



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 07:37 PM UTC

PDB ID : 3HLN / pdb_00003hln
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

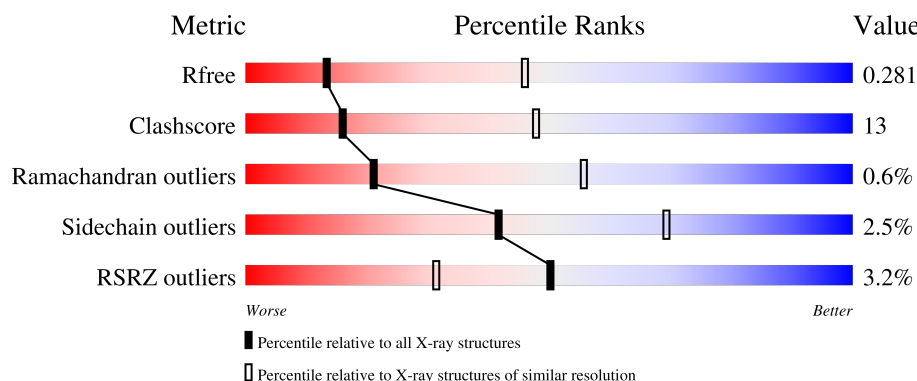
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 ≥ 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 $\leq 5\%$. 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	1	193	 2% 64% 20% 16%
1	2	193	 4% 64% 19% 16%
1	A	193	 2% 58% 25% 16%
1	B	193	 5% 63% 19% 16%
1	C	193	 4% 61% 22% 16%

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Mol	Chain	Length	Quality of chain
1	D	193	
1	E	193	
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

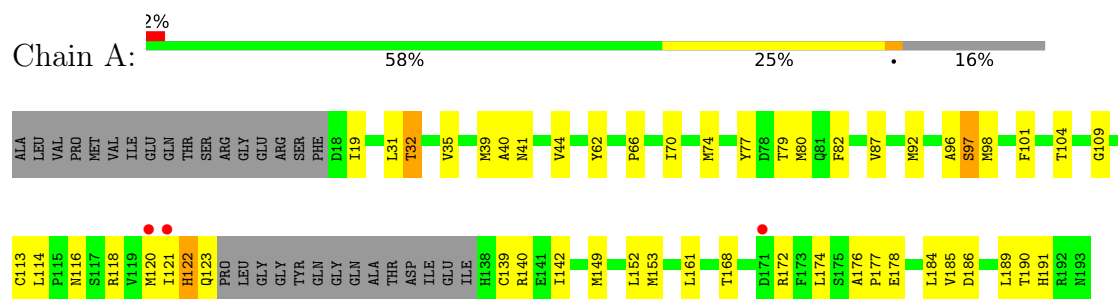
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

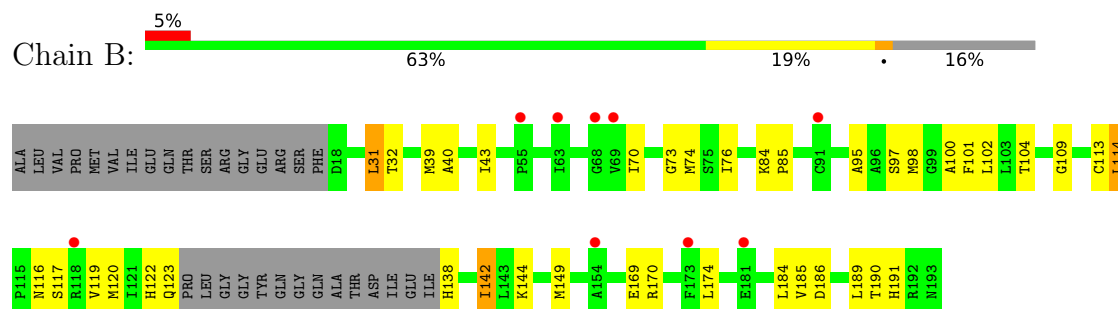
3 Residue-property plots [i](#)

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 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.

