Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2024 – 10:30 AM EDT

PDB ID	:	4JUR
Title	:	Crystal structure of the effector Tae4 from Salmonella typhimurium in complex with the immunity Tai4 from Enterobacter cloacae
Authors	:	Zhang, H.; Gao, Z.Q.; Dong, Y.H.
Deposited on	:	2013-03-25
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

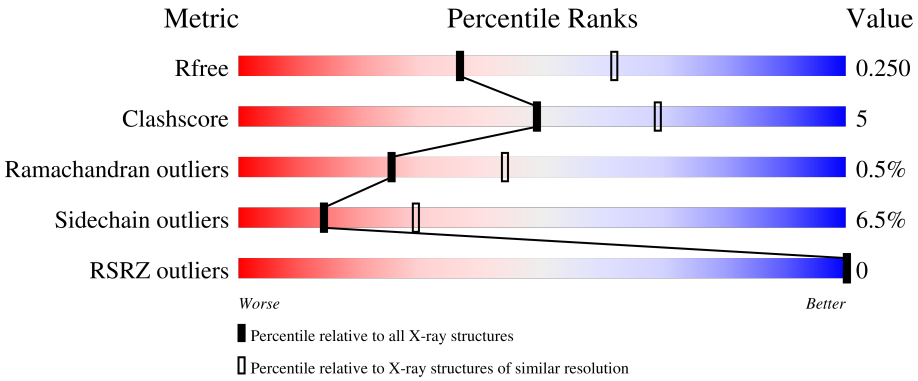
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	176	80% 11% • 9%
1	B	176	79% 11% • 9%
1	C	176	74% 18% 9%
1	D	176	66% 22% • 9%
1	E	176	74% 15% • 9%

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Mol	Chain	Length	Quality of chain
1	F	176	78% 11% • 9%
1	G	176	75% 13% • 9%
1	H	176	74% 16% 10%
2	I	105	74% 15% • 8%
2	J	105	79% 10% • 8%
2	K	105	71% 17% • 8%
2	L	105	72% 19% • 8%
2	M	105	77% 13% • 8%
2	N	105	81% 10% • 8%
2	O	105	77% 13% • 9%
2	P	105	83% 9% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15975 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 Putative cytoplasmic protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	Se	0	0	0
			1241	794	216	224	3	4			
1	B	160	Total	C	N	O	S	Se	0	0	0
			1231	786	217	222	3	3			
1	C	161	Total	C	N	O	S	Se	0	0	0
			1241	792	218	224	3	4			
1	D	160	Total	C	N	O	S	Se	0	0	0
			1234	789	218	221	3	3			
1	E	160	Total	C	N	O	S	Se	0	0	0
			1238	791	219	222	3	3			
1	F	160	Total	C	N	O	S	Se	0	0	0
			1228	785	215	222	3	3			
1	G	160	Total	C	N	O	S	Se	0	0	0
			1230	786	215	223	3	3			
1	H	159	Total	C	N	O	S	Se	0	0	0
			1222	783	215	218	3	3			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP Q93IS4
A	-13	MSE	-	expression tag	UNP Q93IS4
A	-12	ALA	-	expression tag	UNP Q93IS4
A	-11	SER	-	expression tag	UNP Q93IS4
A	-10	MSE	-	expression tag	UNP Q93IS4
A	-9	THR	-	expression tag	UNP Q93IS4
A	-8	GLY	-	expression tag	UNP Q93IS4
A	-7	GLY	-	expression tag	UNP Q93IS4
A	-6	GLN	-	expression tag	UNP Q93IS4
A	-5	GLN	-	expression tag	UNP Q93IS4
A	-4	MSE	-	expression tag	UNP Q93IS4
A	-3	GLY	-	expression tag	UNP Q93IS4
A	-2	ARG	-	expression tag	UNP Q93IS4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q93IS4
A	0	SER	-	expression tag	UNP Q93IS4
B	-14	HIS	-	expression tag	UNP Q93IS4
B	-13	MSE	-	expression tag	UNP Q93IS4
B	-12	ALA	-	expression tag	UNP Q93IS4
B	-11	SER	-	expression tag	UNP Q93IS4
B	-10	MSE	-	expression tag	UNP Q93IS4
B	-9	THR	-	expression tag	UNP Q93IS4
B	-8	GLY	-	expression tag	UNP Q93IS4
B	-7	GLY	-	expression tag	UNP Q93IS4
B	-6	GLN	-	expression tag	UNP Q93IS4
B	-5	GLN	-	expression tag	UNP Q93IS4
B	-4	MSE	-	expression tag	UNP Q93IS4
B	-3	GLY	-	expression tag	UNP Q93IS4
B	-2	ARG	-	expression tag	UNP Q93IS4
B	-1	GLY	-	expression tag	UNP Q93IS4
B	0	SER	-	expression tag	UNP Q93IS4
C	-14	HIS	-	expression tag	UNP Q93IS4
C	-13	MSE	-	expression tag	UNP Q93IS4
C	-12	ALA	-	expression tag	UNP Q93IS4
C	-11	SER	-	expression tag	UNP Q93IS4
C	-10	MSE	-	expression tag	UNP Q93IS4
C	-9	THR	-	expression tag	UNP Q93IS4
C	-8	GLY	-	expression tag	UNP Q93IS4
C	-7	GLY	-	expression tag	UNP Q93IS4
C	-6	GLN	-	expression tag	UNP Q93IS4
C	-5	GLN	-	expression tag	UNP Q93IS4
C	-4	MSE	-	expression tag	UNP Q93IS4
C	-3	GLY	-	expression tag	UNP Q93IS4
C	-2	ARG	-	expression tag	UNP Q93IS4
C	-1	GLY	-	expression tag	UNP Q93IS4
C	0	SER	-	expression tag	UNP Q93IS4
D	-14	HIS	-	expression tag	UNP Q93IS4
D	-13	MSE	-	expression tag	UNP Q93IS4
D	-12	ALA	-	expression tag	UNP Q93IS4
D	-11	SER	-	expression tag	UNP Q93IS4
D	-10	MSE	-	expression tag	UNP Q93IS4
D	-9	THR	-	expression tag	UNP Q93IS4
D	-8	GLY	-	expression tag	UNP Q93IS4
D	-7	GLY	-	expression tag	UNP Q93IS4
D	-6	GLN	-	expression tag	UNP Q93IS4
D	-5	GLN	-	expression tag	UNP Q93IS4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	MSE	-	expression tag	UNP Q93IS4
D	-3	GLY	-	expression tag	UNP Q93IS4
D	-2	ARG	-	expression tag	UNP Q93IS4
D	-1	GLY	-	expression tag	UNP Q93IS4
D	0	SER	-	expression tag	UNP Q93IS4
E	-14	HIS	-	expression tag	UNP Q93IS4
E	-13	MSE	-	expression tag	UNP Q93IS4
E	-12	ALA	-	expression tag	UNP Q93IS4
E	-11	SER	-	expression tag	UNP Q93IS4
E	-10	MSE	-	expression tag	UNP Q93IS4
E	-9	THR	-	expression tag	UNP Q93IS4
E	-8	GLY	-	expression tag	UNP Q93IS4
E	-7	GLY	-	expression tag	UNP Q93IS4
E	-6	GLN	-	expression tag	UNP Q93IS4
E	-5	GLN	-	expression tag	UNP Q93IS4
E	-4	MSE	-	expression tag	UNP Q93IS4
E	-3	GLY	-	expression tag	UNP Q93IS4
E	-2	ARG	-	expression tag	UNP Q93IS4
E	-1	GLY	-	expression tag	UNP Q93IS4
E	0	SER	-	expression tag	UNP Q93IS4
F	-14	HIS	-	expression tag	UNP Q93IS4
F	-13	MSE	-	expression tag	UNP Q93IS4
F	-12	ALA	-	expression tag	UNP Q93IS4
F	-11	SER	-	expression tag	UNP Q93IS4
F	-10	MSE	-	expression tag	UNP Q93IS4
F	-9	THR	-	expression tag	UNP Q93IS4
F	-8	GLY	-	expression tag	UNP Q93IS4
F	-7	GLY	-	expression tag	UNP Q93IS4
F	-6	GLN	-	expression tag	UNP Q93IS4
F	-5	GLN	-	expression tag	UNP Q93IS4
F	-4	MSE	-	expression tag	UNP Q93IS4
F	-3	GLY	-	expression tag	UNP Q93IS4
F	-2	ARG	-	expression tag	UNP Q93IS4
F	-1	GLY	-	expression tag	UNP Q93IS4
F	0	SER	-	expression tag	UNP Q93IS4
G	-14	HIS	-	expression tag	UNP Q93IS4
G	-13	MSE	-	expression tag	UNP Q93IS4
G	-12	ALA	-	expression tag	UNP Q93IS4
G	-11	SER	-	expression tag	UNP Q93IS4
G	-10	MSE	-	expression tag	UNP Q93IS4
G	-9	THR	-	expression tag	UNP Q93IS4
G	-8	GLY	-	expression tag	UNP Q93IS4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLY	-	expression tag	UNP Q93IS4
G	-6	GLN	-	expression tag	UNP Q93IS4
G	-5	GLN	-	expression tag	UNP Q93IS4
G	-4	MSE	-	expression tag	UNP Q93IS4
G	-3	GLY	-	expression tag	UNP Q93IS4
G	-2	ARG	-	expression tag	UNP Q93IS4
G	-1	GLY	-	expression tag	UNP Q93IS4
G	0	SER	-	expression tag	UNP Q93IS4
H	-14	HIS	-	expression tag	UNP Q93IS4
H	-13	MSE	-	expression tag	UNP Q93IS4
H	-12	ALA	-	expression tag	UNP Q93IS4
H	-11	SER	-	expression tag	UNP Q93IS4
H	-10	MSE	-	expression tag	UNP Q93IS4
H	-9	THR	-	expression tag	UNP Q93IS4
H	-8	GLY	-	expression tag	UNP Q93IS4
H	-7	GLY	-	expression tag	UNP Q93IS4
H	-6	GLN	-	expression tag	UNP Q93IS4
H	-5	GLN	-	expression tag	UNP Q93IS4
H	-4	MSE	-	expression tag	UNP Q93IS4
H	-3	GLY	-	expression tag	UNP Q93IS4
H	-2	ARG	-	expression tag	UNP Q93IS4
H	-1	GLY	-	expression tag	UNP Q93IS4
H	0	SER	-	expression tag	UNP Q93IS4

