



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:03 PM UTC

PDB ID : 4K2H / pdb_00004k2h
Title : Crystal structure of C103A mutant of DJ-1 superfamily protein STM1931 from *Salmonella typhimurium*
Authors : Shumilin, I.A.; Niedzialkowska, E.; Domagalski, M.J.; Stam, J.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on : 2013-04-09
Resolution : 2.20 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

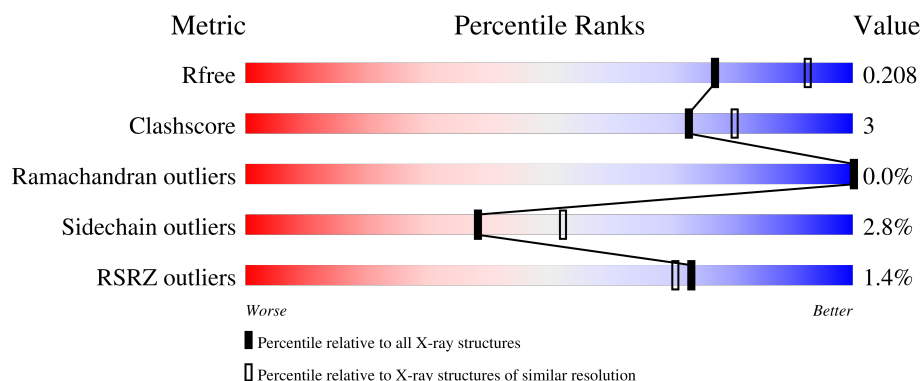
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	188	% 89% 9% ..
1	B	188	% 90% 7% ..
1	C	188	% 90% 9% .
1	D	188	% 91% 7% ..
1	E	188	 91% 7% .

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Mol	Chain	Length	Quality of chain
1	F	188	% 91% 6% ..
1	G	188	% 90% 9% ..
1	H	188	4% 90% 7% ..
1	I	188	2% 92% 6% ..
1	J	188	% 91% 7% .
1	K	188	4% 93% 6% .
1	L	188	4% 87% 10% ..
1	M	188	% 91% 6% ..
1	N	188	% 89% 9% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20792 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 Intracellular protease/amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	1	0
			1390	886	242	257	5			
1	B	185	Total	C	N	O	S	0	2	0
			1397	892	245	255	5			
1	C	185	Total	C	N	O	S	0	2	0
			1396	890	242	259	5			
1	D	186	Total	C	N	O	S	0	3	0
			1404	895	243	261	5			
1	E	185	Total	C	N	O	S	0	2	0
			1398	891	245	257	5			
1	F	185	Total	C	N	O	S	0	1	0
			1390	886	242	257	5			
1	G	186	Total	C	N	O	S	0	1	0
			1398	891	246	256	5			
1	H	185	Total	C	N	O	S	0	0	0
			1385	883	242	255	5			
1	I	185	Total	C	N	O	S	0	9	0
			1446	918	255	267	6			
1	J	185	Total	C	N	O	S	0	2	0
			1396	890	243	258	5			
1	K	185	Total	C	N	O	S	0	2	0
			1399	892	246	256	5			
1	L	185	Total	C	N	O	S	0	2	0
			1396	890	245	256	5			
1	M	185	Total	C	N	O	S	0	3	0
			1404	895	245	259	5			
1	N	185	Total	C	N	O	S	0	2	0
			1396	890	242	259	5			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8ZNU7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP Q8ZNU7
A	0	ALA	-	expression tag	UNP Q8ZNU7
A	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
B	-2	SER	-	expression tag	UNP Q8ZNU7
B	-1	ASN	-	expression tag	UNP Q8ZNU7
B	0	ALA	-	expression tag	UNP Q8ZNU7
B	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
C	-2	SER	-	expression tag	UNP Q8ZNU7
C	-1	ASN	-	expression tag	UNP Q8ZNU7
C	0	ALA	-	expression tag	UNP Q8ZNU7
C	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
D	-2	SER	-	expression tag	UNP Q8ZNU7
D	-1	ASN	-	expression tag	UNP Q8ZNU7
D	0	ALA	-	expression tag	UNP Q8ZNU7
D	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
E	-2	SER	-	expression tag	UNP Q8ZNU7
E	-1	ASN	-	expression tag	UNP Q8ZNU7
E	0	ALA	-	expression tag	UNP Q8ZNU7
E	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
F	-2	SER	-	expression tag	UNP Q8ZNU7
F	-1	ASN	-	expression tag	UNP Q8ZNU7
F	0	ALA	-	expression tag	UNP Q8ZNU7
F	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
G	-2	SER	-	expression tag	UNP Q8ZNU7
G	-1	ASN	-	expression tag	UNP Q8ZNU7
G	0	ALA	-	expression tag	UNP Q8ZNU7
G	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
H	-2	SER	-	expression tag	UNP Q8ZNU7
H	-1	ASN	-	expression tag	UNP Q8ZNU7
H	0	ALA	-	expression tag	UNP Q8ZNU7
H	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
I	-2	SER	-	expression tag	UNP Q8ZNU7
I	-1	ASN	-	expression tag	UNP Q8ZNU7
I	0	ALA	-	expression tag	UNP Q8ZNU7
I	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
J	-2	SER	-	expression tag	UNP Q8ZNU7
J	-1	ASN	-	expression tag	UNP Q8ZNU7
J	0	ALA	-	expression tag	UNP Q8ZNU7
J	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
K	-2	SER	-	expression tag	UNP Q8ZNU7
K	-1	ASN	-	expression tag	UNP Q8ZNU7
K	0	ALA	-	expression tag	UNP Q8ZNU7