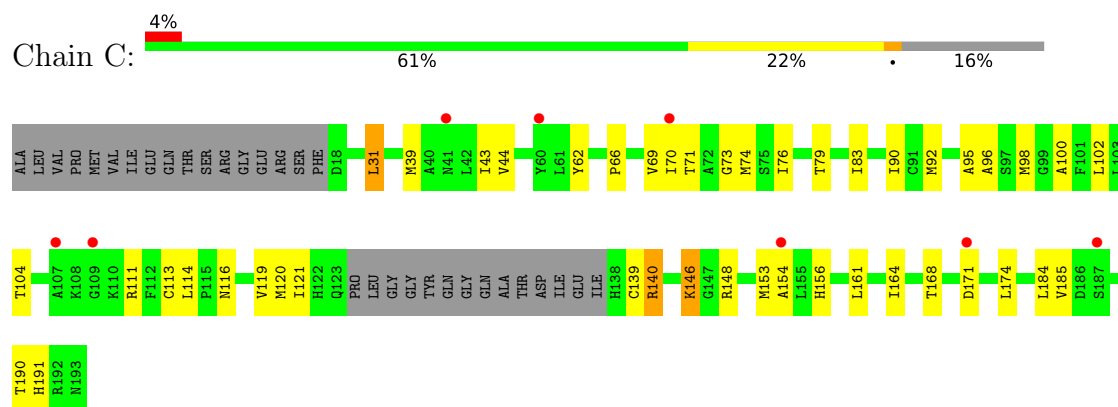
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

