



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 3H43 / pdb_00003h43
Title : N-terminal domain of the proteasome-activating nucleotidase of *Methanocaldococcus jannaschii*
Authors : Jeffrey, P.D.; Zhang, F.; Hu, M.; Tian, G.; Zhang, P.; Finley, D.; Shi, Y.
Deposited on : 2009-04-17
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

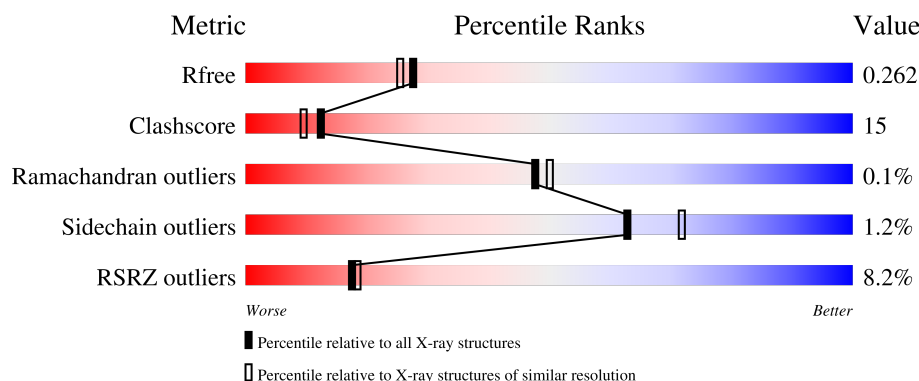
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	85	5% 69% 19% • 11%
1	B	85	7% 61% 25% 5% 9%
1	C	85	6% 78% 8% • 11%
1	D	85	5% 61% 28% 11%
1	E	85	8% 65% 24% • 11%

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Mol	Chain	Length	Quality of chain
1	F	85	
1	G	85	
1	H	85	
1	I	85	
1	J	85	
1	K	85	
1	L	85	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7312 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 Proteasome-activating nucleotidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	B	77	Total	C	N	O	S	Se	0	0	0
			600	378	108	111	1	2			
1	C	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	D	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	E	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	F	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	G	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	H	78	Total	C	N	O	S	Se	0	0	0
			608	384	109	112	1	2			
1	I	79	Total	C	N	O	S	Se	0	0	0
			617	389	110	115	1	2			
1	J	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	K	77	Total	C	N	O	S	Se	0	0	0
			600	379	108	111	1	1			
1	L	79	Total	C	N	O	S	Se	0	0	0
			617	389	110	115	1	2			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	LEU	-	expression tag	UNP Q58576
A	152	GLU	-	expression tag	UNP Q58576
A	153	HIS	-	expression tag	UNP Q58576
A	154	HIS	-	expression tag	UNP Q58576
A	155	HIS	-	expression tag	UNP Q58576

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Chain	Residue	Modelled	Actual	Comment	Reference
A	156	HIS	-	expression tag	UNP Q58576
A	157	HIS	-	expression tag	UNP Q58576
A	158	HIS	-	expression tag	UNP Q58576
B	151	LEU	-	expression tag	UNP Q58576
B	152	GLU	-	expression tag	UNP Q58576
B	153	HIS	-	expression tag	UNP Q58576
B	154	HIS	-	expression tag	UNP Q58576
B	155	HIS	-	expression tag	UNP Q58576
B	156	HIS	-	expression tag	UNP Q58576
B	157	HIS	-	expression tag	UNP Q58576
B	158	HIS	-	expression tag	UNP Q58576
C	151	LEU	-	expression tag	UNP Q58576
C	152	GLU	-	expression tag	UNP Q58576
C	153	HIS	-	expression tag	UNP Q58576
C	154	HIS	-	expression tag	UNP Q58576
C	155	HIS	-	expression tag	UNP Q58576
C	156	HIS	-	expression tag	UNP Q58576
C	157	HIS	-	expression tag	UNP Q58576
C	158	HIS	-	expression tag	UNP Q58576
D	151	LEU	-	expression tag	UNP Q58576
D	152	GLU	-	expression tag	UNP Q58576
D	153	HIS	-	expression tag	UNP Q58576
D	154	HIS	-	expression tag	UNP Q58576
D	155	HIS	-	expression tag	UNP Q58576
D	156	HIS	-	expression tag	UNP Q58576
D	157	HIS	-	expression tag	UNP Q58576
D	158	HIS	-	expression tag	UNP Q58576
E	151	LEU	-	expression tag	UNP Q58576
E	152	GLU	-	expression tag	UNP Q58576
E	153	HIS	-	expression tag	UNP Q58576
E	154	HIS	-	expression tag	UNP Q58576
E	155	HIS	-	expression tag	UNP Q58576
E	156	HIS	-	expression tag	UNP Q58576
E	157	HIS	-	expression tag	UNP Q58576
E	158	HIS	-	expression tag	UNP Q58576
F	151	LEU	-	expression tag	UNP Q58576
F	152	GLU	-	expression tag	UNP Q58576
F	153	HIS	-	expression tag	UNP Q58576
F	154	HIS	-	expression tag	UNP Q58576
F	155	HIS	-	expression tag	UNP Q58576
F	156	HIS	-	expression tag	UNP Q58576
F	157	HIS	-	expression tag	UNP Q58576

