



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:45 AM UTC

PDB ID : 1ELS / pdb_00001els
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

<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

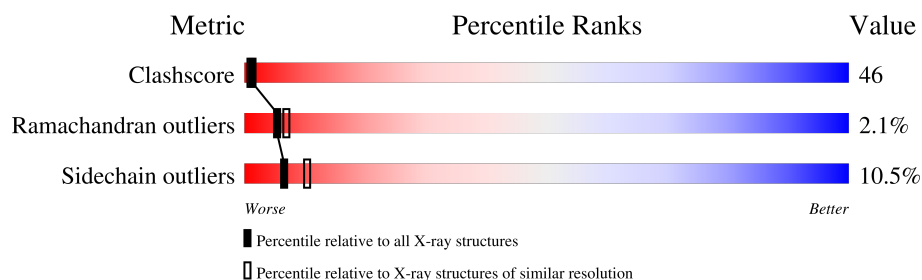
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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	20% 44% 30% 5%

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			

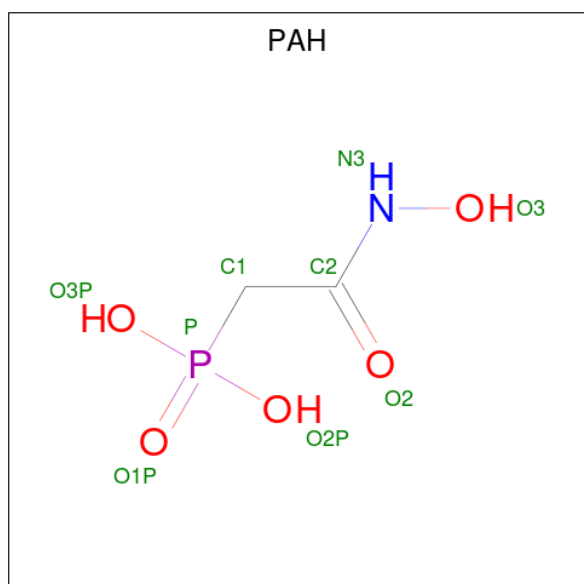
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is PHOSPHONOACETOHYDROXAMIC ACID (CCD ID: 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.

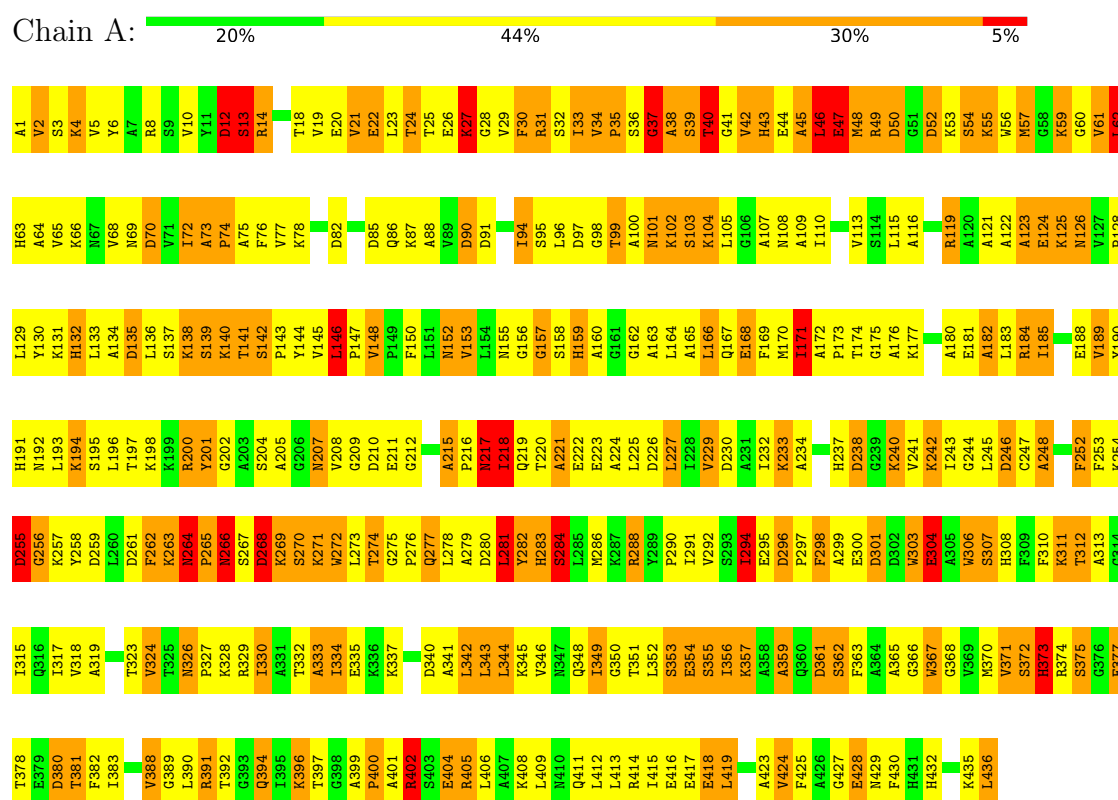
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	343	Total	O	0	0
			343	343		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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) – 2.40	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: MN, PAH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.35	4/3349 (0.1%)	3.10	496/4531 (10.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	GLY	N-CA	7.74	1.51	1.44
1	A	241	VAL	N-CA	-5.69	1.39	1.46
1	A	157	GLY	N-CA	5.44	1.53	1.45
1	A	33	ILE	C-N	-5.01	1.27	1.33

