



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:44 AM UTC

PDB ID : 6LDH / pdb_00006ldh
Title : REFINED CRYSTAL STRUCTURE OF DOGFISH M4 APO-LACTATE DE-HYDROGENASE
Authors : Abad-Zapatero, C.; Rossmann, M.G.
Deposited on : 1987-11-25
Resolution : 2.00 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

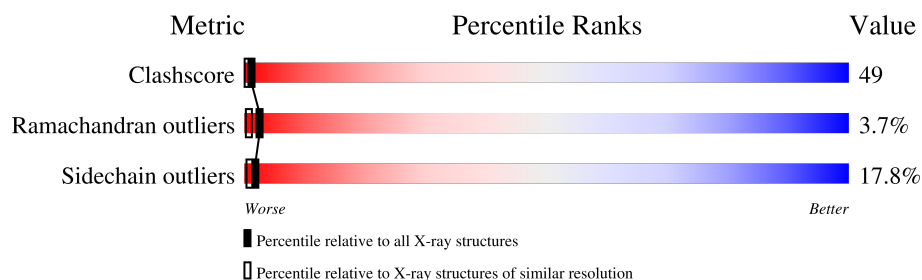
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	330	24% 41% 27% 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2841 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.

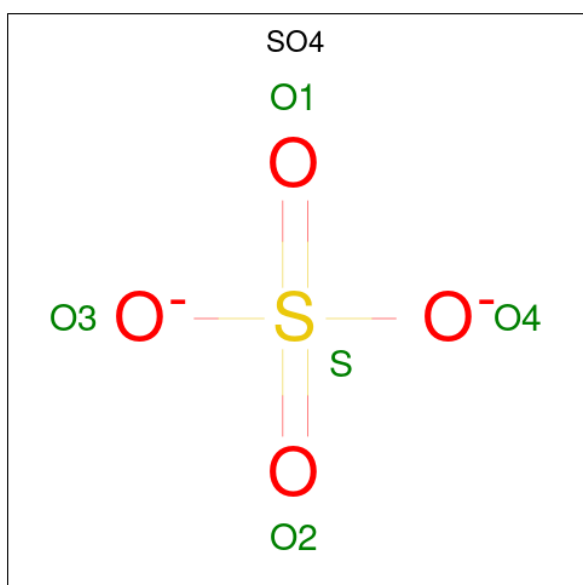
- Molecule 1 is a protein called M4 APO-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2545	1620	439	468	18	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ASN	TRP	conflict	UNP P00341
A	206	VAL	ASN	conflict	UNP P00341
A	208	SER	LEU	conflict	UNP P00341
A	209	ILE	LYS	conflict	UNP P00341
A	210	LYS	GLU	conflict	UNP P00341
A	214	LEU	GLU	conflict	UNP P00341
A	215	ASP	LEU	conflict	UNP P00341
A	308	ASN	ASP	conflict	UNP P00341

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

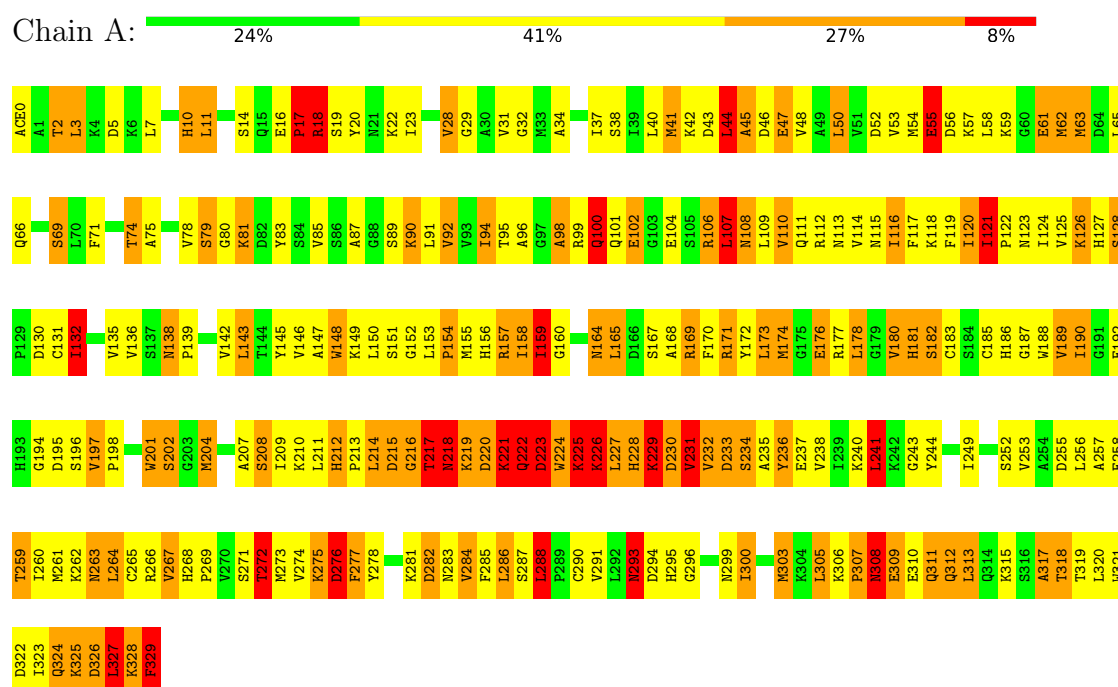
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	286	Total	O	0	0
			286	286		

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: M4 APO-LACTATE DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	F 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	146.80 Å 146.80 Å 155.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2841	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: ACE, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.73	29/2590 (1.1%)	2.78	242/3502 (6.9%)

