



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 04:34 am BST

PDB ID : 4DEJ  
Title : Crystal structure of glutathione transferase-like protein IL0419 (Target EFI-501089) from *Idiomarina loihiensis* L2TR  
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Zencheck, W.D.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Imker, H.J.; Armstrong, R.N.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2012-01-20  
Resolution : 2.90 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

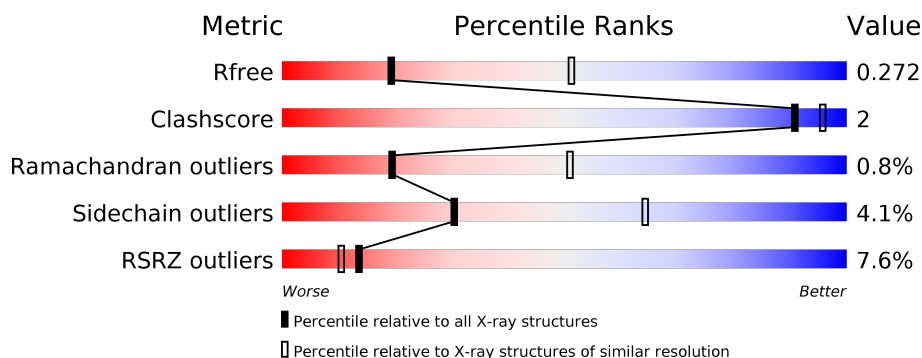
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	231	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>13%</div> </div> </div>
1	B	231	<div> <div></div> <div> <div></div> <div>81%</div> <div>5%</div> <div>13%</div> </div> </div>
1	C	231	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>
1	D	231	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div></div> <div>12%</div> </div> </div>
1	E	231	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>13%</div> </div> </div>
1	F	231	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	231	<div><div></div><div>6%</div><div>78%</div><div>9%</div><div>13%</div></div>
1	H	231	<div><div></div><div>6%</div><div>75%</div><div>12%</div><div>13%</div></div>
1	I	231	<div><div></div><div>5%</div><div>77%</div><div>9%</div><div>13%</div></div>
1	J	231	<div><div></div><div>6%</div><div>77%</div><div>11%</div><div>13%</div></div>
1	K	231	<div><div></div><div>15%</div><div>83%</div><div></div><div>13%</div></div>
1	L	231	<div><div></div><div>13%</div><div>73%</div><div>14%</div><div>13%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19591 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 Glutathione S-transferase related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1639	1051	268	312	8			
1	B	201	Total	C	N	O	S	0	0	0
			1634	1048	267	311	8			
1	C	201	Total	C	N	O	S	0	0	0
			1634	1048	267	311	8			
1	D	203	Total	C	N	O	S	0	0	0
			1653	1058	273	314	8			
1	E	200	Total	C	N	O	S	0	0	0
			1625	1042	265	310	8			
1	F	197	Total	C	N	O	S	0	0	0
			1601	1030	258	305	8			
1	G	201	Total	C	N	O	S	0	0	0
			1625	1044	263	310	8			
1	H	201	Total	C	N	O	S	0	0	0
			1636	1048	269	311	8			
1	I	200	Total	C	N	O	S	0	0	0
			1629	1045	266	310	8			
1	J	202	Total	C	N	O	S	0	0	0
			1643	1053	268	314	8			
1	K	201	Total	C	N	O	S	0	0	0
			1640	1051	270	311	8			
1	L	200	Total	C	N	O	S	0	0	0
			1618	1038	263	309	8			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
A	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
A	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
A	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
A	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
A	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
A	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
A	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
A	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
A	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
A	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
A	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
A	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
A	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
A	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
A	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
B	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
B	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
B	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
B	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
B	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
B	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
B	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
B	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
B	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
B	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
B	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
B	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
B	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
B	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
B	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
B	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
C	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
C	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
C	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
C	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
C	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
C	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
C	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
C	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
C	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
C	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
C	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
C	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
C	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
C	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
C	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
C	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
C	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
D	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
D	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
D	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
D	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
D	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
D	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
D	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
D	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
D	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
D	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
D	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
D	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
D	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
D	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
D	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
D	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
E	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
E	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
E	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
E	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
E	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
E	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
E	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
E	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
E	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
E	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
E	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
E	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
E	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
E	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
E	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
E	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
E	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
F	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
F	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
F	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
F	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
F	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
F	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
F	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
F	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
F	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
F	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
F	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
F	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
F	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
F	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
F	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
F	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
F	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
G	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
G	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
G	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
G	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
G	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
G	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
G	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
G	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
G	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
G	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
G	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
G	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
G	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
G	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
G	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
G	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
G	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
H	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
H	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
H	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
H	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
H	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
H	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
H	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
H	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
H	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
H	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
H	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
H	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
H	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
H	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
H	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
H	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
I	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
I	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
I	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
I	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
I	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
I	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
I	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
I	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
I	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
I	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
I	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
I	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
I	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
I	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
I	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
I	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
J	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
J	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
J	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
J	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
J	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
J	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
J	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
J	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
J	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
J	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
J	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
J	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
J	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
J	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
J	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
J	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
J	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
K	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
K	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
K	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
K	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
K	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
K	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
K	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
K	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
K	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
K	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
K	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
K	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
K	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
K	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
K	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
K	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
L	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
L	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
L	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
L	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
L	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
L	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
L	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
L	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
L	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
L	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
L	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
L	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
L	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
L	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
L	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
L	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
L	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	3	Total O 3 3	0	0
2	C	1	Total O 1 1	0	0
2	E	1	Total O 1 1	0	0

