



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 06:36 AM BST

PDB ID : 6KRM  
Title : Peroxiredoxin from *Aeropyrum pernix* K1 (ApPrx) 0Cys F46A mutant  
Authors : Himiyama, T.; Nakamura, T.  
Deposited on : 2019-08-22  
Resolution : 1.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

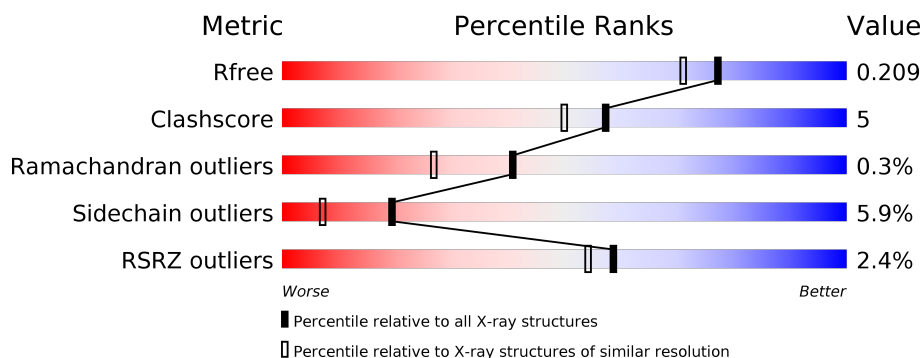
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	250	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 84%, yellow 84%, yellow 96%, green 96%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>84%</span> <span>12% ..</span> </div> </div>
1	B	250	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 83%, yellow 83%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>83%</span> <span>14% .</span> </div> </div>
1	C	250	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 82%, yellow 82%, yellow 95%, green 95%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>82%</span> <span>13% ...</span> </div> </div>
1	D	250	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 85%, yellow 85%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>85%</span> <span>12% ..</span> </div> </div>
1	E	250	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 85%, yellow 85%, yellow 95%, green 95%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>85%</span> <span>10% ...</span> </div> </div>
1	F	250	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 0%, orange 0%, orange 81%, yellow 81%, yellow 95%, green 95%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>81%</span> <span>14% ..</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	250	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>80%</div><div>14%</div><div>...</div></div></div>
1	H	250	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>80%</div><div>15%</div><div>..</div></div></div>
1	I	250	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>83%</div><div>13%</div><div>...</div></div></div>
1	J	250	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>84%</div><div>12%</div><div>..</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21225 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total 1967	C 1262	N 347	O 354	S 4	0	0	0
1	B	244	Total 1967	C 1262	N 347	O 354	S 4	0	0	0
1	C	244	Total 1967	C 1262	N 347	O 354	S 4	0	0	0
1	D	244	Total 1967	C 1262	N 347	O 354	S 4	0	0	0
1	E	244	Total 1967	C 1262	N 347	O 354	S 4	0	0	0
1	F	244	Total 1967	C 1262	N 347	O 354	S 4	0	0	0
1	G	244	Total 1967	C 1262	N 347	O 354	S 4	0	0	0
1	H	244	Total 1967	C 1262	N 347	O 354	S 4	0	0	0
1	I	244	Total 1967	C 1262	N 347	O 354	S 4	0	0	0
1	J	244	Total 1967	C 1262	N 347	O 354	S 4	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9Y9L0
A	46	ALA	PHE	engineered mutation	UNP Q9Y9L0
A	50	SER	CYS	engineered mutation	UNP Q9Y9L0
A	207	SER	CYS	engineered mutation	UNP Q9Y9L0
A	213	SER	CYS	engineered mutation	UNP Q9Y9L0
B	1	MET	-	initiating methionine	UNP Q9Y9L0
B	46	ALA	PHE	engineered mutation	UNP Q9Y9L0
B	50	SER	CYS	engineered mutation	UNP Q9Y9L0
B	207	SER	CYS	engineered mutation	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	213	SER	CYS	engineered mutation	UNP Q9Y9L0
C	1	MET	-	initiating methionine	UNP Q9Y9L0
C	46	ALA	PHE	engineered mutation	UNP Q9Y9L0
C	50	SER	CYS	engineered mutation	UNP Q9Y9L0
C	207	SER	CYS	engineered mutation	UNP Q9Y9L0
C	213	SER	CYS	engineered mutation	UNP Q9Y9L0
D	1	MET	-	initiating methionine	UNP Q9Y9L0
D	46	ALA	PHE	engineered mutation	UNP Q9Y9L0
D	50	SER	CYS	engineered mutation	UNP Q9Y9L0
D	207	SER	CYS	engineered mutation	UNP Q9Y9L0
D	213	SER	CYS	engineered mutation	UNP Q9Y9L0
E	1	MET	-	initiating methionine	UNP Q9Y9L0
E	46	ALA	PHE	engineered mutation	UNP Q9Y9L0
E	50	SER	CYS	engineered mutation	UNP Q9Y9L0
E	207	SER	CYS	engineered mutation	UNP Q9Y9L0
E	213	SER	CYS	engineered mutation	UNP Q9Y9L0
F	1	MET	-	initiating methionine	UNP Q9Y9L0
F	46	ALA	PHE	engineered mutation	UNP Q9Y9L0
F	50	SER	CYS	engineered mutation	UNP Q9Y9L0
F	207	SER	CYS	engineered mutation	UNP Q9Y9L0
F	213	SER	CYS	engineered mutation	UNP Q9Y9L0
G	1	MET	-	initiating methionine	UNP Q9Y9L0
G	46	ALA	PHE	engineered mutation	UNP Q9Y9L0
G	50	SER	CYS	engineered mutation	UNP Q9Y9L0
G	207	SER	CYS	engineered mutation	UNP Q9Y9L0
G	213	SER	CYS	engineered mutation	UNP Q9Y9L0
H	1	MET	-	initiating methionine	UNP Q9Y9L0
H	46	ALA	PHE	engineered mutation	UNP Q9Y9L0
H	50	SER	CYS	engineered mutation	UNP Q9Y9L0
H	207	SER	CYS	engineered mutation	UNP Q9Y9L0
H	213	SER	CYS	engineered mutation	UNP Q9Y9L0
I	1	MET	-	initiating methionine	UNP Q9Y9L0
I	46	ALA	PHE	engineered mutation	UNP Q9Y9L0
I	50	SER	CYS	engineered mutation	UNP Q9Y9L0
I	207	SER	CYS	engineered mutation	UNP Q9Y9L0
I	213	SER	CYS	engineered mutation	UNP Q9Y9L0
J	1	MET	-	initiating methionine	UNP Q9Y9L0
J	46	ALA	PHE	engineered mutation	UNP Q9Y9L0
J	50	SER	CYS	engineered mutation	UNP Q9Y9L0
J	207	SER	CYS	engineered mutation	UNP Q9Y9L0
J	213	SER	CYS	engineered mutation	UNP Q9Y9L0

