



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:42 PM UTC

PDB ID : 5ENL / pdb_00005enl
Title : INHIBITION OF ENOLASE: THE CRYSTAL STRUCTURES OF ENOLASE-CA²⁺-PHOSPHOGLYCERATE AND ENOLASE-ZN²⁺-PHOSPHOGLYCERATE COMPLEXES AT 2.2-ANGSTROMS RESOLUTION
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Deposited on : 1990-11-13
Resolution : 2.20 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

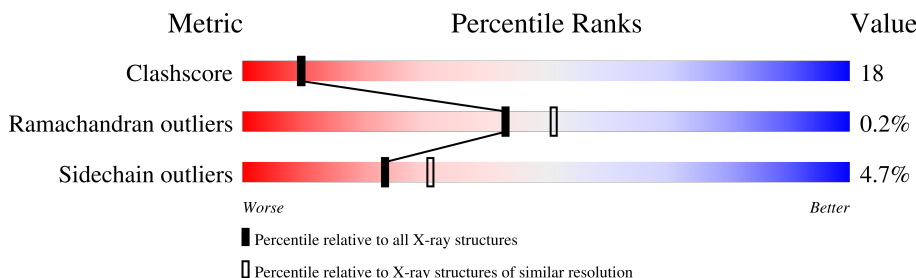
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3656 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
			3289	2076	569	638	6			

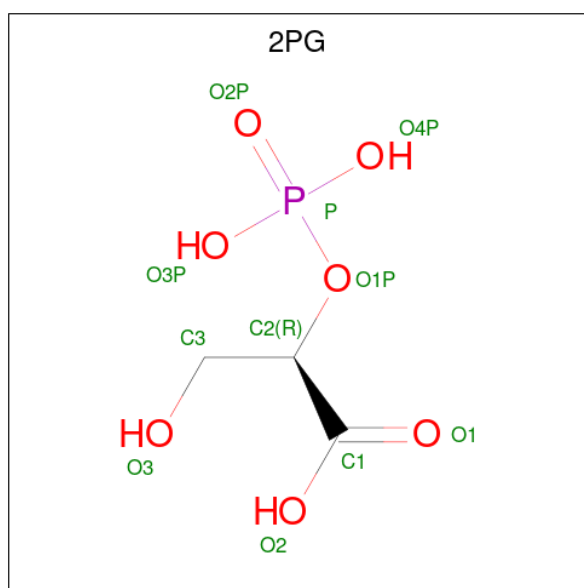
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2-PHOSPHOGLYCERIC ACID (CCD ID: 2PG) (formula: C₃H₇O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 4 is water.

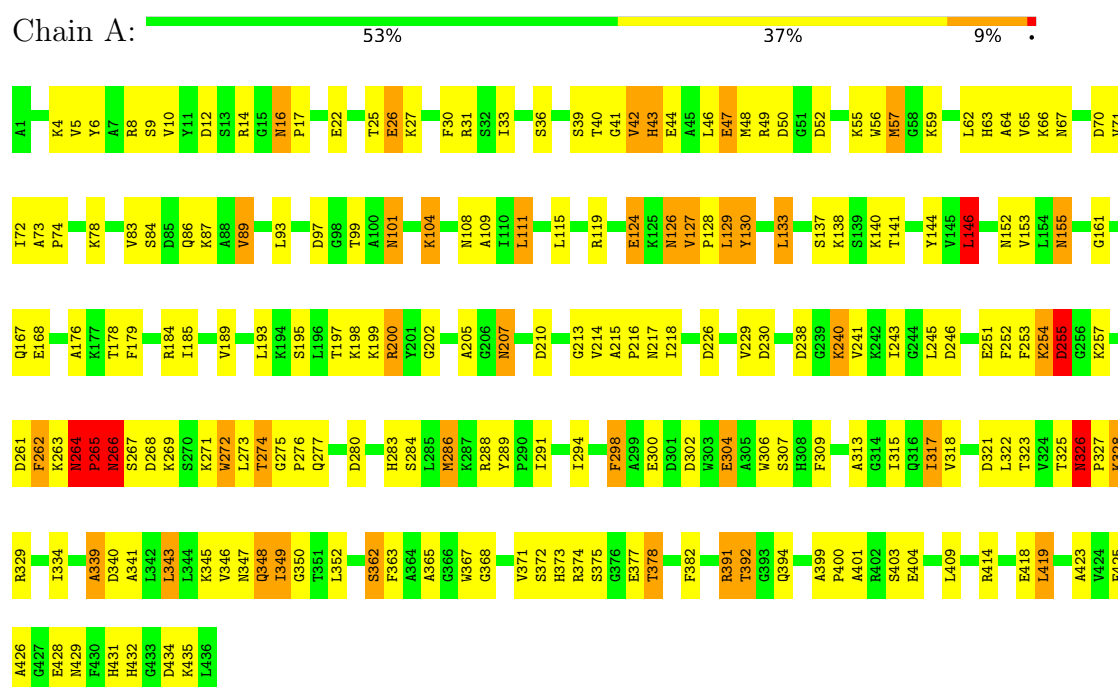
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	355	Total	O	0	0
			355	355		