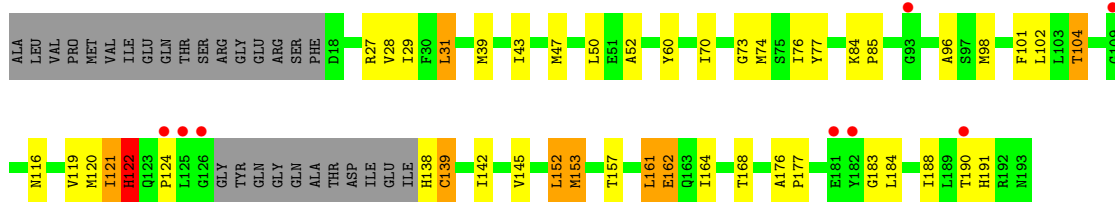


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

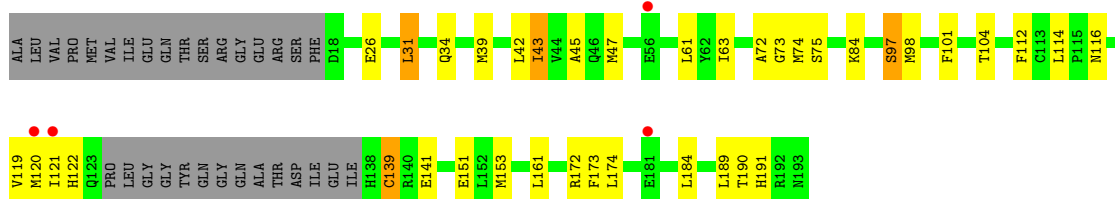


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

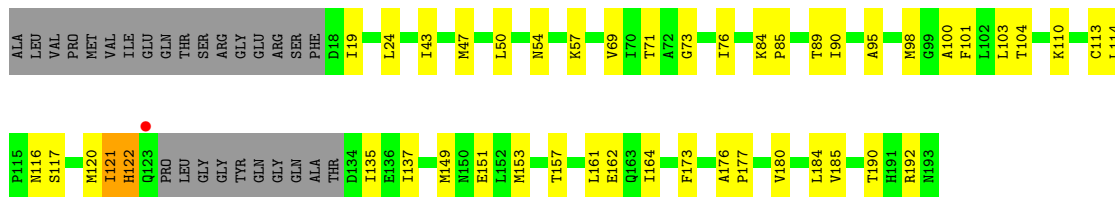




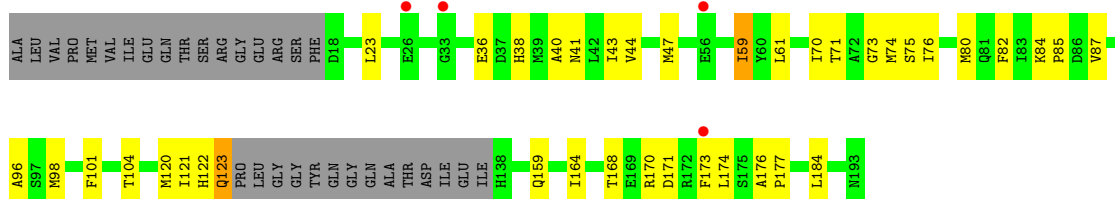
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



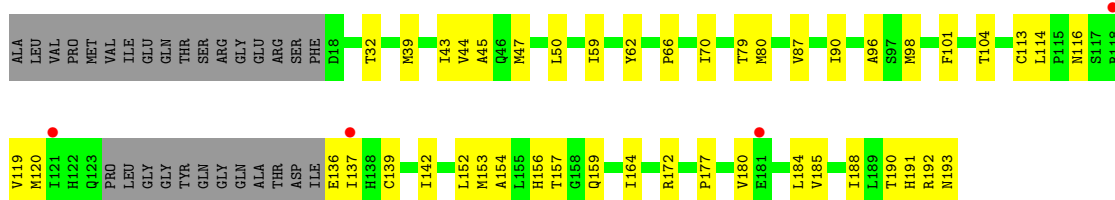
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



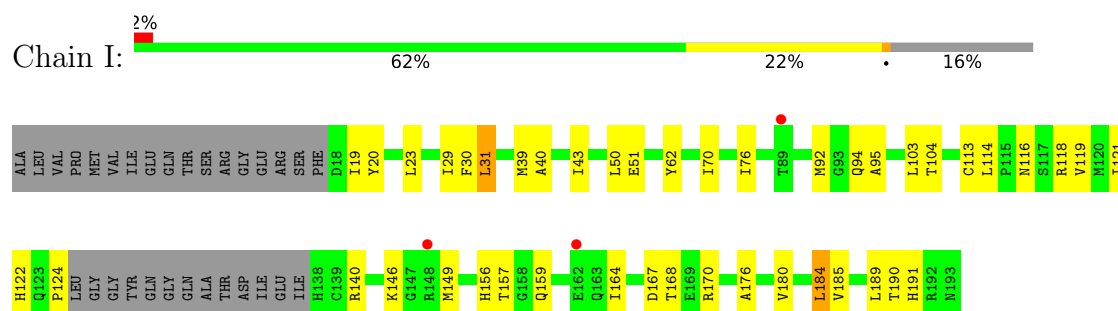
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



