



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:30 PM UTC

PDB ID : 1ILU / pdb_00001ilu
Title : X-RAY CRYSTAL STRUCTURE THE TWO SITE-SPECIFIC MUTANTS
ILE7SER AND PHE110SER OF AZURIN FROM PSEUDOMONAS
AERUGINOSA
Authors : Hammann, C.; Nar, H.; Huber, R.; Messerschmidt, A.
Deposited on : 1995-10-12
Resolution : 2.30 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) : **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

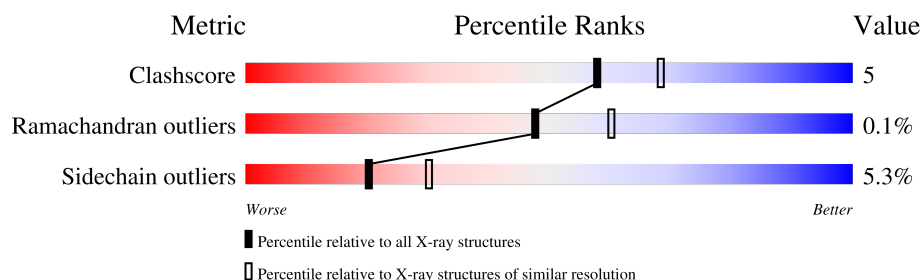
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	128	71% 25% .
1	B	128	80% 20%
1	C	128	77% 21% .
1	D	128	69% 28% .
1	E	128	79% 20% .
1	F	128	84% 13% .
1	G	128	77% 17% 6%
1	H	128	76% 23% .

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Mol	Chain	Length	Quality of chain
1	I	128	 76% 23% .
1	K	128	 66% 34% .
1	L	128	 74% 23% .
1	M	128	 79% 20% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16428 atoms, of which 4072 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 AZURIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	B	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	C	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	D	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	E	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	F	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	G	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	H	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	I	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	K	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	L	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	M	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	SER	PHE	engineered mutation	UNP P00282
B	110	SER	PHE	engineered mutation	UNP P00282
C	110	SER	PHE	engineered mutation	UNP P00282
D	110	SER	PHE	engineered mutation	UNP P00282
E	110	SER	PHE	engineered mutation	UNP P00282

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Chain	Residue	Modelled	Actual	Comment	Reference
F	110	SER	PHE	engineered mutation	UNP P00282
G	110	SER	PHE	engineered mutation	UNP P00282
H	110	SER	PHE	engineered mutation	UNP P00282
I	110	SER	PHE	engineered mutation	UNP P00282
K	110	SER	PHE	engineered mutation	UNP P00282
L	110	SER	PHE	engineered mutation	UNP P00282
M	110	SER	PHE	engineered mutation	UNP P00282

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0
2	G	1	Total Cu 1 1	0	0
2	H	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	K	1	Total Cu 1 1	0	0
2	L	1	Total Cu 1 1	0	0
2	M	1	Total Cu 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	63	Total H O 189 126 63	0	0
3	B	83	Total H O 249 166 83	0	0

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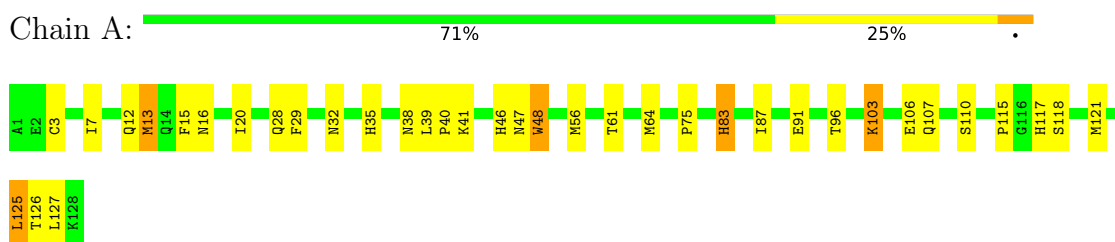
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	63	Total	H	O	0	0
			189	126	63		
3	D	55	Total	H	O	0	0
			165	110	55		
3	E	61	Total	H	O	0	0
			183	122	61		
3	F	47	Total	H	O	0	0
			141	94	47		
3	G	54	Total	H	O	0	0
			162	108	54		
3	H	55	Total	H	O	0	0
			165	110	55		
3	I	52	Total	H	O	0	0
			156	104	52		
3	K	62	Total	H	O	0	0
			186	124	62		
3	L	62	Total	H	O	0	0
			186	124	62		
3	M	59	Total	H	O	0	0
			177	118	59		

3 Residue-property plots

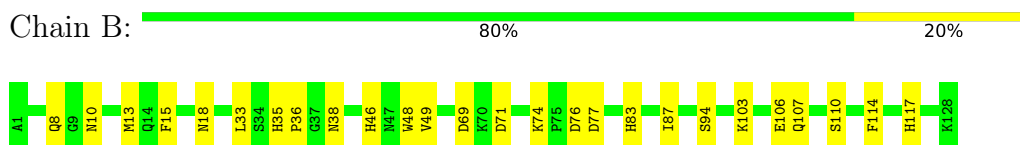
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

