



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:49 PM GMT

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 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)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

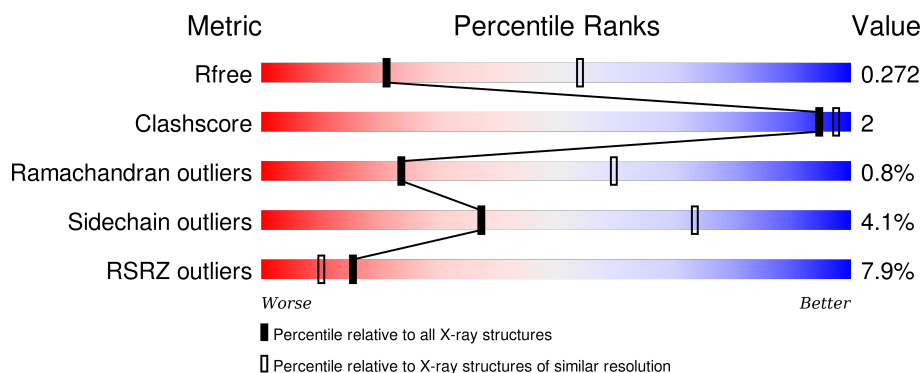
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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. 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>•</div> <div>13%</div> </div> </div>
1	B	231	<div> <div></div> <div> <div>81%</div> <div>5%</div> <div>•</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>•</div> <div>12%</div> </div> </div>
1	E	231	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>•</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	231	
1	G	231	
1	H	231	
1	I	231	
1	J	231	
1	K	231	
1	L	231	

## 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

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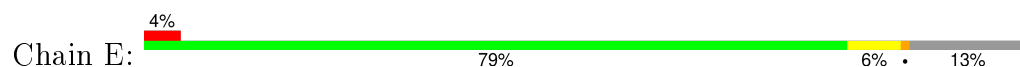
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total 1	O 1	0	0
2	I	2	Total 2	O 2	0	0
2	J	1	Total 1	O 1	0	0
2	L	1	Total 1	O 1	0	0



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

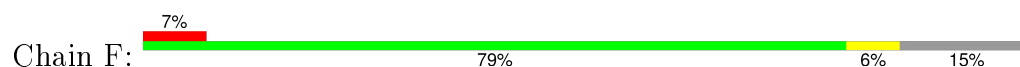
- Molecule 1: Glutathione S-transferase related protein



MET VAL MET MET ALA VAL ALA ALA ASN LYS ARG S9 L20 Q24 Q24 L27 V28 L29 V34 G35 V36 V41 T42 D43 E44 S45 E43 D49 L50 L51 Q52 L53 K60 R66 E67 L68 V69 N72 I75 R83 I118 A123 Y157 I170 A208 GLU

ASN LEU TYR PHE GLN SER HIS HIS HIS HIS ARG HIS TRP SER HIS PRO GLN PHE GLU LYS

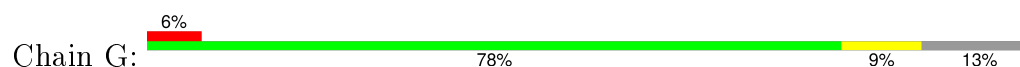
- Molecule 1: Glutathione S-transferase related protein



MET VAL MET MET ALA VAL ALA ALA ASN LYS ARG S9 Q24 L27 V28 L29 V36 V41 E44 S45 L53 K60 V69 N72 W111 N121 I134 S135 L136 I139 V154 Y157 L158 L161 L172 E173 G174 Q175 G176 A177 K178 E179 I180

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

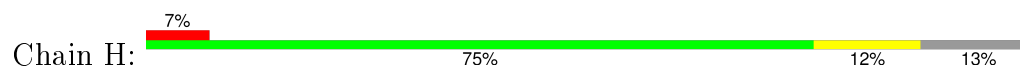
- Molecule 1: Glutathione S-transferase related protein



MET VAL MET MET ALA VAL ALA ALA ASN LYS R8 V36 E44 L53 K60 R66 E67 L68 V69 L70 N72 A73 Q74 E78 R83 E108 Y112 A137 P138 I139 F140 A141 A159 L162 L165 L172 E173 G174 Q175 G176 A177 K178 E179 I180 D195