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Chain	Residue	Modelled	Actual	Comment	Reference
F	158	HIS	-	expression tag	UNP Q58576
G	151	LEU	-	expression tag	UNP Q58576
G	152	GLU	-	expression tag	UNP Q58576
G	153	HIS	-	expression tag	UNP Q58576
G	154	HIS	-	expression tag	UNP Q58576
G	155	HIS	-	expression tag	UNP Q58576
G	156	HIS	-	expression tag	UNP Q58576
G	157	HIS	-	expression tag	UNP Q58576
G	158	HIS	-	expression tag	UNP Q58576
H	151	LEU	-	expression tag	UNP Q58576
H	152	GLU	-	expression tag	UNP Q58576
H	153	HIS	-	expression tag	UNP Q58576
H	154	HIS	-	expression tag	UNP Q58576
H	155	HIS	-	expression tag	UNP Q58576
H	156	HIS	-	expression tag	UNP Q58576
H	157	HIS	-	expression tag	UNP Q58576
H	158	HIS	-	expression tag	UNP Q58576
I	151	LEU	-	expression tag	UNP Q58576
I	152	GLU	-	expression tag	UNP Q58576
I	153	HIS	-	expression tag	UNP Q58576
I	154	HIS	-	expression tag	UNP Q58576
I	155	HIS	-	expression tag	UNP Q58576
I	156	HIS	-	expression tag	UNP Q58576
I	157	HIS	-	expression tag	UNP Q58576
I	158	HIS	-	expression tag	UNP Q58576
J	151	LEU	-	expression tag	UNP Q58576
J	152	GLU	-	expression tag	UNP Q58576
J	153	HIS	-	expression tag	UNP Q58576
J	154	HIS	-	expression tag	UNP Q58576
J	155	HIS	-	expression tag	UNP Q58576
J	156	HIS	-	expression tag	UNP Q58576
J	157	HIS	-	expression tag	UNP Q58576
J	158	HIS	-	expression tag	UNP Q58576
K	151	LEU	-	expression tag	UNP Q58576
K	152	GLU	-	expression tag	UNP Q58576
K	153	HIS	-	expression tag	UNP Q58576
K	154	HIS	-	expression tag	UNP Q58576
K	155	HIS	-	expression tag	UNP Q58576
K	156	HIS	-	expression tag	UNP Q58576
K	157	HIS	-	expression tag	UNP Q58576
K	158	HIS	-	expression tag	UNP Q58576
L	151	LEU	-	expression tag	UNP Q58576

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Chain	Residue	Modelled	Actual	Comment	Reference
L	152	GLU	-	expression tag	UNP Q58576
L	153	HIS	-	expression tag	UNP Q58576
L	154	HIS	-	expression tag	UNP Q58576
L	155	HIS	-	expression tag	UNP Q58576
L	156	HIS	-	expression tag	UNP Q58576
L	157	HIS	-	expression tag	UNP Q58576
L	158	HIS	-	expression tag	UNP Q58576

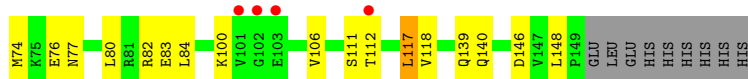
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	8	Total O 8 8	0	0
2	C	18	Total O 18 18	0	0
2	D	21	Total O 21 21	0	0
2	E	8	Total O 8 8	0	0
2	F	6	Total O 6 6	0	0
2	G	12	Total O 12 12	0	0
2	H	11	Total O 11 11	0	0
2	I	10	Total O 10 10	0	0
2	J	8	Total O 8 8	0	0
2	K	11	Total O 11 11	0	0
2	L	10	Total O 10 10	0	0

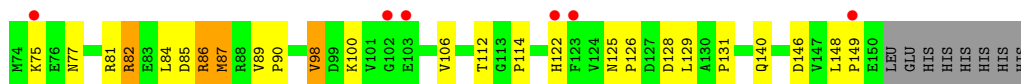
3 Residue-property plots [i](#)

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.

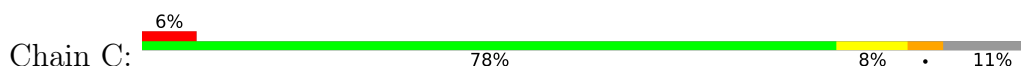
- Molecule 1: Proteasome-activating nucleotidase



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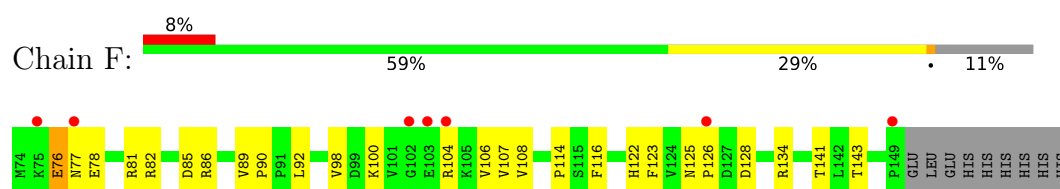
- Molecule 1: Proteasome-activating nucleotidase



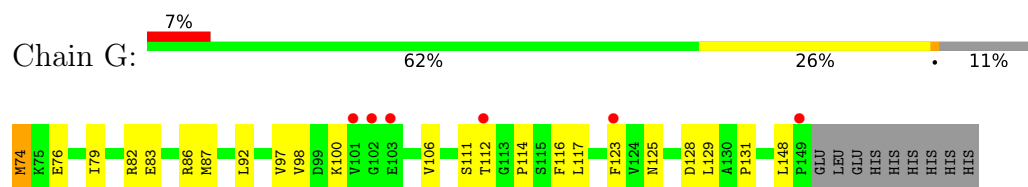
- Molecule 1: Proteasome-activating nucleotidase



