	0.48
1:B:298:PHE:HB2	1:B:306:TRP:CD1	2.48	0.48
1:B:436:LEU:HD12	1:B:436:LEU:HA	1.65	0.48
1:A:17:PRO:HG3	1:A:56:TRP:CD1	2.48	0.47
1:B:42:VAL:HG22	1:B:300:GLU:CD	2.38	0.47
1:B:144:TYR:HB2	1:B:419:LEU:HD13	1.95	0.47
1:A:334:ILE:HD13	1:A:365:ALA:CB	2.45	0.47
1:B:53:LYS:HD3	1:B:53:LYS:N	2.29	0.47
1:B:163:ALA:H	1:B:217:ASN:ND2	2.13	0.47
1:B:274:THR:HG23	1:B:277:GLN:OE1	2.14	0.47
1:A:220:THR:OG1	1:A:223:GLU:HG3	2.15	0.47
1:A:63:HIS:N	1:A:63:HIS:CD2	2.80	0.46
1:A:196:LEU:HA	1:A:196:LEU:HD13	1.50	0.46
1:A:282:TYR:C	1:A:286:MET:HE3	2.40	0.46
1:B:245:LEU:HD12	1:B:294:ILE:HD12	1.96	0.46
1:B:146:LEU:CD1	1:B:416:GLU:HG3	2.45	0.46
1:A:66:LYS:NZ	1:A:70:ASP:OD2	2.35	0.46
1:B:131:LYS:HE3	1:B:135:ASP:OD1	2.15	0.46
1:A:275:GLY:N	1:A:276:PRO:HD2	2.31	0.46
1:A:140:LYS:HD3	1:A:391:ARG:NH2	2.31	0.46
1:B:143:PRO:HG2	1:B:424:VAL:HG23	1.96	0.45
1:A:46:LEU:HG	1:A:47:GLU:N	2.31	0.45
1:A:142:SER:HA	1:A:143:PRO:HA	1.49	0.45
1:A:199:LYS:HB2	1:A:199:LYS:HE3	1.51	0.45
1:B:2:VAL:HG13	1:B:23:LEU:HD23	1.99	0.45
1:A:436:LEU:HA	1:A:436:LEU:HD12	1.77	0.45
1:A:155:ASN:ND2	1:A:213:GLY:H	2.15	0.44
1:B:2:VAL:CG1	1:B:23:LEU:HD21	2.47	0.44
1:B:260:LEU:HD23	1:B:260:LEU:HA	1.59	0.44
1:B:373:HIS:CD2	1:B:373:HIS:H	2.36	0.44
1:A:200:ARG:HB3	1:A:201:TYR:CD2	2.52	0.44
1:A:296:ASP:N	1:A:297:PRO:CD	2.80	0.44
1:B:296:ASP:OD2	1:B:320:ASP:HB3	2.17	0.44
1:B:377:GLU:HB3	1:B:404:GLU:HB2	1.99	0.44
1:A:73:ALA:HB3	1:A:74:PRO:HD3	1.98	0.43
1:B:129:LEU:HG	1:B:133:LEU:HD22	2.00	0.43
1:B:18:THR:OG1	1:B:19:VAL:N	2.51	0.43
1:B:434:ASP:OD1	1:B:435:LYS:HD2	2.18	0.43
1:A:253:PHE:CZ	1:A:256:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLU:CD	1:B:304:GLU:N	2.68	0.43
1:A:422:ASN:HD22	1:A:422:ASN:HA	1.67	0.43
1:A:401:ALA:O	1:A:402:ARG:HB2	2.18	0.43
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.81	0.43
1:B:227:LEU:HD22	1:B:227:LEU:HA	1.62	0.43
1:A:344:LEU:C	1:A:344:LEU:HD23	2.43	0.42
1:B:200:ARG:HD2	1:B:227:LEU:HD21	2.01	0.42
1:B:296:ASP:HA	1:B:306:TRP:CH2	2.54	0.42
1:B:369:VAL:O	1:B:392:THR:HB	2.19	0.42
1:A:4:LYS:HG2	1:A:5:VAL:H	1.82	0.42
1:B:275:GLY:N	1:B:276:PRO:HD2	2.35	0.42
1:A:52:ASP:O	1:A:58:GLY:HA2	2.19	0.42
1:A:140:LYS:HG2	1:A:142:SER:H	1.85	0.42
1:A:155:ASN:HD22	1:A:209:GLY:HA3	1.83	0.42
1:A:133:LEU:HD23	1:A:386:LEU:HA	2.01	0.42
1:B:133:LEU:HD12	1:B:136:LEU:HD12	2.02	0.41
1:B:153:VAL:H	1:B:153:VAL:HG22	1.54	0.41
1:A:369:VAL:O	1:A:392:THR:HB	2.20	0.41
1:A:391:ARG:NH1	1:A:436:LEU:O	2.47	0.41
1:B:289:TYR:O	1:B:291:ILE:N	2.46	0.41
1:A:274:THR:CB	1:A:276:PRO:HD2	2.50	0.41
1:A:167:GLN:NE2	1:A:168:GLU:OE2	2.52	0.41
1:A:259:ASP:OD2	1:A:262:PHE:HA	2.20	0.41
1:A:328:LYS:HD2	4:A:613:HOH:O	2.21	0.41
1:B:199:LYS:HE3	1:B:199:LYS:HB2	1.82	0.41
1:B:344:LEU:HD23	1:B:344:LEU:C	2.45	0.41
1:A:96:LEU:HD12	1:A:96:LEU:HA	1.79	0.41
1:B:97:ASP:CG	1:B:102:LYS:HA	2.45	0.41
1:A:167:GLN:HG2	1:A:168:GLU:HG2	2.02	0.41
1:A:274:THR:OG1	1:A:276:PRO:HD2	2.21	0.41
1:B:289:TYR:HB3	1:B:290:PRO:HD2	2.03	0.41
1:B:406:LEU:HD13	1:B:406:LEU:HA	1.77	0.41
1:A:373:HIS:CD2	1:A:373:HIS:N	2.89	0.40
1:B:378:THR:O	1:B:408:LYS:NZ	2.55	0.40
1:A:35:PRO:HB2	1:A:374:ARG:HG2	2.02	0.40
1:A:373:HIS:CG	1:A:397:THR:HA	2.57	0.40
1:B:144:TYR:CB	1:B:419:LEU:HD13	2.51	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	434/436 (100%)	420 (97%)	13 (3%)	1 (0%)	43	44
1	B	434/436 (100%)	418 (96%)	15 (4%)	1 (0%)	43	44
All	All	868/872 (100%)	838 (96%)	28 (3%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	ARG
1	B	402	ARG