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



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	124.10Å 124.10Å 66.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.148 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3656	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: CA, 2PG

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	1.19	2/3349 (0.1%)	2.34	180/4531 (4.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	GLY	N-CA	5.24	1.51	1.45
1	A	72	ILE	CA-CB	5.22	1.60	1.54

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASN	CA-CB-CG	-13.31	99.29	112.60
1	A	30	PHE	CA-CB-CG	-11.93	101.87	113.80
1	A	255	ASP	CA-C-O	-11.91	106.21	120.98
1	A	8	ARG	NE-CZ-NH1	11.37	132.87	121.50
1	A	298	PHE	CA-CB-CG	-10.79	103.01	113.80
1	A	126	ASN	CA-CB-CG	-10.11	102.49	112.60
1	A	329	ARG	CD-NE-CZ	10.02	138.42	124.40
1	A	161	GLY	N-CA-C	-9.43	98.27	112.41
1	A	8	ARG	NE-CZ-NH2	-9.20	110.92	119.20
1	A	141	THR	CA-C-N	-9.13	111.93	122.52
1	A	141	THR	C-N-CA	-9.13	111.93	122.52
1	A	126	ASN	OD1-CG-ND2	9.02	131.62	122.60
1	A	253	PHE	CA-CB-CG	8.92	122.72	113.80
1	A	140	LYS	CA-CB-CG	8.78	131.67	114.10
1	A	127	VAL	O-C-N	8.75	127.85	121.72
1	A	309	PHE	O-C-N	8.70	132.07	122.15
1	A	12	ASP	CA-CB-CG	8.56	121.16	112.60
1	A	42	VAL	N-CA-C	-8.34	96.19	108.87
1	A	146	LEU	CB-CA-C	8.01	120.16	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ASP	CA-CB-CG	7.91	120.51	112.60
1	A	304	GLU	CA-C-O	-7.90	112.17	120.55
1	A	161	GLY	CA-C-O	-7.86	114.42	122.28
1	A	414	ARG	CD-NE-CZ	-7.86	113.40	124.40
1	A	429	ASN	OD1-CG-ND2	7.81	130.41	122.60
1	A	263	LYS	CA-C-N	7.80	140.84	121.80
1	A	263	LYS	C-N-CA	7.80	140.84	121.80
1	A	184	ARG	CD-NE-CZ	7.70	135.18	124.40
1	A	238	ASP	CA-CB-CG	7.68	120.28	112.60
1	A	59	LYS	O-C-N	7.64	131.75	122.35
1	A	255	ASP	O-C-N	7.52	132.39	122.47
1	A	31	ARG	NE-CZ-NH1	7.51	129.01	121.50
1	A	210	ASP	CA-C-O	-7.49	112.55	120.63
1	A	429	ASN	CA-CB-CG	-7.47	105.13	112.60
1	A	274	THR	CA-C-O	-7.43	113.19	121.89
1	A	36	SER	CB-CA-C	7.39	123.07	109.46
1	A	372	SER	CA-C-O	7.36	129.72	121.11
1	A	246	ASP	N-CA-CB	7.34	122.83	110.87
1	A	289	TYR	O-C-N	7.34	128.11	121.80
1	A	264	ASN	N-CA-C	7.23	125.79	109.81
1	A	155	ASN	OD1-CG-ND2	7.17	129.77	122.60
1	A	349	ILE	CB-CA-C	7.10	118.62	110.88
1	A	391	ARG	CD-NE-CZ	-7.10	114.46	124.40
1	A	245	LEU	O-C-N	7.09	131.96	123.24
1	A	87	LYS	N-CA-CB	6.90	120.26	110.12
1	A	83	VAL	O-C-N	6.90	128.84	121.87
1	A	229	VAL	CB-CA-C	6.89	121.73	112.22
1	A	348	GLN	N-CA-CB	6.87	121.95	110.41
1	A	195	SER	CB-CA-C	-6.85	100.12	110.88
1	A	39	SER	N-CA-C	-6.84	104.82	113.72
1	A	288	ARG	CA-C-O	-6.75	111.37	119.27
1	A	404	GLU	N-CA-C	-6.74	104.32	112.54