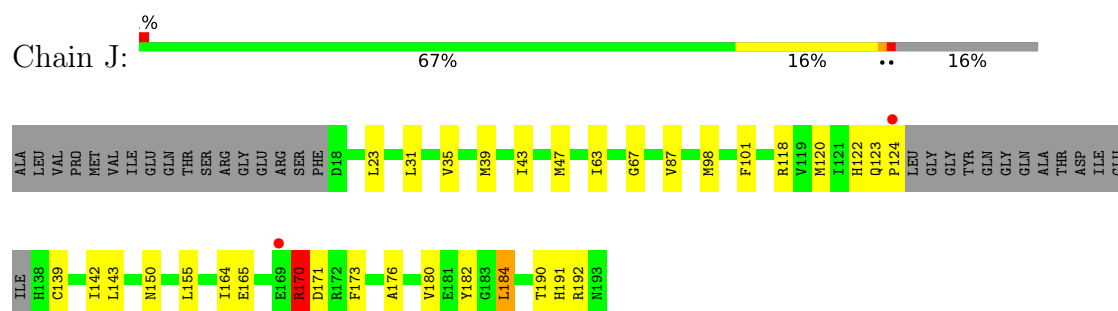
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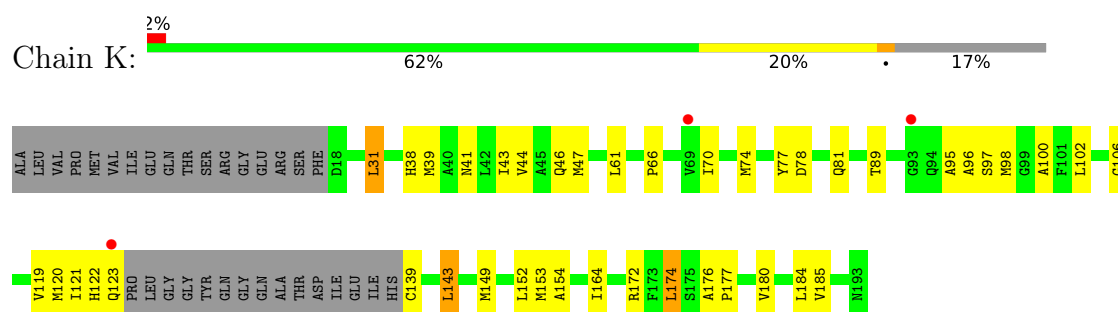
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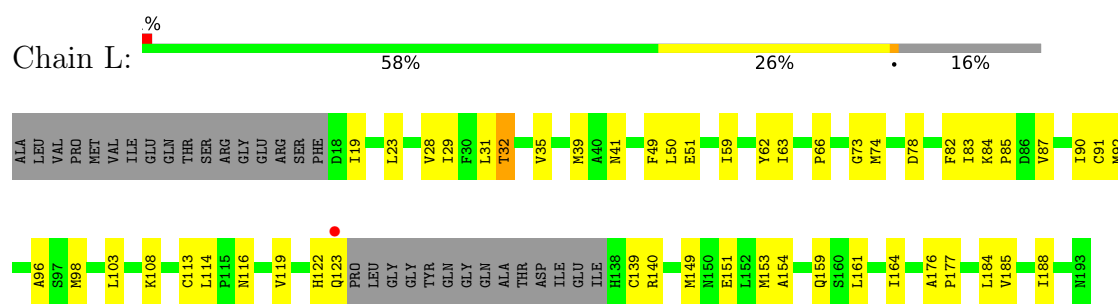
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



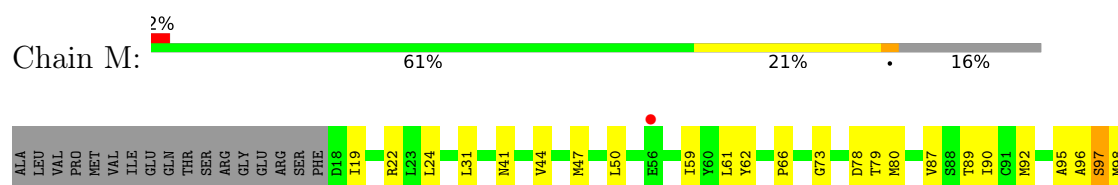
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

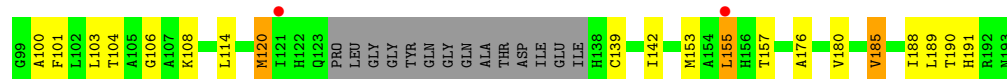


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

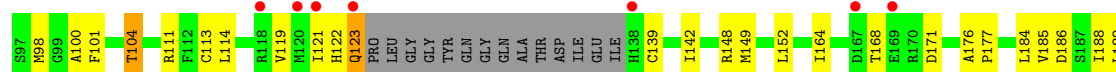
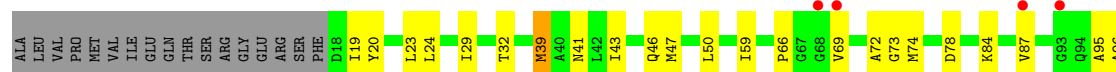


- Molecule 1: ATP-dependent Clp protease proteolytic subunit





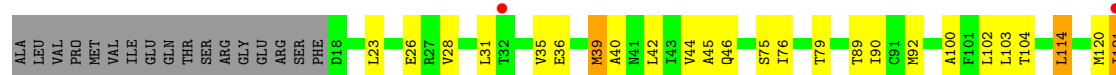
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