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Chain	Residue	Modelled	Actual	Comment	Reference
K	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
L	-2	SER	-	expression tag	UNP Q8ZNU7
L	-1	ASN	-	expression tag	UNP Q8ZNU7
L	0	ALA	-	expression tag	UNP Q8ZNU7
L	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
M	-2	SER	-	expression tag	UNP Q8ZNU7
M	-1	ASN	-	expression tag	UNP Q8ZNU7
M	0	ALA	-	expression tag	UNP Q8ZNU7
M	103	ALA	CYS	engineered mutation	UNP Q8ZNU7
N	-2	SER	-	expression tag	UNP Q8ZNU7
N	-1	ASN	-	expression tag	UNP Q8ZNU7
N	0	ALA	-	expression tag	UNP Q8ZNU7
N	103	ALA	CYS	engineered mutation	UNP Q8ZNU7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	1	Total 1	Zn 1	0	0

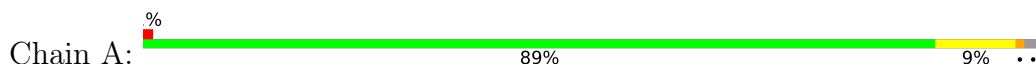
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total 90	O 90	0	0
3	B	143	Total 143	O 143	0	0
3	C	126	Total 126	O 126	0	0
3	D	81	Total 81	O 81	0	0
3	E	110	Total 110	O 110	0	0
3	F	77	Total 77	O 77	0	0
3	G	51	Total 51	O 51	0	0
3	H	56	Total 56	O 56	0	0
3	I	67	Total 67	O 67	0	0
3	J	76	Total 76	O 76	0	0
3	K	47	Total 47	O 47	0	0
3	L	54	Total 54	O 54	0	0
3	M	76	Total 76	O 76	0	0
3	N	129	Total 129	O 129	0	0

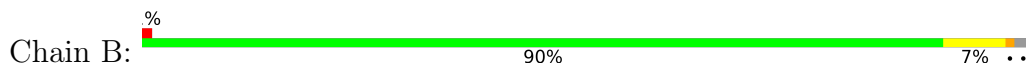
3 Residue-property plots [i](#)

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.