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	97	Total	C	N	O	S	0	0	0
			735	462	124	147	2			
2	J	97	Total	C	N	O	S	0	0	0
			735	463	125	145	2			
2	K	97	Total	C	N	O	S	0	0	0
			739	464	124	149	2			
2	L	97	Total	C	N	O	S	0	0	0
			741	465	125	149	2			
2	M	97	Total	C	N	O	S	0	0	0
			741	466	126	147	2			
2	N	97	Total	C	N	O	S	0	0	0
			736	463	124	147	2			
2	O	96	Total	C	N	O	S	0	0	0
			730	460	123	145	2			
2	P	97	Total	C	N	O	S	0	0	0
			733	462	124	145	2			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	118	HIS	-	expression tag	UNP D5C6F7
I	119	HIS	-	expression tag	UNP D5C6F7
I	120	HIS	-	expression tag	UNP D5C6F7
I	121	HIS	-	expression tag	UNP D5C6F7
I	122	HIS	-	expression tag	UNP D5C6F7
I	123	HIS	-	expression tag	UNP D5C6F7
J	118	HIS	-	expression tag	UNP D5C6F7
J	119	HIS	-	expression tag	UNP D5C6F7
J	120	HIS	-	expression tag	UNP D5C6F7
J	121	HIS	-	expression tag	UNP D5C6F7
J	122	HIS	-	expression tag	UNP D5C6F7
J	123	HIS	-	expression tag	UNP D5C6F7
K	118	HIS	-	expression tag	UNP D5C6F7
K	119	HIS	-	expression tag	UNP D5C6F7
K	120	HIS	-	expression tag	UNP D5C6F7
K	121	HIS	-	expression tag	UNP D5C6F7
K	122	HIS	-	expression tag	UNP D5C6F7
K	123	HIS	-	expression tag	UNP D5C6F7
L	118	HIS	-	expression tag	UNP D5C6F7
L	119	HIS	-	expression tag	UNP D5C6F7
L	120	HIS	-	expression tag	UNP D5C6F7
L	121	HIS	-	expression tag	UNP D5C6F7
L	122	HIS	-	expression tag	UNP D5C6F7
L	123	HIS	-	expression tag	UNP D5C6F7
M	118	HIS	-	expression tag	UNP D5C6F7
M	119	HIS	-	expression tag	UNP D5C6F7
M	120	HIS	-	expression tag	UNP D5C6F7
M	121	HIS	-	expression tag	UNP D5C6F7
M	122	HIS	-	expression tag	UNP D5C6F7
M	123	HIS	-	expression tag	UNP D5C6F7
N	118	HIS	-	expression tag	UNP D5C6F7
N	119	HIS	-	expression tag	UNP D5C6F7
N	120	HIS	-	expression tag	UNP D5C6F7
N	121	HIS	-	expression tag	UNP D5C6F7
N	122	HIS	-	expression tag	UNP D5C6F7
N	123	HIS	-	expression tag	UNP D5C6F7
O	118	HIS	-	expression tag	UNP D5C6F7
O	119	HIS	-	expression tag	UNP D5C6F7
O	120	HIS	-	expression tag	UNP D5C6F7
O	121	HIS	-	expression tag	UNP D5C6F7
O	122	HIS	-	expression tag	UNP D5C6F7
O	123	HIS	-	expression tag	UNP D5C6F7

