



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:48 PM UTC

PDB ID : 7ENL / pdb_00007enl
Title : MECHANISM OF ENOLASE: THE CRYSTAL STRUCTURE OF ENOLASE-MG2+-PHOSPHOGLYCERATE(SLASH) PHOSPHOENOLPYRUVATE COMPLEX AT 2.2-ANGSTROMS RESOLUTION
Authors : Lebioda, L.; Stec, B.
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

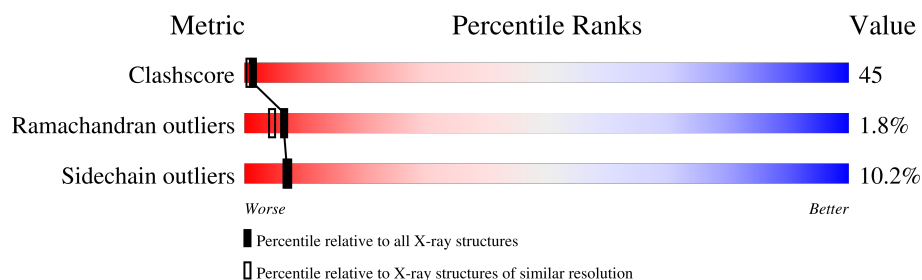
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

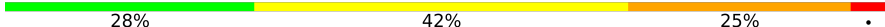
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2PG	A	439	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3648 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			

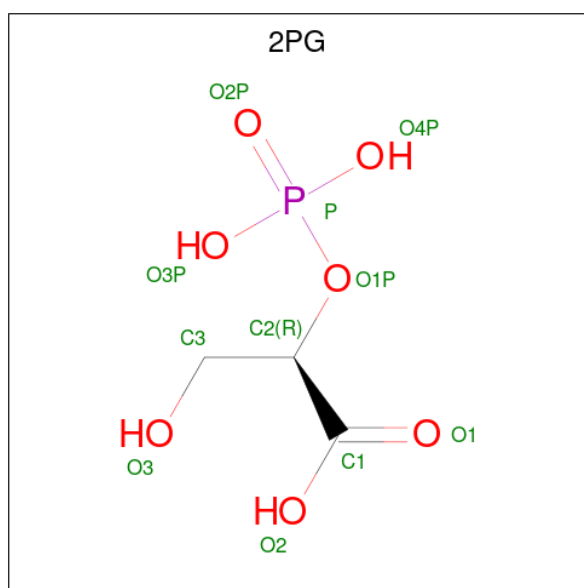
There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	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.

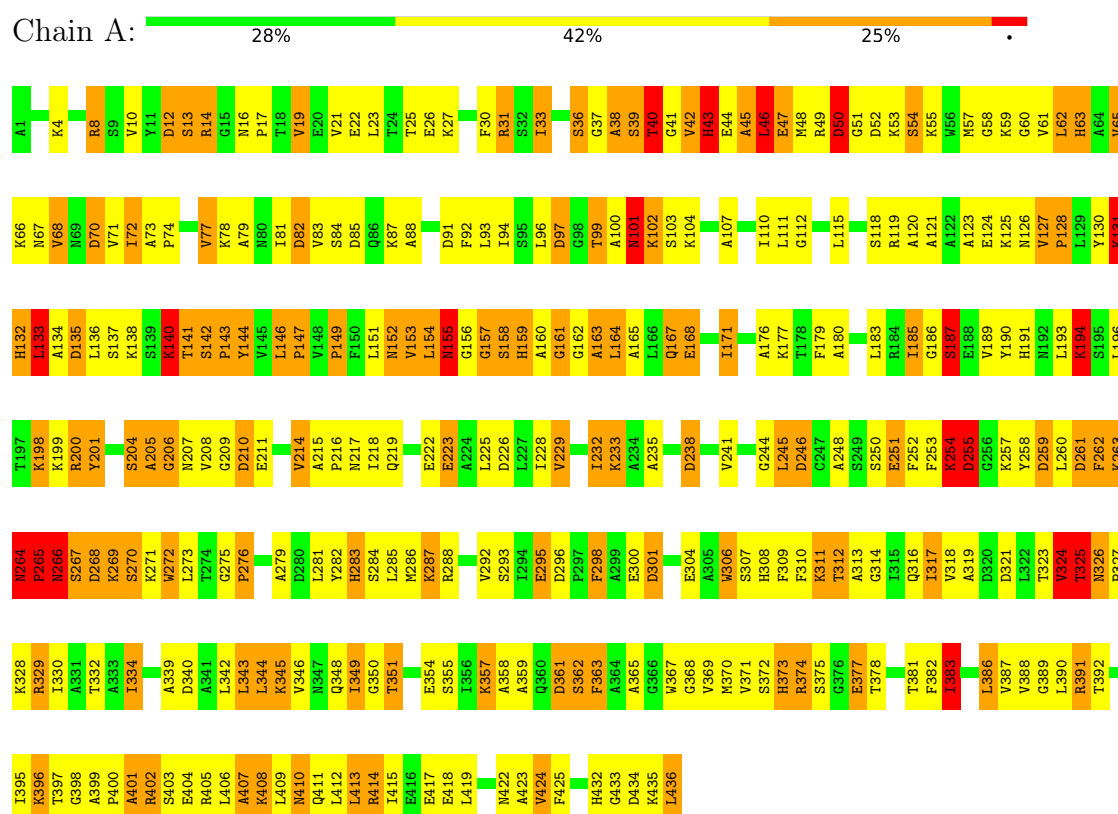
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	347	Total	O	0	0
			347	347		

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



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	122.00Å 122.00Å 67.00Å 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}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3648	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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, 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	1.33	7/3349 (0.2%)	2.86	349/4531 (7.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ILE	N-CA	5.70	1.53	1.46
1	A	296	ASP	N-CA	5.59	1.50	1.46
1	A	415	ILE	CA-CB	5.47	1.61	1.54
1	A	115	LEU	N-CA	5.38	1.53	1.46
1	A	355	SER	C-N	-5.21	1.27	1.33
1	A	412	LEU	C-N	-5.18	1.27	1.33
1	A	332	THR	CA-CB	5.07	1.61	1.53

