



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:36 AM UTC

PDB ID : 7M4S / pdb_00007m4s
Title : Crystal structure of macrocyclase AMdnB from Anabaena sp. PCC 7120
Authors : Li, G.; Bruner, S.D.
Deposited on : 2021-03-22
Resolution : 2.49 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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

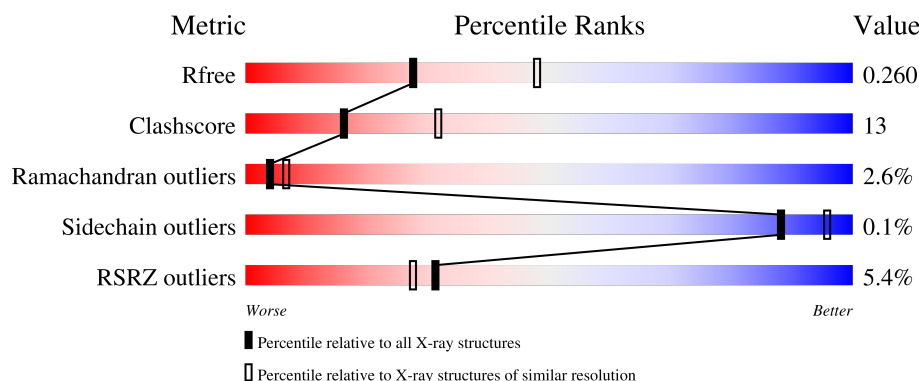
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	360	4% 65% 19% • 14%
1	B	360	5% 61% 23% • 13%
1	C	360	4% 62% 17% •• 18%
1	D	360	5% 56% 21% •• 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9938 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 AMdnB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2533	1624	425	473	11			
1	B	314	Total	C	N	O	S	0	0	0
			2557	1637	432	477	11			
1	C	297	Total	C	N	O	S	0	0	0
			2420	1551	411	449	9			
1	D	292	Total	C	N	O	S	0	0	0
			2381	1530	404	438	9			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP Q8YLC3
A	-32	GLY	-	expression tag	UNP Q8YLC3
A	-31	SER	-	expression tag	UNP Q8YLC3
A	-30	SER	-	expression tag	UNP Q8YLC3
A	-29	HIS	-	expression tag	UNP Q8YLC3
A	-28	HIS	-	expression tag	UNP Q8YLC3
A	-27	HIS	-	expression tag	UNP Q8YLC3
A	-26	HIS	-	expression tag	UNP Q8YLC3
A	-25	HIS	-	expression tag	UNP Q8YLC3
A	-24	HIS	-	expression tag	UNP Q8YLC3
A	-23	SER	-	expression tag	UNP Q8YLC3
A	-22	SER	-	expression tag	UNP Q8YLC3
A	-21	GLY	-	expression tag	UNP Q8YLC3
A	-20	LEU	-	expression tag	UNP Q8YLC3
A	-19	VAL	-	expression tag	UNP Q8YLC3
A	-18	PRO	-	expression tag	UNP Q8YLC3
A	-17	ARG	-	expression tag	UNP Q8YLC3
A	-16	GLY	-	expression tag	UNP Q8YLC3
A	-15	SER	-	expression tag	UNP Q8YLC3
A	-14	HIS	-	expression tag	UNP Q8YLC3
A	-13	MET	-	expression tag	UNP Q8YLC3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP Q8YLC3
A	-11	SER	-	expression tag	UNP Q8YLC3
A	-10	MET	-	expression tag	UNP Q8YLC3
A	-9	THR	-	expression tag	UNP Q8YLC3
A	-8	GLY	-	expression tag	UNP Q8YLC3
A	-7	GLY	-	expression tag	UNP Q8YLC3
A	-6	GLN	-	expression tag	UNP Q8YLC3
A	-5	GLN	-	expression tag	UNP Q8YLC3
A	-4	MET	-	expression tag	UNP Q8YLC3
A	-3	GLY	-	expression tag	UNP Q8YLC3
A	-2	ARG	-	expression tag	UNP Q8YLC3
A	-1	GLY	-	expression tag	UNP Q8YLC3
A	0	SER	-	expression tag	UNP Q8YLC3
B	-33	MET	-	initiating methionine	UNP Q8YLC3
B	-32	GLY	-	expression tag	UNP Q8YLC3
B	-31	SER	-	expression tag	UNP Q8YLC3
B	-30	SER	-	expression tag	UNP Q8YLC3
B	-29	HIS	-	expression tag	UNP Q8YLC3
B	-28	HIS	-	expression tag	UNP Q8YLC3
B	-27	HIS	-	expression tag	UNP Q8YLC3
B	-26	HIS	-	expression tag	UNP Q8YLC3
B	-25	HIS	-	expression tag	UNP Q8YLC3
B	-24	HIS	-	expression tag	UNP Q8YLC3
B	-23	SER	-	expression tag	UNP Q8YLC3
B	-22	SER	-	expression tag	UNP Q8YLC3
B	-21	GLY	-	expression tag	UNP Q8YLC3
B	-20	LEU	-	expression tag	UNP Q8YLC3
B	-19	VAL	-	expression tag	UNP Q8YLC3
B	-18	PRO	-	expression tag	UNP Q8YLC3
B	-17	ARG	-	expression tag	UNP Q8YLC3
B	-16	GLY	-	expression tag	UNP Q8YLC3
B	-15	SER	-	expression tag	UNP Q8YLC3
B	-14	HIS	-	expression tag	UNP Q8YLC3
B	-13	MET	-	expression tag	UNP Q8YLC3
B	-12	ALA	-	expression tag	UNP Q8YLC3
B	-11	SER	-	expression tag	UNP Q8YLC3
B	-10	MET	-	expression tag	UNP Q8YLC3
B	-9	THR	-	expression tag	UNP Q8YLC3
B	-8	GLY	-	expression tag	UNP Q8YLC3
B	-7	GLY	-	expression tag	UNP Q8YLC3
B	-6	GLN	-	expression tag	UNP Q8YLC3
B	-5	GLN	-	expression tag	UNP Q8YLC3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	expression tag	UNP Q8YLC3
B	-3	GLY	-	expression tag	UNP Q8YLC3
B	-2	ARG	-	expression tag	UNP Q8YLC3
B	-1	GLY	-	expression tag	UNP Q8YLC3
B	0	SER	-	expression tag	UNP Q8YLC3
C	-33	MET	-	initiating methionine	UNP Q8YLC3
C	-32	GLY	-	expression tag	UNP Q8YLC3
C	-31	SER	-	expression tag	UNP Q8YLC3
C	-30	SER	-	expression tag	UNP Q8YLC3
C	-29	HIS	-	expression tag	UNP Q8YLC3
C	-28	HIS	-	expression tag	UNP Q8YLC3
C	-27	HIS	-	expression tag	UNP Q8YLC3
C	-26	HIS	-	expression tag	UNP Q8YLC3
C	-25	HIS	-	expression tag	UNP Q8YLC3
C	-24	HIS	-	expression tag	UNP Q8YLC3
C	-23	SER	-	expression tag	UNP Q8YLC3
C	-22	SER	-	expression tag	UNP Q8YLC3
C	-21	GLY	-	expression tag	UNP Q8YLC3
C	-20	LEU	-	expression tag	UNP Q8YLC3
C	-19	VAL	-	expression tag	UNP Q8YLC3
C	-18	PRO	-	expression tag	UNP Q8YLC3
C	-17	ARG	-	expression tag	UNP Q8YLC3
C	-16	GLY	-	expression tag	UNP Q8YLC3
C	-15	SER	-	expression tag	UNP Q8YLC3
C	-14	HIS	-	expression tag	UNP Q8YLC3
C	-13	MET	-	expression tag	UNP Q8YLC3
C	-12	ALA	-	expression tag	UNP Q8YLC3
C	-11	SER	-	expression tag	UNP Q8YLC3
C	-10	MET	-	expression tag	UNP Q8YLC3
C	-9	THR	-	expression tag	UNP Q8YLC3
C	-8	GLY	-	expression tag	UNP Q8YLC3
C	-7	GLY	-	expression tag	UNP Q8YLC3
C	-6	GLN	-	expression tag	UNP Q8YLC3
C	-5	GLN	-	expression tag	UNP Q8YLC3
C	-4	MET	-	expression tag	UNP Q8YLC3
C	-3	GLY	-	expression tag	UNP Q8YLC3
C	-2	ARG	-	expression tag	UNP Q8YLC3
C	-1	GLY	-	expression tag	UNP Q8YLC3
C	0	SER	-	expression tag	UNP Q8YLC3
D	-33	MET	-	initiating methionine	UNP Q8YLC3
D	-32	GLY	-	expression tag	UNP Q8YLC3
D	-31	SER	-	expression tag	UNP Q8YLC3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	SER	-	expression tag	UNP Q8YLC3
D	-29	HIS	-	expression tag	UNP Q8YLC3
D	-28	HIS	-	expression tag	UNP Q8YLC3
D	-27	HIS	-	expression tag	UNP Q8YLC3
D	-26	HIS	-	expression tag	UNP Q8YLC3
D	-25	HIS	-	expression tag	UNP Q8YLC3
D	-24	HIS	-	expression tag	UNP Q8YLC3
D	-23	SER	-	expression tag	UNP Q8YLC3
D	-22	SER	-	expression tag	UNP Q8YLC3
D	-21	GLY	-	expression tag	UNP Q8YLC3
D	-20	LEU	-	expression tag	UNP Q8YLC3
D	-19	VAL	-	expression tag	UNP Q8YLC3
D	-18	PRO	-	expression tag	UNP Q8YLC3
D	-17	ARG	-	expression tag	UNP Q8YLC3
D	-16	GLY	-	expression tag	UNP Q8YLC3
D	-15	SER	-	expression tag	UNP Q8YLC3
D	-14	HIS	-	expression tag	UNP Q8YLC3
D	-13	MET	-	expression tag	UNP Q8YLC3
D	-12	ALA	-	expression tag	UNP Q8YLC3
D	-11	SER	-	expression tag	UNP Q8YLC3
D	-10	MET	-	expression tag	UNP Q8YLC3
D	-9	THR	-	expression tag	UNP Q8YLC3
D	-8	GLY	-	expression tag	UNP Q8YLC3
D	-7	GLY	-	expression tag	UNP Q8YLC3
D	-6	GLN	-	expression tag	UNP Q8YLC3
D	-5	GLN	-	expression tag	UNP Q8YLC3
D	-4	MET	-	expression tag	UNP Q8YLC3
D	-3	GLY	-	expression tag	UNP Q8YLC3
D	-2	ARG	-	expression tag	UNP Q8YLC3
D	-1	GLY	-	expression tag	UNP Q8YLC3
D	0	SER	-	expression tag	UNP Q8YLC3