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Chain	Residue	Modelled	Actual	Comment	Reference
P	118	HIS	-	expression tag	UNP D5C6F7
P	119	HIS	-	expression tag	UNP D5C6F7
P	120	HIS	-	expression tag	UNP D5C6F7
P	121	HIS	-	expression tag	UNP D5C6F7
P	122	HIS	-	expression tag	UNP D5C6F7
P	123	HIS	-	expression tag	UNP D5C6F7

- Molecule 3 is water.

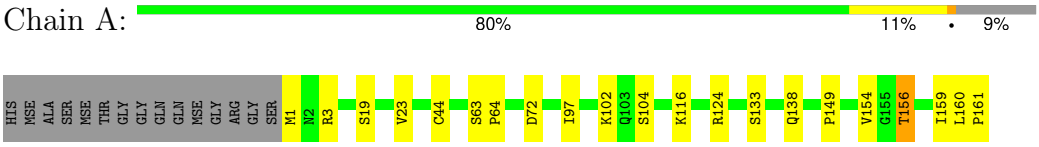
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0
3	B	18	Total O 18 18	0	0
3	C	19	Total O 19 19	0	0
3	D	9	Total O 9 9	0	0
3	E	12	Total O 12 12	0	0
3	F	7	Total O 7 7	0	0
3	G	10	Total O 10 10	0	0
3	H	14	Total O 14 14	0	0
3	I	21	Total O 21 21	0	0
3	J	12	Total O 12 12	0	0
3	K	15	Total O 15 15	0	0
3	L	13	Total O 13 13	0	0
3	M	15	Total O 15 15	0	0
3	N	12	Total O 12 12	0	0
3	O	14	Total O 14 14	0	0
3	P	13	Total O 13 13	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.

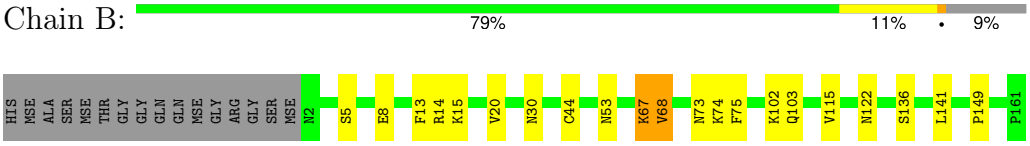
• Molecule 1: Putative cytoplasmic protein

Chain A:



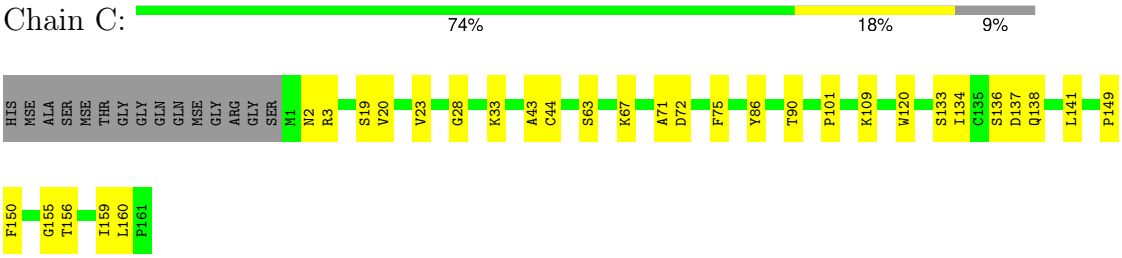
• Molecule 1: Putative cytoplasmic protein

Chain B:



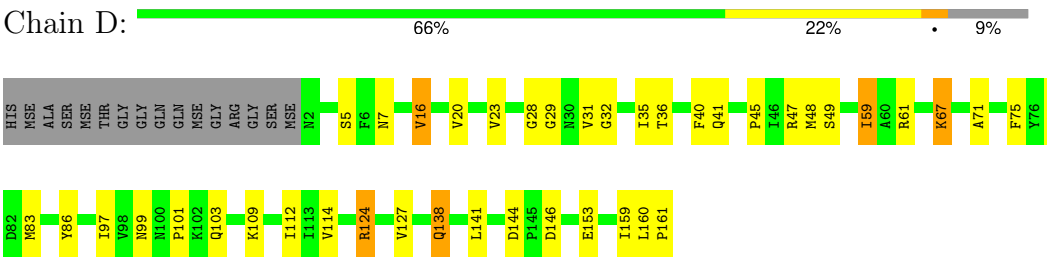
• Molecule 1: Putative cytoplasmic protein

Chain C:



