



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:13 PM GMT

PDB ID : 1ELS
Title : CATALYTIC METAL ION BINDING IN ENOLASE: THE CRYSTAL
STRUCTURE OF ENOLASE-MN2+-PHOSPHONOACETOHYDROXA
MATE COMPLEX AT 2.4 ANGSTROMS RESOLUTION
Authors : Zhang, E.; Hatada, M.; Brewer, J.M.; Lebioda, L.
Deposited on : 1994-04-05
Resolution : 2.40 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

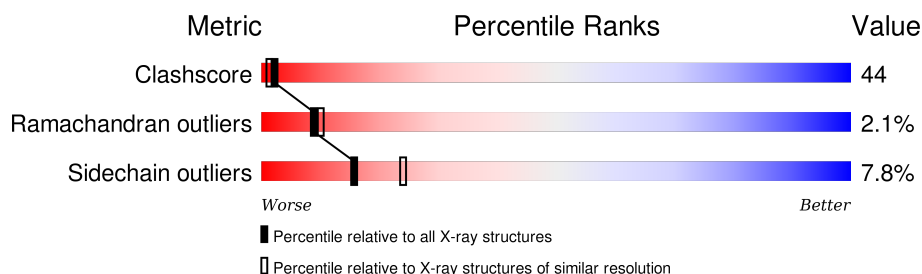
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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	

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	PAH	A	439	-	X	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3643 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			

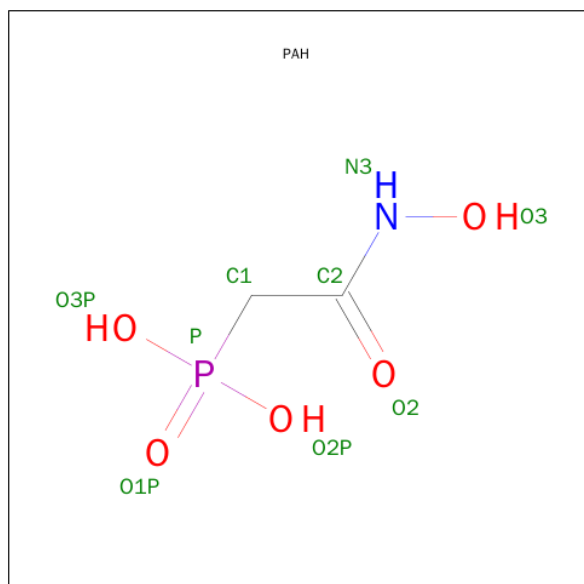
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is PHOSPHONOACETOHYDROXAMIC ACID (three-letter code: PAH) (formula: C₂H₆NO₅P).



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

- Molecule 4 is water.

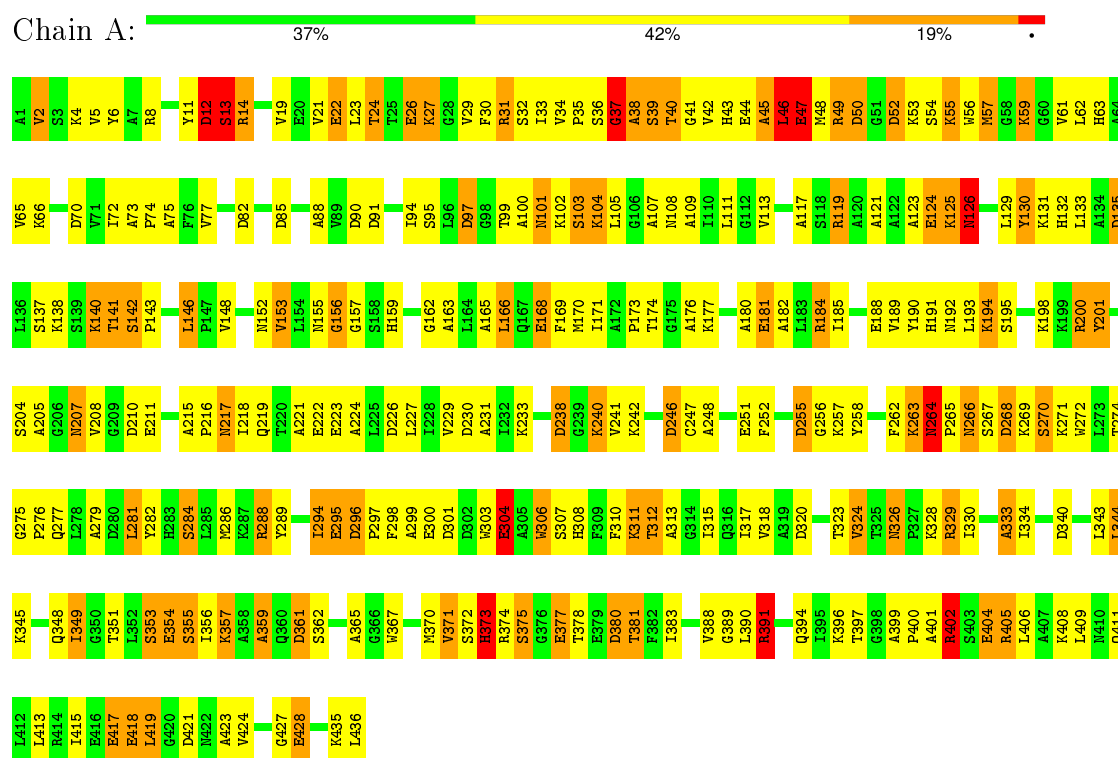
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	343	Total	O	0	0
			343	343		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 will therefore be 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) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3643	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: PAH, MN

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	1.04	2/3349 (0.1%)	2.49	189/4531 (4.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	GLU	CD-OE1	-5.73	1.19	1.25
1	A	377	GLU	CD-OE2	-5.01	1.20	1.25