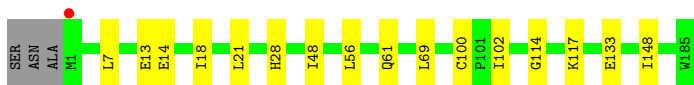
- Molecule 1: Intracellular protease/amidase



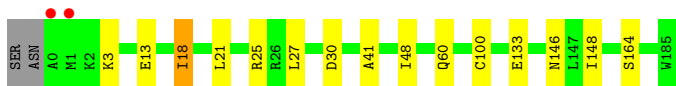
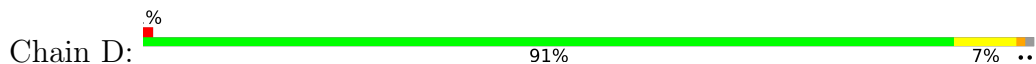
- Molecule 1: Intracellular protease/amidase



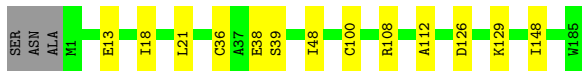
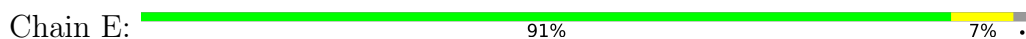
- Molecule 1: Intracellular protease/amidase



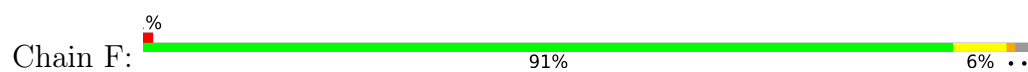
- Molecule 1: Intracellular protease/amidase



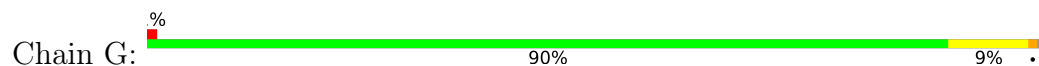
- Molecule 1: Intracellular protease/amidase



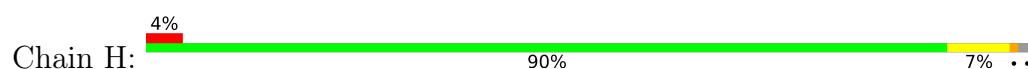
- Molecule 1: Intracellular protease/amidase



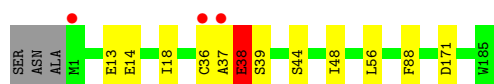
- Molecule 1: Intracellular protease/amidase



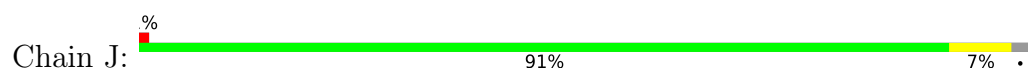
- Molecule 1: Intracellular protease/amidase



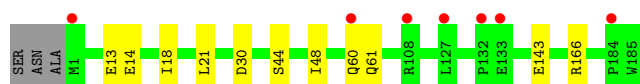
- Molecule 1: Intracellular protease/amidase



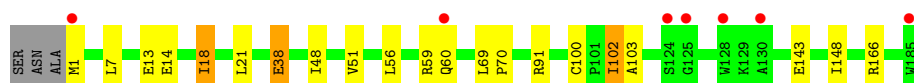
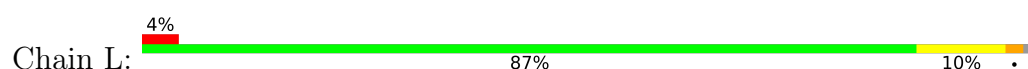
- Molecule 1: Intracellular protease/amidase



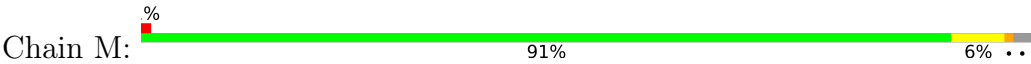
- Molecule 1: Intracellular protease/amidase



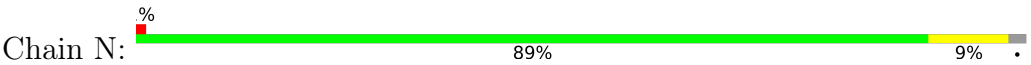
- Molecule 1: Intracellular protease/amidase



