



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 04:53 PM EST

PDB ID : 3ENL
Title : REFINED STRUCTURE OF YEAST APO-ENOLASE AT 2.25
ANGSTROMS RESOLUTION
Authors : Lebioda, L.; Stec, B.
Deposited on : unknown
Resolution : 2.25 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

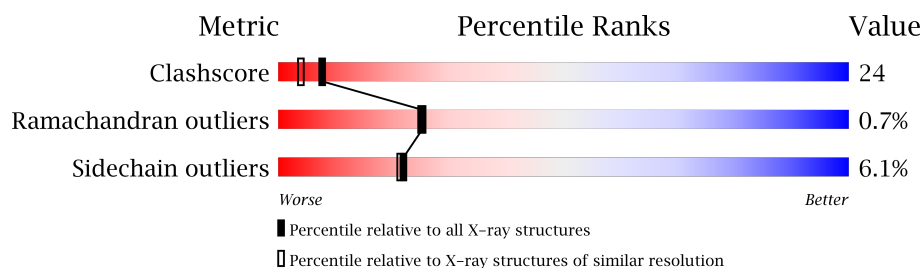
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)

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	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3647 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	3289	2076	569	638	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	SER	LYS	CONFLICT	UNP P00924

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is water.

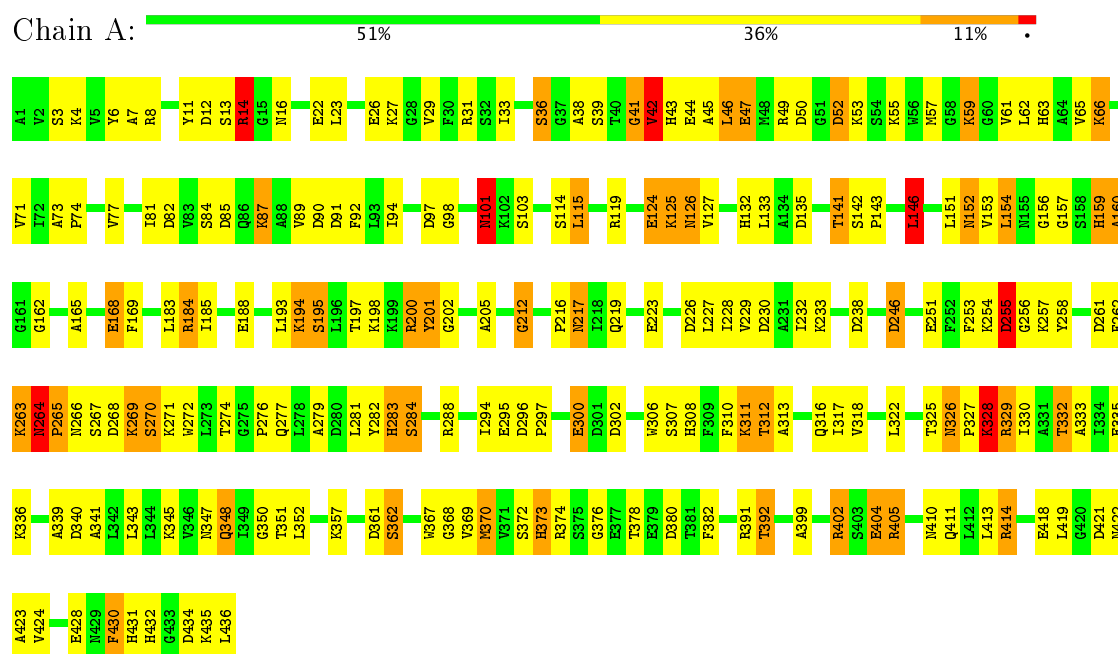
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	353	Total 353	O 353	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.10 Å 124.10 Å 66.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3647	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: SO4

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	1.03	1/3349 (0.0%)	2.39	146/4531 (3.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	ARG	CD-NE	5.09	1.55	1.46