*Continued on next page...*

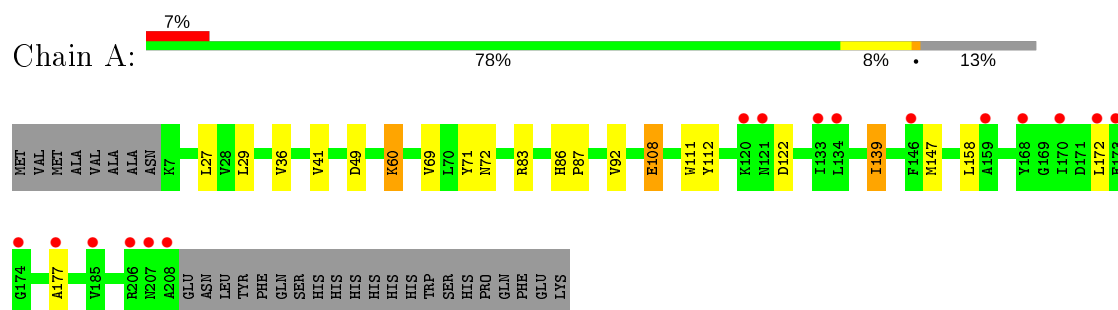
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total 1	O 1	0	0
2	I	2	Total 2	O 2	0	0
2	J	1	Total 1	O 1	0	0
2	L	1	Total 1	O 1	0	0

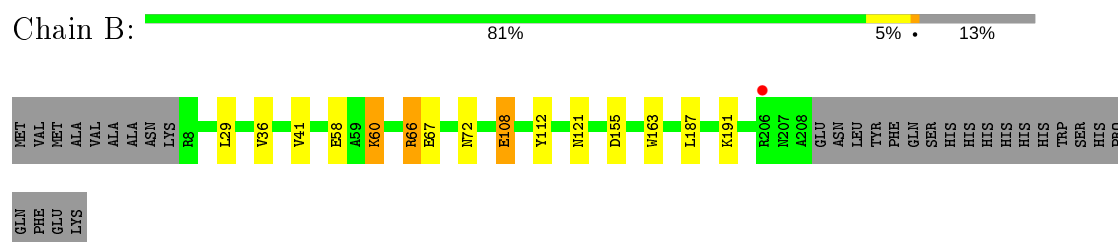
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