● Molecule 1: Intracellular protease/amidase



● Molecule 1: Intracellular protease/amidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.66Å 113.75Å 175.71Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	36.71 – 2.20 36.71 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.8 (36.71-2.20) 94.8 (36.71-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.14Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.205 0.179 , 0.208	Depositor DCC
R_{free} test set	8505 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.0	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	0.97	EDS
Total number of atoms	20792	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9722e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.80	0/1422	0.92	0/1937
1	B	0.87	0/1432	0.93	1/1950 (0.1%)
1	C	0.85	0/1431	0.90	0/1949
1	D	0.76	0/1442	0.88	0/1964
1	E	0.84	0/1433	0.92	0/1951
1	F	0.77	0/1422	0.85	0/1937
1	G	0.66	0/1430	0.82	0/1947
1	H	0.67	0/1414	0.82	0/1926
1	I	0.72	0/1484	0.85	0/2019
1	J	0.76	0/1431	0.86	0/1949
1	K	0.70	0/1434	0.85	0/1952
1	L	0.74	0/1431	0.87	0/1948
1	M	0.73	0/1442	0.84	0/1963
1	N	0.86	0/1431	0.93	1/1949 (0.1%)
All	All	0.77	0/20079	0.87	2/27341 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	CYS	N-CA-C	-6.33	100.79	109.71
1	N	133	GLU	N-CA-C	5.24	117.16	110.61

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	1390	0	1400	9	0
1	B	1397	0	1418	9	0
1	C	1396	0	1406	9	0
1	D	1404	0	1416	10	0
1	E	1398	0	1413	9	0
1	F	1390	0	1400	9	0
1	G	1398	0	1414	12	0
1	H	1385	0	1396	8	0
1	I	1446	0	1459	18	0
1	J	1396	0	1408	10	0
1	K	1399	0	1417	7	0
1	L	1396	0	1414	16	0
1	M	1404	0	1419	9	0
1	N	1396	0	1406	12	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	J	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
2	N	1	0	0	0	0
3	A	90	0	0	1	0
3	B	143	0	0	2	0
3	C	126	0	0	1	0
3	D	81	0	0	1	0
3	E	110	0	0	2	0
3	F	77	0	0	1	0
3	G	51	0	0	0	0
3	H	56	0	0	2	0
3	I	67	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	76	0	0	0	0
3	K	47	0	0	1	0
3	L	54	0	0	0	0
3	M	76	0	0	0	0
3	N	129	0	0	1	0
All	All	20792	0	19786	126	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 3.