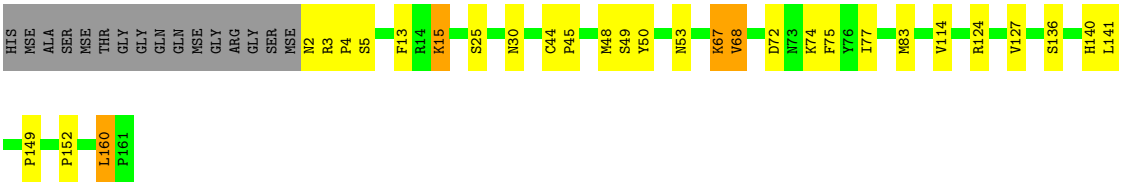
• Molecule 1: Putative cytoplasmic protein

Chain D:



• Molecule 1: Putative cytoplasmic protein

Chain E:

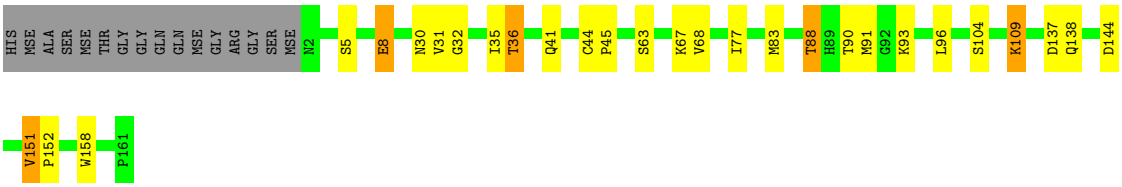


• Molecule 1: Putative cytoplasmic protein

Chain F:

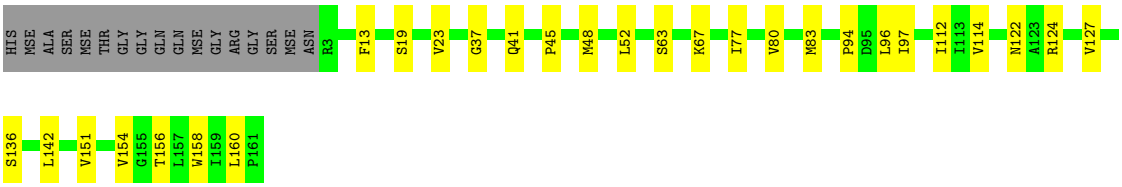
• Molecule 1: Putative cytoplasmic protein

Chain G:



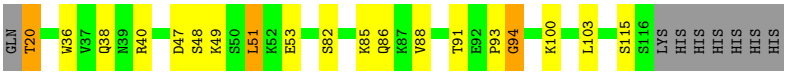
• Molecule 1: Putative cytoplasmic protein

Chain H:



• Molecule 2: Uncharacterized protein

Chain I:

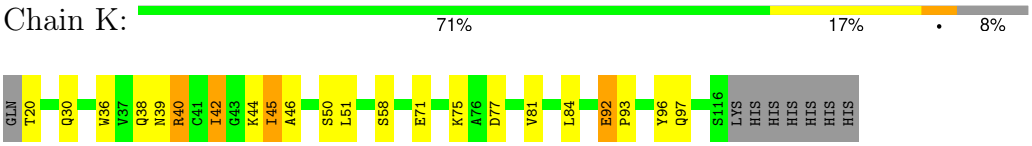


• Molecule 2: Uncharacterized protein

Chain J:

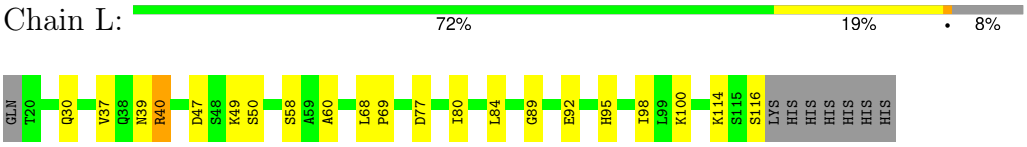
• Molecule 2: Uncharacterized protein

Chain K:



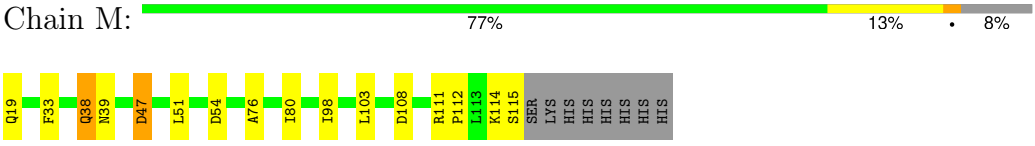
• Molecule 2: Uncharacterized protein

Chain L:



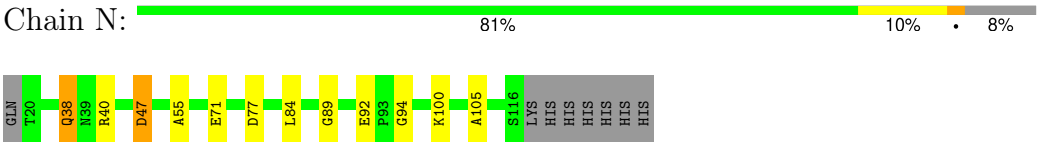
• Molecule 2: Uncharacterized protein

Chain M:



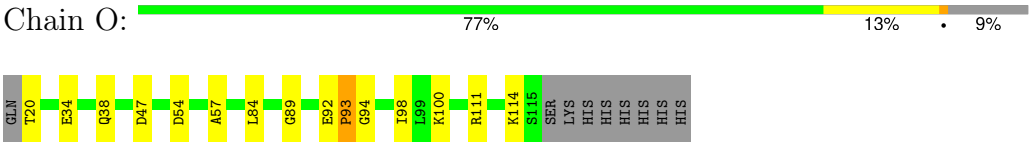
• Molecule 2: Uncharacterized protein

Chain N:



