



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2021 – 02:02 PM EDT

PDB ID : 3HLN  
Title : Crystal structure of ClpP A153C mutant with inter-heptamer disulfide bonds  
Authors : Kimber, M.S.; Yu, A.Y.H.; Borg, M.; Chan, H.S.; Houry, W.A.  
Deposited on : 2009-05-27  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

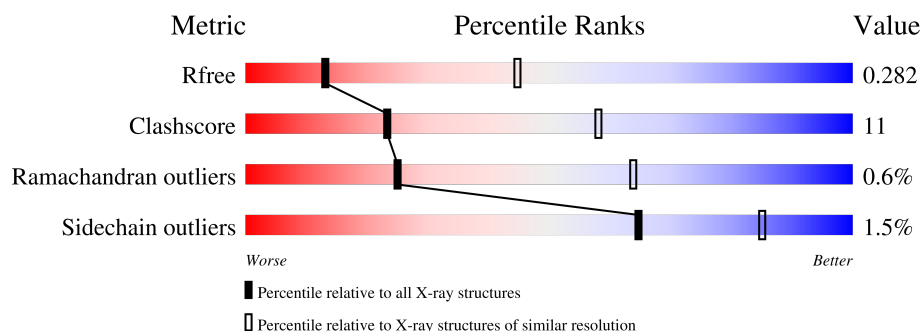
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

















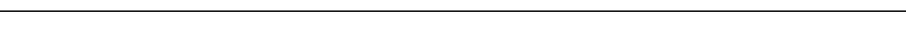
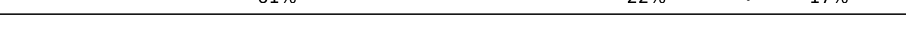





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	1	193	67% 17% • 16%
1	2	193	65% 18% • 16%
1	A	193	62% 20% • 16%
1	B	193	64% 19% • 16%
1	C	193	64% 19% • 16%
1	D	193	63% 20% •• 15%
1	E	193	68% 15% • 16%

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Mol	Chain	Length	Quality of chain
1	F	193	
1	G	193	
1	H	193	
1	I	193	
1	J	193	
1	K	193	
1	L	193	
1	M	193	
1	N	193	
1	O	193	
1	P	193	
1	Q	193	
1	R	193	
1	S	193	
1	T	193	
1	U	193	
1	V	193	
1	W	193	
1	X	193	
1	Y	193	
1	Z	193	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 35844 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	A	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	B	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	C	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	D	165	Total	C	N	O	S	0	0	0
			1294	816	225	241	12			
1	E	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	F	166	Total	C	N	O	S	0	0	0
			1308	824	226	246	12			
1	G	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	H	164	Total	C	N	O	S	0	0	0
			1292	814	224	242	12			
1	I	163	Total	C	N	O	S	0	0	0
			1282	808	223	239	12			
1	J	163	Total	C	N	O	S	0	0	0
			1282	808	223	239	12			
1	K	161	Total	C	N	O	S	0	0	0
			1265	797	219	237	12			
1	L	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	M	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	N	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	O	166	Total	C	N	O	S	0	0	0
			1307	825	226	244	12			
1	P	163	Total	C	N	O	S	0	0	0
			1282	808	223	239	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	R	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	S	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	T	161	Total	C	N	O	S	0	0	0
			1265	797	219	237	12			
1	U	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	V	163	Total	C	N	O	S	0	0	0
			1283	809	223	239	12			
1	W	161	Total	C	N	O	S	0	0	0
			1265	797	219	237	12			
1	X	161	Total	C	N	O	S	0	0	0
			1266	798	220	236	12			
1	Y	163	Total	C	N	O	S	0	0	0
			1283	809	223	239	12			
1	Z	165	Total	C	N	O	S	0	0	0
			1299	819	225	243	12			
1	1	163	Total	C	N	O	S	0	0	0
			1283	809	223	239	12			
1	2	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	CYS	ALA	engineered mutation	UNP P0A6G7
B	139	CYS	ALA	engineered mutation	UNP P0A6G7
C	139	CYS	ALA	engineered mutation	UNP P0A6G7
D	139	CYS	ALA	engineered mutation	UNP P0A6G7
E	139	CYS	ALA	engineered mutation	UNP P0A6G7
F	139	CYS	ALA	engineered mutation	UNP P0A6G7
G	139	CYS	ALA	engineered mutation	UNP P0A6G7
H	139	CYS	ALA	engineered mutation	UNP P0A6G7
I	139	CYS	ALA	engineered mutation	UNP P0A6G7
J	139	CYS	ALA	engineered mutation	UNP P0A6G7
K	139	CYS	ALA	engineered mutation	UNP P0A6G7
L	139	CYS	ALA	engineered mutation	UNP P0A6G7
M	139	CYS	ALA	engineered mutation	UNP P0A6G7
N	139	CYS	ALA	engineered mutation	UNP P0A6G7
O	139	CYS	ALA	engineered mutation	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
P	139	CYS	ALA	engineered mutation	UNP P0A6G7
Q	139	CYS	ALA	engineered mutation	UNP P0A6G7
R	139	CYS	ALA	engineered mutation	UNP P0A6G7
S	139	CYS	ALA	engineered mutation	UNP P0A6G7
T	139	CYS	ALA	engineered mutation	UNP P0A6G7
U	139	CYS	ALA	engineered mutation	UNP P0A6G7
V	139	CYS	ALA	engineered mutation	UNP P0A6G7
W	139	CYS	ALA	engineered mutation	UNP P0A6G7
X	139	CYS	ALA	engineered mutation	UNP P0A6G7
Y	139	CYS	ALA	engineered mutation	UNP P0A6G7
Z	139	CYS	ALA	engineered mutation	UNP P0A6G7
1	139	CYS	ALA	engineered mutation	UNP P0A6G7
2	139	CYS	ALA	engineered mutation	UNP P0A6G7