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0
2	I	1	Total C O 13 6 7	0	0
2	J	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	135	Total O 135 135	0	0
3	B	137	Total O 137 137	0	0

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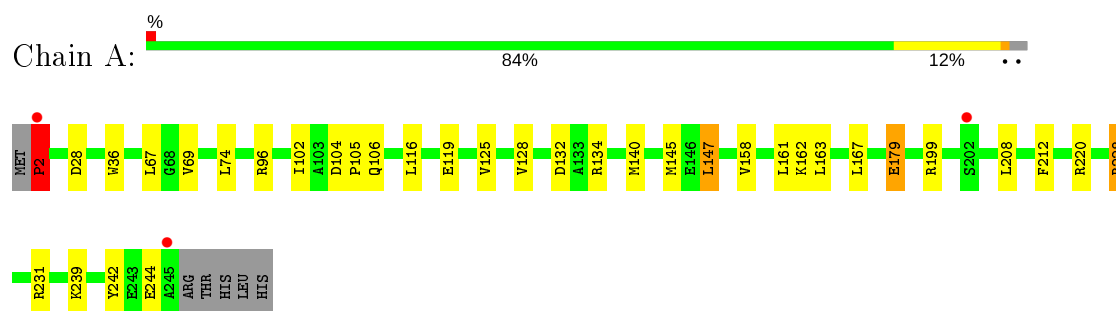
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	150	Total 150	O 150	0	0
3	D	136	Total 136	O 136	0	0
3	E	169	Total 169	O 169	0	0
3	F	153	Total 153	O 153	0	0
3	G	120	Total 120	O 120	0	0
3	H	160	Total 160	O 160	0	0
3	I	139	Total 139	O 139	0	0
3	J	126	Total 126	O 126	0	0

