



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2021 – 12:04 PM EDT

PDB ID : 7M4S
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

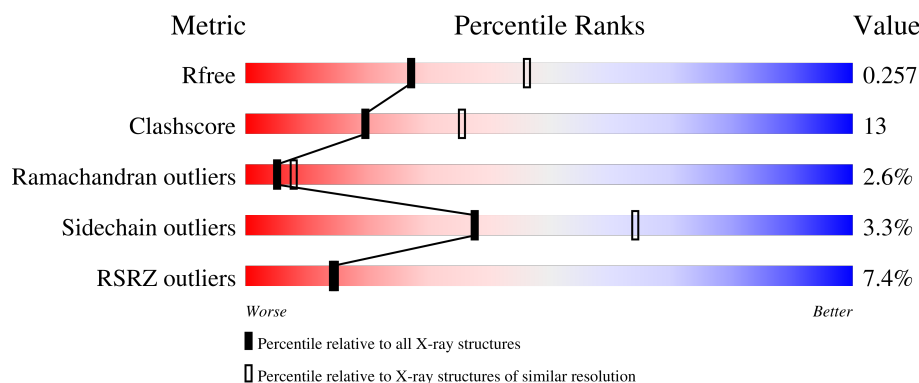
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



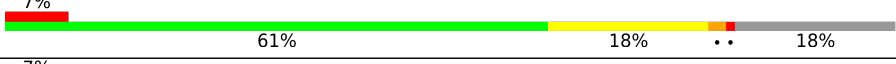

The reported resolution of this entry is 2.49 Å.

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	
1	B	360	
1	C	360	
1	D	360	

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

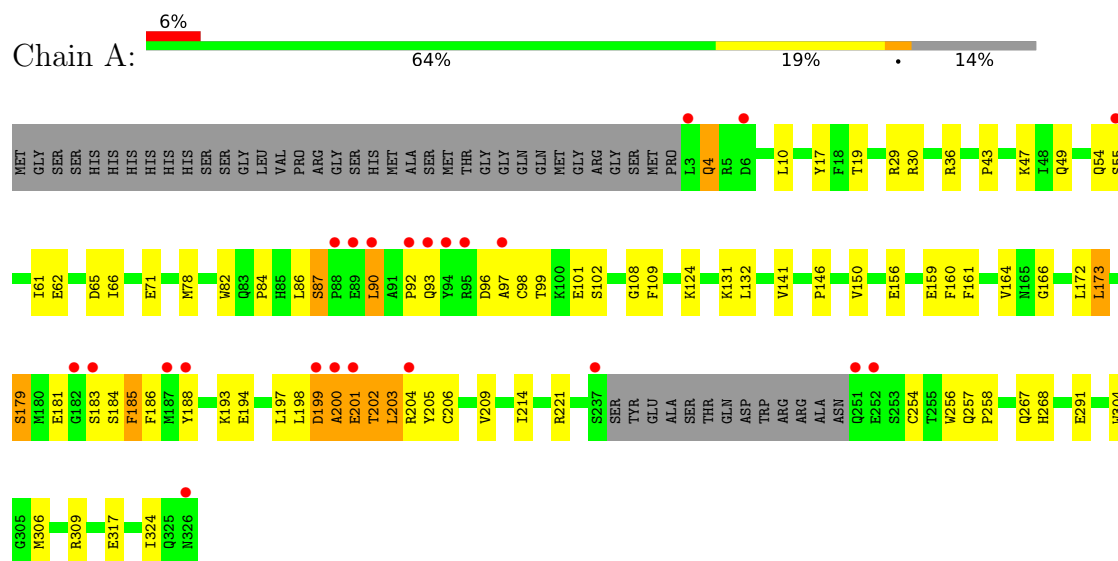
- Molecule 2 is water.