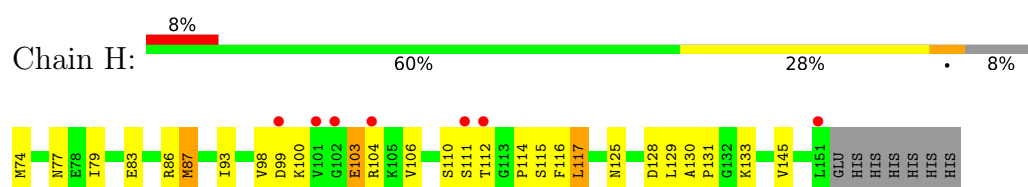
- Molecule 1: Proteasome-activating nucleotidase



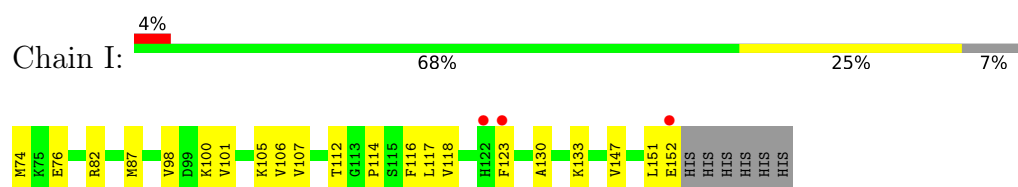
- Molecule 1: Proteasome-activating nucleotidase



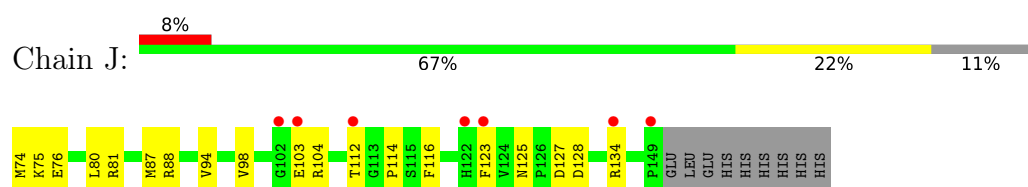
- Molecule 1: Proteasome-activating nucleotidase



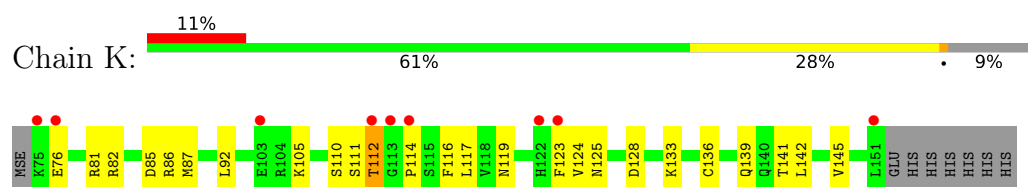
- Molecule 1: Proteasome-activating nucleotidase



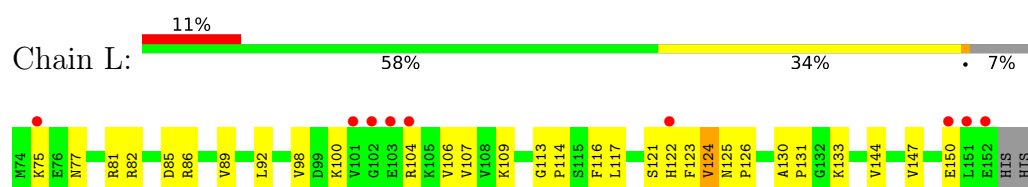
- Molecule 1: Proteasome-activating nucleotidase



- Molecule 1: Proteasome-activating nucleotidase



- Molecule 1: Proteasome-activating nucleotidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.64Å 129.62Å 60.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.89 – 2.10 40.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.89-2.10) 98.8 (40.89-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.10Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.217 , 0.262 0.217 , 0.262	Depositor DCC
R_{free} test set	2931 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7312	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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 [i](#)

5.1 Standard geometry [i](#)

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	0/598	0.99	2/810 (0.2%)
1	B	0.50	0/607	0.98	2/822 (0.2%)
1	C	0.57	0/598	1.00	2/810 (0.2%)
1	D	0.56	0/598	1.02	3/810 (0.4%)
1	E	0.51	0/598	1.02	4/810 (0.5%)
1	F	0.47	0/598	1.04	4/810 (0.5%)
1	G	0.49	0/598	0.95	1/810 (0.1%)
1	H	0.54	0/615	1.02	2/833 (0.2%)
1	I	0.55	0/624	1.04	3/845 (0.4%)
1	J	0.50	0/598	1.00	1/810 (0.1%)
1	K	0.51	0/607	1.02	3/823 (0.4%)
1	L	0.55	0/624	1.03	4/845 (0.5%)
All	All	0.53	0/7263	1.01	31/9838 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	98	VAL	N-CA-C	-8.46	103.58	111.45
1	L	98	VAL	N-CA-C	-7.35	104.62	111.45
1	E	98	VAL	N-CA-C	-7.17	104.86	111.67
1	L	123	PHE	N-CA-C	-6.65	105.14	113.18
1	K	112	THR	N-CA-C	6.58	120.57	112.54
1	F	107	VAL	N-CA-C	-6.37	99.26	108.36
1	E	139	GLN	N-CA-C	6.24	118.08	111.28
1	A	111	SER	N-CA-C	-6.11	105.68	113.01
1	I	130	ALA	N-CA-C	-6.11	102.72	108.22
1	K	139	GLN	N-CA-C	6.09	118.72	111.71
1	J	98	VAL	N-CA-C	-5.96	105.90	111.45
1	H	117	LEU	N-CA-C	-5.91	99.09	108.73
1	F	76	GLU	N-CA-C	-5.91	104.84	111.28
1	E	111	SER	N-CA-C	-5.79	105.47	112.54
1	F	98	VAL	N-CA-C	-5.75	106.10	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	117	LEU	N-CA-C	-5.66	99.51	108.73
1	D	117	LEU	N-CA-C	-5.60	99.61	108.73
1	H	111	SER	N-CA-C	-5.57	106.19	112.87
1	A	117	LEU	N-CA-C	-5.42	99.89	108.73
1	I	118	VAL	N-CA-C	5.40	116.68	108.80
1	D	111	SER	N-CA-C	-5.37	106.68	113.18
1	B	98	VAL	N-CA-C	-5.36	106.47	111.45
1	E	117	LEU	N-CA-C	-5.35	100.01	108.73
1	D	107	VAL	N-CA-C	-5.34	100.72	108.36
1	C	75	LYS	N-CA-C	-5.33	103.36	110.55
1	K	117	LEU	N-CA-C	-5.31	100.08	108.73
1	L	107	VAL	N-CA-C	-5.23	101.05	108.58
1	C	117	LEU	N-CA-C	-5.21	100.25	108.73
1	L	124	VAL	N-CA-C	5.10	115.92	108.53
1	B	75	LYS	N-CA-C	-5.09	106.17	112.38
1	F	123	PHE	N-CA-C	-5.00	107.00	113.01