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	ARG	NE-CZ-NH1	-23.27	108.67	120.30
1	A	8	ARG	NE-CZ-NH1	21.99	131.29	120.30
1	A	49	ARG	NE-CZ-NH1	20.78	130.69	120.30
1	A	49	ARG	NE-CZ-NH2	-16.67	111.96	120.30
1	A	200	ARG	NE-CZ-NH2	-15.29	112.65	120.30
1	A	288	ARG	NE-CZ-NH1	15.12	127.86	120.30
1	A	391	ARG	NH1-CZ-NH2	14.39	135.23	119.40
1	A	211	GLU	OE1-CD-OE2	14.22	140.37	123.30
1	A	50	ASP	CB-CG-OD1	-13.64	106.02	118.30
1	A	304	GLU	OE1-CD-OE2	13.27	139.22	123.30
1	A	340	ASP	CB-CG-OD1	13.11	130.10	118.30
1	A	200	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	A	380	ASP	CB-CG-OD2	11.51	128.66	118.30
1	A	361	ASP	CB-CG-OD2	-11.42	108.02	118.30
1	A	97	ASP	CB-CG-OD1	11.08	128.27	118.30
1	A	405	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	A	8	ARG	NH1-CZ-NH2	-10.67	107.66	119.40
1	A	402	ARG	NE-CZ-NH2	10.43	125.51	120.30
1	A	374	ARG	NE-CZ-NH1	10.36	125.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ARG	CD-NE-CZ	-10.05	109.53	123.60
1	A	12	ASP	CB-CG-OD2	9.97	127.28	118.30
1	A	428	GLU	CA-CB-CG	9.70	134.73	113.40
1	A	279	ALA	N-CA-CB	9.23	123.02	110.10
1	A	170	MET	CG-SD-CE	9.08	114.72	100.20
1	A	184	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	391	ARG	CD-NE-CZ	-8.83	111.24	123.60
1	A	24	THR	CA-CB-CG2	8.78	124.69	112.40
1	A	380	ASP	CB-CG-OD1	-8.76	110.42	118.30
1	A	141	THR	C-N-CA	8.61	143.23	121.70
1	A	37	GLY	N-CA-C	8.57	134.54	113.10
1	A	391	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	402	ARG	NE-CZ-NH1	-8.49	116.05	120.30
1	A	288	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	135	ASP	CB-CG-OD1	-8.39	110.75	118.30
1	A	409	LEU	CB-CA-C	8.37	126.10	110.20
1	A	374	ARG	CD-NE-CZ	8.32	135.25	123.60
1	A	38	ALA	CA-C-O	8.20	137.33	120.10
1	A	288	ARG	CD-NE-CZ	8.16	135.02	123.60
1	A	184	ARG	CD-NE-CZ	-8.09	112.27	123.60
1	A	436	LEU	CA-CB-CG	8.08	133.89	115.30
1	A	181	GLU	OE1-CD-OE2	-8.04	113.65	123.30
1	A	26	GLU	OE1-CD-OE2	8.01	132.91	123.30
1	A	405	ARG	CD-NE-CZ	7.80	134.51	123.60
1	A	135	ASP	CB-CG-OD2	7.68	125.21	118.30
1	A	14	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	A	174	THR	CA-CB-OG1	-7.63	92.98	109.00
1	A	82	ASP	CB-CG-OD1	-7.58	111.48	118.30
1	A	11	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	A	104	LYS	CA-C-O	-7.48	104.40	120.10
1	A	222	GLU	CA-CB-CG	7.42	129.72	113.40
1	A	52	ASP	CB-CG-OD1	-7.37	111.67	118.30
1	A	146	LEU	CB-CA-C	7.36	124.19	110.20
1	A	46	LEU	CB-CA-C	7.34	124.14	110.20
1	A	38	ALA	N-CA-C	7.31	130.73	111.00
1	A	5	VAL	CA-CB-CG1	7.24	121.76	110.90
1	A	281	LEU	CA-CB-CG	7.17	131.78	115.30
1	A	91	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	A	238	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	32	SER	CB-CA-C	7.11	123.60	110.10
1	A	211	GLU	CG-CD-OE2	-7.00	104.30	118.30
1	A	47	GLU	OE1-CD-OE2	6.98	131.67	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ASP	OD1-CG-OD2	-6.93	110.13	123.30
1	A	124	GLU	CG-CD-OE1	-6.86	104.58	118.30
1	A	162	GLY	N-CA-C	-6.85	95.97	113.10
1	A	289	TYR	CB-CG-CD1	6.80	125.08	121.00
1	A	389	GLY	O-C-N	-6.78	111.85	122.70
1	A	119	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	111	LEU	CB-CG-CD2	-6.74	99.55	111.00
1	A	50	ASP	CA-C-N	6.73	129.66	116.20
1	A	329	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	39	SER	C-N-CA	6.63	138.29	121.70
1	A	192	ASN	OD1-CG-ND2	6.62	137.13	121.90
1	A	389	GLY	CA-C-N	6.60	131.72	117.20
1	A	82	ASP	OD1-CG-OD2	6.58	135.80	123.30
1	A	361	ASP	OD1-CG-OD2	6.56	135.77	123.30
1	A	296	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	31	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	A	31	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	A	226	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	142	SER	N-CA-CB	-6.40	100.89	110.50
1	A	377	GLU	CG-CD-OE2	6.35	131.00	118.30
1	A	306	TRP	N-CA-CB	6.31	121.96	110.60
1	A	191	HIS	N-CA-CB	6.31	121.96	110.60
1	A	411	GLN	CG-CD-OE1	6.31	134.22	121.60
1	A	246	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	A	46	LEU	CA-C-O	6.29	133.32	120.10
1	A	344	LEU	CA-CB-CG	6.28	129.75	115.30
1	A	229	VAL	N-CA-CB	6.27	125.29	111.50
1	A	48	MET	CA-CB-CG	-6.27	102.65	113.30
1	A	184	ARG	CA-CB-CG	6.25	127.16	113.40
1	A	311	LYS	CA-CB-CG	6.22	127.08	113.40
