Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2024 – 01:11 PM EST

PDB ID	:	1EBG
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
Authors	:	Wedekind, J.E.; Reed, G.H.; Rayment, I.
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 (i) 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 (i)) were used in the production of this report:

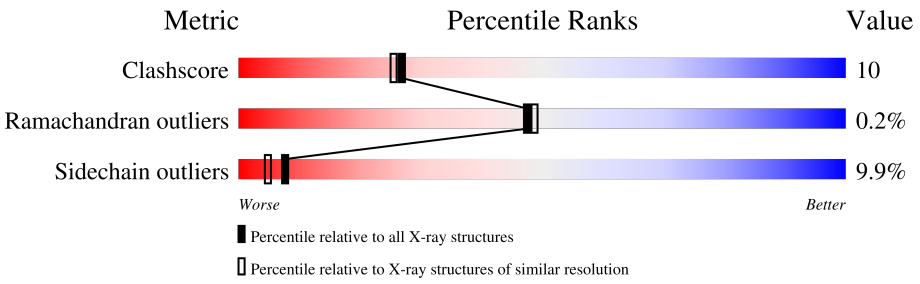
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	70% 24% 5%
1	B	436	66% 27% 7%

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.

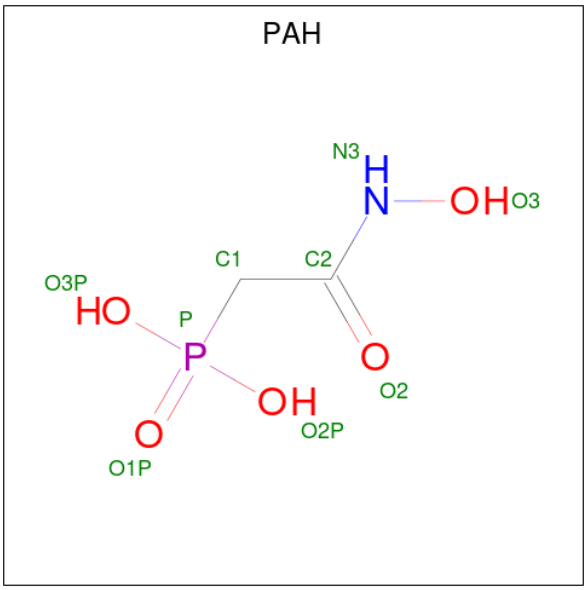
- Molecule 1 is a protein called ENOLASE.

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHONOACETOHYDROXAMIC ACID (three-letter code: PAH) (formula: $C_2H_6NO_5P$).



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

- Molecule 4 is water.

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

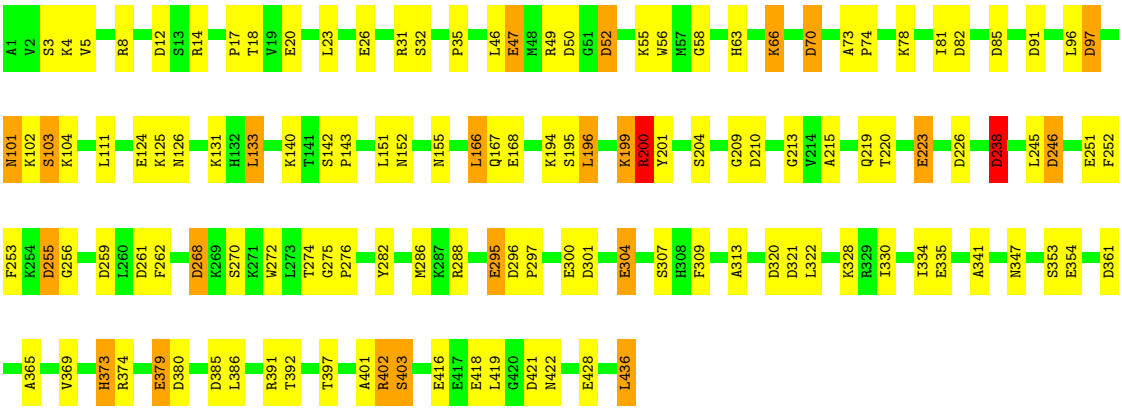
3 Residue-property plots (i)

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.