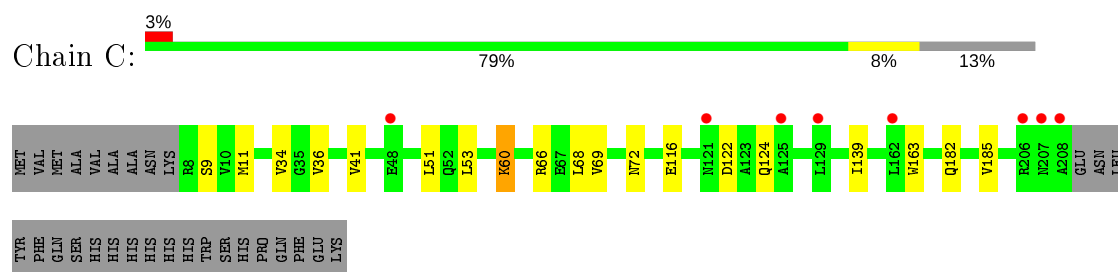
- Molecule 1: Glutathione S-transferase related protein



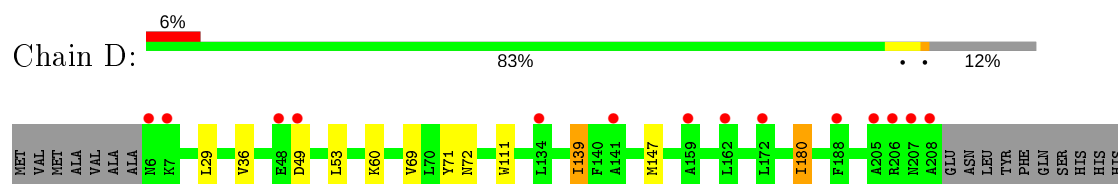
- Molecule 1: Glutathione S-transferase related protein



- Molecule 1: Glutathione S-transferase related protein




- Molecule 1: Glutathione S-transferase related protein



HIS  
HIS  
HIS  
TRP  
SER  
HIS  
HIS  
PRO  
GLN  
PHE  
GLU  
LYS


- Molecule 1: Glutathione S-transferase related protein

Chain E: 

MET VAL MET MET VAL VAL ALA ALA ALA ASN LYS LYS ARG S9 L20 Q24 L27 V28 L29 V34 G35 V36 V41 T42 S45 E48 D49 L50 L51 Q52 L53 K60 R66 E67 L68 V69 W72 I75 R83 I118 A123 Y157 I170 A208 ASN

LEU TYR PHE MET GLN SER SER HIS HIS HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS


- Molecule 1: Glutathione S-transferase related protein

Chain F: 

MET VAL MET MET VAL VAL ALA ALA ALA ASN LYS LYS ARG S9 Q24 L27 V28 L29 V36 V41 E44 S45 L53 K60 V69 W72 W111 N121 L134 S135 L136 I139 V154 Y157 L158 I161 L172 E173 G174 Q175 Q176 A177 K178 E179 I180

V185 E199 A205 ARG ASN ALA ALA ASN ASN LEU TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER HIS HIS HIS HIS HIS HIS HIS


- Molecule 1: Glutathione S-transferase related protein

Chain G: 

MET VAL MET MET VAL VAL ALA ALA ALA ASN LYS R8 V36 E44 L53 K60 R66 E67 L68 V69 W70 Y71 N72 A73 Q74 E78 R83 E108 Y112 A137 P138 I139 F140 A141 A159 L162 L165 L172 E173 G174 Q175 Q176 A177 K178 E179 I180 D195