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ARG	NE-CZ-NH2	32.38	136.49	120.30
1	A	49	ARG	NE-CZ-NH1	25.80	133.20	120.30
1	A	49	ARG	CD-NE-CZ	20.97	152.96	123.60
1	A	340	ASP	CB-CG-OD1	19.40	135.76	118.30
1	A	414	ARG	NE-CZ-NH2	-19.20	110.70	120.30
1	A	329	ARG	CD-NE-CZ	18.64	149.70	123.60
1	A	414	ARG	NE-CZ-NH1	15.94	128.27	120.30
1	A	361	ASP	CB-CG-OD2	-15.58	104.28	118.30
1	A	184	ARG	NE-CZ-NH1	-15.47	112.57	120.30
1	A	8	ARG	NE-CZ-NH1	15.17	127.89	120.30
1	A	119	ARG	NE-CZ-NH2	12.46	126.53	120.30
1	A	288	ARG	NE-CZ-NH2	11.92	126.26	120.30
1	A	329	ARG	NE-CZ-NH1	-11.82	114.39	120.30
1	A	184	ARG	CD-NE-CZ	-11.39	107.66	123.60
1	A	49	ARG	NE-CZ-NH2	-10.67	114.96	120.30
1	A	223	GLU	OE1-CD-OE2	10.56	135.97	123.30
1	A	405	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	A	226	ASP	CB-CG-OD2	-10.27	109.06	118.30
1	A	154	LEU	CA-CB-CG	10.06	138.45	115.30
1	A	391	ARG	NE-CZ-NH1	9.90	125.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLU	OE1-CD-OE2	9.88	135.16	123.30
1	A	255	ASP	CB-CG-OD2	-9.88	109.41	118.30
1	A	340	ASP	CB-CG-OD2	-9.70	109.57	118.30
1	A	329	ARG	NH1-CZ-NH2	-9.36	109.10	119.40
1	A	223	GLU	CG-CD-OE2	-8.91	100.49	118.30
1	A	26	GLU	OE1-CD-OE2	8.72	133.77	123.30
1	A	380	ASP	CB-CG-OD2	8.54	125.99	118.30
1	A	85	ASP	CB-CG-OD1	8.52	125.97	118.30
1	A	41	GLY	N-CA-C	8.45	134.22	113.10
1	A	12	ASP	CB-CG-OD2	8.39	125.85	118.30
1	A	14	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	A	434	ASP	CB-CG-OD1	8.32	125.79	118.30
1	A	246	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	200	ARG	CD-NE-CZ	8.04	134.86	123.60
1	A	269	LYS	N-CA-CB	8.04	125.07	110.60
1	A	8	ARG	NH1-CZ-NH2	-7.92	110.69	119.40
1	A	200	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	A	124	GLU	OE1-CD-OE2	7.89	132.77	123.30
1	A	168	GLU	OE1-CD-OE2	-7.73	114.02	123.30
1	A	124	GLU	CG-CD-OE1	-7.71	102.87	118.30
1	A	282	TYR	CB-CG-CD2	-7.71	116.38	121.00
1	A	226	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	135	ASP	CB-CG-OD2	7.56	125.10	118.30
1	A	372	SER	N-CA-CB	-7.52	99.22	110.50
1	A	325	THR	CA-CB-CG2	7.42	122.79	112.40
1	A	258	TYR	CB-CG-CD2	-7.39	116.56	121.00
1	A	31	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	328	LYS	N-CA-CB	7.30	123.75	110.60
1	A	402	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	263	LYS	CB-CA-C	7.21	124.82	110.40
1	A	184	ARG	CG-CD-NE	-7.20	96.68	111.80
1	A	246	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	119	ARG	CD-NE-CZ	7.04	133.46	123.60
1	A	200	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	328	LYS	CB-CG-CD	6.98	129.75	111.60
1	A	348	GLN	N-CA-CB	6.97	123.15	110.60
1	A	246	ASP	N-CA-CB	6.89	123.01	110.60
1	A	49	ARG	NH1-CZ-NH2	-6.88	111.83	119.40
1	A	418	GLU	CA-CB-CG	6.78	128.32	113.40
1	A	146	LEU	CB-CA-C	6.78	123.07	110.20
1	A	59	LYS	N-CA-CB	6.70	122.67	110.60
1	A	6	TYR	CB-CG-CD1	-6.69	116.98	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASP	CB-CG-OD1	-6.68	112.28	118.30
1	A	279	ALA	N-CA-CB	6.65	119.41	110.10
1	A	391	ARG	NH1-CZ-NH2	-6.63	112.11	119.40
1	A	428	GLU	CB-CG-CD	6.61	132.04	114.20
1	A	125	LYS	CA-CB-CG	6.60	127.92	113.40
1	A	7	ALA	N-CA-CB	6.52	119.22	110.10
1	A	302	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	168	GLU	CG-CD-OE2	6.46	131.22	118.30
1	A	362	SER	O-C-N	6.42	132.98	122.70
1	A	82	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	411	GLN	CG-CD-OE1	6.39	134.38	121.60