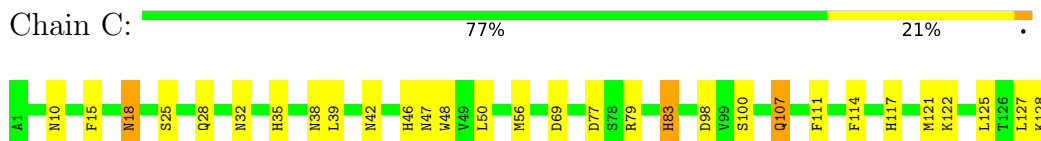
• Molecule 1: AZURIN



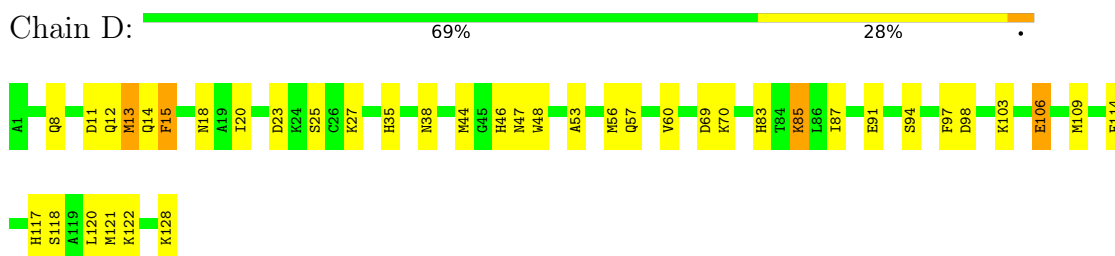
• Molecule 1: AZURIN



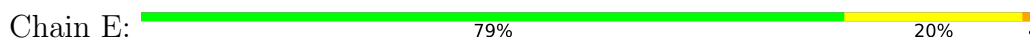
• Molecule 1: AZURIN

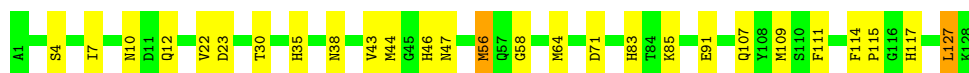


• Molecule 1: AZURIN



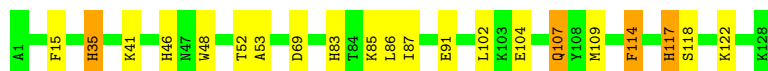
• Molecule 1: AZURIN





- Molecule 1: AZURIN

Chain F: 84% 13%



- Molecule 1: AZURIN

Chain G: 77% 17% 6%



- Molecule 1: AZURIN

Chain H: 76% 23%



- Molecule 1: AZURIN

Chain I: 76% 23%



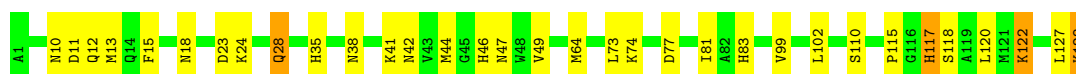
- Molecule 1: AZURIN

Chain K: 66% 34%



- Molecule 1: AZURIN

Chain L: 74% 23%



- Molecule 1: AZURIN

Chain M:

79%

20%

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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.40 Å 170.10 Å 99.70 Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16428	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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:
CU

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	0.93	6/985 (0.6%)	1.80	23/1327 (1.7%)
1	B	0.90	5/985 (0.5%)	1.72	18/1327 (1.4%)
1	C	0.94	5/985 (0.5%)	1.70	19/1327 (1.4%)
1	D	0.90	5/985 (0.5%)	1.72	20/1327 (1.5%)
1	E	0.90	4/985 (0.4%)	1.72	20/1327 (1.5%)
1	F	0.89	4/985 (0.4%)	1.71	15/1327 (1.1%)
1	G	0.92	6/985 (0.6%)	1.77	22/1327 (1.7%)
1	H	0.90	5/985 (0.5%)	1.72	19/1327 (1.4%)
1	I	0.89	4/985 (0.4%)	1.70	17/1327 (1.3%)
1	K	0.87	5/985 (0.5%)	1.69	24/1327 (1.8%)
1	L	0.90	6/985 (0.6%)	1.72	19/1327 (1.4%)
1	M	0.90	6/985 (0.6%)	1.75	20/1327 (1.5%)
All	All	0.90	61/11820 (0.5%)	1.73	236/15924 (1.5%)