All (496) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	THR	CA-C-N	16.32	143.23	123.16
1	A	141	THR	C-N-CA	16.32	143.23	123.16
1	A	192	ASN	OD1-CG-ND2	14.53	137.13	122.60
1	A	38	ALA	N-CA-C	13.68	130.73	109.52
1	A	38	ALA	CA-C-O	13.58	137.33	121.44
1	A	391	ARG	NE-CZ-NH1	-12.84	108.67	121.50
1	A	264	ASN	CA-CB-CG	-12.59	100.01	112.60
1	A	230	ASP	CA-CB-CG	12.58	125.18	112.60
1	A	391	ARG	NH1-CZ-NH2	12.25	135.23	119.30
1	A	6	TYR	CA-C-O	-12.11	107.27	121.44
1	A	108	ASN	CA-CB-CG	12.02	124.62	112.60
1	A	46	LEU	CA-C-O	11.87	133.32	120.38
1	A	349	ILE	CB-CA-C	11.84	122.25	110.65
1	A	146	LEU	CA-C-O	-11.60	110.44	120.19
1	A	104	LYS	CA-C-O	-11.27	104.40	120.51
1	A	354	GLU	CA-C-N	11.09	135.71	120.63
1	A	354	GLU	C-N-CA	11.09	135.71	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	THR	CA-CB-OG1	-11.08	92.98	109.60
1	A	162	GLY	N-CA-C	-10.96	95.97	111.20
1	A	126	ASN	CA-C-O	-10.88	107.49	120.98
1	A	146	LEU	CB-CA-C	10.86	124.19	108.87
1	A	389	GLY	O-C-N	-10.76	111.85	122.18
1	A	290	PRO	CA-C-O	10.71	129.23	121.31
1	A	129	LEU	CA-C-O	-10.70	109.59	120.82
1	A	402	ARG	CD-NE-CZ	-10.62	109.53	124.40
1	A	226	ASP	CA-CB-CG	10.47	123.07	112.60
1	A	340	ASP	CA-C-O	-10.40	108.16	119.08
1	A	217	ASN	OD1-CG-ND2	10.33	132.93	122.60
1	A	428	GLU	CA-CB-CG	10.32	134.73	114.10
1	A	165	ALA	CA-C-O	-9.98	108.14	119.41
1	A	352	LEU	CA-C-O	-9.94	109.89	120.42
1	A	169	PHE	CA-C-O	-9.93	109.98	120.40
1	A	240	LYS	CA-C-N	9.83	135.38	123.19
1	A	240	LYS	C-N-CA	9.83	135.38	123.19
1	A	8	ARG	NE-CZ-NH1	9.79	131.29	121.50
1	A	158	SER	N-CA-C	-9.79	101.27	113.01
1	A	76	PHE	CA-CB-CG	9.74	123.54	113.80
1	A	409	LEU	CB-CA-C	9.70	126.10	110.88
1	A	312	THR	CA-C-O	-9.55	109.24	119.08
1	A	126	ASN	CA-CB-CG	-9.45	103.15	112.60
1	A	391	ARG	CD-NE-CZ	-9.40	111.24	124.40
1	A	406	LEU	CA-C-O	-9.25	108.30	119.49
1	A	86	GLN	OE1-CD-NE2	-9.24	113.36	122.60
1	A	169	PHE	CA-CB-CG	-9.23	104.57	113.80
1	A	396	LYS	CA-C-O	-9.23	110.18	120.70
1	A	49	ARG	NE-CZ-NH1	9.19	130.69	121.50
1	A	126	ASN	OD1-CG-ND2	9.17	131.77	122.60
1	A	405	ARG	CA-C-O	9.15	130.78	120.71
1	A	59	LYS	CA-C-O	-9.12	108.91	119.95
1	A	10	VAL	CA-C-O	-9.02	112.47	121.67
1	A	217	ASN	CA-CB-CG	-9.02	103.58	112.60
1	A	375	SER	O-C-N	9.02	131.68	122.12
1	A	37	GLY	N-CA-C	9.01	134.54	113.18
1	A	374	ARG	CA-C-N	9.01	132.36	120.28
1	A	374	ARG	C-N-CA	9.01	132.36	120.28
1	A	50	ASP	CA-C-O	-8.98	110.93	120.63
1	A	72	ILE	N-CA-C	8.95	119.02	110.42
1	A	8	ARG	NH1-CZ-NH2	-8.95	107.66	119.30
1	A	306	TRP	CA-C-O	-8.95	111.69	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	GLU	CA-C-O	-8.93	109.70	119.97
1	A	135	ASP	CA-CB-CG	8.83	121.43	112.60
1	A	109	ALA	O-C-N	8.83	132.22	122.15
1	A	248	ALA	CA-C-O	-8.78	111.75	122.03
1	A	219	GLN	CA-C-O	-8.77	109.17	119.78
1	A	39	SER	CA-C-N	8.77	138.29	121.54
1	A	39	SER	C-N-CA	8.77	138.29	121.54
1	A	132	HIS	CA-C-O	8.77	129.73	120.70
1	A	280	ASP	CA-CB-CG	8.75	121.35	112.60
1	A	288	ARG	CA-C-O	-8.74	109.05	119.27
1	A	356	ILE	N-CA-C	-8.73	101.20	110.36
1	A	2	VAL	N-CA-CB	-8.69	98.48	110.13
1	A	184	ARG	CD-NE-CZ	-8.66	112.27	124.40
1	A	429	ASN	N-CA-C	-8.65	102.79	112.57
1	A	237	HIS	CA-C-O	-8.60	111.19	121.34
1	A	46	LEU	CA-C-N	8.46	133.60	121.50
1	A	46	LEU	C-N-CA	8.46	133.60	121.50
1	A	300	GLU	CA-C-O	-8.45	110.74	120.20
1	A	148	VAL	N-CA-C	-8.43	101.38	108.63
1	A	42	VAL	N-CA-C	8.39	122.68	111.44
1	A	24	THR	CA-CB-CG2	8.35	124.69	110.50
1	A	271	LYS	N-CA-C	-8.34	103.12	113.38
1	A	46	LEU	CB-CA-C	8.34	124.14	109.72
1	A	159	HIS	CA-CB-CG	-8.32	105.48	113.80
1	A	192	ASN	CA-CB-CG	-8.30	104.30	112.60
1	A	255	ASP	CA-C-O	-8.29	110.54	120.81
1	A	306	TRP	N-CA-CB	8.26	121.96	109.98
1	A	279	ALA	CA-C-O	-8.22	111.00	120.20
1	A	279	ALA	N-CA-CB	8.15	123.02	110.14
1	A	172	ALA	CA-C-O	-8.11	111.09	120.34
1	A	210	ASP	O-C-N	8.07	132.20	122.27
1	A	191	HIS	N-CA-CB	8.05	121.96	110.12
1	A	49	ARG	NE-CZ-NH2	-8.04	111.96	119.20
1	A	432	HIS	CA-CB-CG	8.04	121.84	113.80
1	A	373	HIS	CA-C-N	8.01	136.26	122.81
1	A	373	HIS	C-N-CA	8.01	136.26	122.81
1	A	344	LEU	CA-C-O	-7.97	111.75	120.43
1	A	222	GLU	CB-CG-CD	7.94	126.10	112.60
1	A	261	ASP	CA-CB-CG	7.94	120.54	112.60
