



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:07 PM GMT

PDB ID : 3STA
Title : Crystal structure of ClpP in tetradecameric form from Staphylococcus aureus
Authors : Zhang, J.; Ye, F.; Lan, L.; Jiang, H.; Luo, C.; Yang, C.-G.
Deposited on : 2011-07-09
Resolution : 2.28 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

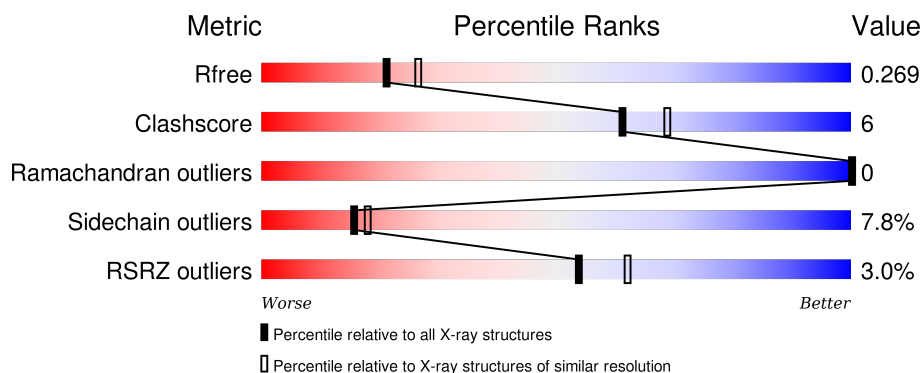
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	197	<div> <div>3%</div> <div>80%13% . .</div> </div>
1	B	197	<div> <div>%</div> <div>80%11% . 8%</div> </div>
1	C	197	<div> <div>2%</div> <div>79%13% . 6%</div> </div>
1	E	197	<div> <div>2%</div> <div>82%11% . 6%</div> </div>
1	F	197	<div> <div>4%</div> <div>81%11% . 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	197	
1	I	197	
1	K	197	
1	L	197	
1	M	197	
1	N	197	
1	S	197	
1	T	197	
1	V	197	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 20755 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	189	Total	C	N	O	S	0	2	0
			1469	922	252	287	8			
1	A	189	Total	C	N	O	S	0	2	0
			1466	921	251	286	8			
1	B	182	Total	C	N	O	S	0	1	0
			1404	886	237	274	7			
1	C	185	Total	C	N	O	S	0	2	0
			1434	904	243	279	8			
1	E	185	Total	C	N	O	S	0	2	0
			1436	905	243	280	8			
1	F	185	Total	C	N	O	S	0	1	0
			1431	901	243	280	7			
1	G	180	Total	C	N	O	S	0	1	0
			1390	878	235	270	7			
1	I	189	Total	C	N	O	S	0	0	0
			1456	913	251	286	6			
1	K	186	Total	C	N	O	S	0	1	0
			1435	903	244	281	7			
1	L	184	Total	C	N	O	S	0	1	0
			1422	896	242	277	7			
1	M	185	Total	C	N	O	S	0	1	0
			1431	901	243	280	7			
1	N	185	Total	C	N	O	S	0	1	0
			1431	901	243	280	7			
1	S	184	Total	C	N	O	S	0	2	0
			1429	901	242	278	8			
1	T	186	Total	C	N	O	S	0	1	0
			1435	903	244	281	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-1	GLY	-	EXPRESSION TAG	UNP P63786

