



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:00 PM UTC

PDB ID : 4G4E / pdb_00004g4e
Title : Crystal structure of the L88A mutant of HslV from Escherichia coli
Authors : Lee, J.W.; Park, E.; Yoo, H.M.; Ha, B.H.; An, J.Y.; Jeon, Y.J.; Seol, J.H.; Eom, S.H.; Chung, C.H.
Deposited on : 2012-07-16
Resolution : 2.89 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:

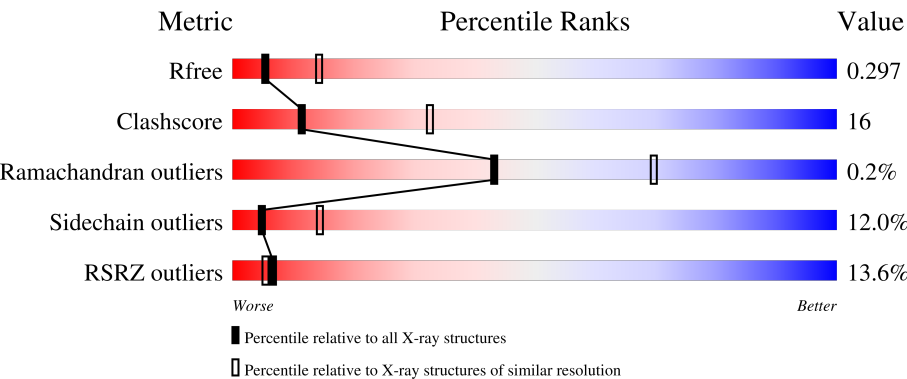
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	174	11% 66% 25% 5%
1	B	174	16% 70% 23%
1	C	174	16% 67% 25% 6%
1	D	174	12% 71% 21% 5%
1	E	174	24% 61% 30% 6%

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Mol	Chain	Length	Quality of chain			
1	F	174	13% 67% 26% 5%			
1	G	174	15% 76% 18%			
1	H	174	12% 72% 22%			
1	I	174	8% 72% 21%			
1	J	174	17% 71% 21% 5%			
1	K	174	7% 70% 23%			
1	L	174	8% 73% 20%			

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15432 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 ATP-dependent protease subunit HslV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	18	0	0
			1286	809	229	245	3			
1	B	169	Total	C	N	O	S	18	0	0
			1286	809	229	245	3			
1	C	169	Total	C	N	O	S	12	0	0
			1286	809	229	245	3			
1	D	169	Total	C	N	O	S	18	0	0
			1286	809	229	245	3			
1	E	169	Total	C	N	O	S	12	0	0
			1286	809	229	245	3			
1	F	169	Total	C	N	O	S	18	0	0
			1286	809	229	245	3			
1	G	169	Total	C	N	O	S	18	0	0
			1286	809	229	245	3			
1	H	169	Total	C	N	O	S	18	0	0
			1286	809	229	245	3			
1	I	169	Total	C	N	O	S	18	0	0
			1286	809	229	245	3			
1	J	169	Total	C	N	O	S	18	0	0
			1286	809	229	245	3			
1	K	169	Total	C	N	O	S	18	0	0
			1286	809	229	245	3			
1	L	169	Total	C	N	O	S	18	0	0
			1286	809	229	245	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	ALA	LEU	engineered mutation	UNP P0A7B8
B	88	ALA	LEU	engineered mutation	UNP P0A7B8
C	88	ALA	LEU	engineered mutation	UNP P0A7B8
D	88	ALA	LEU	engineered mutation	UNP P0A7B8
E	88	ALA	LEU	engineered mutation	UNP P0A7B8

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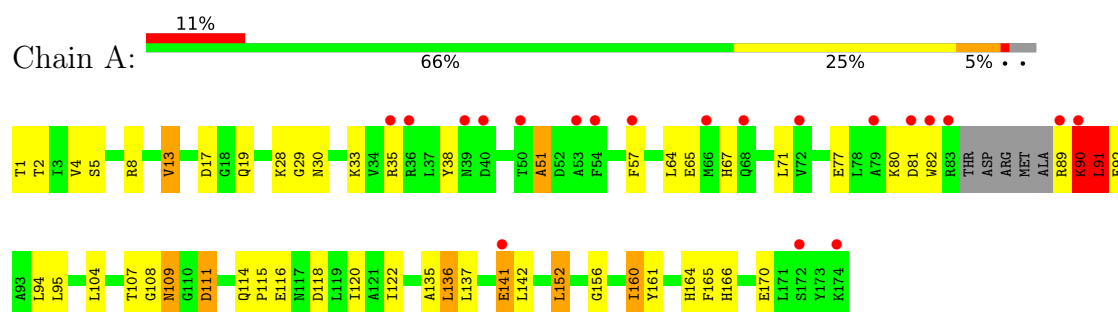
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Chain	Residue	Modelled	Actual	Comment	Reference
F	88	ALA	LEU	engineered mutation	UNP P0A7B8
G	88	ALA	LEU	engineered mutation	UNP P0A7B8
H	88	ALA	LEU	engineered mutation	UNP P0A7B8
I	88	ALA	LEU	engineered mutation	UNP P0A7B8
J	88	ALA	LEU	engineered mutation	UNP P0A7B8
K	88	ALA	LEU	engineered mutation	UNP P0A7B8
L	88	ALA	LEU	engineered mutation	UNP P0A7B8

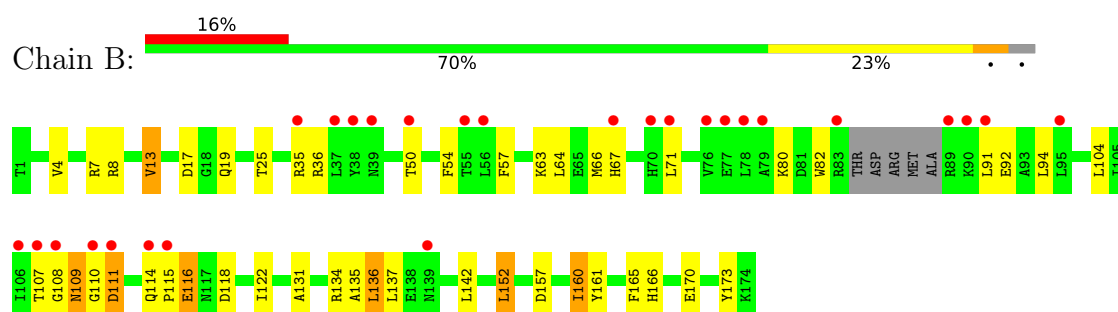
3 Residue-property plots [i](#)

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.

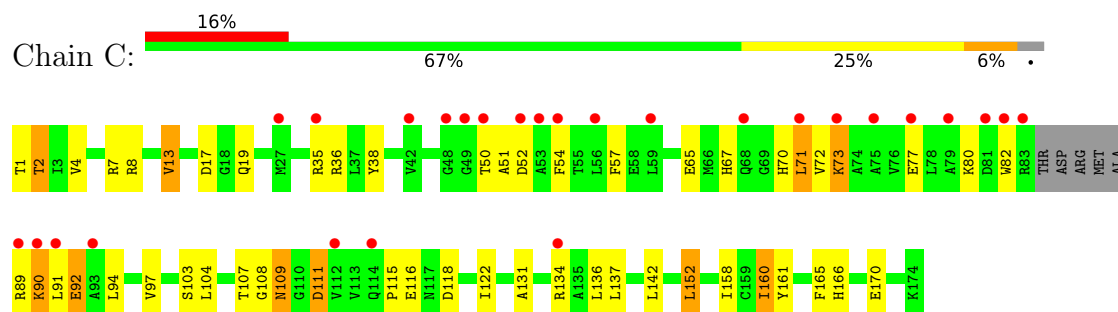
- Molecule 1: ATP-dependent protease subunit HslV



- Molecule 1: ATP-dependent protease subunit HslV

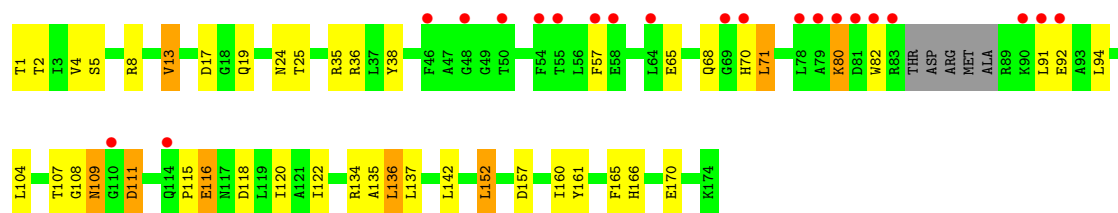


- Molecule 1: ATP-dependent protease subunit HslV

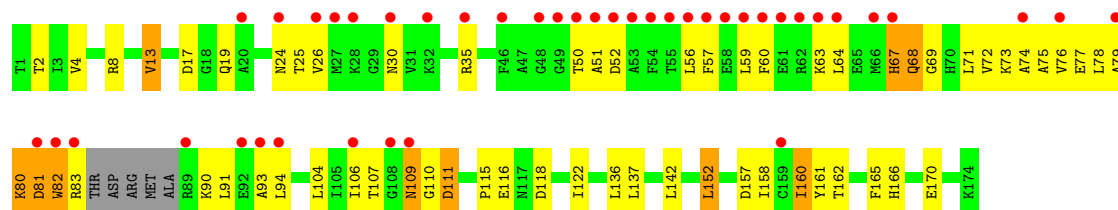


- Molecule 1: ATP-dependent protease subunit HslV

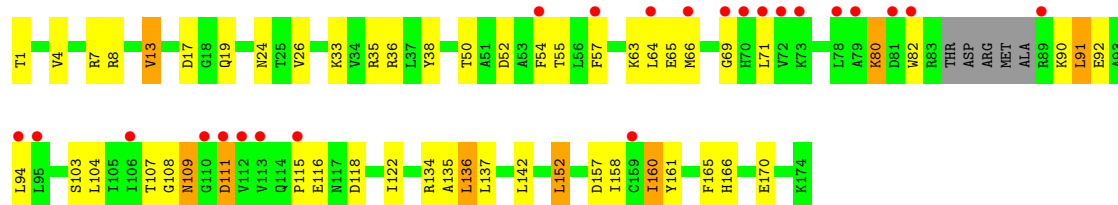




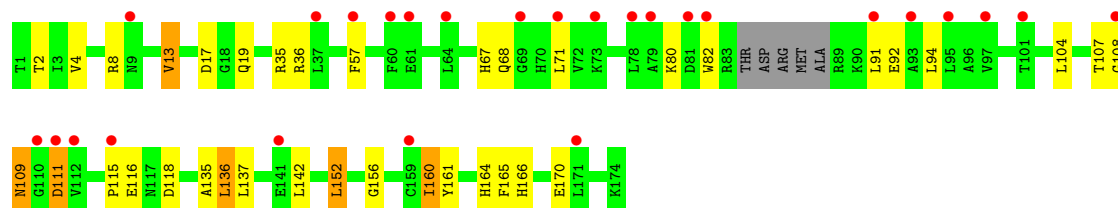
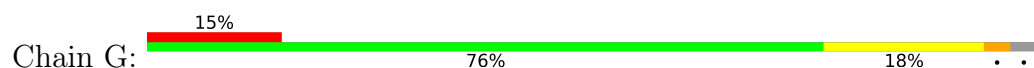
- Molecule 1: ATP-dependent protease subunit HslV



