



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:26 PM GMT

PDB ID : 4EMM
Title : Crystal structure of Staphylococcus aureus ClpP in compact conformation
Authors : Zhang, J.; Liu, H.; Yang, C.-G.
Deposited on : 2012-04-12
Resolution : 2.40 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

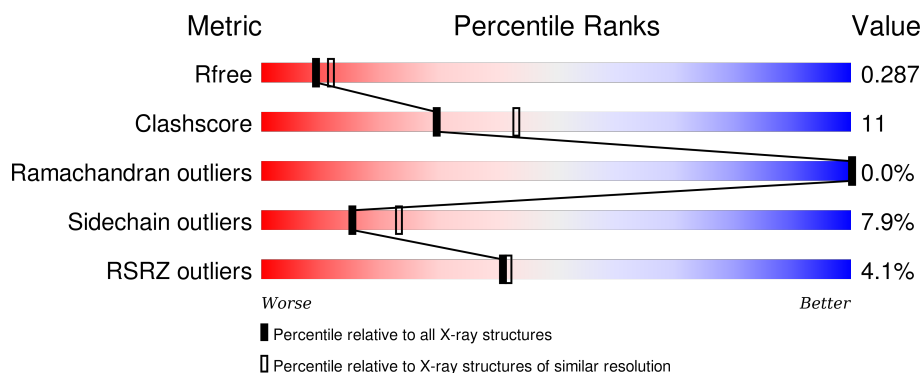
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 ≥ 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	203	<div> <div> <div></div> <div>58%</div> <div>24%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	203	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>22%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	203	<div> <div>7%</div> <div> <div></div> <div>65%</div> <div>18%</div> <div>•</div> <div>15%</div> </div> </div>
1	D	203	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>20%</div> <div>•</div> <div>16%</div> </div> </div>
1	E	203	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>22%</div> <div>•</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	203	
1	G	203	
1	H	203	
1	I	203	
1	J	203	
1	K	203	
1	L	203	
1	M	203	
1	V	203	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18724 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	V	172	Total	C	N	O	S	0	0	0
			1331	843	225	257	6			
1	A	173	Total	C	N	O	S	0	0	0
			1340	848	226	260	6			
1	B	171	Total	C	N	O	S	0	1	0
			1328	841	224	256	7			
1	C	172	Total	C	N	O	S	0	1	0
			1336	847	225	257	7			
1	D	171	Total	C	N	O	S	0	0	0
			1322	838	224	254	6			
1	E	173	Total	C	N	O	S	0	1	0
			1343	851	226	259	7			
1	F	173	Total	C	N	O	S	0	0	0
			1330	842	226	256	6			
1	G	173	Total	C	N	O	S	0	0	0
			1340	848	226	260	6			
1	H	175	Total	C	N	O	S	0	1	0
			1353	857	228	261	7			
1	I	172	Total	C	N	O	S	0	0	0
			1331	843	225	257	6			
1	J	173	Total	C	N	O	S	0	2	0
			1353	856	228	262	7			
1	K	173	Total	C	N	O	S	0	1	0
			1345	852	226	260	7			
1	L	168	Total	C	N	O	S	0	0	0
			1302	824	221	251	6			
1	M	172	Total	C	N	O	S	0	1	0
			1338	848	225	258	7			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	196	LEU	-	EXPRESSION TAG	UNP P63786