1	A	195	SER	CB-CA-C	-7.90	98.80	110.96
1	A	222	GLU	CA-CB-CG	7.81	129.72	114.10
1	A	91	ASP	N-CA-C	-7.81	102.77	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	LEU	O-C-N	7.78	130.08	122.07
1	A	374	ARG	CD-NE-CZ	7.75	135.25	124.40
1	A	344	LEU	CA-C-N	7.75	134.11	122.95
1	A	344	LEU	C-N-CA	7.75	134.11	122.95
1	A	381	THR	CA-CB-OG1	-7.68	98.07	109.60
1	A	301	ASP	CA-CB-CG	-7.67	104.93	112.60
1	A	294	ILE	N-CA-CB	7.63	122.20	111.82
1	A	306	TRP	O-C-N	7.60	130.24	122.03
1	A	20	GLU	CA-C-N	7.60	132.61	123.19
1	A	20	GLU	C-N-CA	7.60	132.61	123.19
1	A	288	ARG	CD-NE-CZ	7.59	135.02	124.40
1	A	229	VAL	N-CA-CB	7.59	125.29	110.95
1	A	152	ASN	CA-C-O	-7.58	111.79	120.58
1	A	23	LEU	N-CA-CB	-7.54	98.72	110.57
1	A	406	LEU	CA-C-N	-7.54	109.42	120.28
1	A	406	LEU	C-N-CA	-7.54	109.42	120.28
1	A	82	ASP	CA-CB-CG	-7.53	105.07	112.60
1	A	146	LEU	N-CA-C	-7.52	100.59	110.07
1	A	20	GLU	CA-C-O	-7.48	112.30	120.30
1	A	372	SER	CA-C-O	7.48	129.85	121.40
1	A	32	SER	CA-C-O	-7.46	112.64	120.99
1	A	335	GLU	CB-CG-CD	7.44	125.24	112.60
1	A	21	VAL	CA-C-O	-7.43	112.60	120.48
1	A	357	LYS	O-C-N	-7.39	114.29	122.12
1	A	397	THR	CA-C-N	7.37	134.06	121.39
1	A	397	THR	C-N-CA	7.37	134.06	121.39
1	A	262	PHE	N-CA-C	-7.33	101.07	110.53
1	A	291	ILE	CA-C-O	-7.32	112.50	120.85
1	A	341	ALA	CA-C-O	-7.31	112.80	120.99
1	A	349	ILE	N-CA-C	-7.28	106.39	113.53
1	A	211	GLU	OE1-CD-OE2	7.28	140.37	122.90
1	A	200	ARG	NE-CZ-NH2	-7.28	112.65	119.20
1	A	273	LEU	CA-C-O	-7.25	112.92	121.11
1	A	405	ARG	CD-NE-CZ	7.22	134.51	124.40
1	A	245	LEU	CA-C-O	-7.22	112.95	121.11
1	A	64	ALA	N-CA-C	-7.21	102.60	111.33
1	A	246	ASP	N-CA-C	-7.21	95.19	108.02
1	A	77	VAL	CB-CA-C	7.17	121.82	112.14
1	A	167	GLN	N-CA-C	7.13	120.09	111.40
1	A	348	GLN	N-CA-CB	7.12	121.65	110.46
1	A	168	GLU	CB-CG-CD	7.12	124.71	112.60
1	A	87	LYS	O-C-N	7.12	130.27	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ASP	CA-C-O	-7.11	111.40	119.79
1	A	223	GLU	O-C-N	7.11	131.01	122.27
1	A	176	ALA	O-C-N	7.07	131.02	122.75
1	A	125	LYS	N-CA-C	-7.04	104.69	113.28
1	A	282	TYR	CA-C-O	-7.03	113.10	120.55
1	A	142	SER	N-CA-CB	-7.02	100.89	111.21
1	A	402	ARG	NE-CZ-NH2	7.01	125.51	119.20
1	A	39	SER	CA-C-O	7.01	130.53	120.51
1	A	371	VAL	CA-C-O	-7.01	113.73	121.23
1	A	333	ALA	CA-C-N	6.97	129.48	120.56
1	A	333	ALA	C-N-CA	6.97	129.48	120.56
1	A	159	HIS	N-CA-C	6.96	121.37	113.02
1	A	375	SER	CB-CA-C	-6.95	99.26	110.79
1	A	380	ASP	CB-CA-C	6.95	121.17	109.84
1	A	134	ALA	N-CA-C	-6.95	103.14	111.69
1	A	46	LEU	N-CA-CB	-6.93	99.68	110.57
1	A	31	ARG	N-CA-CB	-6.92	99.52	111.55
1	A	223	GLU	CA-C-O	-6.91	112.02	119.97
1	A	253	PHE	CA-C-O	-6.90	112.70	120.43
1	A	125	LYS	CA-C-O	6.90	127.39	119.18
1	A	50	ASP	CA-CB-CG	-6.88	105.72	112.60
1	A	177	LYS	N-CA-CB	6.88	120.76	110.65
1	A	74	PRO	CB-CA-C	6.86	123.94	112.62
1	A	241	VAL	CA-C-N	6.84	134.51	122.67
1	A	241	VAL	C-N-CA	6.84	134.51	122.67
1	A	45	ALA	N-CA-C	-6.84	101.04	110.35
1	A	195	SER	O-C-N	6.83	129.13	122.03
1	A	394	GLN	OE1-CD-NE2	-6.81	115.79	122.60
1	A	202	GLY	N-CA-C	-6.81	105.48	111.95
1	A	304	GLU	OE1-CD-OE2	6.80	139.22	122.90
1	A	47	GLU	CB-CG-CD	6.80	124.15	112.60
1	A	425	PHE	CA-C-O	-6.78	112.88	120.54
1	A	176	ALA	CA-C-O	-6.78	114.41	121.87
1	A	229	VAL	CA-C-O	-6.78	112.93	120.25
1	A	409	LEU	N-CA-C	-6.76	103.84	111.07
1	A	298	PHE	CA-CB-CG	-6.73	107.07	113.80
1	A	160	ALA	O-C-N	6.73	131.02	123.48
1	A	356	ILE	CA-C-O	-6.73	114.28	121.27
1	A	411	GLN	CG-CD-OE1	6.71	134.22	120.80
1	A	207	ASN	CB-CG-ND2	6.71	126.47	116.40
1	A	343	LEU	CA-C-O	-6.71	112.71	120.49
1	A	164	LEU	CA-C-O	-6.70	113.66	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	GLY	CA-C-O	-6.70	115.29	121.72
1	A	54	SER	CA-CB-OG	-6.69	97.72	111.10
1	A	5	VAL	CA-CB-CG1	6.68	121.76	110.40
1	A	88	ALA	CA-C-N	6.67	129.10	120.56
1	A	88	ALA	C-N-CA	6.67	129.10	120.56
1	A	61	VAL	CA-C-N	6.65	129.19	120.28
1	A	61	VAL	C-N-CA	6.65	129.19	120.28
1	A	43	HIS	CB-CA-C	-6.64	102.64	111.74
1	A	334	ILE	CA-C-O	-6.64	113.68	121.05
1	A	87	LYS	CA-C-O	-6.64	113.38	120.42
1	A	373	HIS	CA-CB-CG	6.63	120.43	113.80
1	A	188	GLU	O-C-N	-6.62	114.60	122.15
1	A	99	THR	CA-CB-OG1	-6.59	99.71	109.60