1	A	201	TYR	CB-CG-CD2	6.39	124.83	121.00
1	A	265	PRO	C-N-CA	6.38	137.64	121.70
1	A	404	GLU	CG-CD-OE2	-6.37	105.57	118.30
1	A	340	ASP	O-C-N	6.32	132.82	122.70
1	A	352	LEU	CB-CA-C	6.29	122.15	110.20
1	A	47	GLU	CG-CD-OE1	-6.23	105.85	118.30
1	A	402	ARG	CD-NE-CZ	-6.19	114.94	123.60
1	A	351	THR	N-CA-CB	6.14	121.97	110.30
1	A	11	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	A	255	ASP	O-C-N	6.04	133.46	123.20
1	A	36	SER	CB-CA-C	6.02	121.54	110.10
1	A	195	SER	CB-CA-C	-6.02	98.67	110.10
1	A	357	LYS	CD-CE-NZ	-5.98	97.94	111.70
1	A	350	GLY	CA-C-N	5.96	130.32	117.20
1	A	251	GLU	CG-CD-OE1	-5.95	106.39	118.30
1	A	307	SER	CA-CB-OG	-5.92	95.21	111.20
1	A	302	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	46	LEU	CA-C-N	-5.80	104.45	117.20
1	A	115	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	361	ASP	OD1-CG-OD2	5.76	134.24	123.30
1	A	227	LEU	CB-CA-C	5.73	121.08	110.20
1	A	312	THR	N-CA-CB	-5.71	99.44	110.30
1	A	258	TYR	CG-CD1-CE1	-5.70	116.74	121.30
1	A	270	SER	CB-CA-C	5.68	120.89	110.10
1	A	370	MET	CG-SD-CE	5.67	109.28	100.20
1	A	26	GLU	CG-CD-OE1	-5.66	106.98	118.30
1	A	283	HIS	C-N-CA	5.65	135.83	121.70
1	A	284	SER	CB-CA-C	-5.65	99.36	110.10
1	A	22	GLU	O-C-N	5.63	131.72	122.70
1	A	428	GLU	CA-CB-CG	5.59	125.70	113.40
1	A	89	VAL	CA-CB-CG2	5.58	119.27	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	GLY	N-CA-C	5.57	127.02	113.10
1	A	11	TYR	CB-CG-CD1	5.56	124.34	121.00
1	A	55	LYS	O-C-N	5.54	131.56	122.70
1	A	340	ASP	CA-C-O	-5.51	108.52	120.10
1	A	127	VAL	CA-CB-CG2	5.51	119.16	110.90
1	A	188	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	A	45	ALA	CB-CA-C	5.46	118.29	110.10
1	A	421	ASP	CA-CB-CG	5.46	125.41	113.40
1	A	332	THR	CA-CB-CG2	5.44	120.02	112.40
1	A	141	THR	CA-CB-CG2	5.43	120.00	112.40
1	A	294	ILE	N-CA-CB	5.41	123.24	110.80
1	A	156	GLY	N-CA-C	-5.37	99.69	113.10
1	A	333	ALA	CB-CA-C	5.33	118.10	110.10
1	A	436	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	418	GLU	OE1-CD-OE2	5.31	129.67	123.30
1	A	159	HIS	CA-CB-CG	-5.31	104.58	113.60
1	A	311	LYS	CA-CB-CG	-5.28	101.79	113.40
1	A	368	GLY	N-CA-C	-5.27	99.93	113.10
1	A	152	ASN	CB-CG-OD1	-5.26	111.07	121.60
1	A	146	LEU	CA-CB-CG	-5.26	103.21	115.30
1	A	229	VAL	CB-CA-C	5.22	121.33	111.40
1	A	263	LYS	C-N-CA	5.21	134.73	121.70
1	A	160	ALA	O-C-N	5.21	132.05	123.20
1	A	42	VAL	CA-CB-CG1	5.19	118.69	110.90
1	A	230	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	6	TYR	N-CA-CB	-5.18	101.28	110.60
1	A	184	ARG	NH1-CZ-NH2	5.15	125.07	119.40
1	A	311	LYS	O-C-N	-5.15	114.46	122.70
1	A	430	PHE	CB-CG-CD2	5.15	124.41	120.80
1	A	288	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	A	119	ARG	N-CA-CB	5.11	119.79	110.60
1	A	84	SER	O-C-N	5.09	130.85	122.70
1	A	141	THR	CA-CB-OG1	-5.09	98.30	109.00
1	A	169	PHE	O-C-N	5.08	130.83	122.70
1	A	101	ASN	CB-CG-OD1	-5.08	111.44	121.60
1	A	310	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	A	114	SER	N-CA-CB	-5.05	102.93	110.50
1	A	44	GLU	CG-CD-OE1	-5.04	108.22	118.30
1	A	276	PRO	CA-C-N	5.03	128.28	117.20
1	A	316	GLN	CG-CD-OE1	-5.02	111.56	121.60
1	A	212	GLY	CA-C-O	-5.02	111.57	120.60
1	A	217	ASN	CA-CB-CG	-5.01	102.37	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3289	0	3292	160	0
2	A	5	0	0	0	0
3	A	353	0	0	41	1
All	All	3647	0	3292	160	1