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	HIS	CD2-NE2	-7.95	1.29	1.37
1	C	46	HIS	CD2-NE2	-7.08	1.30	1.37
1	F	46	HIS	CD2-NE2	-7.06	1.30	1.37
1	L	117	HIS	CD2-NE2	-7.02	1.30	1.37
1	H	46	HIS	CD2-NE2	-6.86	1.30	1.37
1	H	117	HIS	CD2-NE2	-6.85	1.30	1.37
1	B	83	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	83	HIS	CD2-NE2	-6.80	1.30	1.37
1	I	46	HIS	CD2-NE2	-6.78	1.30	1.37
1	M	35	HIS	CD2-NE2	-6.78	1.30	1.37
1	D	35	HIS	CD2-NE2	-6.74	1.30	1.37
1	G	46	HIS	CD2-NE2	-6.65	1.30	1.37
1	K	83	HIS	CD2-NE2	-6.55	1.30	1.37
1	F	117	HIS	CD2-NE2	-6.54	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	83	HIS	CD2-NE2	-6.51	1.30	1.37
1	L	35	HIS	CD2-NE2	-6.47	1.30	1.37
1	I	35	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	46	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	117	HIS	CD2-NE2	-6.41	1.30	1.37
1	D	117	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	46	HIS	CD2-NE2	-6.38	1.30	1.37
1	H	35	HIS	CD2-NE2	-6.37	1.30	1.37
1	C	117	HIS	CD2-NE2	-6.37	1.30	1.37
1	F	83	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	117	HIS	CD2-NE2	-6.34	1.30	1.37
1	E	46	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	35	HIS	CD2-NE2	-6.22	1.31	1.37
1	E	35	HIS	CD2-NE2	-6.19	1.31	1.37
1	L	46	HIS	CD2-NE2	-6.13	1.31	1.37
1	D	46	HIS	CD2-NE2	-6.12	1.31	1.37
1	G	117	HIS	CD2-NE2	-6.09	1.31	1.37
1	H	117	HIS	CG-ND1	-6.07	1.31	1.38
1	M	46	HIS	CD2-NE2	-6.06	1.31	1.37
1	F	35	HIS	CD2-NE2	-6.03	1.31	1.37
1	E	83	HIS	CD2-NE2	-6.01	1.31	1.37
1	C	83	HIS	CD2-NE2	-5.97	1.31	1.37
1	L	83	HIS	CD2-NE2	-5.94	1.31	1.37
1	M	83	HIS	CD2-NE2	-5.86	1.31	1.37
1	D	117	HIS	CG-ND1	-5.82	1.31	1.38
1	I	117	HIS	CD2-NE2	-5.82	1.31	1.37
1	I	83	HIS	CD2-NE2	-5.82	1.31	1.37
1	G	83	HIS	CD2-NE2	-5.82	1.31	1.37
1	K	46	HIS	CD2-NE2	-5.80	1.31	1.37
1	M	117	HIS	CD2-NE2	-5.79	1.31	1.37
1	K	46	HIS	CG-ND1	-5.77	1.31	1.38
1	K	35	HIS	CD2-NE2	-5.67	1.31	1.37
1	K	117	HIS	CD2-NE2	-5.65	1.31	1.37
1	M	117	HIS	CG-ND1	-5.59	1.32	1.38
1	D	83	HIS	CD2-NE2	-5.58	1.31	1.37
1	G	46	HIS	CG-ND1	-5.55	1.32	1.38
1	G	35	HIS	CD2-NE2	-5.54	1.31	1.37
1	C	46	HIS	CG-ND1	-5.50	1.32	1.38
1	E	117	HIS	CD2-NE2	-5.48	1.31	1.37
1	L	117	HIS	CG-ND1	-5.45	1.32	1.38
1	B	117	HIS	CG-ND1	-5.25	1.32	1.38
1	L	46	HIS	CG-ND1	-5.24	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	117	HIS	CG-ND1	-5.18	1.32	1.38
1	A	107	GLN	CB-CG	-5.17	1.36	1.52
1	M	46	HIS	CG-ND1	-5.15	1.32	1.38
1	B	35	HIS	CD2-NE2	-5.09	1.32	1.37
1	A	117	HIS	CG-ND1	-5.07	1.32	1.38