1	A	266	ASN	CA-C-O	6.59	129.94	120.51
1	A	102	LYS	CA-C-O	-6.59	113.90	121.54
1	A	391	ARG	CB-CA-C	-6.59	103.03	111.86
1	A	104	LYS	O-C-N	6.55	131.30	122.59
1	A	184	ARG	CA-CB-CG	6.53	127.16	114.10
1	A	59	LYS	O-C-N	6.53	130.71	122.22
1	A	244	GLY	CA-C-N	6.53	133.06	122.81
1	A	244	GLY	C-N-CA	6.53	133.06	122.81
1	A	252	PHE	CA-CB-CG	6.52	120.32	113.80
1	A	367	TRP	CA-C-N	6.51	129.72	122.69
1	A	367	TRP	C-N-CA	6.51	129.72	122.69
1	A	311	LYS	CA-CB-CG	6.49	127.08	114.10
1	A	363	PHE	CA-CB-CG	6.47	120.27	113.80
1	A	404	GLU	N-CA-C	-6.47	105.35	113.18
1	A	394	GLN	CA-C-O	-6.47	113.78	120.89
1	A	283	HIS	CA-CB-CG	6.46	120.26	113.80
1	A	18	THR	CA-C-O	-6.46	114.32	121.23
1	A	372	SER	N-CA-C	6.45	118.98	109.24
1	A	47	GLU	CB-CA-C	-6.44	99.34	109.84
1	A	70	ASP	N-CA-C	6.43	121.33	112.90
1	A	201	TYR	CA-CB-CG	-6.43	102.32	113.90
1	A	77	VAL	O-C-N	-6.43	115.63	121.87
1	A	195	SER	CA-C-O	-6.42	114.26	121.00
1	A	32	SER	CB-CA-C	6.41	123.60	109.94
1	A	185	ILE	CB-CG1-CD1	-6.39	100.37	113.80
1	A	75	ALA	O-C-N	6.39	128.99	122.09
1	A	28	GLY	CA-C-N	6.38	130.97	122.93
1	A	28	GLY	C-N-CA	6.38	130.97	122.93
1	A	23	LEU	CA-C-O	-6.38	113.43	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	PHE	CA-C-O	-6.38	113.81	120.70
1	A	33	ILE	CA-C-O	-6.38	113.21	120.67
1	A	288	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	A	90	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	388	VAL	N-CA-CB	6.35	118.26	110.64
1	A	36	SER	CA-C-N	6.35	133.85	121.41
1	A	36	SER	C-N-CA	6.35	133.85	121.41
1	A	189	VAL	CA-C-N	6.34	129.60	120.79
1	A	189	VAL	C-N-CA	6.34	129.60	120.79
1	A	246	ASP	CA-C-O	-6.34	113.49	120.33
1	A	184	ARG	CA-C-O	-6.31	114.37	121.00
1	A	266	ASN	OD1-CG-ND2	6.31	128.91	122.60
1	A	170	MET	CG-SD-CE	6.28	114.72	100.90
1	A	91	ASP	CA-C-O	-6.28	113.89	120.55
1	A	12	ASP	CB-CA-C	6.28	121.53	110.36
1	A	350	GLY	CA-C-O	-6.26	112.07	119.02
1	A	424	VAL	N-CA-C	-6.26	99.20	108.85
1	A	123	ALA	CA-C-N	6.26	129.29	120.28
1	A	123	ALA	C-N-CA	6.26	129.29	120.28
1	A	340	ASP	O-C-N	6.23	129.22	122.05
1	A	355	SER	CA-C-O	6.23	127.31	120.90
1	A	292	VAL	CB-CA-C	-6.22	104.54	110.70
1	A	341	ALA	O-C-N	6.22	130.36	123.33
1	A	375	SER	CA-C-O	-6.22	113.95	120.55
1	A	55	LYS	O-C-N	6.22	130.97	123.26
1	A	253	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	126	ASN	O-C-N	6.19	130.64	122.47
1	A	411	GLN	CG-CD-NE2	-6.19	107.12	116.40
1	A	418	GLU	O-C-N	-6.18	115.10	122.15
1	A	272	TRP	CA-C-O	-6.18	115.00	121.55
1	A	91	ASP	CA-CB-CG	-6.17	106.43	112.60
1	A	299	ALA	CA-C-N	6.17	129.39	120.38
1	A	299	ALA	C-N-CA	6.17	129.39	120.38
1	A	33	ILE	N-CA-C	-6.16	99.61	108.48
1	A	211	GLU	CG-CD-OE2	-6.13	104.30	118.40
1	A	191	HIS	CA-C-O	-6.12	114.07	120.55
1	A	332	THR	CA-C-O	6.08	126.87	120.42
1	A	233	LYS	CA-C-N	6.07	129.03	120.28
1	A	233	LYS	C-N-CA	6.07	129.03	120.28
1	A	327	PRO	CB-CA-C	6.07	120.47	111.85
1	A	169	PHE	O-C-N	6.07	131.13	123.12
1	A	185	ILE	CA-C-N	6.06	126.67	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ILE	C-N-CA	6.06	126.67	119.94
1	A	211	GLU	O-C-N	6.06	129.91	122.34
1	A	128	PRO	N-CA-C	-6.05	101.96	111.34
1	A	209	GLY	CA-C-O	-6.05	115.94	122.47
1	A	248	ALA	O-C-N	6.05	130.13	122.57
1	A	383	ILE	CA-CB-CG1	6.03	120.66	110.40
1	A	300	GLU	N-CA-CB	6.02	119.65	110.14
1	A	124	GLU	CG-CD-OE1	-6.01	104.58	118.40
1	A	69	ASN	N-CA-C	6.00	117.49	111.07
1	A	78	LYS	CA-C-N	5.98	128.78	120.29
1	A	78	LYS	C-N-CA	5.98	128.78	120.29
1	A	277	GLN	N-CA-C	-5.98	104.34	111.69
1	A	183	LEU	N-CA-CB	-5.97	101.35	110.01
1	A	52	ASP	O-C-N	-5.97	114.71	122.77
1	A	5	VAL	N-CA-C	-5.95	99.17	107.80
1	A	335	GLU	N-CA-CB	5.92	119.46	110.28
1	A	73	ALA	N-CA-C	5.92	120.53	112.55
1	A	27	LYS	CA-C-O	-5.91	112.50	119.48
1	A	34	VAL	O-C-N	5.89	127.82	121.10
1	A	419	LEU	N-CA-CB	-5.89	100.08	110.39
1	A	77	VAL	CA-C-N	5.88	130.54	120.72
1	A	77	VAL	C-N-CA	5.88	130.54	120.72
1	A	60	GLY	N-CA-C	-5.88	103.52	112.51
1	A	139	SER	O-C-N	-5.86	116.36	123.10
1	A	174	THR	CA-C-O	5.86	126.58	119.31
1	A	337	LYS	CA-C-O	-5.86	114.87	122.14
1	A	274	THR	CA-C-O	-5.86	115.26	121.88
1	A	145	VAL	CB-CA-C	5.85	119.29	110.63
1	A	210	ASP	CA-CB-CG	-5.84	106.76	112.60