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLU	CB-CG-CD	24.96	155.03	112.60
1	A	265	PRO	CA-N-CD	-16.77	88.53	112.00
1	A	326	ASN	OD1-CG-ND2	14.62	137.22	122.60
1	A	226	ASP	CA-CB-CG	14.08	126.68	112.60
1	A	161	GLY	N-CA-C	13.43	128.95	111.09
1	A	159	HIS	N-CA-C	13.36	129.06	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	LEU	CA-C-N	12.57	138.55	120.95
1	A	46	LEU	C-N-CA	12.57	138.55	120.95
1	A	262	PHE	CA-CB-CG	12.56	126.36	113.80
1	A	264	ASN	CA-C-N	12.37	135.31	119.84
1	A	264	ASN	C-N-CA	12.37	135.31	119.84
1	A	340	ASP	CA-CB-CG	12.04	124.64	112.60
1	A	374	ARG	CD-NE-CZ	11.91	141.07	124.40
1	A	264	ASN	CA-C-O	-11.41	104.53	120.16
1	A	36	SER	CA-CB-OG	11.40	133.90	111.10
1	A	301	ASP	O-C-N	11.24	136.36	122.20
1	A	186	GLY	CA-C-N	11.14	135.21	120.28
1	A	186	GLY	C-N-CA	11.14	135.21	120.28
1	A	372	SER	CA-C-O	11.11	133.96	121.40
1	A	16	ASN	OD1-CG-ND2	-10.35	112.25	122.60
1	A	146	LEU	CB-CA-C	9.88	122.79	108.87
1	A	250	SER	CA-C-O	9.86	131.24	120.10
1	A	142	SER	N-CA-CB	-9.73	99.02	111.09
1	A	42	VAL	N-CA-CB	-9.66	95.29	111.23
1	A	161	GLY	CA-C-O	9.62	131.77	121.96
1	A	168	GLU	CB-CG-CD	9.62	128.95	112.60
1	A	14	ARG	NE-CZ-NH1	-9.53	111.97	121.50
1	A	246	ASP	N-CA-CB	9.46	126.29	110.87
1	A	31	ARG	CD-NE-CZ	-9.41	111.22	124.40
1	A	135	ASP	CA-CB-CG	9.28	121.88	112.60
1	A	141	THR	CA-CB-OG1	-9.26	95.71	109.60
1	A	208	VAL	N-CA-C	9.26	122.44	109.29
1	A	163	ALA	N-CA-C	-9.04	102.41	113.97
1	A	101	ASN	CA-CB-CG	8.90	121.50	112.60
1	A	155	ASN	CA-CB-CG	8.81	121.42	112.60
1	A	316	GLN	O-C-N	8.75	133.70	122.93
1	A	208	VAL	N-CA-CB	-8.72	102.40	112.34
1	A	266	ASN	N-CA-C	-8.69	92.28	110.80
1	A	362	SER	O-C-N	8.47	131.81	122.15
1	A	146	LEU	N-CA-C	-8.47	99.40	110.07
1	A	368	GLY	N-CA-C	-8.46	97.91	112.64
1	A	349	ILE	CB-CA-C	8.46	125.17	111.29
1	A	222	GLU	CA-C-O	8.43	129.67	120.82
1	A	210	ASP	O-C-N	8.42	132.63	122.27
1	A	244	GLY	CA-C-O	-8.37	114.29	121.57
1	A	391	ARG	NE-CZ-NH1	-8.33	113.17	121.50
1	A	363	PHE	CA-CB-CG	8.29	122.09	113.80
1	A	409	LEU	CA-C-N	8.24	131.32	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	LEU	C-N-CA	8.24	131.32	120.28
1	A	8	ARG	NE-CZ-NH1	8.15	129.65	121.50
1	A	404	GLU	N-CA-C	-8.15	102.59	112.54
1	A	251	GLU	CG-CD-OE1	-8.15	99.65	118.40
1	A	167	GLN	OE1-CD-NE2	-8.14	114.46	122.60
1	A	382	PHE	CA-CB-CG	-8.14	105.66	113.80
1	A	401	ALA	CA-C-N	8.05	136.92	121.54
1	A	401	ALA	C-N-CA	8.05	136.92	121.54
1	A	46	LEU	CA-C-O	8.04	130.22	121.05
1	A	12	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	329	ARG	NE-CZ-NH1	8.01	129.51	121.50
1	A	207	ASN	CB-CA-C	7.99	126.06	109.68
1	A	374	ARG	CA-C-N	7.98	130.97	120.28
1	A	374	ARG	C-N-CA	7.98	130.97	120.28
1	A	400	PRO	CA-C-O	7.96	131.68	121.97
1	A	168	GLU	CA-C-O	7.94	129.27	120.70
1	A	214	VAL	N-CA-C	-7.93	101.25	110.21
1	A	47	GLU	CA-C-O	-7.93	111.69	120.81
1	A	140	LYS	CA-CB-CG	7.90	129.90	114.10
1	A	126	ASN	OD1-CG-ND2	7.85	130.45	122.60
1	A	374	ARG	NE-CZ-NH1	7.82	129.32	121.50
1	A	162	GLY	N-CA-C	-7.79	94.72	113.18
1	A	141	THR	CA-CB-CG2	7.76	123.69	110.50
1	A	127	VAL	N-CA-CB	-7.71	106.51	111.83
1	A	97	ASP	CA-CB-CG	-7.68	104.92	112.60
1	A	159	HIS	CA-CB-CG	-7.68	106.12	113.80
1	A	133	LEU	CB-CA-C	7.68	123.90	110.85
1	A	307	SER	O-C-N	7.66	130.24	122.12
1	A	283	HIS	CA-C-N	7.57	131.32	120.79
1	A	283	HIS	C-N-CA	7.57	131.32	120.79
1	A	205	ALA	CA-C-N	7.56	129.87	120.34
1	A	205	ALA	C-N-CA	7.56	129.87	120.34
1	A	85	ASP	CA-C-O	7.55	131.05	122.37
1	A	268	ASP	N-CA-CB	-7.55	97.73	110.49
1	A	357	LYS	N-CA-CB	7.52	121.33	110.06
1	A	194	LYS	CA-C-O	-7.48	113.15	121.00
1	A	287	LYS	CA-CB-CG	-7.47	99.16	114.10
1	A	244	GLY	O-C-N	7.46	129.94	123.37
1	A	340	ASP	O-C-N	7.46	130.65	121.84
1	A	266	ASN	N-CA-CB	7.45	123.08	110.49
1	A	16	ASN	CA-CB-CG	7.45	120.05	112.60
1	A	207	ASN	N-CA-C	-7.43	100.72	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ASP	CA-C-N	7.43	130.24	120.28
1	A	226	ASP	C-N-CA	7.43	130.24	120.28
1	A	300	GLU	N-CA-C	7.38	121.72	112.87
1	A	374	ARG	CG-CD-NE	7.37	128.21	112.00
1	A	391	ARG	CD-NE-CZ	-7.32	114.16	124.40
1	A	386	LEU	CA-C-O	-7.30	113.15	120.82
1	A	43	HIS	N-CA-C	7.28	121.57	111.74
1	A	50	ASP	CA-CB-CG	-7.26	105.34	112.60
1	A	38	ALA	N-CA-C	-7.23	99.45	110.30
1	A	49	ARG	CD-NE-CZ	7.22	134.51	124.40
1	A	269	LYS	N-CA-C	7.20	120.84	108.02
1	A	84	SER	O-C-N	7.17	129.72	122.12
1	A	48	MET	CA-CB-CG	-7.10	99.90	114.10
1	A	255	ASP	N-CA-CB	7.10	122.85	112.13
1	A	155	ASN	O-C-N	7.10	132.23	123.21
1	A	317	ILE	CA-C-O	7.05	128.24	120.48
1	A	252	PHE	CB-CA-C	7.02	122.14	111.18
1	A	168	GLU	CA-CB-CG	7.01	128.13	114.10
1	A	371	VAL	CB-CA-C	7.01	121.30	111.63
1	A	259	ASP	CA-CB-CG	-6.98	105.62	112.60
1	A	190	TYR	O-C-N	6.97	129.25	122.07
1	A	153	VAL	O-C-N	6.94	129.46	122.04
1	A	309	PHE	CA-CB-CG	6.94	120.74	113.80
1	A	167	GLN	CB-CG-CD	6.92	124.37	112.60
1	A	14	ARG	NH1-CZ-NH2	6.92	128.29	119.30