All (126) 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:59[B]:ARG:HG2	1:L:59[B]:ARG:HH21	0.97	1.12
1:I:48:ILE:HD11	1:J:21:LEU:HD22	1.35	1.03
1:L:59[B]:ARG:HH21	1:L:59[B]:ARG:CG	1.75	0.99
1:L:59[B]:ARG:HG2	1:L:59[B]:ARG:NH2	1.80	0.94
1:N:60:GLN:HE21	1:N:61:GLN:HE22	1.18	0.91
1:E:48:ILE:HD11	1:F:21:LEU:HD22	1.55	0.86
1:G:48:ILE:HD11	1:H:21:LEU:HD22	1.60	0.83
1:I:38[A]:GLU:OE2	1:I:39[A]:SER:HB2	1.77	0.83
1:F:41:ALA:HB2	1:J:51:VAL:HG21	1.72	0.71
1:I:36[B]:CYS:SG	1:I:56:LEU:HD22	2.34	0.66
1:I:38[A]:GLU:OE2	1:I:39[A]:SER:N	2.30	0.65
1:A:48:ILE:HD11	1:B:21:LEU:HD22	1.79	0.65
1:D:60:GLN:NE2	1:E:112:ALA:O	2.31	0.63
1:G:48:ILE:HD13	1:H:18:ILE:HD12	1.81	0.63
1:M:48:ILE:HD11	1:N:21:LEU:HD22	1.80	0.62
1:L:59[B]:ARG:CG	1:L:59[B]:ARG:NH2	2.44	0.62
1:B:60:GLN:O	1:B:91:ARG:NH2	2.32	0.62
1:I:48:ILE:HD13	1:J:18:ILE:HD12	1.82	0.61
1:I:48:ILE:HD11	1:J:21:LEU:CD2	2.23	0.59
1:A:38:GLU:H	1:A:38:GLU:CD	2.10	0.59
1:A:14:GLU:HG3	1:A:48:ILE:HD12	1.84	0.59
1:L:38:GLU:H	1:L:38:GLU:CD	2.11	0.59
1:I:38[A]:GLU:OE2	1:I:39[A]:SER:CB	2.50	0.58
1:K:60[B]:GLN:HA	1:K:60[B]:GLN:OE1	2.03	0.57
1:B:117:LYS:HG3	1:B:117:LYS:O	2.05	0.56
1:A:145:GLY:O	1:A:166:ARG:NH1	2.34	0.56
1:G:1:MET:HE3	1:G:1:MET:HA	1.87	0.56
1:I:14:GLU:HG3	1:I:48:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:HIS:CD2	3:C:345:HOH:O	2.59	0.56
1:D:21:LEU:HD23	1:D:21:LEU:C	2.31	0.56
1:M:21:LEU:HD22	1:N:48:ILE:HD11	1.88	0.56
1:F:120:ARG:HD2	3:F:346:HOH:O	2.06	0.55
1:K:143:GLU:OE1	1:K:166:ARG:NH1	2.38	0.54
1:A:100:CYS:HA	1:A:148:ILE:O	2.09	0.53
1:E:21:LEU:C	1:E:21:LEU:HD23	2.33	0.53
1:I:37[B]:ALA:O	1:I:39[B]:SER:N	2.31	0.53
1:K:21:LEU:C	1:K:21:LEU:HD23	2.33	0.53
1:G:100:CYS:HA	1:G:148:ILE:O	2.08	0.53
1:L:60:GLN:O	1:L:91:ARG:NH2	2.42	0.53
1:H:7:LEU:HD12	1:H:69:LEU:CD2	2.39	0.52
1:D:41:ALA:HB2	1:L:51:VAL:HG21	1.91	0.52
1:M:158[A]:ASP:OD1	1:M:183:TYR:OH	2.27	0.52
1:C:100:CYS:HA	1:C:148:ILE:O	2.09	0.52
1:I:37[B]:ALA:C	1:I:39[B]:SER:H	2.16	0.52
1:K:143:GLU:HG3	3:K:331:HOH:O	2.09	0.52
1:C:114:GLY:HA2	1:C:133[B]:GLU:CD	2.35	0.51
1:C:117:LYS:O	1:C:117:LYS:HG3	2.09	0.51
1:J:172:ALA:HB3	1:J:173:PRO:HD3	1.92	0.51
1:A:102:ILE:HG13	1:A:103:ALA:N	2.26	0.51
1:C:21:LEU:HD22	1:D:48:ILE:HD11	1.94	0.50
1:L:14:GLU:HG3	1:L:48:ILE:HD12	1.94	0.49
1:E:100:CYS:HA	1:E:148:ILE:O	2.12	0.49
1:D:21:LEU:HD21	1:D:25:ARG:HD2	1.94	0.49
1:L:102:ILE:HG13	1:L:103:ALA:N	2.28	0.49
1:F:41:ALA:HB2	1:J:51:VAL:CG2	2.43	0.48
1:N:108:ARG:NE	3:N:337:HOH:O	2.46	0.48
1:M:48:ILE:HD12	1:N:18:ILE:HD12	1.95	0.48
1:B:30:ASP:HB3	3:B:428:HOH:O	2.13	0.47
1:E:36:CYS:HB2	3:E:325:HOH:O	2.13	0.47
1:G:21:LEU:C	1:G:21:LEU:HD23	2.38	0.47
1:J:14:GLU:O	1:J:18:ILE:HG12	2.15	0.47
1:C:48:ILE:HD11	1:D:21:LEU:HD22	1.96	0.47
1:M:38:GLU:H	1:M:38:GLU:CD	2.22	0.47
1:L:7:LEU:HD12	1:L:69:LEU:CD2	2.44	0.47
1:C:21:LEU:C	1:C:21:LEU:HD23	2.39	0.47
1:A:21:LEU:C	1:A:21:LEU:HD23	2.41	0.46
1:B:126:ASP:HB2	1:B:129:LYS:HE2	1.96	0.46
1:N:21:LEU:C	1:N:21:LEU:HD23	2.39	0.46
1:C:14:GLU:HG2	1:D:18:ILE:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ILE:HD13	1:F:18:ILE:HD12	1.97	0.46
1:N:14:GLU:O	1:N:18:ILE:HG12	2.15	0.46
1:C:7:LEU:HD12	1:C:69:LEU:CD2	2.45	0.46
1:I:38[B]:GLU:CD	1:I:38[B]:GLU:N	2.73	0.46