1	A	119	ARG	CA-CB-CG	-5.83	102.43	114.10
1	A	362	SER	N-CA-C	-5.82	105.01	111.36
1	A	13	SER	CA-C-N	-5.81	113.53	122.60
1	A	13	SER	C-N-CA	-5.81	113.53	122.60
1	A	281	LEU	N-CA-C	-5.78	104.58	111.69
1	A	13	SER	CA-C-O	-5.78	112.80	119.61
1	A	177	LYS	CA-C-O	-5.77	112.70	119.05
1	A	221	ALA	N-CA-C	-5.76	104.92	111.14
1	A	357	LYS	CA-C-N	5.76	129.06	120.31
1	A	357	LYS	C-N-CA	5.76	129.06	120.31
1	A	319	ALA	CA-C-N	5.74	129.14	121.90
1	A	319	ALA	C-N-CA	5.74	129.14	121.90
1	A	60	GLY	CA-C-O	-5.73	114.25	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	LEU	N-CA-CB	-5.73	101.27	111.08
1	A	183	LEU	O-C-N	-5.73	116.17	122.07
1	A	283	HIS	CA-C-N	5.73	128.75	120.79
1	A	283	HIS	C-N-CA	5.73	128.75	120.79
1	A	48	MET	CA-CB-CG	-5.73	102.65	114.10
1	A	171	ILE	CA-C-O	-5.72	114.13	121.40
1	A	14	ARG	CB-CG-CD	5.71	124.43	111.30
1	A	326	ASN	N-CA-CB	-5.70	101.69	110.01
1	A	62	LEU	CA-C-N	5.70	128.38	120.63
1	A	62	LEU	C-N-CA	5.70	128.38	120.63
1	A	262	PHE	N-CA-CB	5.69	118.57	110.44
1	A	77	VAL	CA-C-O	5.68	126.86	120.95
1	A	102	LYS	N-CA-CB	-5.68	103.38	111.84
1	A	150	PHE	CA-CB-CG	-5.67	108.13	113.80
1	A	278	LEU	N-CA-C	-5.67	105.19	111.36
1	A	35	PRO	CA-C-O	-5.66	110.29	120.60
1	A	259	ASP	N-CA-CB	-5.66	101.91	110.35
1	A	182	ALA	CA-C-O	5.63	126.73	120.82
1	A	126	ASN	CB-CA-C	-5.62	103.98	111.63
1	A	367	TRP	N-CA-CB	-5.61	102.42	110.44
1	A	341	ALA	CA-C-N	-5.60	114.81	122.93
1	A	341	ALA	C-N-CA	-5.60	114.81	122.93
1	A	210	ASP	CA-C-O	-5.59	113.54	119.97
1	A	125	LYS	CA-CB-CG	5.59	125.27	114.10
1	A	197	THR	O-C-N	5.59	128.04	122.12
1	A	412	LEU	CA-C-N	5.58	128.01	120.65
1	A	412	LEU	C-N-CA	5.58	128.01	120.65
1	A	330	ILE	N-CA-C	-5.56	105.19	110.42
1	A	225	LEU	CA-C-N	5.55	128.18	120.29
1	A	225	LEU	C-N-CA	5.55	128.18	120.29
1	A	189	VAL	N-CA-CB	5.55	117.05	110.55
1	A	391	ARG	N-CA-CB	-5.55	103.48	111.91
1	A	265	PRO	CA-C-N	5.54	132.13	121.54
1	A	265	PRO	C-N-CA	5.54	132.13	121.54
1	A	223	GLU	N-CA-CB	5.54	118.87	110.28
1	A	163	ALA	CA-C-O	-5.54	112.79	119.27
1	A	31	ARG	CA-C-N	-5.53	112.06	121.85
1	A	31	ARG	C-N-CA	-5.53	112.06	121.85
1	A	38	ALA	O-C-N	-5.53	115.96	123.15
1	A	404	GLU	CA-C-N	5.52	129.38	121.71
1	A	404	GLU	C-N-CA	5.52	129.38	121.71
1	A	388	VAL	CA-C-O	-5.51	113.87	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	LEU	CA-C-O	-5.51	113.27	120.00
1	A	296	ASP	CB-CA-C	-5.51	106.20	111.00
1	A	348	GLN	O-C-N	5.51	130.24	122.41
1	A	436	LEU	CB-CA-C	5.51	120.56	110.10
1	A	4	LYS	CA-C-N	5.50	130.28	123.12
1	A	4	LYS	C-N-CA	5.50	130.28	123.12
1	A	200	ARG	N-CA-C	5.50	117.08	111.14
1	A	406	LEU	N-CA-C	-5.50	105.67	112.38
1	A	188	GLU	CA-C-O	5.49	126.24	120.42
1	A	414	ARG	CB-CA-C	-5.49	101.68	110.79
1	A	22	GLU	N-CA-CB	5.49	119.89	110.68
1	A	69	ASN	CA-C-N	5.49	131.61	121.52
1	A	69	ASN	C-N-CA	5.49	131.61	121.52
1	A	141	THR	CB-CA-C	-5.49	102.14	111.02
1	A	46	LEU	O-C-N	-5.48	116.82	123.29
1	A	377	GLU	CG-CD-OE2	5.48	131.00	118.40
1	A	75	ALA	CB-CA-C	-5.48	102.24	110.90
1	A	219	GLN	O-C-N	5.48	130.20	122.20
1	A	303	TRP	N-CA-C	5.47	117.95	111.33
1	A	144	TYR	CA-C-O	-5.46	115.27	121.72
1	A	261	ASP	CA-C-O	-5.46	112.70	120.51
1	A	424	VAL	CA-C-O	-5.46	114.12	121.32
1	A	279	ALA	O-C-N	5.45	128.42	122.20
1	A	138	LYS	N-CA-CB	-5.45	103.63	111.91
1	A	402	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	A	238	ASP	CB-CA-C	5.44	119.36	109.62
1	A	400	PRO	CA-C-O	-5.43	117.29	121.31
1	A	172	ALA	O-C-N	5.43	125.95	121.44
1	A	141	THR	O-C-N	-5.43	115.17	122.22
1	A	342	LEU	N-CA-CB	-5.43	101.95	110.69
1	A	142	SER	N-CA-C	5.42	119.77	108.39
1	A	42	VAL	N-CA-CB	-5.41	100.72	110.95
1	A	18	THR	O-C-N	5.41	129.21	123.42
1	A	243	ILE	CA-C-N	5.41	132.01	121.41
1	A	243	ILE	C-N-CA	5.41	132.01	121.41
1	A	436	LEU	N-CA-CB	-5.40	101.32	110.50
1	A	12	ASP	N-CA-CB	-5.40	102.66	110.70
1	A	218	ILE	CA-C-O	-5.39	114.70	121.11
1	A	50	ASP	CB-CG-OD1	-5.38	106.02	118.40
1	A	232	ILE	N-CA-C	-5.38	105.47	110.53
1	A	82	ASP	OD1-CG-OD2	5.38	135.80	122.90
1	A	200	ARG	CA-C-O	-5.37	115.17	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	PRO	O-C-N	5.37	129.40	122.91
1	A	383	ILE	CA-CB-CG2	-5.37	101.38	110.50