L204 A205 R206 A207 A208 GLU ASN LEU TYR PHE SER HIS HIS HIS HIS HIS HIS TRP SER HIS HIS HIS HIS HIS HIS HIS


- Molecule 1: Glutathione S-transferase related protein

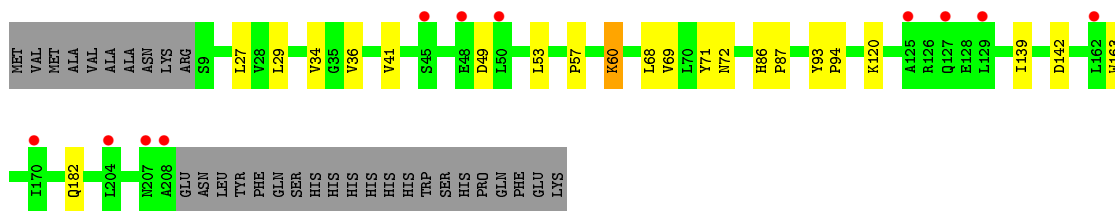
Chain H: 

MET VAL MET MET VAL VAL ALA ALA ALA ASN LYS R8 Q24 L27 V28 L29 V36 E44 D49 L53 K60 V64 D65 R66 Y71 N72 R83 V92 Y93 P94 E108 W111 Y112 K120 N121 D122 A123 Q124 K130 I133 L134 I139 Y157 L158

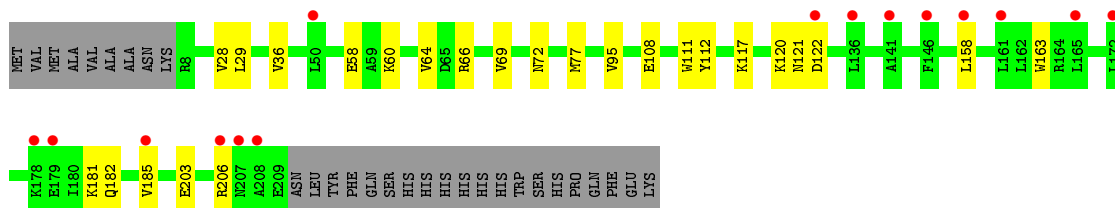
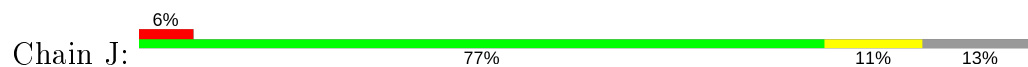
A159 L162 W163 R164 L165 L172 A177 K181 V185 K191 A208 GLU ASN LEU TYR PHE PHE SER HIS HIS HIS HIS HIS TRP SER HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Glutathione S-transferase related protein

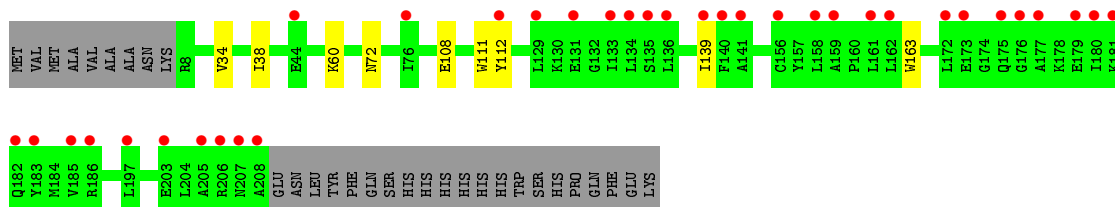
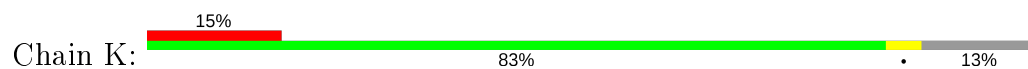
Chain I: 