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	591	0	626	19	0
1	B	600	0	632	35	0
1	C	591	0	626	12	0
1	D	591	0	626	27	0
1	E	591	0	626	21	0
1	F	591	0	626	34	0
1	G	591	0	626	31	0
1	H	608	0	643	27	0
1	I	617	0	649	29	0
1	J	591	0	626	21	0
1	K	600	0	634	24	0
1	L	617	0	649	30	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	0	1	0
2	C	18	0	0	1	0
2	D	21	0	0	2	0
2	E	8	0	0	0	0
2	F	6	0	0	0	0
2	G	12	0	0	1	0
2	H	11	0	0	0	0
2	I	10	0	0	0	0
2	J	8	0	0	0	0
2	K	11	0	0	1	0
2	L	10	0	0	2	0
All	All	7312	0	7589	227	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 15.

All (227) 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:I:100:LYS:HG2	1:I:106:VAL:HG12	1.53	0.90
1:D:112:THR:HG22	1:G:114:PRO:HG3	1.53	0.89
1:J:103:GLU:HG3	1:J:104:ARG:HG3	1.53	0.88
1:I:133:LYS:HE3	1:I:147:VAL:HG11	1.55	0.88
1:I:82:ARG:NH1	1:K:81:ARG:HG2	1.90	0.86
1:L:77:ASN:O	1:L:81:ARG:HG3	1.78	0.83
1:J:88:ARG:HD3	1:J:123:PHE:CE2	2.16	0.80
1:I:82:ARG:HH12	1:K:81:ARG:HG2	1.48	0.79
1:I:133:LYS:HE3	1:I:147:VAL:CG1	2.13	0.78
1:A:112:THR:HA	1:B:114:PRO:HB3	1.67	0.77
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.48	0.77
1:F:77:ASN:HD21	1:F:81:ARG:HH12	1.35	0.74
1:F:100:LYS:NZ	1:F:126:PRO:HB2	2.03	0.73
1:A:74:MSE:HE3	1:A:77:ASN:HD21	1.56	0.70
1:E:81:ARG:HH21	1:F:76:GLU:HG2	1.57	0.70
1:E:146:ASP:OD2	1:H:74:MSE:HG3	1.92	0.70
1:D:82:ARG:HD3	2:D:161:HOH:O	1.92	0.69
1:B:86:ARG:HH22	1:B:87:MSE:HE3	1.58	0.69
1:G:100:LYS:HA	1:G:106:VAL:HG12	1.73	0.69
1:A:148:LEU:HD23	1:D:74:MSE:HE1	1.75	0.68
1:B:86:ARG:HH12	1:B:87:MSE:HG2	1.59	0.68
1:B:77:ASN:HD21	1:B:81:ARG:HH11	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:PHE:HE1	1:L:82:ARG:HH11	1.41	0.67
1:L:133:LYS:HE3	1:L:147:VAL:CG1	2.25	0.66
1:F:82:ARG:HH21	1:F:86:ARG:HH22	1.44	0.65
1:D:100:LYS:HE3	1:D:129:LEU:O	1.98	0.64
1:G:112:THR:HA	1:H:114:PRO:HB3	1.80	0.64
1:G:79:ILE:O	1:G:83:GLU:HG3	1.98	0.64
1:I:123:PHE:CD2	1:L:75:LYS:HE2	2.33	0.64
1:F:82:ARG:HD2	1:G:123:PHE:HE1	1.62	0.64
1:B:82:ARG:NH2	1:C:123:PHE:HZ	1.96	0.64
1:B:82:ARG:CZ	1:C:123:PHE:HZ	2.11	0.64
1:G:86:ARG:HH22	1:H:104:ARG:HB3	1.64	0.64
1:D:112:THR:HG22	1:G:114:PRO:CG	2.25	0.63
1:A:74:MSE:HE1	1:B:77:ASN:HB2	1.81	0.63
1:G:86:ARG:NH2	1:H:104:ARG:HB3	2.12	0.63
1:E:83:GLU:HG2	1:F:122:HIS:CE1	2.34	0.62
1:F:100:LYS:HZ1	1:F:126:PRO:HB2	1.65	0.62
1:J:114:PRO:HG2	1:J:116:PHE:CE1	2.34	0.62
1:I:101:VAL:CG2	1:I:117:LEU:HD11	2.30	0.62
1:I:100:LYS:HG2	1:I:106:VAL:CG1	2.27	0.62
1:B:100:LYS:HE3	1:B:129:LEU:O	2.00	0.61
1:H:86:ARG:NH1	1:H:87:MSE:HE3	2.15	0.61
1:E:86:ARG:CZ	1:F:104:ARG:HD3	2.31	0.61
1:J:125:ASN:HB3	1:J:128:ASP:OD2	2.01	0.61
1:E:106:VAL:HG11	1:E:129:LEU:HD13	1.82	0.61
1:I:82:ARG:NH1	1:K:85:ASP:OD2	2.34	0.60
1:H:86:ARG:HH11	1:H:87:MSE:HE3	1.66	0.60
1:F:86:ARG:HG3	1:F:86:ARG:HH11	1.66	0.60
1:H:100:LYS:HD2	1:H:129:LEU:O	2.01	0.59