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Chain	Residue	Modelled	Actual	Comment	Reference
V	197	GLU	-	EXPRESSION TAG	UNP P63786
V	198	HIS	-	EXPRESSION TAG	UNP P63786
V	199	HIS	-	EXPRESSION TAG	UNP P63786
V	200	HIS	-	EXPRESSION TAG	UNP P63786
V	201	HIS	-	EXPRESSION TAG	UNP P63786
V	202	HIS	-	EXPRESSION TAG	UNP P63786
V	203	HIS	-	EXPRESSION TAG	UNP P63786
A	196	LEU	-	EXPRESSION TAG	UNP P63786
A	197	GLU	-	EXPRESSION TAG	UNP P63786
A	198	HIS	-	EXPRESSION TAG	UNP P63786
A	199	HIS	-	EXPRESSION TAG	UNP P63786
A	200	HIS	-	EXPRESSION TAG	UNP P63786
A	201	HIS	-	EXPRESSION TAG	UNP P63786
A	202	HIS	-	EXPRESSION TAG	UNP P63786
A	203	HIS	-	EXPRESSION TAG	UNP P63786
B	196	LEU	-	EXPRESSION TAG	UNP P63786
B	197	GLU	-	EXPRESSION TAG	UNP P63786
B	198	HIS	-	EXPRESSION TAG	UNP P63786
B	199	HIS	-	EXPRESSION TAG	UNP P63786
B	200	HIS	-	EXPRESSION TAG	UNP P63786
B	201	HIS	-	EXPRESSION TAG	UNP P63786
B	202	HIS	-	EXPRESSION TAG	UNP P63786
B	203	HIS	-	EXPRESSION TAG	UNP P63786
C	196	LEU	-	EXPRESSION TAG	UNP P63786
C	197	GLU	-	EXPRESSION TAG	UNP P63786
C	198	HIS	-	EXPRESSION TAG	UNP P63786
C	199	HIS	-	EXPRESSION TAG	UNP P63786
C	200	HIS	-	EXPRESSION TAG	UNP P63786
C	201	HIS	-	EXPRESSION TAG	UNP P63786
C	202	HIS	-	EXPRESSION TAG	UNP P63786
C	203	HIS	-	EXPRESSION TAG	UNP P63786
D	196	LEU	-	EXPRESSION TAG	UNP P63786
D	197	GLU	-	EXPRESSION TAG	UNP P63786
D	198	HIS	-	EXPRESSION TAG	UNP P63786
D	199	HIS	-	EXPRESSION TAG	UNP P63786
D	200	HIS	-	EXPRESSION TAG	UNP P63786
D	201	HIS	-	EXPRESSION TAG	UNP P63786
D	202	HIS	-	EXPRESSION TAG	UNP P63786
D	203	HIS	-	EXPRESSION TAG	UNP P63786
E	196	LEU	-	EXPRESSION TAG	UNP P63786
E	197	GLU	-	EXPRESSION TAG	UNP P63786
E	198	HIS	-	EXPRESSION TAG	UNP P63786

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Chain	Residue	Modelled	Actual	Comment	Reference
E	199	HIS	-	EXPRESSION TAG	UNP P63786
E	200	HIS	-	EXPRESSION TAG	UNP P63786
E	201	HIS	-	EXPRESSION TAG	UNP P63786
E	202	HIS	-	EXPRESSION TAG	UNP P63786
E	203	HIS	-	EXPRESSION TAG	UNP P63786
F	196	LEU	-	EXPRESSION TAG	UNP P63786
F	197	GLU	-	EXPRESSION TAG	UNP P63786
F	198	HIS	-	EXPRESSION TAG	UNP P63786
F	199	HIS	-	EXPRESSION TAG	UNP P63786
F	200	HIS	-	EXPRESSION TAG	UNP P63786
F	201	HIS	-	EXPRESSION TAG	UNP P63786
F	202	HIS	-	EXPRESSION TAG	UNP P63786
F	203	HIS	-	EXPRESSION TAG	UNP P63786
G	196	LEU	-	EXPRESSION TAG	UNP P63786
G	197	GLU	-	EXPRESSION TAG	UNP P63786
G	198	HIS	-	EXPRESSION TAG	UNP P63786
G	199	HIS	-	EXPRESSION TAG	UNP P63786
G	200	HIS	-	EXPRESSION TAG	UNP P63786
G	201	HIS	-	EXPRESSION TAG	UNP P63786
G	202	HIS	-	EXPRESSION TAG	UNP P63786
G	203	HIS	-	EXPRESSION TAG	UNP P63786
H	196	LEU	-	EXPRESSION TAG	UNP P63786
H	197	GLU	-	EXPRESSION TAG	UNP P63786
H	198	HIS	-	EXPRESSION TAG	UNP P63786
H	199	HIS	-	EXPRESSION TAG	UNP P63786
H	200	HIS	-	EXPRESSION TAG	UNP P63786
H	201	HIS	-	EXPRESSION TAG	UNP P63786
H	202	HIS	-	EXPRESSION TAG	UNP P63786
H	203	HIS	-	EXPRESSION TAG	UNP P63786
I	196	LEU	-	EXPRESSION TAG	UNP P63786
I	197	GLU	-	EXPRESSION TAG	UNP P63786
I	198	HIS	-	EXPRESSION TAG	UNP P63786
I	199	HIS	-	EXPRESSION TAG	UNP P63786
I	200	HIS	-	EXPRESSION TAG	UNP P63786
I	201	HIS	-	EXPRESSION TAG	UNP P63786
I	202	HIS	-	EXPRESSION TAG	UNP P63786
I	203	HIS	-	EXPRESSION TAG	UNP P63786
J	196	LEU	-	EXPRESSION TAG	UNP P63786
J	197	GLU	-	EXPRESSION TAG	UNP P63786
J	198	HIS	-	EXPRESSION TAG	UNP P63786
J	199	HIS	-	EXPRESSION TAG	UNP P63786
J	200	HIS	-	EXPRESSION TAG	UNP P63786