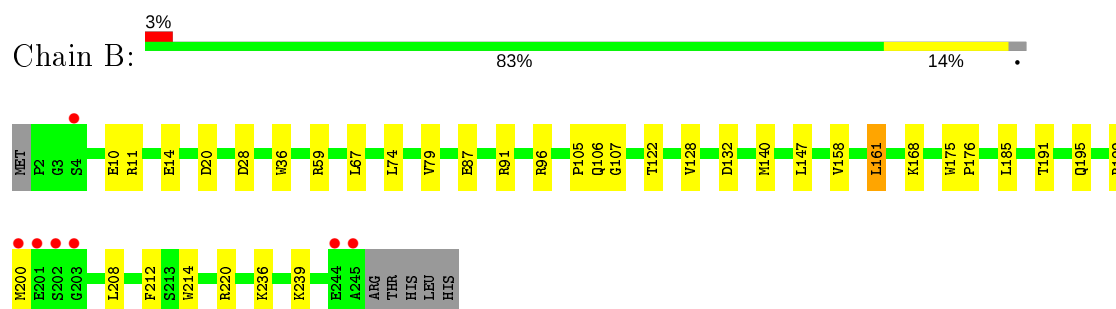
### 3 Residue-property plots [i](#)

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.

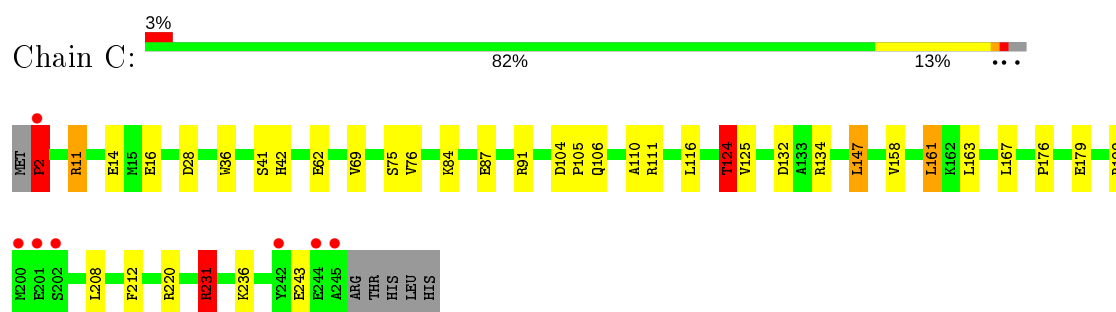
- Molecule 1: Peroxiredoxin



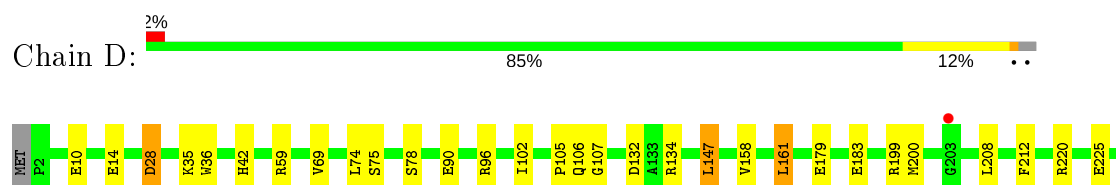
- Molecule 1: Peroxiredoxin



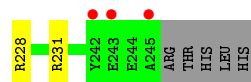
- Molecule 1: Peroxiredoxin



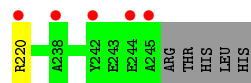
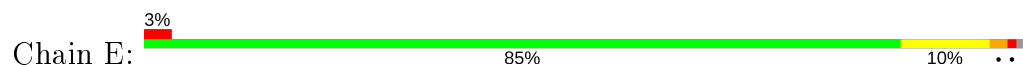
- Molecule 1: Peroxiredoxin



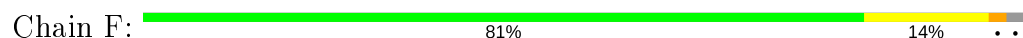




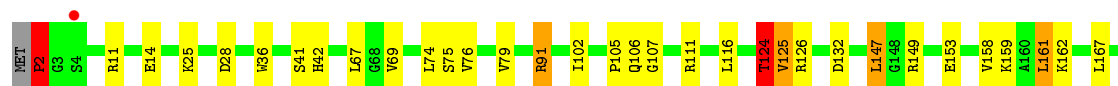
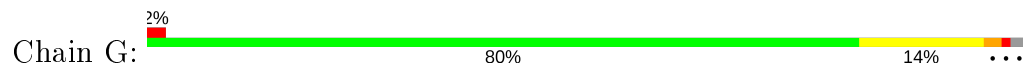
• Molecule 1: Peroxiredoxin