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Chain	Residue	Modelled	Actual	Comment	Reference
V	0	SER	-	EXPRESSION TAG	UNP P63786
A	-1	GLY	-	EXPRESSION TAG	UNP P63786
A	0	SER	-	EXPRESSION TAG	UNP P63786
B	-1	GLY	-	EXPRESSION TAG	UNP P63786
B	0	SER	-	EXPRESSION TAG	UNP P63786
C	-1	GLY	-	EXPRESSION TAG	UNP P63786
C	0	SER	-	EXPRESSION TAG	UNP P63786
E	-1	GLY	-	EXPRESSION TAG	UNP P63786
E	0	SER	-	EXPRESSION TAG	UNP P63786
F	-1	GLY	-	EXPRESSION TAG	UNP P63786
F	0	SER	-	EXPRESSION TAG	UNP P63786
G	-1	GLY	-	EXPRESSION TAG	UNP P63786
G	0	SER	-	EXPRESSION TAG	UNP P63786
I	-1	GLY	-	EXPRESSION TAG	UNP P63786
I	0	SER	-	EXPRESSION TAG	UNP P63786
K	-1	GLY	-	EXPRESSION TAG	UNP P63786
K	0	SER	-	EXPRESSION TAG	UNP P63786
L	-1	GLY	-	EXPRESSION TAG	UNP P63786
L	0	SER	-	EXPRESSION TAG	UNP P63786
M	-1	GLY	-	EXPRESSION TAG	UNP P63786
M	0	SER	-	EXPRESSION TAG	UNP P63786
N	-1	GLY	-	EXPRESSION TAG	UNP P63786
N	0	SER	-	EXPRESSION TAG	UNP P63786
S	-1	GLY	-	EXPRESSION TAG	UNP P63786
S	0	SER	-	EXPRESSION TAG	UNP P63786
T	-1	GLY	-	EXPRESSION TAG	UNP P63786
T	0	SER	-	EXPRESSION TAG	UNP P63786

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	V	58	Total O 58 58	0	0
2	A	53	Total O 53 53	0	0
2	B	59	Total O 59 59	0	0
2	C	57	Total O 57 57	0	0
2	E	42	Total O 42 42	0	0
2	F	48	Total O 48 48	0	0

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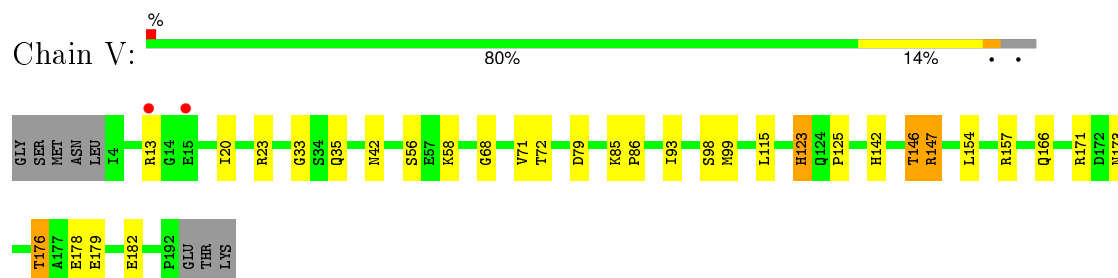
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	52	Total 52	O 52	0	0
2	I	53	Total 53	O 53	0	0
2	K	43	Total 43	O 43	0	0
2	L	27	Total 27	O 27	0	0
2	M	28	Total 28	O 28	0	0
2	N	46	Total 46	O 46	0	0
2	S	64	Total 64	O 64	0	0
2	T	56	Total 56	O 56	0	0

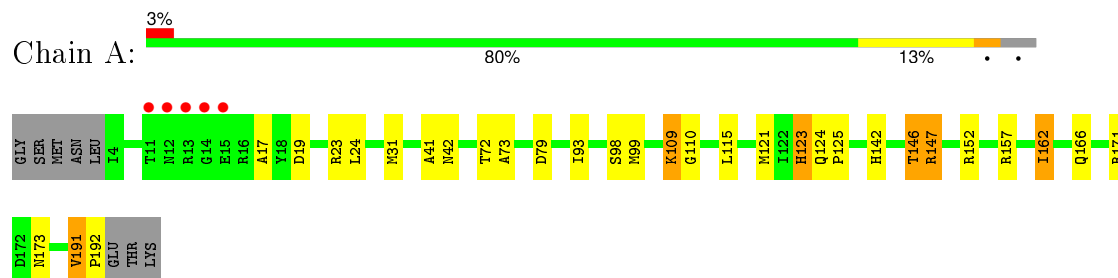
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

