



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 07:59 AM UTC

PDB ID : 3TKR / pdb\_00003tkr  
Title : Crystal structure of full-length human peroxiredoxin 4 with T118E mutation  
Authors : Wang, X.; Wang, L.; Wang, X.; Sun, F.; Wang, C.-C.  
Deposited on : 2011-08-28  
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](mailto:validation@mail.wwpdb.org)

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<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

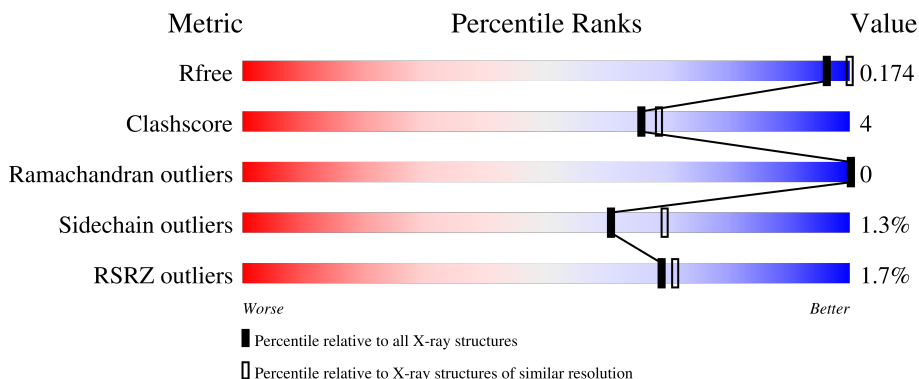
# 1 Overall quality at a glance

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  $\geq 3$ , 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	246	 2% 74% 5% 20%
1	B	246	 2% 76% 2% 20%
1	C	246	 2% 71% 8% 20%
1	D	246	 2% 74% 5% 20%
1	E	246	 2% 73% 7% 20%

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Mol	Chain	Length	Quality of chain
1	F	246	 2% 72% 7% 20%
1	G	246	 % 74% 5% 21%
1	H	246	 % 74% 6% 20%
1	I	246	 % 75% 5% 20%
1	J	246	 % 73% 7% 20%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18082 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 Peroxiredoxin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	197	Total 1624	C 1054	N 269	O 298	S 3	0	7	0
1	I	197	Total 1593	C 1031	N 264	O 295	S 3	0	2	0
1	G	195	Total 1564	C 1012	N 259	O 290	S 3	0	0	0
1	C	197	Total 1615	C 1047	N 269	O 296	S 3	0	6	0
1	F	197	Total 1597	C 1035	N 264	O 295	S 3	0	3	0
1	D	197	Total 1588	C 1028	N 264	O 293	S 3	0	1	0
1	B	197	Total 1593	C 1033	N 264	O 293	S 3	0	2	0
1	H	197	Total 1592	C 1031	N 263	O 295	S 3	0	2	0
1	E	197	Total 1587	C 1029	N 263	O 292	S 3	0	1	0
1	J	197	Total 1594	C 1032	N 263	O 296	S 3	0	2	0