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Chain	Residue	Modelled	Actual	Comment	Reference
J	201	HIS	-	EXPRESSION TAG	UNP P63786
J	202	HIS	-	EXPRESSION TAG	UNP P63786
J	203	HIS	-	EXPRESSION TAG	UNP P63786
K	196	LEU	-	EXPRESSION TAG	UNP P63786
K	197	GLU	-	EXPRESSION TAG	UNP P63786
K	198	HIS	-	EXPRESSION TAG	UNP P63786
K	199	HIS	-	EXPRESSION TAG	UNP P63786
K	200	HIS	-	EXPRESSION TAG	UNP P63786
K	201	HIS	-	EXPRESSION TAG	UNP P63786
K	202	HIS	-	EXPRESSION TAG	UNP P63786
K	203	HIS	-	EXPRESSION TAG	UNP P63786
L	196	LEU	-	EXPRESSION TAG	UNP P63786
L	197	GLU	-	EXPRESSION TAG	UNP P63786
L	198	HIS	-	EXPRESSION TAG	UNP P63786
L	199	HIS	-	EXPRESSION TAG	UNP P63786
L	200	HIS	-	EXPRESSION TAG	UNP P63786
L	201	HIS	-	EXPRESSION TAG	UNP P63786
L	202	HIS	-	EXPRESSION TAG	UNP P63786
L	203	HIS	-	EXPRESSION TAG	UNP P63786
M	196	LEU	-	EXPRESSION TAG	UNP P63786
M	197	GLU	-	EXPRESSION TAG	UNP P63786
M	198	HIS	-	EXPRESSION TAG	UNP P63786
M	199	HIS	-	EXPRESSION TAG	UNP P63786
M	200	HIS	-	EXPRESSION TAG	UNP P63786
M	201	HIS	-	EXPRESSION TAG	UNP P63786
M	202	HIS	-	EXPRESSION TAG	UNP P63786
M	203	HIS	-	EXPRESSION TAG	UNP P63786

- Molecule 2 is water.

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

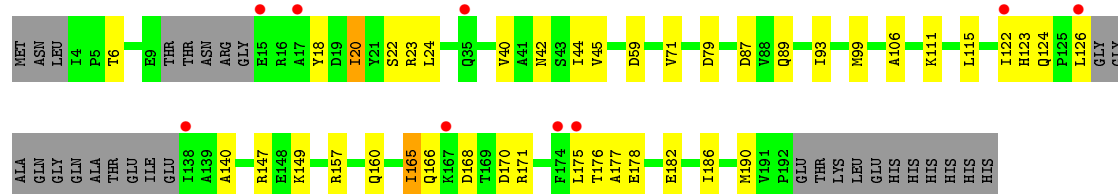
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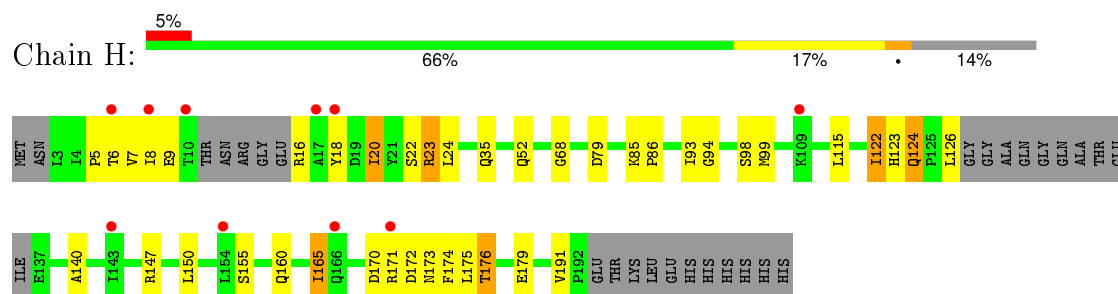
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	2	Total 2	O 2	0	0
2	G	4	Total 4	O 4	0	0
2	H	1	Total 1	O 1	0	0
2	I	3	Total 3	O 3	0	0
2	J	1	Total 1	O 1	0	0
2	K	1	Total 1	O 1	0	0
2	L	3	Total 3	O 3	0	0
2	M	1	Total 1	O 1	0	0