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	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	LYS	N-CA	-9.70	1.33	1.46
1	A	18	ARG	CA-CB	7.95	1.67	1.53
1	A	159	ILE	N-CA	-7.81	1.37	1.46
1	A	180	VAL	C-O	7.01	1.31	1.24
1	A	277	PHE	N-CA	-6.88	1.38	1.46
1	A	187	GLY	N-CA	6.60	1.52	1.45
1	A	159	ILE	C-N	-6.59	1.27	1.33
1	A	260	ILE	CA-CB	6.59	1.61	1.54
1	A	80	GLY	N-CA	6.47	1.51	1.45
1	A	230	ASP	N-CA	6.44	1.54	1.46
1	A	272	THR	CA-CB	6.08	1.64	1.54
1	A	45	ALA	N-CA	5.97	1.53	1.46
1	A	121	ILE	CA-CB	5.96	1.61	1.54
1	A	181	HIS	CE1-NE2	5.90	1.38	1.32
1	A	221	LYS	N-CA	-5.72	1.38	1.46
1	A	165	LEU	C-N	-5.70	1.26	1.33
1	A	95	THR	CA-CB	5.61	1.61	1.53
1	A	32	GLY	C-O	5.57	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	GLY	C-N	-5.40	1.28	1.33
1	A	303	MET	C-N	-5.37	1.26	1.33
1	A	3	LEU	N-CA	5.30	1.52	1.46
1	A	310	GLU	C-N	-5.19	1.27	1.33
1	A	113	ASN	C-O	5.12	1.30	1.24
1	A	217	THR	N-CA	-5.09	1.39	1.46
1	A	268	HIS	CA-C	5.08	1.57	1.52
1	A	204	MET	N-CA	5.08	1.52	1.46
1	A	171	ARG	NE-CZ	-5.07	1.27	1.33
1	A	89	SER	C-N	-5.05	1.26	1.33
1	A	167	SER	C-N	-5.04	1.27	1.34