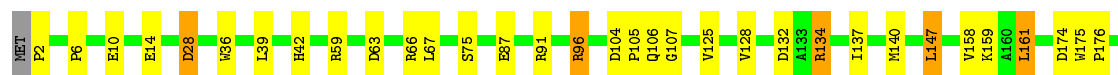
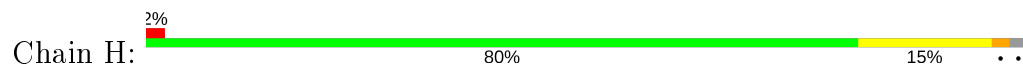
• Molecule 1: Peroxiredoxin



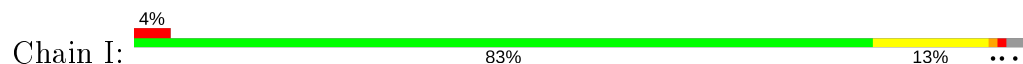
• Molecule 1: Peroxiredoxin

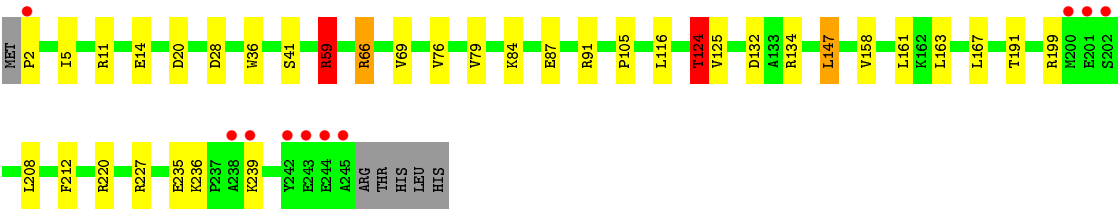


• Molecule 1: Peroxiredoxin

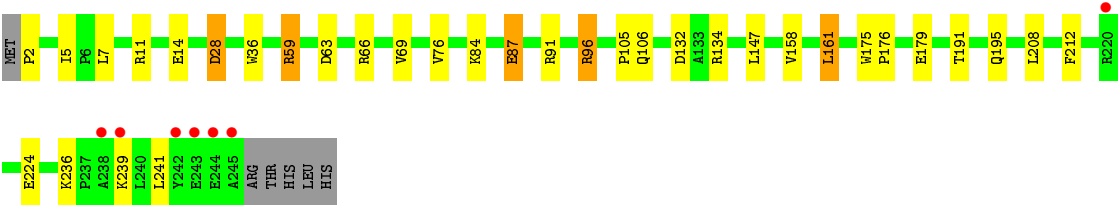
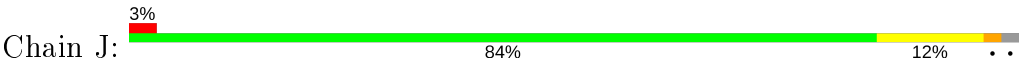


• Molecule 1: Peroxiredoxin





● Molecule 1: Peroxiredoxin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.00Å 103.08Å 104.80Å 105.80° 105.25° 92.53°	Depositor
Resolution (Å)	49.25 – 1.80 49.20 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.25-1.80) 97.0 (49.20-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.163 , 0.198 0.178 , 0.209	Depositor DCC
$R_{free}$ test set	13337 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.77	0/2021	0.99	7/2748 (0.3%)
1	B	0.74	0/2021	0.92	2/2748 (0.1%)
1	C	0.78	1/2021 (0.0%)	0.96	5/2748 (0.2%)
1	D	0.80	1/2021 (0.0%)	0.97	7/2748 (0.3%)
1	E	0.83	2/2021 (0.1%)	1.01	9/2748 (0.3%)
1	F	0.84	2/2021 (0.1%)	0.97	4/2748 (0.1%)
1	G	0.83	1/2021 (0.0%)	0.97	6/2748 (0.2%)
1	H	0.77	0/2021	0.94	4/2748 (0.1%)
1	I	0.77	0/2021	0.94	4/2748 (0.1%)
1	J	0.77	1/2021 (0.0%)	0.93	2/2748 (0.1%)
All	All	0.79	8/20210 (0.0%)	0.96	50/27480 (0.2%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	179	GLU	CD-OE2	13.50	1.40	1.25
1	G	179	GLU	CD-OE2	12.82	1.39	1.25
1	C	179	GLU	CD-OE2	11.75	1.38	1.25
1	F	179	GLU	CD-OE2	8.91	1.35	1.25
1	E	179	GLU	CD-OE2	7.75	1.34	1.25