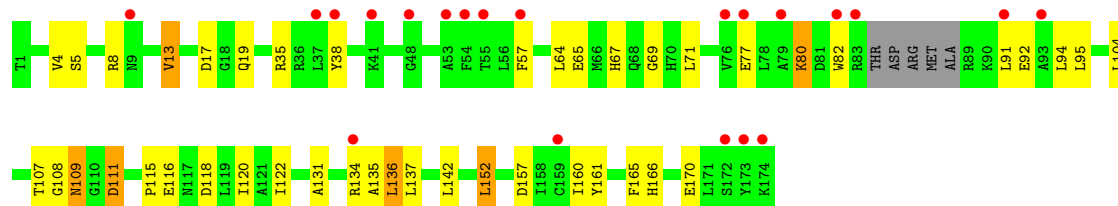
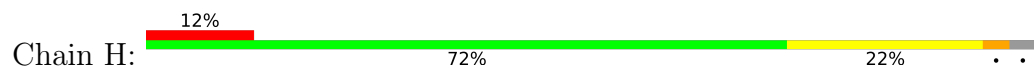
- Molecule 1: ATP-dependent protease subunit HslV



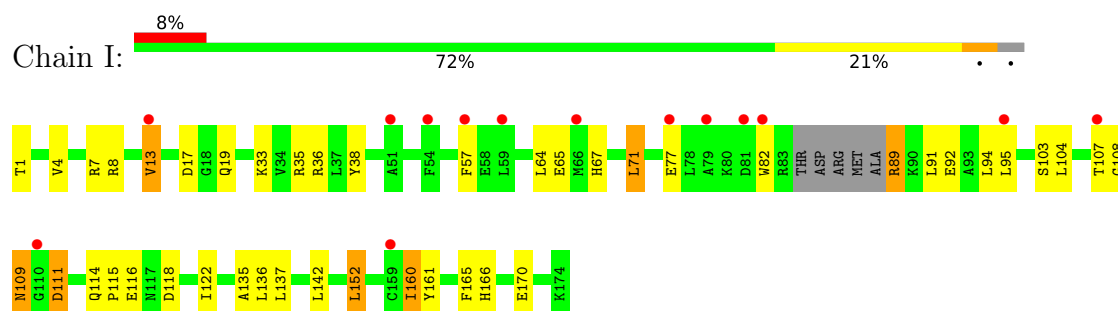
- Molecule 1: ATP-dependent protease subunit HslV



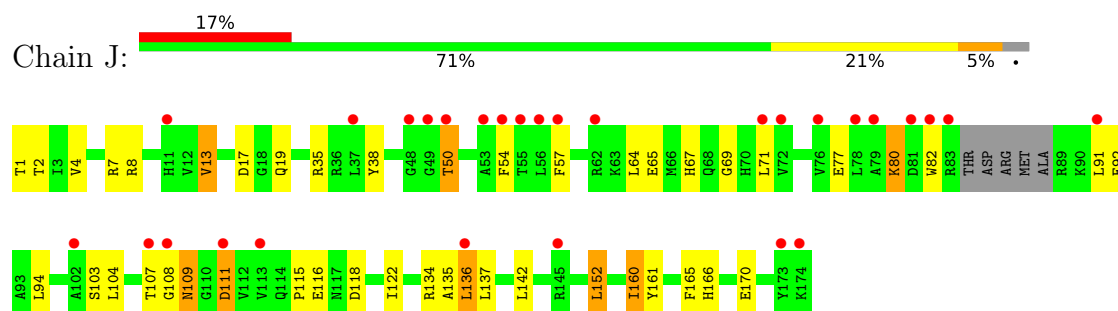
- Molecule 1: ATP-dependent protease subunit HslV



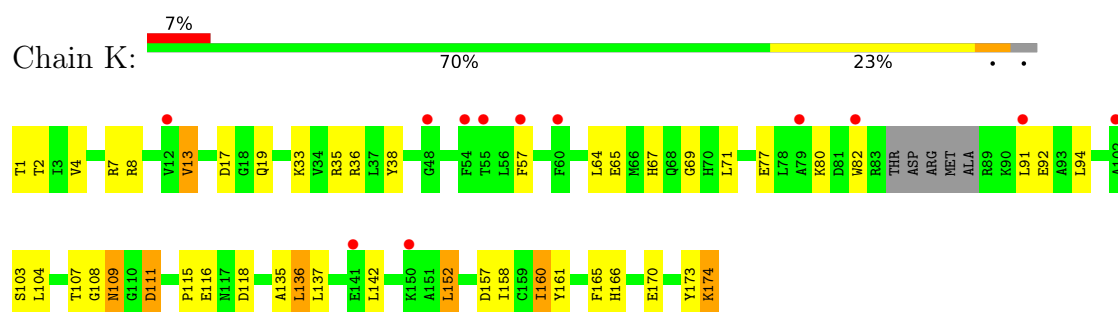
- Molecule 1: ATP-dependent protease subunit HslV



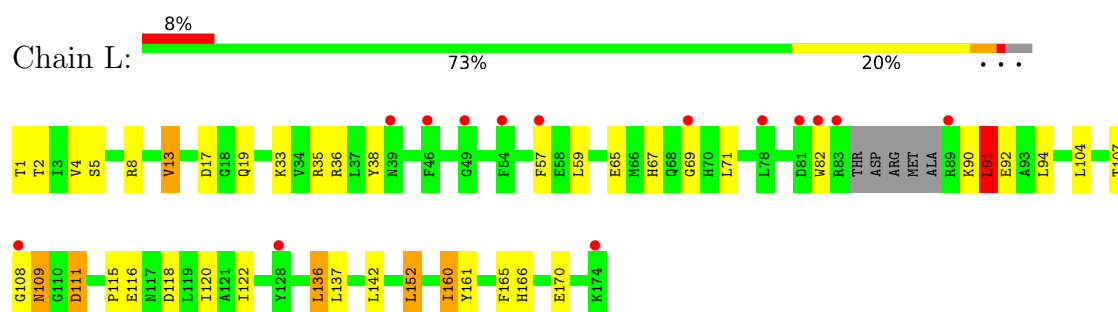
- Molecule 1: ATP-dependent protease subunit HslV



- Molecule 1: ATP-dependent protease subunit HslV



- Molecule 1: ATP-dependent protease subunit HslV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.28Å 167.12Å 90.31Å 90.00° 105.86° 90.00°	Depositor
Resolution (Å)	49.75 – 2.89 49.75 – 2.89	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.75-2.89) 92.7 (49.75-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.258 , 0.293 0.261 , 0.297	Depositor DCC
R_{free} test set	2291 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 79.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15432	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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	0.70	3/1302 (0.2%)	0.99	3/1758 (0.2%)
1	B	0.62	0/1302	0.90	0/1758
1	C	0.60	1/1302 (0.1%)	0.96	4/1758 (0.2%)
1	D	0.55	0/1302	0.90	0/1758
1	E	0.64	0/1302	1.03	6/1758 (0.3%)
1	F	0.52	0/1302	0.88	1/1758 (0.1%)
1	G	0.53	1/1302 (0.1%)	0.87	0/1758
1	H	0.53	0/1302	0.87	1/1758 (0.1%)
1	I	0.50	0/1302	0.90	2/1758 (0.1%)
1	J	0.52	0/1302	0.85	1/1758 (0.1%)
1	K	0.53	1/1302 (0.1%)	0.92	2/1758 (0.1%)
1	L	0.47	0/1302	0.89	0/1758
All	All	0.56	6/15624 (0.0%)	0.92	20/21096 (0.1%)

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	E	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	LYS	C-N	-8.86	1.21	1.33
1	A	51	ALA	CA-CB	-6.13	1.43	1.53
1	K	174	LYS	CA-CB	-6.08	1.41	1.53
1	C	73	LYS	N-CA	5.86	1.53	1.46
1	A	141	GLU	CB-CG	-5.61	1.35	1.52
1	G	2	THR	C-O	-5.38	1.17	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	174	LYS	N-CA-CB	-12.20	89.76	110.50
1	E	80	LYS	CB-CA-C	-9.94	90.64	110.42
1	E	81	ASP	N-CA-CB	-9.85	93.73	109.78
1	E	80	LYS	N-CA-C	9.58	131.21	110.80
1	A	90	LYS	O-C-N	-8.88	110.77	122.59
1	A	91	LEU	CA-C-N	-8.38	110.48	123.13
1	A	91	LEU	C-N-CA	-8.38	110.48	123.13
1	E	68	GLN	N-CA-CB	-7.58	97.68	110.49
1	E	81	ASP	N-CA-C	7.31	123.44	111.37
1	C	73	LYS	N-CA-CB	6.50	121.48	110.49
1	C	92	GLU	N-CA-C	6.18	118.87	107.99
1	I	89	ARG	CA-C-N	-6.00	115.03	122.84
1	I	89	ARG	C-N-CA	-6.00	115.03	122.84
1	E	82	TRP	N-CA-C	-5.77	104.97	112.23
1	C	72	VAL	CA-C-O	-5.69	115.14	121.17
1	K	174	LYS	CA-CB-CG	5.62	125.33	114.10
1	C	2	THR	N-CA-C	5.21	116.56	107.49
1	F	69	GLY	N-CA-C	-5.16	107.94	115.63
1	J	69	GLY	N-CA-C	-5.16	107.95	115.63
1	H	69	GLY	N-CA-C	-5.15	107.95	115.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	LYS	Peptide,Mainchain
1	E	67	HIS	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	1286	0	1303	66	0
1	B	1286	0	1303	40	0
1	C	1286	0	1303	38	0
1	D	1286	0	1303	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1286	0	1303	139	0
1	F	1286	0	1303	48	0
1	G	1286	0	1303	21	0
1	H	1286	0	1303	24	0
1	I	1286	0	1303	25	0
1	J	1286	0	1303	30	0
1	K	1286	0	1303	42	0
1	L	1286	0	1303	39	0
All	All	15432	0	15636	493	0

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 16.