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 24.

All (160) 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:264:ASN:ND2	1:A:265:PRO:HA	1.20	1.41
1:A:264:ASN:HB3	1:A:267:SER:HB2	1.27	1.15
1:A:36:SER:O	3:A:617:HOH:O	1.71	1.08
1:A:264:ASN:ND2	1:A:265:PRO:CA	2.17	1.07
1:A:66:LYS:HE3	3:A:574:HOH:O	1.52	1.06
1:A:41:GLY:CA	1:A:46:LEU:HD21	1.87	1.05
1:A:269:LYS:HB2	3:A:709:HOH:O	1.58	1.03
1:A:268:ASP:HB3	1:A:271:LYS:HD2	1.37	1.02
1:A:264:ASN:HD22	1:A:265:PRO:HA	1.28	0.96
1:A:27:LYS:HE3	1:A:124:GLU:HA	1.45	0.95
1:A:38:ALA:O	1:A:47:GLU:HB3	1.65	0.95
1:A:264:ASN:CG	1:A:265:PRO:HA	1.86	0.95
1:A:327:PRO:HB3	3:A:653:HOH:O	1.66	0.94
1:A:4:LYS:HE2	3:A:604:HOH:O	1.73	0.88
1:A:41:GLY:N	1:A:46:LEU:HD21	1.88	0.87
1:A:152:ASN:HB2	3:A:797:HOH:O	1.74	0.86
1:A:66:LYS:HE2	3:A:505:HOH:O	1.76	0.85
1:A:264:ASN:CB	1:A:267:SER:HB2	2.06	0.83
1:A:73:ALA:HB3	1:A:74:PRO:HD3	1.60	0.81
1:A:233:LYS:HE3	1:A:238:ASP:OD2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:HIS:CD2	3:A:676:HOH:O	2.34	0.80
1:A:432:HIS:HD2	3:A:676:HOH:O	1.64	0.80
1:A:74:PRO:HA	3:A:678:HOH:O	1.82	0.80
1:A:126:ASN:ND2	3:A:669:HOH:O	2.14	0.79
1:A:269:LYS:O	1:A:269:LYS:HG2	1.85	0.76
1:A:27:LYS:CE	1:A:124:GLU:HA	2.15	0.76
1:A:257:LYS:HG3	3:A:619:HOH:O	1.84	0.76
1:A:41:GLY:HA2	1:A:46:LEU:HD21	1.67	0.75
1:A:313:ALA:HB1	1:A:317:ILE:HD11	1.67	0.75
1:A:268:ASP:CB	1:A:271:LYS:HD2	2.15	0.74
1:A:268:ASP:HB3	1:A:271:LYS:CD	2.18	0.73
1:A:265:PRO:HB2	3:A:745:HOH:O	1.90	0.72
1:A:327:PRO:CB	3:A:653:HOH:O	2.28	0.71
1:A:53:LYS:HG2	3:A:472:HOH:O	1.91	0.70
1:A:271:LYS:HB2	3:A:751:HOH:O	1.92	0.69
1:A:74:PRO:O	3:A:678:HOH:O	2.10	0.68
1:A:255:ASP:N	3:A:711:HOH:O	2.26	0.68
1:A:327:PRO:CG	3:A:653:HOH:O	2.42	0.67
1:A:264:ASN:CG	1:A:265:PRO:CA	2.58	0.66
1:A:41:GLY:HA3	1:A:46:LEU:HD21	1.73	0.66
1:A:228:ILE:O	1:A:232:ILE:HG13	1.96	0.66
1:A:33:ILE:HG22	1:A:378:THR:HG21	1.76	0.66
1:A:328:LYS:HG2	1:A:329:ARG:N	2.12	0.65
1:A:217:ASN:N	1:A:217:ASN:HD22	1.94	0.65
1:A:332:THR:HG22	1:A:336:LYS:HD2	1.77	0.64