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	231	ARG	NE-CZ-NH1	-12.68	113.96	120.30
1	D	231	ARG	NE-CZ-NH1	-11.38	114.61	120.30
1	D	199	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	C	2	PRO	CA-N-CD	-9.71	97.91	111.50
1	A	2	PRO	CA-N-CD	-9.57	98.10	111.50

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	1967	0	1955	18	0
1	B	1967	0	1955	22	0
1	C	1967	0	1955	26	0
1	D	1967	0	1955	20	0
1	E	1967	0	1955	16	0
1	F	1967	0	1955	26	0
1	G	1967	0	1955	27	0
1	H	1967	0	1955	29	0
1	I	1967	0	1955	18	0
1	J	1967	0	1955	27	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	1	0
2	G	13	0	5	0	0
2	H	13	0	5	0	0
2	I	13	0	5	0	0
2	J	13	0	5	0	0
3	A	135	0	0	3	0
3	B	137	0	0	2	0
3	C	150	0	0	2	0
3	D	136	0	0	0	0
3	E	169	0	0	1	0
3	F	153	0	0	6	0
3	G	120	0	0	4	0
3	H	160	0	0	3	0
3	I	139	0	0	0	0
3	J	126	0	0	4	0
All	All	21225	0	19600	192	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 5.

The worst 5 of 192 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:59:ARG:NH1	1:J:179:GLU:OE2	1.99	0.95
1:F:225:GLU:HG2	3:F:500:HOH:O	1.68	0.91
1:I:11:ARG:NH1	1:I:14:GLU:OE1	2.02	0.91
1:C:91:ARG:NH1	3:C:401:HOH:O	2.05	0.89
1:B:11:ARG:NH1	1:B:14:GLU:OE2	2.10	0.83

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	242/250 (97%)	237 (98%)	4 (2%)	1 (0%)	34	21
1	B	242/250 (97%)	239 (99%)	3 (1%)	0	100	100
1	C	242/250 (97%)	236 (98%)	5 (2%)	1 (0%)	34	21
1	D	242/250 (97%)	237 (98%)	5 (2%)	0	100	100
1	E	242/250 (97%)	239 (99%)	2 (1%)	1 (0%)	34	21
1	F	242/250 (97%)	238 (98%)	3 (1%)	1 (0%)	34	21
1	G	242/250 (97%)	236 (98%)	5 (2%)	1 (0%)	34	21
1	H	242/250 (97%)	239 (99%)	2 (1%)	1 (0%)	34	21
1	I	242/250 (97%)	238 (98%)	3 (1%)	1 (0%)	34	21
1	J	242/250 (97%)	237 (98%)	5 (2%)	0	100	100
All	All	2420/2500 (97%)	2376 (98%)	37 (2%)	7 (0%)	41	27

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	243	GLU

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Mol	Chain	Res	Type
1	H	125	VAL
1	G	125	VAL
1	E	125	VAL
1	F	125	VAL

### 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	209/215 (97%)	195 (93%)	14 (7%)	16	5
1	B	209/215 (97%)	200 (96%)	9 (4%)	29	14
1	C	209/215 (97%)	193 (92%)	16 (8%)	13	4
1	D	209/215 (97%)	201 (96%)	8 (4%)	33	18
1	E	209/215 (97%)	195 (93%)	14 (7%)	16	5
1	F	209/215 (97%)	195 (93%)	14 (7%)	16	5
1	G	209/215 (97%)	196 (94%)	13 (6%)	18	6
1	H	209/215 (97%)	201 (96%)	8 (4%)	33	18
1	I	209/215 (97%)	190 (91%)	19 (9%)	9	2
1	J	209/215 (97%)	200 (96%)	9 (4%)	29	14
All	All	2090/2150 (97%)	1966 (94%)	124 (6%)	19	7