1	A	255	ASP	CA-C-O	-6.88	113.10	121.28
1	A	301	ASP	CA-CB-CG	-6.86	105.74	112.60
1	A	179	PHE	CA-CB-CG	-6.83	106.97	113.80
1	A	162	GLY	O-C-N	6.82	131.56	122.70
1	A	49	ARG	NE-CZ-NH2	-6.80	113.08	119.20
1	A	72	ILE	N-CA-C	6.79	116.94	110.42
1	A	325	THR	CA-C-N	6.79	130.70	121.74
1	A	325	THR	C-N-CA	6.79	130.70	121.74
1	A	47	GLU	N-CA-CB	-6.78	99.75	109.85
1	A	49	ARG	CA-C-O	-6.73	113.43	120.70
1	A	27	LYS	CA-CB-CG	-6.70	100.70	114.10
1	A	226	ASP	N-CA-C	-6.70	104.06	111.36
1	A	326	ASN	N-CA-CB	-6.68	101.68	110.17
1	A	388	VAL	CA-C-N	6.66	127.49	120.03
1	A	388	VAL	C-N-CA	6.66	127.49	120.03
1	A	296	ASP	O-C-N	6.66	124.59	121.53
1	A	351	THR	O-C-N	6.65	130.98	123.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ASN	CB-CG-ND2	6.64	126.37	116.40
1	A	187	SER	CA-C-N	6.63	129.06	120.44
1	A	187	SER	C-N-CA	6.63	129.06	120.44
1	A	33	ILE	CA-C-O	-6.63	113.34	120.36
1	A	279	ALA	O-C-N	6.63	129.14	122.12
1	A	304	GLU	CA-C-O	-6.63	113.53	120.55
1	A	99	THR	CB-CA-C	6.61	122.48	109.66
1	A	258	TYR	O-C-N	6.59	130.92	123.27
1	A	254	LYS	CA-C-N	6.59	131.49	122.19
1	A	254	LYS	C-N-CA	6.59	131.49	122.19
1	A	180	ALA	CA-C-N	6.58	131.84	120.58
1	A	180	ALA	C-N-CA	6.58	131.84	120.58
1	A	372	SER	CA-CB-OG	6.57	124.25	111.10
1	A	157	GLY	CA-C-N	6.53	129.69	120.28
1	A	157	GLY	C-N-CA	6.53	129.69	120.28
1	A	171	ILE	CB-CA-C	6.53	120.35	110.62
1	A	126	ASN	O-C-N	6.53	131.28	122.59
1	A	262	PHE	CB-CA-C	6.51	120.54	109.80
1	A	319	ALA	CB-CA-C	6.51	120.87	110.19
1	A	406	LEU	O-C-N	6.50	129.83	122.22
1	A	301	ASP	CA-C-O	-6.47	112.29	119.34
1	A	255	ASP	CB-CA-C	-6.46	102.56	111.73
1	A	408	LYS	CA-C-N	6.45	128.93	120.28
1	A	408	LYS	C-N-CA	6.45	128.93	120.28
1	A	158	SER	N-CA-C	6.45	119.12	111.71
1	A	374	ARG	N-CA-C	-6.42	99.70	109.85
1	A	51	GLY	N-CA-C	-6.41	107.08	115.47
1	A	312	THR	N-CA-CB	-6.41	100.86	111.49
1	A	357	LYS	CA-C-O	-6.39	113.72	120.63
1	A	10	VAL	CA-C-O	-6.38	114.74	121.44
1	A	425	PHE	CA-CB-CG	-6.38	107.42	113.80
1	A	351	THR	N-CA-CB	6.35	123.35	111.53
1	A	85	ASP	CA-C-N	6.33	128.67	120.44
1	A	85	ASP	C-N-CA	6.33	128.67	120.44
1	A	389	GLY	O-C-N	6.33	128.31	122.17
1	A	201	TYR	N-CA-C	6.30	121.91	113.72
1	A	19	VAL	CA-CB-CG1	6.29	121.10	110.40
1	A	27	LYS	CA-C-N	-6.29	112.48	122.92
1	A	27	LYS	C-N-CA	-6.29	112.48	122.92
1	A	265	PRO	N-CA-C	6.28	125.41	112.47
1	A	288	ARG	CB-CG-CD	6.28	125.73	111.30
1	A	63	HIS	CA-C-O	6.26	127.35	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	GLU	CA-CB-CG	6.25	126.61	114.10
1	A	400	PRO	O-C-N	-6.25	113.24	122.12
1	A	84	SER	N-CA-CB	6.21	119.26	110.12
1	A	424	VAL	N-CA-C	-6.21	99.29	108.85
1	A	389	GLY	CA-C-O	-6.20	114.72	120.80
1	A	124	GLU	CG-CD-OE1	-6.17	104.20	118.40
1	A	187	SER	CB-CA-C	6.14	120.99	110.79
1	A	334	ILE	CA-C-O	-6.12	114.26	121.05
1	A	436	LEU	N-CA-CB	-6.10	100.12	110.50
1	A	411	GLN	CA-C-O	-6.09	114.42	120.70
1	A	342	LEU	CA-C-O	-6.09	113.74	120.38
1	A	206	GLY	N-CA-C	6.07	122.97	113.86
1	A	31	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	A	229	VAL	CA-C-N	6.05	128.39	120.28
1	A	229	VAL	C-N-CA	6.05	128.39	120.28
1	A	185	ILE	CA-CB-CG2	6.05	120.79	110.50
1	A	156	GLY	N-CA-C	-6.05	98.85	113.18
1	A	343	LEU	CA-C-N	-6.04	114.74	122.77
1	A	343	LEU	C-N-CA	-6.04	114.74	122.77
1	A	223	GLU	CG-CD-OE2	-6.03	104.54	118.40
1	A	264	ASN	O-C-N	6.01	128.24	121.32
1	A	285	LEU	CA-C-N	6.01	128.61	120.38
1	A	285	LEU	C-N-CA	6.01	128.61	120.38
1	A	128	PRO	CA-C-O	-6.01	114.34	121.67
1	A	68	VAL	CB-CA-C	-5.97	104.05	111.94
1	A	46	LEU	CB-CA-C	5.96	119.60	109.53
1	A	8	ARG	NH1-CZ-NH2	-5.95	111.56	119.30
1	A	134	ALA	N-CA-C	-5.95	104.79	111.28
1	A	414	ARG	N-CA-C	5.94	117.75	111.28
1	A	346	VAL	N-CA-C	5.93	117.39	110.62
1	A	232	ILE	CA-C-N	5.92	128.46	120.65
1	A	232	ILE	C-N-CA	5.92	128.46	120.65
1	A	401	ALA	CA-C-O	-5.92	112.22	120.21
1	A	144	TYR	O-C-N	5.91	129.68	123.06
1	A	350	GLY	CA-C-O	-5.89	112.69	119.10
1	A	137	SER	CA-C-O	-5.88	112.19	119.18
1	A	204	SER	CA-CB-OG	-5.87	99.37	111.10
1	A	8	ARG	CD-NE-CZ	5.87	132.61	124.40
1	A	344	LEU	O-C-N	5.86	129.90	123.22
1	A	296	ASP	N-CA-CB	-5.85	105.17	111.66
1	A	25	THR	CA-C-O	-5.84	114.91	121.40
1	A	413	LEU	N-CA-C	-5.84	103.89	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	VAL	CA-C-N	5.84	128.11	120.28
1	A	77	VAL	C-N-CA	5.84	128.11	120.28
1	A	158	SER	N-CA-CB	-5.83	101.24	110.22
1	A	14	ARG	CD-NE-CZ	-5.83	116.23	124.40
1	A	30	PHE	CA-CB-CG	-5.82	107.98	113.80
1	A	383	ILE	CA-C-O	-5.82	112.20	119.70
1	A	396	LYS	CB-CA-C	5.81	120.10	110.74
1	A	120	ALA	N-CA-C	-5.80	105.09	111.82
1	A	70	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	88	ALA	O-C-N	5.77	128.24	122.12
1	A	65	VAL	N-CA-CB	5.76	117.29	110.55
1	A	50	ASP	CA-C-O	-5.76	114.41	120.63
1	A	154	LEU	CB-CA-C	5.74	118.98	110.14
1	A	417	GLU	OE1-CD-OE2	5.73	136.65	122.90
1	A	326	ASN	CA-C-O	5.72	123.01	119.29
1	A	82	ASP	CA-CB-CG	-5.71	106.89	112.60