1	A	43	HIS	CA-CB-CG	-6.65	107.15	113.80
1	A	10	VAL	CA-C-O	-6.65	112.47	120.78
1	A	253	PHE	O-C-N	6.65	130.80	123.22
1	A	215	ALA	O-C-N	6.63	126.03	121.19
1	A	309	PHE	CA-C-O	-6.63	113.39	120.42
1	A	108	ASN	CA-CB-CG	6.60	119.20	112.60
1	A	72	ILE	N-CA-C	6.52	116.55	110.42
1	A	251	GLU	CG-CD-OE1	-6.39	103.69	118.40
1	A	176	ALA	O-C-N	6.37	130.11	122.85
1	A	178	THR	O-C-N	6.36	130.41	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	LYS	CA-C-O	-6.36	112.22	119.78
1	A	70	ASP	CA-C-N	-6.35	116.74	122.97
1	A	70	ASP	C-N-CA	-6.35	116.74	122.97
1	A	414	ARG	NE-CZ-NH2	-6.35	113.48	119.20
1	A	426	ALA	CA-C-O	-6.33	113.11	120.20
1	A	368	GLY	N-CA-C	-6.33	102.89	112.89
1	A	352	LEU	CB-CA-C	6.33	120.90	110.90
1	A	419	LEU	CA-C-O	-6.29	112.73	119.97
1	A	184	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	A	49	ARG	NE-CZ-NH2	-6.26	113.57	119.20
1	A	226	ASP	CA-C-N	6.21	128.59	120.28
1	A	226	ASP	C-N-CA	6.21	128.59	120.28
1	A	217	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	A	214	VAL	CB-CA-C	6.20	118.41	111.59
1	A	286	MET	CA-C-O	-6.14	113.91	120.42
1	A	283	HIS	CA-CB-CG	-6.14	107.66	113.80
1	A	371	VAL	N-CA-C	-6.14	100.86	109.21
1	A	84	SER	N-CA-CB	6.09	119.71	110.28
1	A	262	PHE	CA-CB-CG	6.07	119.87	113.80
1	A	265	PRO	CA-C-N	6.03	133.06	121.54
1	A	265	PRO	C-N-CA	6.03	133.06	121.54
1	A	307	SER	CA-CB-OG	-6.03	99.05	111.10
1	A	59	LYS	CA-CB-CG	-5.99	102.11	114.10
1	A	185	ILE	CB-CG1-CD1	-5.99	101.23	113.80
1	A	425	PHE	CA-C-O	-5.96	113.80	120.54
1	A	318	VAL	CA-C-O	5.95	126.93	120.57
1	A	124	GLU	CB-CG-CD	5.94	122.70	112.60
1	A	195	SER	O-C-N	5.93	128.18	122.07
1	A	426	ALA	O-C-N	5.93	128.96	122.20
1	A	50	ASP	CA-C-O	-5.89	114.30	120.55
1	A	49	ARG	CD-NE-CZ	5.85	132.59	124.40
1	A	291	ILE	CA-C-N	5.85	128.64	122.14
1	A	291	ILE	C-N-CA	5.85	128.64	122.14
1	A	189	VAL	N-CA-CB	5.83	117.37	110.55
1	A	30	PHE	O-C-N	5.80	130.13	123.29
1	A	339	ALA	CA-C-O	-5.80	114.91	120.94
1	A	409	LEU	CA-C-N	5.77	128.01	120.28
1	A	409	LEU	C-N-CA	5.77	128.01	120.28
1	A	343	LEU	N-CA-C	-5.72	99.87	108.96
1	A	284	SER	N-CA-CB	-5.71	101.73	110.01
1	A	130	TYR	CA-C-O	-5.71	114.50	120.55
1	A	14	ARG	NE-CZ-NH2	-5.69	114.08	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	SER	O-C-N	5.69	129.45	122.34
1	A	200	ARG	N-CA-C	5.69	119.39	112.23
1	A	167	GLN	N-CA-C	5.68	118.68	111.69
1	A	78	LYS	CA-C-O	-5.68	114.53	120.55
1	A	371	VAL	O-C-N	5.68	129.42	122.72
1	A	280	ASP	N-CA-CB	5.66	118.44	110.12
1	A	272	TRP	CA-C-O	-5.61	115.44	121.56
1	A	119	ARG	CA-C-N	5.57	127.74	120.28
1	A	119	ARG	C-N-CA	5.57	127.74	120.28
1	A	217	ASN	CB-CA-C	5.56	120.45	111.05
1	A	243	ILE	CA-C-O	5.56	127.17	120.67
1	A	403	SER	CA-C-O	-5.55	112.77	119.49