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q13162
A	-10	ARG	-	expression tag	UNP Q13162
A	-9	GLY	-	expression tag	UNP Q13162
A	-8	SER	-	expression tag	UNP Q13162
A	-7	HIS	-	expression tag	UNP Q13162
A	-6	HIS	-	expression tag	UNP Q13162
A	-5	HIS	-	expression tag	UNP Q13162
A	-4	HIS	-	expression tag	UNP Q13162
A	-3	HIS	-	expression tag	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	expression tag	UNP Q13162
A	-1	GLY	-	expression tag	UNP Q13162
A	0	SER	-	expression tag	UNP Q13162
A	118	GLU	THR	engineered mutation	UNP Q13162
I	-11	MET	-	expression tag	UNP Q13162
I	-10	ARG	-	expression tag	UNP Q13162
I	-9	GLY	-	expression tag	UNP Q13162
I	-8	SER	-	expression tag	UNP Q13162
I	-7	HIS	-	expression tag	UNP Q13162
I	-6	HIS	-	expression tag	UNP Q13162
I	-5	HIS	-	expression tag	UNP Q13162
I	-4	HIS	-	expression tag	UNP Q13162
I	-3	HIS	-	expression tag	UNP Q13162
I	-2	HIS	-	expression tag	UNP Q13162
I	-1	GLY	-	expression tag	UNP Q13162
I	0	SER	-	expression tag	UNP Q13162
I	118	GLU	THR	engineered mutation	UNP Q13162
G	-11	MET	-	expression tag	UNP Q13162
G	-10	ARG	-	expression tag	UNP Q13162
G	-9	GLY	-	expression tag	UNP Q13162
G	-8	SER	-	expression tag	UNP Q13162
G	-7	HIS	-	expression tag	UNP Q13162
G	-6	HIS	-	expression tag	UNP Q13162
G	-5	HIS	-	expression tag	UNP Q13162
G	-4	HIS	-	expression tag	UNP Q13162
G	-3	HIS	-	expression tag	UNP Q13162
G	-2	HIS	-	expression tag	UNP Q13162
G	-1	GLY	-	expression tag	UNP Q13162
G	0	SER	-	expression tag	UNP Q13162
G	118	GLU	THR	engineered mutation	UNP Q13162
C	-11	MET	-	expression tag	UNP Q13162
C	-10	ARG	-	expression tag	UNP Q13162
C	-9	GLY	-	expression tag	UNP Q13162
C	-8	SER	-	expression tag	UNP Q13162
C	-7	HIS	-	expression tag	UNP Q13162
C	-6	HIS	-	expression tag	UNP Q13162
C	-5	HIS	-	expression tag	UNP Q13162
C	-4	HIS	-	expression tag	UNP Q13162
C	-3	HIS	-	expression tag	UNP Q13162
C	-2	HIS	-	expression tag	UNP Q13162
C	-1	GLY	-	expression tag	UNP Q13162
C	0	SER	-	expression tag	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
C	118	GLU	THR	engineered mutation	UNP Q13162
F	-11	MET	-	expression tag	UNP Q13162
F	-10	ARG	-	expression tag	UNP Q13162
F	-9	GLY	-	expression tag	UNP Q13162
F	-8	SER	-	expression tag	UNP Q13162
F	-7	HIS	-	expression tag	UNP Q13162
F	-6	HIS	-	expression tag	UNP Q13162
F	-5	HIS	-	expression tag	UNP Q13162
F	-4	HIS	-	expression tag	UNP Q13162
F	-3	HIS	-	expression tag	UNP Q13162
F	-2	HIS	-	expression tag	UNP Q13162
F	-1	GLY	-	expression tag	UNP Q13162
F	0	SER	-	expression tag	UNP Q13162
F	118	GLU	THR	engineered mutation	UNP Q13162
D	-11	MET	-	expression tag	UNP Q13162
D	-10	ARG	-	expression tag	UNP Q13162
D	-9	GLY	-	expression tag	UNP Q13162
D	-8	SER	-	expression tag	UNP Q13162
D	-7	HIS	-	expression tag	UNP Q13162
D	-6	HIS	-	expression tag	UNP Q13162
D	-5	HIS	-	expression tag	UNP Q13162
D	-4	HIS	-	expression tag	UNP Q13162
D	-3	HIS	-	expression tag	UNP Q13162
D	-2	HIS	-	expression tag	UNP Q13162
D	-1	GLY	-	expression tag	UNP Q13162
D	0	SER	-	expression tag	UNP Q13162
D	118	GLU	THR	engineered mutation	UNP Q13162
B	-11	MET	-	expression tag	UNP Q13162
B	-10	ARG	-	expression tag	UNP Q13162
B	-9	GLY	-	expression tag	UNP Q13162
B	-8	SER	-	expression tag	UNP Q13162
B	-7	HIS	-	expression tag	UNP Q13162
B	-6	HIS	-	expression tag	UNP Q13162
B	-5	HIS	-	expression tag	UNP Q13162
B	-4	HIS	-	expression tag	UNP Q13162
B	-3	HIS	-	expression tag	UNP Q13162
B	-2	HIS	-	expression tag	UNP Q13162
B	-1	GLY	-	expression tag	UNP Q13162
B	0	SER	-	expression tag	UNP Q13162
B	118	GLU	THR	engineered mutation	UNP Q13162
H	-11	MET	-	expression tag	UNP Q13162
H	-10	ARG	-	expression tag	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	GLY	-	expression tag	UNP Q13162
H	-8	SER	-	expression tag	UNP Q13162
H	-7	HIS	-	expression tag	UNP Q13162
H	-6	HIS	-	expression tag	UNP Q13162
H	-5	HIS	-	expression tag	UNP Q13162
H	-4	HIS	-	expression tag	UNP Q13162
H	-3	HIS	-	expression tag	UNP Q13162
H	-2	HIS	-	expression tag	UNP Q13162
H	-1	GLY	-	expression tag	UNP Q13162
H	0	SER	-	expression tag	UNP Q13162
H	118	GLU	THR	engineered mutation	UNP Q13162
E	-11	MET	-	expression tag	UNP Q13162
E	-10	ARG	-	expression tag	UNP Q13162
E	-9	GLY	-	expression tag	UNP Q13162
E	-8	SER	-	expression tag	UNP Q13162
E	-7	HIS	-	expression tag	UNP Q13162
E	-6	HIS	-	expression tag	UNP Q13162
E	-5	HIS	-	expression tag	UNP Q13162
E	-4	HIS	-	expression tag	UNP Q13162
E	-3	HIS	-	expression tag	UNP Q13162
E	-2	HIS	-	expression tag	UNP Q13162
E	-1	GLY	-	expression tag	UNP Q13162
E	0	SER	-	expression tag	UNP Q13162
E	118	GLU	THR	engineered mutation	UNP Q13162
J	-11	MET	-	expression tag	UNP Q13162
J	-10	ARG	-	expression tag	UNP Q13162
J	-9	GLY	-	expression tag	UNP Q13162
J	-8	SER	-	expression tag	UNP Q13162
J	-7	HIS	-	expression tag	UNP Q13162
J	-6	HIS	-	expression tag	UNP Q13162
J	-5	HIS	-	expression tag	UNP Q13162
J	-4	HIS	-	expression tag	UNP Q13162
J	-3	HIS	-	expression tag	UNP Q13162
J	-2	HIS	-	expression tag	UNP Q13162
J	-1	GLY	-	expression tag	UNP Q13162
J	0	SER	-	expression tag	UNP Q13162
J	118	GLU	THR	engineered mutation	UNP Q13162