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

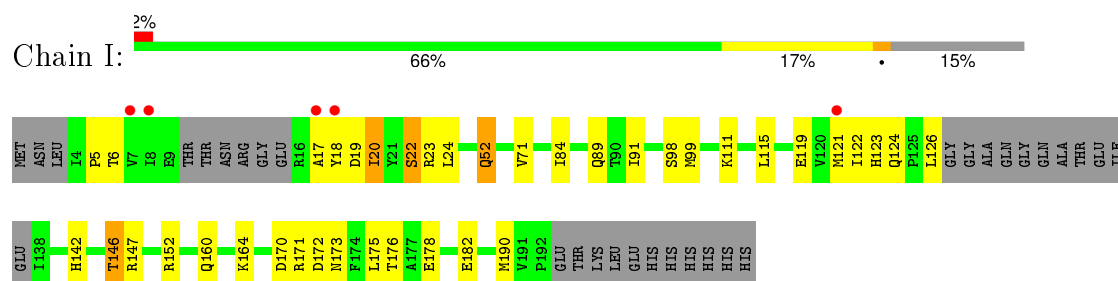




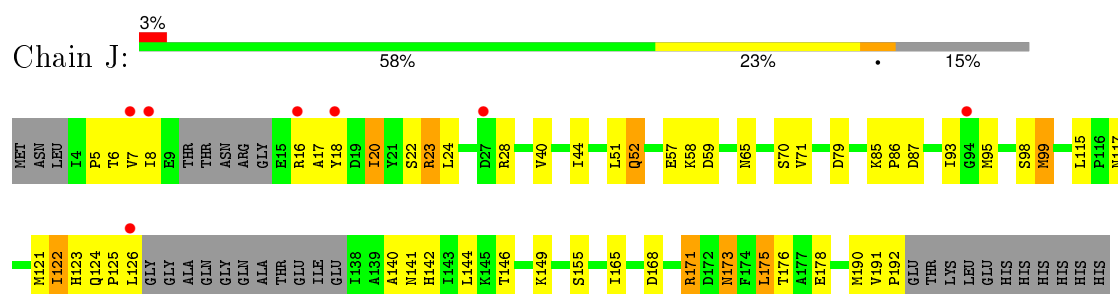
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



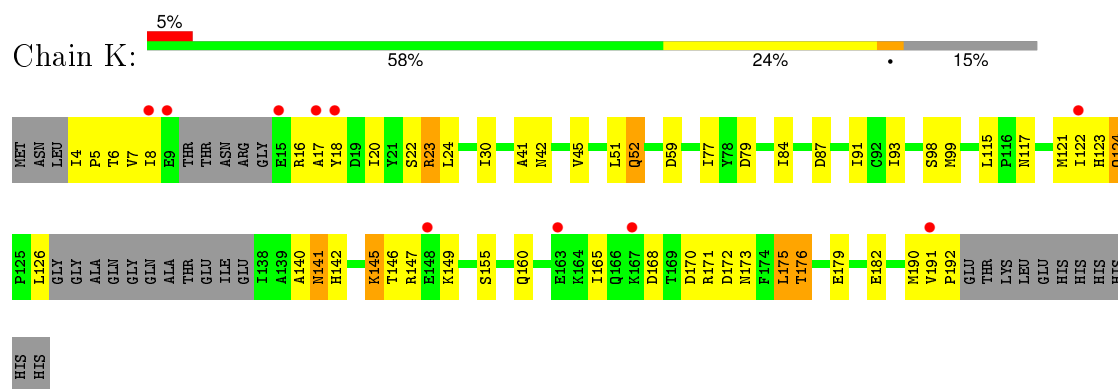
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