1	A	421	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	82	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	31	ARG	N-CA-CB	-6.16	99.52	110.60
1	A	340	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	348	GLN	N-CA-CB	6.14	121.65	110.60
1	A	6	TYR	CA-C-O	-6.11	107.27	120.10
1	A	85	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	264	ASN	CA-CB-CG	-6.08	100.01	113.40
1	A	418	GLU	OE1-CD-OE2	6.08	130.60	123.30
1	A	126	ASN	CA-C-O	-6.00	107.49	120.10
1	A	371	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	A	109	ALA	O-C-N	5.95	132.22	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	SER	CB-CA-C	-5.95	98.80	110.10
1	A	210	ASP	O-C-N	5.94	132.20	122.70
1	A	2	VAL	N-CA-CB	-5.92	98.48	111.50
1	A	156	GLY	CA-C-N	5.86	127.92	116.20
1	A	246	ASP	N-CA-C	-5.86	95.19	111.00
1	A	13	SER	CB-CA-C	-5.85	98.99	110.10
1	A	300	GLU	CG-CD-OE2	5.85	130.00	118.30
1	A	23	LEU	N-CA-CB	-5.84	98.72	110.40
1	A	201	TYR	CA-CB-CG	-5.83	102.32	113.40
1	A	373	HIS	C-N-CA	5.83	136.26	121.70
1	A	299	ALA	CB-CA-C	5.75	118.73	110.10
1	A	130	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	A	130	TYR	CB-CG-CD2	5.73	124.44	121.00
1	A	377	GLU	OE1-CD-OE2	-5.73	116.42	123.30
1	A	163	ALA	CB-CA-C	-5.72	101.52	110.10
1	A	375	SER	CB-CA-C	-5.71	99.26	110.10
1	A	294	ILE	CG1-CB-CG2	-5.70	98.85	111.40
1	A	289	TYR	CG-CD2-CE2	5.70	125.86	121.30
1	A	165	ALA	CA-C-O	-5.70	108.14	120.10
1	A	340	ASP	CA-C-O	-5.69	108.16	120.10
1	A	180	ALA	N-CA-CB	-5.68	102.15	110.10
1	A	52	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	333	ALA	CB-CA-C	5.65	118.58	110.10
1	A	417	GLU	CG-CD-OE1	-5.65	107.00	118.30
1	A	177	LYS	N-CA-CB	5.65	120.76	110.60
1	A	405	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
1	A	406	LEU	CA-C-O	-5.62	108.30	120.10
1	A	324	VAL	CA-CB-CG1	5.61	119.31	110.90
1	A	354	GLU	C-N-CA	5.61	135.71	121.70
1	A	397	THR	C-N-CA	5.60	134.06	122.30
1	A	124	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	207	ASN	CB-CG-OD1	-5.58	110.44	121.60
1	A	168	GLU	CG-CD-OE2	5.58	129.46	118.30
1	A	12	ASP	CB-CA-C	5.57	121.53	110.40
1	A	47	GLU	CB-CA-C	-5.53	99.34	110.40
1	A	45	ALA	N-CA-CB	5.51	117.81	110.10
1	A	36	SER	C-N-CA	5.50	133.85	122.30
1	A	38	ALA	CB-CA-C	-5.50	101.85	110.10
1	A	77	VAL	CB-CA-C	5.49	121.82	111.40
1	A	240	LYS	C-N-CA	5.47	135.38	121.70
1	A	436	LEU	CB-CA-C	5.46	120.56	110.20
1	A	295	GLU	CG-CD-OE1	-5.43	107.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	LYS	CA-CB-CG	5.40	125.27	113.40
1	A	19	VAL	CA-CB-CG1	5.39	118.99	110.90
1	A	380	ASP	CB-CA-C	5.38	121.17	110.40
1	A	104	LYS	O-C-N	5.37	131.30	122.70
1	A	359	ALA	N-CA-CB	-5.36	102.59	110.10
1	A	46	LEU	N-CA-CB	-5.36	99.68	110.40
1	A	146	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	A	428	GLU	CG-CD-OE1	-5.36	107.59	118.30
1	A	230	ASP	CA-CB-CG	5.36	125.18	113.40
1	A	153	VAL	CA-CB-CG2	5.35	118.92	110.90
1	A	279	ALA	CB-CA-C	-5.34	102.08	110.10
1	A	59	LYS	CA-C-O	-5.33	108.91	120.10
1	A	349	ILE	CB-CA-C	5.33	122.25	111.60
1	A	169	PHE	O-C-N	5.27	131.13	122.70
1	A	288	ARG	CA-C-O	-5.26	109.05	120.10
1	A	231	ALA	CB-CA-C	5.26	117.99	110.10
1	A	357	LYS	O-C-N	-5.26	114.29	122.70
1	A	75	ALA	CB-CA-C	-5.24	102.24	110.10
1	A	219	GLN	CA-C-O	-5.21	109.17	120.10
1	A	381	THR	CA-CB-OG1	-5.20	98.07	109.00
1	A	176	ALA	O-C-N	5.20	131.02	122.70
1	A	223	GLU	O-C-N	5.20	131.01	122.70
1	A	55	LYS	O-C-N	5.17	130.97	122.70
1	A	312	THR	CA-C-O	-5.17	109.24	120.10
1	A	22	GLU	CB-CA-C	-5.17	100.07	110.40
1	A	22	GLU	N-CA-CB	5.16	119.89	110.60
1	A	419	LEU	N-CA-CB	-5.16	100.08	110.40
1	A	50	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	241	VAL	C-N-CA	5.12	134.51	121.70
1	A	320	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	251	GLU	CG-CD-OE1	-5.10	108.09	118.30
1	A	108	ASN	CA-CB-CG	5.10	124.62	113.40
1	A	417	GLU	CG-CD-OE2	5.10	128.49	118.30
1	A	117	ALA	N-CA-CB	-5.09	102.97	110.10
1	A	405	ARG	CA-C-O	5.08	130.78	120.10
1	A	383	ILE	CA-CB-CG1	5.08	120.66	111.00
1	A	88	ALA	N-CA-CB	5.07	117.20	110.10
1	A	188	GLU	O-C-N	-5.06	114.60	122.70
1	A	251	GLU	CG-CD-OE2	5.06	128.42	118.30
1	A	229	VAL	CG1-CB-CG2	5.03	118.95	110.90
1	A	300	GLU	N-CA-CB	5.03	119.65	110.60
1	A	419	LEU	CB-CG-CD2	-5.02	102.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	LEU	CA-C-O	-5.00	109.59	120.10
1	A	165	ALA	CA-C-N	5.00	128.21	117.20