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	232	Total 232 O 232	0	0

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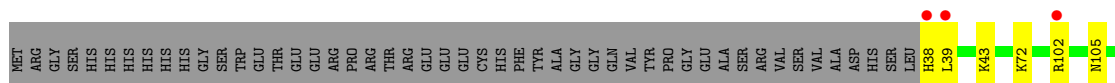
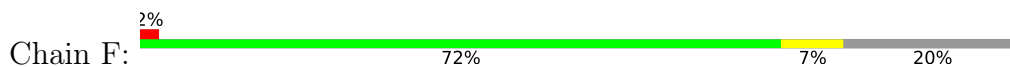
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	I	216	Total 216	O 216	0	0
2	G	226	Total 226	O 226	0	0
2	C	228	Total 228	O 228	0	0
2	F	215	Total 215	O 215	0	0
2	D	220	Total 220	O 220	0	0
2	B	226	Total 226	O 226	0	0
2	H	233	Total 233	O 233	0	0
2	E	176	Total 176	O 176	0	0
2	J	163	Total 163	O 163	0	0

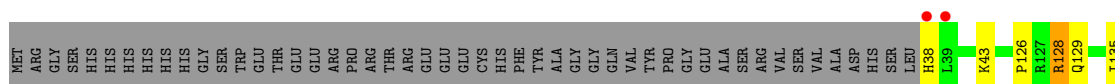
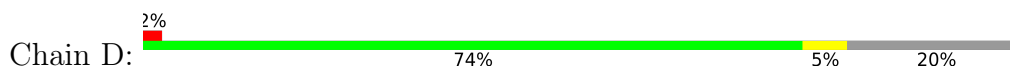




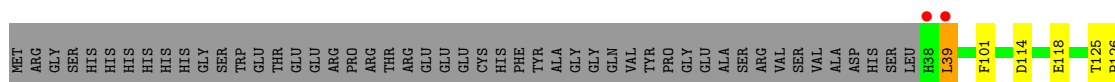
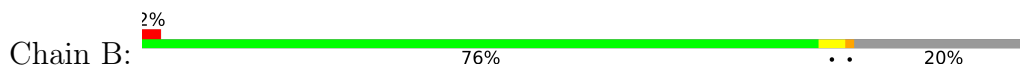
- Molecule 1: Peroxiredoxin-4