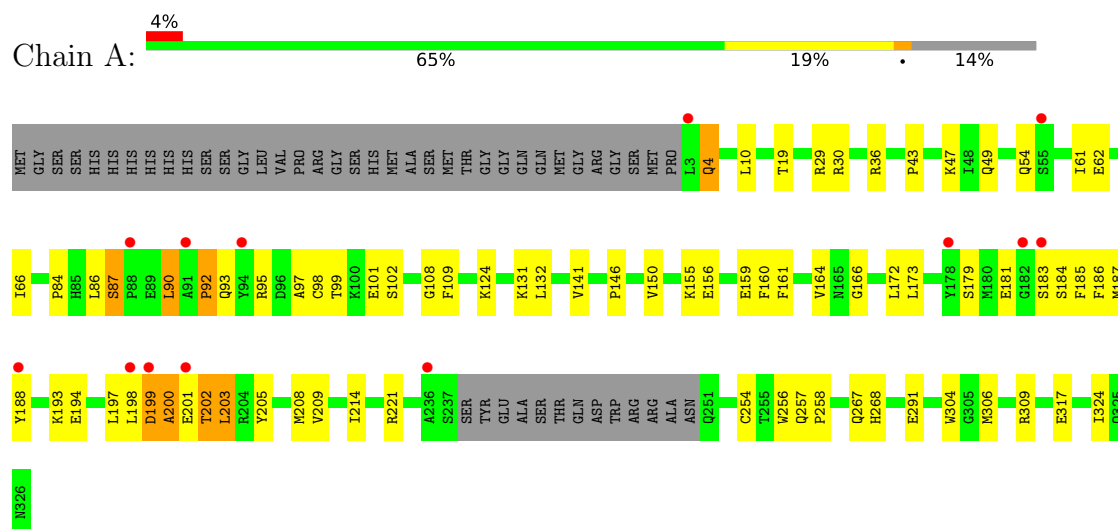
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	9	Total O 9 9	0	0
2	C	16	Total O 16 16	0	0
2	D	8	Total O 8 8	0	0