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	3291	288	5
2	A	2	0	0	0	0
3	A	9	0	3	9	0
4	A	343	0	0	111	6
All	All	3643	0	3294	290	6

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 44.

All (290) 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:142:SER:HA	4:A:586:HOH:O	1.33	1.23
1:A:255:ASP:HB3	4:A:708:HOH:O	1.39	1.18
1:A:435:LYS:HE3	4:A:694:HOH:O	1.43	1.17
1:A:227:LEU:HB2	4:A:597:HOH:O	1.52	1.08
1:A:345:LYS:NZ	3:A:439:PAH:H12	1.66	1.08
1:A:57:MET:SD	4:A:692:HOH:O	2.08	1.08
1:A:264:ASN:HB3	1:A:265:PRO:HA	1.29	1.07
1:A:264:ASN:CG	1:A:266:ASN:H	1.59	1.05
1:A:146:LEU:HD12	1:A:423:ALA:HB1	1.38	1.03
1:A:345:LYS:HZ1	3:A:439:PAH:H12	1.23	1.00
1:A:66:LYS:HE2	4:A:504:HOH:O	1.58	1.00
1:A:141:THR:O	4:A:586:HOH:O	1.80	1.00
1:A:157:GLY:CA	4:A:758:HOH:O	2.11	0.98
1:A:47:GLU:HB3	4:A:448:HOH:O	1.60	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASN:HA	4:A:785:HOH:O	1.63	0.98
1:A:14:ARG:HH11	1:A:375:SER:HB3	1.30	0.96
1:A:94:ILE:HG23	4:A:684:HOH:O	1.65	0.96
1:A:282:TYR:O	1:A:286:MET:HE2	1.66	0.96
1:A:345:LYS:NZ	3:A:439:PAH:C1	2.28	0.95
1:A:157:GLY:HA2	4:A:758:HOH:O	1.64	0.95
1:A:262:PHE:O	1:A:263:LYS:HB2	1.69	0.93
1:A:326:ASN:O	1:A:330:ILE:HG13	1.70	0.92
1:A:41:GLY:O	1:A:44:GLU:OE2	1.91	0.89
1:A:4:LYS:HE2	4:A:600:HOH:O	1.71	0.89
1:A:264:ASN:HB3	1:A:265:PRO:CA	2.04	0.87
1:A:152:ASN:HB2	4:A:753:HOH:O	1.73	0.87
1:A:345:LYS:HZ3	3:A:439:PAH:C1	1.87	0.87
1:A:257:LYS:HD2	4:A:614:HOH:O	1.75	0.86
1:A:43:HIS:HA	4:A:727:HOH:O	1.75	0.86
1:A:46:LEU:C	1:A:46:LEU:HD23	1.98	0.83
1:A:268:ASP:OD2	1:A:271:LYS:HE3	1.77	0.83
1:A:313:ALA:CB	1:A:317:ILE:HD11	2.08	0.83
1:A:131:LYS:HD3	1:A:131:LYS:O	1.79	0.82
1:A:52:ASP:C	1:A:52:ASP:OD1	2.16	0.82
1:A:373:HIS:HD2	1:A:405:ARG:HH11	1.28	0.81
1:A:61:VAL:O	1:A:65:VAL:HG23	1.79	0.81
1:A:301:ASP:HB2	4:A:446:HOH:O	1.79	0.81
1:A:156:GLY:O	4:A:758:HOH:O	1.99	0.80
1:A:269:LYS:HD3	4:A:705:HOH:O	1.84	0.78
1:A:146:LEU:CD1	1:A:423:ALA:HB1	2.13	0.77
1:A:399:ALA:HB1	1:A:400:PRO:HD2	1.65	0.77
1:A:255:ASP:O	4:A:708:HOH:O	2.02	0.77
1:A:66:LYS:O	1:A:70:ASP:HB2	1.84	0.77
1:A:143:PRO:HG2	1:A:424:VAL:HG13	1.64	0.77
1:A:307:SER:O	4:A:581:HOH:O	2.04	0.76
1:A:14:ARG:NH1	1:A:375:SER:HB3	2.00	0.76
1:A:417:GLU:OE2	4:A:566:HOH:O	2.04	0.76
1:A:62:LEU:O	1:A:66:LYS:HG3	1.86	0.75
1:A:373:HIS:CD2	1:A:405:ARG:HH11	2.04	0.75
1:A:38:ALA:CB	1:A:40:THR:HG23	2.16	0.75
1:A:52:ASP:CB	4:A:579:HOH:O	2.34	0.75
1:A:264:ASN:CA	4:A:785:HOH:O	2.28	0.75
1:A:38:ALA:N	4:A:611:HOH:O	2.20	0.74
1:A:30:PHE:CE2	1:A:123:ALA:HB2	2.22	0.74
1:A:262:PHE:O	1:A:263:LYS:CB	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ALA:HB1	1:A:317:ILE:HD11	1.71	0.73
1:A:304:GLU:HB2	4:A:474:HOH:O	1.88	0.73
1:A:264:ASN:CG	1:A:266:ASN:N	2.40	0.73
1:A:56:TRP:CH2	4:A:651:HOH:O	2.42	0.72
1:A:152:ASN:O	1:A:399:ALA:HB2	1.88	0.72
1:A:345:LYS:HZ1	3:A:439:PAH:C1	1.95	0.72
1:A:46:LEU:HD13	1:A:103:SER:HB3	1.71	0.71
1:A:56:TRP:HH2	4:A:651:HOH:O	1.73	0.71
1:A:40:THR:HG22	4:A:752:HOH:O	1.88	0.71
1:A:143:PRO:CG	1:A:424:VAL:HG13	2.20	0.71
1:A:362:SER:O	1:A:367:TRP:HB2	1.91	0.71
1:A:73:ALA:HB1	4:A:619:HOH:O	1.90	0.70