L204 A205 R206 L207 A208 GLU ASN LYS LEU TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER PRO GLN PHE GLU LYS

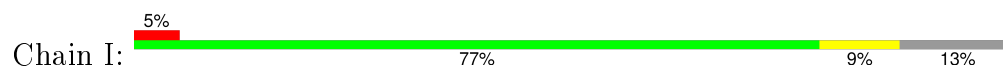
- Molecule 1: Glutathione S-transferase related protein



MET VAL MET MET ALA VAL ALA ALA ASN LYS R8 D18 Q24 L27 V28 L29 V36 E44 D49 L53 K60 V64 D65 R66 Y71 N72 Y77 R83 Y92 Y93 P94 E108 W111 Y112 K120 N121 D122 A123 Q124 K130 I133 I134 I139

Y157 L158 A159 L162 W163 W164 L165 L172 A177 K181 V185 K191 A207 A208 GLU ASN TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER PRO GLN PHE GLU LYS

- 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	2357 reflections (3.10%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 86599 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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

All (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
1	L	163	TRP	CD2-CE2	5.17	1.47	1.41
1	K	111	TRP	CD2-CE2	5.11	1.47	1.41
1	C	163	TRP	CD2-CE2	5.09	1.47	1.41
1	H	111	TRP	CD2-CE2	5.08	1.47	1.41
1	B	163	TRP	CD2-CE2	5.07	1.47	1.41
1	K	163	TRP	CD2-CE2	5.07	1.47	1.41
1	L	111	TRP	CD2-CE2	5.07	1.47	1.41
1	I	163	TRP	CD2-CE2	5.06	1.47	1.41
1	J	163	TRP	CD2-CE2	5.04	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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:172:LEU:HB2	1:A:177:ALA:HB1	1.88	0.55
1:B:29:LEU:HD13	1:B:36:VAL:HG11	1.88	0.55
1:A:108:GLU:HA	1:A:112:TYR:HB2	1.89	0.55
1:A:41:VAL:HG23	1:A:60:LYS:HE3	1.89	0.54
1:C:53:LEU:HB3	1:C:69:VAL:HG21	1.89	0.53
1:J:117:LYS:HB3	1:J:122:ASP:OD2	2.08	0.53
1:D:139:ILE:HD13	1:D:147:MET:HG3	1.91	0.53
1:A:29:LEU:HD13	1:A:36:VAL:HG11	1.89	0.52
1:J:29:LEU:HD13	1:J:36:VAL:HG11	1.91	0.52
1:L:53:LEU:HB3	1:L:69:VAL:HG21	1.92	0.52
1:E:42:THR:HG23	1:E:45:SER:H	1.76	0.51
1:I:41:VAL:HG23	1:I:60:LYS:HE3	1.93	0.50
1:D:29:LEU:HD13	1:D:36:VAL:HG11	1.94	0.50
1:F:29:LEU:HD13	1:F:36:VAL:HG11	1.93	0.50
1:D:53:LEU:HB3	1:D:69:VAL:HG21	1.94	0.50
1:G:108:GLU:HA	1:G:112:TYR:HB2	1.94	0.49
1:I:53:LEU:HB3	1:I:69:VAL:HG21	1.93	0.49
1:F:53:LEU:HB3	1:F:69:VAL:HG21	1.93	0.49
1:L:24:GLN:HE21	1:L:157:TYR:HA	1.78	0.48
1:G:53:LEU:HB3	1:G:69:VAL:HG21	1.95	0.48
1:H:24:GLN:HE21	1:H:157:TYR:HA	1.79	0.47
1:J:108:GLU:HA	1:J:112:TYR:HB2	1.96	0.47
1:E:34:VAL:HG12	1:L:34:VAL:HG13	1.97	0.47
1:A:139:ILE:HD13	1:A:147:MET:HG3	1.96	0.46
1:C:11:MET:HB2	1:C:36:VAL:HG12	1.97	0.46