All (493) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TRP:CZ2	1:A:91:LEU:HB2	1.37	1.55
1:E:56:LEU:HD11	1:E:82:TRP:CE3	1.49	1.47
1:E:80:LYS:CG	1:E:81:ASP:H	1.20	1.39
1:A:89:ARG:CB	1:A:90:LYS:HD2	1.55	1.33
1:E:80:LYS:HD2	1:E:81:ASP:CG	1.50	1.33
1:E:82:TRP:CH2	1:E:93:ALA:HB3	1.68	1.25
1:E:56:LEU:CD1	1:E:82:TRP:CE3	2.23	1.20
1:E:63:LYS:CE	1:E:77:GLU:HB3	1.70	1.20
1:E:56:LEU:HD11	1:E:82:TRP:CZ3	1.78	1.19
1:E:56:LEU:CD1	1:E:82:TRP:CZ3	2.25	1.18
1:E:82:TRP:HE1	1:E:91:LEU:CB	1.55	1.17
1:A:82:TRP:CZ2	1:A:91:LEU:CB	2.29	1.14
1:K:1:THR:HG23	1:K:33:LYS:HZ2	1.03	1.13
1:C:89:ARG:O	1:C:90:LYS:HG3	1.48	1.13
1:E:82:TRP:CZ3	1:E:93:ALA:HB3	1.84	1.13
1:L:82:TRP:CZ2	1:L:91:LEU:HB2	1.82	1.12
1:A:90:LYS:CD	1:A:90:LYS:H	1.48	1.11
1:E:82:TRP:HE1	1:E:91:LEU:HB2	1.07	1.11
1:A:90:LYS:H	1:A:90:LYS:CE	1.64	1.11
1:E:80:LYS:HG3	1:E:81:ASP:N	1.22	1.10
1:F:82:TRP:HE1	1:F:90:LYS:HA	1.17	1.10
1:A:89:ARG:HB3	1:A:90:LYS:CD	1.83	1.09
1:E:80:LYS:HD2	1:E:81:ASP:OD1	1.52	1.09
1:D:68:GLN:HB2	1:D:70:HIS:CD2	1.89	1.07
1:E:60:PHE:HB2	1:E:78:LEU:HD22	1.35	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:TRP:CH2	1:E:93:ALA:CB	2.37	1.06
1:K:1:THR:HG23	1:K:33:LYS:NZ	1.70	1.06
1:E:80:LYS:CD	1:E:81:ASP:CG	2.30	1.05
1:A:90:LYS:N	1:A:90:LYS:HE3	1.76	1.01
1:E:56:LEU:CG	1:E:82:TRP:CE3	2.44	1.00
1:E:80:LYS:O	1:E:83:ARG:HB2	1.61	1.00
1:E:56:LEU:HD21	1:E:82:TRP:CE3	1.96	0.99
1:A:82:TRP:HZ2	1:A:91:LEU:CB	1.70	0.99
1:A:1:THR:HG23	1:A:17:ASP:OD1	1.62	0.99
1:I:82:TRP:CZ2	1:I:91:LEU:HB2	1.97	0.99
1:E:63:LYS:HE2	1:E:77:GLU:CB	1.93	0.98
1:E:75:ALA:HB1	1:E:106:ILE:HD11	1.42	0.98
1:E:80:LYS:HD2	1:E:81:ASP:OD2	1.64	0.97
1:E:75:ALA:CB	1:E:106:ILE:HD11	1.95	0.96
1:K:1:THR:CG2	1:K:33:LYS:NZ	2.27	0.96
1:E:63:LYS:HE2	1:E:77:GLU:HB3	0.97	0.95
1:A:90:LYS:CD	1:A:90:LYS:N	2.30	0.94
1:E:56:LEU:HD11	1:E:82:TRP:HE3	1.16	0.94
1:E:77:GLU:O	1:E:80:LYS:HG2	1.67	0.94
1:E:82:TRP:NE1	1:E:91:LEU:HB2	1.82	0.94
1:A:90:LYS:CE	1:A:90:LYS:N	2.30	0.94
1:E:52:ASP:HB3	1:E:82:TRP:CZ2	2.03	0.93
1:E:82:TRP:NE1	1:E:91:LEU:CB	2.31	0.93
1:E:56:LEU:CD1	1:E:82:TRP:HZ3	1.78	0.92
1:E:56:LEU:HG	1:E:82:TRP:CZ3	2.03	0.92
1:L:82:TRP:HZ2	1:L:91:LEU:HB2	1.32	0.92
1:E:56:LEU:CG	1:E:82:TRP:CZ3	2.52	0.92
1:E:63:LYS:HB3	1:E:74:ALA:HA	1.53	0.91
1:E:67:HIS:CD2	1:E:73:LYS:HE3	2.08	0.89
1:E:63:LYS:HE3	1:E:77:GLU:OE1	1.74	0.88
1:L:1:THR:HG23	1:L:17:ASP:OD1	1.73	0.88
1:C:89:ARG:O	1:C:90:LYS:CG	2.23	0.87
1:E:56:LEU:CD1	1:E:82:TRP:HE3	1.76	0.87
1:E:56:LEU:CD2	1:E:82:TRP:CE3	2.57	0.86
1:E:80:LYS:HG3	1:E:81:ASP:CB	2.05	0.86
1:A:89:ARG:HB3	1:A:90:LYS:HD2	0.86	0.86
1:C:134:ARG:HH22	1:E:157:ASP:HB3	1.39	0.86
1:E:67:HIS:O	1:E:68:GLN:HB2	1.74	0.85
1:A:90:LYS:H	1:A:90:LYS:HE3	1.35	0.85
1:A:90:LYS:HD2	1:A:90:LYS:H	1.26	0.83
1:E:82:TRP:HH2	1:E:93:ALA:CB	1.88	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ALA:HB1	1:E:106:ILE:CD1	2.10	0.81
1:E:82:TRP:HE1	1:E:91:LEU:HB3	1.46	0.81
1:B:135:ALA:HB1	1:H:136:LEU:HD13	1.63	0.79
1:E:60:PHE:HB2	1:E:78:LEU:CD2	2.13	0.78
1:E:56:LEU:HD21	1:E:82:TRP:HE3	1.48	0.78
1:A:90:LYS:O	1:A:91:LEU:C	2.21	0.78
1:E:80:LYS:CD	1:E:81:ASP:OD1	2.30	0.78
1:I:82:TRP:HZ2	1:I:91:LEU:HB2	1.49	0.77
1:A:91:LEU:N	1:A:91:LEU:HD23	2.00	0.77
1:E:82:TRP:NE1	1:E:91:LEU:HB3	1.98	0.76
1:L:82:TRP:CZ2	1:L:91:LEU:CB	2.68	0.76
1:E:52:ASP:HB3	1:E:82:TRP:CH2	2.20	0.76
1:E:60:PHE:HE1	1:E:75:ALA:CA	1.99	0.75
1:K:1:THR:HG23	1:K:17:ASP:OD1	1.86	0.75
1:K:1:THR:CG2	1:K:33:LYS:HZ3	1.99	0.75
1:E:82:TRP:O	1:E:83:ARG:C	2.30	0.74
1:A:1:THR:HG23	1:A:33:LYS:HZ2	1.52	0.74
1:E:59:LEU:HD21	1:E:81:ASP:HB3	1.71	0.73
1:A:90:LYS:HD2	1:A:90:LYS:N	1.99	0.73
1:F:82:TRP:HE1	1:F:90:LYS:CA	2.00	0.73
1:D:82:TRP:CZ2	1:D:91:LEU:HB2	2.24	0.72
1:E:59:LEU:HB3	1:E:78:LEU:HD13	1.70	0.72
1:E:79:ALA:HB1	1:E:110:GLY:O	1.88	0.72
1:C:134:ARG:NH2	1:E:157:ASP:HB3	2.06	0.71
1:H:82:TRP:CZ2	1:H:91:LEU:HB2	2.26	0.71
1:F:52:ASP:HB3	1:F:91:LEU:HB3	1.73	0.71
1:E:63:LYS:CE	1:E:77:GLU:CB	2.59	0.71
1:E:80:LYS:CG	1:E:81:ASP:CG	2.64	0.71
1:K:82:TRP:CZ2	1:K:91:LEU:HB2	2.26	0.71
1:F:52:ASP:HB3	1:F:91:LEU:CB	2.21	0.70
1:L:91:LEU:HD23	1:L:91:LEU:H	1.55	0.70
1:E:80:LYS:HG3	1:E:81:ASP:CA	2.21	0.70
1:A:28:LYS:NZ	1:B:114:GLN:O	2.23	0.70
1:C:134:ARG:HH22	1:E:157:ASP:CB	2.05	0.70
1:G:82:TRP:CZ2	1:G:91:LEU:HB2	2.27	0.70
1:F:91:LEU:HD12	1:F:91:LEU:H	1.57	0.70
1:K:1:THR:CG2	1:K:33:LYS:HZ2	1.86	0.69
1:E:80:LYS:CG	1:E:81:ASP:N	1.98	0.69
1:E:82:TRP:HH2	1:E:93:ALA:HB2	1.56	0.69
1:E:80:LYS:O	1:E:83:ARG:CB	2.39	0.69
1:B:82:TRP:CZ2	1:B:91:LEU:HB2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASP:OD1	1:B:111:ASP:N	2.25	0.69
1:A:136:LEU:HD13	1:G:135:ALA:HB1	1.75	0.69
1:L:91:LEU:HD23	1:L:91:LEU:N	2.08	0.68
1:E:56:LEU:CD2	1:E:82:TRP:HE3	1.99	0.68
1:F:111:ASP:OD1	1:F:111:ASP:N	2.26	0.68
1:I:111:ASP:OD1	1:I:111:ASP:N	2.26	0.68
1:J:82:TRP:CZ2	1:J:91:LEU:HB2	2.29	0.68
1:L:111:ASP:OD1	1:L:111:ASP:N	2.27	0.68
1:D:111:ASP:OD1	1:D:111:ASP:N	2.27	0.67
1:D:1:THR:HG22	1:D:2:THR:N	2.09	0.67
1:J:135:ALA:HB1	1:K:136:LEU:HD13	1.76	0.67
1:J:111:ASP:N	1:J:111:ASP:OD1	2.28	0.67
1:E:56:LEU:HD12	1:E:82:TRP:HZ3	1.56	0.67
1:E:111:ASP:N	1:E:111:ASP:OD1	2.26	0.67
1:K:1:THR:HG21	1:K:33:LYS:HD3	1.76	0.67
1:L:1:THR:HG23	1:L:33:LYS:HZ2	1.58	0.67
1:E:80:LYS:CD	1:E:81:ASP:OD2	2.40	0.66
1:H:111:ASP:OD1	1:H:111:ASP:N	2.28	0.66
1:E:60:PHE:CE1	1:E:75:ALA:CA	2.78	0.66
1:K:111:ASP:OD1	1:K:111:ASP:N	2.28	0.66
1:E:67:HIS:NE2	1:E:73:LYS:HE3	2.11	0.66
1:A:111:ASP:OD1	1:A:111:ASP:N	2.26	0.65
1:E:63:LYS:CB	1:E:74:ALA:HA	2.24	0.65
1:L:82:TRP:CH2	1:L:108:GLY:HA2	2.32	0.65
1:C:111:ASP:N	1:C:111:ASP:OD1	2.27	0.65
1:H:82:TRP:CH2	1:H:108:GLY:HA2	2.32	0.65
1:A:51:ALA:HB2	1:B:110:GLY:O	1.97	0.64
1:E:60:PHE:HE1	1:E:75:ALA:N	1.95	0.64
1:E:80:LYS:HG3	1:E:81:ASP:CG	2.22	0.64
1:G:111:ASP:OD1	1:G:111:ASP:N	2.28	0.64
1:A:1:THR:HG22	1:A:2:THR:N	2.11	0.64
1:E:63:LYS:CD	1:E:77:GLU:CB	2.76	0.64
1:F:82:TRP:CH2	1:F:108:GLY:HA2	2.32	0.64
1:E:63:LYS:CD	1:E:77:GLU:HB3	2.28	0.64
1:A:82:TRP:CH2	1:A:108:GLY:HA2	2.33	0.64
1:I:82:TRP:CH2	1:I:108:GLY:HA2	2.33	0.63
1:K:82:TRP:CH2	1:K:108:GLY:HA2	2.33	0.63
1:G:82:TRP:CH2	1:G:108:GLY:HA2	2.34	0.63
1:D:68:GLN:HB2	1:D:70:HIS:HD2	1.62	0.63
1:D:82:TRP:CH2	1:D:108:GLY:HA2	2.34	0.62
1:B:82:TRP:CH2	1:B:108:GLY:HA2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:THR:HG21	1:A:33:LYS:HD3	1.81	0.62
1:A:1:THR:CG2	1:A:33:LYS:NZ	2.63	0.62
1:C:89:ARG:C	1:C:90:LYS:HG3	2.23	0.62
1:K:1:THR:CG2	1:K:17:ASP:OD1	2.48	0.62
1:A:82:TRP:CE2	1:A:91:LEU:HB2	2.23	0.62
1:C:82:TRP:CH2	1:C:108:GLY:HA2	2.34	0.62
1:F:82:TRP:HZ2	1:F:91:LEU:O	1.83	0.62
1:D:136:LEU:HD13	1:F:135:ALA:HB1	1.81	0.61
1:B:160:ILE:HD11	1:C:19:GLN:OE1	2.00	0.61
1:D:68:GLN:CB	1:D:70:HIS:CD2	2.77	0.61
1:E:60:PHE:CE1	1:E:75:ALA:N	2.69	0.60
1:K:1:THR:HG21	1:K:33:LYS:NZ	2.16	0.60
1:E:160:ILE:HB	1:F:24:ASN:O	2.01	0.60
1:E:82:TRP:CE2	1:E:91:LEU:HB3	2.36	0.60
1:B:131:ALA:HB3	1:H:131:ALA:HB3	1.83	0.60
1:D:19:GLN:NE2	1:D:161:TYR:C	2.59	0.60