1	A	361	ASP	OD1-CG-OD2	5.36	135.77	122.90
1	A	96	LEU	CD1-CG-CD2	-5.36	99.01	110.80
1	A	126	ASN	CB-CG-ND2	-5.36	108.37	116.40
1	A	31	ARG	N-CA-C	5.35	117.82	109.52
1	A	115	LEU	N-CA-C	-5.35	105.01	112.45
1	A	68	VAL	N-CA-C	-5.35	105.88	110.74
1	A	388	VAL	N-CA-C	-5.35	105.88	110.74
1	A	234	ALA	O-C-N	-5.34	115.97	122.22
1	A	298	PHE	CA-C-O	-5.34	115.38	121.68
1	A	299	ALA	N-CA-C	5.34	117.58	110.53
1	A	74	PRO	N-CA-C	-5.34	106.11	113.53
1	A	368	GLY	N-CA-C	-5.33	102.40	112.10
1	A	12	ASP	OD1-CG-OD2	-5.32	110.13	122.90
1	A	185	ILE	CA-CB-CG2	5.32	119.54	110.50
1	A	254	LYS	CA-C-O	-5.30	113.76	120.28
1	A	45	ALA	N-CA-CB	5.29	117.81	110.04
1	A	167	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	212	GLY	CA-C-O	-5.29	113.15	119.07
1	A	326	ASN	OD1-CG-ND2	5.28	127.88	122.60
1	A	382	PHE	CA-CB-CG	-5.28	108.52	113.80
1	A	110	ILE	N-CA-C	5.27	115.49	110.53
1	A	22	GLU	CB-CA-C	-5.27	100.07	109.71
1	A	196	LEU	N-CA-C	-5.27	105.54	111.28
1	A	182	ALA	O-C-N	-5.26	116.65	122.07
1	A	307	SER	CA-CB-OG	-5.26	100.59	111.10
1	A	6	TYR	O-C-N	5.25	129.98	123.15
1	A	87	LYS	N-CA-C	-5.25	105.64	111.36
1	A	268	ASP	CA-C-O	-5.24	114.94	120.92
1	A	324	VAL	CA-CB-CG1	5.24	119.31	110.40
1	A	371	VAL	N-CA-C	-5.23	102.84	109.58
1	A	31	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	A	184	ARG	CA-C-N	5.22	127.34	120.60
1	A	184	ARG	C-N-CA	5.22	127.34	120.60
1	A	284	SER	CA-C-N	5.22	127.53	120.38
1	A	284	SER	C-N-CA	5.22	127.53	120.38
1	A	288	ARG	O-C-N	5.21	129.60	122.46
1	A	380	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	220	THR	CA-C-O	-5.21	115.53	121.68
1	A	242	LYS	CA-C-O	5.20	128.49	121.89
1	A	201	TYR	N-CA-C	5.18	119.88	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASN	CB-CG-OD1	-5.18	110.44	120.80
1	A	94	ILE	CA-CB-CG2	5.16	119.28	110.50
1	A	147	PRO	N-CA-C	5.16	120.38	111.77
1	A	307	SER	N-CA-C	5.15	117.56	111.33
1	A	70	ASP	N-CA-CB	-5.15	102.61	110.33
1	A	170	MET	N-CA-CB	-5.14	102.28	111.08
1	A	238	ASP	N-CA-CB	5.14	117.59	110.04
1	A	85	ASP	CA-C-N	5.13	129.40	120.68
1	A	85	ASP	C-N-CA	5.13	129.40	120.68
1	A	382	PHE	CA-C-O	-5.13	115.18	120.92
1	A	430	PHE	CA-C-N	5.13	129.34	121.19
1	A	430	PHE	C-N-CA	5.13	129.34	121.19
1	A	159	HIS	CB-CA-C	-5.12	101.26	110.37
1	A	175	GLY	CA-C-N	5.12	129.51	120.87
1	A	175	GLY	C-N-CA	5.12	129.51	120.87
1	A	359	ALA	N-CA-CB	-5.11	102.59	110.16
1	A	243	ILE	CA-C-O	5.11	127.78	121.75
1	A	416	GLU	O-C-N	5.11	127.61	122.09
1	A	222	GLU	CA-C-O	5.11	126.14	120.63
1	A	1	ALA	CA-C-O	-5.10	112.12	120.80
1	A	43	HIS	CA-CB-CG	-5.10	108.70	113.80
1	A	37	GLY	CA-C-O	-5.10	111.69	120.57
1	A	256	GLY	CA-C-N	5.10	131.38	122.81
1	A	256	GLY	C-N-CA	5.10	131.38	122.81
1	A	326	ASN	CB-CA-C	5.09	115.66	109.85
1	A	349	ILE	CA-C-N	5.09	131.81	121.93
1	A	349	ILE	C-N-CA	5.09	131.81	121.93
1	A	404	GLU	O-C-N	5.09	129.86	122.43
1	A	215	ALA	O-C-N	5.09	125.87	121.34
1	A	210	ASP	N-CA-C	5.09	117.72	111.82
1	A	340	ASP	CB-CG-OD1	5.09	130.10	118.40
1	A	184	ARG	N-CA-C	-5.08	105.43	110.97
1	A	52	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	230	ASP	N-CA-C	-5.08	105.83	111.36
1	A	296	ASP	CA-C-N	5.07	124.38	118.85
1	A	296	ASP	C-N-CA	5.07	124.38	118.85
1	A	116	ALA	CA-C-N	5.07	127.58	120.28
1	A	116	ALA	C-N-CA	5.07	127.58	120.28
1	A	230	ASP	N-CA-CB	5.07	117.66	110.16
1	A	366	GLY	O-C-N	5.06	128.86	122.43
1	A	22	GLU	N-CA-C	-5.06	100.65	108.90
1	A	136	LEU	N-CA-C	5.06	118.22	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ALA	N-CA-CB	-5.06	102.15	110.14
1	A	19	VAL	CA-CB-CG1	5.05	118.99	110.40
1	A	47	GLU	CA-C-O	-5.05	114.93	120.69
1	A	40	THR	N-CA-C	5.04	121.54	110.80
1	A	300	GLU	CG-CD-OE2	5.04	130.00	118.40
1	A	48	MET	N-CA-C	5.04	116.82	108.20
1	A	416	GLU	N-CA-CB	5.04	117.37	110.07
1	A	132	HIS	CA-CB-CG	5.03	118.83	113.80
1	A	98	GLY	CA-C-O	-5.03	113.30	119.69
1	A	436	LEU	CA-CB-CG	5.03	133.89	116.30
1	A	25	THR	O-C-N	-5.02	117.04	122.92
1	A	402	ARG	CA-C-O	-5.02	113.33	120.51
1	A	47	GLU	N-CA-CB	-5.02	102.17	109.95
1	A	119	ARG	CB-CA-C	-5.01	102.33	110.85
1	A	153	VAL	CA-CB-CG2	5.01	118.92	110.40
1	A	227	LEU	CA-C-N	5.01	128.91	120.29
1	A	227	LEU	C-N-CA	5.01	128.91	120.29