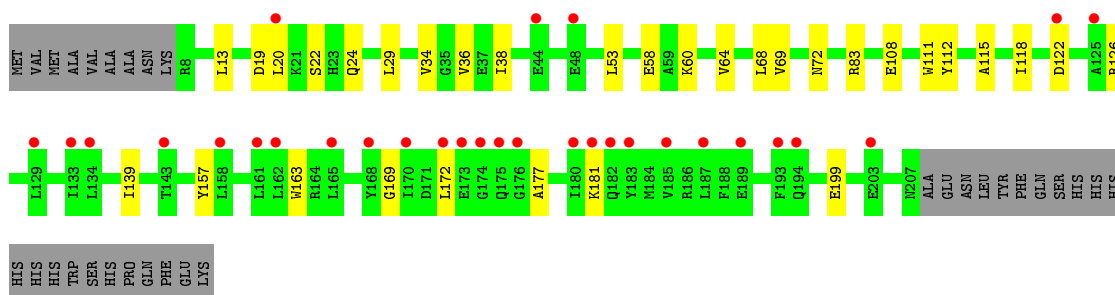
- Molecule 1: Glutathione S-transferase related protein



- Molecule 1: Glutathione S-transferase related protein



- Molecule 1: Glutathione S-transferase related protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.36Å 156.99Å 244.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 48.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.90) 99.1 (48.10-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.207 , 0.275 0.210 , 0.272	Depositor DCC
$R_{free}$ test set	2617 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.9	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 75.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19591	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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

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	0.43	1/1675 (0.1%)	0.62	0/2271
1	B	0.43	1/1670 (0.1%)	0.64	0/2264
1	C	0.42	1/1670 (0.1%)	0.62	0/2264
1	D	0.43	1/1689 (0.1%)	0.61	0/2289
1	E	0.43	0/1661	0.63	0/2253
1	F	0.43	1/1637 (0.1%)	0.60	0/2220
1	G	0.43	0/1661	0.62	0/2253
1	H	0.44	2/1672 (0.1%)	0.61	0/2267
1	I	0.42	1/1665 (0.1%)	0.61	0/2257
1	J	0.43	2/1679 (0.1%)	0.59	0/2276
1	K	0.43	2/1676 (0.1%)	0.60	0/2271
1	L	0.43	2/1654 (0.1%)	0.59	0/2245
All	All	0.43	14/20009 (0.1%)	0.61	0/27130

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	111	TRP	CD2-CE2	5.29	1.47	1.41
1	A	111	TRP	CD2-CE2	5.27	1.47	1.41
1	F	111	TRP	CD2-CE2	5.26	1.47	1.41
1	D	111	TRP	CD2-CE2	5.19	1.47	1.41
1	H	163	TRP	CD2-CE2	5.18	1.47	1.41

There are no bond angle outliers.

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	1639	0	1627	6	0
1	B	1634	0	1625	5	0
1	C	1634	0	1625	3	0
1	D	1653	0	1644	4	0
1	E	1625	0	1612	7	0
1	F	1601	0	1593	4	0
1	G	1625	0	1610	5	0
1	H	1636	0	1625	6	0
1	I	1629	0	1623	7	0
1	J	1643	0	1631	10	0
1	K	1640	0	1636	2	0
1	L	1618	0	1594	11	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	I	2	0	0	0	0
2	J	1	0	0	0	0
2	L	1	0	0	0	0
All	All	19591	0	19445	67	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 2.

The worst 5 of 67 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:J:121:ASN:O	1:J:121:ASN:ND2	2.30	0.64
1:I:29:LEU:HD13	1:I:36:VAL:HG11	1.85	0.57
1:E:29:LEU:HD13	1:E:36:VAL:HG11	1.87	0.56
1:J:120:LYS:O	1:J:121:ASN:HB3	2.06	0.56
1:L:29:LEU:HD13	1:L:36:VAL:HG11	1.88	0.56