1:B:160:ILE:HG13	1:C:160:ILE:O	2.02	0.60
1:L:1:THR:HG21	1:L:33:LYS:HD3	1.83	0.60
1:L:1:THR:HG22	1:L:2:THR:N	2.17	0.60
1:E:72:VAL:O	1:E:76:VAL:HG23	2.01	0.60
1:B:25:THR:HA	1:C:158:ILE:O	2.01	0.60
1:E:24:ASN:O	1:F:160:ILE:HB	2.02	0.59
1:C:1:THR:HG22	1:C:2:THR:N	2.16	0.59
1:E:75:ALA:CB	1:E:106:ILE:CD1	2.76	0.59
1:E:67:HIS:CD2	1:E:73:LYS:CE	2.84	0.59
1:L:1:THR:CG2	1:L:33:LYS:NZ	2.65	0.59
1:A:141:GLU:CD	1:A:141:GLU:N	2.59	0.59
1:E:60:PHE:HE1	1:E:75:ALA:HB2	1.66	0.59
1:F:90:LYS:HD3	1:F:109:ASN:HA	1.84	0.59
1:A:141:GLU:CD	1:A:141:GLU:H	2.10	0.58
1:J:82:TRP:CH2	1:J:108:GLY:HA2	2.38	0.58
1:E:60:PHE:HE1	1:E:75:ALA:CB	2.17	0.58
1:E:63:LYS:HD2	1:E:77:GLU:HG3	1.85	0.58
1:D:82:TRP:HZ2	1:D:91:LEU:HB2	1.67	0.58
1:A:1:THR:HG23	1:A:33:LYS:NZ	2.19	0.58
1:L:19:GLN:NE2	1:L:161:TYR:C	2.61	0.58
1:F:55:THR:HG21	1:F:91:LEU:HD21	1.86	0.58
1:A:82:TRP:HZ2	1:A:91:LEU:HB2	0.80	0.58
1:E:79:ALA:O	1:E:83:ARG:HG3	2.03	0.58
1:C:19:GLN:NE2	1:C:161:TYR:C	2.63	0.57
1:E:60:PHE:CE1	1:E:75:ALA:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ASN:N	1:F:109:ASN:OD1	2.37	0.57
1:E:60:PHE:CE1	1:E:75:ALA:HA	2.38	0.57
1:K:82:TRP:HZ2	1:K:91:LEU:HB2	1.69	0.56
1:E:109:ASN:OD1	1:E:109:ASN:N	2.37	0.56
1:F:82:TRP:CZ2	1:F:91:LEU:O	2.57	0.56
1:D:109:ASN:N	1:D:109:ASN:OD1	2.38	0.56
1:E:80:LYS:C	1:E:83:ARG:HB2	2.29	0.56
1:H:109:ASN:OD1	1:H:109:ASN:N	2.39	0.56
1:D:1:THR:CG2	1:D:2:THR:N	2.69	0.56
1:J:19:GLN:NE2	1:J:161:TYR:C	2.63	0.56
1:G:82:TRP:HZ2	1:G:91:LEU:HB2	1.70	0.56
1:G:156:GLY:C	1:G:164:HIS:HE1	2.13	0.56
1:B:82:TRP:HZ2	1:B:91:LEU:HB2	1.70	0.55
1:A:1:THR:CG2	1:A:17:ASP:OD1	2.48	0.55
1:J:109:ASN:OD1	1:J:109:ASN:N	2.39	0.55
1:J:160:ILE:HG13	1:L:160:ILE:O	2.07	0.55
1:E:59:LEU:HD21	1:E:81:ASP:CB	2.34	0.55
1:F:52:ASP:CB	1:F:91:LEU:HB3	2.37	0.55
1:C:109:ASN:OD1	1:C:109:ASN:N	2.39	0.55
1:E:13:VAL:HG12	1:E:170:GLU:HG3	1.89	0.55
1:F:13:VAL:HG12	1:F:170:GLU:HG3	1.89	0.55
1:J:8:ARG:NH1	1:J:142:LEU:O	2.40	0.55
1:K:19:GLN:NE2	1:K:161:TYR:C	2.65	0.55
1:A:19:GLN:NE2	1:A:161:TYR:C	2.65	0.55
1:B:134:ARG:HH22	1:H:157:ASP:CB	2.20	0.54
1:K:109:ASN:N	1:K:109:ASN:OD1	2.39	0.54
1:A:13:VAL:HG12	1:A:170:GLU:HG3	1.90	0.54
1:A:109:ASN:N	1:A:109:ASN:OD1	2.40	0.54
1:B:25:THR:HG22	1:C:158:ILE:HG22	1.88	0.54
1:E:63:LYS:HG3	1:E:77:GLU:HB2	1.88	0.54
1:I:109:ASN:N	1:I:109:ASN:OD1	2.40	0.54
1:F:82:TRP:CZ2	1:F:91:LEU:HD12	2.43	0.54
1:L:1:THR:HG23	1:L:33:LYS:NZ	2.21	0.54
1:E:60:PHE:CD1	1:E:75:ALA:HA	2.43	0.54
1:B:13:VAL:HG12	1:B:170:GLU:HG3	1.90	0.54
1:E:19:GLN:NE2	1:E:161:TYR:C	2.65	0.54
1:B:109:ASN:OD1	1:B:109:ASN:N	2.39	0.54
1:E:82:TRP:CH2	1:E:93:ALA:HB2	2.30	0.54
1:G:109:ASN:OD1	1:G:109:ASN:N	2.41	0.54
1:L:82:TRP:HZ2	1:L:91:LEU:CB	2.11	0.54
1:C:13:VAL:HG12	1:C:170:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:VAL:HG12	1:G:170:GLU:HG3	1.90	0.54
1:H:82:TRP:HZ2	1:H:91:LEU:HB2	1.69	0.54
1:A:8:ARG:NH1	1:A:142:LEU:O	2.39	0.53
1:D:116:GLU:HG3	1:E:30:ASN:ND2	2.23	0.53
1:J:134:ARG:HH22	1:K:157:ASP:CB	2.20	0.53
1:L:13:VAL:HG12	1:L:170:GLU:HG3	1.89	0.53
1:E:67:HIS:O	1:E:69:GLY:N	2.41	0.53
1:A:89:ARG:CB	1:A:90:LYS:CD	2.42	0.53
1:F:19:GLN:NE2	1:F:161:TYR:C	2.67	0.53
1:C:89:ARG:HD2	1:C:91:LEU:HD12	1.90	0.53
1:H:19:GLN:NE2	1:H:161:TYR:C	2.67	0.53
1:E:63:LYS:CE	1:E:77:GLU:OE1	2.51	0.53
1:E:80:LYS:HG3	1:E:81:ASP:HB2	1.86	0.53
1:F:91:LEU:H	1:F:91:LEU:CD1	2.13	0.53
1:E:90:LYS:C	1:E:91:LEU:HG	2.34	0.53
1:K:13:VAL:HG12	1:K:170:GLU:HG3	1.90	0.53
1:A:1:THR:CG2	1:A:2:THR:N	2.72	0.52
1:E:82:TRP:CZ2	1:E:91:LEU:HB3	2.44	0.52
1:F:82:TRP:NE1	1:F:90:LYS:HA	2.02	0.52
1:A:51:ALA:HB2	1:B:111:ASP:HA	1.91	0.52
1:A:156:GLY:C	1:A:164:HIS:HE1	2.17	0.52
1:J:13:VAL:HG12	1:J:170:GLU:HG3	1.91	0.52
1:A:28:LYS:HD2	1:B:114:GLN:O	2.09	0.52
1:K:1:THR:HG21	1:K:33:LYS:CD	2.39	0.52
1:E:2:THR:OG1	1:E:162:THR:HG21	2.10	0.52
1:B:19:GLN:NE2	1:B:161:TYR:C	2.68	0.52
1:E:52:ASP:OD1	1:E:91:LEU:HD22	2.09	0.52
1:K:1:THR:HG22	1:K:2:THR:H	1.75	0.51
1:E:8:ARG:NH1	1:E:142:LEU:O	2.41	0.51
1:D:13:VAL:HG12	1:D:170:GLU:HG3	1.93	0.51
1:E:80:LYS:HG3	1:E:81:ASP:H	0.37	0.51
1:L:67:HIS:C	1:L:69:GLY:H	2.18	0.51
1:E:63:LYS:HD2	1:E:77:GLU:CG	2.40	0.51
1:F:91:LEU:HD12	1:F:91:LEU:N	2.25	0.51
1:A:135:ALA:HB1	1:G:136:LEU:HD13	1.93	0.51
1:B:17:ASP:HA	1:B:165:PHE:O	2.11	0.51
1:D:157:ASP:CB	1:F:134:ARG:HH22	2.24	0.51
1:D:19:GLN:HE22	1:D:161:TYR:C	2.19	0.51
1:F:8:ARG:NH1	1:F:142:LEU:O	2.40	0.51
1:L:90:LYS:O	1:L:91:LEU:O	2.29	0.51
1:J:17:ASP:HA	1:J:165:PHE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:PRO:HG2	1:L:118:ASP:HA	1.94	0.50
1:A:17:ASP:HA	1:A:165:PHE:O	2.12	0.50
1:E:56:LEU:CG	1:E:82:TRP:HE3	2.05	0.50
1:E:56:LEU:HD22	1:E:78:LEU:HD11	1.92	0.50
1:F:52:ASP:HB3	1:F:91:LEU:HB2	1.93	0.50
1:J:82:TRP:HZ2	1:J:91:LEU:HB2	1.73	0.50
1:E:26:VAL:N	1:F:158:ILE:O	2.37	0.50
1:E:115:PRO:HG2	1:E:118:ASP:HA	1.94	0.50
1:G:17:ASP:HA	1:G:165:PHE:O	2.12	0.50
1:I:13:VAL:HG12	1:I:170:GLU:HG3	1.93	0.50
1:H:17:ASP:HA	1:H:165:PHE:O	2.11	0.50
1:E:52:ASP:CB	1:E:82:TRP:CH2	2.92	0.50
1:K:8:ARG:NH1	1:K:142:LEU:O	2.43	0.50
1:H:13:VAL:HG12	1:H:170:GLU:HG3	1.94	0.49
1:C:17:ASP:HA	1:C:165:PHE:O	2.11	0.49
1:L:8:ARG:NH1	1:L:142:LEU:O	2.43	0.49
1:B:63:LYS:HA	1:B:66:MET:HB3	1.94	0.49
1:C:8:ARG:NH1	1:C:142:LEU:O	2.40	0.49
1:C:82:TRP:HZ2	1:C:91:LEU:O	1.95	0.49
1:D:134:ARG:HH22	1:F:157:ASP:HB3	1.77	0.49
1:J:115:PRO:HG2	1:J:118:ASP:HA	1.94	0.49
1:F:17:ASP:HA	1:F:165:PHE:O	2.12	0.49
1:H:152:LEU:HD13	1:H:166:HIS:CE1	2.48	0.49
1:I:19:GLN:NE2	1:I:161:TYR:C	2.71	0.49
1:E:25:THR:HA	1:F:158:ILE:O	2.13	0.49
1:A:1:THR:HG22	1:A:2:THR:H	1.78	0.48
1:C:115:PRO:HG2	1:C:118:ASP:HA	1.94	0.48
1:E:90:LYS:O	1:E:91:LEU:HG	2.12	0.48
1:A:91:LEU:HD23	1:A:91:LEU:H	1.77	0.48
1:D:1:THR:O	1:D:2:THR:OG1	2.30	0.48
1:I:17:ASP:HA	1:I:165:PHE:O	2.13	0.48
1:C:1:THR:O	1:C:2:THR:OG1	2.30	0.48
1:L:109:ASN:OD1	1:L:109:ASN:N	2.46	0.48
1:B:80:LYS:HE3	1:B:80:LYS:HB3	1.62	0.48
1:D:135:ALA:HB1	1:F:136:LEU:HD13	1.94	0.48
1:H:8:ARG:NH1	1:H:142:LEU:O	2.43	0.48
1:L:17:ASP:HA	1:L:165:PHE:O	2.13	0.48
1:E:17:ASP:HA	1:E:165:PHE:O	2.13	0.48
1:H:115:PRO:HG2	1:H:118:ASP:HA	1.94	0.48
1:J:136:LEU:HD13	1:K:135:ALA:HB1	1.96	0.48
1:L:1:THR:CG2	1:L:2:THR:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ASP:HA	1:D:165:PHE:O	2.14	0.48
1:E:35:ARG:HG3	1:E:57:PHE:HE2	1.79	0.48
1:G:19:GLN:NE2	1:G:161:TYR:C	2.71	0.48
1:G:80:LYS:HE3	1:G:80:LYS:HB3	1.61	0.48
1:J:1:THR:HG22	1:J:2:THR:N	2.29	0.48
1:J:160:ILE:HD11	1:L:19:GLN:OE1	2.13	0.48
1:K:1:THR:HG22	1:K:2:THR:N	2.29	0.48
1:E:56:LEU:HG	1:E:82:TRP:CE3	2.31	0.47
1:I:115:PRO:HG2	1:I:118:ASP:HA	1.96	0.47
1:A:28:LYS:CE	1:B:114:GLN:O	2.61	0.47
1:E:63:LYS:HD2	1:E:77:GLU:CB	2.43	0.47
1:D:115:PRO:HG2	1:D:118:ASP:HA	1.96	0.47
1:C:7:ARG:NH2	1:C:103:SER:OG	2.46	0.47
1:I:35:ARG:HG3	1:I:57:PHE:HE2	1.80	0.47
1:L:1:THR:OG1	1:L:33:LYS:NZ	2.47	0.47
1:L:67:HIS:O	1:L:69:GLY:N	2.47	0.47
1:E:64:LEU:HA	1:E:74:ALA:HB2	1.97	0.47
1:I:152:LEU:HD13	1:I:166:HIS:CE1	2.49	0.47