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

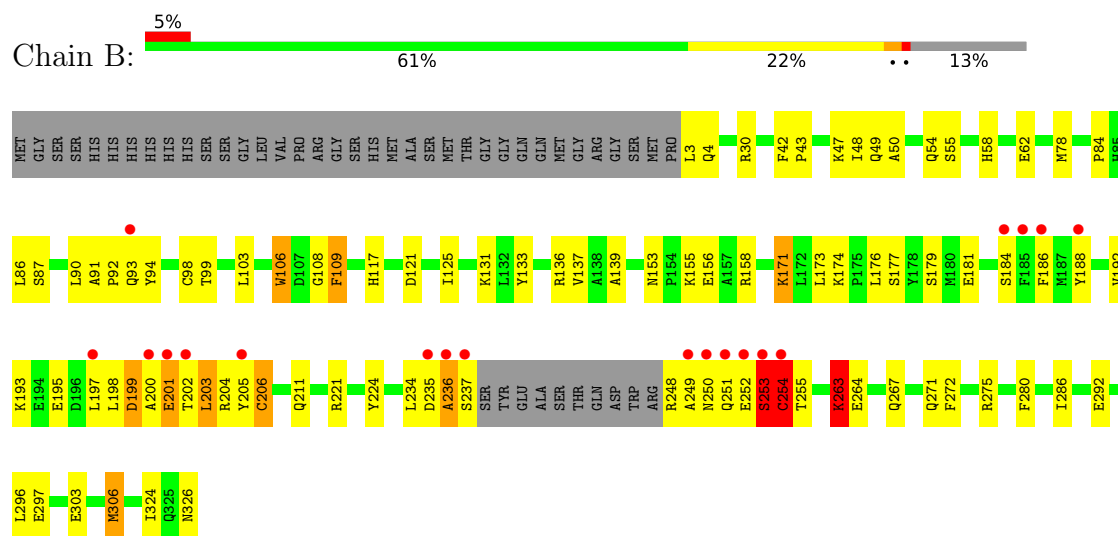
3 Residue-property plots [i](#)