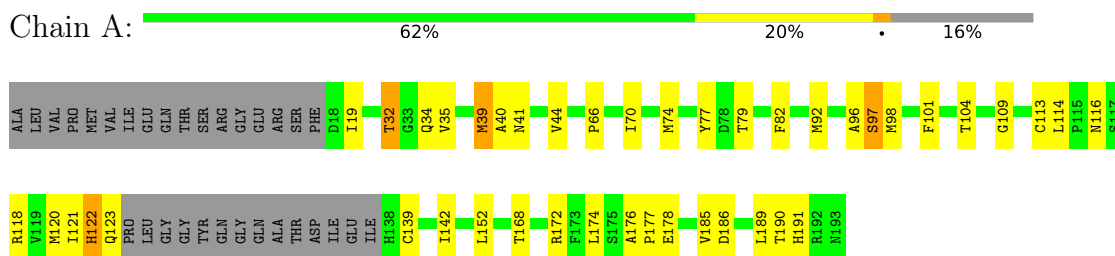
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	2	Total Ca 2 2	0	0
2	I	2	Total Ca 2 2	0	0
2	J	3	Total Ca 3 3	0	0
2	M	1	Total Ca 1 1	0	0
2	T	1	Total Ca 1 1	0	0
2	V	1	Total Ca 1 1	0	0
2	Z	1	Total Ca 1 1	0	0
2	1	1	Total Ca 1 1	0	0
2	2	1	Total Ca 1 1	0	0

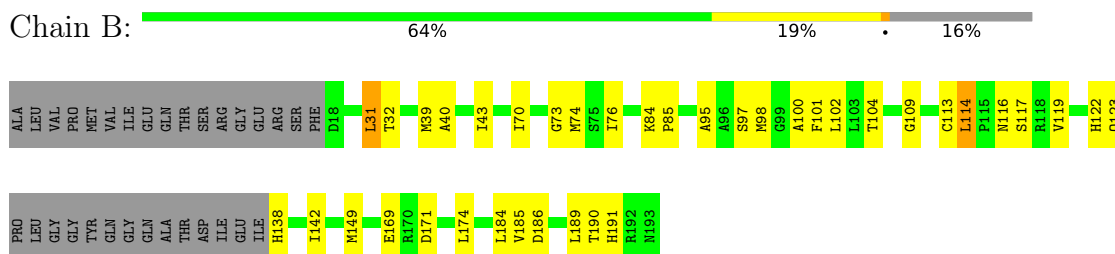
### 3 Residue-property plots [i](#)

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. 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. 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.