1:L:108:GLU:HA	1:L:112:TYR:HB2	1.97	0.46
1:E:72:ASN:HB3	1:E:75:ILE:HD12	1.98	0.45
1:L:115:ALA:HA	1:L:118:ILE:HD12	1.98	0.45
1:C:41:VAL:HG23	1:C:60:LYS:HE3	1.98	0.45
1:H:29:LEU:HD13	1:H:36:VAL:HG11	1.98	0.45
1:L:126:ARG:HE	1:L:169:GLY:HA3	1.82	0.45
1:I:34:VAL:HG12	1:K:34:VAL:HG13	1.99	0.45
1:B:41:VAL:HG23	1:B:60:LYS:HE3	1.98	0.45
1:B:155:ASP:HB3	1:B:187:LEU:HD11	2.00	0.44
1:A:86:HIS:HA	1:A:87:PRO:HA	1.91	0.44
1:L:172:LEU:HD22	1:L:177:ALA:HB1	2.00	0.44
1:J:203:GLU:HG3	1:J:206:ARG:HH11	1.82	0.44
1:H:172:LEU:HB3	1:H:177:ALA:HB1	1.98	0.44
1:F:41:VAL:HG23	1:F:60:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:93:TYR:HA	1:I:94:PRO:HD3	1.87	0.43
1:E:41:VAL:HG23	1:E:60:LYS:HE3	1.99	0.43
1:L:64:VAL:HG22	1:L:69:VAL:HG23	2.01	0.42
1:J:28:VAL:HG21	1:J:77:MET:HG2	2.01	0.42
1:E:24:GLN:HE21	1:E:157:TYR:HA	1.84	0.42
1:I:68:LEU:HD22	1:J:95:VAL:HG13	2.01	0.42
1:K:108:GLU:HA	1:K:112:TYR:HB2	2.02	0.42
1:G:162:LEU:HA	1:G:165:LEU:HD13	2.01	0.42
1:L:13:LEU:HD23	1:L:38:ILE:HG12	2.01	0.42
1:H:53:LEU:HD13	1:H:64:VAL:HG21	2.01	0.42
1:J:120:LYS:O	1:J:121:ASN:CB	2.65	0.42
1:G:137:ALA:HA	1:G:140:PHE:HD2	1.85	0.42
1:B:66:ARG:HB2	1:B:67:GLU:H	1.73	0.42
1:G:74:GLN:HE21	1:G:78:GLU:HG3	1.84	0.41
1:H:93:TYR:HA	1:H:94:PRO:HD3	1.92	0.41
1:J:64:VAL:HG22	1:J:69:VAL:HG23	2.01	0.41
1:I:86:HIS:HA	1:I:87:PRO:HA	1.94	0.41
1:F:24:GLN:HE21	1:F:157:TYR:HA	1.85	0.41
1:H:108:GLU:HA	1:H:112:TYR:HB2	2.02	0.41
1:L:19:ASP:HB3	1:L:22:SER:HB2	2.03	0.41
1:D:180:ILE:HG12	1:D:180:ILE:H	1.69	0.41
1:E:53:LEU:HB3	1:E:69:VAL:HG21	2.03	0.40
1:B:108:GLU:HA	1:B:112:TYR:HB2	2.03	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	200/231 (87%)	191 (96%)	8 (4%)	1 (0%)	34 71
1	B	199/231 (86%)	195 (98%)	2 (1%)	2 (1%)	19 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	199/231 (86%)	189 (95%)	8 (4%)	2 (1%)	19	54
1	D	201/231 (87%)	195 (97%)	5 (2%)	1 (0%)	34	71
1	E	198/231 (86%)	194 (98%)	2 (1%)	2 (1%)	19	54
1	F	195/231 (84%)	189 (97%)	5 (3%)	1 (0%)	34	71
1	G	199/231 (86%)	192 (96%)	5 (2%)	2 (1%)	19	54
1	H	199/231 (86%)	193 (97%)	3 (2%)	3 (2%)	13	42
1	I	198/231 (86%)	191 (96%)	5 (2%)	2 (1%)	19	54
1	J	200/231 (87%)	194 (97%)	4 (2%)	2 (1%)	19	54
1	K	199/231 (86%)	188 (94%)	10 (5%)	1 (0%)	34	71
1	L	198/231 (86%)	190 (96%)	7 (4%)	1 (0%)	34	71
All	All	2385/2772 (86%)	2301 (96%)	64 (3%)	20 (1%)	24	60