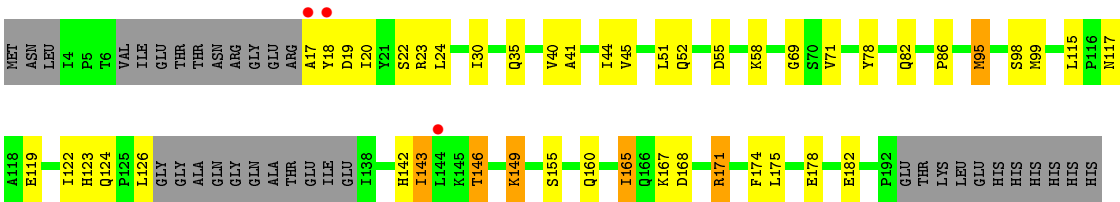


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

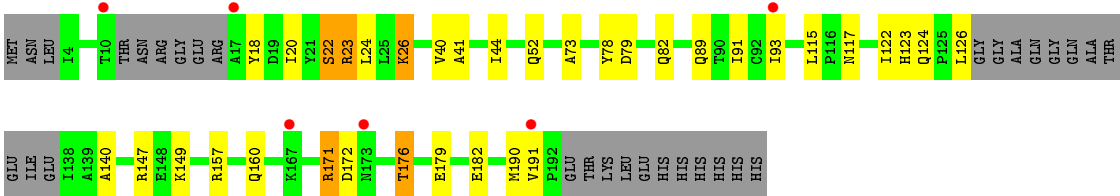


- Molecule 1: ATP-dependent Clp protease proteolytic subunit





● Molecule 1: ATP-dependent Clp protease proteolytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.38Å 170.05Å 96.33Å 90.00° 102.87° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 49.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-2.40) 95.6 (49.06-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.286 0.239 , 0.287	Depositor DCC
R_{free} test set	5664 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.8	EDS
Estimated twinning fraction	0.286 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 112766 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18724	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.53	0/1357	0.67	0/1831
1	B	0.59	0/1348	0.68	0/1818
1	C	0.50	0/1356	0.63	0/1829
1	D	0.55	0/1339	0.68	0/1807
1	E	0.52	0/1363	0.65	0/1839
1	F	0.52	0/1347	0.63	0/1817
1	G	0.50	0/1357	0.64	0/1831
1	H	0.49	0/1373	0.61	0/1853
1	I	0.52	0/1348	0.65	0/1819
1	J	0.57	0/1373	0.68	1/1852 (0.1%)
1	K	0.48	0/1365	0.63	0/1841
1	L	0.51	0/1319	0.65	0/1779
1	M	0.50	0/1358	0.61	0/1832
1	V	0.60	0/1348	0.71	0/1819
All	All	0.53	0/18951	0.65	1/25567 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	175	LEU	CA-CB-CG	5.74	128.49	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	172	ASP	Peptide

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	1340	0	1351	57	0
1	B	1328	0	1343	53	0
1	C	1336	0	1354	32	0
1	D	1322	0	1339	30	0
1	E	1343	0	1361	44	0
1	F	1330	0	1345	34	0
1	G	1340	0	1351	31	0
1	H	1353	0	1365	28	0
1	I	1331	0	1345	28	0
1	J	1353	0	1365	45	0
1	K	1345	0	1360	42	0
1	L	1302	0	1317	35	0
1	M	1338	0	1359	22	0
1	V	1331	0	1345	49	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	4	0	0	1	0
2	F	2	0	0	0	0
2	G	4	0	0	1	0
2	H	1	0	0	0	0
2	I	3	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	3	0	0	0	0
2	M	1	0	0	0	0
2	V	4	0	0	0	0
All	All	18724	0	18900	422	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 11.