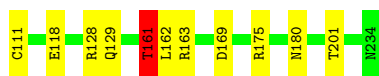
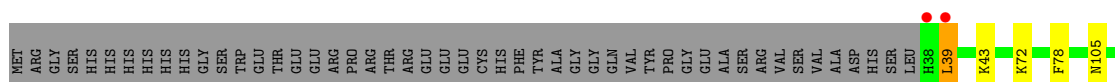
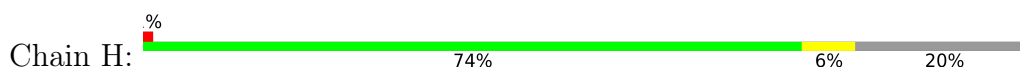
- Molecule 1: Peroxiredoxin-4



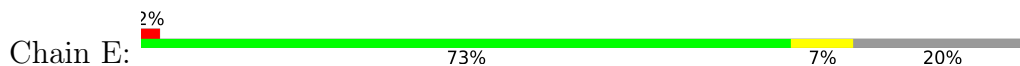
- Molecule 1: Peroxiredoxin-4

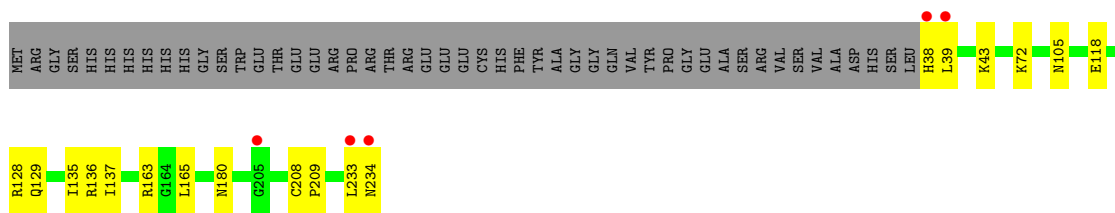


- Molecule 1: Peroxiredoxin-4

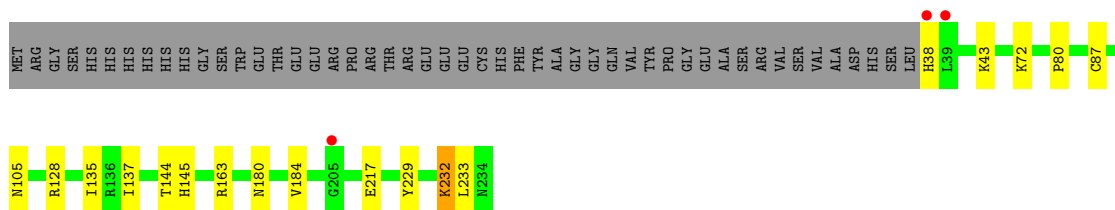
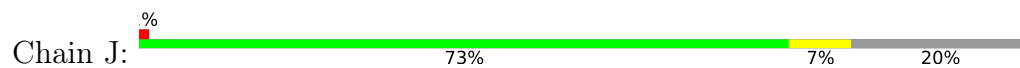


- Molecule 1: Peroxiredoxin-4





- Molecule 1: Peroxiredoxin-4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.71Å 139.12Å 178.97Å 90.00° 96.32° 90.00°	Depositor
Resolution (Å)	46.00 – 2.10 46.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (46.00-2.10) 98.0 (46.00-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.40 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, $R_{free}$	0.150 , 0.178 0.148 , 0.174	Depositor DCC
$R_{free}$ test set	8544 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtrriage
Anisotropy	0.538	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18082	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.49 % 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 6.7729e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.49	0/1687	0.72	0/2285
1	B	0.45	0/1641	0.72	0/2226
1	C	0.44	0/1675	0.72	1/2271 (0.0%)
1	D	0.44	0/1633	0.75	0/2214
1	E	0.41	0/1632	0.72	0/2213
1	F	0.50	1/1648 (0.1%)	0.73	1/2233 (0.0%)
1	G	0.45	0/1605	0.71	0/2176
1	H	0.47	0/1640	0.77	1/2224 (0.0%)
1	I	0.45	0/1641	0.72	0/2226
1	J	0.41	0/1642	0.70	1/2226 (0.0%)
All	All	0.45	1/16444 (0.0%)	0.73	4/22294 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	102	ARG	C-O	-5.28	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	102	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	H	161	THR	N-CA-CB	-5.30	102.30	110.56
1	C	81	LEU	N-CA-C	5.25	116.92	108.32
1	J	184	VAL	N-CA-C	5.06	115.14	107.75