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	LEU	CA-C-N	28.77	176.49	121.54
1	A	327	LEU	C-N-CA	28.77	176.49	121.54
1	A	115	ASN	CA-CB-CG	16.64	129.24	112.60
1	A	276	ASP	CA-C-N	14.40	143.69	122.95
1	A	276	ASP	C-N-CA	14.40	143.69	122.95
1	A	195	ASP	CA-CB-CG	14.15	126.75	112.60
1	A	310	GLU	CB-CG-CD	13.71	135.92	112.60
1	A	18	ARG	NE-CZ-NH1	13.46	134.96	121.50
1	A	220	ASP	CA-C-N	12.19	144.82	121.54
1	A	220	ASP	C-N-CA	12.19	144.82	121.54
1	A	218	ASN	CA-CB-CG	-12.04	100.56	112.60
1	A	18	ARG	NE-CZ-NH2	-11.96	108.43	119.20
1	A	164	ASN	CA-CB-CG	11.60	124.20	112.60
1	A	208	SER	CA-CB-OG	11.22	133.55	111.10
1	A	18	ARG	N-CA-C	11.22	128.67	108.48
1	A	127	HIS	CA-CB-CG	-10.95	102.85	113.80
1	A	18	ARG	CB-CA-C	-10.40	92.11	109.80
1	A	216	GLY	N-CA-C	-10.26	100.20	114.67
1	A	308	ASN	CA-C-N	10.13	134.41	120.63
1	A	308	ASN	C-N-CA	10.13	134.41	120.63
1	A	233	ASP	CA-CB-CG	9.93	122.53	112.60
1	A	324	GLN	CA-C-O	9.93	134.71	120.51
1	A	221	LYS	N-CA-C	9.65	131.35	110.80
1	A	110	VAL	CB-CA-C	9.47	125.28	112.22
1	A	18	ARG	N-CA-CB	-9.43	95.06	110.71
1	A	326	ASP	CA-CB-CG	9.14	121.74	112.60
1	A	48	VAL	CB-CA-C	9.01	122.58	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	MET	CA-C-N	8.79	137.47	122.26
1	A	41	MET	C-N-CA	8.79	137.47	122.26
1	A	115	ASN	OD1-CG-ND2	-8.72	113.88	122.60
1	A	11	LEU	N-CA-C	-8.68	98.83	110.55
1	A	99	ARG	CD-NE-CZ	8.58	136.41	124.40
1	A	284	VAL	CA-C-N	8.58	134.56	122.72
1	A	284	VAL	C-N-CA	8.58	134.56	122.72
1	A	171	ARG	CD-NE-CZ	8.30	136.02	124.40
1	A	228	HIS	CA-C-N	8.19	131.92	120.29
1	A	228	HIS	C-N-CA	8.19	131.92	120.29
1	A	215	ASP	CA-CB-CG	8.17	120.77	112.60
1	A	10	HIS	CA-C-O	8.17	130.54	121.06
1	A	282	ASP	CA-C-N	8.11	135.54	122.32
1	A	282	ASP	C-N-CA	8.11	135.54	122.32
1	A	263	ASN	CA-C-O	-8.09	112.45	121.84
1	A	223	ASP	CA-C-N	8.07	136.96	121.54
1	A	223	ASP	C-N-CA	8.07	136.96	121.54
1	A	231	VAL	N-CA-C	-7.97	103.04	110.53
1	A	268	HIS	CA-CB-CG	-7.94	105.86	113.80
1	A	299	ASN	OD1-CG-ND2	7.88	130.47	122.60
1	A	10	HIS	CA-CB-CG	-7.87	105.94	113.80
1	A	89	SER	CA-C-N	7.77	133.69	120.71
1	A	89	SER	C-N-CA	7.77	133.69	120.71
1	A	277	PHE	CB-CA-C	-7.61	99.45	111.17
1	A	61	GLU	CA-C-N	7.46	130.28	120.28
1	A	61	GLU	C-N-CA	7.46	130.28	120.28
1	A	310	GLU	CA-CB-CG	7.43	128.96	114.10
1	A	299	ASN	O-C-N	7.41	130.70	123.29
1	A	324	GLN	CB-CA-C	7.32	124.98	110.42
1	A	294	ASP	CA-CB-CG	7.28	119.88	112.60
1	A	138	ASN	CB-CA-C	7.28	119.74	108.61
1	A	143	LEU	CB-CA-C	7.24	124.58	110.67
1	A	327	LEU	O-C-N	-7.24	112.96	122.59
1	A	174	MET	CA-C-N	7.13	128.01	120.03
1	A	174	MET	C-N-CA	7.13	128.01	120.03
1	A	178	LEU	CA-C-O	-7.10	111.29	119.60
1	A	48	VAL	CA-CB-CG1	7.06	122.40	110.40
1	A	123	ASN	CA-CB-CG	7.06	119.66	112.60
1	A	32	GLY	CA-C-O	-7.02	113.04	120.90
1	A	174	MET	CA-C-O	6.98	128.37	120.90
1	A	236	TYR	N-CA-C	-6.92	103.84	112.90
1	A	327	LEU	CA-C-O	6.88	130.36	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ASP	CB-CA-C	6.83	121.50	110.09
1	A	288	LEU	O-C-N	6.81	126.62	121.85
1	A	224	TRP	N-CA-CB	6.81	122.00	110.49
1	A	307	PRO	CA-C-N	6.80	129.71	120.54
1	A	307	PRO	C-N-CA	6.80	129.71	120.54
1	A	169	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	A	154	PRO	CA-C-O	-6.78	113.70	121.36
1	A	176	GLU	CA-C-N	6.78	129.91	120.29
1	A	176	GLU	C-N-CA	6.78	129.91	120.29
1	A	92	VAL	O-C-N	6.77	130.57	123.26
1	A	192	GLU	CB-CG-CD	6.76	124.09	112.60
1	A	106	ARG	CD-NE-CZ	-6.75	114.95	124.40
1	A	232	VAL	CA-C-N	6.74	131.80	120.88
1	A	232	VAL	C-N-CA	6.74	131.80	120.88
1	A	276	ASP	CA-C-O	6.71	129.50	121.65
1	A	229	LYS	CA-C-N	-6.69	111.50	122.54
1	A	229	LYS	C-N-CA	-6.69	111.50	122.54
1	A	318	THR	O-C-N	6.65	129.83	122.11
1	A	329	PHE	CA-CB-CG	-6.64	107.16	113.80
1	A	272	THR	OG1-CB-CG2	6.62	122.54	109.30
1	A	132	ILE	CB-CA-C	6.59	120.83	110.81
1	A	11	LEU	CB-CA-C	6.57	122.84	109.76
1	A	303	MET	N-CA-C	-6.55	102.08	110.53
1	A	309	GLU	CB-CG-CD	6.55	123.74	112.60
1	A	264	LEU	CA-C-O	-6.55	112.06	119.79
1	A	98	ALA	CA-C-O	-6.53	113.69	121.66
1	A	226	LYS	O-C-N	6.53	129.64	122.20
1	A	216	GLY	CA-C-N	6.53	134.01	121.54
1	A	216	GLY	C-N-CA	6.53	134.01	121.54
1	A	313	LEU	O-C-N	6.52	129.14	122.09
1	A	217	THR	CB-CA-C	-6.49	97.50	110.42
1	A	128	SER	O-C-N	6.49	126.69	121.17
1	A	255	ASP	CA-CB-CG	-6.49	106.11	112.60
1	A	47	GLU	CG-CD-OE1	6.48	133.30	118.40
1	A	225	LYS	CB-CG-CD	6.48	126.21	111.30
1	A	173	LEU	CA-C-O	-6.47	113.69	120.55
1	A	135	VAL	CA-C-O	6.43	128.18	120.65
1	A	17	PRO	CA-C-O	6.43	128.63	121.43
1	A	310	GLU	CG-CD-OE1	6.43	133.18	118.40
1	A	136	VAL	CA-C-N	6.42	129.96	120.90
1	A	136	VAL	C-N-CA	6.42	129.96	120.90
1	A	173	LEU	CB-CA-C	6.42	121.46	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	TRP	CA-C-N	6.41	129.39	120.29
1	A	321	TRP	C-N-CA	6.41	129.39	120.29
1	A	100	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	A	328	LYS	N-CA-CB	6.36	121.24	110.49
1	A	324	GLN	CA-C-N	6.35	131.25	121.53
1	A	324	GLN	C-N-CA	6.35	131.25	121.53
1	A	59	LYS	CA-CB-CG	-6.35	101.40	114.10
1	A	63	MET	O-C-N	6.30	128.90	122.09
1	A	201	TRP	O-C-N	6.30	128.80	122.12
1	A	157	ARG	CD-NE-CZ	-6.28	115.61	124.40
1	A	121	ILE	N-CA-C	6.27	122.41	108.88