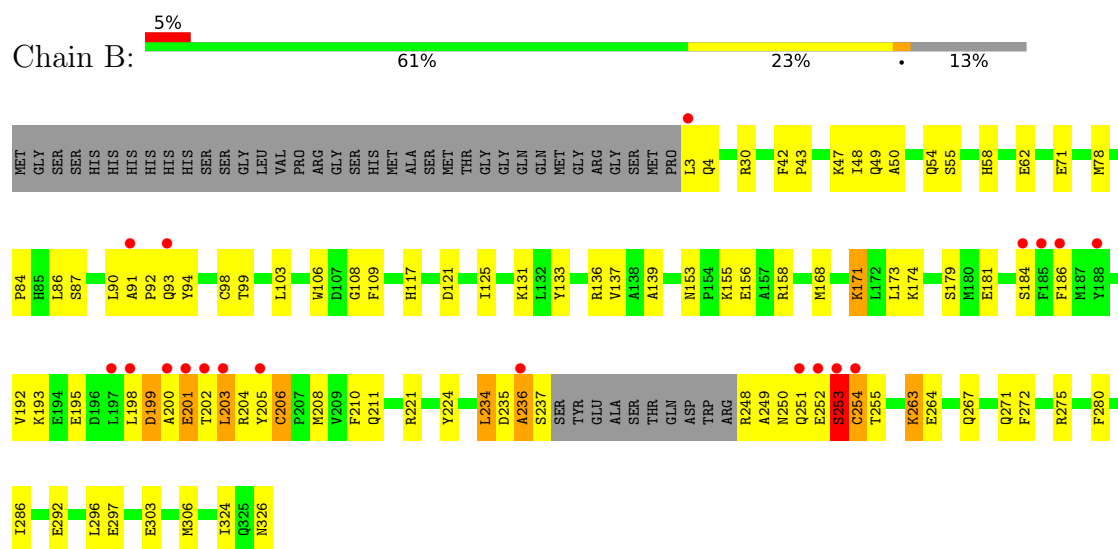
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