1:A:347:ASN:OD1	1:A:374:ARG:NH1	2.29	0.63
1:A:125:LYS:HE3	1:A:132:HIS:CE1	2.34	0.63
1:A:50:ASP:OD2	1:A:62:LEU:HB2	1.99	0.63
1:A:264:ASN:HB2	1:A:267:SER:N	2.13	0.63
1:A:52:ASP:C	1:A:52:ASP:OD1	2.33	0.62
1:A:39:SER:HA	1:A:47:GLU:O	2.00	0.62
1:A:194:LYS:O	1:A:198:LYS:HG3	2.00	0.61
1:A:41:GLY:N	1:A:46:LEU:CD2	2.63	0.61
1:A:345:LYS:HB2	1:A:348:GLN:HG3	1.83	0.61
1:A:77:VAL:HB	3:A:678:HOH:O	2.02	0.60
1:A:326:ASN:HB3	1:A:329:ARG:HB2	1.84	0.60
1:A:332:THR:O	1:A:336:LYS:HG3	2.03	0.58
1:A:27:LYS:HE3	1:A:124:GLU:CA	2.27	0.58
1:A:300:GLU:O	1:A:322:LEU:HD12	2.05	0.57
1:A:313:ALA:CB	1:A:317:ILE:CD1	2.83	0.57
1:A:313:ALA:HB1	1:A:317:ILE:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:HIS:ND1	1:A:405:ARG:NH1	2.52	0.56
1:A:33:ILE:HD11	3:A:508:HOH:O	2.03	0.56
1:A:146:LEU:HD12	1:A:423:ALA:HB1	1.87	0.56
1:A:71:VAL:HG21	3:A:655:HOH:O	2.04	0.56
1:A:261:ASP:HA	3:A:734:HOH:O	2.04	0.56
1:A:312:THR:CG2	3:A:628:HOH:O	2.54	0.56
1:A:197:THR:HG22	1:A:205:ALA:HB1	1.86	0.56
1:A:435:LYS:HD2	3:A:699:HOH:O	2.05	0.56
1:A:143:PRO:HG2	1:A:424:VAL:HG13	1.88	0.55
1:A:328:LYS:HD2	3:A:529:HOH:O	2.07	0.54
1:A:87:LYS:HE2	1:A:91:ASP:OD2	2.07	0.54
1:A:308:HIS:O	1:A:311:LYS:HB2	2.08	0.53
1:A:217:ASN:N	1:A:217:ASN:ND2	2.55	0.53
1:A:219:GLN:HG2	3:A:591:HOH:O	2.07	0.53
1:A:73:ALA:HB3	1:A:74:PRO:CD	2.36	0.53
1:A:281:LEU:HD23	1:A:281:LEU:C	2.29	0.52
1:A:4:LYS:HE2	3:A:471:HOH:O	2.09	0.52
1:A:212:GLY:HA3	1:A:399:ALA:HB3	1.91	0.52
1:A:313:ALA:CB	1:A:317:ILE:HD11	2.36	0.52
1:A:39:SER:CB	1:A:47:GLU:O	2.58	0.51
1:A:264:ASN:CB	1:A:267:SER:CB	2.85	0.51
1:A:317:ILE:O	1:A:339:ALA:HB1	2.10	0.51
1:A:253:PHE:CZ	1:A:256:GLY:HA2	2.45	0.50
1:A:59:LYS:HE3	3:A:558:HOH:O	2.12	0.50
1:A:274:THR:OG1	1:A:277:GLN:HG3	2.10	0.50
1:A:281:LEU:O	1:A:281:LEU:HD23	2.12	0.50
1:A:125:LYS:HE3	1:A:132:HIS:ND1	2.27	0.50
1:A:200:ARG:HB3	3:A:763:HOH:O	2.11	0.50
1:A:162:GLY:HA2	1:A:219:GLN:HE22	1.77	0.49
1:A:61:VAL:O	1:A:65:VAL:HG23	2.12	0.49
1:A:63:HIS:CD2	3:A:679:HOH:O	2.66	0.49