1	A	14	SER	CA-C-O	-6.26	114.58	121.28
1	A	117	PHE	O-C-N	6.25	129.95	122.27
1	A	208	SER	N-CA-CB	6.24	121.03	110.49
1	A	110	VAL	CA-CB-CG1	6.21	120.96	110.40
1	A	79	SER	CA-C-N	-6.18	113.11	121.27
1	A	79	SER	C-N-CA	-6.18	113.11	121.27
1	A	50	LEU	CA-CB-CG	6.17	137.89	116.30
1	A	218	ASN	CA-C-O	6.15	129.31	120.51
1	A	111	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	A	264	LEU	N-CA-C	6.12	119.94	112.23
1	A	180	VAL	CB-CA-C	6.11	120.22	110.82
1	A	276	ASP	O-C-N	-6.08	115.28	122.58
1	A	107	LEU	O-C-N	6.04	128.62	122.09
1	A	121	ILE	N-CA-CB	-6.03	102.77	111.21
1	A	116	ILE	CA-C-O	6.03	127.15	120.46
1	A	62	MET	O-C-N	5.97	128.45	122.12
1	A	208	SER	O-C-N	5.97	130.53	122.59
1	A	189	VAL	N-CA-C	-5.96	99.16	107.80
1	A	170	PHE	CB-CA-C	5.94	120.20	110.88
1	A	18	ARG	NH1-CZ-NH2	-5.93	111.59	119.30
1	A	147	ALA	N-CA-C	-5.90	104.93	111.36
1	A	18	ARG	CA-CB-CG	-5.89	102.31	114.10
1	A	31	VAL	CA-C-N	5.89	126.36	119.94
1	A	31	VAL	C-N-CA	5.89	126.36	119.94
1	A	218	ASN	CA-C-N	5.87	132.75	121.54
1	A	218	ASN	C-N-CA	5.87	132.75	121.54
1	A	259	THR	N-CA-CB	5.86	118.72	109.82
1	A	119	PHE	CA-CB-CG	-5.84	107.95	113.80
1	A	222	GLN	N-CA-CB	5.84	120.37	110.49
1	A	81	LYS	N-CA-C	-5.82	104.90	112.23
1	A	196	SER	O-C-N	5.82	129.69	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	VAL	CB-CA-C	5.81	119.44	110.96
1	A	214	LEU	CA-C-O	-5.80	113.80	120.24
1	A	120	ILE	CA-C-N	5.79	132.84	122.13
1	A	120	ILE	C-N-CA	5.79	132.84	122.13
1	A	215	ASP	O-C-N	5.74	131.66	122.42
1	A	174	MET	CB-CA-C	-5.73	101.65	110.81
1	A	177	ARG	CA-C-N	-5.72	110.99	121.52
1	A	177	ARG	C-N-CA	-5.72	110.99	121.52
1	A	159	ILE	O-C-N	5.70	129.33	123.18
1	A	69	SER	CA-C-N	5.68	128.67	120.38
1	A	69	SER	C-N-CA	5.68	128.67	120.38
1	A	308	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	61	GLU	O-C-N	5.64	128.58	122.15
1	A	148	TRP	CA-CB-CG	-5.64	102.88	113.60
1	A	221	LYS	CA-C-N	5.62	132.28	121.54
1	A	221	LYS	C-N-CA	5.62	132.28	121.54
1	A	55	GLU	CG-CD-OE2	-5.61	105.49	118.40
1	A	102	GLU	CA-CB-CG	5.59	125.28	114.10
1	A	272	THR	CB-CA-C	-5.59	99.23	110.30
1	A	187	GLY	N-CA-C	-5.58	101.09	111.14
1	A	217	THR	CA-CB-CG2	5.55	119.94	110.50
1	A	329	PHE	CA-C-O	-5.55	111.36	120.80
1	A	101	GLN	CA-C-O	5.50	128.83	121.78
1	A	138	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	169	ARG	CB-CG-CD	5.50	123.94	111.30
1	A	117	PHE	CA-C-O	-5.49	113.66	119.97
1	A	305	LEU	O-C-N	5.48	129.08	122.94
1	A	170	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	328	LYS	CA-C-O	5.46	128.31	120.51
1	A	317	ALA	CA-C-N	5.45	129.72	120.88
1	A	317	ALA	C-N-CA	5.45	129.72	120.88
1	A	281	LYS	CA-C-O	-5.45	113.14	119.14
1	A	312	GLN	CA-C-N	5.45	127.85	120.44
1	A	312	GLN	C-N-CA	5.45	127.85	120.44
1	A	16	GLU	CB-CG-CD	5.45	121.86	112.60
1	A	288	LEU	CA-C-O	-5.44	114.36	119.91
1	A	148	TRP	CA-C-N	5.44	127.57	120.28
1	A	148	TRP	C-N-CA	5.44	127.57	120.28
1	A	303	MET	CA-C-N	5.43	132.24	123.33
1	A	303	MET	C-N-CA	5.43	132.24	123.33
1	A	94	ILE	CB-CG1-CD1	-5.43	102.40	113.80
1	A	43	ASP	CB-CG-OD1	5.42	130.88	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ASN	OD1-CG-ND2	5.41	128.01	122.60
1	A	59	LYS	N-CA-CB	5.40	118.05	110.12
1	A	132	ILE	CA-C-O	-5.39	114.57	120.72
1	A	29	GLY	CA-C-O	-5.39	116.03	121.64
1	A	227	LEU	CB-CA-C	5.37	121.66	110.32
1	A	287	SER	CA-C-N	5.37	133.35	122.45
1	A	287	SER	C-N-CA	5.37	133.35	122.45
1	A	169	ARG	CA-C-O	5.36	126.19	120.24
1	A	325	LYS	CA-CB-CG	5.35	124.81	114.10
1	A	267	VAL	O-C-N	5.34	129.45	122.94
1	A	19	SER	CA-C-O	-5.31	114.42	120.32
1	A	295	HIS	CA-C-N	5.31	129.73	121.72
1	A	295	HIS	C-N-CA	5.31	129.73	121.72
1	A	182	SER	CA-C-O	-5.30	113.08	119.49
1	A	16	GLU	CG-CD-OE1	5.29	130.56	118.40
1	A	96	ALA	O-C-N	5.28	129.52	123.29
1	A	148	TRP	CA-C-O	5.25	126.84	121.07
1	A	299	ASN	CA-C-O	-5.25	115.67	121.28
1	A	65	LEU	CA-C-O	-5.24	115.32	120.82
1	A	44	LEU	CA-C-N	-5.23	113.37	122.37
1	A	44	LEU	C-N-CA	-5.23	113.37	122.37
1	A	132	ILE	CA-CB-CG2	5.23	119.39	110.50
1	A	202	SER	CA-C-O	-5.21	112.29	119.12
1	A	229	LYS	O-C-N	5.21	128.09	122.15
1	A	272	THR	O-C-N	5.21	130.07	122.94
1	A	295	HIS	CA-CB-CG	-5.20	108.60	113.80
1	A	59	LYS	O-C-N	5.19	127.62	122.12
1	A	123	ASN	CB-CG-ND2	5.17	124.15	116.40
1	A	177	ARG	N-CA-CB	5.15	117.78	110.16
1	A	34	ALA	O-C-N	5.15	128.40	122.17
1	A	154	PRO	N-CA-C	-5.14	103.03	111.15
1	A	197	VAL	O-C-N	5.14	126.04	121.57
1	A	152	GLY	CA-C-O	5.13	124.70	118.86
1	A	196	SER	CA-C-O	-5.12	113.54	120.15
1	A	253	VAL	CA-C-O	-5.10	115.25	120.71
1	A	90	LYS	N-CA-C	-5.10	105.18	111.40
1	A	28	VAL	CB-CA-C	5.09	119.64	111.29
1	A	275	LYS	CA-C-N	5.08	129.40	122.34
1	A	275	LYS	C-N-CA	5.08	129.40	122.34
1	A	293	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	241	LEU	N-CA-CB	-5.05	101.85	110.33
1	A	310	GLU	CG-CD-OE2	-5.05	106.78	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ALA	N-CA-C	5.04	116.85	111.36
1	A	100	GLN	N-CA-CB	5.03	118.99	110.49
1	A	71	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	313	LEU	CA-C-N	5.03	127.02	120.28
1	A	313	LEU	C-N-CA	5.03	127.02	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	2545	0	2613	252	13
2	A	10	0	0	1	0
3	A	286	0	0	35	5
All	All	2841	0	2613	252	16