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	ASP	CA-CB-CG	9.56	122.16	112.60
1	A	32	ASN	OD1-CG-ND2	-9.01	113.59	122.60
1	L	47	ASN	CA-CB-CG	8.99	121.59	112.60
1	F	117	HIS	N-CA-C	8.85	122.04	111.33
1	E	47	ASN	CA-CB-CG	8.49	121.09	112.60
1	A	35	HIS	CB-CG-CD2	-8.34	120.36	131.20
1	G	69	ASP	CA-CB-CG	8.28	120.88	112.60
1	G	107	GLN	OE1-CD-NE2	-8.21	114.39	122.60
1	C	69	ASP	CA-CB-CG	8.02	120.62	112.60
1	H	35	HIS	CB-CG-CD2	-8.01	120.79	131.20
1	G	14	GLN	OE1-CD-NE2	-7.73	114.87	122.60
1	D	38	ASN	CA-CB-CG	7.72	120.33	112.60
1	M	35	HIS	CB-CG-CD2	-7.72	121.16	131.20
1	C	18	ASN	CA-CB-CG	7.70	120.30	112.60
1	K	43	VAL	N-CA-C	-7.69	105.67	111.90
1	K	32	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	L	35	HIS	CB-CG-CD2	-7.35	121.64	131.20
1	E	46	HIS	CB-CG-CD2	-7.26	121.76	131.20
1	E	23	ASP	CA-CB-CG	7.24	119.84	112.60
1	C	47	ASN	CA-CB-CG	7.24	119.83	112.60
1	A	3	CYS	N-CA-C	7.20	121.80	113.38
1	F	46	HIS	ND1-CG-CD2	7.10	113.20	106.10
1	E	56	MET	CG-SD-CE	-7.09	85.30	100.90
1	I	122	LYS	CB-CA-C	-7.04	97.83	110.36
1	A	35	HIS	CB-CG-ND1	7.02	133.24	122.70
1	F	35	HIS	CB-CG-CD2	-7.01	122.08	131.20
1	G	32	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	C	46	HIS	CB-CG-CD2	-6.98	122.13	131.20
1	D	117	HIS	ND1-CG-CD2	6.94	113.04	106.10
1	C	35	HIS	CB-CG-CD2	-6.93	122.19	131.20
1	E	35	HIS	CB-CG-CD2	-6.92	122.21	131.20
1	D	35	HIS	CB-CG-CD2	-6.89	122.24	131.20
1	G	46	HIS	CB-CG-CD2	-6.86	122.28	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	38	ASN	CA-CB-CG	6.85	119.45	112.60
1	M	11	ASP	CA-CB-CG	6.77	119.37	112.60
1	E	46	HIS	ND1-CG-CD2	6.77	112.87	106.10
1	I	23	ASP	CA-CB-CG	6.77	119.37	112.60
1	L	18	ASN	CA-CB-CG	6.76	119.36	112.60
1	A	46	HIS	CB-CG-CD2	-6.75	122.43	131.20
1	A	117	HIS	ND1-CG-CD2	6.72	112.83	106.10
1	D	57	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	E	43	VAL	N-CA-C	-6.68	106.49	111.90
1	M	35	HIS	CB-CG-ND1	6.63	132.64	122.70
1	K	117	HIS	ND1-CG-CD2	6.62	112.72	106.10
1	A	46	HIS	ND1-CG-CD2	6.58	112.68	106.10
1	H	35	HIS	CB-CG-ND1	6.58	132.56	122.70
1	E	10	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	C	38	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	H	47	ASN	CA-CB-CG	6.56	119.16	112.60
1	D	18	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	I	46	HIS	ND1-CG-CD2	6.53	112.63	106.10
1	K	71	ASP	CA-CB-CG	6.53	119.13	112.60
1	C	46	HIS	ND1-CG-CD2	6.53	112.63	106.10
1	G	2	GLU	N-CA-C	-6.50	98.02	108.55
1	K	46	HIS	ND1-CG-CD2	6.49	112.59	106.10
1	D	69	ASP	CA-CB-CG	6.47	119.07	112.60
1	E	117	HIS	N-CA-C	6.46	119.15	111.33
1	M	47	ASN	CA-CB-CG	6.45	119.05	112.60
1	G	46	HIS	ND1-CG-CD2	6.44	112.54	106.10
1	F	46	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	L	128	LYS	CA-CB-CG	6.39	126.88	114.10
1	F	117	HIS	ND1-CG-CD2	6.39	112.49	106.10
1	E	35	HIS	CB-CG-ND1	6.38	132.27	122.70
1	G	28	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	C	35	HIS	CB-CG-ND1	6.33	132.20	122.70
1	G	77	ASP	N-CA-C	-6.29	100.34	109.59
1	I	46	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	I	35	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	K	118	SER	N-CA-C	6.27	119.78	111.75
1	B	18	ASN	CA-CB-CG	6.27	118.87	112.60
1	L	35	HIS	CB-CG-ND1	6.25	132.08	122.70
1	I	117	HIS	ND1-CG-CD2	6.21	112.31	106.10
1	L	28	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	G	10	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	L	46	HIS	ND1-CG-CD2	6.17	112.27	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	122	LYS	CA-CB-CG	6.16	126.43	114.10
1	C	32	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	E	91	GLU	N-CA-C	6.16	118.49	110.43
1	F	114	PHE	CA-C-N	6.15	126.17	119.90
1	F	114	PHE	C-N-CA	6.15	126.17	119.90
1	C	28	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	L	117	HIS	ND1-CG-CD2	6.14	112.25	106.10