1:A:345:LYS:HZ3	3:A:439:PAH:H11	1.56	0.70
1:A:168:GLU:OE1	1:A:396:LYS:HE3	1.90	0.70
1:A:401:ALA:O	1:A:402:ARG:HB2	1.92	0.70
1:A:255:ASP:N	4:A:706:HOH:O	2.24	0.69
1:A:50:ASP:OD2	1:A:62:LEU:HB2	1.92	0.69
1:A:264:ASN:C	1:A:264:ASN:OD1	2.27	0.68
1:A:200:ARG:O	4:A:765:HOH:O	2.11	0.68
1:A:264:ASN:CB	1:A:265:PRO:HA	2.12	0.68
1:A:377:GLU:OE2	4:A:749:HOH:O	2.12	0.68
1:A:381:THR:CG2	4:A:507:HOH:O	2.42	0.67
1:A:4:LYS:HG2	4:A:470:HOH:O	1.93	0.67
1:A:313:ALA:CB	1:A:317:ILE:CD1	2.73	0.66
1:A:282:TYR:C	1:A:286:MET:HE2	2.16	0.65
1:A:131:LYS:HD3	1:A:131:LYS:C	2.17	0.65
1:A:294:ILE:HG13	1:A:315:ILE:HD11	1.79	0.65
1:A:153:VAL:HB	1:A:193:LEU:HD23	1.78	0.65
1:A:313:ALA:HB3	1:A:317:ILE:CD1	2.27	0.65
1:A:38:ALA:CB	1:A:40:THR:CG2	2.75	0.65
1:A:157:GLY:C	4:A:758:HOH:O	2.32	0.64
1:A:344:LEU:HD22	1:A:371:VAL:HG22	1.78	0.64
1:A:131:LYS:NZ	1:A:135:ASP:OD2	2.30	0.64
1:A:282:TYR:HB3	1:A:286:MET:HE1	1.79	0.64
1:A:14:ARG:CZ	4:A:573:HOH:O	2.46	0.63
1:A:268:ASP:OD1	1:A:268:ASP:C	2.36	0.63
1:A:373:HIS:CD2	1:A:405:ARG:NH1	2.66	0.63
1:A:94:ILE:HA	4:A:684:HOH:O	1.98	0.63
1:A:345:LYS:NZ	3:A:439:PAH:H11	2.10	0.63
1:A:296:ASP:HA	1:A:306:TRP:CH2	2.33	0.63
1:A:119:ARG:NH1	4:A:603:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASP:O	1:A:408:LYS:HE3	1.98	0.63
1:A:264:ASN:CB	4:A:785:HOH:O	2.46	0.63
1:A:38:ALA:HB1	1:A:40:THR:HG23	1.81	0.62
1:A:349:ILE:HD13	1:A:354:GLU:HB3	1.80	0.62
1:A:159:HIS:CD2	4:A:576:HOH:O	2.53	0.62
1:A:142:SER:CA	4:A:586:HOH:O	2.10	0.62
1:A:166:LEU:N	1:A:166:LEU:HD23	2.15	0.62
1:A:41:GLY:HA3	4:A:613:HOH:O	1.99	0.61
1:A:63:HIS:O	1:A:66:LYS:N	2.32	0.61
1:A:101:ASN:C	1:A:101:ASN:HD22	2.02	0.61
1:A:66:LYS:HD2	4:A:685:HOH:O	2.01	0.61
3:A:439:PAH:O2P	4:A:768:HOH:O	2.16	0.61
1:A:100:ALA:O	4:A:736:HOH:O	2.16	0.60
1:A:66:LYS:CD	4:A:685:HOH:O	2.50	0.60
1:A:143:PRO:HA	4:A:586:HOH:O	2.02	0.59
1:A:153:VAL:HG11	1:A:171:ILE:HG12	1.84	0.59
1:A:399:ALA:HB1	1:A:400:PRO:CD	2.31	0.59
1:A:428:GLU:OE2	4:A:744:HOH:O	2.16	0.59
1:A:264:ASN:CB	1:A:265:PRO:CA	2.75	0.59
1:A:143:PRO:CG	1:A:424:VAL:CG1	2.81	0.58
1:A:262:PHE:CD2	1:A:263:LYS:HG3	2.38	0.58
1:A:123:ALA:HB1	4:A:663:HOH:O	2.03	0.58
1:A:13:SER:HB2	4:A:524:HOH:O	2.04	0.58
1:A:42:VAL:HG23	1:A:43:HIS:CE1	2.37	0.58
1:A:246:ASP:HA	1:A:295:GLU:HB3	1.86	0.58
1:A:4:LYS:HE3	4:A:764:HOH:O	2.03	0.57
1:A:159:HIS:CD2	1:A:159:HIS:N	2.69	0.57
1:A:53:LYS:HG3	4:A:676:HOH:O	2.04	0.57
1:A:94:ILE:CA	4:A:684:HOH:O	2.53	0.57
1:A:38:ALA:HB1	1:A:40:THR:CG2	2.34	0.57
1:A:45:ALA:HB1	1:A:107:ALA:HB2	1.87	0.57
1:A:303:TRP:HZ2	1:A:329:ARG:HH21	1.53	0.56
1:A:53:LYS:CG	4:A:676:HOH:O	2.52	0.56
1:A:256:GLY:N	4:A:706:HOH:O	2.03	0.56
1:A:353:SER:O	1:A:357:LYS:HB2	2.04	0.56
1:A:240:LYS:HE3	4:A:778:HOH:O	2.06	0.56
1:A:275:GLY:N	1:A:276:PRO:CD	2.69	0.56
1:A:49:ARG:NH1	1:A:59:LYS:O	2.36	0.56
1:A:38:ALA:HB2	1:A:40:THR:CG2	2.37	0.55
1:A:200:ARG:HB3	4:A:765:HOH:O	2.06	0.55
1:A:46:LEU:C	1:A:46:LEU:CD2	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:CG2	4:A:684:HOH:O	2.35	0.55
1:A:97:ASP:OD2	1:A:99:THR:OG1	2.23	0.55
1:A:152:ASN:ND2	4:A:753:HOH:O	2.40	0.55
1:A:101:ASN:HB3	4:A:519:HOH:O	2.06	0.55