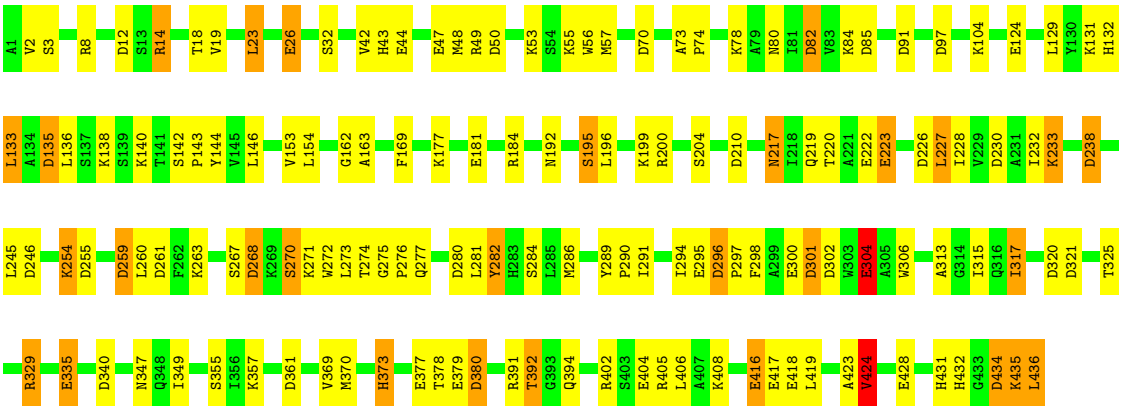
• Molecule 1: ENOLASE

Chain A: 70% 24% 5%



• Molecule 1: ENOLASE

Chain B: 66% 27% 7%



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.07	16/3352 (0.5%)	1.39	54/4534 (1.2%)
1	B	1.05	17/3352 (0.5%)	1.42	62/4534 (1.4%)
All	All	1.06	33/6704 (0.5%)	1.41	116/9068 (1.3%)

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 (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	416	GLU	CD-OE2	8.25	1.34	1.25
1	B	335	GLU	CD-OE1	7.28	1.33	1.25
1	A	295	GLU	CD-OE2	7.18	1.33	1.25
1	B	417	GLU	CD-OE1	7.17	1.33	1.25
1	A	304	GLU	CD-OE1	7.00	1.33	1.25
1	A	379	GLU	CD-OE1	6.96	1.33	1.25
1	A	416	GLU	CD-OE2	6.91	1.33	1.25
1	B	295	GLU	CD-OE2	6.88	1.33	1.25
1	B	47	GLU	CD-OE1	6.77	1.33	1.25
1	B	304	GLU	CD-OE1	6.69	1.33	1.25
1	A	335	GLU	CD-OE1	-6.34	1.18	1.25
1	A	418	GLU	CD-OE1	6.31	1.32	1.25
1	A	124	GLU	CD-OE2	6.31	1.32	1.25
1	A	47	GLU	CD-OE2	-6.14	1.18	1.25
1	A	251	GLU	CD-OE2	6.09	1.32	1.25
1	B	428	GLU	CD-OE2	6.05	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	428	GLU	CD-OE2	6.02	1.32	1.25
1	B	181	GLU	CD-OE2	5.97	1.32	1.25
1	B	26	GLU	CD-OE1	5.90	1.32	1.25
1	B	222	GLU	CD-OE2	5.88	1.32	1.25
1	B	329	ARG	CZ-NH2	5.86	1.40	1.33
1	A	26	GLU	CD-OE1	5.82	1.32	1.25
1	B	379	GLU	CD-OE1	-5.81	1.19	1.25
1	A	354	GLU	CD-OE2	5.71	1.31	1.25
1	B	405	ARG	CZ-NH1	5.67	1.40	1.33
1	B	223	GLU	CD-OE2	5.53	1.31	1.25
1	A	47	GLU	CD-OE1	5.46	1.31	1.25
1	A	223	GLU	CD-OE1	5.46	1.31	1.25
1	B	44	GLU	CD-OE2	5.45	1.31	1.25
1	A	335	GLU	CD-OE2	5.41	1.31	1.25
1	A	20	GLU	CD-OE1	-5.37	1.19	1.25
1	B	124	GLU	CD-OE2	5.36	1.31	1.25
1	B	14	ARG	CD-NE	-5.33	1.37	1.46