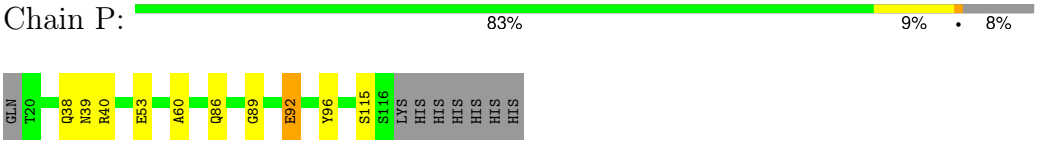
• Molecule 2: Uncharacterized protein

Chain O:



• Molecule 2: Uncharacterized protein

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.95Å 89.12Å 271.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.19 – 2.50 46.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.19-2.50) 98.9 (46.19-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.07 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.207 , 0.261 0.198 , 0.250	Depositor DCC
R_{free} test set	3772 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 19.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.467 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15975	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.47	0/1273	0.58	0/1728
1	B	0.48	0/1263	0.60	0/1716
1	C	0.47	0/1273	0.61	0/1729
1	D	0.45	0/1266	0.63	0/1719
1	E	0.48	0/1270	0.62	0/1723
1	F	0.43	0/1260	0.58	0/1712
1	G	0.42	0/1262	0.58	0/1715
1	H	0.46	0/1254	0.58	0/1703
2	I	0.53	0/747	0.62	1/1014 (0.1%)
2	J	0.53	0/747	0.63	0/1014
2	K	0.50	0/751	0.61	0/1019
2	L	0.56	0/753	0.59	0/1021
2	M	0.53	0/753	0.60	0/1021
2	N	0.51	0/748	0.57	0/1015
2	O	0.51	0/742	0.60	0/1007
2	P	0.53	0/745	0.60	0/1011
All	All	0.48	0/16107	0.60	1/21867 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	94	GLY	N-CA-C	5.02	125.65	113.10