• Molecule 1: AMdnB protein

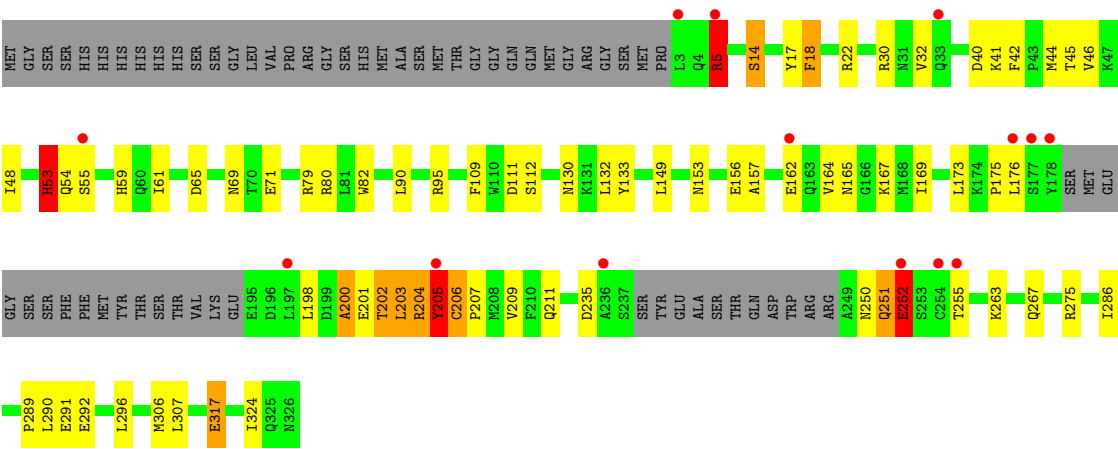


• Molecule 1: AMdnB protein

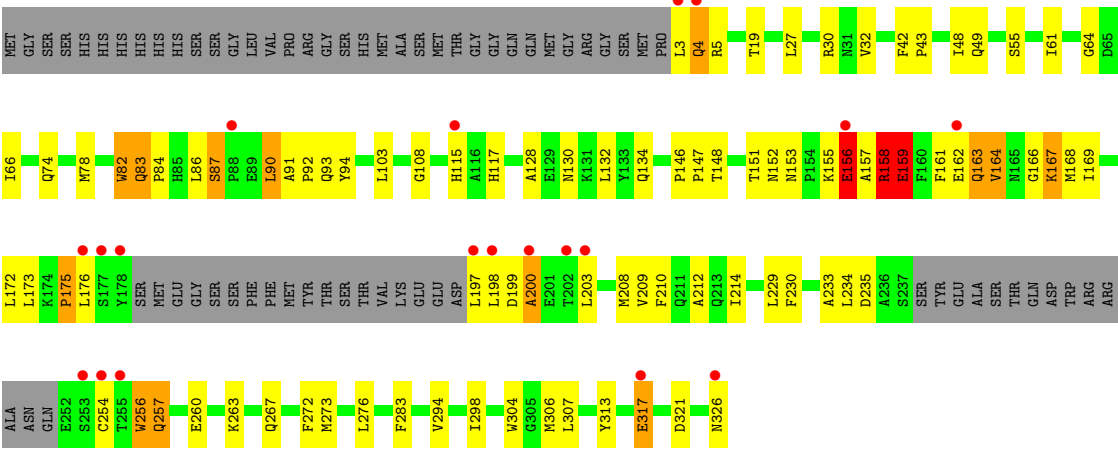


• Molecule 1: AMdnB protein





• Molecule 1: AMdnB protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.48Å 132.46Å 83.01Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	41.50 – 2.49 41.50 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.7 (41.50-2.49) 97.6 (41.50-2.49)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.48Å)	Xtriage
Refinement program	PHENIX v1.19.2	Depositor
R, R_{free}	0.199 , 0.258 0.201 , 0.260	Depositor DCC
R_{free} test set	2342 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9938	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.50	0/2596	0.91	13/3529 (0.4%)
1	B	0.57	1/2620 (0.0%)	0.99	26/3561 (0.7%)
1	C	0.51	1/2479 (0.0%)	0.99	20/3372 (0.6%)
1	D	0.57	1/2440 (0.0%)	1.02	24/3319 (0.7%)
All	All	0.54	3/10135 (0.0%)	0.98	83/13781 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	4
1	D	0	4
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	GLN	CB-CG	-5.77	1.35	1.52
1	B	155	LYS	CD-CE	-5.33	1.36	1.52
1	C	5	ARG	CB-CG	-5.15	1.37	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	317	GLU	CA-CB-CG	-14.66	84.79	114.10
1	C	5	ARG	CD-NE-CZ	12.83	142.36	124.40
1	C	203	LEU	CA-C-O	-10.74	105.15	120.51
1	D	156	GLU	CB-CA-C	-10.21	92.01	110.70
1	A	203	LEU	CA-C-N	-9.96	106.10	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	LEU	C-N-CA	-9.96	106.10	122.54
1	A	291	GLU	CA-CB-CG	-9.66	94.78	114.10
1	B	263	LYS	N-CA-CB	9.45	124.93	110.28
1	D	83	GLN	CB-CG-CD	-9.16	97.03	112.60
1	B	263	LYS	CA-CB-CG	9.07	132.24	114.10
1	B	202	THR	OG1-CB-CG2	-8.94	91.42	109.30
1	A	256	TRP	CA-C-N	-8.77	107.16	123.65
1	A	256	TRP	C-N-CA	-8.77	107.16	123.65
1	D	159	GLU	CA-CB-CG	8.73	131.57	114.10
1	B	263	LYS	CB-CG-CD	8.44	130.72	111.30
1	C	5	ARG	CG-CD-NE	-8.14	94.08	112.00
1	B	263	LYS	CB-CA-C	-8.02	95.26	110.67
1	C	5	ARG	NE-CZ-NH2	-7.87	112.12	119.20
1	D	156	GLU	CA-CB-CG	7.86	129.83	114.10
1	C	252	GLU	CB-CG-CD	-7.86	99.24	112.60
1	D	159	GLU	CB-CA-C	7.64	122.22	109.38
1	D	167	LYS	CG-CD-CE	7.61	128.81	111.30
1	C	252	GLU	CA-CB-CG	7.59	129.29	114.10
1	B	202	THR	N-CA-CB	7.55	123.25	110.49
1	B	92	PRO	CA-C-N	-7.43	107.08	121.58
1	B	92	PRO	C-N-CA	-7.43	107.08	121.58
1	B	202	THR	CB-CA-C	-7.04	96.40	110.42
1	D	163	GLN	CA-CB-CG	-7.03	100.04	114.10
1	B	201	GLU	CA-C-N	7.00	134.90	121.54
1	B	201	GLU	C-N-CA	7.00	134.90	121.54
1	D	260	GLU	N-CA-CB	6.72	121.12	110.57
1	B	235	ASP	N-CA-CB	6.53	119.82	109.51
1	B	234	LEU	CA-C-N	-6.42	111.51	121.02
1	B	234	LEU	C-N-CA	-6.42	111.51	121.02
1	D	260	GLU	CB-CA-C	-6.33	98.78	109.72
1	B	253	SER	CB-CA-C	-6.30	97.89	110.42
1	B	235	ASP	CB-CA-C	-6.24	101.17	110.16
1	A	159	GLU	CA-CB-CG	6.16	126.41	114.10
1	C	205	TYR	CB-CG-CD2	-6.13	111.61	120.80
1	C	203	LEU	CA-C-N	6.12	128.96	120.63
1	C	203	LEU	C-N-CA	6.12	128.96	120.63
1	A	93	GLN	N-CA-CB	-6.03	100.07	110.32
1	B	171	LYS	CB-CG-CD	-6.03	97.43	111.30
1	B	171	LYS	CG-CD-CE	-5.90	97.73	111.30
1	D	82	TRP	CA-C-N	-5.89	112.94	122.48
1	D	82	TRP	C-N-CA	-5.89	112.94	122.48
1	D	257	GLN	CA-CB-CG	5.83	125.77	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	LYS	N-CA-CB	-5.80	100.63	111.13
1	A	92	PRO	CA-C-N	5.76	129.82	120.60
1	A	92	PRO	C-N-CA	5.76	129.82	120.60
1	B	292	GLU	CA-CB-CG	5.74	125.58	114.10
1	D	164	VAL	N-CA-CB	-5.73	101.77	111.23
1	B	253	SER	N-CA-C	5.73	123.00	110.80
1	C	5	ARG	CB-CG-CD	5.72	124.45	111.30
1	C	205	TYR	CA-CB-CG	-5.71	103.62	113.90
1	D	83	GLN	N-CA-C	5.68	116.66	110.13
1	B	203	LEU	CA-CB-CG	5.68	136.17	116.30
1	B	93	GLN	N-CA-CB	5.62	119.85	110.41
1	B	71	GLU	CA-CB-CG	-5.59	102.92	114.10
1	D	167	LYS	CA-CB-CG	-5.51	103.09	114.10
1	C	53	HIS	CB-CA-C	-5.50	102.70	111.17
1	A	93	GLN	CA-CB-CG	5.45	125.01	114.10
1	C	204	ARG	CB-CA-C	-5.43	102.53	110.95
1	A	90	LEU	CB-CG-CD1	5.36	126.78	110.70
1	C	252	GLU	N-CA-CB	-5.36	101.44	110.49
1	A	155	LYS	CG-CD-CE	5.32	123.54	111.30
1	D	159	GLU	N-CA-C	-5.30	106.76	114.12
1	B	92	PRO	N-CA-C	5.28	121.02	113.47
1	D	164	VAL	CB-CA-C	5.26	119.92	111.29
1	C	200	ALA	CA-C-N	-5.24	114.42	122.60
1	C	200	ALA	C-N-CA	-5.24	114.42	122.60
1	D	256	TRP	CA-C-N	5.23	140.10	121.59
1	D	256	TRP	C-N-CA	5.23	140.10	121.59
1	D	317	GLU	CA-CB-CG	5.15	124.41	114.10
1	C	205	TYR	CE1-CZ-OH	5.13	135.29	119.90
1	C	202	THR	N-CA-C	-5.09	105.85	111.71
1	A	95	ARG	CB-CG-CD	-5.07	99.64	111.30
1	D	257	GLN	N-CA-CB	-5.07	102.09	109.90
1	B	98	CYS	CA-CB-SG	-5.07	102.75	114.40
1	D	115	HIS	N-CA-CB	5.06	118.78	110.39
1	C	14	SER	CB-CA-C	-5.05	102.41	110.79
1	D	167	LYS	CD-CE-NZ	-5.03	95.81	111.90
1	D	55	SER	CB-CA-C	-5.00	99.25	110.21

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	A	201	GLU	Peptide
1	B	199	ASP	Peptide
1	C	205	TYR	Sidechain
1	C	255	THR	Peptide
1	C	5	ARG	Sidechain
1	C	53	HIS	Sidechain
1	D	156	GLU	Sidechain
1	D	157	ALA	Peptide
1	D	158	ARG	Peptide
1	D	159	GLU	Peptide

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	2533	0	2467	55	1
1	B	2557	0	2492	86	1
1	C	2420	0	2362	73	0
1	D	2381	0	2332	74	0
2	A	14	0	0	0	0
2	B	9	0	0	1	0
2	C	16	0	0	0	0
2	D	8	0	0	0	0
All	All	9938	0	9653	256	1

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 13.