1	A	326	ASN	OD1-CG-ND2	5.55	128.15	122.60
1	A	168	GLU	CB-CG-CD	5.54	122.03	112.60
1	A	401	ALA	CA-C-O	-5.54	114.79	120.89
1	A	198	LYS	O-C-N	5.53	127.99	122.12
1	A	26	GLU	CB-CA-C	-5.50	99.61	110.27
1	A	198	LYS	CA-C-O	-5.49	114.73	120.55
1	A	31	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	321	ASP	CA-C-O	-5.49	112.85	119.49
1	A	317	ILE	CB-CG1-CD1	-5.48	102.28	113.80
1	A	280	ASP	CA-C-O	-5.48	114.75	120.55
1	A	302	ASP	O-C-N	5.45	129.52	122.71
1	A	8	ARG	CD-NE-CZ	5.45	132.03	124.40
1	A	87	LYS	CA-C-O	-5.45	114.78	120.55
1	A	202	GLY	CA-C-O	5.45	125.76	122.22
1	A	414	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	A	241	VAL	O-C-N	5.42	129.11	123.26
1	A	47	GLU	CB-CA-C	5.41	119.42	109.46
1	A	350	GLY	N-CA-C	5.40	121.50	115.08
1	A	64	ALA	O-C-N	5.39	127.70	122.09
1	A	326	ASN	CA-C-N	5.39	125.47	119.32
1	A	326	ASN	C-N-CA	5.39	125.47	119.32
1	A	363	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	93	LEU	CA-C-N	5.38	127.34	120.56
1	A	93	LEU	C-N-CA	5.38	127.34	120.56
1	A	409	LEU	CA-C-O	-5.37	114.86	120.55
1	A	146	LEU	N-CA-C	-5.35	103.32	110.07
1	A	328	LYS	N-CA-C	-5.33	105.55	111.36
1	A	266	ASN	CA-CB-CG	5.33	117.92	112.60
1	A	348	GLN	OE1-CD-NE2	5.32	127.92	122.60
1	A	394	GLN	OE1-CD-NE2	-5.31	117.29	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	VAL	N-CA-C	5.30	115.53	108.11
1	A	89	VAL	CA-C-O	5.30	126.78	121.17
1	A	362	SER	O-C-N	5.29	127.80	122.09
1	A	251	GLU	OE1-CD-OE2	5.27	135.55	122.90
1	A	434	ASP	O-C-N	5.25	128.36	122.22
1	A	111	LEU	CA-C-O	-5.23	115.33	120.82
1	A	199	LYS	N-CA-CB	5.23	117.59	110.01
1	A	214	VAL	N-CA-C	-5.23	104.35	110.05
1	A	71	VAL	O-C-N	5.22	125.82	121.85
1	A	22	GLU	O-C-N	5.22	129.42	123.31
1	A	87	LYS	O-C-N	5.22	127.65	122.12
1	A	298	PHE	O-C-N	5.22	129.93	123.15
1	A	65	VAL	O-C-N	5.21	127.19	121.83
1	A	62	LEU	O-C-N	5.20	127.63	122.12
1	A	179	PHE	CA-CB-CG	-5.20	108.60	113.80
1	A	109	ALA	CA-C-N	5.19	127.20	120.56
1	A	109	ALA	C-N-CA	5.19	127.20	120.56
1	A	9	SER	CA-C-O	-5.19	114.81	120.36
1	A	323	THR	N-CA-C	5.17	120.59	113.97
1	A	67	ASN	O-C-N	5.17	127.59	122.12
1	A	207	ASN	CA-CB-CG	-5.16	107.44	112.60
1	A	129	LEU	CA-C-O	-5.14	115.40	120.90
1	A	87	LYS	CB-CA-C	-5.14	102.26	110.79
1	A	378	THR	CA-CB-CG2	5.12	119.19	110.50
1	A	392	THR	CA-CB-OG1	-5.11	101.93	109.60
1	A	47	GLU	OE1-CD-OE2	5.11	135.15	122.90
1	A	346	VAL	CA-C-O	-5.10	115.74	121.05
1	A	16	ASN	CB-CA-C	5.10	116.41	108.61
1	A	25	THR	N-CA-C	-5.08	101.69	108.86
1	A	341	ALA	O-C-N	5.08	129.27	123.48
1	A	230	ASP	O-C-N	5.08	127.30	122.07
1	A	255	ASP	CB-CA-C	-5.07	104.74	111.63
1	A	50	ASP	CA-CB-CG	-5.05	107.55	112.60
1	A	321	ASP	O-C-N	5.02	128.92	122.39
1	A	179	PHE	N-CA-C	-5.02	105.70	111.07