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

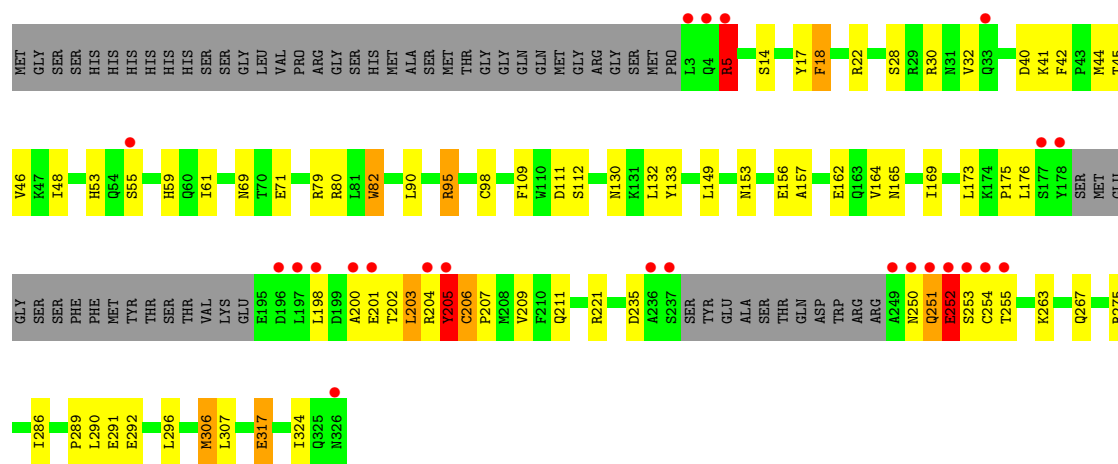


• Molecule 1: AMdnB protein

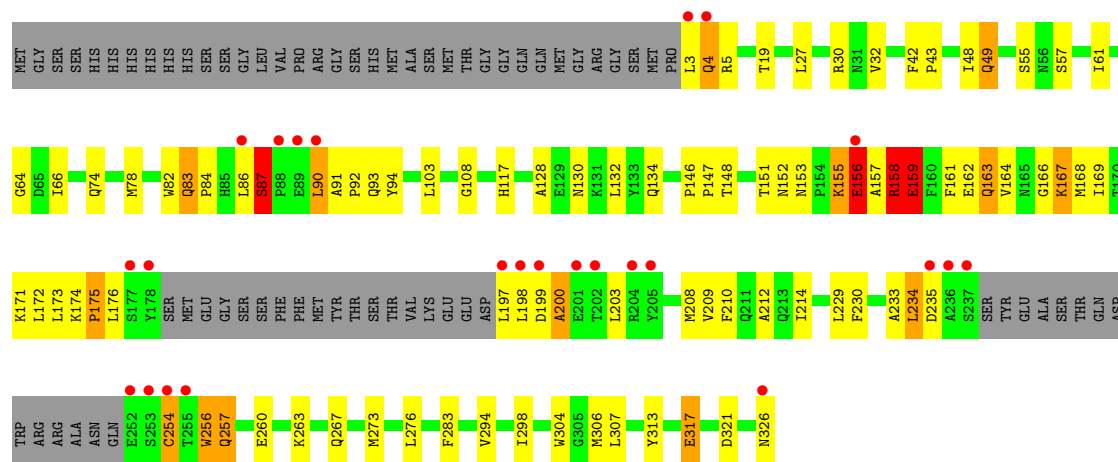


• Molecule 1: AMdnB protein





• 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) 97.7 (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 0.199 , 0.257	Depositor DCC
R_{free} test set	2339 reflections (5.17%)	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)	0.33 , 40.1	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	0.57	2/2596 (0.1%)	0.84	10/3529 (0.3%)
1	B	0.63	4/2620 (0.2%)	0.93	22/3561 (0.6%)
1	C	0.61	2/2479 (0.1%)	1.01	17/3372 (0.5%)
1	D	0.63	3/2440 (0.1%)	0.92	16/3319 (0.5%)
All	All	0.61	11/10135 (0.1%)	0.93	65/13781 (0.5%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	205	TYR	CD1-CE1	8.73	1.52	1.39
1	A	71	GLU	CB-CG	6.51	1.64	1.52
1	A	71	GLU	CG-CD	6.46	1.61	1.51
1	D	83	GLN	CB-CG	-6.45	1.35	1.52
1	B	155	LYS	CD-CE	-5.91	1.36	1.51
1	B	98	CYS	CB-SG	-5.85	1.72	1.81
1	C	5	ARG	CB-CG	-5.76	1.37	1.52
1	B	171	LYS	CB-CG	-5.58	1.37	1.52
1	D	159	GLU	CG-CD	5.39	1.60	1.51
1	D	159	GLU	CB-CG	5.33	1.62	1.52
1	B	155	LYS	CE-NZ	-5.25	1.35	1.49