1	B	117	HIS	ND1-CG-CD2	6.13	112.23	106.10
1	E	117	HIS	ND1-CG-CD2	6.12	112.22	106.10
1	M	42	ASN	CA-CB-CG	6.12	118.72	112.60
1	M	46	HIS	ND1-CG-CD2	6.11	112.21	106.10
1	D	117	HIS	N-CA-C	6.11	118.72	111.33
1	H	46	HIS	CB-CG-CD2	-6.10	123.27	131.20
1	C	10	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	G	117	HIS	ND1-CG-CD2	6.08	112.18	106.10
1	K	35	HIS	CB-CG-CD2	-6.08	123.30	131.20
1	H	117	HIS	ND1-CG-CD2	6.07	112.17	106.10
1	M	71	ASP	CA-CB-CG	6.07	118.67	112.60
1	F	35	HIS	CB-CG-ND1	6.06	131.79	122.70
1	H	97	PHE	CA-CB-CG	6.04	119.84	113.80
1	H	98	ASP	CA-CB-CG	6.00	118.60	112.60
1	K	27	LYS	N-CA-C	-6.00	104.66	111.14
1	A	16	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	K	18	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	A	61	THR	CA-CB-OG1	-5.97	100.64	109.60
1	L	35	HIS	CA-CB-CG	5.93	119.73	113.80
1	L	46	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	G	114	PHE	CA-C-N	5.89	126.23	119.93
1	G	114	PHE	C-N-CA	5.89	126.23	119.93
1	D	47	ASN	CA-CB-CG	5.88	118.48	112.60
1	K	18	ASN	CA-CB-CG	5.85	118.45	112.60
1	K	38	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	K	39	LEU	CA-C-N	5.83	125.81	120.21
1	K	39	LEU	C-N-CA	5.83	125.81	120.21
1	M	114	PHE	CA-C-N	5.81	126.15	119.93
1	M	114	PHE	C-N-CA	5.81	126.15	119.93
1	M	42	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	B	46	HIS	ND1-CG-CD2	5.80	111.91	106.10
1	M	48	TRP	CG-CD2-CE3	5.80	139.70	133.90
1	L	10	ASN	CA-CB-CG	5.79	118.39	112.60
1	L	122	LYS	CA-CB-CG	5.79	125.68	114.10
1	G	35	HIS	CB-CG-CD2	-5.78	123.68	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	42	ASN	CA-CB-CG	5.77	118.37	112.60
1	L	41	LYS	N-CA-C	5.77	118.04	111.11
1	D	46	HIS	ND1-CG-CD2	5.76	111.86	106.10
1	M	13	MET	CA-CB-CG	5.75	125.61	114.10
1	C	39	LEU	N-CA-C	5.73	118.20	110.29
1	B	46	HIS	CB-CG-CD2	-5.73	123.76	131.20
1	B	76	ASP	CA-CB-CG	5.71	118.31	112.60
1	G	12	GLN	CA-CB-CG	5.71	125.52	114.10
1	I	71	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	110	SER	CA-CB-OG	-5.70	99.71	111.10
1	K	40	PRO	N-CA-C	5.70	119.19	111.22
1	C	117	HIS	ND1-CG-CD2	5.69	111.79	106.10
1	M	8	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	D	106	GLU	N-CA-C	-5.66	100.55	109.50
1	A	12	GLN	N-CA-C	-5.66	106.27	112.72
1	D	35	HIS	CB-CG-ND1	5.66	131.19	122.70
1	C	77	ASP	CA-CB-CG	5.64	118.24	112.60
1	K	16	ASN	CA-CB-CG	5.63	118.23	112.60
1	G	107	GLN	CG-CD-NE2	5.62	124.84	116.40
1	F	48	TRP	CE2-CD2-CG	-5.62	100.45	107.20
1	G	48	TRP	CG-CD2-CE3	5.62	139.52	133.90
1	H	46	HIS	ND1-CG-CD2	5.62	111.72	106.10
1	G	35	HIS	CB-CG-ND1	5.61	131.12	122.70
1	A	13	MET	CA-CB-CG	5.61	125.32	114.10
1	F	48	TRP	CG-CD2-CE3	5.61	139.50	133.90
1	L	12	GLN	N-CA-C	-5.58	104.90	112.26
1	A	38	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	H	83	HIS	CB-CG-CD2	-5.55	123.99	131.20
1	D	23	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	35	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	M	126	THR	CA-CB-OG1	-5.54	101.30	109.60
1	E	12	GLN	CA-C-N	5.52	130.79	122.68
1	E	12	GLN	C-N-CA	5.52	130.79	122.68
1	F	83	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	K	23	ASP	CA-CB-CG	5.51	118.11	112.60
1	K	117	HIS	CG-CD2-NE2	-5.50	101.70	107.20
1	G	12	GLN	N-CA-C	-5.49	105.90	112.59
1	B	48	TRP	CG-CD2-CE3	5.49	139.38	133.90
1	A	39	LEU	CA-C-N	5.48	125.79	119.92
1	A	39	LEU	C-N-CA	5.48	125.79	119.92
1	H	55	ASP	N-CA-C	5.46	119.95	113.28
1	K	16	ASN	OD1-CG-ND2	-5.46	117.14	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	PHE	CA-C-N	5.45	126.66	119.84
1	B	114	PHE	C-N-CA	5.45	126.66	119.84
1	H	56	MET	N-CA-C	5.45	117.66	111.11
1	C	114	PHE	CA-C-N	5.44	125.75	119.93
1	C	114	PHE	C-N-CA	5.44	125.75	119.93
1	L	23	ASP	CA-CB-CG	5.42	118.02	112.60