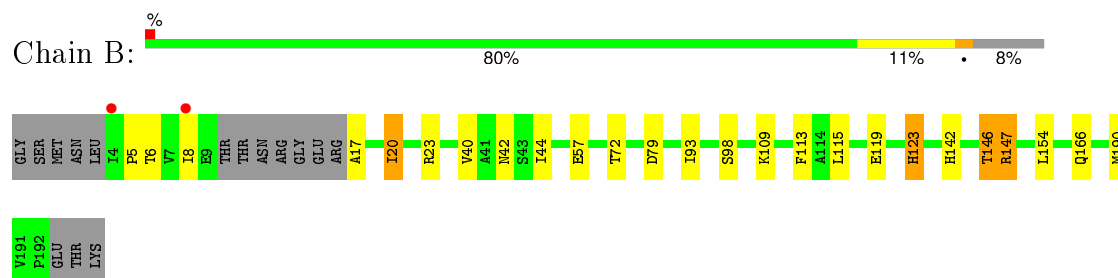
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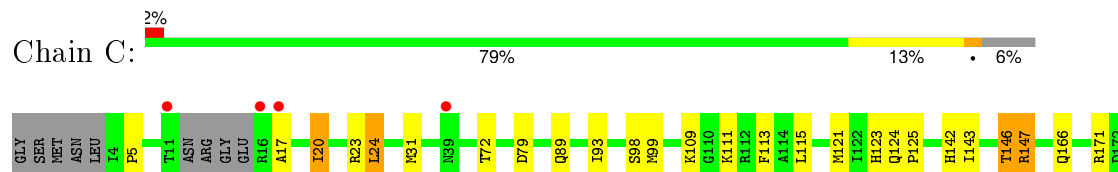
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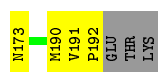


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

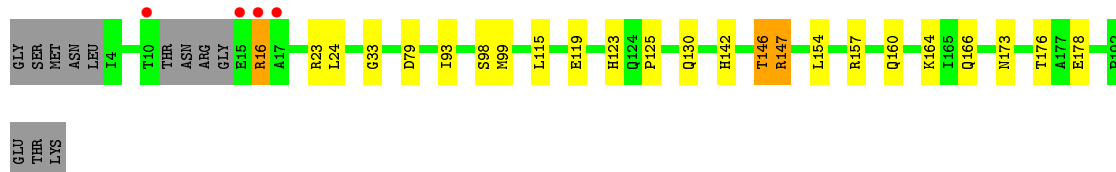
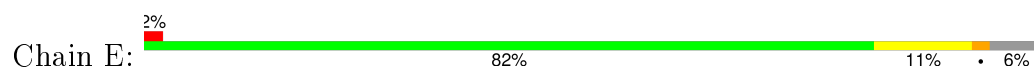


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

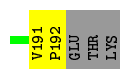
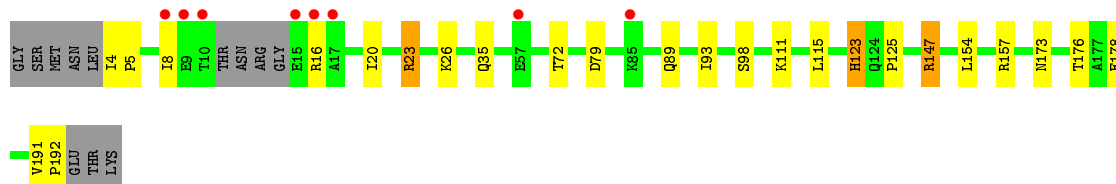
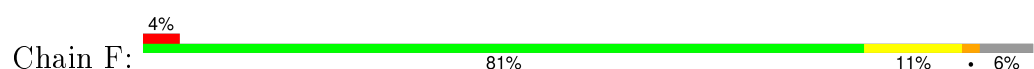