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	ARG	NE-CZ-NH2	-16.36	112.12	120.30
1	C	205	TYR	CB-CG-CD2	-15.70	111.58	121.00
1	C	5	ARG	CD-NE-CZ	13.40	142.36	123.60
1	C	317	GLU	CA-CB-CG	-13.01	84.79	113.40
1	C	205	TYR	CB-CG-CD1	12.07	128.25	121.00
1	A	90	LEU	CB-CG-CD1	9.28	126.78	111.00
1	D	156	GLU	CB-CA-C	-9.20	92.01	110.40
1	B	203	LEU	CA-CB-CG	9.08	136.17	115.30
1	B	263	LYS	CA-CB-CG	8.56	132.24	113.40
1	A	291	GLU	CA-CB-CG	-8.46	94.78	113.40
1	C	5	ARG	CG-CD-NE	-8.44	94.08	111.80
1	D	159	GLU	CA-CB-CG	8.26	131.57	113.40
1	B	202	THR	OG1-CB-CG2	-8.08	91.42	110.00
1	B	263	LYS	N-CA-CB	7.96	124.93	110.60
1	B	263	LYS	CB-CA-C	-7.57	95.26	110.40
1	D	156	GLU	CA-CB-CG	7.47	129.83	113.40
1	A	90	LEU	CB-CG-CD2	-7.40	98.42	111.00
1	D	256	TRP	C-N-CA	7.36	140.10	121.70
1	B	263	LYS	CB-CG-CD	7.35	130.72	111.60
1	B	197	LEU	CB-CG-CD2	-7.24	98.70	111.00
1	C	252	GLU	CA-CB-CG	7.22	129.29	113.40
1	C	203	LEU	CA-C-O	-7.12	105.15	120.10
1	D	167	LYS	CD-CE-NZ	-6.91	95.81	111.70
1	C	205	TYR	CG-CD1-CE1	-6.88	115.80	121.30
1	B	202	THR	N-CA-CB	6.82	123.25	110.30
1	B	263	LYS	CD-CE-NZ	-6.49	96.78	111.70
1	B	253	SER	CB-CA-C	-6.43	97.89	110.10
1	B	98	CYS	CA-CB-SG	-6.25	102.75	114.00
1	A	203	LEU	C-N-CA	-6.24	106.10	121.70
1	A	204	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	155	LYS	CD-CE-NZ	-6.23	97.37	111.70
1	C	252	GLU	OE1-CD-OE2	6.12	130.64	123.30
1	D	163	GLN	CA-CB-CG	-6.07	100.04	113.40
1	A	159	GLU	CA-CB-CG	5.91	126.41	113.40
1	D	159	GLU	CB-CA-C	5.91	122.22	110.40
1	B	92	PRO	C-N-CA	-5.85	107.08	121.70
1	D	260	GLU	N-CA-CB	5.84	121.12	110.60
1	A	93	GLN	N-CA-CB	-5.83	100.11	110.60
1	A	256	TRP	C-N-CA	-5.82	107.16	121.70
1	D	260	GLU	CB-CA-C	-5.81	98.78	110.40
1	C	203	LEU	CA-C-N	5.77	129.89	117.20
1	D	158	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	55	SER	CB-CA-C	-5.71	99.25	110.10
1	A	173	LEU	CA-CB-CG	5.70	128.42	115.30
1	D	167	LYS	CG-CD-CE	5.64	128.81	111.90
1	B	202	THR	CB-CA-C	-5.63	96.40	111.60
1	D	257	GLN	CA-CB-CG	5.62	125.77	113.40
1	C	205	TYR	CE1-CZ-OH	5.62	135.27	120.10
1	D	83	GLN	CB-CG-CD	-5.60	97.03	111.60
1	C	252	GLU	CB-CG-CD	-5.54	99.24	114.20
1	B	292	GLU	CA-CB-CG	5.54	125.58	113.40
1	B	171	LYS	N-CA-CB	-5.54	100.63	110.60
1	B	171	LYS	CB-CG-CD	-5.45	97.43	111.60
1	B	201	GLU	C-N-CA	5.28	134.90	121.70
1	A	93	GLN	CA-CB-CG	5.28	125.01	113.40
1	B	176	LEU	CA-CB-CG	5.23	127.32	115.30
1	C	203	LEU	CA-CB-CG	5.21	127.28	115.30
1	C	317	GLU	CG-CD-OE1	-5.20	107.90	118.30
1	B	93	GLN	N-CA-CB	5.14	119.85	110.60
1	C	205	TYR	CA-CB-CG	-5.13	103.65	113.40
1	B	235	ASP	N-CA-CB	5.12	119.82	110.60
1	C	252	GLU	N-CA-CB	-5.09	101.44	110.60
1	D	234	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	177	SER	CB-CA-C	-5.08	100.45	110.10
1	D	317	GLU	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	PHE	Peptide
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	51	1
1	B	2557	0	2492	91	1
1	C	2420	0	2362	69	0
1	D	2381	0	2332	69	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	249	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 (249) 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:263:LYS:HG3	1:B:267:GLN:HE21	0.96	1.06
1:B:94:TYR:HB3	1:C:205:TYR:OH	1.56	1.04
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: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:B:78:MET:HE3	1:B:125:ILE:HD13	1.55	0.89
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:B:78:MET:HE2	1:B:125:ILE:HD13	1.61	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:252:GLU:CD	1:B:306:MET:HE2	2.08	0.74
1:A:306:MET:SD	1:C:290:LEU:HD22	2.26	0.74
1:D:83:GLN:HB3	1:D:84:PRO:HD2	1.69	0.73
1:B:78:MET:HE2	1:B:125:ILE:CD1	2.18	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:B:252:GLU:CD	1:B:306:MET:CE	2.61	0.69
1:B:78:MET:CE	1:B:125:ILE:CD1	2.69	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:303:GLU:HG3	1:B:306:MET:HE3	1.75	0.67