1	D	14	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	M	118	SER	N-CA-C	5.40	119.36	112.34
1	M	14	GLN	CA-CB-CG	5.40	124.89	114.10
1	I	39	LEU	CA-C-N	5.39	125.37	120.03
1	I	39	LEU	C-N-CA	5.39	125.37	120.03
1	D	114	PHE	CA-C-N	5.39	125.65	119.83
1	D	114	PHE	C-N-CA	5.39	125.65	119.83
1	F	102	LEU	N-CA-C	5.38	117.52	107.99
1	B	13	MET	CA-CB-CG	5.38	124.85	114.10
1	I	10	ASN	CA-CB-CG	5.36	117.96	112.60
1	C	38	ASN	CA-CB-CG	5.34	117.94	112.60
1	K	44	MET	N-CA-CB	-5.34	105.39	111.79
1	M	48	TRP	CE2-CD2-CG	-5.34	100.80	107.20
1	D	46	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	D	117	HIS	CG-CD2-NE2	-5.30	101.90	107.20
1	G	48	TRP	CE2-CD2-CG	-5.30	100.84	107.20
1	A	56	MET	N-CA-C	5.29	120.05	111.37
1	I	3	CYS	N-CA-C	5.29	119.03	112.47
1	E	71	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	48	TRP	CE2-CD2-CG	-5.27	100.87	107.20
1	H	114	PHE	CA-C-N	5.27	126.43	119.84
1	H	114	PHE	C-N-CA	5.27	126.43	119.84
1	M	10	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	I	28	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	M	44	MET	O-C-N	-5.25	116.98	122.18
1	B	38	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	47	ASN	CA-CB-CG	5.24	117.84	112.60
1	L	11	ASP	CA-CB-CG	5.24	117.84	112.60
1	E	56	MET	N-CA-C	5.23	117.38	111.11
1	L	12	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	D	98	ASP	CA-CB-CG	5.19	117.79	112.60
1	F	46	HIS	CG-CD2-NE2	-5.19	102.01	107.20
1	B	15	PHE	O-C-N	-5.19	117.09	122.96
1	K	35	HIS	CB-CG-ND1	5.18	130.47	122.70
1	D	48	TRP	CB-CG-CD1	-5.18	119.13	126.90
1	F	107	GLN	OE1-CD-NE2	-5.18	117.42	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	48	TRP	CB-CG-CD1	-5.17	119.14	126.90
1	B	15	PHE	N-CA-C	-5.16	102.85	110.48
1	B	10	ASN	CA-CB-CG	5.14	117.74	112.60
1	K	48	TRP	N-CA-C	-5.13	99.92	108.34
1	G	66	SER	N-CA-C	5.13	119.25	113.15
1	C	114	PHE	CA-C-O	-5.12	115.41	119.71
1	I	35	HIS	CB-CG-ND1	5.12	130.38	122.70
1	C	42	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	E	83	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	H	48	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	H	67	GLY	N-CA-C	5.10	118.51	112.33
1	E	114	PHE	CA-C-N	5.09	125.00	119.76
1	E	114	PHE	C-N-CA	5.09	125.00	119.76
1	B	48	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	A	35	HIS	CA-CB-CG	5.06	118.86	113.80
1	K	97	PHE	CA-CB-CG	5.05	118.85	113.80
1	H	125	LEU	N-CA-C	-5.05	100.22	108.76
1	A	40	PRO	CA-C-N	5.04	127.55	120.28
1	A	40	PRO	C-N-CA	5.04	127.55	120.28
1	B	71	ASP	CA-CB-CG	5.04	117.64	112.60
1	K	38	ASN	CB-CG-ND2	5.04	123.96	116.40
1	A	16	ASN	CB-CG-ND2	5.04	123.96	116.40
1	A	41	LYS	N-CA-C	5.04	117.50	111.71
1	H	10	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	B	38	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	K	110	SER	N-CA-C	-5.03	101.67	109.72
1	H	11	ASP	CA-CB-CG	5.03	117.63	112.60
1	M	69	ASP	CA-CB-CG	5.02	117.62	112.60
1	H	28	GLN	OE1-CD-NE2	-5.01	117.58	122.60
1	I	74	LYS	CA-C-N	5.01	125.29	119.93
1	I	74	LYS	C-N-CA	5.01	125.29	119.93
1	L	15	PHE	N-CA-C	-5.01	102.35	110.32
1	D	15	PHE	N-CA-C	-5.01	102.35	110.32
1	E	7	ILE	CB-CA-C	5.01	118.21	110.50
1	I	48	TRP	CE2-CD2-CG	-5.00	101.20	107.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	969	220	949	9	0
1	B	969	220	948	7	0
1	C	969	220	948	5	1
1	D	969	220	948	14	1
1	E	969	220	948	8	0
1	F	969	220	948	5	0
1	G	969	220	948	7	1
1	H	969	220	948	8	0
1	I	969	220	948	11	1
1	K	969	220	948	16	0
1	L	969	220	948	9	0
1	M	969	220	948	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
3	A	63	126	0	1	0
3	B	83	166	0	2	0
3	C	63	126	0	1	0
3	D	55	110	0	4	1
3	E	61	122	0	3	0
3	F	47	94	0	1	0
3	G	54	108	0	3	0
3	H	55	110	0	2	0
3	I	52	104	0	0	0
3	K	62	124	0	2	1
3	L	62	124	0	2	0
3	M	59	118	0	1	0
All	All	12356	4072	11377	104	3