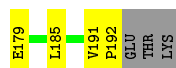
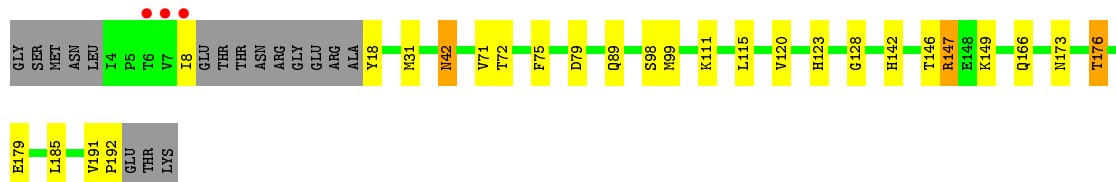
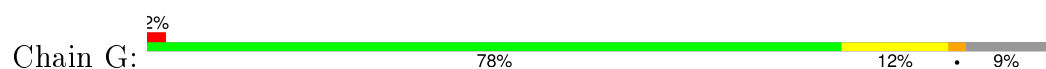
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



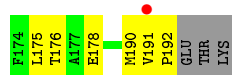
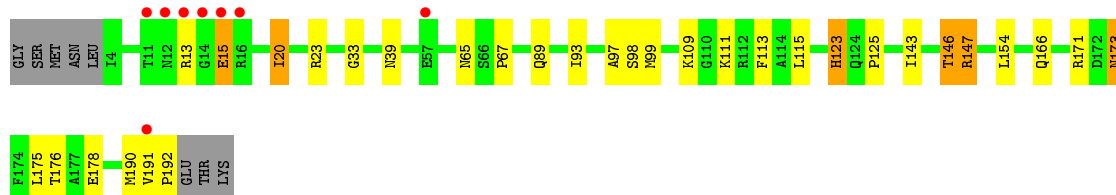
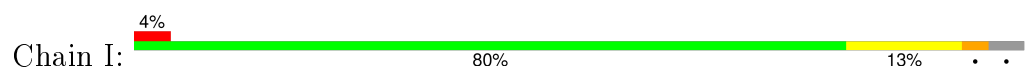
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



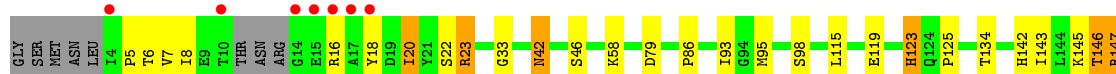
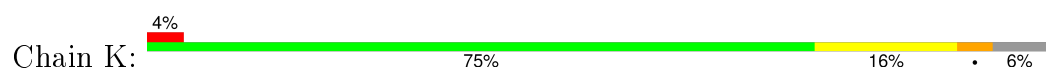
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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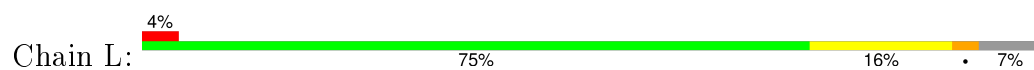


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

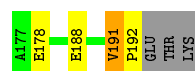
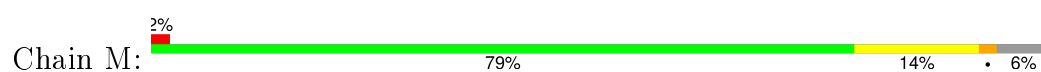




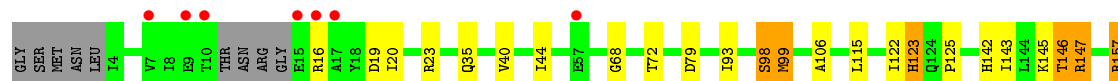
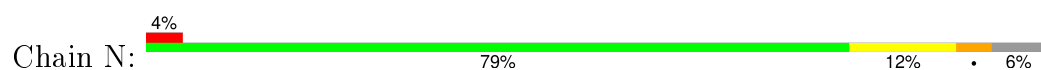
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