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	1241	0	1202	8	0
1	B	1231	0	1187	9	0
1	C	1241	0	1198	14	0
1	D	1234	0	1195	30	0
1	E	1238	0	1207	14	0
1	F	1228	0	1185	10	0
1	G	1230	0	1184	14	0
1	H	1222	0	1180	16	0
2	I	735	0	718	9	0
2	J	735	0	719	10	0
2	K	739	0	722	11	0
2	L	741	0	729	9	0
2	M	741	0	730	9	0
2	N	736	0	720	6	0
2	O	730	0	715	9	0
2	P	733	0	718	7	0
3	A	16	0	0	0	0
3	B	18	0	0	0	0
3	C	19	0	0	0	0
3	D	9	0	0	0	0
3	E	12	0	0	0	0
3	F	7	0	0	0	0
3	G	10	0	0	0	0
3	H	14	0	0	0	0
3	I	21	0	0	1	0
3	J	12	0	0	0	0
3	K	15	0	0	0	0
3	L	13	0	0	0	0
3	M	15	0	0	0	0
3	N	12	0	0	0	0
3	O	14	0	0	0	0
3	P	13	0	0	0	0
All	All	15975	0	15309	164	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.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:SER:HB3	1:D:83:MSE:HE1	1.69	0.72
1:H:112:ILE:HG13	1:H:160:LEU:HD11	1.71	0.72
1:D:16:VAL:HG22	1:D:23:VAL:HG23	1.73	0.70
2:K:44:LYS:NZ	2:K:77:ASP:OD1	2.25	0.70
1:H:122:ASN:HD21	2:I:91:THR:HG22	1.58	0.69
1:D:48:MSE:HG3	1:D:127:VAL:HG12	1.77	0.66
1:A:3:ARG:NH1	1:A:159:ILE:O	2.29	0.64
1:C:20:VAL:HG13	1:C:43:ALA:HB2	1.79	0.63
1:G:77:ILE:HB	1:G:83:MSE:HE2	1.79	0.63
2:I:82:SER:O	2:I:85:LYS:HG2	1.99	0.63
1:D:81:ASN:OD1	1:D:124:ARG:NH1	2.32	0.63
1:F:53:ASN:HB3	1:F:74:LYS:HD3	1.82	0.62
1:D:114:VAL:HG22	1:D:127:VAL:HG22	1.82	0.61
1:G:96:LEU:HD22	1:G:109:LYS:HE2	1.82	0.61
1:D:67:LYS:HD3	1:D:75:PHE:HB3	1.82	0.60
1:A:1:MSE:HE1	1:A:161:PRO:HG3	1.83	0.60
2:M:108:ASP:OD1	2:M:111:ARG:NH2	2.34	0.60
1:D:31:VAL:O	1:D:35:ILE:HG12	2.02	0.59
2:L:40:ARG:NH1	2:L:77:ASP:OD1	2.36	0.59
1:H:77:ILE:HB	1:H:83:MSE:HE2	1.85	0.59
1:C:137:ASP:OD1	1:C:138:GLN:N	2.36	0.59
1:D:45:PRO:O	1:D:83:MSE:HE3	2.02	0.59
1:E:67:LYS:HD3	1:E:75:PHE:HB3	1.85	0.58
1:H:45:PRO:O	1:H:83:MSE:HE3	2.03	0.58
1:D:61:ARG:HB2	1:D:75:PHE:CE2	2.40	0.57
1:D:28:GLY:HA3	1:D:71:ALA:HB2	1.87	0.57
1:D:103:GLN:NE2	1:D:144:ASP:OD1	2.37	0.57
2:K:44:LYS:HE2	2:K:81:VAL:HG22	1.86	0.57
2:J:111:ARG:HH21	2:P:115:SER:HB3	1.70	0.56
2:J:23:ASP:O	2:J:26:THR:HB	2.06	0.55
1:H:13:PHE:CE2	1:H:136:SER:HB3	2.42	0.55
2:K:30:GLN:OE1	2:O:111:ARG:NH1	2.38	0.55
1:D:28:GLY:HA3	1:D:71:ALA:H	1.72	0.55
2:I:48:SER:HB2	2:I:51:LEU:H	1.72	0.54
2:I:88:VAL:HG13	2:I:100:LYS:HE2	1.89	0.54
2:J:98:ILE:HD13	2:N:55:ALA:HB2	1.89	0.54
1:A:116:LYS:HD3	1:A:124:ARG:NH1	2.22	0.53
2:I:86:GLN:NE2	3:I:212:HOH:O	2.37	0.53
1:F:111:GLY:HA2	1:F:160:LEU:HB2	1.91	0.53
2:K:45:ILE:HD13	2:K:97:GLN:HB3	1.90	0.53
2:O:34:GLU:OE2	2:O:114:LYS:NZ	2.42	0.53
1:E:114:VAL:HG22	1:E:127:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:GLN:NE2	2:O:57:ALA:HA	2.23	0.52
1:D:35:ILE:HD13	1:D:40:PHE:HB2	1.91	0.52
1:D:109:LYS:HD3	1:D:159:ILE:HD11	1.91	0.52
1:F:60:ALA:O	1:F:67:LYS:NZ	2.43	0.52
1:D:97:ILE:HD12	1:G:93:LYS:HA	1.92	0.52
1:D:28:GLY:HA3	1:D:71:ALA:CB	2.39	0.52
1:D:77:ILE:HB	1:D:83:MSE:HE2	1.92	0.52
1:D:32:GLY:O	1:D:36:THR:HG23	2.10	0.51
2:J:111:ARG:HG2	2:J:114:LYS:HE2	1.92	0.51
1:B:53:ASN:HB3	1:B:74:LYS:HD3	1.91	0.51
1:C:109:LYS:HD3	1:C:159:ILE:HD11	1.93	0.51
1:C:28:GLY:HA3	1:C:71:ALA:HB2	1.93	0.50
1:B:67:LYS:HD3	1:B:75:PHE:HB3	1.92	0.50
1:C:3:ARG:NH1	1:C:159:ILE:O	2.41	0.50
1:F:93:LYS:HA	1:H:97:ILE:HD12	1.94	0.50
1:D:16:VAL:HG13	1:D:47:ARG:HG2	1.94	0.49
1:H:41:GLN:HG3	2:P:60:ALA:HB2	1.94	0.49
1:F:137:ASP:OD1	1:F:138:GLN:N	2.40	0.49
1:E:45:PRO:O	1:E:83:MSE:HE3	2.11	0.49
1:D:41:GLN:HG3	2:L:60:ALA:HB2	1.93	0.49
2:O:84:LEU:HD12	2:O:100:LYS:HD2	1.93	0.49
1:E:13:PHE:CD2	1:E:136:SER:HB2	2.48	0.49
2:J:111:ARG:NH2	2:P:115:SER:HB3	2.27	0.49
1:E:53:ASN:HB3	1:E:74:LYS:HD3	1.95	0.49
1:H:114:VAL:HG22	1:H:127:VAL:HG22	1.95	0.48
2:K:42:ILE:HG21	2:L:98:ILE:HD12	1.95	0.48
1:D:112:ILE:HG13	1:D:160:LEU:HD11	1.94	0.48
1:H:48:MSE:HG3	1:H:127:VAL:HG12	1.95	0.48
2:L:37:VAL:HG13	2:L:80:ILE:HD11	1.96	0.48
2:O:92:GLU:HA	2:O:93:PRO:HD2	1.64	0.48
1:G:31:VAL:O	1:G:35:ILE:HG12	2.13	0.48
2:K:39:ASN:ND2	2:K:58:SER:HB3	2.29	0.48
2:M:98:ILE:HG12	2:O:54:ASP:OD1	2.13	0.48
2:M:47:ASP:OD1	2:M:47:ASP:N	2.44	0.48
2:P:92:GLU:HG2	2:P:96:TYR:OH	2.14	0.48
1:G:45:PRO:O	1:G:83:MSE:HE3	2.14	0.47
1:D:138:GLN:HE21	1:D:146:ASP:CG	2.17	0.47
1:G:77:ILE:HB	1:G:83:MSE:CE	2.45	0.47
1:C:101:PRO:HB2	1:C:141:LEU:HD22	1.96	0.47
1:B:13:PHE:CD2	1:B:136:SER:HB2	2.50	0.47
1:E:77:ILE:HB	1:E:83:MSE:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PRO:HG3	2:P:89:GLY:HA3	1.97	0.46