1	A	82	ASP	CA-C-O	-5.70	113.83	120.62
1	A	84	SER	CA-C-N	5.70	130.71	122.16
1	A	84	SER	C-N-CA	5.70	130.71	122.16
1	A	314	GLY	CA-C-N	5.70	130.78	123.03
1	A	314	GLY	C-N-CA	5.70	130.78	123.03
1	A	266	ASN	CA-C-O	5.68	128.63	120.51
1	A	406	LEU	N-CA-C	-5.68	105.18	111.71
1	A	244	GLY	N-CA-C	-5.67	102.14	111.38
1	A	383	ILE	CB-CG1-CD1	5.66	125.69	113.80
1	A	374	ARG	NH1-CZ-NH2	-5.66	111.94	119.30
1	A	310	PHE	O-C-N	5.65	128.84	122.22
1	A	235	ALA	N-CA-C	-5.65	106.23	113.01
1	A	179	PHE	CA-C-O	5.65	126.52	120.70
1	A	410	ASN	CA-C-O	5.64	126.53	120.55
1	A	276	PRO	CA-C-N	5.64	128.30	120.29
1	A	276	PRO	C-N-CA	5.64	128.30	120.29
1	A	329	ARG	CD-NE-CZ	-5.63	116.52	124.40
1	A	328	LYS	N-CA-CB	5.60	118.13	110.01
1	A	130	TYR	CA-C-O	5.60	126.47	120.20
1	A	417	GLU	CG-CD-OE1	-5.60	105.52	118.40
1	A	47	GLU	CB-CA-C	-5.59	100.94	109.89
1	A	118	SER	CA-C-N	5.58	130.12	120.58
1	A	118	SER	C-N-CA	5.58	130.12	120.58
1	A	131	LYS	CA-C-N	5.58	127.75	120.28
1	A	131	LYS	C-N-CA	5.58	127.75	120.28
1	A	414	ARG	NH1-CZ-NH2	5.57	126.54	119.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	SER	O-C-N	5.56	129.61	123.33
1	A	38	ALA	CA-C-O	-5.56	114.80	120.80
1	A	101	ASN	CB-CG-ND2	5.54	124.71	116.40
1	A	141	THR	CA-C-O	5.53	125.96	120.32
1	A	334	ILE	O-C-N	5.51	127.63	121.90
1	A	42	VAL	N-CA-C	-5.51	97.89	109.34
1	A	126	ASN	CB-CG-ND2	-5.50	108.16	116.40
1	A	60	GLY	N-CA-C	-5.49	106.29	112.33
1	A	31	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	A	397	THR	CB-CA-C	5.49	119.85	110.85
1	A	17	PRO	CA-C-O	5.49	130.59	120.60
1	A	12	ASP	CA-C-N	5.49	129.46	120.63
1	A	12	ASP	C-N-CA	5.49	129.46	120.63
1	A	179	PHE	N-CA-C	-5.46	105.24	111.14
1	A	115	LEU	CB-CA-C	5.46	120.69	110.70
1	A	365	ALA	CA-C-O	5.44	125.72	119.35
1	A	404	GLU	CA-C-O	5.44	126.08	119.38
1	A	298	PHE	CA-CB-CG	-5.44	108.36	113.80
1	A	63	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	A	323	THR	CA-C-O	-5.42	113.09	119.05
1	A	301	ASP	N-CA-C	-5.41	104.96	113.02
1	A	229	VAL	CA-C-O	-5.41	114.78	120.57
1	A	147	PRO	CB-CA-C	-5.39	102.66	111.56
1	A	272	TRP	CB-CA-C	5.39	118.38	109.70
1	A	12	ASP	CA-C-O	-5.38	115.06	121.89
1	A	349	ILE	CB-CG1-CD1	-5.38	102.50	113.80
1	A	407	ALA	CA-C-O	-5.38	114.82	120.63
1	A	187	SER	N-CA-CB	-5.38	102.22	110.12
1	A	102	LYS	CB-CG-CD	5.36	123.63	111.30
1	A	232	ILE	CB-CG1-CD1	5.34	125.02	113.80
1	A	43	HIS	CB-CA-C	-5.34	104.15	111.73
1	A	214	VAL	CB-CA-C	5.33	117.42	111.45
1	A	283	HIS	N-CA-CB	5.32	118.04	110.06
1	A	21	VAL	CA-C-N	5.31	130.48	122.99
1	A	21	VAL	C-N-CA	5.31	130.48	122.99
1	A	131	LYS	N-CA-CB	-5.31	102.30	110.16
1	A	261	ASP	CA-C-N	-5.30	113.09	122.74
1	A	261	ASP	C-N-CA	-5.30	113.09	122.74
1	A	358	ALA	N-CA-C	5.30	117.97	111.82
1	A	91	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	138	LYS	CA-CB-CG	5.28	124.66	114.10
1	A	304	GLU	N-CA-C	5.28	117.03	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	370	MET	N-CA-C	-5.27	100.14	108.73
1	A	373	HIS	CA-CB-CG	5.27	119.07	113.80
1	A	167	GLN	CG-CD-NE2	5.25	124.27	116.40
1	A	49	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	A	411	GLN	CB-CG-CD	5.24	121.51	112.60
1	A	436	LEU	CB-CA-C	5.22	120.03	110.10
1	A	149	PRO	N-CA-CB	-5.21	97.78	103.25
1	A	306	TRP	CA-C-N	5.21	127.51	120.38
1	A	306	TRP	C-N-CA	5.21	127.51	120.38
1	A	62	LEU	CA-C-N	5.20	127.70	120.63
1	A	62	LEU	C-N-CA	5.20	127.70	120.63
1	A	308	HIS	N-CA-C	5.20	117.03	111.36
1	A	371	VAL	N-CA-C	-5.20	102.38	109.55
1	A	45	ALA	N-CA-CB	5.19	117.67	109.83
1	A	83	VAL	CA-C-N	5.18	127.22	120.28
1	A	83	VAL	C-N-CA	5.18	127.22	120.28
1	A	125	LYS	CB-CG-CD	-5.18	99.39	111.30
1	A	340	ASP	CA-C-O	-5.17	113.11	118.65
1	A	238	ASP	N-CA-C	-5.17	102.62	110.28
1	A	200	ARG	N-CA-C	5.16	118.04	111.69
1	A	125	LYS	CA-C-N	5.16	131.40	121.54
1	A	125	LYS	C-N-CA	5.16	131.40	121.54
1	A	413	LEU	CA-C-O	-5.16	115.39	121.07
1	A	323	THR	O-C-N	5.15	128.68	122.35
1	A	345	LYS	CA-C-N	5.14	127.78	120.53
1	A	345	LYS	C-N-CA	5.14	127.78	120.53
1	A	12	ASP	CB-CA-C	5.13	119.33	110.45
1	A	147	PRO	N-CA-CB	-5.12	97.87	103.25
1	A	49	ARG	N-CA-C	5.09	117.70	109.40
1	A	63	HIS	CA-C-N	5.09	128.46	120.82
1	A	63	HIS	C-N-CA	5.09	128.46	120.82
1	A	130	TYR	CB-CG-CD2	-5.09	113.17	120.80
1	A	362	SER	N-CA-CB	5.09	117.69	110.16
1	A	328	LYS	N-CA-C	-5.08	105.63	111.07
1	A	132	HIS	CA-C-N	5.08	127.51	120.29
1	A	132	HIS	C-N-CA	5.08	127.51	120.29
1	A	141	THR	CA-C-N	5.08	128.12	122.74
1	A	141	THR	C-N-CA	5.08	128.12	122.74
1	A	261	ASP	O-C-N	5.08	130.57	122.81
1	A	152	ASN	CA-C-O	-5.06	114.59	120.62
1	A	40	THR	CB-CA-C	5.06	120.49	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	GLU	CA-C-O	5.04	128.43	121.88
1	A	198	LYS	CA-C-O	5.04	125.89	120.55
1	A	42	VAL	CB-CA-C	5.02	119.53	111.29
1	A	245	LEU	O-C-N	5.02	129.42	123.24
1	A	295	GLU	CG-CD-OE1	-5.02	106.86	118.40
1	A	42	VAL	O-C-N	-5.01	116.31	122.57
1	A	391	ARG	N-CA-CB	-5.00	104.58	112.13