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 49.

All (252) 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:219:LYS:HE2	3:A:400:HOH:O	1.31	1.27
1:A:54:MET:HE1	3:A:398:HOH:O	1.33	1.20
1:A:273:MET:CE	1:A:275:LYS:HB2	1.70	1.20
1:A:107:LEU:HD11	1:A:325:LYS:HE3	1.20	1.15
1:A:62:MET:HE2	1:A:78:VAL:HA	1.32	1.08
1:A:62:MET:HE3	1:A:79:SER:N	1.70	1.05
1:A:210:LYS:HG2	1:A:213:PRO:CD	1.87	1.05
1:A:62:MET:HE3	1:A:79:SER:H	1.13	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:HG23	1:A:228:HIS:HE1	1.20	1.03
1:A:57:LYS:HE3	3:A:570:HOH:O	1.59	1.02
1:A:100:GLN:HB2	1:A:109:LEU:HD22	1.36	1.02
1:A:273:MET:HE1	1:A:283:ASN:HA	1.38	1.02
1:A:273:MET:HE3	1:A:275:LYS:HB2	1.03	1.01
1:A:81:LYS:O	3:A:430:HOH:O	1.77	1.01
1:A:303:MET:HE3	1:A:305:LEU:HD21	1.45	0.98
1:A:312:GLN:HG2	3:A:525:HOH:O	1.62	0.98
1:A:197:VAL:HG23	1:A:228:HIS:CE1	1.99	0.98
1:A:210:LYS:HG2	1:A:213:PRO:HD3	1.47	0.97
1:A:210:LYS:HB3	1:A:213:PRO:HG2	1.50	0.93
1:A:230:ASP:HA	1:A:233:ASP:HB2	1.51	0.92
1:A:0:ACE:H2	1:A:5:ASP:HB3	1.50	0.92
1:A:288:LEU:HD23	1:A:300:ILE:CD1	2.01	0.91
1:A:17:PRO:HA	1:A:18:ARG:HD3	1.52	0.91
1:A:273:MET:HE3	1:A:275:LYS:CB	1.98	0.90
1:A:62:MET:CE	1:A:78:VAL:HA	2.03	0.88
1:A:284:VAL:HG11	1:A:317:ALA:HA	1.57	0.86
1:A:212:HIS:O	1:A:217:THR:HA	1.74	0.86
1:A:0:ACE:CH3	1:A:5:ASP:HB3	2.06	0.86
1:A:58:LEU:HD23	3:A:438:HOH:O	1.74	0.85
1:A:327:LEU:HD22	3:A:549:HOH:O	1.77	0.85
1:A:210:LYS:HG2	1:A:213:PRO:HD2	1.58	0.85
1:A:57:LYS:HG3	3:A:570:HOH:O	1.76	0.84
1:A:229:LYS:HG2	3:A:536:HOH:O	1.77	0.84
1:A:226:LYS:HD3	3:A:535:HOH:O	1.78	0.83
1:A:107:LEU:CD1	1:A:325:LYS:HE3	2.08	0.83
1:A:142:VAL:O	1:A:146:VAL:HG23	1.80	0.81
1:A:236:TYR:C	1:A:240:LYS:HE2	2.05	0.81
1:A:98:ALA:HB1	1:A:112:ARG:NH1	1.96	0.81
1:A:194:GLY:H	1:A:197:VAL:CG1	1.94	0.79
1:A:210:LYS:HZ1	1:A:212:HIS:HB3	1.48	0.79
1:A:83:TYR:HE2	1:A:124:ILE:HD11	1.48	0.79
1:A:190:ILE:C	1:A:190:ILE:HD13	2.06	0.79
1:A:107:LEU:HD11	1:A:325:LYS:CE	2.09	0.77
1:A:83:TYR:OH	1:A:120:ILE:HG23	1.84	0.77
1:A:263:ASN:OD1	1:A:293:ASN:HB2	1.85	0.77
1:A:274:VAL:HG21	1:A:286:LEU:HD12	1.64	0.77
1:A:210:LYS:HB3	1:A:213:PRO:CG	2.15	0.76
1:A:236:TYR:O	1:A:240:LYS:HE2	1.86	0.75
1:A:218:ASN:OD1	1:A:219:LYS:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:CB	1:A:109:LEU:HD22	2.18	0.74
1:A:210:LYS:CG	1:A:213:PRO:CD	2.66	0.74
1:A:181:HIS:HD2	1:A:183:CYS:SG	2.11	0.74
1:A:181:HIS:CD2	1:A:183:CYS:SG	2.82	0.73
1:A:210:LYS:C	1:A:213:PRO:HD2	2.14	0.73
1:A:210:LYS:O	1:A:213:PRO:HD2	1.89	0.73
1:A:210:LYS:NZ	1:A:212:HIS:HB3	2.03	0.73
1:A:216:GLY:O	1:A:217:THR:HG23	1.89	0.72
1:A:230:ASP:O	1:A:234:SER:HB2	1.89	0.71
1:A:215:ASP:HB3	1:A:217:THR:O	1.90	0.71
1:A:312:GLN:CG	3:A:525:HOH:O	2.31	0.69
1:A:83:TYR:CE2	1:A:124:ILE:HD11	2.27	0.69
1:A:20:TYR:O	1:A:90:LYS:HD3	1.93	0.68
1:A:100:GLN:HB2	1:A:109:LEU:CD2	2.20	0.68
1:A:165:LEU:CD2	1:A:249:ILE:HG12	2.23	0.68
1:A:194:GLY:N	1:A:197:VAL:HG13	2.08	0.68
1:A:46:ASP:OD2	3:A:593:HOH:O	2.12	0.67
1:A:186:HIS:ND1	2:A:330:SO4:O1	2.23	0.67
1:A:53:VAL:HA	1:A:81:LYS:HD2	1.75	0.67
1:A:215:ASP:C	1:A:217:THR:H	2.01	0.66
1:A:308:ASN:ND2	3:A:404:HOH:O	2.27	0.66
1:A:194:GLY:H	1:A:197:VAL:HG11	1.58	0.66
1:A:278:TYR:HE2	1:A:288:LEU:HD21	1.61	0.66
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.61	0.66
1:A:18:ARG:O	1:A:18:ARG:CG	2.41	0.66
1:A:273:MET:CE	1:A:275:LYS:CB	2.62	0.66
1:A:194:GLY:N	1:A:197:VAL:CG1	2.58	0.65
1:A:264:LEU:HB3	1:A:266:ARG:HG3	1.79	0.65
1:A:225:LYS:HG3	3:A:560:HOH:O	1.97	0.64
1:A:210:LYS:CG	1:A:213:PRO:HD2	2.29	0.63
1:A:94:ILE:HD13	1:A:121:ILE:HD11	1.80	0.62
1:A:232:VAL:HG23	3:A:594:HOH:O	2.00	0.62
1:A:2:THR:HG22	1:A:5:ASP:H	1.65	0.62
1:A:259:THR:HG23	1:A:264:LEU:HB2	1.82	0.62
1:A:318:THR:HG23	1:A:319:THR:N	2.15	0.62
1:A:329:PHE:CD2	1:A:329:PHE:O	2.53	0.62
1:A:57:LYS:CG	3:A:570:HOH:O	2.41	0.61
1:A:155:MET:O	3:A:584:HOH:O	2.16	0.61
1:A:230:ASP:O	1:A:234:SER:CB	2.48	0.61
1:A:273:MET:HE2	1:A:275:LYS:HB2	1.79	0.60
1:A:0:ACE:CH3	1:A:5:ASP:CB	2.78	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:ND2	3:A:452:HOH:O	2.35	0.59
1:A:212:HIS:CD2	1:A:218:ASN:H	2.21	0.59
1:A:315:LYS:O	1:A:318:THR:HG22	2.01	0.59
1:A:173:LEU:HD12	1:A:231:VAL:HG23	1.84	0.59
1:A:323:ILE:O	1:A:325:LYS:N	2.34	0.59
1:A:106:ARG:O	1:A:110:VAL:HG23	2.03	0.59
1:A:190:ILE:O	1:A:198:PRO:HD2	2.03	0.59
1:A:258:GLU:HG3	1:A:262:LYS:HD2	1.84	0.58
1:A:181:HIS:CD2	1:A:183:CYS:H	2.21	0.58
1:A:309:GLU:OE2	3:A:528:HOH:O	2.17	0.58
1:A:40:LEU:HD23	1:A:74:THR:HG21	1.85	0.57
1:A:217:THR:O	1:A:218:ASN:HB2	2.03	0.57
1:A:307:PRO:O	1:A:311:GLN:HB2	2.03	0.57
1:A:312:GLN:NE2	3:A:408:HOH:O	2.37	0.57
1:A:109:LEU:HD12	1:A:109:LEU:O	2.04	0.57
1:A:233:ASP:O	1:A:236:TYR:N	2.29	0.57
1:A:98:ALA:HB1	1:A:112:ARG:HH12	1.68	0.57
1:A:125:VAL:HG21	1:A:151:SER:HB2	1.85	0.57
1:A:318:THR:CG2	1:A:319:THR:H	2.17	0.57
1:A:121:ILE:HB	1:A:122:PRO:HD3	1.86	0.57
1:A:132:ILE:CD1	1:A:159:ILE:HG13	2.35	0.56
1:A:210:LYS:NZ	1:A:212:HIS:CB	2.68	0.56
1:A:18:ARG:HG2	1:A:18:ARG:O	2.05	0.56
1:A:197:VAL:O	1:A:228:HIS:NE2	2.39	0.56
1:A:288:LEU:HB3	1:A:300:ILE:HD11	1.87	0.56
1:A:194:GLY:O	1:A:197:VAL:HG22	2.06	0.56
1:A:257:ALA:O	1:A:261:MET:HG2	2.06	0.56
1:A:38:SER:O	1:A:42:LYS:HB2	2.06	0.55
1:A:229:LYS:HD2	3:A:535:HOH:O	2.06	0.55
1:A:22:LYS:HE3	1:A:47:GLU:OE2	2.06	0.55
1:A:212:HIS:HB3	1:A:213:PRO:HD3	1.88	0.55
1:A:225:LYS:HZ3	1:A:226:LYS:NZ	2.05	0.55
1:A:106:ARG:HG3	3:A:508:HOH:O	2.06	0.54
1:A:219:LYS:HZ3	1:A:219:LYS:HB3	1.71	0.54
1:A:23:ILE:HD12	1:A:45:ALA:HB2	1.88	0.54