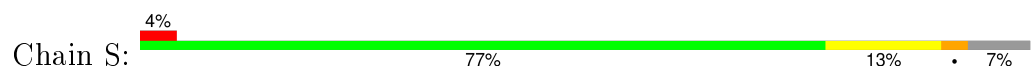
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



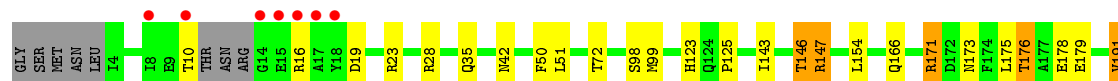
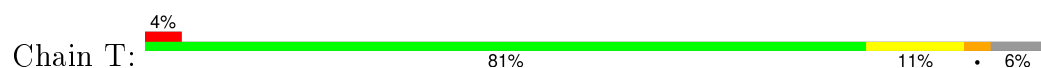
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



PL92
GLU
THR
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.57Å 96.29Å 192.61Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.28 41.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-2.28) 95.1 (41.94-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.269 0.224 , 0.269	Depositor DCC
R_{free} test set	6879 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.3	EDS
Estimated twinning fraction	0.013 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.013 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.018 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.020 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.017 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 148037 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20755	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/1491	0.53	0/2012
1	B	0.36	0/1425	0.54	0/1923
1	C	0.35	0/1458	0.52	0/1967
1	E	0.34	0/1460	0.50	0/1969
1	F	0.34	0/1452	0.50	0/1959
1	G	0.35	0/1411	0.50	0/1904
1	I	0.35	0/1475	0.51	0/1992
1	K	0.35	0/1456	0.50	0/1964
1	L	0.34	0/1443	0.51	0/1947
1	M	0.33	0/1452	0.50	0/1959
1	N	0.34	0/1452	0.50	0/1959
1	S	0.36	0/1453	0.53	0/1959
1	T	0.34	0/1456	0.51	0/1964
1	V	0.35	0/1491	0.53	0/2012
All	All	0.35	0/20375	0.51	0/27490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1466	0	1483	21	0
1	B	1404	0	1418	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1434	0	1454	15	0
1	E	1436	0	1453	12	0
1	F	1431	0	1444	16	0
1	G	1390	0	1407	20	0
1	I	1456	0	1465	20	0
1	K	1435	0	1447	27	0
1	L	1422	0	1438	27	0
1	M	1431	0	1444	16	0
1	N	1431	0	1444	16	0
1	S	1429	0	1446	22	0
1	T	1435	0	1447	15	0
1	V	1469	0	1482	20	0
2	A	53	0	0	3	0
2	B	59	0	0	1	0
2	C	57	0	0	0	0
2	E	42	0	0	1	0
2	F	48	0	0	1	0
2	G	52	0	0	3	0
2	I	53	0	0	0	0
2	K	43	0	0	0	0
2	L	27	0	0	0	0
2	M	28	0	0	0	0
2	N	46	0	0	0	0
2	S	64	0	0	1	0
2	T	56	0	0	0	0
2	V	58	0	0	1	0
All	All	20755	0	20272	223	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 6.

The worst 5 of 223 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:S:23:ARG:HG2	1:S:23:ARG:HH11	1.22	1.00
1:A:152:ARG:HA	1:A:162:ILE:HD11	1.46	0.97
1:N:98:SER:HB3	1:N:123:HIS:CE1	2.02	0.95
1:S:191:VAL:HG22	1:S:192:PRO:HA	1.53	0.91
1:T:191:VAL:HG22	1:T:192:PRO:HA	1.57	0.85