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	ASN	Peptide,Mainchain

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	293	2
2	A	1	0	0	0	0
3	A	11	0	3	4	0
4	A	347	0	0	94	2
All	All	3648	0	3296	296	2

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 45.

All (296) 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:158:SER:HB2	4:A:576:HOH:O	1.14	1.24
1:A:47:GLU:HG3	1:A:47:GLU:O	1.42	1.14
1:A:57:MET:O	4:A:471:HOH:O	1.68	1.10
1:A:66:LYS:HE2	4:A:504:HOH:O	1.51	1.09
1:A:140:LYS:HB3	1:A:391:ARG:NH1	1.75	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:HIS:HA	1:A:286:MET:HE3	1.39	1.01
1:A:57:MET:SD	4:A:692:HOH:O	2.21	0.99
1:A:73:ALA:HB1	4:A:619:HOH:O	1.64	0.98
1:A:313:ALA:HB1	1:A:317:ILE:HD11	1.45	0.96
1:A:47:GLU:O	1:A:47:GLU:CG	2.08	0.96
1:A:152:ASN:ND2	1:A:168:GLU:HB3	1.81	0.95
1:A:46:LEU:HD13	1:A:103:SER:CB	1.97	0.95
1:A:62:LEU:O	4:A:571:HOH:O	1.85	0.94
1:A:14:ARG:NH1	1:A:375:SER:OG	2.01	0.94
1:A:391:ARG:NH2	1:A:436:LEU:OXT	2.01	0.94
1:A:325:THR:O	1:A:349:ILE:HD12	1.68	0.93
1:A:348:GLN:NE2	4:A:644:HOH:O	1.96	0.93
1:A:155:ASN:ND2	4:A:621:HOH:O	2.00	0.93
1:A:37:GLY:HA2	1:A:374:ARG:HB3	1.52	0.91
1:A:301:ASP:OD2	4:A:515:HOH:O	1.89	0.90
1:A:152:ASN:OD1	1:A:155:ASN:ND2	2.05	0.89
1:A:152:ASN:O	1:A:399:ALA:HB2	1.72	0.88
1:A:71:VAL:O	1:A:74:PRO:HG2	1.73	0.88
1:A:43:HIS:HE1	4:A:515:HOH:O	1.57	0.88
1:A:269:LYS:O	1:A:269:LYS:HD3	1.71	0.88
1:A:142:SER:HA	4:A:586:HOH:O	1.73	0.87
1:A:264:ASN:CG	1:A:266:ASN:H	1.83	0.86
1:A:41:GLY:HA2	4:A:613:HOH:O	1.75	0.86
1:A:4:LYS:HE2	4:A:600:HOH:O	1.76	0.86
1:A:155:ASN:OD1	1:A:209:GLY:HA3	1.76	0.86
1:A:199:LYS:HG3	4:A:669:HOH:O	1.76	0.86
1:A:163:ALA:HB1	1:A:261:ASP:HA	1.60	0.83
1:A:41:GLY:O	1:A:44:GLU:OE2	1.95	0.83
1:A:313:ALA:CB	1:A:317:ILE:HD11	2.07	0.83
1:A:46:LEU:HD13	1:A:103:SER:HB3	1.61	0.83
1:A:435:LYS:HE2	4:A:694:HOH:O	1.78	0.83
1:A:152:ASN:HD21	1:A:168:GLU:HB3	1.44	0.82
1:A:164:LEU:N	1:A:219:GLN:O	2.12	0.82
1:A:54:SER:O	1:A:55:LYS:HG3	1.79	0.81
1:A:168:GLU:OE2	4:A:525:HOH:O	1.96	0.81
1:A:158:SER:HB3	4:A:523:HOH:O	1.80	0.81
1:A:251:GLU:OE1	4:A:522:HOH:O	1.98	0.81
1:A:41:GLY:O	1:A:44:GLU:HG2	1.80	0.80
1:A:13:SER:HB2	4:A:524:HOH:O	1.81	0.80
1:A:82:ASP:HB2	4:A:557:HOH:O	1.82	0.80
1:A:39:SER:O	1:A:40:THR:HG23	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:CE	4:A:614:HOH:O	2.30	0.79
1:A:387:VAL:HG23	1:A:392:THR:OG1	1.82	0.78
1:A:38:ALA:HB1	4:A:760:HOH:O	1.83	0.78
1:A:63:HIS:CD2	4:A:688:HOH:O	2.36	0.78
1:A:260:LEU:HD12	1:A:273:LEU:HD11	1.66	0.77
1:A:264:ASN:ND2	1:A:266:ASN:O	2.18	0.77
1:A:257:LYS:HE2	4:A:614:HOH:O	1.85	0.77
1:A:264:ASN:CB	1:A:266:ASN:H	1.98	0.76
3:A:439:2PG:O1	3:A:439:2PG:O3	2.01	0.76
1:A:4:LYS:CE	4:A:600:HOH:O	2.32	0.76
1:A:164:LEU:HB3	4:A:702:HOH:O	1.85	0.75
1:A:361:ASP:OD1	4:A:735:HOH:O	2.04	0.75
1:A:327:PRO:HG2	4:A:648:HOH:O	1.87	0.75
1:A:66:LYS:HE3	4:A:688:HOH:O	1.87	0.75
1:A:62:LEU:O	1:A:66:LYS:HG3	1.87	0.74
1:A:46:LEU:C	1:A:46:LEU:HD23	2.12	0.74
1:A:283:HIS:CA	1:A:286:MET:HE3	2.16	0.73
1:A:52:ASP:C	1:A:52:ASP:OD1	2.27	0.73
1:A:146:LEU:HD12	1:A:423:ALA:HB1	1.71	0.73
1:A:100:ALA:O	4:A:736:HOH:O	2.05	0.73
1:A:348:GLN:OE1	4:A:644:HOH:O	2.07	0.73
1:A:66:LYS:HG2	4:A:571:HOH:O	1.88	0.72
1:A:262:PHE:O	1:A:263:LYS:HB2	1.89	0.72
1:A:4:LYS:HE3	4:A:764:HOH:O	1.90	0.71
1:A:200:ARG:O	4:A:765:HOH:O	2.06	0.71
1:A:326:ASN:C	1:A:326:ASN:HD22	1.98	0.71
1:A:37:GLY:CA	1:A:374:ARG:HB3	2.20	0.70
1:A:264:ASN:HB3	1:A:266:ASN:H	1.57	0.69
1:A:50:ASP:N	1:A:50:ASP:OD1	2.17	0.69
1:A:94:ILE:HG23	4:A:684:HOH:O	1.92	0.68
1:A:176:ALA:O	4:A:670:HOH:O	2.11	0.68
1:A:260:LEU:HD11	1:A:281:LEU:HD23	1.75	0.68
1:A:45:ALA:HB1	1:A:107:ALA:HB2	1.76	0.67
1:A:313:ALA:CB	1:A:317:ILE:CD1	2.73	0.67
1:A:111:LEU:HB2	4:A:754:HOH:O	1.95	0.67
1:A:264:ASN:HB3	1:A:265:PRO:HA	1.75	0.67
1:A:73:ALA:N	1:A:74:PRO:HD2	2.10	0.67
1:A:257:LYS:HE3	4:A:614:HOH:O	1.94	0.67
1:A:348:GLN:CD	4:A:644:HOH:O	2.28	0.67
1:A:283:HIS:HE1	1:A:312:THR:O	1.77	0.66
1:A:325:THR:OG1	1:A:348:GLN:NE2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASP:OD1	1:A:272:TRP:NE1	2.29	0.66
1:A:301:ASP:OD1	4:A:510:HOH:O	2.14	0.66
1:A:102:LYS:NZ	1:A:354:GLU:OE1	2.29	0.66
1:A:43:HIS:CE1	4:A:515:HOH:O	2.38	0.66
1:A:131:LYS:NZ	1:A:135:ASP:OD2	2.30	0.65
1:A:214:VAL:HG23	1:A:216:PRO:HD3	1.79	0.65
1:A:419:LEU:O	4:A:560:HOH:O	2.13	0.65