1:A:153:VAL:HB	1:A:193:LEU:CD2	2.36	0.55
1:A:301:ASP:N	4:A:446:HOH:O	2.37	0.54
1:A:351:THR:OG1	1:A:354:GLU:HB2	2.08	0.54
1:A:33:ILE:HG22	1:A:378:THR:HG21	1.89	0.54
1:A:38:ALA:HB1	1:A:40:THR:OG1	2.08	0.54
1:A:137:SER:O	1:A:138:LYS:HB2	2.07	0.54
1:A:39:SER:HB2	4:A:668:HOH:O	2.08	0.54
1:A:143:PRO:HG2	1:A:424:VAL:CG1	2.34	0.53
1:A:217:ASN:HB3	4:A:617:HOH:O	2.07	0.53
1:A:282:TYR:C	1:A:286:MET:CE	2.77	0.53
1:A:124:GLU:HB2	4:A:715:HOH:O	2.08	0.53
1:A:73:ALA:HB3	1:A:74:PRO:HD3	1.91	0.53
1:A:159:HIS:HE1	4:A:730:HOH:O	1.91	0.53
1:A:70:ASP:CG	4:A:687:HOH:O	2.47	0.52
1:A:97:ASP:OD2	1:A:102:LYS:HA	2.09	0.52
1:A:14:ARG:NH1	1:A:375:SER:CB	2.71	0.52
1:A:190:TYR:O	1:A:193:LEU:HB3	2.10	0.52
1:A:52:ASP:HB3	4:A:579:HOH:O	2.03	0.52
1:A:44:GLU:HA	4:A:465:HOH:O	2.10	0.52
1:A:264:ASN:ND2	1:A:266:ASN:C	2.63	0.51
1:A:334:ILE:HD13	1:A:365:ALA:HB2	1.91	0.51
1:A:30:PHE:CZ	1:A:123:ALA:CB	2.94	0.51
1:A:269:LYS:O	1:A:270:SER:CB	2.58	0.51
1:A:101:ASN:HA	4:A:519:HOH:O	2.10	0.51
1:A:326:ASN:HD22	1:A:326:ASN:C	2.08	0.51
1:A:90:ASP:OD2	1:A:353:SER:OG	2.23	0.51
1:A:194:LYS:O	1:A:198:LYS:HG3	2.11	0.50
1:A:257:LYS:HB3	1:A:272:TRP:HB3	1.93	0.50
1:A:39:SER:HB3	4:A:606:HOH:O	2.09	0.50
1:A:264:ASN:CG	4:A:785:HOH:O	2.50	0.50
1:A:72:ILE:HD11	1:A:105:LEU:HD13	1.94	0.49
1:A:143:PRO:HG3	1:A:424:VAL:CG1	2.42	0.49
1:A:4:LYS:CE	4:A:600:HOH:O	2.43	0.49
1:A:417:GLU:CD	4:A:566:HOH:O	2.48	0.49
1:A:157:GLY:C	1:A:159:HIS:H	2.15	0.49
1:A:153:VAL:CG1	1:A:171:ILE:HG12	2.42	0.49
1:A:295:GLU:HA	1:A:318:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:THR:HG23	4:A:623:HOH:O	2.12	0.49
1:A:4:LYS:CE	4:A:764:HOH:O	2.60	0.48
1:A:31:ARG:O	4:A:603:HOH:O	2.20	0.48
1:A:40:THR:HB	4:A:520:HOH:O	2.12	0.48
1:A:262:PHE:HD2	4:A:703:HOH:O	1.97	0.48
1:A:30:PHE:CE2	1:A:123:ALA:CB	2.95	0.48
1:A:264:ASN:CB	1:A:266:ASN:H	2.26	0.48
1:A:252:PHE:HB3	1:A:262:PHE:CD1	2.49	0.48
1:A:52:ASP:OD1	1:A:54:SER:N	2.41	0.48
1:A:405:ARG:HA	1:A:405:ARG:HD3	1.65	0.48
1:A:349:ILE:CD1	1:A:354:GLU:HB3	2.41	0.48
1:A:50:ASP:OD1	1:A:50:ASP:N	2.40	0.48
1:A:227:LEU:HD13	4:A:597:HOH:O	2.13	0.48
1:A:156:GLY:C	4:A:758:HOH:O	2.49	0.48
1:A:173:PRO:HG2	1:A:182:ALA:HB1	1.95	0.48
1:A:281:LEU:O	1:A:284:SER:HB2	2.14	0.48
1:A:419:LEU:HA	4:A:560:HOH:O	2.14	0.47
1:A:101:ASN:ND2	1:A:103:SER:OG	2.43	0.47
1:A:113:VAL:HG12	1:A:113:VAL:O	2.14	0.47
1:A:334:ILE:HD13	1:A:365:ALA:CB	2.44	0.47
1:A:152:ASN:O	1:A:399:ALA:CB	2.62	0.47
1:A:148:VAL:HG21	1:A:427:GLY:O	2.14	0.47
1:A:274:THR:OG1	1:A:277:GLN:HG3	2.15	0.47
1:A:119:ARG:CZ	4:A:603:HOH:O	2.63	0.47
1:A:157:GLY:C	1:A:159:HIS:N	2.66	0.46
1:A:12:ASP:O	1:A:14:ARG:N	2.47	0.46
1:A:155:ASN:OD1	4:A:621:HOH:O	2.21	0.46
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.78	0.46
1:A:268:ASP:CG	1:A:271:LYS:HE3	2.33	0.46
1:A:72:ILE:HG13	1:A:105:LEU:HD13	1.97	0.46
1:A:310:PHE:CD1	1:A:310:PHE:C	2.89	0.46
1:A:50:ASP:CB	4:A:500:HOH:O	2.64	0.46
1:A:61:VAL:HA	4:A:569:HOH:O	2.15	0.46
1:A:390:LEU:O	1:A:391:ARG:HB3	2.15	0.46
1:A:294:ILE:HG21	1:A:294:ILE:HD12	1.59	0.45
1:A:41:GLY:CA	4:A:613:HOH:O	2.60	0.45
1:A:101:ASN:CB	4:A:519:HOH:O	2.63	0.45
1:A:157:GLY:O	1:A:263:LYS:HE3	2.16	0.45