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	163	LEU
1	F	199	ARG
1	I	239	LYS
1	E	167	LEU
1	F	28	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	204	GLN
1	F	123	HIS
1	J	195	GLN
1	F	106	GLN
1	F	195	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CIT	D	301	-	3,12,12	1.40	1 (33%)	3,17,17	1.57	0
2	CIT	H	301	-	3,12,12	1.86	1 (33%)	3,17,17	1.53	1 (33%)
2	CIT	I	301	-	3,12,12	1.80	1 (33%)	3,17,17	1.12	0
2	CIT	J	301	-	3,12,12	1.58	1 (33%)	3,17,17	1.26	0
2	CIT	E	301	-	3,12,12	2.31	1 (33%)	3,17,17	1.64	1 (33%)
2	CIT	F	301	-	3,12,12	1.88	1 (33%)	3,17,17	1.48	1 (33%)
2	CIT	G	301	-	3,12,12	1.75	1 (33%)	3,17,17	1.26	0
2	CIT	A	301	-	3,12,12	1.56	1 (33%)	3,17,17	0.96	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CIT	B	301	-	3,12,12	1.39	1 (33%)	3,17,17	1.27	1 (33%)
2	CIT	C	301	-	3,12,12	1.67	1 (33%)	3,17,17	1.29	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	D	301	-	-	3/6/16/16	-
2	CIT	H	301	-	-	3/6/16/16	-
2	CIT	I	301	-	-	3/6/16/16	-
2	CIT	J	301	-	-	3/6/16/16	-
2	CIT	E	301	-	-	3/6/16/16	-
2	CIT	F	301	-	-	3/6/16/16	-
2	CIT	G	301	-	-	3/6/16/16	-
2	CIT	A	301	-	-	3/6/16/16	-
2	CIT	B	301	-	-	5/6/16/16	-
2	CIT	C	301	-	-	3/6/16/16	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	CIT	C4-C3	-3.75	1.49	1.54
2	H	301	CIT	C2-C3	-3.09	1.50	1.54
2	F	301	CIT	C4-C3	-3.07	1.50	1.54
2	I	301	CIT	C2-C3	-2.94	1.50	1.54
2	G	301	CIT	C4-C3	-2.87	1.50	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	CIT	C4-C3-C2	-2.66	102.22	109.33
2	H	301	CIT	C4-C3-C2	-2.61	102.34	109.33
2	B	301	CIT	C4-C3-C2	-2.13	103.63	109.33
2	F	301	CIT	C4-C3-C2	-2.11	103.67	109.33
2	C	301	CIT	C4-C3-C2	-2.10	103.70	109.33

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	CIT	C2-C3-C4-C5
2	D	301	CIT	O7-C3-C4-C5
2	D	301	CIT	C6-C3-C4-C5
2	H	301	CIT	C2-C3-C4-C5
2	H	301	CIT	O7-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	CIT	1	0

## 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, 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	244/250 (97%)	-0.31	3 (1%) 79 76	15, 22, 44, 73	0
1	B	244/250 (97%)	-0.36	7 (2%) 51 46	16, 23, 43, 82	0
1	C	244/250 (97%)	-0.32	7 (2%) 51 46	15, 23, 44, 94	0
1	D	244/250 (97%)	-0.25	4 (1%) 72 68	16, 23, 44, 83	0
1	E	244/250 (97%)	-0.44	7 (2%) 51 46	13, 19, 40, 82	0
1	F	244/250 (97%)	-0.33	1 (0%) 92 90	13, 20, 39, 79	0
1	G	244/250 (97%)	-0.27	6 (2%) 57 52	15, 24, 43, 68	0
1	H	244/250 (97%)	-0.44	6 (2%) 57 52	14, 22, 44, 80	0
1	I	244/250 (97%)	-0.34	10 (4%) 37 31	15, 23, 44, 86	0
1	J	244/250 (97%)	-0.26	7 (2%) 51 46	16, 25, 47, 80	0
All	All	2440/2500 (97%)	-0.33	58 (2%) 59 54	13, 23, 44, 94	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	245	ALA	4.8
1	I	2	PRO	4.6
1	B	245	ALA	4.5
1	E	245	ALA	4.3
1	I	244	GLU	4.3

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CIT	D	301	13/13	0.91	0.11	20,31,43,45	0
2	CIT	G	301	13/13	0.91	0.10	19,29,37,38	0
2	CIT	A	301	13/13	0.91	0.12	19,28,40,40	0
2	CIT	E	301	13/13	0.92	0.11	16,24,36,38	0
2	CIT	I	301	13/13	0.92	0.11	19,32,41,41	0
2	CIT	J	301	13/13	0.92	0.10	20,32,42,43	0
2	CIT	H	301	13/13	0.93	0.11	19,29,38,45	0
2	CIT	B	301	13/13	0.93	0.10	21,32,42,45	0
2	CIT	C	301	13/13	0.93	0.10	19,31,41,41	0
2	CIT	F	301	13/13	0.94	0.10	17,28,37,37	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.