1:N:19:VAL:HG11	1:N:156:VAL:HG13	1.97	0.46
1:H:38:GLU:HG2	3:H:306:HOH:O	2.15	0.46
1:N:172:ALA:HB3	1:N:173:PRO:HD3	1.97	0.46
1:I:38[A]:GLU:CD	1:I:39[A]:SER:N	2.74	0.46
1:B:39:SER:CB	3:B:379:HOH:O	2.64	0.45
1:B:59[A]:ARG:HG2	1:B:59[A]:ARG:HH21	1.82	0.45
1:E:126:ASP:HB2	1:E:129:LYS:HE3	1.98	0.45
1:I:14:GLU:HB3	1:I:44:SER:CB	2.47	0.45
1:G:14:GLU:HB3	1:G:44:SER:HB2	1.99	0.45
1:M:145:GLY:O	1:M:166:ARG:NH1	2.37	0.44
1:H:129:LYS:HB3	3:H:318:HOH:O	2.17	0.44
1:M:14:GLU:HB3	1:M:44:SER:HB2	2.00	0.44
1:F:38:GLU:HG3	3:I:363:HOH:O	2.17	0.44
1:G:14:GLU:HB3	1:G:44:SER:CB	2.47	0.44
1:D:146:ASN:HB3	3:D:351:HOH:O	2.17	0.44
1:F:143:GLU:OE2	1:F:166:ARG:NH2	2.50	0.44
1:H:172:ALA:HB3	1:H:173:PRO:HD3	1.99	0.43
1:I:37[B]:ALA:C	1:I:39[B]:SER:N	2.76	0.43
1:K:14:GLU:HB3	1:K:44:SER:HB2	2.00	0.43
1:N:100:CYS:HA	1:N:148:ILE:O	2.18	0.43
1:M:14:GLU:HB3	1:M:44:SER:CB	2.49	0.43
1:M:3:LYS:HA	1:M:30:ASP:O	2.19	0.43
1:N:9:ALA:O	1:N:10:PRO:C	2.60	0.43
1:I:38[B]:GLU:CD	1:I:38[B]:GLU:H	2.26	0.42
1:D:27:LEU:HD13	1:D:164:SER:HB3	2.00	0.42
1:A:74:GLN:HG3	3:A:349:HOH:O	2.20	0.42
1:G:18:ILE:HD12	1:H:48:ILE:CD1	2.50	0.42
1:G:40:ARG:HD2	1:G:52:ALA:O	2.20	0.42
1:K:48:ILE:HD11	1:L:21:LEU:HD22	2.01	0.42
1:L:143:GLU:OE2	1:L:166:ARG:NH2	2.49	0.42
1:H:100:CYS:HA	1:H:148:ILE:O	2.20	0.42
1:J:114:GLY:HA2	1:J:133:GLU:CD	2.45	0.41
1:L:70:PRO:HA	1:L:102:ILE:HG23	2.01	0.41
1:E:38:GLU:H	1:E:38:GLU:CD	2.28	0.41
1:G:47:ASP:O	1:G:49:PRO:HD3	2.20	0.41
1:G:133:GLU:O	1:G:133:GLU:CD	2.63	0.41
1:L:100:CYS:HA	1:L:148:ILE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38[A]:GLU:OE2	1:I:39[A]:SER:CA	2.69	0.41
1:A:7:LEU:HD12	1:A:69:LEU:CD2	2.51	0.41
1:D:100:CYS:HA	1:D:148:ILE:O	2.20	0.41
1:J:116:LEU:HD23	1:J:116:LEU:HA	1.94	0.41
1:L:56:LEU:O	1:L:60:GLN:HG3	2.21	0.41
1:B:100:CYS:HA	1:B:148:ILE:O	2.21	0.41
1:B:138:ASP:OD1	1:B:138:ASP:C	2.62	0.41
1:E:108[A]:ARG:NH2	3:E:391:HOH:O	2.38	0.41
1:I:14:GLU:CD	1:I:14:GLU:H	2.29	0.41
1:K:14:GLU:HG2	1:L:18:ILE:HG23	2.02	0.41
1:N:14:GLU:HG3	1:N:48:ILE:HD12	2.03	0.41
1:F:56:LEU:HD11	1:F:88:PHE:CD1	2.56	0.41
1:F:14:GLU:HB3	1:F:44:SER:CB	2.51	0.40
1:G:18:ILE:HD13	1:G:18:ILE:HA	1.86	0.40
1:I:56:LEU:HD11	1:I:88:PHE:CG	2.57	0.40
1:J:100:CYS:HA	1:J:148:ILE:O	2.22	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	184/188 (98%)	177 (96%)	7 (4%)	0	100	100
1	B	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
1	C	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
1	D	187/188 (100%)	183 (98%)	4 (2%)	0	100	100
1	E	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
1	F	184/188 (98%)	179 (97%)	5 (3%)	0	100	100
1	G	185/188 (98%)	179 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	183/188 (97%)	177 (97%)	6 (3%)	0	100	100
1	I	192/188 (102%)	183 (95%)	7 (4%)	2 (1%)	12	11
1	J	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
1	K	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
1	L	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
1	M	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	N	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
All	All	2596/2632 (99%)	2521 (97%)	73 (3%)	2 (0%)	100	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	38[A]	GLU
1	I	38[B]	GLU