1:A:13:SER:OG	1:A:404:GLU:HG3	2.17	0.45
1:A:215:ALA:N	4:A:512:HOH:O	2.21	0.45
1:A:201:TYR:HB2	1:A:205:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASN:HB3	1:A:329:ARG:HG3	1.98	0.45
1:A:294:ILE:HD13	1:A:294:ILE:HG23	1.59	0.45
1:A:121:ALA:HB3	1:A:132:HIS:NE2	2.31	0.45
1:A:233:LYS:NZ	1:A:238:ASP:OD2	2.40	0.45
1:A:185:ILE:O	1:A:189:VAL:HG23	2.16	0.45
1:A:22:GLU:HB3	1:A:29:VAL:HG12	1.97	0.45
1:A:343:LEU:HD23	1:A:345:LYS:HE3	1.99	0.45
1:A:216:PRO:HG2	1:A:218:ILE:HG13	1.98	0.45
1:A:37:GLY:HA2	4:A:573:HOH:O	2.16	0.45
1:A:370:MET:HA	1:A:394:GLN:HG3	1.98	0.45
1:A:396:LYS:NZ	4:A:653:HOH:O	2.49	0.45
1:A:269:LYS:CD	4:A:705:HOH:O	2.53	0.45
1:A:323:THR:O	1:A:324:VAL:C	2.54	0.45
1:A:38:ALA:CA	4:A:611:HOH:O	2.65	0.45
1:A:157:GLY:HA3	4:A:521:HOH:O	2.17	0.44
1:A:37:GLY:HA3	1:A:375:SER:HB2	1.98	0.44
1:A:308:HIS:HB2	4:A:750:HOH:O	2.17	0.44
1:A:388:VAL:HG21	1:A:415:ILE:HG21	1.98	0.44
1:A:41:GLY:HA3	1:A:324:VAL:CG1	2.48	0.44
1:A:38:ALA:HB2	1:A:40:THR:HG21	1.99	0.44
1:A:252:PHE:HB3	1:A:262:PHE:CE1	2.53	0.44
1:A:101:ASN:ND2	1:A:101:ASN:C	2.68	0.44
1:A:140:LYS:HB3	1:A:391:ARG:NH1	2.33	0.44
1:A:297:PRO:HB2	1:A:298:PHE:CD2	2.52	0.44
1:A:345:LYS:NZ	4:A:674:HOH:O	2.39	0.43
1:A:402:ARG:O	1:A:405:ARG:HB2	2.18	0.43
1:A:171:ILE:HA	1:A:242:LYS:O	2.17	0.43
1:A:46:LEU:O	1:A:46:LEU:HD23	2.17	0.43
1:A:381:THR:HG21	4:A:507:HOH:O	2.12	0.43
1:A:119:ARG:CD	4:A:603:HOH:O	2.66	0.43
1:A:355:SER:O	1:A:356:ILE:C	2.57	0.43
1:A:72:ILE:CG1	1:A:105:LEU:HD13	2.49	0.43
1:A:146:LEU:CD1	1:A:423:ALA:CB	2.91	0.42
1:A:52:ASP:CG	4:A:579:HOH:O	2.56	0.42
1:A:247:CYS:O	1:A:248:ALA:C	2.56	0.42
1:A:204:SER:HB2	4:A:700:HOH:O	2.18	0.42
1:A:184:ARG:HD3	1:A:184:ARG:HH11	1.58	0.42
1:A:274:THR:HB	4:A:637:HOH:O	2.20	0.42
1:A:26:GLU:HG2	1:A:27:LYS:HG2	2.01	0.42
1:A:21:VAL:HG11	1:A:113:VAL:HA	2.02	0.42
1:A:44:GLU:OE1	4:A:468:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ALA:O	1:A:224:ALA:HB3	2.19	0.42
1:A:142:SER:N	4:A:586:HOH:O	2.29	0.42
1:A:181:GLU:O	1:A:185:ILE:HG13	2.19	0.42
1:A:12:ASP:C	1:A:14:ARG:N	2.73	0.42
1:A:4:LYS:NZ	4:A:764:HOH:O	2.32	0.42
1:A:2:VAL:HA	1:A:24:THR:O	2.20	0.42
1:A:42:VAL:CG2	4:A:515:HOH:O	2.67	0.42
3:A:439:PAH:C2	4:A:653:HOH:O	2.68	0.41
1:A:101:ASN:CA	4:A:519:HOH:O	2.67	0.41
1:A:361:ASP:HB3	4:A:478:HOH:O	2.20	0.41
1:A:62:LEU:HD23	1:A:62:LEU:HA	1.81	0.41
1:A:47:GLU:CB	4:A:448:HOH:O	2.37	0.41
1:A:34:VAL:C	1:A:35:PRO:O	2.56	0.41
1:A:252:PHE:O	1:A:258:TYR:HA	2.20	0.41
1:A:269:LYS:NZ	4:A:705:HOH:O	2.27	0.41
1:A:130:TYR:OH	1:A:418:GLU:OE2	2.24	0.41
1:A:344:LEU:CD1	1:A:359:ALA:HB2	2.50	0.41
1:A:297:PRO:HD2	1:A:306:TRP:CH2	2.55	0.41
1:A:42:VAL:HG23	1:A:43:HIS:ND1	2.35	0.41
1:A:185:ILE:HG21	1:A:185:ILE:HD13	1.36	0.41
1:A:54:SER:O	1:A:55:LYS:HG3	2.20	0.41
1:A:38:ALA:HB2	1:A:40:THR:HG23	1.98	0.41
1:A:157:GLY:O	4:A:758:HOH:O	2.22	0.40
1:A:52:ASP:OD1	1:A:53:LYS:N	2.52	0.40
1:A:294:ILE:HG13	1:A:315:ILE:CD1	2.50	0.40
1:A:125:LYS:O	1:A:126:ASN:CB	2.66	0.40
1:A:264:ASN:OD1	1:A:266:ASN:N	2.41	0.40
1:A:113:VAL:CG1	1:A:113:VAL:O	2.68	0.40
1:A:330:ILE:O	1:A:333:ALA:HB3	2.22	0.40
1:A:390:LEU:O	1:A:391:ARG:CB	2.68	0.40