1:K:110:SER:HB2	2:K:162:HOH:O	2.01	0.59
1:G:74:MSE:HE2	1:G:74:MSE:HA	1.85	0.59
1:E:105:LYS:HE2	1:E:119:ASN:OD1	2.03	0.59
1:B:86:ARG:NH2	1:B:140:GLN:HE22	2.00	0.59
1:L:85:ASP:O	1:L:89:VAL:HG13	2.02	0.59
1:J:125:ASN:HD21	1:J:127:ASP:HB3	1.68	0.58
1:E:114:PRO:HG2	1:E:116:PHE:CE1	2.39	0.58
1:I:112:THR:HA	1:J:114:PRO:HB3	1.86	0.58
1:E:100:LYS:HE2	1:E:129:LEU:O	2.04	0.57
1:E:114:PRO:HG3	1:J:112:THR:HG22	1.87	0.57
1:F:78:GLU:HG2	1:G:123:PHE:HE2	1.69	0.57
1:C:86:ARG:NH2	1:D:120:VAL:O	2.38	0.57
1:L:133:LYS:NZ	1:L:150:GLU:HG3	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:133:LYS:NZ	1:L:150:GLU:CG	2.67	0.56
1:J:75:LYS:HE3	1:K:124:VAL:HG22	1.87	0.56
1:B:90:PRO:CG	1:I:105:LYS:HE3	2.36	0.56
1:E:112:THR:HG22	1:F:114:PRO:HB3	1.87	0.56
1:J:74:MSE:HE1	1:L:117:LEU:CD2	2.36	0.56
1:F:82:ARG:HE	1:F:86:ARG:NH1	2.04	0.56
1:F:82:ARG:HH21	1:F:86:ARG:NH2	2.03	0.56
1:K:76:GLU:HG2	1:L:77:ASN:ND2	2.20	0.55
1:J:74:MSE:HE1	1:L:117:LEU:HD21	1.89	0.55
1:F:77:ASN:ND2	1:F:81:ARG:HH12	2.03	0.55
1:E:100:LYS:HG2	1:E:106:VAL:HG12	1.88	0.55
1:L:77:ASN:OD1	1:L:81:ARG:HD2	2.07	0.55
1:I:87:MSE:O	1:J:87:MSE:HE1	2.06	0.54
1:F:77:ASN:OD1	1:F:81:ARG:NH1	2.41	0.54
1:F:141:THR:OG1	1:F:143:THR:HG22	2.08	0.54
1:G:114:PRO:HG2	1:G:116:PHE:CE1	2.43	0.54
1:I:114:PRO:HG2	1:I:116:PHE:CZ	2.42	0.54
1:E:125:ASN:OD1	1:E:127:ASP:HB2	2.08	0.53
1:L:124:VAL:HG21	1:L:144:VAL:HG12	1.90	0.53
1:A:84:LEU:HD13	1:B:84:LEU:HD23	1.91	0.53
1:F:106:VAL:HG23	1:F:108:VAL:HG13	1.90	0.53
1:L:133:LYS:HE3	1:L:147:VAL:HG11	1.90	0.53
1:D:112:THR:CA	1:G:114:PRO:HB3	2.39	0.52
1:K:125:ASN:HB3	1:K:128:ASP:OD2	2.09	0.52
1:B:82:ARG:NH1	1:B:82:ARG:HG2	2.24	0.52
1:D:124:VAL:HG21	1:D:144:VAL:HG12	1.92	0.52
1:D:98:VAL:O	1:D:131:PRO:HB3	2.10	0.51
1:J:125:ASN:HD22	1:J:128:ASP:CG	2.18	0.51
1:B:86:ARG:NH1	1:B:87:MSE:HG2	2.24	0.51
2:C:163:HOH:O	1:D:77:ASN:HB2	2.09	0.51
1:B:100:LYS:HA	1:B:106:VAL:HG12	1.93	0.51
1:C:114:PRO:HG2	1:C:116:PHE:CZ	2.46	0.51
1:B:148:LEU:HD22	1:B:149:PRO:HD2	1.92	0.51
1:C:122:HIS:CD2	1:C:122:HIS:H	2.28	0.51
1:F:100:LYS:HZ2	1:F:126:PRO:HB2	1.76	0.51
1:L:121:SER:HA	2:L:160:HOH:O	2.10	0.51
1:K:76:GLU:CG	1:L:77:ASN:ND2	2.74	0.51
1:D:112:THR:HA	1:G:114:PRO:HB3	1.93	0.50
1:F:114:PRO:HG2	1:F:116:PHE:CE1	2.46	0.50
1:I:74:MSE:HE1	1:I:82:ARG:HH21	1.75	0.50
1:F:134:ARG:HG2	1:F:134:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:75:LYS:HD2	1:K:145:VAL:O	2.12	0.50
1:K:128:ASP:O	1:K:133:LYS:HD3	2.11	0.50
1:G:125:ASN:HB3	1:G:128:ASP:OD2	2.12	0.50
1:I:123:PHE:HD2	1:L:75:LYS:HE2	1.75	0.50
1:A:148:LEU:HD23	1:D:74:MSE:CE	2.41	0.49
1:F:77:ASN:HD21	1:F:81:ARG:NH1	2.07	0.49
1:D:86:ARG:O	1:D:89:VAL:HG22	2.12	0.49
1:L:114:PRO:HG2	1:L:116:PHE:CE1	2.46	0.49
1:L:133:LYS:HZ3	1:L:150:GLU:CG	2.25	0.49
1:B:125:ASN:HB3	1:B:128:ASP:OD1	2.12	0.49