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 5.

All (104) 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:L:13:MET:HE2	1:L:120:LEU:HD12	1.62	0.79
1:I:46:HIS:CE1	1:I:121:MET:HE1	2.25	0.70
1:I:32:ASN:HB3	1:I:92:LYS:HZ2	1.58	0.67
1:I:46:HIS:CG	1:I:121:MET:HE1	2.33	0.64
1:G:87:ILE:HB	1:G:91:GLU:HB2	1.81	0.63
1:M:34:SER:HB3	1:M:92:LYS:HD2	1.79	0.63
1:I:32:ASN:HB3	1:I:92:LYS:NZ	2.14	0.62
1:B:33:LEU:HD13	3:B:3007:HOH:O	2.00	0.61
1:D:13:MET:HG3	1:D:120:LEU:HD12	1.82	0.61
1:A:64:MET:HG3	1:A:115:PRO:HB3	1.84	0.60
1:I:64:MET:HG3	1:I:115:PRO:HG3	1.83	0.60
1:A:20:ILE:HB	1:A:125:LEU:HD12	1.85	0.59
1:H:21:THR:HG22	1:H:128:LYS:HG2	1.84	0.58
1:E:64:MET:HE2	1:E:115:PRO:HB3	1.86	0.57
1:B:8:GLN:HE21	1:B:36:PRO:HG2	1.70	0.57
1:C:56:MET:HG3	1:C:111:PHE:CE1	2.41	0.55
1:F:41:LYS:HD3	1:F:86:LEU:HD23	1.89	0.55
1:I:13:MET:HE2	1:I:120:LEU:HD12	1.88	0.55
1:D:20:ILE:HD11	3:D:1911:HOH:O	2.07	0.55
1:K:60:VAL:HG12	1:K:64:MET:HE3	1.89	0.55
1:D:15:PHE:CD1	1:D:121:MET:HE2	2.42	0.54
1:M:13:MET:HE2	1:M:120:LEU:HD23	1.89	0.54
1:H:7:ILE:HB	3:H:2554:HOH:O	2.09	0.53
1:D:118:SER:HB3	3:D:570:HOH:O	2.09	0.52
1:K:56:MET:O	1:K:60:VAL:HG23	2.10	0.52
1:M:23:ASP:HA	1:M:128:LYS:HB3	1.90	0.52
1:A:87:ILE:HB	1:A:91:GLU:HB2	1.92	0.52
1:D:60:VAL:HG22	3:D:570:HOH:O	2.10	0.51
1:G:18:ASN:HB3	3:G:3103:HOH:O	2.08	0.51
1:K:33:LEU:O	1:K:92:LYS:HD2	2.10	0.51
1:E:56:MET:SD	1:E:109:MET:HE3	2.51	0.51
1:I:46:HIS:ND1	1:I:121:MET:HE1	2.24	0.51
1:L:99:VAL:HG13	3:L:2808:HOH:O	2.11	0.51
1:G:76:ASP:HA	3:G:3115:HOH:O	2.11	0.50
1:E:44:MET:HE2	3:E:1313:HOH:O	2.11	0.50
1:E:85:LYS:HB2	3:E:1542:HOH:O	2.12	0.50
1:G:29:PHE:O	1:G:96:THR:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:LEU:HD12	1:H:127:LEU:HD21	1.94	0.49
1:K:21:THR:HG22	1:K:126:THR:HB	1.94	0.49
1:K:87:ILE:HB	1:K:91:GLU:HB2	1.95	0.49
1:K:13:MET:HG3	1:K:120:LEU:HD12	1.95	0.49
1:D:97:PHE:HB2	3:D:3127:HOH:O	2.13	0.48
1:B:103:LYS:HE2	1:B:106:GLU:HB2	1.95	0.48
1:I:46:HIS:CD2	1:I:121:MET:HE1	2.48	0.48
1:A:103:LYS:HZ3	1:A:106:GLU:HB2	1.78	0.48
1:L:64:MET:HG3	1:L:115:PRO:HB3	1.95	0.47
1:F:53:ALA:HA	1:F:109:MET:HG2	1.95	0.47
1:A:28:GLN:HB3	1:A:96:THR:HG22	1.96	0.47
1:D:15:PHE:CE1	1:D:121:MET:HE2	2.50	0.47
1:B:107:GLN:HA	3:B:2926:HOH:O	2.14	0.47
1:M:16:ASN:ND2	3:M:2510:HOH:O	2.48	0.46
1:E:56:MET:HG3	1:E:111:PHE:CE1	2.50	0.46
1:K:53:ALA:HA	1:K:109:MET:HG2	1.96	0.46
1:D:56:MET:O	1:D:60:VAL:HG23	2.14	0.46
1:H:127:LEU:HD13	3:H:2645:HOH:O	2.15	0.46
1:K:104:GLU:HB2	3:K:2324:HOH:O	2.16	0.45
1:L:13:MET:HE1	1:L:117:HIS:HA	1.97	0.45
1:L:24:LYS:HB2	1:L:128:LYS:OXT	2.16	0.45
1:I:64:MET:HE3	1:I:64:MET:HB2	1.84	0.45
1:K:20:ILE:O	1:K:125:LEU:HA	2.17	0.45
1:A:29:PHE:O	1:A:96:THR:HA	2.17	0.45
1:F:87:ILE:HB	1:F:91:GLU:HB2	1.99	0.44
1:H:4:SER:HA	1:H:30:THR:O	2.17	0.44
1:K:49:VAL:O	1:K:110:SER:HA	2.17	0.44
1:L:49:VAL:O	1:L:110:SER:HA	2.16	0.44
1:C:15:PHE:CE1	1:C:121:MET:HE2	2.51	0.44
1:K:8:GLN:HG2	1:K:34:SER:OG	2.16	0.44
1:B:74:LYS:O	1:B:77:ASP:HB2	2.17	0.44
1:D:11:ASP:O	1:D:44:MET:HE3	2.18	0.44
1:F:104:GLU:HB2	3:F:2748:HOH:O	2.17	0.44
1:K:92:LYS:HE2	3:K:630:HOH:O	2.17	0.44
1:D:118:SER:O	1:D:122:LYS:HE3	2.18	0.43
1:G:75:PRO:HA	3:G:1831:HOH:O	2.18	0.43
1:H:7:ILE:HD11	1:H:15:PHE:HB3	2.00	0.43
1:H:21:THR:HA	1:H:126:THR:O	2.18	0.43
1:I:87:ILE:HB	1:I:91:GLU:HB2	2.00	0.43
1:K:29:PHE:O	1:K:96:THR:HA	2.18	0.43
1:M:1:ALA:HB3	1:M:4:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:MET:HG3	1:H:115:PRO:HG3	2.00	0.43
1:B:33:LEU:HG	1:B:87:ILE:HD11	2.00	0.43
1:L:13:MET:CE	1:L:117:HIS:HA	2.49	0.43
1:A:15:PHE:CE1	1:A:121:MET:HE2	2.54	0.42
1:D:87:ILE:HB	1:D:91:GLU:HB2	2.01	0.42
1:G:48:TRP:O	1:G:83:HIS:HA	2.19	0.42
1:D:85:LYS:HB2	1:D:85:LYS:NZ	2.34	0.42
1:D:11:ASP:HA	1:D:44:MET:HG2	2.02	0.42
1:A:64:MET:HB2	3:A:578:HOH:O	2.18	0.42
1:L:102:LEU:HD12	3:L:2808:HOH:O	2.19	0.42
1:G:49:VAL:O	1:G:110:SER:HA	2.20	0.42
1:C:48:TRP:O	1:C:83:HIS:HA	2.20	0.41
1:C:107:GLN:HA	3:C:2058:HOH:O	2.20	0.41
1:K:64:MET:HE2	1:K:115:PRO:HA	2.01	0.41
1:B:49:VAL:O	1:B:110:SER:HA	2.20	0.41
1:E:58:GLY:HA2	3:E:2905:HOH:O	2.20	0.41
1:I:64:MET:HE2	1:I:115:PRO:HA	2.03	0.41
1:K:33:LEU:HG	1:K:87:ILE:HD11	2.02	0.41
1:F:114:PHE:O	1:F:117:HIS:HB2	2.21	0.41
1:E:22:VAL:O	1:E:127:LEU:HD23	2.20	0.41
1:K:31:VAL:O	1:K:94:SER:HA	2.21	0.41
1:D:53:ALA:HA	1:D:109:MET:HG3	2.04	0.40
1:A:48:TRP:O	1:A:83:HIS:HA	2.21	0.40
1:E:4:SER:HA	1:E:30:THR:O	2.21	0.40
1:L:74:LYS:NZ	1:L:77:ASP:HA	2.37	0.40
1:C:50:LEU:HD13	1:C:125:LEU:HD13	2.04	0.40