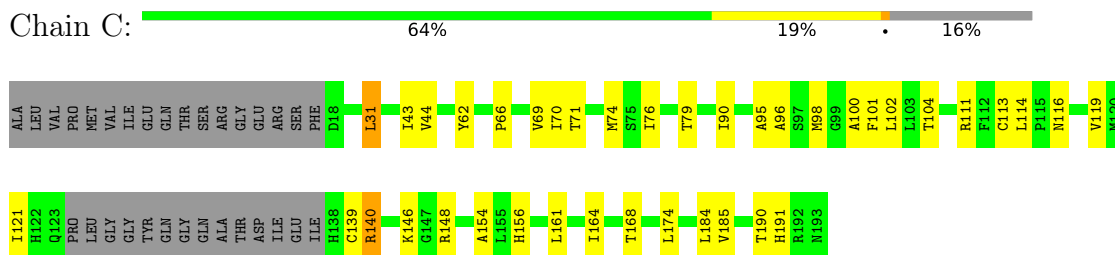
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



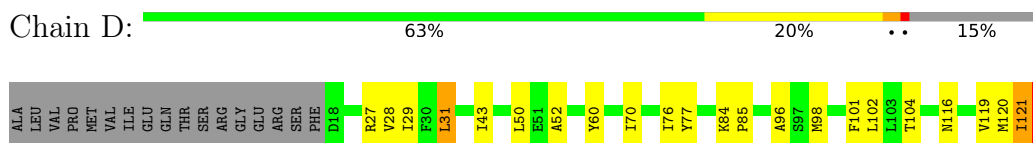
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

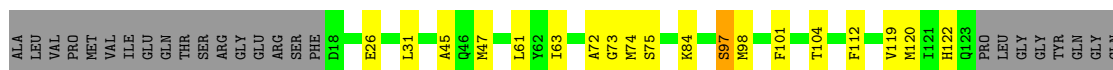


- Molecule 1: ATP-dependent Clp protease proteolytic subunit





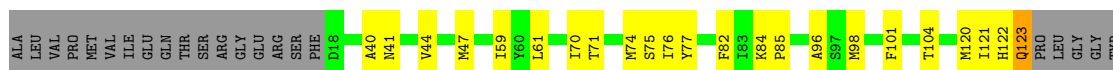
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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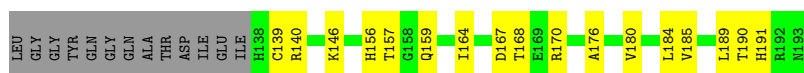
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit







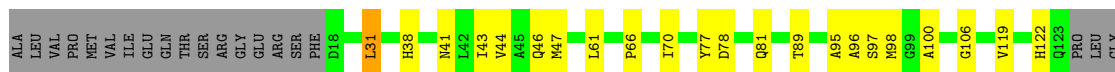
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J: 69% 15% 16%



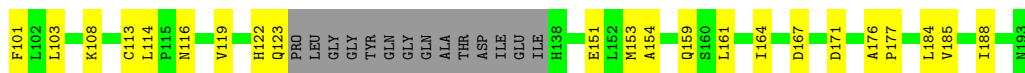
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K: 65% 18% 17%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L: 59% 25% 16%



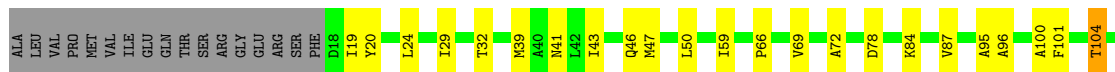
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M: 64% 19% 16%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

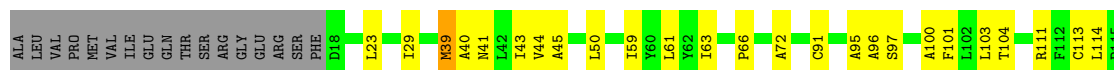
Chain N: 61% 22% 16%





- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain O: 64% 21% 14%



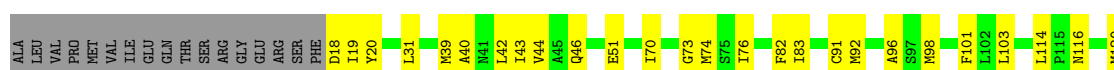
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain P: 62% 22% 16%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q: 64% 19% 16%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain R: 65% 19% 16%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain S: 61% 23% 16%





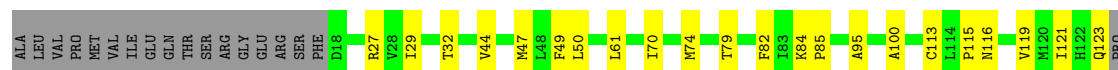
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



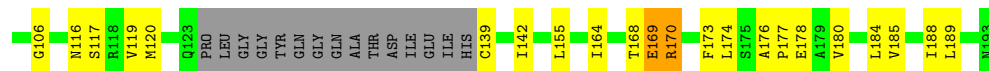
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