1:L:19:GLN:HE22	1:L:161:TYR:C	2.23	0.47
1:E:59:LEU:HB3	1:E:78:LEU:CD1	2.40	0.47
1:B:8:ARG:NH1	1:B:142:LEU:O	2.42	0.47
1:E:160:ILE:CD1	1:F:26:VAL:HG23	2.45	0.47
1:G:115:PRO:HG2	1:G:118:ASP:HA	1.96	0.47
1:F:115:PRO:HG2	1:F:118:ASP:HA	1.96	0.47
1:A:35:ARG:HG3	1:A:57:PHE:HE2	1.79	0.47
1:K:115:PRO:HG2	1:K:118:ASP:HA	1.97	0.47
1:A:29:GLY:N	1:B:116:GLU:OE2	2.42	0.46
1:K:17:ASP:HA	1:K:165:PHE:O	2.14	0.46
1:A:1:THR:CG2	1:A:2:THR:H	2.28	0.46
1:C:35:ARG:HG3	1:C:57:PHE:HE2	1.80	0.46
1:D:111:ASP:N	1:E:51:ALA:HB2	2.30	0.46
1:D:111:ASP:CA	1:E:51:ALA:HB2	2.46	0.46
1:E:19:GLN:HE22	1:E:161:TYR:C	2.23	0.46
1:B:135:ALA:HB1	1:H:136:LEU:CD1	2.38	0.46
1:D:111:ASP:HB3	1:E:50:THR:HB	1.98	0.46
1:A:80:LYS:HD2	1:A:81:ASP:N	2.31	0.46
1:C:52:ASP:OD1	1:C:91:LEU:HB3	2.15	0.46
1:E:63:LYS:CG	1:E:77:GLU:HB2	2.46	0.46
1:E:152:LEU:HD13	1:E:166:HIS:CE1	2.51	0.46
1:L:35:ARG:HG3	1:L:57:PHE:HE2	1.81	0.46
1:A:29:GLY:H	1:B:116:GLU:CD	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LYS:HB3	1:C:80:LYS:HE3	1.65	0.46
1:B:35:ARG:HG3	1:B:57:PHE:HE2	1.81	0.46
1:J:80:LYS:HB3	1:J:80:LYS:HE3	1.60	0.46
1:C:1:THR:CG2	1:C:2:THR:N	2.79	0.45
1:E:60:PHE:CB	1:E:78:LEU:HD22	2.25	0.45
1:K:152:LEU:HD13	1:K:166:HIS:CE1	2.51	0.45
1:K:173:TYR:CD1	1:K:174:LYS:N	2.84	0.45
1:H:35:ARG:HG3	1:H:57:PHE:HE2	1.82	0.45
1:L:1:THR:CG2	1:L:33:LYS:HZ3	2.28	0.45
1:B:115:PRO:HG2	1:B:118:ASP:HA	1.97	0.45
1:E:59:LEU:CB	1:E:78:LEU:HD13	2.43	0.45
1:L:90:LYS:O	1:L:91:LEU:C	2.59	0.45
1:B:36:ARG:NH2	1:B:170:GLU:O	2.49	0.45
1:D:35:ARG:HG3	1:D:57:PHE:HE2	1.81	0.45
1:D:80:LYS:HB3	1:D:80:LYS:HE3	1.65	0.45
1:G:8:ARG:NH1	1:G:142:LEU:O	2.45	0.45
1:G:35:ARG:HG3	1:G:57:PHE:HE2	1.82	0.45
1:J:160:ILE:HG23	1:L:160:ILE:HG13	1.99	0.45
1:D:136:LEU:CD1	1:F:135:ALA:HB1	2.47	0.45
1:I:135:ALA:HB1	1:L:136:LEU:HD13	1.99	0.45
1:A:30:ASN:CG	1:B:116:GLU:HG3	2.42	0.45
1:F:80:LYS:HE3	1:F:80:LYS:HB3	1.61	0.45
1:K:19:GLN:HE22	1:K:161:TYR:C	2.25	0.45
1:K:36:ARG:NH2	1:K:170:GLU:O	2.50	0.45
1:L:152:LEU:HD13	1:L:166:HIS:CE1	2.52	0.45
1:A:90:LYS:O	1:A:91:LEU:O	2.35	0.44
1:A:160:ILE:HG22	1:A:161:TYR:CD2	2.52	0.44
1:B:136:LEU:HD13	1:H:135:ALA:HB1	1.99	0.44
1:D:111:ASP:CG	1:E:51:ALA:HB2	2.42	0.44
1:L:36:ARG:NH2	1:L:170:GLU:O	2.50	0.44
1:E:52:ASP:OD1	1:E:91:LEU:CD2	2.65	0.44
1:A:1:THR:CG2	1:A:33:LYS:HZ3	2.30	0.44
1:A:19:GLN:HE22	1:A:161:TYR:C	2.24	0.44
1:B:152:LEU:HD13	1:B:166:HIS:CE1	2.52	0.44
1:C:19:GLN:HE22	1:C:161:TYR:C	2.25	0.44
1:E:83:ARG:HA	1:E:109:ASN:O	2.18	0.44
1:C:131:ALA:HB2	1:E:158:ILE:HD12	2.00	0.44
1:E:77:GLU:O	1:E:80:LYS:CG	2.53	0.44
1:I:8:ARG:NH1	1:I:142:LEU:O	2.44	0.44
1:C:38:TYR:HE1	1:C:65:GLU:HG3	1.83	0.44
1:G:67:HIS:C	1:G:68:GLN:HG3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:ILE:HG13	1:I:160:ILE:O	2.18	0.44
1:I:64:LEU:HD23	1:I:64:LEU:HA	1.86	0.44
1:J:19:GLN:HE22	1:J:161:TYR:C	2.26	0.44
1:G:36:ARG:NH2	1:G:170:GLU:O	2.51	0.43
1:I:1:THR:HG23	1:I:33:LYS:NZ	2.33	0.43
1:K:1:THR:HG21	1:K:33:LYS:HZ3	1.75	0.43
1:H:38:TYR:HE1	1:H:65:GLU:HG3	1.83	0.43
1:K:64:LEU:HD23	1:K:64:LEU:HA	1.86	0.43
1:B:157:ASP:HB3	1:H:134:ARG:HH22	1.83	0.43
1:B:19:GLN:HE22	1:B:161:TYR:C	2.26	0.43
1:C:70:HIS:CE1	1:C:73:LYS:H	2.35	0.43
1:D:8:ARG:NH1	1:D:142:LEU:O	2.44	0.43
1:E:80:LYS:HA	1:E:83:ARG:HD2	1.99	0.43
1:K:7:ARG:NH2	1:K:103:SER:OG	2.47	0.43
1:C:152:LEU:HD13	1:C:166:HIS:CE1	2.54	0.43
1:E:83:ARG:HG3	1:E:110:GLY:HA3	2.01	0.43
1:K:35:ARG:HG3	1:K:57:PHE:HE2	1.83	0.43
1:A:5:SER:HB3	1:A:120:ILE:HB	2.01	0.42
1:B:7:ARG:NH1	1:B:173:TYR:OH	2.48	0.42
1:I:36:ARG:NH2	1:I:170:GLU:O	2.52	0.42
1:A:38:TYR:HE1	1:A:65:GLU:HG3	1.84	0.42
1:F:64:LEU:HD23	1:F:64:LEU:HA	1.86	0.42
1:I:7:ARG:NH2	1:I:103:SER:OG	2.47	0.42
1:I:114:GLN:HA	1:I:115:PRO:HD2	1.92	0.42
1:K:38:TYR:HE1	1:K:65:GLU:HG3	1.85	0.42
1:E:52:ASP:HB3	1:E:82:TRP:HZ2	1.75	0.42
1:L:59:LEU:HD12	1:L:59:LEU:HA	1.88	0.42
1:E:59:LEU:HD12	1:E:59:LEU:HA	1.88	0.42
1:H:67:HIS:CE1	1:H:77:GLU:HG3	2.55	0.42
1:I:67:HIS:CE1	1:I:77:GLU:HG3	2.55	0.42
1:J:152:LEU:HD13	1:J:166:HIS:CE1	2.54	0.42
1:B:64:LEU:HD23	1:B:64:LEU:HA	1.86	0.42
1:C:67:HIS:CE1	1:C:77:GLU:HG3	2.55	0.42
1:J:35:ARG:HG3	1:J:57:PHE:HE2	1.83	0.42
1:J:50:THR:O	1:J:54:PHE:HB2	2.20	0.42
1:D:5:SER:HB3	1:D:120:ILE:HB	2.00	0.42
1:F:38:TYR:HE1	1:F:65:GLU:HG3	1.85	0.42
1:A:152:LEU:HD13	1:A:166:HIS:CE1	2.54	0.42
1:F:36:ARG:NH2	1:F:170:GLU:O	2.53	0.42
1:J:135:ALA:HB1	1:K:136:LEU:CD1	2.47	0.42
1:J:160:ILE:HA	1:J:160:ILE:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:67:HIS:CE1	1:K:77:GLU:HG3	2.55	0.42
1:L:5:SER:HB3	1:L:120:ILE:HB	2.01	0.42
1:H:5:SER:HB3	1:H:120:ILE:HB	2.02	0.42
1:J:38:TYR:HE1	1:J:65:GLU:HG3	1.84	0.42
1:K:80:LYS:HB3	1:K:80:LYS:HE3	1.64	0.42
1:A:115:PRO:HG2	1:A:118:ASP:HA	2.01	0.41
1:K:173:TYR:HD1	1:K:174:LYS:H	1.63	0.41
1:B:50:THR:O	1:B:54:PHE:HB2	2.20	0.41
1:D:134:ARG:HH22	1:F:157:ASP:CB	2.32	0.41
1:I:38:TYR:HE1	1:I:65:GLU:HG3	1.86	0.41
1:L:38:TYR:HE1	1:L:65:GLU:HG3	1.84	0.41
1:A:136:LEU:CD1	1:G:135:ALA:HB1	2.48	0.41
1:J:64:LEU:HD23	1:J:64:LEU:HA	1.86	0.41
1:D:25:THR:HA	1:K:158:ILE:O	2.21	0.41
1:D:38:TYR:HE1	1:D:65:GLU:HG3	1.85	0.41
1:F:50:THR:O	1:F:54:PHE:HB2	2.21	0.41
1:G:152:LEU:HD13	1:G:166:HIS:CE1	2.55	0.41
1:D:71:LEU:HD23	1:D:71:LEU:HA	1.88	0.41
1:D:116:GLU:HG3	1:E:30:ASN:CG	2.45	0.41
1:D:152:LEU:HD13	1:D:166:HIS:CE1	2.56	0.41
1:C:71:LEU:HD11	1:C:97:VAL:HG12	2.03	0.41
1:D:157:ASP:HB3	1:F:134:ARG:HH22	1.84	0.41
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.88	0.41
1:A:90:LYS:HB3	1:A:90:LYS:HE2	1.47	0.41
1:F:1:THR:HG23	1:F:33:LYS:NZ	2.36	0.41
1:H:64:LEU:HD23	1:H:64:LEU:HA	1.88	0.41
1:B:160:ILE:HD12	1:B:160:ILE:HA	1.81	0.41
1:F:55:THR:HG21	1:F:91:LEU:CD2	2.50	0.41
1:I:82:TRP:NE1	1:I:89:ARG:O	2.53	0.41
1:F:7:ARG:NH2	1:F:103:SER:OG	2.49	0.41
1:F:152:LEU:HD13	1:F:166:HIS:CE1	2.56	0.41
1:G:19:GLN:HE22	1:G:161:TYR:C	2.29	0.41
1:I:71:LEU:HD23	1:I:71:LEU:HA	1.87	0.41
1:J:67:HIS:CE1	1:J:77:GLU:HG3	2.55	0.41
1:C:36:ARG:NH2	1:C:170:GLU:O	2.54	0.41
1:D:36:ARG:NH2	1:D:170:GLU:O	2.54	0.41
1:F:63:LYS:HA	1:F:66:MET:HB3	2.02	0.41
1:J:7:ARG:NH2	1:J:103:SER:OG	2.49	0.41
1:C:50:THR:O	1:C:54:PHE:HB2	2.21	0.40
1:F:35:ARG:HG3	1:F:57:PHE:HE2	1.85	0.40
1:L:160:ILE:HG22	1:L:161:TYR:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HD12	1:A:160:ILE:HA	1.89	0.40
1:B:160:ILE:HG23	1:C:160:ILE:HG13	2.02	0.40
1:E:24:ASN:C	1:F:160:ILE:HB	2.46	0.40
1:E:79:ALA:O	1:E:83:ARG:CG	2.68	0.40
1:I:19:GLN:HE22	1:I:161:TYR:C	2.29	0.40
1:A:67:HIS:CE1	1:A:77:GLU:HG3	2.57	0.40
1:C:51:ALA:HB2	1:H:111:ASP:HA	2.03	0.40
1:D:24:ASN:O	1:K:160:ILE:HB	2.22	0.40
1:F:19:GLN:HE22	1:F:161:TYR:C	2.29	0.40
1:H:80:LYS:HE3	1:H:80:LYS:HB3	1.64	0.40
1:K:160:ILE:HA	1:K:160:ILE:HD12	1.89	0.40
1:E:59:LEU:CD2	1:E:81:ASP:HB3	2.44	0.40
1:J:1:THR:CG2	1:J:2:THR:N	2.84	0.40
1:A:114:GLN:HA	1:A:115:PRO:HD2	1.94	0.40
1:B:66:MET:HG2	1:B:67:HIS:ND1	2.36	0.40
1:I:111:ASP:OD2	1:J:50:THR:HB	2.20	0.40
1:K:67:HIS:O	1:K:69:GLY:N	2.54	0.40