1:B:198:LEU:O	1:B:200:ALA:N	2.29	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
1:B:91:ALA:O	1:B:94:TYR:HB2	1.98	0.63
1:B:303:GLU:HG3	1:B:306:MET:CE	2.28	0.62
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:248:ARG:HH22	1:B:297:GLU:HG2	1.70	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:B:198:LEU:C	1:B:200:ALA:H	2.09	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:D:273:MET:HE2	1:D:273:MET:HA	1.86	0.55
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: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
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: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:273:MET:HE3	1:D:298:ILE:HD12	1.91	0.53
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:C:250:ASN:C	1:C:252:GLU:N	2.62	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:C:250:ASN:O	1:C:251:GLN:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLU:OE2	1:C:162:GLU:HA	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: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
1:D:197:LEU:O	1:D:197:LEU:CD1	2.60	0.50
1:B:121:ASP:OD1	2:B:401:HOH:O	2.20	0.49
1:B:49:GLN:HE21	1:C:156:GLU:CD	2.16	0.49
1:D:172:LEU:HD11	1:D:203:LEU:HD13	1.93	0.49
1:D:168:MET:HE2	1:D:210:PHE:HB3	1.93	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:86:LEU:HB3	1:B:90:LEU:HD22	1.94	0.48
1:D:162:GLU:C	1:D:163:GLN:HG2	2.29	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:D:30:ARG:HH21	1:D:321:ASP:CG	2.17	0.48
1:B:234:LEU:O	1:B:234:LEU:HG	2.13	0.48
1:B:237:SER:HA	1:B:254:CYS:HG	1.79	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:B:271:GLN:O	1:B:275:ARG:HG3	2.14	0.48
1:C:250:ASN:C	1:C:252:GLU:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:PHE:O	1:C:22:ARG:HG3	2.14	0.47
1:A:309:ARG:HH21	1:C:291:GLU:CD	2.18	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:B:201:GLU:C	1:B:203:LEU:H	2.17	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: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: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: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:D:156:GLU:C	1:D:159:GLU:H	2.18	0.45
1:B:252:GLU:OE2	1:B:306:MET:HE2	2.15	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:B:306:MET:CE	1:B:306:MET:H	2.30	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:A:62:GLU:HA	1:A:66:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:MET:SD	1:B:78:MET:C	2.96	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:B:42:PHE:CD1	1:B:43:PRO:HA	2.53	0.44
1:B:153:ASN:HB3	1:B:156:GLU:HG3	2.00	0.43
1:B:252:GLU:CG	1:B:306:MET:HE2	2.48	0.43
1:D:199:ASP:O	1:D:200:ALA:HB2	2.18	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:D:273:MET:HE3	1:D:283:PHE:CZ	2.54	0.43
1:B:136:ARG:HD3	1:C:111:ASP:OD2	2.18	0.43
1:A:221:ARG:HD3	1:A:306:MET:HE1	2.00	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
1:B:198:LEU:C	1:B:200:ALA:N	2.72	0.42
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:78:MET:HE3	1:B:125:ILE:CD1	2.38	0.42
1:B:137:VAL:HG12	1:B:272:PHE:CD1	2.53	0.42
1:B:252:GLU:CD	1:B:306:MET:HE1	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:128:ALA:HB1	1:D:276:LEU:HD13	2.02	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:49:GLN:NE2	1:C:156:GLU:CD	2.74	0.41
1:B:306:MET:HE2	1:B:306:MET:HB3	1.71	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:175:PRO:C	1:D:176:LEU:HG	2.41	0.41
1:D:86:LEU:HD23	1:D:86:LEU:HA	1.69	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:198:LEU:O	1:C:202:THR:OG1	2.28	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
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%)	4	5
1	B	310/360 (86%)	284 (92%)	19 (6%)	7 (2%)	6	10
1	C	291/360 (81%)	274 (94%)	11 (4%)	6 (2%)	7	11
1	D	286/360 (79%)	266 (93%)	12 (4%)	8 (3%)	5	7
All	All	1194/1440 (83%)	1107 (93%)	56 (5%)	31 (3%)	5	8