All (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
1	H	66	ARG
1	H	120	LYS
1	J	66	ARG
1	K	72	ASN
1	L	72	ASN
1	B	66	ARG
1	D	72	ASN
1	E	72	ASN
1	G	72	ASN
1	H	72	ASN
1	I	72	ASN
1	J	72	ASN
1	C	66	ARG
1	C	72	ASN
1	I	120	LYS

### 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	178/206 (86%)	167 (94%)	11 (6%)	23	55
1	B	178/206 (86%)	173 (97%)	5 (3%)	51	84
1	C	178/206 (86%)	167 (94%)	11 (6%)	23	55
1	D	180/206 (87%)	175 (97%)	5 (3%)	51	84
1	E	177/206 (86%)	172 (97%)	5 (3%)	51	84
1	F	175/206 (85%)	170 (97%)	5 (3%)	50	83
1	G	176/206 (85%)	166 (94%)	10 (6%)	25	59
1	H	178/206 (86%)	168 (94%)	10 (6%)	26	60
1	I	178/206 (86%)	170 (96%)	8 (4%)	34	70
1	J	179/206 (87%)	173 (97%)	6 (3%)	44	79
1	K	179/206 (87%)	176 (98%)	3 (2%)	68	91
1	L	175/206 (85%)	166 (95%)	9 (5%)	29	65
All	All	2131/2472 (86%)	2043 (96%)	88 (4%)	37	73

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	49	ASP
1	A	60	LYS
1	A	69	VAL
1	A	71	TYR
1	A	83	ARG
1	A	92	VAL
1	A	108	GLU
1	A	122	ASP
1	A	139	ILE
1	A	158	LEU
1	B	58	GLU
1	B	60	LYS
1	B	108	GLU

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Mol	Chain	Res	Type
1	B	121	ASN
1	B	191	LYS
1	C	9	SER
1	C	34	VAL
1	C	51	LEU
1	C	60	LYS
1	C	68	LEU
1	C	116	GLU
1	C	122	ASP
1	C	124	GLN
1	C	139	ILE
1	C	182	GLN
1	C	185	VAL
1	D	49	ASP
1	D	60	LYS
1	D	71	TYR
1	D	139	ILE
1	D	180	ILE
1	E	27	LEU
1	E	42	THR
1	E	49	ASP
1	E	60	LYS
1	E	83	ARG
1	F	27	LEU
1	F	60	LYS
1	F	121	ASN
1	F	139	ILE
1	F	158	LEU
1	G	36	VAL
1	G	60	LYS
1	G	68	LEU
1	G	71	TYR
1	G	83	ARG
1	G	108	GLU
1	G	139	ILE
1	G	172	LEU
1	G	175	GLN
1	G	195	ASP
1	H	8	ARG
1	H	27	LEU
1	H	49	ASP
1	H	60	LYS

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Mol	Chain	Res	Type
1	H	71	TYR
1	H	83	ARG
1	H	92	VAL
1	H	122	ASP
1	H	139	ILE
1	H	191	LYS
1	I	27	LEU
1	I	49	ASP
1	I	57	PRO
1	I	60	LYS
1	I	71	TYR
1	I	139	ILE
1	I	142	ASP
1	I	182	GLN
1	J	58	GLU
1	J	60	LYS
1	J	158	LEU
1	J	181	LYS
1	J	182	GLN
1	J	185	VAL
1	K	38	ILE
1	K	60	LYS
1	K	139	ILE
1	L	20	LEU
1	L	58	GLU
1	L	60	LYS
1	L	68	LEU
1	L	83	ARG
1	L	122	ASP
1	L	139	ILE
1	L	181	LYS
1	L	199	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	B	24	GLN
1	B	127	GLN
1	E	24	GLN
1	F	24	GLN
1	F	182	GLN