All (256) 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:B:263:LYS:HG3	1:B:267:GLN:NE2	1.54	1.20
1:B:78:MET:HE3	1:B:125:ILE:HD13	1.22	1.17
1:B:263:LYS:HG3	1:B:267:GLN:HE21	0.96	1.06
1:B:303:GLU:HG3	1:B:306:MET:HE1	1.35	1.04
1:B:94:TYR:HB3	1:C:205:TYR:OH	1.56	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:MET:CE	1:B:125:ILE:HD13	1.89	1.02
1:A:49:GLN:HG3	1:D:156:GLU:OE2	1.60	1.02
1:B:78:MET:HE3	1:B:125:ILE:CD1	1.90	1.02
1:B:252:GLU:CD	1:B:306:MET:HE2	1.86	1.00
1:B:131:LYS:NZ	1:B:297:GLU:OE2	2.00	0.94
1:C:30:ARG:NH1	1:C:317:GLU:OE1	2.02	0.91
1:C:204:ARG:HB2	1:C:205:TYR:CD1	2.05	0.91
1:D:83:GLN:OE1	1:D:103:LEU:HD21	1.74	0.87
1:D:162:GLU:O	1:D:163:GLN:HG2	1.74	0.87
1:B:236:ALA:O	1:B:255:THR:OG1	1.95	0.85
1:B:94:TYR:CB	1:C:205:TYR:OH	2.23	0.85
1:A:257:GLN:HB3	1:A:258:PRO:HD2	1.59	0.84
1:B:94:TYR:CG	1:C:205:TYR:OH	2.30	0.84
1:D:3:LEU:O	1:D:4:GLN:HG2	1.79	0.81
1:A:197:LEU:O	1:A:199:ASP:N	2.18	0.76
1:C:252:GLU:OE2	1:C:306:MET:HB3	1.86	0.74
1:C:14:SER:OG	1:C:40:ASP:OD2	2.05	0.74
1:B:263:LYS:CG	1:B:267:GLN:NE2	2.44	0.74
1:C:201:GLU:O	1:C:204:ARG:HG3	1.87	0.74
1:A:306:MET:SD	1:C:290:LEU:HD22	2.26	0.74
1:B:252:GLU:CD	1:B:306:MET:CE	2.61	0.74
1:B:303:GLU:CG	1:B:306:MET:HE1	2.16	0.73
1:D:83:GLN:HB3	1:D:84:PRO:HD2	1.69	0.73
1:B:200:ALA:HA	1:B:204:ARG:HB2	1.71	0.72
1:C:250:ASN:O	1:C:252:GLU:N	2.22	0.72
1:D:30:ARG:HH22	1:D:317:GLU:HG2	1.54	0.72
1:C:204:ARG:HE	1:C:205:TYR:HE1	1.37	0.71
1:C:5:ARG:NH1	1:C:71:GLU:HB2	2.05	0.70
1:D:273:MET:HE2	1:D:273:MET:HA	1.75	0.69
1:D:3:LEU:O	1:D:4:GLN:CG	2.41	0.68
1:D:19:THR:HG23	1:D:304:TRP:CZ2	2.28	0.68
1:B:58:HIS:CE1	1:D:92:PRO:HG2	2.29	0.67
1:B:198:LEU:O	1:B:200:ALA:N	2.29	0.65
1:B:306:MET:H	1:B:306:MET:HE3	1.61	0.65
1:B:195:GLU:O	1:B:199:ASP:HB2	1.96	0.65
1:D:164:VAL:O	1:D:167:LYS:HB2	1.96	0.64
1:B:87:SER:HB3	1:B:90:LEU:HD13	1.80	0.64
1:A:146:PRO:HB3	1:A:214:ILE:HD11	1.78	0.63
1:B:252:GLU:HG3	1:B:306:MET:HB3	1.79	0.63
1:A:200:ALA:O	1:A:203:LEU:N	2.31	0.63
1:B:158:ARG:NH2	1:B:201:GLU:OE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ALA:O	1:B:94:TYR:HB2	1.98	0.63
1:C:175:PRO:HG2	1:C:176:LEU:HD12	1.81	0.62
1:C:251:GLN:O	1:C:252:GLU:HB2	1.95	0.62
1:D:86:LEU:O	1:D:87:SER:HB3	1.98	0.62
1:A:161:PHE:CZ	1:A:166:GLY:HA2	2.35	0.61
1:D:197:LEU:HD13	1:D:197:LEU:O	2.00	0.61
1:B:198:LEU:C	1:B:200:ALA:H	2.09	0.61
1:B:205:TYR:HE1	1:C:44:MET:HG3	1.66	0.60
1:D:156:GLU:O	1:D:159:GLU:N	2.29	0.60
1:A:132:LEU:HD21	1:A:150:VAL:HG21	1.82	0.60
1:D:168:MET:HE2	1:D:210:PHE:HB3	1.84	0.60
1:B:158:ARG:HH22	1:B:201:GLU:HB3	1.66	0.60
1:D:173:LEU:HG	1:D:209:VAL:HG21	1.84	0.59
1:D:198:LEU:HD12	1:D:199:ASP:H	1.68	0.58
1:C:5:ARG:NH1	1:C:71:GLU:CB	2.66	0.58
1:B:94:TYR:CD2	1:C:205:TYR:OH	2.50	0.58
1:B:200:ALA:CA	1:B:204:ARG:HB2	2.33	0.58
1:D:306:MET:HG2	1:D:307:LEU:HD23	1.86	0.58
1:A:267:GLN:O	1:A:267:GLN:NE2	2.37	0.57
1:C:250:ASN:C	1:C:252:GLU:N	2.62	0.57
1:B:248:ARG:HH22	1:B:297:GLU:HG2	1.70	0.57
1:C:250:ASN:O	1:C:251:GLN:C	2.48	0.57
1:A:203:LEU:O	1:A:203:LEU:HG	2.05	0.56
1:A:257:GLN:HB3	1:A:258:PRO:CD	2.34	0.56
1:A:202:THR:HA	1:A:205:TYR:CZ	2.40	0.56
1:D:152:ASN:HB3	1:D:208:MET:CE	2.35	0.56
1:A:156:GLU:HG3	1:D:49:GLN:HG2	1.87	0.56
1:A:141:VAL:O	1:A:268:HIS:ND1	2.37	0.56
1:C:69:ASN:OD1	1:C:71:GLU:HG2	2.06	0.56
1:D:155:LYS:O	1:D:158:ARG:HB3	2.06	0.56
1:D:161:PHE:CZ	1:D:166:GLY:HA2	2.41	0.56
1:A:202:THR:HA	1:A:205:TYR:CE2	2.41	0.55
1:C:263:LYS:O	1:C:267:GLN:HG3	2.06	0.55
1:A:30:ARG:HD3	1:A:324:ILE:HD13	1.88	0.55
1:A:202:THR:O	1:A:205:TYR:N	2.40	0.55
1:D:27:LEU:O	1:D:32:VAL:HG12	2.05	0.55
1:B:237:SER:HA	1:B:254:CYS:SG	2.47	0.54
1:A:221:ARG:HD3	1:A:306:MET:HE1	1.89	0.54
1:B:49:GLN:HE21	1:C:156:GLU:CD	2.16	0.54