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	200/231 (87%)	191 (96%)	8 (4%)	1 (0%)	29	61
1	B	199/231 (86%)	195 (98%)	2 (1%)	2 (1%)	15	45
1	C	199/231 (86%)	189 (95%)	8 (4%)	2 (1%)	15	45
1	D	201/231 (87%)	195 (97%)	5 (2%)	1 (0%)	29	61
1	E	198/231 (86%)	194 (98%)	2 (1%)	2 (1%)	15	45
1	F	195/231 (84%)	189 (97%)	5 (3%)	1 (0%)	29	61
1	G	199/231 (86%)	192 (96%)	5 (2%)	2 (1%)	15	45
1	H	199/231 (86%)	193 (97%)	3 (2%)	3 (2%)	10	34
1	I	198/231 (86%)	191 (96%)	5 (2%)	2 (1%)	15	45
1	J	200/231 (87%)	194 (97%)	4 (2%)	2 (1%)	15	45
1	K	199/231 (86%)	188 (94%)	10 (5%)	1 (0%)	29	61
1	L	198/231 (86%)	190 (96%)	7 (4%)	1 (0%)	29	61
All	All	2385/2772 (86%)	2301 (96%)	64 (3%)	20 (1%)	19	51

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	B	72	ASN
1	E	66	ARG
1	F	72	ASN
1	G	66	ARG

### 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	178/206 (86%)	167 (94%)	11 (6%)	18	47
1	B	178/206 (86%)	173 (97%)	5 (3%)	43	76
1	C	178/206 (86%)	167 (94%)	11 (6%)	18	47
1	D	180/206 (87%)	175 (97%)	5 (3%)	43	76
1	E	177/206 (86%)	172 (97%)	5 (3%)	43	76
1	F	175/206 (85%)	170 (97%)	5 (3%)	42	76
1	G	176/206 (85%)	166 (94%)	10 (6%)	20	51
1	H	178/206 (86%)	168 (94%)	10 (6%)	21	52
1	I	178/206 (86%)	170 (96%)	8 (4%)	27	61
1	J	179/206 (87%)	173 (97%)	6 (3%)	37	71
1	K	179/206 (87%)	176 (98%)	3 (2%)	60	86
1	L	175/206 (85%)	166 (95%)	9 (5%)	24	56
All	All	2131/2472 (86%)	2043 (96%)	88 (4%)	30	64

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	121	ASN
1	G	172	LEU
1	L	60	LYS
1	F	139	ILE
1	G	68	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	24	GLN
1	H	119	GLN
1	J	121	ASN
1	G	182	GLN
1	J	182	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates 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, 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	202/231 (87%)	0.60	16 (7%) 12 10	57, 94, 148, 176	0
1	B	201/231 (87%)	0.31	1 (0%) 91 91	47, 77, 123, 184	0
1	C	201/231 (87%)	0.39	8 (3%) 38 33	56, 93, 142, 173	0
1	D	203/231 (87%)	0.56	14 (6%) 16 13	63, 95, 144, 173	0
1	E	200/231 (86%)	0.50	9 (4%) 33 29	56, 84, 140, 184	0
1	F	197/231 (85%)	0.63	16 (8%) 12 9	59, 103, 151, 169	0
1	G	201/231 (87%)	0.69	14 (6%) 16 12	55, 100, 149, 180	0
1	H	201/231 (87%)	0.52	15 (7%) 14 11	69, 105, 150, 169	0
1	I	200/231 (86%)	0.46	11 (5%) 25 21	67, 101, 147, 188	0
1	J	202/231 (87%)	0.53	15 (7%) 14 11	68, 104, 149, 187	0
1	K	201/231 (87%)	0.96	35 (17%) 1 1	76, 124, 163, 180	0
1	L	200/231 (86%)	0.85	30 (15%) 2 1	76, 126, 165, 182	0
All	All	2409/2772 (86%)	0.58	184 (7%) 13 10	47, 100, 155, 188	0

The worst 5 of 184 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	208	ALA	8.0
1	G	207	ASN	6.9
1	L	183	TYR	6.3
1	D	6	ASN	6.0
1	K	185	VAL	6.0

### 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 carbohydrates 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.