1:A:272:THR:O	1:A:285:PHE:HA	2.07	0.54
1:A:110:VAL:O	1:A:114:VAL:HG23	2.08	0.54
1:A:100:GLN:HA	1:A:104:GLU:OE1	2.08	0.54
1:A:326:ASP:O	1:A:327:LEU:HB2	2.07	0.54
1:A:174:MET:O	1:A:178:LEU:N	2.34	0.54
1:A:94:ILE:CD1	1:A:121:ILE:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:O	1:A:252:SER:HB3	2.08	0.53
1:A:306:LYS:O	1:A:309:GLU:HB2	2.08	0.53
1:A:66:GLN:O	1:A:69:SER:OG	2.14	0.53
1:A:202:SER:O	1:A:210:LYS:HD2	2.08	0.53
1:A:267:VAL:HA	1:A:290:CYS:O	2.09	0.53
1:A:154:PRO:HB2	1:A:156:HIS:CD2	2.44	0.53
1:A:210:LYS:HE3	1:A:213:PRO:HD3	1.89	0.53
1:A:318:THR:HG23	1:A:319:THR:H	1.73	0.53
1:A:121:ILE:O	1:A:125:VAL:HG23	2.09	0.53
1:A:325:LYS:O	1:A:325:LYS:HG2	2.09	0.52
1:A:132:ILE:HD11	1:A:159:ILE:HG13	1.91	0.52
1:A:233:ASP:C	1:A:235:ALA:N	2.66	0.52
1:A:0:ACE:H2	1:A:5:ASP:CB	2.33	0.52
1:A:142:VAL:HG22	1:A:320:LEU:CD2	2.39	0.52
1:A:214:LEU:C	1:A:216:GLY:H	2.17	0.52
1:A:188:TRP:CZ3	1:A:269:PRO:HD3	2.45	0.52
1:A:112:ARG:O	1:A:116:ILE:HG13	2.08	0.52
1:A:126:LYS:O	1:A:126:LYS:HG3	2.09	0.52
1:A:62:MET:HE1	3:A:479:HOH:O	2.10	0.51
1:A:229:LYS:HE2	3:A:462:HOH:O	2.09	0.51
1:A:210:LYS:CB	1:A:213:PRO:HD2	2.40	0.51
1:A:210:LYS:NZ	3:A:531:HOH:O	2.41	0.51
1:A:318:THR:CG2	1:A:319:THR:N	2.71	0.51
1:A:186:HIS:O	1:A:204:MET:HA	2.11	0.51
1:A:52:ASP:OD1	1:A:54:MET:HE2	2.10	0.51
1:A:110:VAL:HG22	1:A:139:PRO:HG3	1.91	0.50
1:A:243:GLY:O	1:A:244:TYR:HB3	2.11	0.50
1:A:106:ARG:O	1:A:110:VAL:CG2	2.59	0.50
1:A:57:LYS:O	1:A:61:GLU:HG2	2.11	0.50
1:A:62:MET:CE	1:A:79:SER:H	2.04	0.50
1:A:219:LYS:HB3	1:A:219:LYS:NZ	2.26	0.50
1:A:219:LYS:NZ	1:A:219:LYS:CB	2.75	0.50
1:A:110:VAL:HG11	1:A:142:VAL:HG11	1.93	0.50
1:A:83:TYR:CE2	1:A:124:ILE:CD1	2.93	0.49
1:A:157:ARG:C	1:A:158:ILE:HG12	2.37	0.49
1:A:288:LEU:HD23	1:A:300:ILE:HD11	1.92	0.49
1:A:288:LEU:HD23	1:A:300:ILE:HD12	1.90	0.49
1:A:22:LYS:HG3	1:A:47:GLU:HB3	1.95	0.49
1:A:318:THR:CB	3:A:608:HOH:O	2.60	0.49
1:A:190:ILE:HD13	1:A:190:ILE:O	2.13	0.48
1:A:165:LEU:O	1:A:168:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:MET:CE	1:A:305:LEU:HD21	2.30	0.48
1:A:110:VAL:CG1	1:A:142:VAL:HG11	2.43	0.48
1:A:63:MET:CE	3:A:381:HOH:O	2.62	0.48
1:A:320:LEU:O	1:A:324:GLN:HG3	2.14	0.48
1:A:164:ASN:O	3:A:484:HOH:O	2.20	0.47
1:A:190:ILE:C	1:A:190:ILE:CD1	2.78	0.47
1:A:18:ARG:HG2	1:A:18:ARG:NH1	2.26	0.47
1:A:145:TYR:O	1:A:148:TRP:HB3	2.14	0.47
1:A:0:ACE:H1	1:A:5:ASP:CB	2.45	0.47
1:A:217:THR:OG1	1:A:218:ASN:N	2.40	0.47
1:A:110:VAL:HG11	1:A:323:ILE:HG21	1.97	0.46
1:A:210:LYS:CE	1:A:213:PRO:HD3	2.45	0.46
1:A:278:TYR:CE2	1:A:288:LEU:HD21	2.47	0.46
1:A:58:LEU:HG	1:A:79:SER:HB2	1.97	0.46
1:A:130:ASP:HA	1:A:157:ARG:HH12	1.80	0.46
1:A:210:LYS:CB	1:A:213:PRO:CD	2.93	0.46
1:A:229:LYS:HE3	1:A:229:LYS:HB2	1.32	0.46
1:A:318:THR:HA	3:A:608:HOH:O	2.15	0.46
1:A:153:LEU:HB2	1:A:158:ILE:HD11	1.96	0.46
1:A:288:LEU:HB3	1:A:300:ILE:CD1	2.45	0.46
1:A:288:LEU:HD23	1:A:300:ILE:HD13	1.92	0.46
1:A:44:LEU:HD11	1:A:258:GLU:HB2	1.98	0.46
1:A:329:PHE:O	1:A:329:PHE:CG	2.68	0.46
1:A:233:ASP:C	1:A:235:ALA:H	2.22	0.46
1:A:165:LEU:HB3	3:A:519:HOH:O	2.16	0.45
1:A:210:LYS:CG	1:A:213:PRO:HD3	2.31	0.45
1:A:171:ARG:HD3	1:A:186:HIS:HA	1.99	0.45
1:A:50:LEU:O	1:A:79:SER:HA	2.17	0.45
1:A:325:LYS:HE2	1:A:325:LYS:HB3	1.54	0.45
1:A:171:ARG:CD	1:A:185:CYS:O	2.65	0.45
1:A:171:ARG:HD2	1:A:185:CYS:O	2.17	0.45
1:A:264:LEU:HD13	1:A:266:ARG:HD3	1.97	0.45
1:A:145:TYR:OH	1:A:149:LYS:NZ	2.49	0.45
1:A:172:TYR:HA	1:A:182:SER:HB3	1.99	0.45
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.73	0.45
1:A:100:GLN:HG3	1:A:104:GLU:HB3	1.98	0.44
1:A:83:TYR:HD2	1:A:124:ILE:HD13	1.82	0.44
1:A:142:VAL:HG22	1:A:320:LEU:HD22	1.98	0.44
1:A:165:LEU:HD22	1:A:249:ILE:HG12	1.95	0.44
1:A:210:LYS:HB3	1:A:213:PRO:CD	2.47	0.44
1:A:178:LEU:HD11	1:A:211:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:HE3	1:A:213:PRO:HG3	2.00	0.44
1:A:237:GLU:HA	1:A:240:LYS:HE3	1.98	0.44
1:A:237:GLU:O	1:A:241:LEU:HB2	2.17	0.44
1:A:229:LYS:O	1:A:232:VAL:HG12	2.18	0.44
1:A:63:MET:HE3	3:A:381:HOH:O	2.17	0.43
1:A:92:VAL:HG21	1:A:124:ILE:CG2	2.48	0.43
1:A:62:MET:CE	1:A:78:VAL:CA	2.86	0.43
1:A:288:LEU:CB	1:A:300:ILE:HD11	2.49	0.43
1:A:312:GLN:HG2	3:A:557:HOH:O	2.18	0.43
1:A:114:VAL:O	1:A:118:LYS:HG3	2.18	0.43
1:A:225:LYS:NZ	1:A:226:LYS:CE	2.81	0.43
1:A:261:MET:HB3	1:A:261:MET:HE3	1.64	0.42
1:A:277:PHE:O	1:A:278:TYR:HB2	2.18	0.42
1:A:265:CYS:HA	1:A:291:VAL:HG13	2.00	0.42
1:A:28:VAL:HG22	1:A:52:ASP:HB2	2.02	0.42
1:A:313:LEU:HA	1:A:313:LEU:HD12	1.72	0.42
1:A:83:TYR:CD2	1:A:124:ILE:HD13	2.55	0.42
1:A:210:LYS:HZ2	1:A:212:HIS:CB	2.32	0.42
1:A:128:SER:HB3	1:A:131:CYS:HB3	2.01	0.41
1:A:28:VAL:HG11	1:A:50:LEU:HD13	2.02	0.41
1:A:223:ASP:HB3	3:A:349:HOH:O	2.19	0.41
1:A:62:MET:CE	3:A:479:HOH:O	2.67	0.41
1:A:212:HIS:CD2	1:A:218:ASN:N	2.86	0.41
1:A:276:ASP:OD1	1:A:276:ASP:O	2.38	0.41
1:A:160:GLY:HA3	1:A:271:SER:HB3	2.01	0.41
1:A:52:ASP:OD1	1:A:54:MET:CE	2.69	0.41
1:A:54:MET:CE	3:A:398:HOH:O	2.20	0.41
1:A:61:GLU:OE2	1:A:61:GLU:HA	2.19	0.41
1:A:94:ILE:HD13	1:A:94:ILE:HG21	1.88	0.41
1:A:7:LEU:O	1:A:7:LEU:HG	2.21	0.41
1:A:189:VAL:HG13	1:A:197:VAL:HB	2.03	0.40
1:A:83:TYR:CD2	1:A:124:ILE:CD1	3.04	0.40
1:A:173:LEU:HD12	1:A:231:VAL:CG2	2.48	0.40
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.82	0.40
1:A:305:LEU:HD12	1:A:313:LEU:HD22	2.04	0.40
1:A:55:GLU:HB2	1:A:56:ASP:H	1.71	0.40
1:A:201:TRP:CD1	1:A:219:LYS:HG2	2.57	0.40
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.76	0.40
1:A:204:MET:HE2	1:A:204:MET:HB3	1.85	0.40