1:B:249:ALA:HB1	1:B:253:SER:OG	2.08	0.54
1:C:80:ARG:HD2	1:C:82:TRP:CH2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ALA:HB1	1:B:204:ARG:NE	2.23	0.54
1:C:306:MET:HG2	1:C:307:LEU:N	2.21	0.54
1:B:286:ILE:HG12	1:B:296:LEU:HD11	1.89	0.54
1:D:162:GLU:C	1:D:163:GLN:HG2	2.29	0.53
1:A:150:VAL:HG22	1:A:209:VAL:HG22	1.91	0.53
1:C:90:LEU:O	1:C:95:ARG:NE	2.34	0.53
1:D:30:ARG:HH21	1:D:321:ASP:CG	2.17	0.53
1:B:201:GLU:C	1:B:203:LEU:H	2.17	0.53
1:C:250:ASN:C	1:C:252:GLU:H	2.18	0.52
1:D:91:ALA:HB3	1:D:94:TYR:HD1	1.74	0.52
1:A:183:SER:OG	1:A:184:SER:N	2.39	0.52
1:B:48:ILE:HD12	1:B:109:PHE:CE1	2.43	0.52
1:B:204:ARG:HD2	1:B:206:CYS:O	2.09	0.52
1:A:97:ALA:HB1	1:D:203:LEU:HD21	1.90	0.52
1:A:47:LYS:HD2	1:D:153:ASN:HB2	1.92	0.52
1:A:309:ARG:HH21	1:C:291:GLU:CD	2.18	0.52
1:A:29:ARG:NH2	1:A:317:GLU:OE2	2.42	0.52
1:B:108:GLY:HA3	1:C:132:LEU:HD12	1.91	0.52
1:D:82:TRP:HH2	1:D:197:LEU:CD2	2.23	0.52
1:B:263:LYS:HE3	1:B:264:GLU:OE2	2.10	0.52
1:C:162:GLU:OE2	1:C:162:GLU:HA	2.10	0.52
1:C:252:GLU:OE2	1:C:306:MET:HE3	2.10	0.52
1:A:49:GLN:CG	1:D:156:GLU:OE2	2.48	0.51
1:A:188:TYR:HA	1:C:165:ASN:HB3	1.91	0.51
1:B:205:TYR:HE1	1:C:44:MET:CG	2.22	0.51
1:C:198:LEU:O	1:C:202:THR:OG1	2.28	0.51
1:A:108:GLY:HA3	1:D:132:LEU:HD12	1.92	0.51
1:D:168:MET:HG2	1:D:169:ILE:N	2.26	0.51
1:A:4:GLN:O	1:A:4:GLN:HG2	2.11	0.51
1:A:84:PRO:HD2	1:A:99:THR:HG23	1.92	0.51
1:B:205:TYR:O	1:B:206:CYS:HB2	2.10	0.51
1:D:43:PRO:HD3	1:D:84:PRO:HB3	1.94	0.50
1:B:3:LEU:N	1:B:4:GLN:OE1	2.45	0.50
1:B:103:LEU:HD23	1:B:106:TRP:HD1	1.75	0.50
1:D:91:ALA:HB1	1:D:93:GLN:NE2	2.26	0.50
1:D:151:THR:O	1:D:208:MET:HA	2.11	0.50
1:A:306:MET:SD	1:C:290:LEU:CD2	2.99	0.50
1:A:131:LYS:HE3	1:A:173:LEU:O	2.12	0.50
1:B:94:TYR:HE1	1:C:198:LEU:HG	1.76	0.50
1:A:172:LEU:HD11	1:C:164:VAL:HG12	1.93	0.50
1:B:184:SER:HA	1:B:186:PHE:HD1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LEU:O	1:D:197:LEU:CD1	2.60	0.50
1:D:156:GLU:C	1:D:159:GLU:H	2.18	0.50
1:B:121:ASP:OD1	2:B:401:HOH:O	2.20	0.49
1:D:172:LEU:HD11	1:D:203:LEU:HD13	1.93	0.49
1:B:78:MET:SD	1:B:78:MET:C	2.96	0.49
1:A:61:ILE:HG13	1:A:109:PHE:CZ	2.47	0.49
1:B:4:GLN:OE1	1:B:4:GLN:N	2.28	0.49
1:B:252:GLU:OE1	1:B:306:MET:HE2	2.13	0.49
1:B:86:LEU:HB3	1:B:90:LEU:HD22	1.94	0.48
1:B:192:VAL:HG12	1:B:193:LYS:H	1.78	0.48
1:D:234:LEU:HD13	1:D:256:TRP:CH2	2.48	0.48
1:C:80:ARG:HD2	1:C:82:TRP:CZ3	2.48	0.48
1:B:234:LEU:O	1:B:234:LEU:HG	2.13	0.48
1:B:47:LYS:NZ	1:C:153:ASN:HB2	2.29	0.48
1:D:214:ILE:HG21	1:D:294:VAL:HG21	1.96	0.48
1:B:253:SER:O	1:B:254:CYS:HB2	2.13	0.48
1:D:273:MET:HE3	1:D:283:PHE:HZ	1.79	0.48
1:B:271:GLN:O	1:B:275:ARG:HG3	2.14	0.48
1:D:158:ARG:HA	1:D:158:ARG:NE	2.28	0.48
1:B:49:GLN:NE2	1:C:156:GLU:OE1	2.43	0.47
1:D:273:MET:HE1	1:D:298:ILE:HD12	1.96	0.47
1:C:18:PHE:O	1:C:22:ARG:HG3	2.14	0.47
1:B:252:GLU:OE2	1:B:306:MET:CE	2.62	0.47
1:C:204:ARG:HB2	1:C:205:TYR:CG	2.48	0.47
1:C:109:PHE:O	1:C:112:SER:HB3	2.14	0.47
1:D:146:PRO:O	1:D:148:THR:HG23	2.15	0.47
1:B:171:LYS:HE2	1:B:248:ARG:HE	1.80	0.47
1:C:169:ILE:HG13	1:C:211:GLN:O	2.15	0.47
1:A:193:LYS:O	1:A:197:LEU:HG	2.15	0.46
1:B:200:ALA:O	1:B:204:ARG:N	2.48	0.46
1:D:117:HIS:CG	1:D:326:ASN:HA	2.50	0.46
1:C:306:MET:HG2	1:C:307:LEU:HD23	1.98	0.46
1:A:87:SER:HB3	1:A:90:LEU:HD13	1.97	0.46
1:B:47:LYS:HB2	1:B:62:GLU:HB3	1.96	0.46
1:B:200:ALA:HB1	1:B:204:ARG:CZ	2.45	0.46
1:D:130:ASN:O	1:D:134:GLN:HG3	2.16	0.46
1:B:84:PRO:HG2	1:B:99:THR:HG23	1.98	0.46
1:B:30:ARG:HD3	1:B:324:ILE:HD13	1.98	0.46
1:C:48:ILE:HD13	1:C:61:ILE:HG22	1.96	0.46
1:D:273:MET:HE1	1:D:298:ILE:CD1	2.45	0.46
1:B:49:GLN:NE2	1:C:156:GLU:CD	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:HIS:CG	1:B:326:ASN:HA	2.50	0.46