1:D:101:PRO:HB2	1:D:141:LEU:HD22	1.96	0.46
1:B:149:PRO:HG3	2:N:89:GLY:HA3	1.97	0.46
1:C:63:SER:O	1:C:67:LYS:NZ	2.46	0.46
1:G:137:ASP:OD1	1:G:138:GLN:N	2.38	0.46
1:H:19:SER:O	1:H:23:VAL:HG23	2.16	0.46
2:J:38:GLN:HG3	2:J:39:ASN:N	2.31	0.46
2:N:38:GLN:HB3	2:N:105:ALA:HB2	1.96	0.46
1:F:120:TRP:CE2	1:F:150:PHE:HB2	2.50	0.46
1:F:160:LEU:HA	1:F:161:PRO:HD3	1.70	0.46
1:G:32:GLY:O	1:G:36:THR:HG23	2.16	0.46
1:F:160:LEU:HA	1:F:160:LEU:HD12	1.83	0.46
2:K:36:TRP:CZ2	2:K:40:ARG:HG3	2.50	0.46
1:A:63:SER:HA	1:A:64:PRO:HD3	1.80	0.46
1:F:116:LYS:HD2	1:F:124:ARG:NH1	2.31	0.45
1:G:63:SER:HB3	1:G:67:LYS:HE2	1.99	0.45
1:C:19:SER:O	1:C:23:VAL:HG23	2.16	0.45
2:I:36:TRP:CH2	2:I:40:ARG:HD2	2.50	0.45
1:D:59:ILE:HG23	1:D:86:TYR:CE1	2.52	0.45
1:E:149:PRO:HG3	2:O:89:GLY:HA3	1.99	0.45
2:J:47:ASP:OD1	2:J:47:ASP:N	2.49	0.45
1:D:28:GLY:HA3	1:D:71:ALA:N	2.32	0.44
1:D:61:ARG:HD3	1:D:75:PHE:CZ	2.52	0.44
1:E:4:PRO:O	1:E:160:LEU:HG	2.16	0.44
1:B:15:LYS:HB3	1:B:15:LYS:HE2	1.66	0.44
1:C:149:PRO:HG3	2:L:89:GLY:HA3	2.00	0.44
2:L:30:GLN:HG2	2:L:114:LYS:HD2	2.00	0.44
2:M:33:PHE:CD2	2:M:114:LYS:HG2	2.52	0.44
2:M:38:GLN:HG3	2:M:39:ASN:N	2.33	0.44
1:F:114:VAL:HG22	1:F:127:VAL:HG22	1.99	0.44
1:C:86:TYR:CE2	1:C:90:THR:HG21	2.53	0.44
1:H:63:SER:HB2	1:H:67:LYS:HE2	1.99	0.43
1:C:33:LYS:HE2	1:C:33:LYS:HB3	1.68	0.43
1:C:101:PRO:HG3	1:C:155:GLY:N	2.33	0.43
1:D:99:ASN:O	1:D:153:GLU:O	2.35	0.43
1:H:94:PRO:HA	1:H:158:TRP:CD1	2.54	0.43
1:E:30:ASN:HB2	1:E:68:VAL:HG13	2.01	0.43
2:J:39:ASN:ND2	2:J:62:TRP:HE1	2.17	0.42
1:A:19:SER:O	1:A:23:VAL:HG23	2.18	0.42
2:M:54:ASP:OD1	2:O:98:ILE:HG12	2.19	0.42
2:N:47:ASP:OD1	2:N:47:ASP:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:HIS:O	1:E:152:PRO:HG3	2.20	0.42
1:E:141:LEU:HD23	1:E:141:LEU:HA	1.82	0.42
2:L:68:LEU:HA	2:L:69:PRO:HD3	1.90	0.42
1:E:72:ASP:OD2	1:E:74:LYS:HD2	2.18	0.42
1:G:5:SER:OG	1:G:8:GLU:HB2	2.19	0.42
2:I:20:THR:HG22	2:P:86:GLN:NE2	2.34	0.42
1:B:30:ASN:HB2	1:B:68:VAL:HG13	2.00	0.42
2:M:76:ALA:O	2:M:80:ILE:HG13	2.19	0.42
1:C:67:LYS:HD2	1:C:75:PHE:HB3	2.01	0.42
1:D:20:VAL:HG12	1:D:35:ILE:HD12	2.00	0.42
1:E:49:SER:OG	1:E:83:MSE:HE1	2.19	0.42
1:D:160:LEU:HA	1:D:161:PRO:HD3	1.82	0.42
1:G:30:ASN:HB2	1:G:68:VAL:HG13	2.02	0.42
1:A:102:LYS:HE3	1:A:104:SER:OG	2.20	0.41
1:E:15:LYS:HD2	1:E:50:TYR:OH	2.19	0.41
2:K:46:ALA:HB1	2:K:51:LEU:HB3	2.01	0.41
2:K:84:LEU:HD23	2:K:84:LEU:HA	1.79	0.41
2:M:51:LEU:HA	2:M:51:LEU:HD12	1.80	0.41
2:O:84:LEU:HD12	2:O:84:LEU:HA	1.91	0.41
1:H:37:GLY:O	2:P:40:ARG:NH2	2.52	0.41
1:H:67:LYS:HB3	1:H:67:LYS:HE3	1.89	0.41
2:N:84:LEU:HD23	2:N:100:LYS:HD2	2.03	0.41
1:B:103:GLN:HG3	1:B:141:LEU:HD12	2.02	0.41
2:L:84:LEU:HD23	2:L:100:LYS:HD2	2.03	0.41
1:C:120:TRP:CE2	1:C:150:PHE:HB2	2.55	0.41
1:G:88:THR:HG23	1:G:158:TRP:HZ2	1.85	0.41
2:L:39:ASN:HD22	2:L:58:SER:HB3	1.86	0.41
1:G:151:VAL:HA	1:G:152:PRO:HD3	1.81	0.40
1:H:122:ASN:ND2	2:I:91:THR:HG22	2.31	0.40
2:J:76:ALA:O	2:J:80:ILE:HG13	2.21	0.40
1:B:122:ASN:O	2:J:64:GLU:HG2	2.21	0.40
1:D:20:VAL:HA	1:D:23:VAL:HG12	2.03	0.40
2:I:49:LYS:O	2:I:53:GLU:HG3	2.21	0.40
2:K:92:GLU:HA	2:K:93:PRO:HD2	1.92	0.40
2:M:108:ASP:O	2:M:112:PRO:HD3	2.21	0.40
1:A:97:ILE:HG12	1:A:156:THR:HB	2.03	0.40
1:B:141:LEU:HD23	1:B:141:LEU:HA	1.90	0.40
1:H:142:LEU:HD23	1:H:142:LEU:HA	1.96	0.40
2:K:92:GLU:HB2	2:K:96:TYR:OH	2.22	0.40
2:N:40:ARG:NE	2:N:77:ASP:OD1	2.42	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	159/176 (90%)	153 (96%)	5 (3%)	1 (1%)	22 39
1	B	158/176 (90%)	153 (97%)	5 (3%)	0	100 100
1	C	159/176 (90%)	150 (94%)	7 (4%)	2 (1%)	10 19
1	D	158/176 (90%)	146 (92%)	10 (6%)	2 (1%)	10 19
1	E	158/176 (90%)	154 (98%)	4 (2%)	0	100 100
1	F	158/176 (90%)	150 (95%)	8 (5%)	0	100 100
1	G	158/176 (90%)	153 (97%)	5 (3%)	0	100 100
1	H	157/176 (89%)	148 (94%)	9 (6%)	0	100 100
2	I	95/105 (90%)	92 (97%)	1 (1%)	2 (2%)	5 10
2	J	95/105 (90%)	94 (99%)	1 (1%)	0	100 100
2	K	95/105 (90%)	94 (99%)	1 (1%)	0	100 100
2	L	95/105 (90%)	95 (100%)	0	0	100 100
2	M	95/105 (90%)	92 (97%)	3 (3%)	0	100 100
2	N	95/105 (90%)	94 (99%)	0	1 (1%)	12 23
2	O	94/105 (90%)	91 (97%)	1 (1%)	2 (2%)	5 10
2	P	95/105 (90%)	95 (100%)	0	0	100 100
All	All	2024/2248 (90%)	1954 (96%)	60 (3%)	10 (0%)	25 44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	ASN
2	I	93	PRO
2	I	94	GLY
1	C	72	ASP
1	D	29	GLY
1	A	72	ASP