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	189/197 (96%)	184 (97%)	5 (3%)	0	100	100
1	B	179/197 (91%)	175 (98%)	4 (2%)	0	100	100
1	C	183/197 (93%)	180 (98%)	3 (2%)	0	100	100
1	E	183/197 (93%)	180 (98%)	3 (2%)	0	100	100
1	F	182/197 (92%)	179 (98%)	3 (2%)	0	100	100
1	G	177/197 (90%)	174 (98%)	3 (2%)	0	100	100
1	I	187/197 (95%)	184 (98%)	3 (2%)	0	100	100
1	K	183/197 (93%)	180 (98%)	3 (2%)	0	100	100
1	L	181/197 (92%)	179 (99%)	2 (1%)	0	100	100
1	M	182/197 (92%)	176 (97%)	6 (3%)	0	100	100
1	N	182/197 (92%)	179 (98%)	3 (2%)	0	100	100
1	S	182/197 (92%)	179 (98%)	3 (2%)	0	100	100
1	T	183/197 (93%)	181 (99%)	2 (1%)	0	100	100
1	V	189/197 (96%)	187 (99%)	2 (1%)	0	100	100
All	All	2562/2758 (93%)	2517 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	158/164 (96%)	144 (91%)	14 (9%)	12	13
1	B	151/164 (92%)	141 (93%)	10 (7%)	21	25
1	C	155/164 (94%)	142 (92%)	13 (8%)	14	15
1	E	155/164 (94%)	144 (93%)	11 (7%)	18	21
1	F	154/164 (94%)	145 (94%)	9 (6%)	25	31
1	G	150/164 (92%)	142 (95%)	8 (5%)	28	35
1	I	156/164 (95%)	143 (92%)	13 (8%)	14	15
1	K	154/164 (94%)	143 (93%)	11 (7%)	18	21
1	L	153/164 (93%)	137 (90%)	16 (10%)	8	8
1	M	154/164 (94%)	144 (94%)	10 (6%)	21	26
1	N	154/164 (94%)	139 (90%)	15 (10%)	10	11
1	S	154/164 (94%)	142 (92%)	12 (8%)	16	18
1	T	154/164 (94%)	140 (91%)	14 (9%)	12	12
1	V	158/164 (96%)	145 (92%)	13 (8%)	14	16
All	All	2160/2296 (94%)	1991 (92%)	169 (8%)	16	18

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	173	ASN
1	K	123	HIS
1	T	23	ARG
1	I	15	GLU
1	I	147	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	39	ASN
1	I	151	ASN
1	T	35	GLN
1	G	82	GLN
1	G	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	189/197 (95%)	0.01	5 (2%) 59 67	20, 25, 46, 55	0
1	B	182/197 (92%)	-0.12	2 (1%) 82 86	19, 25, 36, 60	0
1	C	185/197 (93%)	0.07	4 (2%) 65 72	18, 26, 43, 56	0
1	E	185/197 (93%)	0.02	4 (2%) 65 72	23, 30, 44, 57	0
1	F	185/197 (93%)	0.15	8 (4%) 39 47	24, 31, 45, 64	0
1	G	180/197 (91%)	-0.04	3 (1%) 73 79	22, 29, 37, 61	0
1	I	189/197 (95%)	0.13	8 (4%) 40 47	20, 27, 51, 59	0
1	K	186/197 (94%)	0.07	7 (3%) 44 52	23, 30, 52, 62	0
1	L	184/197 (93%)	0.33	8 (4%) 39 47	28, 34, 51, 75	0
1	M	185/197 (93%)	0.16	4 (2%) 65 72	27, 33, 47, 56	0
1	N	185/197 (93%)	0.05	7 (3%) 44 52	24, 29, 44, 59	0
1	S	184/197 (93%)	0.01	8 (4%) 39 47	20, 25, 42, 63	0
1	T	186/197 (94%)	-0.02	7 (3%) 44 52	20, 25, 48, 62	0
1	V	189/197 (95%)	-0.09	2 (1%) 82 86	19, 25, 43, 52	0
All	All	2594/2758 (94%)	0.05	77 (2%) 54 62	18, 28, 48, 75	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	17	ALA	7.6
1	L	10	THR	7.0
1	L	9	GLU	6.8
1	L	8	ILE	6.8
1	L	16	ARG	6.4

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.