1:C:275:ARG:HG2	1:C:275:ARG:HH11	1.81	0.46
1:B:208:MET:HE2	1:B:210:PHE:CZ	2.51	0.46
1:C:250:ASN:ND2	1:C:251:GLN:H	2.14	0.46
1:C:59:HIS:CD2	1:C:112:SER:HB2	2.51	0.45
1:D:175:PRO:C	1:D:176:LEU:HG	2.41	0.45
1:B:179:SER:HB2	1:B:181:GLU:H	1.81	0.45
1:D:152:ASN:HB3	1:D:208:MET:HE2	1.97	0.45
1:B:3:LEU:HD12	1:B:3:LEU:O	2.16	0.45
1:B:139:ALA:HB1	1:C:55:SER:N	2.31	0.45
1:B:50:ALA:HA	1:B:58:HIS:O	2.16	0.45
1:B:136:ARG:NH1	1:C:111:ASP:OD1	2.49	0.45
1:D:5:ARG:HB3	1:D:74:GLN:HB3	1.98	0.45
1:C:173:LEU:HD21	1:C:209:VAL:HG21	1.98	0.45
1:B:224:TYR:O	1:B:280:PHE:HA	2.16	0.45
1:C:149:LEU:HD23	1:C:157:ALA:HA	1.98	0.45
1:D:64:GLY:O	1:D:66:ILE:HD12	2.17	0.45
1:A:61:ILE:HD11	1:A:109:PHE:CE2	2.53	0.44
1:A:160:PHE:O	1:A:164:VAL:HG22	2.16	0.44
1:B:168:MET:HE3	1:B:210:PHE:CD1	2.52	0.44
1:D:78:MET:HE3	1:D:78:MET:O	2.17	0.44
1:A:62:GLU:HA	1:A:66:ILE:O	2.18	0.44
1:D:233:ALA:O	1:D:257:GLN:HB2	2.17	0.44
1:A:84:PRO:HG3	1:A:102:SER:HB2	1.98	0.44
1:A:202:THR:HG22	1:A:205:TYR:CE2	2.52	0.44
1:D:90:LEU:HD12	1:D:91:ALA:H	1.82	0.44
1:A:172:LEU:HD23	1:A:208:MET:HE1	1.98	0.44
1:B:42:PHE:CD1	1:B:43:PRO:HA	2.53	0.44
1:D:272:PHE:HD2	1:D:273:MET:HE3	1.83	0.44
1:B:153:ASN:HB3	1:B:156:GLU:HG3	2.00	0.43
1:D:199:ASP:O	1:D:200:ALA:HB2	2.18	0.43
1:B:252:GLU:CG	1:B:306:MET:HE2	2.46	0.43
1:D:158:ARG:O	1:D:161:PHE:HB3	2.18	0.43
1:C:5:ARG:NE	1:C:71:GLU:O	2.52	0.43
1:B:136:ARG:HD3	1:C:111:ASP:OD2	2.18	0.43
1:A:172:LEU:CD2	1:A:208:MET:HE1	2.49	0.43
1:C:200:ALA:O	1:C:203:LEU:HD12	2.17	0.43
1:B:54:GLN:HB3	1:B:55:SER:H	1.61	0.43
1:C:130:ASN:O	1:C:133:TYR:HB3	2.18	0.43
1:A:132:LEU:HD12	1:D:108:GLY:HA3	2.01	0.43
1:A:179:SER:HB2	1:C:292:GLU:OE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:MET:HE3	1:D:283:PHE:CZ	2.53	0.43
1:D:263:LYS:O	1:D:267:GLN:HG3	2.19	0.42
1:A:86:LEU:O	1:A:87:SER:CB	2.67	0.42
1:B:137:VAL:HG12	1:B:272:PHE:CD1	2.53	0.42
1:C:53:HIS:O	1:C:54:GLN:C	2.63	0.42
1:A:254:CYS:HB2	1:C:289:PRO:HG3	1.99	0.42
1:C:41:LYS:HB3	1:C:45:THR:HB	2.02	0.42
1:C:80:ARG:HB3	1:C:82:TRP:CZ3	2.55	0.42
1:A:43:PRO:HB3	1:D:208:MET:HE1	2.00	0.42
1:A:124:LYS:HA	1:A:124:LYS:HD3	1.77	0.42
1:B:221:ARG:NH2	1:B:250:ASN:HD21	2.17	0.42
1:C:286:ILE:HG12	1:C:296:LEU:HD11	2.01	0.42
1:D:172:LEU:HD21	1:D:203:LEU:HB2	1.99	0.42
1:D:42:PHE:CD1	1:D:43:PRO:HA	2.55	0.42
1:A:187:MET:HE3	1:C:167:LYS:NZ	2.35	0.42
1:C:41:LYS:HA	1:C:41:LYS:HD3	1.79	0.42
1:D:229:LEU:HD13	1:D:229:LEU:HA	1.83	0.42
1:A:19:THR:HB	1:A:304:TRP:CZ2	2.55	0.42
1:A:87:SER:CB	1:A:90:LEU:HD13	2.50	0.42
1:B:106:TRP:HA	1:B:106:TRP:CE3	2.55	0.42
1:C:206:CYS:N	1:C:207:PRO:HD3	2.34	0.42
1:A:161:PHE:CE2	1:A:166:GLY:HA2	2.55	0.41
1:C:206:CYS:N	1:C:207:PRO:CD	2.83	0.41
1:B:171:LYS:NZ	1:B:211:GLN:OE1	2.53	0.41
1:D:173:LEU:HD23	1:D:173:LEU:HA	1.82	0.41
1:C:252:GLU:CD	1:C:306:MET:HB3	2.45	0.41
1:D:128:ALA:HB1	1:D:276:LEU:HD13	2.02	0.41
1:A:221:ARG:HH21	1:A:306:MET:HE1	1.85	0.41
1:C:79:ARG:HG3	1:C:80:ARG:HG2	2.03	0.41
1:D:161:PHE:HD1	1:D:168:MET:SD	2.43	0.41
1:B:186:PHE:HB3	1:B:248:ARG:O	2.21	0.41
1:C:5:ARG:HH11	1:C:71:GLU:HB2	1.80	0.41
1:A:10:LEU:HB2	1:A:36:ARG:HA	2.03	0.41
1:B:158:ARG:HH22	1:B:201:GLU:CB	2.31	0.41
1:D:128:ALA:O	1:D:134:GLN:NE2	2.49	0.41
1:D:86:LEU:HD23	1:D:86:LEU:HA	1.69	0.41
1:D:91:ALA:HB1	1:D:93:GLN:CD	2.46	0.41
1:D:230:PHE:HB3	1:D:313:TYR:CD2	2.56	0.41
1:A:98:CYS:HA	1:A:101:GLU:HB2	2.02	0.40
1:C:95:ARG:HH21	1:C:95:ARG:HG2	1.86	0.40
1:C:32:VAL:HG21	1:C:324:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ILE:HD11	1:D:61:ILE:HD12	2.04	0.40
1:D:147:PRO:HD2	1:D:212:ALA:HB3	2.01	0.40
1:B:198:LEU:HA	1:B:198:LEU:HD12	1.72	0.40
1:C:42:PHE:HB2	1:C:46:VAL:HB	2.03	0.40
1:D:158:ARG:HA	1:D:158:ARG:HE	1.87	0.40