All (3) 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:D:70:LYS:HZ2	3:D:1944:HOH:H2[1_455]	1.32	0.28
1:C:79:ARG:HH12	3:K:2351:HOH:H1[2_646]	1.34	0.26
1:G:12:GLN:HE21	1:I:85:LYS:HZ3[1_554]	1.34	0.26

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	126/128 (98%)	117 (93%)	9 (7%)	0	100	100
1	B	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
1	C	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
1	D	126/128 (98%)	122 (97%)	3 (2%)	1 (1%)	16	20
1	E	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
1	F	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
1	G	126/128 (98%)	118 (94%)	7 (6%)	1 (1%)	16	20
1	H	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
1	I	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
1	K	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
1	L	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
1	M	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
All	All	1512/1536 (98%)	1450 (96%)	60 (4%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	3	CYS
1	D	13	MET

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	110/110 (100%)	102 (93%)	8 (7%)	13	18
1	B	110/110 (100%)	109 (99%)	1 (1%)	70	84
1	C	110/110 (100%)	102 (93%)	8 (7%)	13	18
1	D	110/110 (100%)	101 (92%)	9 (8%)	10	14
1	E	110/110 (100%)	107 (97%)	3 (3%)	39	58
1	F	110/110 (100%)	103 (94%)	7 (6%)	16	23
1	G	110/110 (100%)	101 (92%)	9 (8%)	10	14
1	H	110/110 (100%)	104 (94%)	6 (6%)	19	28
1	I	110/110 (100%)	102 (93%)	8 (7%)	13	18
1	K	110/110 (100%)	109 (99%)	1 (1%)	70	84
1	L	110/110 (100%)	102 (93%)	8 (7%)	13	18
1	M	110/110 (100%)	108 (98%)	2 (2%)	51	70
All	All	1320/1320 (100%)	1250 (95%)	70 (5%)	20	30

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	13	MET
1	A	75	PRO
1	A	103	LYS
1	A	118	SER
1	A	125	LEU
1	A	126	THR
1	A	127	LEU
1	B	94	SER
1	C	18	ASN
1	C	25	SER
1	C	98	ASP
1	C	100	SER
1	C	107	GLN
1	C	122	LYS
1	C	127	LEU
1	C	128	LYS
1	D	8	GLN
1	D	12	GLN
1	D	25	SER
1	D	27	LYS
1	D	85	LYS

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Mol	Chain	Res	Type
1	D	94	SER
1	D	103	LYS
1	D	106	GLU
1	D	128	LYS
1	E	38	ASN
1	E	107	GLN
1	E	127	LEU
1	F	15	PHE
1	F	35	HIS
1	F	52	THR
1	F	69	ASP
1	F	85	LYS
1	F	107	GLN
1	F	118	SER
1	G	2	GLU
1	G	6	ASP
1	G	28	GLN
1	G	69	ASP
1	G	74	LYS
1	G	76	ASP
1	G	100	SER
1	G	107	GLN
1	G	122	LYS
1	H	7	ILE
1	H	25	SER
1	H	34	SER
1	H	78	SER
1	H	120	LEU
1	H	128	LYS
1	I	38	ASN
1	I	100	SER
1	I	101	LYS
1	I	103	LYS
1	I	106	GLU
1	I	118	SER
1	I	125	LEU
1	I	128	LYS
1	K	122	LYS
1	L	28	GLN
1	L	38	ASN
1	L	44	MET
1	L	73	LEU

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Mol	Chain	Res	Type
1	L	81	ILE
1	L	118	SER
1	L	122	LYS
1	L	127	LEU
1	M	85	LYS
1	M	126	THR

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	8	GLN
1	A	107	GLN
1	B	8	GLN
1	B	18	ASN
1	C	8	GLN
1	D	28	GLN
1	D	32	ASN
1	F	12	GLN
1	G	32	ASN
1	H	8	GLN
1	I	18	ASN
1	K	57	GLN
1	L	8	GLN
1	L	12	GLN
1	L	42	ASN
1	M	28	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

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

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.