1:C:87:MSE:HE3	1:D:145:VAL:HG12	1.95	0.49
1:I:112:THR:HG22	1:J:114:PRO:HG3	1.94	0.49
1:F:78:GLU:HG2	1:G:123:PHE:CE2	2.47	0.49
1:K:112:THR:CG2	1:L:113:GLY:C	2.86	0.49
1:G:111:SER:CB	1:H:115:SER:H	2.26	0.49
1:H:103:GLU:CD	1:H:103:GLU:H	2.20	0.49
1:A:117:LEU:HD23	1:F:92:LEU:HD12	1.94	0.48
1:D:114:PRO:HG2	1:D:116:PHE:CE1	2.48	0.48
1:A:74:MSE:CE	1:B:77:ASN:HB2	2.42	0.48
1:B:112:THR:HA	1:I:114:PRO:HB3	1.95	0.48
1:I:101:VAL:HG21	1:I:117:LEU:HD11	1.95	0.48
1:B:82:ARG:CG	1:B:82:ARG:HH11	2.27	0.48
1:D:112:THR:N	1:G:114:PRO:HB3	2.28	0.47
1:H:110:SER:C	1:H:112:THR:N	2.71	0.47
1:E:100:LYS:HA	1:E:106:VAL:HG12	1.97	0.47
1:J:94:VAL:HG12	1:J:134:ARG:NH1	2.29	0.47
1:H:100:LYS:HA	1:H:106:VAL:HG23	1.96	0.47
1:H:125:ASN:HB3	1:H:128:ASP:OD2	2.14	0.47
1:E:112:THR:CG2	1:F:114:PRO:HB3	2.44	0.47
1:F:82:ARG:NH2	1:F:86:ARG:NH2	2.63	0.47
1:I:114:PRO:HG2	1:I:116:PHE:CE1	2.49	0.47
1:E:77:ASN:HD21	1:F:76:GLU:CG	2.28	0.47
1:I:107:VAL:CG2	1:I:117:LEU:HD13	2.45	0.47
1:A:112:THR:CA	1:B:114:PRO:HB3	2.42	0.47
1:A:146:ASP:OD2	1:D:74:MSE:HB3	2.15	0.47
1:A:76:GLU:H	1:A:76:GLU:CD	2.23	0.46
1:E:81:ARG:HB3	1:G:82:ARG:NH2	2.29	0.46
1:B:82:ARG:HG2	1:B:82:ARG:HH11	1.80	0.46
1:L:86:ARG:O	1:L:89:VAL:HG22	2.16	0.46
1:A:100:LYS:HG2	1:A:106:VAL:HG12	1.96	0.46
1:E:74:MSE:O	1:E:78:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:151:LEU:O	1:I:152:GLU:HB2	2.16	0.46
1:A:140:GLN:HE22	1:D:86:ARG:CZ	2.28	0.46
1:K:141:THR:O	1:K:142:LEU:HB2	2.16	0.46
1:F:125:ASN:HB3	1:F:128:ASP:OD2	2.16	0.46
1:I:76:GLU:OE2	1:J:81:ARG:NH2	2.49	0.46
1:J:114:PRO:HG2	1:J:116:PHE:HE1	1.80	0.46
1:C:122:HIS:CD2	1:C:122:HIS:N	2.84	0.46
1:B:85:ASP:O	1:B:89:VAL:HG13	2.15	0.45
1:L:133:LYS:HE3	1:L:147:VAL:HG12	1.97	0.45
1:B:86:ARG:NH1	2:B:159:HOH:O	2.48	0.45
1:D:112:THR:HG22	1:G:114:PRO:CB	2.46	0.45
1:G:92:LEU:HD12	1:H:117:LEU:HD23	1.98	0.45
1:A:82:ARG:NH2	1:C:74:MSE:CG	2.80	0.45
1:G:98:VAL:O	1:G:131:PRO:HB3	2.17	0.45
1:K:112:THR:HG22	1:L:113:GLY:C	2.42	0.45
1:K:86:ARG:CD	1:L:104:ARG:HH22	2.29	0.45
1:B:82:ARG:NH2	1:C:123:PHE:CZ	2.82	0.45
1:D:114:PRO:HG2	1:D:116:PHE:HE1	1.81	0.45
1:F:82:ARG:CD	1:G:123:PHE:HE1	2.30	0.45
1:E:146:ASP:OD2	1:H:74:MSE:CG	2.61	0.44
1:H:112:THR:HA	1:K:114:PRO:HB3	1.98	0.44
1:K:86:ARG:CD	1:L:104:ARG:NH2	2.80	0.44
1:G:86:ARG:CZ	1:H:104:ARG:HD3	2.48	0.44
1:B:148:LEU:CD2	1:B:149:PRO:HD2	2.47	0.44
1:H:110:SER:C	1:H:112:THR:H	2.24	0.44
1:E:77:ASN:HD21	1:F:76:GLU:HG3	1.81	0.44
1:C:76:GLU:OE2	1:D:81:ARG:NH2	2.47	0.44
1:D:74:MSE:O	1:D:75:LYS:HD3	2.18	0.44
1:D:125:ASN:HB3	1:D:128:ASP:OD2	2.17	0.44
1:J:76:GLU:O	1:J:80:LEU:HG	2.18	0.44
1:K:87:MSE:HG3	2:L:160:HOH:O	2.18	0.44
1:I:74:MSE:HE3	1:K:82:ARG:NH2	2.33	0.44
1:K:111:SER:OG	1:L:109:LYS:HE3	2.18	0.43
1:I:107:VAL:HG22	1:I:117:LEU:HD13	2.00	0.43
1:L:130:ALA:O	1:L:131:PRO:C	2.59	0.43