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1624	0	1631	23	0
1	B	1593	0	1587	7	0
1	C	1615	0	1621	16	0
1	D	1588	0	1576	14	0
1	E	1587	0	1579	13	0
1	F	1597	0	1592	14	0
1	G	1564	0	1550	12	0
1	H	1592	0	1581	16	0
1	I	1593	0	1580	21	0
1	J	1594	0	1580	10	0
2	A	232	0	0	4	0
2	B	226	0	0	1	0
2	C	228	0	0	4	0
2	D	220	0	0	2	0
2	E	176	0	0	2	0
2	F	215	0	0	1	0
2	G	226	0	0	1	0
2	H	233	0	0	4	0
2	I	216	0	0	3	0
2	J	163	0	0	0	0
All	All	18082	0	15877	120	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 4.

All (120) 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:D:128:ARG:HH11	1:D:128:ARG:HG2	1.32	0.95
1:I:39:LEU:HB3	2:I:1749:HOH:O	1.69	0.93
1:G:43:LYS:HE3	1:C:38:HIS:HB2	1.50	0.92
1:H:201[B]:THR:HG23	2:H:454:HOH:O	1.69	0.90
1:A:43:LYS:HE3	1:I:38:HIS:HB2	1.52	0.90
1:H:128:ARG:HH12	1:H:129:GLN:HE21	1.20	0.87
1:E:43:LYS:HE3	1:J:38:HIS:HB2	1.57	0.86
1:F:38:HIS:HB2	1:D:43:LYS:HE2	1.57	0.84
1:I:128:ARG:HH11	1:I:128:ARG:HG3	1.46	0.80
1:H:128:ARG:NH1	1:H:129:GLN:HE21	1.79	0.79
1:I:201:THR:HG23	2:I:271:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:THR:HG23	1:H:162:LEU:O	1.84	0.76
1:D:128:ARG:HH11	1:D:128:ARG:CG	1.99	0.75
1:G:234:ASN:HB2	1:C:128:ARG:HG2	1.74	0.69
1:H:78:PHE:HB3	1:H:161:THR:HG21	1.76	0.66
1:C:201[B]:THR:HG23	2:C:862:HOH:O	1.96	0.65
1:I:128:ARG:HG3	1:I:128:ARG:NH1	2.11	0.64
1:C:128:ARG:HG3	2:C:261:HOH:O	1.96	0.64
1:D:128:ARG:HG2	1:D:128:ARG:NH1	2.10	0.63
1:H:128:ARG:NE	2:H:1698:HOH:O	2.33	0.61
1:G:234:ASN:CB	1:C:128:ARG:HG2	2.31	0.61
1:D:128:ARG:CZ	2:D:1908:HOH:O	2.48	0.61
1:A:234:ASN:HB2	1:I:128:ARG:HG2	1.83	0.60
1:B:101:PHE:CE2	1:B:192:LEU:HD13	2.35	0.60
1:G:40:SER:N	2:G:2070:HOH:O	2.36	0.58
1:H:161:THR:HB	2:H:235:HOH:O	2.04	0.58
1:C:101:PHE:CE2	1:C:192:LEU:HD13	2.39	0.58
1:H:39:LEU:H	1:H:39:LEU:HD23	1.67	0.57
1:F:233:LEU:HD13	1:F:234:ASN:ND2	2.19	0.57
1:A:136:ARG:NE	2:A:1918:HOH:O	2.38	0.56
1:D:128:ARG:NH2	2:D:1908:HOH:O	2.39	0.56
1:A:38:HIS:HB2	1:I:43:LYS:HD2	1.90	0.54
1:H:39:LEU:HD23	1:H:39:LEU:N	2.23	0.54
1:A:135:ILE:HG13	1:A:137:ILE:H	1.73	0.54
1:A:72[B]:LYS:HG2	1:A:105:ASN:OD1	2.08	0.54
1:A:136:ARG:NH2	2:A:1918:HOH:O	2.40	0.54
1:E:39:LEU:HD12	2:E:2053:HOH:O	2.08	0.54