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	300	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	3296	302	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 46.

All (302) 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:264:ASN:CG	1:A:266:ASN:H	1.59	1.10
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:345:LYS:HZ1	3:A:439:PAH:H12	1.13	1.08
1:A:264:ASN:HB3	1:A:265:PRO:HA	1.29	1.07
1:A:146:LEU:HD12	1:A:423:ALA:HB1	1.38	1.03
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
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: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:345:LYS:HZ1	3:A:439:PAH:C1	1.80	0.93
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:4:LYS:HE2	4:A:600:HOH:O	1.71	0.89
1:A:41:GLY:O	1:A:44:GLU:OE2	1.91	0.89
1:A:46:LEU:C	1:A:46:LEU:HD23	1.98	0.88
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:52:ASP:C	1:A:52:ASP:OD1	2.16	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: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:O	1:A:131:LYS:HD3	1.79	0.82
1:A:61:VAL:O	1:A:65:VAL:HG23	1.79	0.81
1:A:373:HIS:HD2	1:A:405:ARG:HH11	1.28	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:264:ASN:CG	1:A:266:ASN:N	2.40	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:66:LYS:O	1:A:70:ASP:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASP:O	4:A:708:HOH:O	2.02	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:30:PHE:CE2	1:A:123:ALA:HB2	2.22	0.74
1:A:38:ALA:N	4:A:611:HOH:O	2.20	0.74
1:A:262:PHE:O	1:A:263:LYS:CB	2.35	0.74
1:A:304:GLU:HB2	4:A:474:HOH:O	1.88	0.73
1:A:313:ALA:HB1	1:A:317:ILE:HD11	1.71	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:264:ASN:C	1:A:264:ASN:OD1	2.27	0.71
1:A:46:LEU:HD13	1:A:103:SER:HB3	1.71	0.71
1:A:282:TYR:O	1:A:286:MET:HE3	1.91	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: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:131:LYS:HD3	1:A:131:LYS:C	2.17	0.69
1:A:157:GLY:C	4:A:758:HOH:O	2.32	0.69
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:200:ARG:O	4:A:765:HOH:O	2.11	0.68
1:A:268:ASP:C	1:A:268:ASP:OD1	2.36	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:283:HIS:HA	1:A:286:MET:HE3	1.75	0.67
1:A:345:LYS:HZ3	3:A:439:PAH:C1	2.03	0.67
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:282:TYR:C	1:A:286:MET:HE3	2.19	0.66
1:A:101:ASN:C	1:A:101:ASN:HD22	2.02	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ALA:CB	1:A:317:ILE:CD1	2.73	0.66
1:A:345:LYS:NZ	3:A:439:PAH:H11	2.10	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:38:ALA:CB	1:A:40:THR:CG2	2.75	0.65
1:A:313:ALA:HB3	1:A:317:ILE:CD1	2.27	0.65
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:14:ARG:CZ	4:A:573:HOH:O	2.46	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: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
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:282:TYR:HB3	1:A:286:MET:HE2	1.82	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: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:46:LEU:C	1:A:46:LEU:CD2	2.74	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:282:TYR:C	1:A:286:MET:CE	2.77	0.58
1:A:70:ASP:CG	4:A:687:HOH:O	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HE3	4:A:764:HOH:O	2.03	0.57
1:A:53:LYS:HG3	4:A:676:HOH:O	2.04	0.57
1:A:159:HIS:CD2	1:A:159:HIS:N	2.69	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:53:LYS:CG	4:A:676:HOH:O	2.52	0.56
1:A:303:TRP:HZ2	1:A:329:ARG:HH21	1.53	0.56
1:A:256:GLY:N	4:A:706:HOH:O	2.03	0.56
1:A:264:ASN:ND2	1:A:266:ASN:C	2.63	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:49:ARG:NH1	1:A:59:LYS:O	2.36	0.56
1:A:275:GLY:N	1:A:276:PRO:CD	2.69	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: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:101:ASN:HB3	4:A:519:HOH:O	2.06	0.55
1:A:152:ASN:ND2	4:A:753:HOH:O	2.40	0.55
1:A:153:VAL:HB	1:A:193:LEU:CD2	2.36	0.55
1:A:264:ASN:CG	4:A:785:HOH:O	2.50	0.55
1:A:326:ASN:C	1:A:326:ASN:HD22	2.08	0.54
1:A:156:GLY:C	4:A:758:HOH:O	2.49	0.54
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:417:GLU:CD	4:A:566:HOH:O	2.48	0.54
1:A:38:ALA:HB1	1:A:40:THR:OG1	2.08	0.54
1:A:39:SER:HB2	4:A:668:HOH:O	2.08	0.54
1:A:137:SER:O	1:A:138:LYS:HB2	2.07	0.54
1:A:345:LYS:NZ	4:A:674:HOH:O	2.39	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: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:157:GLY:C	1:A:159:HIS:H	2.15	0.53
1:A:159:HIS:HE1	4:A:730:HOH:O	1.91	0.53
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:268:ASP:CG	1:A:271:LYS:HE3	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TYR:O	1:A:286:MET:CE	2.57	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: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:310:PHE:CD1	1:A:310:PHE:C	2.89	0.51
1:A:90:ASP:OD2	1:A:353:SER:OG	2.23	0.51
1:A:157:GLY:C	1:A:159:HIS:N	2.66	0.50
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:72:ILE:HD11	1:A:105:LEU:HD13	1.94	0.49
1:A:4:LYS:CE	4:A:600:HOH:O	2.43	0.49
1:A:143:PRO:HG3	1:A:424:VAL:CG1	2.42	0.49
1:A:323:THR:O	1:A:324:VAL:C	2.54	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
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:30:PHE:CE2	1:A:123:ALA:CB	2.95	0.48
1:A:262:PHE:HD2	4:A:703:HOH:O	1.97	0.48
1:A:52:ASP:OD1	1:A:54:SER:N	2.41	0.48
1:A:252:PHE:HB3	1:A:262:PHE:CD1	2.49	0.48
1:A:264:ASN:CB	1:A:266:ASN:H	2.26	0.48
1:A:349:ILE:CD1	1:A:354:GLU:HB3	2.41	0.48
1:A:405:ARG:HA	1:A:405:ARG:HD3	1.65	0.48
1:A:50:ASP:N	1:A:50:ASP:OD1	2.40	0.48
1:A:355:SER:O	1:A:356:ILE:C	2.57	0.48
1:A:173:PRO:HG2	1:A:182:ALA:HB1	1.95	0.48
1:A:227:LEU:HD13	4:A:597:HOH:O	2.13	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:O	1:A:113:VAL:HG12	2.14	0.47
1:A:247:CYS:O	1:A:248:ALA:C	2.56	0.47
1:A:52:ASP:CG	4:A:579:HOH:O	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ILE:HD13	1:A:365:ALA:CB	2.44	0.47
1:A:148:VAL:HG21	1:A:427:GLY:O	2.14	0.47
1:A:152:ASN:O	1:A:399:ALA:CB	2.62	0.47
1:A:274:THR:OG1	1:A:277:GLN:HG3	2.15	0.47
1:A:283:HIS:CA	1:A:286:MET:HE3	2.42	0.47
1:A:345:LYS:HZ3	3:A:439:PAH:H11	1.73	0.47
1:A:119:ARG:CZ	4:A:603:HOH:O	2.63	0.47
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:HA	1:A:413:LEU:HD23	1.78	0.46
1:A:72:ILE:HG13	1:A:105:LEU:HD13	1.97	0.46
1:A:48:MET:HE3	1:A:48:MET:HB2	1.78	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:HD12	1:A:294:ILE:HG21	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:13:SER:OG	1:A:404:GLU:HG3	2.17	0.45
1:A:34:VAL:C	1:A:35:PRO:O	2.56	0.45
1:A:157:GLY:O	1:A:263:LYS:HE3	2.16	0.45
1:A:201:TYR:HB2	1:A:205:ALA:CB	2.46	0.45
1:A:215:ALA:N	4:A:512:HOH:O	2.21	0.45
1:A:121:ALA:HB3	1:A:132:HIS:NE2	2.31	0.45
1:A:185:ILE:O	1:A:189:VAL:HG23	2.16	0.45
1:A:233:LYS:NZ	1:A:238:ASP:OD2	2.40	0.45
1:A:294:ILE:HG23	1:A:294:ILE:HD13	1.59	0.45
1:A:326:ASN:HB3	1:A:329:ARG:HG3	1.98	0.45
1:A:22:GLU:HB3	1:A:29:VAL:HG12	1.97	0.45
1:A:216:PRO:HG2	1:A:218:ILE:HG13	1.98	0.45
1:A:343:LEU:HD23	1:A:345:LYS:HE3	1.99	0.45
1:A:12:ASP:C	1:A:14:ARG:N	2.73	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:269:LYS:CD	4:A:705:HOH:O	2.53	0.45
1:A:396:LYS:NZ	4:A:653:HOH:O	2.49	0.45
1:A:38:ALA:CA	4:A:611:HOH:O	2.65	0.45
1:A:101:ASN:C	1:A:101:ASN:ND2	2.68	0.45
1:A:37:GLY:HA3	1:A:375:SER:HB2	1.98	0.44
1:A:157:GLY:HA3	4:A:521:HOH:O	2.17	0.44
1:A:308:HIS:HB2	4:A:750:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:VAL:HG21	1:A:415:ILE:HG21	1.98	0.44
1:A:246:ASP:OD1	1:A:246:ASP:C	2.60	0.44
1:A:38:ALA:HB2	1:A:40:THR:HG21	1.99	0.44
1:A:41:GLY:HA3	1:A:324:VAL:CG1	2.48	0.44
1:A:139:SER:O	1:A:140:LYS:C	2.59	0.44
1:A:252:PHE:HB3	1:A:262:PHE:CE1	2.53	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:122:ALA:O	1:A:123:ALA:C	2.61	0.43
1:A:131:LYS:NZ	1:A:135:ASP:CG	2.76	0.43
1:A:171:ILE:HA	1:A:242:LYS:O	2.17	0.43
1:A:402:ARG:O	1:A:405:ARG:HB2	2.18	0.43
1:A:46:LEU:HD23	1:A:46:LEU:O	2.17	0.43
1:A:119:ARG:CD	4:A:603:HOH:O	2.66	0.43
1:A:381:THR:HG21	4:A:507:HOH:O	2.12	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:184:ARG:HH11	1:A:184:ARG:HD3	1.58	0.42
1:A:204:SER:HB2	4:A:700:HOH:O	2.18	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
1:A:221:ALA:O	1:A:224:ALA:HB3	2.19	0.42
1:A:181:GLU:O	1:A:185:ILE:HG13	2.19	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
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
3:A:439:PAH:C2	4:A:653:HOH:O	2.68	0.41
1:A:62:LEU:HD23	1:A:62:LEU:HA	1.81	0.41
1:A:326:ASN:C	1:A:326:ASN:ND2	2.74	0.41
1:A:47:GLU:CB	4:A:448:HOH:O	2.37	0.41
1:A:131:LYS:C	1:A:131:LYS:CD	2.90	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:297:PRO:HD2	1:A:306:TRP:CH2	2.55	0.41
1:A:344:LEU:CD1	1:A:359:ALA:HB2	2.50	0.41
1:A:12:ASP:C	1:A:14:ARG:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:ALA:HB2	1:A:40:THR:HG23	1.98	0.41
1:A:54:SER:O	1:A:55:LYS:HG3	2.20	0.41
1:A:435:LYS:C	1:A:436:LEU:OXT	2.62	0.41
1:A:52:ASP:OD1	1:A:53:LYS:N	2.52	0.40
1:A:157:GLY:O	4:A:758:HOH:O	2.22	0.40
1:A:125:LYS:O	1:A:126:ASN:CB	2.66	0.40
1:A:294:ILE:HG13	1:A:315:ILE:CD1	2.50	0.40
1:A:113:VAL:O	1:A:113:VAL:CG1	2.68	0.40
1:A:200:ARG:C	4:A:765:HOH:O	2.59	0.40
1:A:264:ASN:OD1	1:A:266:ASN:N	2.41	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%)	5 7