1:A:165:ALA:HA	1:A:262:PHE:HE1	1.78	0.49
1:A:143:PRO:CG	1:A:424:VAL:HG13	2.44	0.48
1:A:216:PRO:C	1:A:217:ASN:HD22	2.16	0.48
1:A:246:ASP:HA	1:A:295:GLU:HB3	1.96	0.48
1:A:101:ASN:ND2	1:A:103:SER:OG	2.46	0.48
1:A:143:PRO:HB2	1:A:422:ASN:O	2.13	0.48
1:A:297:PRO:HD2	1:A:306:TRP:CH2	2.48	0.48
1:A:152:ASN:O	1:A:399:ALA:HB2	2.14	0.48
1:A:42:VAL:HG11	3:A:618:HOH:O	2.13	0.48
1:A:42:VAL:HG12	1:A:43:HIS:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:HIS:HD2	3:A:679:HOH:O	1.97	0.47
1:A:269:LYS:CG	1:A:269:LYS:O	2.55	0.47
1:A:369:VAL:O	1:A:392:THR:HB	2.14	0.47
1:A:152:ASN:ND2	1:A:168:GLU:HB3	2.29	0.47
1:A:162:GLY:O	1:A:263:LYS:HE3	2.14	0.47
1:A:42:VAL:HG12	1:A:43:HIS:H	1.79	0.47
1:A:159:HIS:O	1:A:160:ALA:HB2	2.14	0.47
1:A:410:ASN:O	1:A:414:ARG:HG3	2.14	0.46
1:A:97:ASP:C	3:A:764:HOH:O	2.54	0.46
1:A:268:ASP:OD1	1:A:270:SER:HB2	2.16	0.46
1:A:261:ASP:O	1:A:264:ASN:HB3	2.16	0.46
1:A:272:TRP:N	1:A:272:TRP:CD1	2.81	0.46
1:A:362:SER:O	1:A:367:TRP:HB2	2.15	0.46
1:A:153:VAL:HB	1:A:193:LEU:HD23	1.98	0.45
1:A:326:ASN:HA	1:A:327:PRO:HD3	1.81	0.45
1:A:201:TYR:HB2	1:A:205:ALA:CB	2.46	0.45
1:A:254:LYS:O	1:A:255:ASP:HB2	2.15	0.45
1:A:73:ALA:N	1:A:74:PRO:HD2	2.32	0.45
1:A:413:LEU:HA	1:A:413:LEU:HD23	1.85	0.44
1:A:269:LYS:HG3	1:A:272:TRP:CD2	2.52	0.44
1:A:318:VAL:HG22	1:A:341:ALA:HB3	1.98	0.44
1:A:115:LEU:HD22	1:A:382:PHE:CZ	2.52	0.44
1:A:125:LYS:O	1:A:126:ASN:CB	2.65	0.44
1:A:141:THR:O	3:A:589:HOH:O	2.21	0.44
1:A:312:THR:HG21	3:A:628:HOH:O	2.15	0.44
1:A:264:ASN:CG	1:A:265:PRO:C	2.76	0.44
1:A:81:ILE:HD11	1:A:92:PHE:CG	2.53	0.43
1:A:184:ARG:HD3	1:A:184:ARG:HH11	1.09	0.43
1:A:90:ASP:O	1:A:94:ILE:HG13	2.19	0.43
1:A:326:ASN:HD22	1:A:327:PRO:CD	2.32	0.43
1:A:14:ARG:HD2	1:A:376:GLY:HA2	1.99	0.43
1:A:185:ILE:HG21	1:A:185:ILE:HD13	1.69	0.43
1:A:39:SER:HB2	1:A:47:GLU:O	2.18	0.43
1:A:142:SER:HA	1:A:143:PRO:HA	1.64	0.42
1:A:257:LYS:HE3	1:A:269:LYS:HE2	2.02	0.42
1:A:38:ALA:C	1:A:47:GLU:HB3	2.35	0.42
1:A:343:LEU:HD12	1:A:370:MET:HB3	2.00	0.42