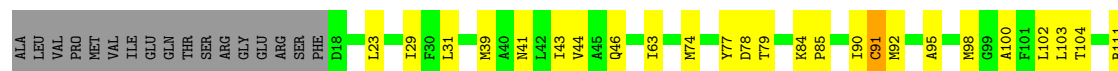
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.30Å 182.30Å 476.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.22 – 3.20 42.21 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (42.22-3.20) 97.5 (42.21-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.213 , 0.253 0.270 , 0.282	Depositor DCC
$R_{free}$ test set	7454 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	105.3	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	35844	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1	0.37	0/1302	0.52	0/1750
1	2	0.39	0/1294	0.57	0/1739
1	A	0.38	0/1294	0.53	0/1739
1	B	0.40	0/1294	0.57	0/1739
1	C	0.36	0/1294	0.55	0/1739
1	D	0.40	0/1314	0.58	0/1767
1	E	0.36	0/1294	0.58	0/1739
1	F	0.37	0/1327	0.54	0/1784
1	G	0.35	0/1294	0.54	0/1739
1	H	0.34	0/1311	0.50	0/1762
1	I	0.37	0/1302	0.53	0/1751
1	J	0.38	0/1302	0.55	0/1751
1	K	0.35	0/1283	0.55	0/1724
1	L	0.35	0/1294	0.53	0/1739
1	M	0.34	0/1294	0.50	0/1739
1	N	0.35	0/1294	0.51	0/1739
1	O	0.41	0/1327	0.57	0/1785
1	P	0.36	0/1302	0.54	0/1751
1	Q	0.36	0/1294	0.53	0/1739
1	R	0.35	0/1294	0.49	0/1739
1	S	0.37	0/1294	0.51	0/1739
1	T	0.36	0/1283	0.50	0/1724
1	U	0.38	0/1294	0.52	0/1739
1	V	0.37	0/1302	0.53	0/1750
1	W	0.38	0/1283	0.53	0/1724
1	X	0.35	0/1285	0.53	0/1727
1	Y	0.38	0/1302	0.55	0/1750
1	Z	0.40	0/1319	0.55	0/1774
All	All	0.37	0/36366	0.54	0/48881

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	J	0	1
1	W	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	170	ARG	Peptide
1	W	170	ARG	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	1	1283	0	1296	24	0
1	2	1275	0	1284	29	0
1	A	1275	0	1284	36	0
1	B	1275	0	1284	28	0
1	C	1275	0	1284	32	0
1	D	1294	0	1305	33	0
1	E	1275	0	1284	25	0
1	F	1308	0	1316	33	0
1	G	1275	0	1284	29	0
1	H	1292	0	1301	45	0
1	I	1282	0	1291	37	0
1	J	1282	0	1291	21	0
1	K	1265	0	1277	30	0
1	L	1275	0	1284	37	0
1	M	1275	0	1284	35	0
1	N	1275	0	1284	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1307	0	1320	43	0
1	P	1282	0	1291	44	0
1	Q	1275	0	1284	34	0
1	R	1275	0	1285	25	0
1	S	1275	0	1284	35	0
1	T	1265	0	1277	32	0
1	U	1275	0	1285	30	0
1	V	1283	0	1295	29	0
1	W	1265	0	1278	38	0
1	X	1266	0	1276	40	0
1	Y	1283	0	1295	30	0
1	Z	1299	0	1309	38	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
2	E	2	0	0	0	0
2	I	2	0	0	0	0
2	J	3	0	0	0	0
2	M	1	0	0	0	0
2	T	1	0	0	0	0
2	V	1	0	0	0	0
2	Z	1	0	0	0	0
All	All	35844	0	36112	813	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 813 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:I:103:LEU:HD11	1:I:185:VAL:CG1	1.94	0.98
1:A:139:CYS:O	1:A:142:ILE:HG22	1.62	0.98
1:C:104:THR:HG22	1:C:156:HIS:HB3	1.48	0.95
1:U:176:ALA:HB1	1:U:188:ILE:HD12	1.49	0.93
1:I:103:LEU:HD11	1:I:185:VAL:HG12	1.51	0.93