All (16) 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:329:PHE:CE1	1:A:329:PHE:CE1[32_555]	0.72	1.48
1:A:329:PHE:CE1	1:A:329:PHE:CZ[32_555]	1.37	0.83
1:A:329:PHE:CB	3:A:419:HOH:O[32_555]	1.39	0.81
1:A:329:PHE:CD1	1:A:329:PHE:CZ[32_555]	1.42	0.78
3:A:364:HOH:O	3:A:364:HOH:O[32_555]	1.61	0.59
3:A:590:HOH:O	3:A:590:HOH:O[14_555]	1.66	0.54
1:A:108:ASN:ND2	1:A:329:PHE:CD2[32_555]	1.88	0.32
1:A:329:PHE:O	1:A:329:PHE:CE2[32_555]	1.88	0.32
1:A:329:PHE:CD1	1:A:329:PHE:CE1[32_555]	1.98	0.22
1:A:108:ASN:OD1	1:A:329:PHE:O[32_555]	2.00	0.20
1:A:329:PHE:CZ	1:A:329:PHE:CZ[32_555]	2.04	0.16
3:A:576:HOH:O	3:A:596:HOH:O[27_555]	2.08	0.12
1:A:329:PHE:CG	1:A:329:PHE:CZ[32_555]	2.11	0.09
1:A:188:TRP:NE1	1:A:207:ALA:O[14_555]	2.16	0.04
1:A:126:LYS:O	3:A:602:HOH:O[27_555]	2.19	0.01
1:A:329:PHE:C	1:A:329:PHE:CE2[32_555]	2.19	0.01