All (6) 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:207:ASN:C	4:A:630:HOH:O[8_666]	0.80	1.40
1:A:207:ASN:CA	4:A:630:HOH:O[8_666]	1.06	1.14
1:A:208:VAL:N	4:A:630:HOH:O[8_666]	1.40	0.80
1:A:288:ARG:NH2	4:A:672:HOH:O[4_565]	1.72	0.48
1:A:207:ASN:O	4:A:630:HOH:O[8_666]	2.00	0.20
4:A:705:HOH:O	4:A:763:HOH:O[5_655]	2.15	0.05

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%)	394 (91%)	31 (7%)	9 (2%)	9 10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	264	ASN
1	A	270	SER
1	A	37	GLY
1	A	263	LYS
1	A	267	SER
1	A	13	SER
1	A	402	ARG
1	A	104	LYS

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%)	317 (92%)	27 (8%)	16 24

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	27	LYS

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Mol	Chain	Res	Type
1	A	46	LEU
1	A	47	GLU
1	A	57	MET
1	A	95	SER
1	A	101	ASN
1	A	103	SER
1	A	126	ASN
1	A	133	LEU
1	A	140	LYS
1	A	166	LEU
1	A	194	LYS
1	A	217	ASN
1	A	255	ASP
1	A	266	ASN
1	A	268	ASP
1	A	284	SER
1	A	304	GLU
1	A	311	LYS
1	A	326	ASN
1	A	328	LYS
1	A	353	SER
1	A	355	SER
1	A	372	SER
1	A	373	HIS
1	A	391	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	152	ASN
1	A	155	ASN
1	A	266	ASN
1	A	326	ASN
1	A	348	GLN
1	A	373	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are 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	PAH	A	439	2	8,8,8	6.57	5 (62%)	11,11,11	5.77	8 (72%)

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	439	2	-	2/7/7/7	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	439	PAH	P-O1P	-3.20	1.43	1.50
3	A	439	PAH	C1-C2	-2.12	1.47	1.52
3	A	439	PAH	O2-C2	2.25	1.28	1.23
3	A	439	PAH	P-C1	4.53	1.86	1.79
3	A	439	PAH	C2-N3	17.47	1.50	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	439	PAH	O2-C2-N3	-6.13	116.29	123.53
3	A	439	PAH	O2-C2-C1	-3.53	111.61	120.92
3	A	439	PAH	O2P-P-C1	-3.39	99.53	107.01
3	A	439	PAH	O2P-P-O1P	-3.16	104.32	112.40
3	A	439	PAH	O3P-P-O1P	3.08	120.28	112.40
3	A	439	PAH	C1-C2-N3	5.64	125.91	114.59
3	A	439	PAH	P-C1-C2	8.86	136.01	114.41
3	A	439	PAH	O3-N3-C2	13.08	139.34	119.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	439	PAH	C1-C2-N3-O3
3	A	439	PAH	O2-C2-N3-O3

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	439	PAH	9	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.