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	142/143 (99%)	137 (96%)	5 (4%)	32	43
1	B	143/143 (100%)	140 (98%)	3 (2%)	47	63
1	C	143/143 (100%)	138 (96%)	5 (4%)	32	43
1	D	144/143 (101%)	139 (96%)	5 (4%)	32	43
1	E	143/143 (100%)	140 (98%)	3 (2%)	47	63
1	F	142/143 (99%)	139 (98%)	3 (2%)	47	63
1	G	142/143 (99%)	137 (96%)	5 (4%)	32	43
1	H	141/143 (99%)	136 (96%)	5 (4%)	32	43
1	I	148/143 (104%)	143 (97%)	5 (3%)	32	44
1	J	143/143 (100%)	140 (98%)	3 (2%)	47	63
1	K	143/143 (100%)	139 (97%)	4 (3%)	38	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	143/143 (100%)	138 (96%)	5 (4%)	32	43
1	M	144/143 (101%)	139 (96%)	5 (4%)	32	43
1	N	143/143 (100%)	142 (99%)	1 (1%)	76	87
All	All	2004/2002 (100%)	1947 (97%)	57 (3%)	38	52

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	18	ILE
1	A	22	ASP
1	A	30	ASP
1	A	102	ILE
1	B	13	GLU
1	B	39	SER
1	B	61	GLN
1	C	13	GLU
1	C	18	ILE
1	C	56	LEU
1	C	61	GLN
1	C	102	ILE
1	D	3	LYS
1	D	13	GLU
1	D	18	ILE
1	D	30	ASP
1	D	133	GLU
1	E	13	GLU
1	E	18	ILE
1	E	39	SER
1	F	3	LYS
1	F	13	GLU
1	F	18	ILE
1	G	13	GLU
1	G	38	GLU
1	G	40	ARG
1	G	56	LEU
1	G	74	GLN
1	H	13	GLU
1	H	18	ILE
1	H	22	ASP
1	H	47	ASP

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Mol	Chain	Res	Type
1	H	133	GLU
1	I	13	GLU
1	I	18	ILE
1	I	38[A]	GLU
1	I	38[B]	GLU
1	I	171	ASP
1	J	13	GLU
1	J	31	VAL
1	J	38	GLU
1	K	13	GLU
1	K	18	ILE
1	K	30	ASP
1	K	61	GLN
1	L	1	MET
1	L	13	GLU
1	L	18	ILE
1	L	38	GLU
1	L	102	ILE
1	M	13	GLU
1	M	18	ILE
1	M	30	ASP
1	M	48	ILE
1	M	56	LEU
1	N	13	GLU

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	60	GLN
1	A	61	GLN
1	B	177	GLN
1	C	177	GLN
1	D	74	GLN
1	D	177	GLN
1	F	60	GLN
1	F	61	GLN
1	I	74	GLN
1	I	177	GLN
1	J	61	GLN
1	L	74	GLN
1	M	177	GLN
1	M	180	HIS