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	344/344 (100%)	310 (90%)	34 (10%)	7	5
1	B	344/344 (100%)	307 (89%)	37 (11%)	6	4
All	All	688/688 (100%)	617 (90%)	71 (10%)	7	4

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	23	LEU
1	A	32	SER
1	A	53	LYS

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Mol	Chain	Res	Type
1	A	55	LYS
1	A	66	LYS
1	A	81	ILE
1	A	84	LYS
1	A	101	ASN
1	A	103	SER
1	A	108	ASN
1	A	111	LEU
1	A	125	LYS
1	A	126	ASN
1	A	131	LYS
1	A	133	LEU
1	A	151	LEU
1	A	166	LEU
1	A	194	LYS
1	A	195	SER
1	A	196	LEU
1	A	199	LYS
1	A	200	ARG
1	A	204	SER
1	A	219	GLN
1	A	238	ASP
1	A	255	ASP
1	A	304	GLU
1	A	307	SER
1	A	317	ILE
1	A	347	ASN
1	A	379	GLU
1	A	403	SER
1	A	436	LEU
1	B	3	SER
1	B	23	LEU
1	B	26	GLU
1	B	32	SER
1	B	55	LYS
1	B	57	MET
1	B	82	ASP
1	B	133	LEU
1	B	138	LYS
1	B	140	LYS
1	B	142	SER
1	B	166	LEU

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Mol	Chain	Res	Type
1	B	177	LYS
1	B	195	SER
1	B	196	LEU
1	B	204	SER
1	B	227	LEU
1	B	229	VAL
1	B	233	LYS
1	B	254	LYS
1	B	255	ASP
1	B	270	SER
1	B	281	LEU
1	B	284	SER
1	B	304	GLU
1	B	317	ILE
1	B	335	GLU
1	B	347	ASN
1	B	349	ILE
1	B	355	SER
1	B	357	LYS
1	B	392	THR
1	B	396	LYS
1	B	417	GLU
1	B	418	GLU
1	B	424	VAL
1	B	436	LEU

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

Mol	Chain	Res	Type
1	A	63	HIS
1	A	67	ASN
1	A	101	ASN
1	A	126	ASN
1	A	155	ASN
1	A	219	GLN
1	A	422	ASN
1	B	43	HIS
1	B	80	ASN
1	B	126	ASN
1	B	152	ASN
1	B	217	ASN
1	B	316	GLN

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Mol	Chain	Res	Type
1	B	394	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 6 ligands modelled in this entry, 4 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
3	PAH	A	440	2	8,8,8	2.29	3 (37%)	10,11,11	2.20	3 (30%)
3	PAH	B	440	2	8,8,8	1.57	2 (25%)	10,11,11	1.62	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PAH	A	440	2	-	1/7/7/7	-
3	PAH	B	440	2	-	5/7/7/7	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	440	PAH	P-C1	4.84	1.87	1.79
3	A	440	PAH	O2-C2	3.46	1.30	1.23
3	B	440	PAH	O2-C2	3.05	1.29	1.23
3	A	440	PAH	P-O1P	2.16	1.54	1.50
3	B	440	PAH	P-C1	-2.06	1.76	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	440	PAH	C1-C2-N3	4.02	119.37	114.87
3	A	440	PAH	O3-N3-C2	-3.93	113.98	119.79
3	B	440	PAH	C1-C2-N3	3.48	118.77	114.87
3	A	440	PAH	O2-C2-N3	-3.08	119.49	123.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	440	PAH	C2-C1-P-O1P
3	B	440	PAH	C2-C1-P-O3P
3	B	440	PAH	C1-C2-N3-O3
3	B	440	PAH	O2-C2-N3-O3
3	B	440	PAH	C2-C1-P-O2P
3	A	440	PAH	C2-C1-P-O1P

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

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.