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
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

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Mol	Chain	Res	Type
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%)	266 (96%)	10 (4%)	35	61
1	B	278/315 (88%)	272 (98%)	6 (2%)	52	77
1	C	262/315 (83%)	252 (96%)	10 (4%)	33	58
1	D	258/315 (82%)	249 (96%)	9 (4%)	36	62
All	All	1074/1260 (85%)	1039 (97%)	35 (3%)	38	64

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

Mol	Chain	Res	Type
1	A	17	TYR
1	A	55	SER
1	A	65	ASP
1	A	78	MET
1	A	82	TRP
1	A	96	ASP
1	A	179	SER
1	A	185	PHE
1	A	201	GLU
1	A	206	CYS
1	B	106	TRP
1	B	109	PHE
1	B	188	TYR
1	B	254	CYS
1	B	263	LYS
1	B	306	MET
1	C	5	ARG
1	C	28	SER
1	C	82	TRP
1	C	95	ARG

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Mol	Chain	Res	Type
1	C	98	CYS
1	C	205	TYR
1	C	221	ARG
1	C	253	SER
1	C	254	CYS
1	C	306	MET
1	D	49	GLN
1	D	57	SER
1	D	78	MET
1	D	87	SER
1	D	155	LYS
1	D	158	ARG
1	D	171	LYS
1	D	174	LYS
1	D	254	CYS

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

Mol	Chain	Res	Type
1	B	49	GLN
1	B	267	GLN
1	C	49	GLN
1	C	250	ASN
1	C	257	GLN
1	D	59	HIS
1	D	163	GLN

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 monosaccharides 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%)	0.15	23 (7%)	14 15	30, 46, 82, 109	0
1	B	314/360 (87%)	0.15	19 (6%)	21 22	28, 42, 79, 94	0
1	C	297/360 (82%)	0.24	24 (8%)	12 12	29, 47, 87, 108	0
1	D	292/360 (81%)	0.28	24 (8%)	11 11	30, 50, 87, 108	0
All	All	1214/1440 (84%)	0.20	90 (7%)	14 15	28, 46, 85, 109	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	SER	9.6
1	A	199	ASP	9.4
1	C	177	SER	8.7
1	A	55	SER	7.5
1	C	205	TYR	6.9
1	B	202	THR	6.4
1	A	88	PRO	6.4
1	C	178	TYR	6.3
1	C	197	LEU	6.1
1	D	178	TYR	5.9
1	D	253	SER	5.9
1	D	254	CYS	5.9
1	B	200	ALA	5.8
1	B	254	CYS	5.6
1	D	197	LEU	5.3
1	B	188	TYR	5.3
1	C	252	GLU	5.2
1	C	250	ASN	5.1
1	D	199	ASP	5.1
1	C	251	GLN	5.1
1	A	89	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	198	LEU	5.0
1	D	88	PRO	4.9
1	C	255	THR	4.8
1	A	237	SER	4.8
1	D	4	GLN	4.4
1	A	251	GLN	4.4
1	B	93	GLN	4.3
1	C	254	CYS	4.0
1	D	205	TYR	3.9
1	A	3	LEU	3.9
1	B	201	GLU	3.8
1	D	156	GLU	3.8
1	B	236	ALA	3.7
1	B	186	PHE	3.6
1	D	252	GLU	3.6
1	D	255	THR	3.5
1	A	93	GLN	3.5
1	B	184	SER	3.5
1	B	250	ASN	3.5
1	A	326	ASN	3.4
1	B	249	ALA	3.4
1	D	236	ALA	3.3
1	C	3	LEU	3.3
1	A	94	TYR	3.3
1	C	236	ALA	3.3
1	B	197	LEU	3.2
1	B	251	GLN	3.2
1	A	6	ASP	3.2
1	A	95	ARG	3.2
1	A	92	PRO	3.2
1	C	237	SER	3.1
1	D	326	ASN	3.1
1	B	252	GLU	3.1
1	C	196	ASP	3.1
1	C	201	GLU	3.1
1	D	198	LEU	3.0
1	C	253	SER	3.0
1	C	55	SER	3.0
1	D	89	GLU	3.0
1	B	235	ASP	2.9
1	A	182	GLY	2.9
1	C	326	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	90	LEU	2.8
1	D	3	LEU	2.8
1	C	249	ALA	2.8
1	B	185	PHE	2.7
1	D	177	SER	2.7
1	B	237	SER	2.7
1	A	201	GLU	2.6
1	D	237	SER	2.6
1	B	205	TYR	2.6
1	A	252	GLU	2.6
1	C	5	ARG	2.4
1	A	200	ALA	2.4
1	D	202	THR	2.3
1	A	188	TYR	2.3
1	D	235	ASP	2.3
1	A	183	SER	2.2
1	D	204	ARG	2.2
1	C	4	GLN	2.2
1	D	201	GLU	2.2
1	A	204	ARG	2.2
1	A	97	ALA	2.2
1	A	187	MET	2.1
1	C	200	ALA	2.1
1	D	90	LEU	2.1
1	C	204	ARG	2.1
1	C	33	GLN	2.0
1	D	86	LEU	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 monosaccharides 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.