1:A:155:ASN:CG	4:A:621:HOH:O	2.38	0.65
1:A:196:LEU:O	1:A:200:ARG:HG3	1.96	0.65
1:A:163:ALA:O	1:A:164:LEU:C	2.40	0.65
1:A:268:ASP:O	1:A:272:TRP:NE1	2.30	0.65
1:A:73:ALA:HB3	1:A:74:PRO:CD	2.27	0.65
1:A:238:ASP:HB2	4:A:695:HOH:O	1.98	0.64
1:A:41:GLY:C	1:A:42:VAL:O	2.39	0.64
1:A:119:ARG:O	4:A:508:HOH:O	2.15	0.63
1:A:4:LYS:CE	4:A:764:HOH:O	2.46	0.63
1:A:391:ARG:HG2	1:A:434:ASP:HA	1.80	0.62
1:A:123:ALA:HB1	4:A:663:HOH:O	1.99	0.62
1:A:4:LYS:NZ	4:A:600:HOH:O	2.24	0.62
1:A:111:LEU:O	1:A:112:GLY:C	2.41	0.62
1:A:262:PHE:O	1:A:263:LYS:CB	2.48	0.61
1:A:12:ASP:OD2	1:A:36:SER:HB2	2.01	0.61
1:A:136:LEU:O	4:A:770:HOH:O	2.16	0.61
1:A:42:VAL:HG12	4:A:761:HOH:O	2.01	0.61
1:A:153:VAL:HB	1:A:193:LEU:HD23	1.83	0.61
1:A:266:ASN:O	1:A:268:ASP:N	2.34	0.61
1:A:41:GLY:HA3	1:A:324:VAL:HG11	1.83	0.60
1:A:143:PRO:HG3	1:A:424:VAL:CG1	2.32	0.60
1:A:101:ASN:ND2	4:A:728:HOH:O	2.35	0.60
1:A:343:LEU:HD23	1:A:345:LYS:HE3	1.84	0.59
1:A:260:LEU:CD1	1:A:273:LEU:HD11	2.32	0.59
1:A:104:LYS:HG3	4:A:677:HOH:O	2.03	0.59
1:A:31:ARG:NH1	4:A:486:HOH:O	2.34	0.59
1:A:141:THR:HG22	4:A:484:HOH:O	2.02	0.58
1:A:153:VAL:HB	1:A:193:LEU:CD2	2.33	0.58
1:A:232:ILE:HD13	1:A:241:VAL:HG12	1.84	0.58
1:A:225:LEU:HD21	1:A:245:LEU:HD21	1.86	0.58
1:A:82:ASP:HA	4:A:503:HOH:O	2.03	0.58
1:A:157:GLY:HA3	4:A:521:HOH:O	2.03	0.58
1:A:168:GLU:OE1	1:A:396:LYS:HE3	2.03	0.58
1:A:143:PRO:HG3	1:A:424:VAL:HG13	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:CG	1:A:391:ARG:O	2.52	0.57
1:A:152:ASN:HB2	4:A:753:HOH:O	2.02	0.57
1:A:52:ASP:O	1:A:58:GLY:HA2	2.05	0.57
1:A:141:THR:HB	1:A:144:TYR:CZ	2.39	0.57
1:A:391:ARG:HG2	1:A:391:ARG:O	2.04	0.57
1:A:41:GLY:O	1:A:44:GLU:CG	2.51	0.57
1:A:46:LEU:HD13	1:A:103:SER:HB2	1.86	0.57
1:A:255:ASP:HB3	4:A:708:HOH:O	2.05	0.57
1:A:283:HIS:CE1	1:A:312:THR:O	2.56	0.57
1:A:164:LEU:HD23	4:A:702:HOH:O	2.05	0.56
1:A:62:LEU:O	1:A:66:LYS:CG	2.53	0.56
1:A:311:LYS:HB3	1:A:312:THR:HG23	1.86	0.56
1:A:264:ASN:CG	1:A:266:ASN:N	2.61	0.56
1:A:321:ASP:OD1	4:A:464:HOH:O	2.17	0.56
1:A:47:GLU:HB2	4:A:440:HOH:O	2.04	0.56
1:A:47:GLU:O	1:A:47:GLU:HG2	2.02	0.56
1:A:163:ALA:O	1:A:165:ALA:N	2.39	0.55
1:A:295:GLU:OE1	1:A:396:LYS:NZ	2.38	0.55
1:A:37:GLY:O	1:A:38:ALA:C	2.49	0.55
1:A:343:LEU:CD2	1:A:345:LYS:HE3	2.37	0.55
1:A:50:ASP:OD2	1:A:62:LEU:HB2	2.06	0.55
1:A:61:VAL:O	1:A:65:VAL:HG23	2.06	0.55
1:A:369:VAL:O	1:A:392:THR:HB	2.07	0.55
1:A:253:PHE:C	1:A:254:LYS:HG3	2.32	0.55
1:A:215:ALA:N	4:A:512:HOH:O	2.36	0.55
1:A:232:ILE:HD13	1:A:241:VAL:CG1	2.36	0.55
1:A:228:ILE:O	1:A:232:ILE:HG13	2.06	0.54
1:A:33:ILE:HG22	1:A:378:THR:HG21	1.90	0.54
1:A:44:GLU:HA	4:A:465:HOH:O	2.08	0.54
1:A:233:LYS:HE3	1:A:238:ASP:OD2	2.07	0.54
1:A:330:ILE:HG22	1:A:334:ILE:HD12	1.89	0.54
1:A:131:LYS:NZ	1:A:135:ASP:CG	2.66	0.53
1:A:327:PRO:HD3	1:A:349:ILE:CD1	2.38	0.53
1:A:46:LEU:C	1:A:46:LEU:CD2	2.81	0.53
1:A:93:LEU:HB3	1:A:110:ILE:HG23	1.90	0.53
1:A:183:LEU:O	1:A:187:SER:HB3	2.08	0.53
1:A:269:LYS:O	1:A:269:LYS:CD	2.50	0.53
1:A:4:LYS:HG2	4:A:470:HOH:O	2.09	0.53
1:A:4:LYS:HB3	4:A:763:HOH:O	2.09	0.53
1:A:326:ASN:C	1:A:326:ASN:ND2	2.67	0.53
1:A:140:LYS:HB3	1:A:391:ARG:HH12	1.71	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:HIS:O	1:A:66:LYS:N	2.43	0.52
1:A:63:HIS:O	1:A:67:ASN:N	2.41	0.52
1:A:292:VAL:O	4:A:639:HOH:O	2.19	0.52
1:A:327:PRO:HD3	1:A:349:ILE:HD11	1.92	0.52
1:A:410:ASN:O	1:A:414:ARG:HG3	2.09	0.52
1:A:146:LEU:CD1	1:A:423:ALA:HB1	2.39	0.52
1:A:152:ASN:HD22	1:A:168:GLU:HB3	1.70	0.51
1:A:264:ASN:ND2	1:A:266:ASN:C	2.68	0.51
1:A:87:LYS:HE2	4:A:733:HOH:O	2.09	0.51
1:A:422:ASN:HB2	4:A:560:HOH:O	2.09	0.51
1:A:185:ILE:O	1:A:189:VAL:HG23	2.11	0.51
1:A:63:HIS:HB2	4:A:569:HOH:O	2.10	0.50
1:A:363:PHE:HZ	1:A:392:THR:HG22	1.76	0.50
1:A:43:HIS:CE1	1:A:329:ARG:NH2	2.80	0.50
1:A:435:LYS:CE	4:A:694:HOH:O	2.44	0.50
1:A:260:LEU:CD1	1:A:281:LEU:HD23	2.40	0.50
1:A:211:GLU:HB2	4:A:621:HOH:O	2.10	0.50
1:A:264:ASN:HB3	1:A:266:ASN:N	2.25	0.50
1:A:282:TYR:HB3	1:A:286:MET:HE2	1.94	0.49
1:A:383:ILE:HG13	1:A:395:ILE:HD11	1.94	0.49
1:A:131:LYS:HD3	1:A:131:LYS:C	2.38	0.49
1:A:287:LYS:NZ	4:A:748:HOH:O	2.27	0.49
1:A:4:LYS:HD3	4:A:469:HOH:O	2.10	0.49
1:A:57:MET:HB2	4:A:555:HOH:O	2.13	0.49
1:A:111:LEU:HD22	4:A:754:HOH:O	2.11	0.49
1:A:102:LYS:HE2	1:A:351:THR:HG23	1.94	0.49
1:A:362:SER:O	1:A:367:TRP:HB2	2.12	0.49