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	3293	116	1
2	A	1	0	0	0	0
3	A	11	0	4	2	0
4	A	355	0	0	28	3
All	All	3656	0	3297	117	3

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 18.

All (117) 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:435:LYS:HE3	4:A:698:HOH:O	1.40	1.21
1:A:264:ASN:HD22	1:A:267:SER:HA	1.21	1.02
1:A:264:ASN:ND2	1:A:267:SER:HA	1.79	0.96
1:A:200:ARG:HB3	4:A:770:HOH:O	1.70	0.91
1:A:432:HIS:HD2	4:A:675:HOH:O	1.53	0.91
1:A:63:HIS:HD2	1:A:66:LYS:NZ	1.69	0.89
1:A:326:ASN:HD21	1:A:328:LYS:HG3	1.41	0.85
1:A:313:ALA:CB	1:A:317:ILE:HD11	2.08	0.84
1:A:57:MET:SD	4:A:696:HOH:O	2.37	0.83
1:A:138:LYS:HE3	4:A:775:HOH:O	1.83	0.78
1:A:326:ASN:C	1:A:326:ASN:HD22	1.91	0.78
1:A:63:HIS:CD2	1:A:66:LYS:NZ	2.51	0.77
1:A:41:GLY:CA	1:A:46:LEU:HD21	2.16	0.76
1:A:432:HIS:CD2	4:A:675:HOH:O	2.32	0.76
1:A:42:VAL:O	4:A:731:HOH:O	2.04	0.75
1:A:255:ASP:HB3	4:A:712:HOH:O	1.92	0.69
1:A:268:ASP:OD2	1:A:271:LYS:HE2	1.92	0.69
1:A:63:HIS:HD2	1:A:66:LYS:HZ2	1.41	0.68
1:A:63:HIS:HD2	1:A:66:LYS:HZ3	1.39	0.67
1:A:4:LYS:HE2	1:A:6:TYR:HB2	1.77	0.66
1:A:41:GLY:HA3	1:A:46:LEU:HD21	1.78	0.66
1:A:152:ASN:HB2	4:A:758:HOH:O	1.96	0.66
1:A:326:ASN:ND2	1:A:328:LYS:HG3	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLY:O	4:A:650:HOH:O	2.12	0.65
1:A:257:LYS:HE3	4:A:618:HOH:O	1.95	0.65
1:A:240:LYS:NZ	4:A:783:HOH:O	2.30	0.64
1:A:138:LYS:HE3	4:A:776:HOH:O	1.96	0.64
1:A:264:ASN:HB2	1:A:267:SER:HB2	1.80	0.64
1:A:313:ALA:HB1	1:A:317:ILE:HD11	1.79	0.63
1:A:428:GLU:OE1	4:A:629:HOH:O	2.15	0.63
1:A:73:ALA:HB3	1:A:74:PRO:HD3	1.79	0.63
1:A:63:HIS:CD2	1:A:66:LYS:HZ2	2.13	0.62
1:A:264:ASN:OD1	1:A:264:ASN:C	2.41	0.62
1:A:313:ALA:HB3	1:A:317:ILE:HD11	1.81	0.61
1:A:146:LEU:CD1	1:A:423:ALA:HB1	2.31	0.61
1:A:99:THR:HB	4:A:732:HOH:O	2.00	0.60
1:A:261:ASP:OD2	1:A:264:ASN:ND2	2.34	0.60
3:A:442:2PG:O3	4:A:514:HOH:O	1.99	0.60
1:A:273:LEU:HD22	1:A:277:GLN:HB2	1.83	0.60
1:A:41:GLY:N	1:A:46:LEU:HD21	2.16	0.59
1:A:4:LYS:HD2	4:A:768:HOH:O	2.02	0.59
1:A:298:PHE:HB2	1:A:306:TRP:CD1	2.38	0.58
1:A:44:GLU:N	4:A:521:HOH:O	2.38	0.57
1:A:273:LEU:HD22	1:A:277:GLN:CB	2.35	0.56
1:A:268:ASP:OD2	1:A:271:LYS:CE	2.54	0.56
1:A:264:ASN:OD1	1:A:264:ASN:O	2.24	0.56
1:A:152:ASN:HD21	1:A:155:ASN:ND2	2.05	0.55
1:A:4:LYS:HD3	4:A:471:HOH:O	2.06	0.55
1:A:261:ASP:HA	4:A:578:HOH:O	2.05	0.55
1:A:264:ASN:ND2	1:A:267:SER:CA	2.64	0.55
1:A:129:LEU:HG	1:A:133:LEU:HD22	1.89	0.54
1:A:399:ALA:HB1	1:A:400:PRO:HD2	1.90	0.54
1:A:43:HIS:C	4:A:521:HOH:O	2.51	0.53
1:A:264:ASN:HB3	1:A:265:PRO:CA	2.39	0.53
1:A:273:LEU:CD2	1:A:277:GLN:HB2	2.39	0.53
1:A:257:LYS:HG3	4:A:618:HOH:O	2.09	0.53