1:F:146:GLN:HG3	2:F:1889:HOH:O	2.08	0.53
1:A:72[A]:LYS:HG2	1:A:105:ASN:OD1	2.09	0.53
1:F:128:ARG:HG2	1:D:234:ASN:HB2	1.90	0.52
1:A:128[A]:ARG:HH11	1:I:234:ASN:C	2.18	0.52
1:G:128:ARG:HE	1:C:234:ASN:C	2.18	0.52
1:E:128:ARG:HH12	1:E:129:GLN:HE21	1.58	0.52
1:A:234:ASN:HB2	1:I:128:ARG:CG	2.40	0.52
1:J:135:ILE:HG13	1:J:137:ILE:H	1.75	0.51
1:A:146[A]:GLN:NE2	2:A:1338:HOH:O	2.43	0.51
1:E:234:ASN:HB2	1:J:128:ARG:HG2	1.92	0.50
1:C:135:ILE:HD12	2:C:371:HOH:O	2.11	0.50
1:E:72:LYS:HG2	1:E:105:ASN:OD1	2.11	0.50
1:A:234:ASN:OXT	1:I:128:ARG:NH1	2.45	0.49
1:H:72:LYS:HG2	1:H:105:ASN:OD1	2.12	0.49
1:F:135:ILE:HG13	1:F:137:ILE:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:HIS:CB	1:D:43:LYS:HE2	2.37	0.48
1:F:72[B]:LYS:HG2	1:F:105:ASN:OD1	2.13	0.48
1:J:72:LYS:HG2	1:J:105:ASN:OD1	2.13	0.48
1:J:229:TYR:CZ	1:J:233:LEU:HD22	2.49	0.48
1:A:128[A]:ARG:HD2	1:I:234:ASN:O	2.14	0.48
1:G:163:ARG:HB2	1:G:180:ASN:HB2	1.96	0.48
1:C:144:THR:O	1:C:145:HIS:HB2	2.14	0.48
1:H:128:ARG:HH12	1:H:129:GLN:NE2	2.01	0.48
1:A:72[B]:LYS:HE2	1:A:72[B]:LYS:HB2	1.38	0.47
1:C:136[A]:ARG:NH1	2:C:2116:HOH:O	2.48	0.47
1:B:101:PHE:CZ	1:B:192:LEU:HD13	2.50	0.46
1:G:118:GLU:OE2	1:B:114:ASP:OD1	2.34	0.46
1:C:163:ARG:HB2	1:C:180:ASN:HB2	1.98	0.46
1:I:70:ARG:NH1	2:I:834:HOH:O	2.25	0.45
1:G:72:LYS:HG2	1:G:105:ASN:OD1	2.16	0.45
1:A:114:ASP:OD1	1:H:118:GLU:OE1	2.35	0.45
1:H:43:LYS:NZ	2:H:2163:HOH:O	2.49	0.45
1:F:233:LEU:H	1:F:233:LEU:HD12	1.82	0.45
1:E:136:ARG:NH1	2:E:1798:HOH:O	2.25	0.45
1:I:46:LYS:HA	1:I:46:LYS:HD2	1.85	0.45
1:A:136:ARG:CZ	2:A:1918:HOH:O	2.64	0.44
1:D:182:LEU:N	1:D:183:PRO:CD	2.80	0.44
1:H:163:ARG:HB2	1:H:180:ASN:HB2	1.98	0.44
1:G:114:ASP:OD1	1:B:118:GLU:OE1	2.36	0.44
1:G:135:ILE:HG12	1:G:137:ILE:H	1.82	0.44
1:E:38:HIS:HB2	1:J:43:LYS:HD2	1.99	0.44
1:A:70:ARG:HH11	1:A:70:ARG:HG3	1.82	0.44
1:G:183:PRO:HB2	1:C:201[B]:THR:HG21	2.00	0.44
1:F:72[A]:LYS:HG2	1:F:105:ASN:OD1	2.17	0.44
1:F:144:THR:O	1:F:145:HIS:HB2	2.18	0.43
1:D:163:ARG:HB2	1:D:180:ASN:HB2	1.99	0.43
1:E:165:LEU:C	1:E:165:LEU:HD23	2.44	0.43
1:E:135:ILE:HG12	1:E:137:ILE:H	1.83	0.43
1:E:163:ARG:HB2	1:E:180:ASN:HB2	2.00	0.43
1:B:163:ARG:HB2	1:B:180:ASN:HB2	2.01	0.43
1:D:126:PRO:HG2	1:D:129[B]:GLN:NE2	2.34	0.43