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Mol	Chain	Res	Type
1	G	182	GLN
1	H	24	GLN
1	H	119	GLN
1	I	24	GLN
1	I	119	GLN
1	J	52	GLN
1	J	121	ASN
1	J	182	GLN
1	K	182	GLN
1	L	24	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 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%)	0.63	16 (7%) 15 10	57, 94, 148, 176	0
1	B	201/231 (87%)	0.33	1 (0%) 91 90	47, 77, 123, 184	0
1	C	201/231 (87%)	0.41	8 (3%) 42 35	56, 93, 142, 173	0
1	D	203/231 (87%)	0.58	15 (7%) 17 11	63, 95, 144, 173	0
1	E	200/231 (86%)	0.52	10 (5%) 32 26	56, 84, 140, 184	0
1	F	197/231 (85%)	0.65	16 (8%) 15 9	59, 103, 151, 169	0
1	G	201/231 (87%)	0.71	14 (6%) 19 13	55, 100, 149, 180	0
1	H	201/231 (87%)	0.54	17 (8%) 13 8	69, 105, 150, 169	0
1	I	200/231 (86%)	0.49	12 (6%) 25 18	67, 101, 147, 188	0
1	J	202/231 (87%)	0.56	16 (7%) 15 10	68, 104, 149, 187	0
1	K	201/231 (87%)	0.99	36 (17%) 2 1	76, 124, 163, 180	0
1	L	200/231 (86%)	0.88	30 (15%) 3 2	76, 126, 165, 182	0
All	All	2409/2772 (86%)	0.61	191 (7%) 15 10	47, 100, 155, 188	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	208	ALA	7.6
1	G	207	ASN	7.1
1	D	6	ASN	6.4
1	L	183	TYR	6.4
1	K	185	VAL	6.1
1	L	168	TYR	6.0
1	A	121	ASN	6.0
1	K	172	LEU	5.7
1	G	173	GLU	5.4
1	L	162	LEU	5.2
1	A	173	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	207	ASN	4.9
1	C	121	ASN	4.7
1	L	175	GLN	4.6
1	E	48	GLU	4.6
1	F	176	GLY	4.6
1	D	206	ARG	4.4
1	F	180	ILE	4.4
1	L	125	ALA	4.3
1	J	207	ASN	4.3
1	L	176	GLY	4.2
1	L	158	LEU	4.2
1	L	165	LEU	4.2
1	L	129	LEU	4.1
1	L	172	LEU	4.1
1	H	134	LEU	4.1
1	J	208	ALA	4.0
1	G	208	ALA	4.0
1	J	136	LEU	3.9
1	G	174	GLY	3.9
1	I	45	SER	3.9
1	G	140	PHE	3.9
1	K	156	CYS	3.8
1	G	141	ALA	3.7
1	D	48	GLU	3.7
1	A	207	ASN	3.7
1	D	205	ALA	3.6
1	D	208	ALA	3.6
1	L	161	LEU	3.5
1	K	181	LYS	3.5
1	I	207	ASN	3.5
1	L	44	GLU	3.5
1	L	133	ILE	3.5
1	K	131	GLU	3.4
1	E	123	ALA	3.4
1	K	162	LEU	3.4
1	K	183	TYR	3.4
1	A	174	GLY	3.3
1	L	173	GLU	3.3
1	I	127	GLN	3.3
1	L	187	LEU	3.3
1	E	50	LEU	3.3
1	J	185	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	44	GLU	3.3
1	G	204	LEU	3.3
1	K	206	ARG	3.3
1	K	180	ILE	3.2
1	D	172	LEU	3.2
1	A	134	LEU	3.2
1	I	208	ALA	3.2
1	K	175	GLN	3.2
1	L	122	ASP	3.1
1	D	162	LEU	3.1
1	F	44	GLU	3.1
1	C	206	ARG	3.1
1	A	172	LEU	3.1
1	E	45	SER	3.1