1:A:326:ASN:C	1:A:326:ASN:ND2	2.61	0.52
1:A:264:ASN:HB3	1:A:266:ASN:N	2.24	0.52
1:A:294:ILE:HG13	1:A:315:ILE:HD11	1.92	0.52
1:A:66:LYS:HD3	4:A:689:HOH:O	2.08	0.52
1:A:41:GLY:N	1:A:46:LEU:CD2	2.73	0.51
1:A:153:VAL:HB	1:A:193:LEU:HD23	1.92	0.51
1:A:340:ASP:O	1:A:431:HIS:HE1	1.94	0.51
1:A:275:GLY:N	1:A:276:PRO:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:HIS:CD2	1:A:66:LYS:HZ3	2.24	0.50
1:A:33:ILE:HG22	1:A:378:THR:HG21	1.94	0.49
1:A:42:VAL:HG22	1:A:43:HIS:CE1	2.47	0.49
1:A:327:PRO:HG3	4:A:652:HOH:O	2.12	0.49
1:A:317:ILE:O	1:A:339:ALA:HB1	2.13	0.49
1:A:343:LEU:HD23	1:A:345:LYS:HE3	1.94	0.49
1:A:66:LYS:HE2	4:A:505:HOH:O	2.12	0.48
1:A:268:ASP:HB3	1:A:271:LYS:CD	2.43	0.48
1:A:111:LEU:HD22	1:A:347:ASN:HA	1.95	0.48
1:A:375:SER:HB2	3:A:442:2PG:O3P	2.13	0.48
1:A:115:LEU:HD22	1:A:382:PHE:CZ	2.49	0.47
1:A:254:LYS:O	1:A:255:ASP:HB2	2.13	0.47
1:A:130:TYR:OH	1:A:418:GLU:OE2	2.14	0.47
1:A:216:PRO:HG2	1:A:218:ILE:CD1	2.45	0.47
1:A:104:LYS:C	1:A:104:LYS:HD3	2.39	0.47
1:A:153:VAL:HB	1:A:193:LEU:CD2	2.44	0.47
1:A:146:LEU:HD13	1:A:423:ALA:HB1	1.96	0.47
1:A:97:ASP:OD1	1:A:104:LYS:HB3	2.15	0.46
1:A:269:LYS:HG3	1:A:272:TRP:CD2	2.50	0.46
1:A:264:ASN:HD22	1:A:267:SER:CA	2.10	0.46
1:A:56:TRP:C	1:A:57:MET:HG2	2.40	0.46
1:A:27:LYS:HD2	1:A:124:GLU:HA	1.98	0.45
1:A:66:LYS:HG3	4:A:574:HOH:O	2.17	0.45
1:A:86:GLN:O	1:A:89:VAL:HB	2.17	0.45
1:A:362:SER:O	1:A:367:TRP:HB2	2.17	0.45
1:A:345:LYS:HB2	1:A:348:GLN:HG3	1.98	0.45
1:A:274:THR:OG1	1:A:277:GLN:HG3	2.16	0.45
1:A:48:MET:HE3	1:A:48:MET:HB2	1.81	0.44
1:A:55:LYS:HE3	4:A:695:HOH:O	2.16	0.44
1:A:252:PHE:HB3	1:A:262:PHE:CD1	2.52	0.44
1:A:373:HIS:CD2	1:A:373:HIS:C	2.95	0.44
1:A:273:LEU:CD2	1:A:277:GLN:CB	2.94	0.44
1:A:26:GLU:HG2	1:A:27:LYS:HG3	2.00	0.44
1:A:334:ILE:HD13	1:A:365:ALA:HB2	2.00	0.44
1:A:152:ASN:O	1:A:399:ALA:HB2	2.18	0.43
1:A:343:LEU:HD12	1:A:343:LEU:HA	1.93	0.43
1:A:261:ASP:O	1:A:264:ASN:HB2	2.19	0.43
1:A:325:THR:O	1:A:349:ILE:HD12	2.19	0.43
1:A:286:MET:HE1	1:A:313:ALA:O	2.18	0.43
1:A:73:ALA:HB3	1:A:74:PRO:CD	2.48	0.43
1:A:300:GLU:O	1:A:322:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HG2	1:A:5:VAL:N	2.34	0.43
1:A:197:THR:HG22	1:A:205:ALA:HB1	2.01	0.43
1:A:391:ARG:HH11	1:A:391:ARG:HD3	1.55	0.42
1:A:326:ASN:HA	1:A:327:PRO:HD3	1.86	0.42
1:A:101:ASN:ND2	1:A:101:ASN:H	2.17	0.41
1:A:216:PRO:HG2	1:A:218:ILE:HD12	2.00	0.41
1:A:345:LYS:NZ	4:A:716:HOH:O	2.53	0.41
1:A:16:ASN:HA	1:A:17:PRO:HD3	1.89	0.41
1:A:374:ARG:O	1:A:377:GLU:HG2	2.20	0.41
1:A:144:TYR:HB2	1:A:419:LEU:HD13	2.03	0.40
1:A:52:ASP:OD1	1:A:52:ASP:C	2.65	0.40
1:A:127:VAL:HB	1:A:128:PRO:CD	2.52	0.40