1:A:152:ASN:ND2	3:A:797:HOH:O	2.52	0.42
1:A:157:GLY:C	1:A:159:HIS:H	2.23	0.42
1:A:23:LEU:O	1:A:29:VAL:HA	2.20	0.42
1:A:313:ALA:CB	1:A:317:ILE:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASP:OD1	1:A:50:ASP:N	2.52	0.41
1:A:202:GLY:O	1:A:205:ALA:HB3	2.20	0.41
1:A:283:HIS:HE1	1:A:312:THR:O	2.04	0.41
1:A:152:ASN:CB	3:A:797:HOH:O	2.50	0.41
1:A:332:THR:O	1:A:335:GLU:HB3	2.21	0.41
1:A:73:ALA:N	1:A:74:PRO:CD	2.83	0.41
1:A:326:ASN:OD1	1:A:328:LYS:HE3	2.20	0.41
1:A:3:SER:O	1:A:4:LYS:HB2	2.20	0.41
1:A:327:PRO:HA	1:A:330:ILE:HB	2.03	0.41
1:A:16:ASN:ND2	3:A:558:HOH:O	2.48	0.41
1:A:184:ARG:NH1	3:A:540:HOH:O	2.53	0.41
1:A:430:PHE:CD1	1:A:431:HIS:N	2.89	0.41
1:A:183:LEU:HA	1:A:183:LEU:HD12	1.84	0.41
1:A:296:ASP:HA	1:A:306:TRP:CH2	2.56	0.41
1:A:13:SER:CB	1:A:404:GLU:HG3	2.51	0.40
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.90	0.40
1:A:66:LYS:HG3	3:A:680:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:474:HOH:O	3:A:665:HOH:O[4_564]	2.09	0.11

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%)	414 (95%)	17 (4%)	3 (1%)	25	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	264	ASN
1	A	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%)	323 (94%)	21 (6%)	22	21

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	57	MET
1	A	66	LYS
1	A	87	LYS
1	A	101	ASN
1	A	126	ASN
1	A	133	LEU
1	A	146	LEU
1	A	151	LEU
1	A	154	LEU
1	A	194	LYS
1	A	195	SER
1	A	255	ASP
1	A	264	ASN
1	A	266	ASN
1	A	284	SER
1	A	300	GLU
1	A	326	ASN
1	A	328	LYS
1	A	373	HIS
1	A	392	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	43	HIS
1	A	101	ASN
1	A	152	ASN
1	A	155	ASN
1	A	217	ASN
1	A	219	GLN
1	A	266	ASN

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 ⓘ

1 ligand is modelled in this entry.

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	$\# Z > 2$
2	SO4	A	444	-	4,4,4	0.73	0	6,6,6	1.20	0

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
2	SO4	A	444	-	-	0/0/0/0	0/0/0/0

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.