There are no symmetry-related clashes.

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	165/174 (95%)	154 (93%)	10 (6%)	1 (1%)	21	48
1	B	165/174 (95%)	153 (93%)	12 (7%)	0	100	100
1	C	165/174 (95%)	154 (93%)	10 (6%)	1 (1%)	21	48
1	D	165/174 (95%)	155 (94%)	10 (6%)	0	100	100
1	E	165/174 (95%)	153 (93%)	12 (7%)	0	100	100
1	F	165/174 (95%)	156 (94%)	9 (6%)	0	100	100
1	G	165/174 (95%)	156 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	165/174 (95%)	155 (94%)	10 (6%)	0	100	100
1	I	165/174 (95%)	156 (94%)	9 (6%)	0	100	100
1	J	165/174 (95%)	154 (93%)	11 (7%)	0	100	100
1	K	165/174 (95%)	154 (93%)	11 (7%)	0	100	100
1	L	165/174 (95%)	153 (93%)	11 (7%)	1 (1%)	21	48
All	All	1980/2088 (95%)	1853 (94%)	124 (6%)	3 (0%)	43	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	LYS
1	C	90	LYS
1	L	91	LEU

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	131/135 (97%)	113 (86%)	18 (14%)	3	10
1	B	131/135 (97%)	116 (88%)	15 (12%)	5	16
1	C	131/135 (97%)	116 (88%)	15 (12%)	5	16
1	D	131/135 (97%)	115 (88%)	16 (12%)	5	14
1	E	131/135 (97%)	117 (89%)	14 (11%)	6	19
1	F	131/135 (97%)	114 (87%)	17 (13%)	4	11
1	G	131/135 (97%)	117 (89%)	14 (11%)	6	19
1	H	131/135 (97%)	114 (87%)	17 (13%)	4	11
1	I	131/135 (97%)	115 (88%)	16 (12%)	5	14
1	J	131/135 (97%)	114 (87%)	17 (13%)	4	11
1	K	131/135 (97%)	117 (89%)	14 (11%)	6	19
1	L	131/135 (97%)	115 (88%)	16 (12%)	5	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1572/1620 (97%)	1383 (88%)	189 (12%)	5 14