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	1	159/193 (82%)	155 (98%)	4 (2%)	0	100	100
1	2	158/193 (82%)	154 (98%)	3 (2%)	1 (1%)	25	64
1	A	158/193 (82%)	151 (96%)	5 (3%)	2 (1%)	12	47
1	B	158/193 (82%)	148 (94%)	8 (5%)	2 (1%)	12	47
1	C	158/193 (82%)	152 (96%)	5 (3%)	1 (1%)	25	64
1	D	161/193 (83%)	150 (93%)	8 (5%)	3 (2%)	8	39
1	E	158/193 (82%)	149 (94%)	8 (5%)	1 (1%)	25	64
1	F	162/193 (84%)	155 (96%)	6 (4%)	1 (1%)	25	64
1	G	158/193 (82%)	149 (94%)	8 (5%)	1 (1%)	25	64
1	H	160/193 (83%)	151 (94%)	9 (6%)	0	100	100
1	I	159/193 (82%)	150 (94%)	9 (6%)	0	100	100
1	J	159/193 (82%)	147 (92%)	12 (8%)	0	100	100
1	K	157/193 (81%)	146 (93%)	10 (6%)	1 (1%)	25	64
1	L	158/193 (82%)	148 (94%)	9 (6%)	1 (1%)	25	64
1	M	158/193 (82%)	146 (92%)	11 (7%)	1 (1%)	25	64
1	N	158/193 (82%)	147 (93%)	11 (7%)	0	100	100
1	O	162/193 (84%)	151 (93%)	9 (6%)	2 (1%)	13	49
1	P	159/193 (82%)	151 (95%)	8 (5%)	0	100	100
1	Q	158/193 (82%)	151 (96%)	6 (4%)	1 (1%)	25	64
1	R	158/193 (82%)	147 (93%)	11 (7%)	0	100	100
1	S	158/193 (82%)	144 (91%)	12 (8%)	2 (1%)	12	47
1	T	157/193 (81%)	150 (96%)	5 (3%)	2 (1%)	12	47
1	U	158/193 (82%)	146 (92%)	11 (7%)	1 (1%)	25	64
1	V	159/193 (82%)	150 (94%)	9 (6%)	0	100	100
1	W	157/193 (81%)	148 (94%)	8 (5%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	157/193 (81%)	144 (92%)	13 (8%)	0	100	100
1	Y	159/193 (82%)	147 (92%)	11 (7%)	1 (1%)	25	64
1	Z	161/193 (83%)	147 (91%)	14 (9%)	0	100	100
All	All	4442/5404 (82%)	4174 (94%)	243 (6%)	25 (1%)	25	64

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	122	HIS
1	Q	122	HIS
1	B	169	GLU
1	E	97	SER
1	M	97	SER

### 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	1	140/164 (85%)	139 (99%)	1 (1%)	84	94
1	2	139/164 (85%)	135 (97%)	4 (3%)	42	74
1	A	139/164 (85%)	136 (98%)	3 (2%)	52	79
1	B	139/164 (85%)	135 (97%)	4 (3%)	42	74
1	C	139/164 (85%)	137 (99%)	2 (1%)	67	86
1	D	141/164 (86%)	136 (96%)	5 (4%)	36	69
1	E	139/164 (85%)	136 (98%)	3 (2%)	52	79
1	F	143/164 (87%)	142 (99%)	1 (1%)	84	94
1	G	139/164 (85%)	137 (99%)	2 (1%)	67	86
1	H	141/164 (86%)	141 (100%)	0	100	100
1	I	140/164 (85%)	136 (97%)	4 (3%)	42	74
1	J	140/164 (85%)	138 (99%)	2 (1%)	67	86
1	K	138/164 (84%)	136 (99%)	2 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	139/164 (85%)	137 (99%)	2 (1%)	67	86
1	M	139/164 (85%)	138 (99%)	1 (1%)	84	94
1	N	139/164 (85%)	136 (98%)	3 (2%)	52	79
1	O	143/164 (87%)	138 (96%)	5 (4%)	36	69
1	P	140/164 (85%)	139 (99%)	1 (1%)	84	94
1	Q	139/164 (85%)	135 (97%)	4 (3%)	42	74
1	R	139/164 (85%)	138 (99%)	1 (1%)	84	94
1	S	139/164 (85%)	138 (99%)	1 (1%)	84	94
1	T	138/164 (84%)	136 (99%)	2 (1%)	67	86
1	U	139/164 (85%)	139 (100%)	0	100	100
1	V	140/164 (85%)	140 (100%)	0	100	100
1	W	138/164 (84%)	137 (99%)	1 (1%)	84	94
1	X	138/164 (84%)	135 (98%)	3 (2%)	52	79
1	Y	140/164 (85%)	138 (99%)	2 (1%)	67	86
1	Z	142/164 (87%)	141 (99%)	1 (1%)	84	94
All	All	3909/4592 (85%)	3849 (98%)	60 (2%)	65	85

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	167	ASP
1	1	39	MET
1	O	41	ASN
1	Z	155	LEU
1	2	187	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	34	GLN
1	T	41	ASN
1	O	163	GLN
1	Q	193	ASN
1	U	41	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.