1:A:140:GLN:HE22	1:D:86:ARG:NE	2.17	0.43
1:H:114:PRO:HG2	1:H:116:PHE:CE1	2.54	0.43
1:A:82:ARG:NH2	1:C:74:MSE:HG3	2.33	0.43
1:D:109:LYS:HE2	2:D:160:HOH:O	2.19	0.43
1:E:77:ASN:OD1	1:F:77:ASN:HB2	2.18	0.43
1:B:98:VAL:O	1:B:131:PRO:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:92:LEU:HD13	1:K:136:CYS:HB3	1.99	0.43
1:K:105:LYS:NZ	1:K:119:ASN:OD1	2.39	0.43
1:B:86:ARG:HH21	1:B:140:GLN:HE22	1.66	0.43
1:B:90:PRO:HG2	1:I:105:LYS:HE3	2.01	0.43
1:B:100:LYS:HE2	1:B:126:PRO:O	2.18	0.43
1:D:82:ARG:HH11	1:D:82:ARG:HG2	1.83	0.43
1:F:85:ASP:O	1:F:89:VAL:HG13	2.19	0.43
1:E:146:ASP:OD2	1:H:74:MSE:HA	2.19	0.42
1:L:104:ARG:CZ	1:L:122:HIS:NE2	2.82	0.42
1:A:76:GLU:O	1:A:80:LEU:HG	2.19	0.42
1:G:100:LYS:HD3	1:G:129:LEU:O	2.19	0.42
1:L:100:LYS:HA	1:L:106:VAL:HG12	2.01	0.42
1:B:86:ARG:HH11	1:B:86:ARG:CB	2.26	0.42
1:C:117:LEU:HD23	1:L:92:LEU:HD12	2.02	0.42
1:F:125:ASN:HA	1:F:126:PRO:HD2	1.89	0.42
1:I:100:LYS:HA	1:I:106:VAL:HG12	2.01	0.42
1:H:130:ALA:O	1:H:131:PRO:C	2.62	0.42
1:J:88:ARG:HD3	1:J:123:PHE:CD2	2.55	0.42
1:F:134:ARG:HG2	1:F:134:ARG:NH1	2.35	0.41
1:D:112:THR:CG2	1:G:114:PRO:HB3	2.50	0.41
1:G:86:ARG:NE	2:G:46:HOH:O	2.34	0.41
1:A:83:GLU:HG2	1:B:122:HIS:CG	2.55	0.41
1:L:125:ASN:HA	1:L:126:PRO:HD2	1.93	0.41
1:B:82:ARG:NH1	1:B:82:ARG:CG	2.83	0.41
1:G:148:LEU:HD23	1:G:148:LEU:HA	1.93	0.41
1:H:79:ILE:O	1:H:83:GLU:HG2	2.21	0.41
1:H:114:PRO:HG2	1:H:116:PHE:HE1	1.85	0.41
1:H:130:ALA:O	1:H:133:LYS:HB2	2.20	0.41
1:B:86:ARG:NH2	1:B:87:MSE:HE3	2.30	0.41
1:G:87:MSE:HE3	1:H:145:VAL:HG12	2.02	0.41
1:H:98:VAL:HG12	1:H:99:ASP:OD1	2.21	0.41
1:J:88:ARG:HD3	1:J:123:PHE:CZ	2.56	0.41
1:G:76:GLU:OE2	1:H:77:ASN:HB2	2.20	0.41
1:G:97:VAL:O	1:G:131:PRO:HA	2.21	0.40
1:I:74:MSE:HE3	1:K:82:ARG:CZ	2.50	0.40
1:G:74:MSE:HA	1:G:74:MSE:CE	2.51	0.40
1:K:123:PHE:HE1	1:K:145:VAL:O	2.03	0.40
1:I:112:THR:HG22	1:J:114:PRO:CB	2.51	0.40
1:A:118:VAL:HA	1:F:90:PRO:HB3	2.03	0.40
1:B:100:LYS:HE2	1:B:129:LEU:HB2	2.03	0.40
1:H:93:ILE:HG12	1:K:116:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	74/85 (87%)	71 (96%)	2 (3%)	1 (1%)	9	5
1	B	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
1	C	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
1	D	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
1	E	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
1	F	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
1	G	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
1	H	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
1	I	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
1	J	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
1	K	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
1	L	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
All	All	898/1020 (88%)	872 (97%)	25 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	GLN