1:A:187:SER:O	1:A:191:HIS:ND1	2.45	0.49
1:A:74:PRO:O	1:A:78:LYS:HD2	2.12	0.49
1:A:432:HIS:HD2	4:A:671:HOH:O	1.96	0.49
1:A:41:GLY:HA3	1:A:324:VAL:CG1	2.42	0.48
1:A:218:ILE:HG23	1:A:223:GLU:HG2	1.94	0.48
1:A:403:SER:O	1:A:407:ALA:CB	2.61	0.48
1:A:398:GLY:HA3	1:A:405:ARG:HD2	1.95	0.48
1:A:73:ALA:HB3	1:A:74:PRO:HD2	1.95	0.48
1:A:41:GLY:O	1:A:44:GLU:CD	2.56	0.48
1:A:45:ALA:CB	1:A:107:ALA:HB2	2.43	0.47
1:A:57:MET:CB	4:A:555:HOH:O	2.63	0.47
1:A:260:LEU:CD1	1:A:273:LEU:CD1	2.92	0.47
1:A:158:SER:CB	4:A:576:HOH:O	2.00	0.47
1:A:185:ILE:HG21	1:A:185:ILE:HD13	1.59	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ARG:O	1:A:377:GLU:HG2	2.14	0.47
1:A:152:ASN:O	1:A:399:ALA:CB	2.53	0.47
1:A:66:LYS:CE	4:A:688:HOH:O	2.57	0.47
1:A:161:GLY:O	1:A:217:ASN:OD1	2.32	0.46
1:A:357:LYS:O	1:A:357:LYS:HG2	2.15	0.46
1:A:131:LYS:NZ	1:A:135:ASP:OD1	2.41	0.46
1:A:196:LEU:HD22	1:A:200:ARG:NH2	2.30	0.46
1:A:225:LEU:O	1:A:229:VAL:HG22	2.15	0.46
1:A:248:ALA:HB1	4:A:654:HOH:O	2.16	0.46
1:A:66:LYS:CE	4:A:504:HOH:O	2.30	0.46
1:A:144:TYR:O	1:A:423:ALA:HA	2.16	0.46
1:A:275:GLY:N	1:A:276:PRO:CD	2.79	0.46
1:A:159:HIS:HE2	1:A:210:ASP:CG	2.23	0.46
1:A:312:THR:CG2	4:A:623:HOH:O	2.64	0.45
1:A:101:ASN:ND2	1:A:103:SER:HB3	2.32	0.45
1:A:73:ALA:CB	1:A:74:PRO:CD	2.90	0.45
1:A:325:THR:O	1:A:349:ILE:CD1	2.52	0.45
1:A:68:VAL:HA	1:A:72:ILE:HB	1.99	0.45
1:A:281:LEU:O	1:A:281:LEU:HD12	2.17	0.45
1:A:387:VAL:CG2	1:A:392:THR:OG1	2.59	0.45
1:A:43:HIS:ND1	1:A:329:ARG:NH2	2.65	0.45
1:A:26:GLU:OE1	1:A:26:GLU:N	2.44	0.45
1:A:362:SER:HB3	1:A:367:TRP:HB2	1.99	0.45
1:A:4:LYS:CB	4:A:763:HOH:O	2.64	0.45
1:A:390:LEU:O	1:A:391:ARG:HB3	2.16	0.44
1:A:298:PHE:HB2	1:A:306:TRP:CD1	2.52	0.44
1:A:259:ASP:OD1	1:A:272:TRP:CD1	2.71	0.44
1:A:378:THR:O	1:A:408:LYS:NZ	2.50	0.44
1:A:46:LEU:HD22	1:A:103:SER:HA	1.99	0.44
1:A:132:HIS:O	1:A:135:ASP:HB2	2.17	0.44
1:A:46:LEU:CD1	1:A:103:SER:HB2	2.47	0.44
1:A:70:ASP:O	1:A:74:PRO:HG3	2.18	0.44
1:A:233:LYS:CE	1:A:238:ASP:OD2	2.65	0.44
1:A:432:HIS:O	1:A:433:GLY:C	2.60	0.44
1:A:317:ILE:HG21	4:A:709:HOH:O	2.17	0.44
1:A:67:ASN:O	1:A:71:VAL:HB	2.18	0.44
1:A:167:GLN:HE22	3:A:439:2PG:H31	1.82	0.44
1:A:330:ILE:HG22	1:A:334:ILE:CD1	2.48	0.43
1:A:262:PHE:C	1:A:263:LYS:HG3	2.43	0.43
1:A:97:ASP:O	1:A:99:THR:HG23	2.19	0.43
1:A:218:ILE:HD13	1:A:218:ILE:HG21	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:NZ	4:A:615:HOH:O	2.52	0.43
1:A:248:ALA:CB	4:A:654:HOH:O	2.66	0.43
1:A:46:LEU:CD1	1:A:103:SER:CB	2.82	0.43
1:A:42:VAL:CG1	4:A:761:HOH:O	2.62	0.43
1:A:143:PRO:HG3	1:A:424:VAL:HG11	2.00	0.43
3:A:439:2PG:C1	4:A:525:HOH:O	2.67	0.43
1:A:271:LYS:C	4:A:622:HOH:O	2.62	0.42
1:A:363:PHE:CZ	1:A:392:THR:HG22	2.54	0.42
1:A:8:ARG:HH12	1:A:22:GLU:CD	2.26	0.42
1:A:204:SER:OG	1:A:205:ALA:N	2.52	0.42
1:A:271:LYS:CB	4:A:622:HOH:O	2.66	0.42
1:A:387:VAL:O	1:A:387:VAL:HG22	2.19	0.42
1:A:133:LEU:HD23	1:A:386:LEU:HA	2.01	0.42
1:A:31:ARG:HH11	1:A:31:ARG:HD2	1.51	0.42
1:A:201:TYR:HB2	1:A:205:ALA:CB	2.49	0.42
1:A:204:SER:C	1:A:206:GLY:H	2.26	0.42
1:A:295:GLU:HA	1:A:318:VAL:HB	2.01	0.42
1:A:121:ALA:HB3	1:A:132:HIS:NE2	2.35	0.42
1:A:177:LYS:HD2	1:A:177:LYS:HA	1.85	0.42
1:A:59:LYS:HD2	4:A:555:HOH:O	2.19	0.42
1:A:39:SER:O	1:A:40:THR:CG2	2.61	0.42
1:A:194:LYS:HG2	1:A:198:LYS:HE3	2.02	0.42
1:A:326:ASN:HD22	1:A:327:PRO:N	2.18	0.42
1:A:381:THR:OG1	4:A:507:HOH:O	2.18	0.41
1:A:401:ALA:O	1:A:402:ARG:HB2	2.19	0.41
1:A:41:GLY:O	1:A:42:VAL:C	2.63	0.41
1:A:168:GLU:HG3	1:A:246:ASP:HB3	2.02	0.41
1:A:317:ILE:O	1:A:339:ALA:HB1	2.20	0.41
1:A:344:LEU:CD1	1:A:359:ALA:HB2	2.49	0.41
1:A:373:HIS:CE1	1:A:405:ARG:HH11	2.36	0.41
1:A:46:LEU:HD13	1:A:103:SER:CA	2.49	0.41
1:A:267:SER:HB3	1:A:272:TRP:CH2	2.56	0.41
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.84	0.41
1:A:143:PRO:CG	1:A:424:VAL:HG13	2.49	0.41
1:A:282:TYR:C	1:A:286:MET:CE	2.94	0.40
1:A:77:VAL:HB	4:A:673:HOH:O	2.20	0.40
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.90	0.40
1:A:159:HIS:CE1	1:A:210:ASP:H	2.40	0.40
3:A:439:2PG:H2	4:A:525:HOH:O	2.21	0.40
1:A:266:ASN:HD22	1:A:266:ASN:HA	1.37	0.40
1:A:127:VAL:HB	1:A:128:PRO:HD2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HB3	1:A:392:THR:HG23	2.03	0.40
1:A:92:PHE:CD1	1:A:92:PHE:C	2.99	0.40
1:A:101:ASN:HD21	1:A:103:SER:HB3	1.86	0.40
1:A:267:SER:HB3	1:A:272:TRP:CZ2	2.56	0.40