1:J:80:PRO:HD2	1:J:87:CYS:SG	2.59	0.43
1:A:163:ARG:HB2	1:A:180:ASN:HB2	2.01	0.42
1:C:220:ILE:HG22	1:C:222[B]:ASP:OD1	2.20	0.42
1:D:128:ARG:CG	1:D:128:ARG:NH1	2.68	0.42
1:J:144:THR:O	1:J:145:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:ILE:HG12	1:G:136:ARG:N	2.35	0.42
1:J:163:ARG:HB2	1:J:180:ASN:HB2	2.00	0.42
1:F:43:LYS:HE2	1:D:38:HIS:HB2	2.01	0.42
1:C:166:PHE:HB3	1:C:174[A]:LEU:HD21	2.02	0.42
1:I:43:LYS:HE3	1:I:43:LYS:HB3	1.90	0.42
1:F:163:ARG:HB2	1:F:180:ASN:HB2	2.02	0.42
1:H:169:ASP:OD2	1:H:175:ARG:HD3	2.19	0.42
1:C:165:LEU:HD23	1:C:165:LEU:C	2.45	0.41
1:I:114:ASP:OD1	1:E:118:GLU:OE1	2.37	0.41
1:B:125:THR:HA	1:B:126:PRO:HD3	1.95	0.41
1:I:70:ARG:HH11	1:I:70:ARG:HB3	1.85	0.41
1:D:217:GLU:OE2	1:D:232:LYS:HE3	2.20	0.41
1:B:39:LEU:HD12	2:B:1289:HOH:O	2.20	0.41
1:I:163:ARG:HB2	1:I:180:ASN:HB2	2.02	0.41
1:A:234:ASN:OXT	1:I:128:ARG:HD3	2.21	0.41
1:F:229:TYR:O	1:F:233:LEU:HD12	2.19	0.41
1:A:70:ARG:HH11	1:A:70:ARG:CG	2.33	0.41
1:C:72:LYS:HG2	1:C:105:ASN:OD1	2.20	0.41
1:F:182:LEU:N	1:F:183:PRO:CD	2.84	0.41
1:A:128[A]:ARG:CG	1:I:234:ASN:HB2	2.51	0.41
1:I:78:PHE:HA	1:I:111:CYS:O	2.21	0.40
1:H:78:PHE:HA	1:H:111:CYS:O	2.21	0.40
1:J:217[B]:GLU:OE1	1:J:232:LYS:HD2	2.22	0.40
1:E:208:CYS:HA	1:E:209:PRO:HD3	1.86	0.40
1:A:70:ARG:CG	1:A:70:ARG:NH1	2.84	0.40
1:A:128[A]:ARG:HG2	1:I:234:ASN:HB2	2.03	0.40
1:E:128:ARG:NH1	1:E:129:GLN:HE21	2.17	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	202/246 (82%)	195 (96%)	7 (4%)	0	100	100
1	B	197/246 (80%)	189 (96%)	8 (4%)	0	100	100
1	C	201/246 (82%)	193 (96%)	8 (4%)	0	100	100
1	D	196/246 (80%)	188 (96%)	8 (4%)	0	100	100
1	E	196/246 (80%)	188 (96%)	8 (4%)	0	100	100
1	F	198/246 (80%)	189 (96%)	9 (4%)	0	100	100
1	G	193/246 (78%)	185 (96%)	8 (4%)	0	100	100
1	H	197/246 (80%)	188 (95%)	9 (5%)	0	100	100
1	I	197/246 (80%)	190 (96%)	7 (4%)	0	100	100
1	J	197/246 (80%)	189 (96%)	8 (4%)	0	100	100
All	All	1974/2460 (80%)	1894 (96%)	80 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	179/213 (84%)	175 (98%)	4 (2%)	45	53
1	B	174/213 (82%)	171 (98%)	3 (2%)	53	62
1	C	178/213 (84%)	171 (96%)	7 (4%)	28	31
1	D	173/213 (81%)	170 (98%)	3 (2%)	53	62
1	E	173/213 (81%)	172 (99%)	1 (1%)	78	86