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Mol	Chain	Res	Type
1	N	61	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](#)

Of 14 ligands modelled in this entry, 14 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 [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	185/188 (98%)	-0.27	1 (0%) 87 85	23, 35, 53, 71	1 (0%)
1	B	185/188 (98%)	-0.31	1 (0%) 87 85	18, 30, 48, 76	2 (1%)
1	C	185/188 (98%)	-0.28	1 (0%) 87 85	20, 31, 46, 73	2 (1%)
1	D	186/188 (98%)	-0.23	2 (1%) 78 76	23, 36, 58, 92	3 (1%)
1	E	185/188 (98%)	-0.32	0 100 100	20, 32, 49, 62	2 (1%)
1	F	185/188 (98%)	-0.06	1 (0%) 87 85	25, 39, 65, 80	1 (0%)
1	G	186/188 (98%)	0.16	2 (1%) 78 76	28, 46, 80, 99	1 (0%)
1	H	185/188 (98%)	0.49	7 (3%) 44 41	31, 49, 83, 100	0
1	I	185/188 (98%)	0.01	3 (1%) 70 67	16, 40, 62, 78	9 (4%)
1	J	185/188 (98%)	-0.13	1 (0%) 87 85	25, 39, 64, 81	2 (1%)
1	K	185/188 (98%)	0.20	7 (3%) 44 41	27, 48, 87, 101	2 (1%)
1	L	185/188 (98%)	0.27	7 (3%) 44 41	25, 46, 83, 99	2 (1%)
1	M	185/188 (98%)	-0.09	1 (0%) 87 85	25, 39, 62, 80	3 (1%)
1	N	185/188 (98%)	-0.25	2 (1%) 78 76	20, 33, 50, 74	2 (1%)
All	All	2592/2632 (98%)	-0.06	36 (1%) 73 71	16, 38, 70, 101	32 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.2
1	H	172	ALA	4.1
1	L	1	MET	3.9
1	D	0	ALA	3.8
1	J	1	MET	3.4
1	K	1	MET	3.4
1	H	1	MET	3.3
1	I	1	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.1
1	G	0	ALA	3.0
1	G	1	MET	3.0
1	M	1	MET	3.0
1	K	133	GLU	3.0
1	N	1	MET	3.0
1	L	60	GLN	2.8
1	H	130	ALA	2.6
1	K	127	LEU	2.6
1	L	185	TRP	2.6
1	L	128	TRP	2.6
1	A	1	MET	2.6
1	C	1	MET	2.5
1	L	125	GLY	2.5
1	K	132	PRO	2.4
1	F	1	MET	2.4
1	H	135	VAL	2.4
1	H	127	LEU	2.4
1	I	37[A]	ALA	2.3
1	I	36[A]	CYS	2.2
1	L	124	SER	2.2
1	K	108[A]	ARG	2.1
1	H	124	SER	2.1
1	H	134	GLY	2.1
1	L	130	ALA	2.0
1	K	60[A]	GLN	2.0
1	K	184	PRO	2.0
1	N	108	ARG	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	C	201	1/1	0.99	0.02	35,35,35,35	0
2	ZN	D	201	1/1	0.99	0.02	30,30,30,30	0
2	ZN	G	201	1/1	0.99	0.02	47,47,47,47	0
2	ZN	K	201	1/1	0.99	0.02	43,43,43,43	0
2	ZN	L	201	1/1	0.99	0.02	38,38,38,38	0
2	ZN	N	201	1/1	0.99	0.02	37,37,37,37	0
2	ZN	A	201	1/1	1.00	0.02	30,30,30,30	0
2	ZN	H	201	1/1	1.00	0.02	43,43,43,43	0
2	ZN	I	201	1/1	1.00	0.02	39,39,39,39	0
2	ZN	J	201	1/1	1.00	0.02	40,40,40,40	0
2	ZN	B	201	1/1	1.00	0.02	34,34,34,34	0
2	ZN	E	201	1/1	1.00	0.02	36,36,36,36	0
2	ZN	M	201	1/1	1.00	0.02	33,33,33,33	0
2	ZN	F	201	1/1	1.00	0.03	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.