The worst 5 of 422 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:A:42:ASN:HD22	1:B:31[A]:MET:CE	1.60	1.13
1:B:149:LYS:HE3	1:K:117:ASN:HD22	1.23	1.02
1:D:149:LYS:HE3	1:F:117:ASN:HD22	1.21	1.00
1:J:117:ASN:HD22	1:L:149:LYS:HE2	1.21	0.98
1:M:176:THR:HG22	1:M:179:GLU:H	1.26	0.98

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	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
1	B	166/203 (82%)	162 (98%)	4 (2%)	0	100	100
1	C	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
1	D	165/203 (81%)	159 (96%)	6 (4%)	0	100	100
1	E	168/203 (83%)	165 (98%)	3 (2%)	0	100	100
1	F	167/203 (82%)	163 (98%)	4 (2%)	0	100	100
1	G	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
1	H	170/203 (84%)	166 (98%)	3 (2%)	1 (1%)	30	43
1	I	166/203 (82%)	162 (98%)	4 (2%)	0	100	100
1	J	169/203 (83%)	166 (98%)	3 (2%)	0	100	100
1	K	168/203 (83%)	164 (98%)	4 (2%)	0	100	100
1	L	162/203 (80%)	159 (98%)	3 (2%)	0	100	100
1	M	167/203 (82%)	161 (96%)	6 (4%)	0	100	100
1	V	166/203 (82%)	162 (98%)	4 (2%)	0	100	100
All	All	2335/2842 (82%)	2281 (98%)	53 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	94	GLY

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	145/171 (85%)	135 (93%)	10 (7%)	19	30
1	B	144/171 (84%)	134 (93%)	10 (7%)	19	30
1	C	145/171 (85%)	136 (94%)	9 (6%)	23	35
1	D	143/171 (84%)	131 (92%)	12 (8%)	14	20
1	E	146/171 (85%)	131 (90%)	15 (10%)	9	13
1	F	143/171 (84%)	136 (95%)	7 (5%)	31	48
1	G	145/171 (85%)	138 (95%)	7 (5%)	31	49
1	H	146/171 (85%)	131 (90%)	15 (10%)	9	13
1	I	144/171 (84%)	133 (92%)	11 (8%)	16	25
1	J	147/171 (86%)	133 (90%)	14 (10%)	11	15
1	K	146/171 (85%)	136 (93%)	10 (7%)	20	31
1	L	141/171 (82%)	129 (92%)	12 (8%)	13	20
1	M	146/171 (85%)	132 (90%)	14 (10%)	10	15
1	V	144/171 (84%)	130 (90%)	14 (10%)	10	15
All	All	2025/2394 (85%)	1865 (92%)	160 (8%)	15	23

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	24	LEU
1	H	122	ILE
1	M	22	SER
1	F	146	THR
1	G	166	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	151	ASN
1	G	82	GLN
1	L	160	GLN
1	E	173	ASN
1	F	123	HIS

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, 95th 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	173/203 (85%)	0.52	3 (1%) 73 72	36, 49, 66, 85	0
1	B	171/203 (84%)	0.58	6 (3%) 48 48	35, 46, 61, 79	0
1	C	172/203 (84%)	0.72	14 (8%) 15 14	40, 53, 69, 90	0
1	D	171/203 (84%)	0.54	5 (2%) 55 54	37, 49, 63, 71	0
1	E	173/203 (85%)	0.69	6 (3%) 48 48	37, 49, 68, 92	0
1	F	173/203 (85%)	0.67	12 (6%) 20 19	37, 51, 70, 79	0
1	G	173/203 (85%)	0.58	9 (5%) 31 31	39, 51, 68, 80	0
1	H	175/203 (86%)	0.60	10 (5%) 27 27	40, 52, 69, 87	0
1	I	172/203 (84%)	0.52	5 (2%) 55 54	37, 49, 67, 92	0
1	J	173/203 (85%)	0.49	7 (4%) 42 43	35, 48, 72, 83	0
1	K	173/203 (85%)	0.60	10 (5%) 26 27	39, 53, 72, 88	0
1	L	168/203 (82%)	0.50	3 (1%) 71 71	38, 50, 62, 73	0
1	M	172/203 (84%)	0.58	6 (3%) 48 48	38, 53, 66, 82	0
1	V	172/203 (84%)	0.48	2 (1%) 81 81	30, 46, 59, 76	0
All	All	2411/2842 (84%)	0.58	98 (4%) 41 42	30, 50, 68, 92	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	ALA	7.5
1	L	17	ALA	6.8
1	K	122	ILE	6.0
1	B	17	ALA	5.6
1	I	17	ALA	5.2

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.