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Mol	Chain	Res	Type
2	O	94	GLY
1	D	138	GLN
2	O	93	PRO
2	N	94	GLY

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	132/138 (96%)	126 (96%)	6 (4%)	23 46
1	B	131/138 (95%)	121 (92%)	10 (8%)	11 22
1	C	132/138 (96%)	126 (96%)	6 (4%)	23 46
1	D	131/138 (95%)	124 (95%)	7 (5%)	19 38
1	E	133/138 (96%)	122 (92%)	11 (8%)	9 19
1	F	131/138 (95%)	122 (93%)	9 (7%)	13 26
1	G	131/138 (95%)	121 (92%)	10 (8%)	11 22
1	H	128/138 (93%)	121 (94%)	7 (6%)	18 37
2	I	79/90 (88%)	73 (92%)	6 (8%)	11 22
2	J	78/90 (87%)	73 (94%)	5 (6%)	14 30
2	K	80/90 (89%)	71 (89%)	9 (11%)	4 9
2	L	81/90 (90%)	74 (91%)	7 (9%)	8 18
2	M	80/90 (89%)	75 (94%)	5 (6%)	15 30
2	N	79/90 (88%)	75 (95%)	4 (5%)	20 40
2	O	78/90 (87%)	75 (96%)	3 (4%)	28 53
2	P	78/90 (87%)	74 (95%)	4 (5%)	20 40
All	All	1682/1824 (92%)	1573 (94%)	109 (6%)	14 29

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	CYS
1	A	133	SER
1	A	138	GLN
1	A	154	VAL
1	A	156	THR
1	A	160	LEU
1	B	5	SER
1	B	8	GLU
1	B	14	ARG
1	B	20	VAL
1	B	44	CYS
1	B	67	LYS
1	B	68	VAL
1	B	73	ASN
1	B	102	LYS
1	B	115	VAL
1	C	44	CYS
1	C	133	SER
1	C	134	ILE
1	C	136	SER
1	C	156	THR
1	C	160	LEU
1	D	5	SER
1	D	7	ASN
1	D	16	VAL
1	D	59	ILE
1	D	67	LYS
1	D	80	VAL
1	D	124	ARG
1	E	2	ASN
1	E	3	ARG
1	E	5	SER
1	E	15	LYS
1	E	25	SER
1	E	44	CYS
1	E	48	MSE
1	E	67	LYS
1	E	68	VAL
1	E	124	ARG
1	E	160	LEU
1	F	2	ASN
1	F	33	LYS
1	F	44	CYS

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Mol	Chain	Res	Type
1	F	67	LYS
1	F	88	THR
1	F	109	LYS
1	F	138	GLN
1	F	144	ASP
1	F	160	LEU
1	G	8	GLU
1	G	36	THR
1	G	44	CYS
1	G	88	THR
1	G	90	THR
1	G	91	MSE
1	G	104	SER
1	G	109	LYS
1	G	144	ASP
1	G	151	VAL
1	H	52	LEU
1	H	80	VAL
1	H	96	LEU
1	H	124	ARG
1	H	151	VAL
1	H	154	VAL
1	H	156	THR
2	I	20	THR
2	I	38	GLN
2	I	47	ASP
2	I	51	LEU
2	I	103	LEU
2	I	115	SER
2	J	26	THR
2	J	38	GLN
2	J	47	ASP
2	J	51	LEU
2	J	92	GLU
2	K	20	THR
2	K	38	GLN
2	K	40	ARG
2	K	42	ILE
2	K	45	ILE
2	K	50	SER
2	K	71	GLU
2	K	75	LYS

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Mol	Chain	Res	Type
2	K	92	GLU
2	L	40	ARG
2	L	47	ASP
2	L	49	LYS
2	L	50	SER
2	L	92	GLU
2	L	95	HIS
2	L	116	SER
2	M	19	GLN
2	M	38	GLN
2	M	47	ASP
2	M	103	LEU
2	M	115	SER
2	N	38	GLN
2	N	47	ASP
2	N	71	GLU
2	N	92	GLU
2	O	20	THR
2	O	38	GLN
2	O	47	ASP
2	P	38	GLN
2	P	39	ASN
2	P	53	GLU
2	P	92	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	38	GLN
2	J	39	ASN
2	K	38	GLN
2	K	39	ASN
2	L	39	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	157/176 (89%)	-1.34	0	100	100	37, 48, 63, 78	0
1	B	157/176 (89%)	-1.30	0	100	100	39, 49, 62, 73	0
1	C	157/176 (89%)	-1.33	0	100	100	38, 49, 63, 76	0
1	D	157/176 (89%)	-1.30	0	100	100	40, 50, 63, 71	0
1	E	157/176 (89%)	-1.26	0	100	100	40, 49, 62, 74	0
1	F	157/176 (89%)	-1.22	0	100	100	45, 54, 66, 71	0
1	G	157/176 (89%)	-1.24	0	100	100	45, 54, 66, 76	0
1	H	156/176 (88%)	-1.27	0	100	100	39, 50, 61, 73	0
2	I	97/105 (92%)	-1.36	0	100	100	32, 43, 63, 70	0
2	J	97/105 (92%)	-1.32	0	100	100	32, 46, 66, 72	0
2	K	97/105 (92%)	-1.33	0	100	100	31, 43, 62, 68	0
2	L	97/105 (92%)	-1.39	0	100	100	34, 45, 59, 65	0
2	M	97/105 (92%)	-1.26	0	100	100	33, 46, 68, 73	0
2	N	97/105 (92%)	-1.34	0	100	100	35, 48, 65, 73	0
2	O	96/105 (91%)	-1.33	0	100	100	36, 48, 64, 74	0
2	P	97/105 (92%)	-1.36	0	100	100	34, 44, 60, 69	0
All	All	2030/2248 (90%)	-1.30	0	100	100	31, 49, 64, 78	0

There are no RSRZ outliers to report.

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.