All (1) 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:194:GLU:OE2	1:B:133:TYR:OH[1_455]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/360 (85%)	283 (92%)	14 (5%)	10 (3%)	3	4
1	B	310/360 (86%)	284 (92%)	19 (6%)	7 (2%)	5	8
1	C	291/360 (81%)	274 (94%)	11 (4%)	6 (2%)	5	9
1	D	286/360 (79%)	266 (93%)	12 (4%)	8 (3%)	4	6
All	All	1194/1440 (83%)	1107 (93%)	56 (5%)	31 (3%)	4	7

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	198	LEU
1	A	199	ASP
1	B	173	LEU
1	B	236	ALA

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Mol	Chain	Res	Type
1	B	253	SER
1	B	254	CYS
1	C	252	GLU
1	D	4	GLN
1	D	90	LEU
1	D	175	PRO
1	D	200	ALA
1	A	92	PRO
1	B	251	GLN
1	C	17	TYR
1	C	18	PHE
1	C	251	GLN
1	D	87	SER
1	D	254	CYS
1	D	235	ASP
1	A	4	GLN
1	A	181	GLU
1	A	185	PHE
1	D	158	ARG
1	A	200	ALA
1	A	202	THR
1	B	206	CYS
1	C	235	ASP
1	A	54	GLN
1	C	206	CYS
1	B	174	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	276/315 (88%)	276 (100%)	0	100	100
1	B	278/315 (88%)	278 (100%)	0	100	100
1	C	262/315 (83%)	261 (100%)	1 (0%)	84	93
1	D	258/315 (82%)	258 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1074/1260 (85%)	1073 (100%)	1 (0%)	88 96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	65	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
1	A	257	GLN
1	B	49	GLN
1	B	85	HIS
1	B	163	GLN
1	B	267	GLN
1	B	326	ASN
1	C	49	GLN
1	C	115	HIS
1	C	218	GLN
1	C	250	ASN
1	C	257	GLN
1	C	268	HIS
1	D	58	HIS
1	D	59	HIS
1	D	163	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	311/360 (86%)	0.18	13 (4%) 40 36	30, 46, 82, 109	0
1	B	314/360 (87%)	0.13	19 (6%) 27 23	28, 42, 79, 94	0
1	C	297/360 (82%)	0.19	14 (4%) 36 32	29, 47, 87, 108	0
1	D	292/360 (81%)	0.26	19 (6%) 25 22	30, 50, 87, 108	0
All	All	1214/1440 (84%)	0.19	65 (5%) 31 27	28, 46, 85, 109	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	205	TYR	6.1
1	A	55	SER	4.6
1	C	178	TYR	4.4
1	A	3	LEU	4.2
1	D	156	GLU	4.2
1	D	326	ASN	3.9
1	B	253	SER	3.9
1	B	186	PHE	3.8
1	D	178	TYR	3.8
1	C	197	LEU	3.7
1	A	199	ASP	3.6
1	B	188	TYR	3.6
1	B	198	LEU	3.6
1	C	255	THR	3.5
1	B	184	SER	3.5
1	C	3	LEU	3.5
1	A	188	TYR	3.5
1	C	55	SER	3.3
1	C	176	LEU	3.2
1	D	198	LEU	3.1
1	B	252	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	5	ARG	3.0
1	B	197	LEU	2.9
1	C	177	SER	2.8
1	D	255	THR	2.8
1	B	203	LEU	2.7
1	B	200	ALA	2.7
1	B	201	GLU	2.7
1	B	202	THR	2.7
1	D	3	LEU	2.6
1	A	88	PRO	2.5
1	D	88	PRO	2.5
1	D	177	SER	2.5
1	D	197	LEU	2.5
1	D	115	HIS	2.5
1	A	94	TYR	2.4
1	B	93	GLN	2.4
1	B	185	PHE	2.4
1	A	178	TYR	2.4
1	D	200	ALA	2.4
1	C	252	GLU	2.4
1	B	3	LEU	2.4
1	B	91	ALA	2.4
1	A	198	LEU	2.3
1	B	254	CYS	2.3
1	C	162	GLU	2.3
1	D	254	CYS	2.3
1	B	251	GLN	2.3
1	D	176	LEU	2.3
1	A	201	GLU	2.3
1	D	253	SER	2.2
1	A	236	ALA	2.2
1	D	202	THR	2.2
1	A	91	ALA	2.1
1	D	317	GLU	2.1
1	C	33	GLN	2.1
1	B	236	ALA	2.1
1	A	182	GLY	2.1
1	D	203	LEU	2.1
1	D	162	GLU	2.1
1	D	4	GLN	2.1
1	A	183	SER	2.1
1	C	236	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	254	CYS	2.0
1	B	205	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.