All (3) 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)
4:A:730:HOH:O	4:A:730:HOH:O[8_666]	1.65	0.55
4:A:709:HOH:O	4:A:768:HOH:O[5_655]	1.80	0.40
1:A:207:ASN:ND2	4:A:761:HOH:O[8_666]	2.18	0.02

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%)	418 (96%)	15 (4%)	1 (0%)	43 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	ASN

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%)	328 (95%)	16 (5%)	23	31

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	47	GLU
1	A	57	MET
1	A	101	ASN
1	A	104	LYS
1	A	126	ASN
1	A	133	LEU
1	A	146	LEU
1	A	240	LYS
1	A	254	LYS
1	A	255	ASP
1	A	265	PRO
1	A	266	ASN
1	A	304	GLU
1	A	326	ASN
1	A	392	THR

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	16	ASN
1	A	43	HIS
1	A	63	HIS
1	A	101	ASN
1	A	155	ASN
1	A	207	ASN
1	A	217	ASN
1	A	264	ASN
1	A	266	ASN

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Mol	Chain	Res	Type
1	A	326	ASN
1	A	348	GLN
1	A	432	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	2PG	A	442	2	9,10,10	1.22	2 (22%)	12,14,14	2.09	3 (25%)

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	2PG	A	442	2	-	5/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	442	2PG	O1-C1	2.52	1.29	1.22
3	A	442	2PG	P-O4P	-2.13	1.46	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	442	2PG	O1-C1-C2	-5.35	111.29	122.85
3	A	442	2PG	O2-C1-C2	2.94	120.36	112.71
3	A	442	2PG	O3-C3-C2	2.32	117.63	111.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	442	2PG	O1-C1-C2-O1P
3	A	442	2PG	O2-C1-C2-O1P
3	A	442	2PG	C1-C2-C3-O3
3	A	442	2PG	O1P-C2-C3-O3
3	A	442	2PG	C2-O1P-P-O2P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	442	2PG	2	0

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.