1	K	129	LEU	3.1
1	D	49	ASP	3.0
1	A	133	ILE	3.0
1	G	206	ARG	3.0
1	H	121	ASN	3.0
1	F	161	LEU	3.0
1	L	181	LYS	3.0
1	F	177	ALA	3.0
1	F	174	GLY	2.9
1	A	146	PHE	2.9
1	L	48	GLU	2.9
1	G	44	GLU	2.9
1	K	203	GLU	2.9
1	K	140	PHE	2.9
1	A	208	ALA	2.9
1	D	207	ASN	2.9
1	F	199	GLU	2.8
1	A	168	TYR	2.8
1	F	185	VAL	2.8
1	L	185	VAL	2.8
1	K	133	ILE	2.8
1	A	170	ILE	2.8
1	E	67	GLU	2.8
1	I	204	LEU	2.8
1	F	45	SER	2.7
1	J	172	LEU	2.7
1	K	134	LEU	2.7
1	I	170	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	134	LEU	2.7
1	K	182	GLN	2.7
1	L	174	GLY	2.7
1	F	172	LEU	2.7
1	J	178	LYS	2.7
1	K	136	LEU	2.7
1	J	179	GLU	2.6
1	H	133	ILE	2.6
1	G	178	LYS	2.6
1	K	186	ARG	2.6
1	K	141	ALA	2.6
1	K	177	ALA	2.6
1	K	173	GLU	2.6
1	F	134	LEU	2.6
1	L	143	THR	2.6
1	K	179	GLU	2.6
1	G	159	ALA	2.6
1	C	125	ALA	2.5
1	D	159	ALA	2.5
1	D	134	LEU	2.5
1	D	141	ALA	2.5
1	L	180	ILE	2.5
1	C	48	GLU	2.5
1	I	50	LEU	2.5
1	I	129	LEU	2.5
1	K	139	ILE	2.5
1	B	206	ARG	2.4
1	J	122	ASP	2.4
1	K	76	ILE	2.4
1	L	193	PHE	2.4
1	L	203	GLU	2.4
1	I	48	GLU	2.4
1	K	197	LEU	2.4
1	G	175	GLN	2.4
1	K	205	ALA	2.4
1	G	176	GLY	2.4
1	E	20	LEU	2.3
1	C	129	LEU	2.3
1	H	162	LEU	2.3
1	A	120	LYS	2.3
1	H	53	LEU	2.3
1	J	206	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	181	LYS	2.3
1	J	158	LEU	2.3
1	F	121	ASN	2.3
1	J	141	ALA	2.3
1	K	176	GLY	2.3
1	C	162	LEU	2.3
1	F	136	LEU	2.3
1	C	208	ALA	2.3
1	D	188	PHE	2.3
1	F	173	GLU	2.3
1	H	165	LEU	2.3
1	K	161	LEU	2.3
1	A	177	ALA	2.2
1	L	170	ILE	2.2
1	D	7	LYS	2.2
1	J	146	PHE	2.2
1	H	185	VAL	2.2
1	I	162	LEU	2.2
1	L	20	LEU	2.2
1	H	158	LEU	2.2
1	J	161	LEU	2.2
1	I	125	ALA	2.2
1	L	182	GLN	2.2
1	A	185	VAL	2.2
1	E	51	LEU	2.2
1	F	178	LYS	2.2
1	K	207	ASN	2.2
1	G	180	ILE	2.2
1	A	206	ARG	2.2
1	H	130	LYS	2.1
1	H	124	GLN	2.1
1	H	208	ALA	2.1
1	E	170	ILE	2.1
1	A	159	ALA	2.1
1	H	44	GLU	2.1
1	K	112	TYR	2.1
1	J	165	LEU	2.1
1	E	44	GLU	2.1
1	J	50	LEU	2.1
1	D	175	GLN	2.1
1	K	165	LEU	2.1
1	I	140	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	60	LYS	2.1
1	L	189	GLU	2.1
1	K	135	SER	2.0
1	H	18	ASP	2.0
1	H	207	ASN	2.0
1	L	194	GLN	2.0
1	F	154	VAL	2.0
1	H	177	ALA	2.0
1	K	39	THR	2.0
1	H	159	ALA	2.0
1	E	118	ILE	2.0
1	K	158	LEU	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 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.