1	F	175/213 (82%)	173 (99%)	2 (1%)	65	74
1	G	170/213 (80%)	169 (99%)	1 (1%)	78	86
1	H	174/213 (82%)	172 (99%)	2 (1%)	65	74
1	I	174/213 (82%)	173 (99%)	1 (1%)	78	86
1	J	174/213 (82%)	173 (99%)	1 (1%)	78	86
All	All	1744/2130 (82%)	1719 (99%)	25 (1%)	61	67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	135	ILE
1	A	157[A]	ASP
1	A	157[B]	ASP
1	I	70	ARG
1	G	135	ILE
1	C	174[A]	LEU
1	C	174[B]	LEU
1	C	192	LEU
1	C	222[A]	ASP
1	C	222[B]	ASP
1	C	232	LYS
1	C	233	LEU
1	F	39	LEU
1	F	233	LEU
1	D	128	ARG
1	D	135	ILE
1	D	231	ASP
1	B	39	LEU
1	B	192	LEU
1	B	232	LYS
1	H	39	LEU
1	H	161	THR
1	E	233	LEU
1	J	232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	I	204	HIS
1	C	234	ASN
1	F	38	HIS
1	F	234	ASN
1	D	146	GLN
1	H	129	GLN
1	H	146	GLN
1	H	196	GLN
1	E	129	GLN
1	E	204	HIS
1	J	129	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	197/246 (80%)	-0.60	3 (1%) 72 74	9, 17, 35, 65	7 (3%)
1	B	197/246 (80%)	-0.62	4 (2%) 65 67	11, 18, 38, 56	2 (1%)
1	C	197/246 (80%)	-0.62	4 (2%) 65 67	9, 17, 37, 64	6 (3%)
1	D	197/246 (80%)	-0.58	4 (2%) 65 67	12, 18, 36, 64	1 (0%)
1	E	197/246 (80%)	-0.33	5 (2%) 58 61	14, 23, 46, 62	1 (0%)
1	F	197/246 (80%)	-0.61	4 (2%) 65 67	12, 18, 35, 64	3 (1%)
1	G	195/246 (79%)	-0.65	2 (1%) 79 81	11, 18, 35, 49	0
1	H	197/246 (80%)	-0.65	2 (1%) 79 81	11, 16, 35, 64	2 (1%)
1	I	197/246 (80%)	-0.64	3 (1%) 72 74	12, 17, 37, 60	2 (1%)
1	J	197/246 (80%)	-0.40	3 (1%) 72 74	14, 23, 43, 58	2 (1%)
All	All	1968/2460 (80%)	-0.57	34 (1%) 69 71	9, 19, 38, 65	26 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	LEU	5.9
1	B	39	LEU	5.3
1	I	38	HIS	5.2
1	D	39	LEU	5.1
1	H	39	LEU	4.8
1	F	39	LEU	4.6
1	E	39	LEU	4.5
1	A	38	HIS	4.2
1	E	233	LEU	3.9
1	F	233	LEU	3.7
1	F	38	HIS	3.7
1	D	233	LEU	3.6
1	C	233	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	38	HIS	3.5
1	D	38	HIS	3.4
1	C	38	HIS	3.3
1	G	234	ASN	3.3
1	J	39	LEU	3.3
1	H	38	HIS	3.2
1	B	38	HIS	3.2
1	E	38	HIS	3.2
1	I	39	LEU	3.2
1	J	205	GLY	3.1
1	C	39	LEU	3.1
1	E	205	GLY	3.0
1	G	233	LEU	2.6
1	B	233	LEU	2.5
1	C	234	ASN	2.3
1	D	234	ASN	2.3
1	B	234	ASN	2.3
1	I	128	ARG	2.3
1	E	234	ASN	2.2
1	A	233	LEU	2.0
1	F	102	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.