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	13	VAL
1	A	71	LEU
1	A	90	LYS
1	A	91	LEU
1	A	92	GLU
1	A	94	LEU
1	A	95	LEU
1	A	104	LEU
1	A	107	THR
1	A	109	ASN
1	A	111	ASP
1	A	116	GLU
1	A	122	ILE
1	A	136	LEU
1	A	137	LEU
1	A	152	LEU
1	A	160	ILE
1	B	4	VAL
1	B	13	VAL
1	B	71	LEU
1	B	92	GLU
1	B	94	LEU
1	B	104	LEU
1	B	107	THR
1	B	109	ASN
1	B	111	ASP
1	B	116	GLU
1	B	122	ILE
1	B	136	LEU
1	B	137	LEU
1	B	152	LEU
1	B	160	ILE
1	C	4	VAL
1	C	13	VAL
1	C	71	LEU
1	C	92	GLU

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Mol	Chain	Res	Type
1	C	94	LEU
1	C	104	LEU
1	C	107	THR
1	C	109	ASN
1	C	111	ASP
1	C	116	GLU
1	C	122	ILE
1	C	136	LEU
1	C	137	LEU
1	C	152	LEU
1	C	160	ILE
1	D	4	VAL
1	D	13	VAL
1	D	71	LEU
1	D	80	LYS
1	D	92	GLU
1	D	94	LEU
1	D	104	LEU
1	D	107	THR
1	D	109	ASN
1	D	111	ASP
1	D	116	GLU
1	D	122	ILE
1	D	136	LEU
1	D	137	LEU
1	D	152	LEU
1	D	160	ILE
1	E	4	VAL
1	E	13	VAL
1	E	71	LEU
1	E	94	LEU
1	E	104	LEU
1	E	107	THR
1	E	109	ASN
1	E	111	ASP
1	E	116	GLU
1	E	122	ILE
1	E	136	LEU
1	E	137	LEU
1	E	152	LEU
1	E	160	ILE
1	F	4	VAL

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Mol	Chain	Res	Type
1	F	13	VAL
1	F	71	LEU
1	F	80	LYS
1	F	91	LEU
1	F	92	GLU
1	F	94	LEU
1	F	104	LEU
1	F	107	THR
1	F	109	ASN
1	F	111	ASP
1	F	116	GLU
1	F	122	ILE
1	F	136	LEU
1	F	137	LEU
1	F	152	LEU
1	F	160	ILE
1	G	4	VAL
1	G	13	VAL
1	G	71	LEU
1	G	92	GLU
1	G	94	LEU
1	G	104	LEU
1	G	107	THR
1	G	109	ASN
1	G	111	ASP
1	G	116	GLU
1	G	136	LEU
1	G	137	LEU
1	G	152	LEU
1	G	160	ILE
1	H	4	VAL
1	H	13	VAL
1	H	71	LEU
1	H	80	LYS
1	H	92	GLU
1	H	94	LEU
1	H	95	LEU
1	H	104	LEU
1	H	107	THR
1	H	109	ASN
1	H	111	ASP
1	H	116	GLU

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Mol	Chain	Res	Type
1	H	122	ILE
1	H	136	LEU
1	H	137	LEU
1	H	152	LEU
1	H	160	ILE
1	I	4	VAL
1	I	13	VAL
1	I	71	LEU
1	I	92	GLU
1	I	94	LEU
1	I	95	LEU
1	I	104	LEU
1	I	107	THR
1	I	109	ASN
1	I	111	ASP
1	I	116	GLU
1	I	122	ILE
1	I	136	LEU
1	I	137	LEU
1	I	152	LEU
1	I	160	ILE
1	J	4	VAL
1	J	13	VAL
1	J	50	THR
1	J	71	LEU
1	J	80	LYS
1	J	92	GLU
1	J	94	LEU
1	J	104	LEU
1	J	107	THR
1	J	109	ASN
1	J	111	ASP
1	J	116	GLU
1	J	122	ILE
1	J	136	LEU
1	J	137	LEU
1	J	152	LEU
1	J	160	ILE
1	K	4	VAL
1	K	13	VAL
1	K	71	LEU
1	K	92	GLU

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Mol	Chain	Res	Type
1	K	94	LEU
1	K	104	LEU
1	K	107	THR
1	K	109	ASN
1	K	111	ASP
1	K	116	GLU
1	K	136	LEU
1	K	137	LEU
1	K	152	LEU
1	K	160	ILE
1	L	4	VAL
1	L	13	VAL
1	L	71	LEU
1	L	91	LEU
1	L	92	GLU
1	L	94	LEU
1	L	104	LEU
1	L	107	THR
1	L	109	ASN
1	L	111	ASP
1	L	116	GLU
1	L	122	ILE
1	L	136	LEU
1	L	137	LEU
1	L	152	LEU
1	L	160	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	139	ASN
1	B	19	GLN
1	D	19	GLN
1	D	67	HIS
1	D	70	HIS
1	D	139	ASN
1	E	19	GLN
1	G	19	GLN
1	G	67	HIS
1	H	19	GLN
1	H	67	HIS