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 ⓘ

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%)	308 (90%)	36 (10%)	6 10

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	12	ASP
1	A	13	SER
1	A	27	LYS
1	A	46	LEU
1	A	47	GLU
1	A	57	MET
1	A	62	LEU
1	A	95	SER
1	A	101	ASN
1	A	103	SER
1	A	133	LEU
1	A	140	LYS
1	A	146	LEU
1	A	166	LEU
1	A	171	ILE

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Mol	Chain	Res	Type
1	A	194	LYS
1	A	217	ASN
1	A	218	ILE
1	A	229	VAL
1	A	255	ASP
1	A	266	ASN
1	A	268	ASP
1	A	269	LYS
1	A	281	LEU
1	A	284	SER
1	A	294	ILE
1	A	304	GLU
1	A	311	LYS
1	A	328	LYS
1	A	342	LEU
1	A	346	VAL
1	A	353	SER
1	A	372	SER
1	A	373	HIS
1	A	392	THR

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	101	ASN
1	A	152	ASN
1	A	155	ASN
1	A	219	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	6.35	5 (62%)	10,11,11	5.98	7 (70%)

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	-	5/7/7/7	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	439	PAH	C2-N3	16.78	1.50	1.32
3	A	439	PAH	P-C1	4.23	1.86	1.79
3	A	439	PAH	P-O1P	-3.52	1.43	1.50
3	A	439	PAH	O2-C2	2.39	1.28	1.23
3	A	439	PAH	C1-C2	-2.17	1.47	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	439	PAH	O3-N3-C2	13.23	139.34	119.79
3	A	439	PAH	C1-C2-N3	9.87	125.91	114.87
3	A	439	PAH	O2-C2-N3	-5.69	116.29	123.27
3	A	439	PAH	O2-C2-C1	-4.24	111.61	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	439	PAH	O2P-P-C1	-3.48	99.53	106.84
3	A	439	PAH	O2P-P-O1P	-3.12	104.32	112.39
3	A	439	PAH	O3P-P-O1P	3.05	120.28	112.39

There are no chirality outliers.

All (5) 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
3	A	439	PAH	C2-C1-P-O2P
3	A	439	PAH	C2-C1-P-O3P
3	A	439	PAH	C2-C1-P-O1P

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

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.