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	14	ARG	NE-CZ-NH2	-14.54	113.03	120.30
1	B	340	ASP	CB-CG-OD2	-11.86	107.63	118.30
1	A	14	ARG	NE-CZ-NH2	-11.51	114.54	120.30
1	B	97	ASP	CB-CG-OD2	-11.35	108.08	118.30
1	B	391	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	A	91	ASP	CB-CG-OD2	-9.43	109.81	118.30
1	A	321	ASP	CB-CG-OD2	-9.38	109.86	118.30
1	B	340	ASP	CB-CG-OD1	9.29	126.66	118.30
1	B	226	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	B	405	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	14	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	321	ASP	CB-CG-OD1	8.98	126.39	118.30
1	A	361	ASP	CB-CG-OD1	8.98	126.38	118.30
1	A	52	ASP	CB-CG-OD1	-8.69	110.48	118.30
1	A	12	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	B	85	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	A	12	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	97	ASP	CB-CG-OD1	7.83	125.34	118.30
1	A	380	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	255	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	A	238	ASP	CB-CG-OD2	-7.68	111.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	91	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	B	280	ASP	CB-CG-OD1	7.64	125.17	118.30
1	B	135	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	B	85	ASP	CB-CG-OD1	7.40	124.96	118.30
1	B	135	ASP	CB-CG-OD1	7.37	124.93	118.30
1	B	12	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	97	ASP	CB-CG-OD1	7.24	124.82	118.30
1	B	184	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	B	12	ASP	CB-CG-OD1	7.18	124.76	118.30
1	B	329	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	B	301	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	49	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	8	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	B	82	ASP	CB-CG-OD1	6.92	124.53	118.30
1	B	361	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	A	403	SER	N-CA-CB	6.85	120.78	110.50
1	A	91	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	226	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	B	246	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	A	246	ASP	N-CA-CB	6.77	122.79	110.60
1	A	85	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	97	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	B	296	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	50	ASP	CB-CG-OD1	6.68	124.32	118.30
1	B	434	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	B	70	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	302	ASP	CB-CG-OD2	6.60	124.24	118.30
1	B	361	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	301	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	85	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	A	261	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	200	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	434	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	210	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	B	184	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	49	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	52	ASP	N-CA-CB	-6.20	99.43	110.60
1	A	226	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	380	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	A	361	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	A	320	ASP	CB-CG-OD1	6.15	123.83	118.30
1	B	226	ASP	CB-CG-OD1	6.14	123.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	14	ARG	CB-CA-C	-6.11	98.17	110.40
1	A	210	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	385	ASP	CB-CG-OD1	-6.11	112.81	118.30
1	B	238	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	259	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	50	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	421	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	50	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	302	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	B	380	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	238	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	82	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	238	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	230	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	B	261	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	385	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	8	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	268	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	B	246	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	391	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	268	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	A	301	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	259	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	91	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	341	ALA	N-CA-CB	5.68	118.06	110.10
1	A	210	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	210	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	261	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	245	LEU	CB-CA-C	-5.60	99.56	110.20
1	B	268	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	246	ASP	N-CA-CB	5.57	120.62	110.60
1	A	313	ALA	CB-CA-C	5.56	118.44	110.10
1	B	280	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	70	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	215	ALA	N-CA-CB	-5.50	102.40	110.10
1	B	230	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	424	VAL	CB-CA-C	-5.45	101.05	111.40
1	B	49	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	31	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	82	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	288	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	296	ASP	CB-CG-OD1	5.35	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	321	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	B	282	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	A	18	THR	N-CA-CB	5.18	120.13	110.30
1	B	48	MET	N-CA-CB	-5.16	101.31	110.60
1	A	353	SER	N-CA-CB	5.12	118.17	110.50
1	A	421	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	82	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	B	70	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	200	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	273	LEU	CB-CA-C	-5.02	100.65	110.20
1	B	184	ARG	CA-CB-CG	-5.02	102.36	113.40

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 (i)