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Mol	Chain	Res	Type
1	I	67	HIS
1	J	67	HIS
1	K	67	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	169/174 (97%)	0.65	20 (11%) 9 8	19, 49, 116, 248	3 (1%)
1	B	169/174 (97%)	0.94	27 (15%) 5 4	17, 53, 162, 220	3 (1%)
1	C	169/174 (97%)	0.87	27 (15%) 5 4	19, 52, 144, 213	2 (1%)
1	D	169/174 (97%)	0.70	21 (12%) 8 7	23, 51, 133, 278	3 (1%)
1	E	169/174 (97%)	1.38	42 (24%) 2 1	23, 59, 214, 380	2 (1%)
1	F	169/174 (97%)	0.78	23 (13%) 7 5	25, 61, 167, 227	3 (1%)
1	G	169/174 (97%)	0.86	26 (15%) 5 4	21, 67, 164, 253	3 (1%)
1	H	169/174 (97%)	0.76	21 (12%) 8 7	15, 62, 142, 225	3 (1%)
1	I	169/174 (97%)	0.75	14 (8%) 17 14	24, 72, 144, 262	3 (1%)
1	J	169/174 (97%)	0.98	29 (17%) 4 3	31, 73, 164, 219	3 (1%)
1	K	169/174 (97%)	0.83	12 (7%) 22 17	29, 73, 153, 235	3 (1%)
1	L	169/174 (97%)	0.73	14 (8%) 17 14	37, 68, 146, 232	3 (1%)
All	All	2028/2088 (97%)	0.85	276 (13%) 7 5	15, 61, 162, 380	34 (1%)

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	50	THR	7.9
1	E	56	LEU	7.9
1	E	60	PHE	7.2
1	E	55	THR	6.3
1	E	57	PHE	6.0
1	E	93	ALA	5.7
1	B	79	ALA	5.4
1	E	49	GLY	5.3
1	I	79	ALA	5.3
1	E	54	PHE	5.3
1	C	56	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	110	GLY	5.2
1	A	174	LYS	5.2
1	C	89	ARG	4.9
1	D	79	ALA	4.9
1	H	57	PHE	4.8
1	F	159	CYS	4.8
1	J	108	GLY	4.8
1	D	82	TRP	4.8
1	D	91	LEU	4.7
1	C	82	TRP	4.7
1	E	79	ALA	4.6
1	B	55	THR	4.6
1	E	46	PHE	4.5
1	J	76	VAL	4.5
1	I	57	PHE	4.5
1	E	159	CYS	4.4
1	G	159	CYS	4.4
1	E	82	TRP	4.4
1	I	82	TRP	4.3
1	L	82	TRP	4.3
1	F	79	ALA	4.3
1	E	30	ASN	4.3
1	D	57	PHE	4.2
1	E	59	LEU	4.2
1	K	57	PHE	4.2
1	A	53	ALA	4.1
1	G	112	VAL	4.1
1	C	77	GLU	4.1
1	C	91	LEU	4.0
1	B	76	VAL	4.0
1	L	57	PHE	4.0
1	F	78	LEU	4.0
1	G	110	GLY	3.9
1	J	56	LEU	3.9
1	G	111	ASP	3.9
1	D	81	ASP	3.8
1	D	114	GLN	3.8
1	K	82	TRP	3.8
1	D	48	GLY	3.8
1	K	141	GLU	3.7
1	E	28	LYS	3.7
1	D	83	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	108	GLY	3.6
1	E	92	GLU	3.6
1	F	72	VAL	3.6
1	F	71	LEU	3.6
1	C	48	GLY	3.5
1	F	110	GLY	3.5
1	H	37	LEU	3.5
1	G	9	ASN	3.5
1	E	53	ALA	3.5
1	J	79	ALA	3.5
1	A	57	PHE	3.4
1	C	54	PHE	3.4
1	G	93	ALA	3.4
1	K	60	PHE	3.4
1	L	54	PHE	3.4
1	F	64	LEU	3.4
1	J	91	LEU	3.3
1	C	71	LEU	3.3
1	D	54	PHE	3.3
1	B	107	THR	3.3
1	G	95	LEU	3.3
1	E	26	VAL	3.3
1	E	27	MET	3.2
1	G	79	ALA	3.2
1	D	64	LEU	3.2
1	G	78	LEU	3.2
1	L	83	ARG	3.2
1	B	114	GLN	3.2
1	E	48	GLY	3.2
1	J	81	ASP	3.2
1	E	76	VAL	3.2
1	C	114	GLN	3.2
1	J	53	ALA	3.2
1	E	81	ASP	3.1
1	C	59	LEU	3.1
1	D	55	THR	3.1
1	G	115	PRO	3.1
1	G	82	TRP	3.1
1	D	70	HIS	3.1
1	F	106	ILE	3.1
1	E	106	ILE	3.0
1	J	54	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	71	LEU	3.0
1	G	91	LEU	3.0
1	E	58	GLU	3.0
1	E	63	LYS	3.0
1	G	64	LEU	3.0
1	K	55	THR	3.0
1	H	54	PHE	3.0
1	E	83	ARG	2.9
1	G	81	ASP	2.9
1	F	69	GLY	2.9
1	C	52	ASP	2.9
1	I	159	CYS	2.9
1	G	108	GLY	2.9
1	C	93	ALA	2.9
1	I	13	VAL	2.9
1	C	79	ALA	2.8
1	C	83	ARG	2.8
1	C	27	MET	2.8
1	D	50	THR	2.8
1	J	113	VAL	2.8
1	K	54	PHE	2.8
1	G	171	LEU	2.8
1	A	50	THR	2.8
1	D	90	LYS	2.8
1	B	35	ARG	2.8
1	J	82	TRP	2.8
1	F	57	PHE	2.8
1	H	38	TYR	2.8
1	E	66	MET	2.8
1	G	73	LYS	2.8
1	D	92	GLU	2.7
1	E	51	ALA	2.7
1	L	49	GLY	2.7
1	E	74	ALA	2.7
1	F	54	PHE	2.7
1	J	57	PHE	2.7
1	I	110	GLY	2.7
1	F	115	PRO	2.7
1	J	145	ARG	2.7
1	E	64	LEU	2.7
1	H	82	TRP	2.7
1	E	52	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	81	ASP	2.7
1	A	40	ASP	2.7
1	B	95	LEU	2.7
1	G	37	LEU	2.7
1	B	38	TYR	2.6
1	J	62	ARG	2.6
1	A	141	GLU	2.6
1	C	81	ASP	2.6
1	G	57	PHE	2.6
1	B	91	LEU	2.6
1	I	107	THR	2.6
1	K	91	LEU	2.6
1	A	39	ASN	2.6
1	G	141	GLU	2.6
1	H	77	GLU	2.6
1	H	48	GLY	2.6
1	J	71	LEU	2.6
1	B	106	ILE	2.6
1	C	112	VAL	2.6
1	H	76	VAL	2.6
1	B	70	HIS	2.5
1	G	69	GLY	2.5
1	J	78	LEU	2.5
1	B	50	THR	2.5
1	E	94	LEU	2.5
1	B	89	ARG	2.5
1	C	50	THR	2.5
1	E	108	GLY	2.5
1	C	53	ALA	2.5
1	E	20	ALA	2.5
1	H	83	ARG	2.5
1	A	36	ARG	2.4
1	E	89	ARG	2.4
1	F	82	TRP	2.4
1	I	54	PHE	2.4
1	A	68	GLN	2.4
1	G	101	THR	2.4
1	J	136	LEU	2.4
1	I	81	ASP	2.4
1	D	80	LYS	2.4
1	L	174	LYS	2.4
1	K	79	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	50	THR	2.4
1	B	37	LEU	2.4
1	B	39	ASN	2.4
1	F	112	VAL	2.4
1	G	61	GLU	2.4
1	C	42	VAL	2.4
1	C	75	ALA	2.4
1	H	55	THR	2.4
1	B	56	LEU	2.4
1	E	109	ASN	2.3
1	B	111	ASP	2.3
1	F	95	LEU	2.3
1	A	90	LYS	2.3
1	A	89	ARG	2.3
1	J	48	GLY	2.3
1	F	111	ASP	2.3
1	B	78	LEU	2.3
1	H	174	LYS	2.3
1	F	89	ARG	2.3
1	J	83	ARG	2.3
1	C	49	GLY	2.3
1	D	69	GLY	2.3
1	B	77	GLU	2.3
1	I	66	MET	2.3
1	B	90	LYS	2.3
1	C	134	ARG	2.3
1	E	35	ARG	2.3
1	B	108	GLY	2.3
1	K	48	GLY	2.3
1	A	66	MET	2.3
1	I	95	LEU	2.3
1	J	111	ASP	2.3
1	F	70	HIS	2.3
1	B	83	ARG	2.3
1	J	55	THR	2.3
1	I	77	GLU	2.2
1	D	78	LEU	2.2
1	F	94	LEU	2.2
1	A	81	ASP	2.2
1	C	35	ARG	2.2
1	A	172	SER	2.2
1	J	49	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	51	ALA	2.2
1	A	83	ARG	2.2
1	B	115	PRO	2.2
1	I	59	LEU	2.2
1	B	67	HIS	2.2
1	E	67	HIS	2.2
1	K	150	LYS	2.2
1	J	37	LEU	2.2
1	D	58	GLU	2.2
1	F	113	VAL	2.2
1	C	73	LYS	2.2
1	H	173	TYR	2.2
1	J	173	TYR	2.2
1	H	172	SER	2.2
1	H	79	ALA	2.2
1	B	139	ASN	2.1
1	L	78	LEU	2.1
1	A	72	VAL	2.1
1	H	41	LYS	2.1
1	J	107	THR	2.1
1	B	71	LEU	2.1
1	H	91	LEU	2.1
1	E	62	ARG	2.1
1	H	134	ARG	2.1
1	C	68	GLN	2.1
1	C	90	LYS	2.1
1	G	97	VAL	2.1
1	H	9	ASN	2.1
1	J	174	LYS	2.1
1	L	39	ASN	2.1
1	L	69	GLY	2.1
1	G	60	PHE	2.1
1	H	159	CYS	2.1
1	K	12	VAL	2.1
1	D	46	PHE	2.1
1	A	79	ALA	2.1
1	E	61	GLU	2.1
1	A	54	PHE	2.0
1	L	89	ARG	2.0
1	F	81	ASP	2.0
1	J	102	ALA	2.0
1	K	102	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	82	TRP	2.0
1	E	32	LYS	2.0
1	J	11	HIS	2.0
1	A	35	ARG	2.0
1	E	24	ASN	2.0
1	D	110	GLY	2.0
1	L	46	PHE	2.0
1	H	53	ALA	2.0
1	H	93	ALA	2.0
1	F	73	LYS	2.0
1	F	66	MET	2.0
1	L	128	TYR	2.0
1	J	72	VAL	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.