All (2) 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)
1:A:79:ALA:O	4:A:643:HOH:O[3_644]	2.14	0.06
1:A:79:ALA:CA	4:A:643:HOH:O[3_644]	2.15	0.05

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%)	392 (90%)	34 (8%)	8 (2%)	6 4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	LYS
1	A	265	PRO
1	A	267	SER
1	A	270	SER
1	A	164	LEU
1	A	402	ARG
1	A	160	ALA
1	A	324	VAL

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%)	309 (90%)	35 (10%)	7 7

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	19	VAL
1	A	23	LEU
1	A	39	SER
1	A	40	THR
1	A	43	HIS
1	A	46	LEU
1	A	50	ASP
1	A	53	LYS
1	A	54	SER
1	A	81	ILE
1	A	96	LEU
1	A	101	ASN
1	A	131	LYS
1	A	133	LEU
1	A	140	LYS
1	A	143	PRO
1	A	147	PRO
1	A	149	PRO
1	A	151	LEU
1	A	154	LEU
1	A	155	ASN
1	A	171	ILE
1	A	187	SER
1	A	194	LYS
1	A	233	LYS
1	A	254	LYS
1	A	255	ASP
1	A	266	ASN
1	A	270	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	284	SER
1	A	311	LYS
1	A	324	VAL
1	A	325	THR
1	A	383	ILE

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

Mol	Chain	Res	Type
1	A	43	HIS
1	A	101	ASN
1	A	167	GLN
1	A	207	ASN
1	A	266	ASN
1	A	283	HIS
1	A	326	ASN
1	A	432	HIS

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 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	439	2	9,10,10	1.52	2 (22%)	12,14,14	1.48	4 (33%)

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	439	2	-	7/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	439	2PG	P-O4P	-2.69	1.44	1.54
3	A	439	2PG	O1-C1	2.36	1.29	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	439	2PG	O1-C1-C2	-2.61	117.22	122.85
3	A	439	2PG	O4P-P-O3P	2.12	115.75	107.80
3	A	439	2PG	O1P-C2-C1	-2.06	107.37	111.66
3	A	439	2PG	O3-C3-C2	2.01	116.83	111.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	439	2PG	O2-C1-C2-O1P
3	A	439	2PG	C1-C2-C3-O3
3	A	439	2PG	O1P-C2-C3-O3
3	A	439	2PG	C3-C2-O1P-P
3	A	439	2PG	O1-C1-C2-C3
3	A	439	2PG	O2-C1-C2-C3
3	A	439	2PG	C2-O1P-P-O3P

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	439	2PG	4	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.