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	60	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	135	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 (135) 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:ND2	1:A:101:ASN:H	1.54	1.03
1:A:101:ASN:N	1:A:101:ASN:HD22	1.55	0.99
1:A:101:ASN:H	1:A:101:ASN:HD22	0.92	0.88
1:A:238:ASP:HB2	4:A:614:HOH:O	1.77	0.82
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:B:304:GLU:H	1:B:304:GLU:CD	1.90	0.74
1:A:4:LYS:HG2	1:A:5:VAL:N	2.03	0.72
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:ND2	1:A:101:ASN:N	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:B:286:MET:CE	1:B:315:ILE:HD11	2.30	0.62
1:A:246:ASP:HA	1:A:295:GLU:HB3	1.81	0.62
1:B:313:ALA:HB1	1:B:317:ILE:CD1	2.31	0.61
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:HIS:CD2	1:B:432:HIS:NE2	2.78	0.52
1:B:56:TRP:C	1:B:57:MET:HG2	2.29	0.52
1:B:286:MET:HE2	1:B:315:ILE:HD11	1.92	0.52
1:B:78:LYS:HG3	1:B:78:LYS:O	2.09	0.51
1:A:268:ASP:OD2	1:A:270:SER:OG	2.29	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: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:286:MET:HE1	1:A:309:PHE:HZ	1.78	0.47
1:A:17:PRO:HG3	1:A:56:TRP:CD1	2.48	0.47
1:B:144:TYR:HB2	1:B:419:LEU:HD13	1.95	0.47
1:B:286:MET:HE1	1:B:315:ILE:HD11	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:66:LYS:NZ	1:A:70:ASP:OD2	2.35	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:B:192:ASN:O	1:B:195:SER:OG	2.29	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:B:268:ASP:OD2	1:B:270:SER:OG	2.34	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
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:42:VAL:HG22	1:B:300:GLU:CD	2.38	0.43
1:B:227:LEU:HD22	1:B:227:LEU:HA	1.62	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LYS:HE3	1:B:199:LYS:HB2	1.82	0.41
1:A:96:LEU:HD12	1:A:96:LEU:HA	1.79	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 (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	434/436 (100%)	420 (97%)	13 (3%)	1 (0%)	47 49
1	B	434/436 (100%)	418 (96%)	15 (4%)	1 (0%)	47 49
All	All	868/872 (100%)	838 (96%)	28 (3%)	2 (0%)	47 49

All (2) Ramachandran outliers are listed below:

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

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	344/344 (100%)	312 (91%)	32 (9%)	9 6
1	B	344/344 (100%)	308 (90%)	36 (10%)	7 4
All	All	688/688 (100%)	620 (90%)	68 (10%)	8 5

All (68) 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	55	LYS
1	A	66	LYS
1	A	81	ILE
1	A	101	ASN
1	A	103	SER
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	152	ASN
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

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Mol	Chain	Res	Type
1	A	347	ASN
1	A	373	HIS
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	80	ASN
1	B	133	LEU
1	B	138	LYS
1	B	140	LYS
1	B	142	SER
1	B	177	LYS
1	B	195	SER
1	B	196	LEU
1	B	204	SER
1	B	217	ASN
1	B	227	LEU
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	329	ARG
1	B	335	GLU
1	B	347	ASN
1	B	349	ILE
1	B	355	SER
1	B	357	LYS
1	B	373	HIS
1	B	392	THR
1	B	418	GLU
1	B	424	VAL
1	B	435	LYS
1	B	436	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

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	152	ASN
1	A	155	ASN
1	A	422	ASN
1	B	43	HIS
1	B	80	ASN
1	B	167	GLN
1	B	217	ASN
1	B	422	ASN

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 monosaccharides 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	2.23	3 (37%)	10,11,11	2.19	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PAH	B	440	2	8,8,8	1.54	1 (12%)	10,11,11	1.60	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	-	0/7/7/7	-
3	PAH	B	440	2	-	5/7/7/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	440	PAH	P-C1	4.69	1.87	1.79
3	A	440	PAH	O2-C2	3.37	1.30	1.23
3	B	440	PAH	O2-C2	2.97	1.29	1.23
3	A	440	PAH	P-O1P	2.09	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	440	PAH	C1-C2-N3	3.99	119.37	115.08
3	A	440	PAH	O3-N3-C2	-3.93	113.98	119.79
3	B	440	PAH	C1-C2-N3	3.43	118.77	115.08
3	A	440	PAH	O2-C2-N3	-3.08	119.49	123.27

There are no chirality outliers.

All (5) 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

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.