5.3.2 Protein sidechains [i](#)

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	71/78 (91%)	71 (100%)	0	100	100
1	B	72/78 (92%)	68 (94%)	4 (6%)	19	18
1	C	71/78 (91%)	69 (97%)	2 (3%)	38	43
1	D	71/78 (91%)	71 (100%)	0	100	100
1	E	71/78 (91%)	70 (99%)	1 (1%)	59	67
1	F	71/78 (91%)	71 (100%)	0	100	100
1	G	71/78 (91%)	70 (99%)	1 (1%)	59	67
1	H	73/78 (94%)	71 (97%)	2 (3%)	39	45
1	I	74/78 (95%)	74 (100%)	0	100	100
1	J	71/78 (91%)	71 (100%)	0	100	100
1	K	72/78 (92%)	72 (100%)	0	100	100
1	L	74/78 (95%)	74 (100%)	0	100	100
All	All	862/936 (92%)	852 (99%)	10 (1%)	63	72

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	82	ARG
1	B	86	ARG
1	B	87	MSE
1	B	146	ASP
1	C	76	GLU
1	C	122	HIS
1	E	77	ASN
1	G	74	MSE
1	H	87	MSE
1	H	103	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	B	77	ASN
1	B	139	GLN
1	B	140	GLN
1	C	122	HIS

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Mol	Chain	Res	Type
1	C	139	GLN
1	D	139	GLN
1	E	139	GLN
1	I	119	ASN
1	J	125	ASN
1	J	139	GLN
1	J	140	GLN
1	K	139	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 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	74/85 (87%)	0.27	4 (5%) 31 33	20, 32, 58, 72	0
1	B	75/85 (88%)	0.38	6 (8%) 18 19	19, 34, 61, 81	0
1	C	74/85 (87%)	-0.00	5 (6%) 23 25	18, 27, 46, 64	0
1	D	74/85 (87%)	0.25	4 (5%) 31 33	18, 31, 50, 63	0
1	E	74/85 (87%)	0.44	7 (9%) 14 14	18, 33, 59, 88	0
1	F	74/85 (87%)	0.62	7 (9%) 14 14	21, 38, 69, 91	0
1	G	74/85 (87%)	0.35	6 (8%) 18 19	20, 35, 61, 74	0
1	H	76/85 (89%)	0.37	7 (9%) 14 15	19, 34, 58, 67	0
1	I	77/85 (90%)	0.08	3 (3%) 43 45	16, 30, 56, 78	0
1	J	74/85 (87%)	0.60	7 (9%) 14 14	21, 38, 61, 74	0
1	K	76/85 (89%)	0.36	9 (11%) 9 9	20, 33, 58, 76	0
1	L	77/85 (90%)	0.46	9 (11%) 9 9	18, 33, 64, 82	0
All	All	899/1020 (88%)	0.35	74 (8%) 17 18	16, 33, 60, 91	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	103	GLU	5.0
1	H	112	THR	4.7
1	K	75	LYS	4.6
1	E	112	THR	4.1
1	C	123	PHE	3.9
1	D	149	PRO	3.8
1	J	122	HIS	3.7
1	H	151	LEU	3.7
1	K	112	THR	3.7
1	J	149	PRO	3.7
1	A	102	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	111	SER	3.6
1	D	112	THR	3.5
1	L	101	VAL	3.3
1	H	102	GLY	3.3
1	E	111	SER	3.2
1	C	149	PRO	3.2
1	L	102	GLY	3.1
1	I	123	PHE	3.1
1	K	113	GLY	3.0
1	L	75	LYS	3.0
1	C	101	VAL	2.9
1	A	112	THR	2.9
1	J	112	THR	2.9
1	E	99	ASP	2.9
1	F	104	ARG	2.9
1	E	101	VAL	2.8
1	K	114	PRO	2.8
1	L	151	LEU	2.8
1	F	77	ASN	2.8
1	F	75	LYS	2.7
1	H	101	VAL	2.7
1	J	123	PHE	2.7
1	I	152	GLU	2.7
1	G	112	THR	2.6
1	K	122	HIS	2.6
1	A	101	VAL	2.6
1	C	134	ARG	2.6
1	D	102	GLY	2.5
1	G	102	GLY	2.5
1	F	149	PRO	2.5
1	B	75	LYS	2.4
1	H	104	ARG	2.4
1	E	149	PRO	2.4
1	C	99	ASP	2.4
1	G	101	VAL	2.4
1	L	104	ARG	2.4
1	B	149	PRO	2.4
1	F	126	PRO	2.3
1	L	152	GLU	2.3
1	L	103	GLU	2.3
1	L	150	GLU	2.3
1	B	122	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	76	GLU	2.3
1	K	151	LEU	2.3
1	G	149	PRO	2.2
1	K	76	GLU	2.2
1	H	99	ASP	2.2
1	B	123	PHE	2.2
1	K	123	PHE	2.2
1	G	103	GLU	2.2
1	K	103	GLU	2.1
1	B	102	GLY	2.1
1	D	101	VAL	2.1
1	L	122	HIS	2.1
1	E	77	ASN	2.1
1	B	103	GLU	2.1
1	G	123	PHE	2.1
1	J	134	ARG	2.0
1	F	102	GLY	2.0
1	A	103	GLU	2.0
1	F	103	GLU	2.0
1	I	122	HIS	2.0
1	J	102	GLY	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.