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	328/330 (99%)	289 (88%)	27 (8%)	12 (4%)	2 1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	A	217	THR
1	A	218	ASN
1	A	221	LYS
1	A	222	GLN
1	A	223	ASP
1	A	327	LEU
1	A	87	ALA

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Mol	Chain	Res	Type
1	A	234	SER
1	A	100	GLN
1	A	219	LYS
1	A	224	TRP

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	286/286 (100%)	235 (82%)	51 (18%)	2 1

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	LEU
1	A	10	HIS
1	A	11	LEU
1	A	17	PRO
1	A	18	ARG
1	A	37	ILE
1	A	41	MET
1	A	44	LEU
1	A	55	GLU
1	A	74	THR
1	A	85	VAL
1	A	91	LEU
1	A	102	GLU
1	A	107	LEU
1	A	108	ASN
1	A	121	ILE
1	A	126	LYS
1	A	132	ILE
1	A	150	LEU
1	A	158	ILE
1	A	159	ILE

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Mol	Chain	Res	Type
1	A	169	ARG
1	A	176	GLU
1	A	180	VAL
1	A	190	ILE
1	A	209	ILE
1	A	212	HIS
1	A	220	ASP
1	A	221	LYS
1	A	222	GLN
1	A	225	LYS
1	A	226	LYS
1	A	229	LYS
1	A	231	VAL
1	A	238	VAL
1	A	241	LEU
1	A	256	LEU
1	A	272	THR
1	A	276	ASP
1	A	282	ASP
1	A	286	LEU
1	A	288	LEU
1	A	293	ASN
1	A	300	ILE
1	A	308	ASN
1	A	311	GLN
1	A	322	ASP
1	A	327	LEU
1	A	328	LYS
1	A	329	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	127	HIS
1	A	181	HIS
1	A	205	ASN
1	A	228	HIS
1	A	293	ASN

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	330	-	4,4,4	0.73	0	6,6,6	0.70	0
2	SO4	A	331	-	4,4,4	0.78	0	6,6,6	0.37	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	330	SO4	1	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.