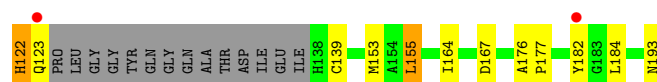
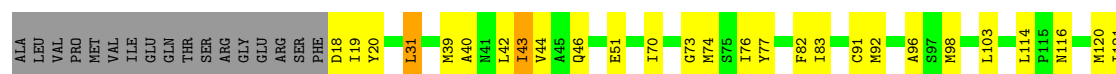
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



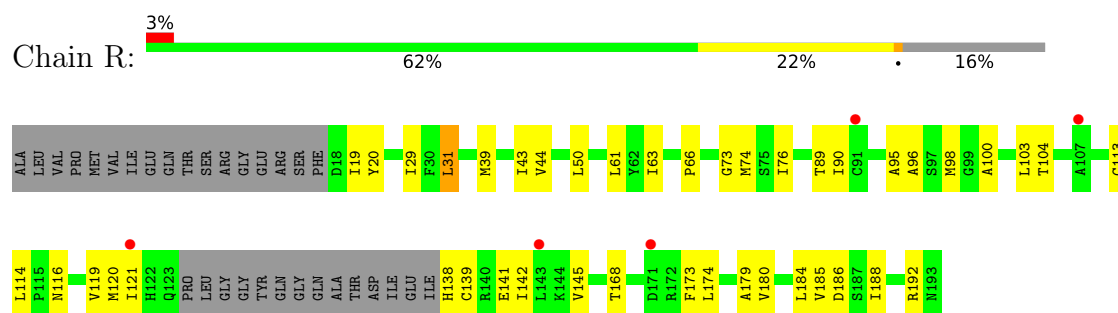
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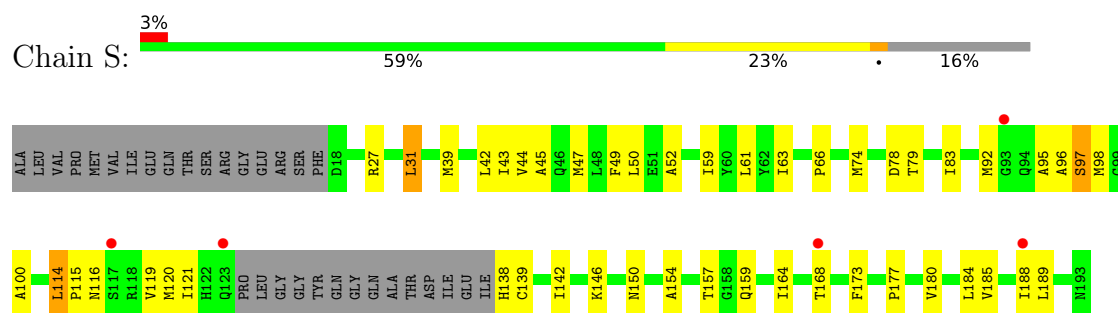
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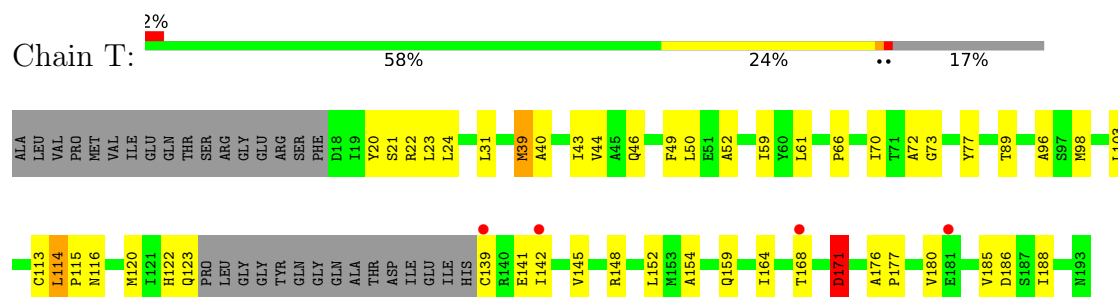
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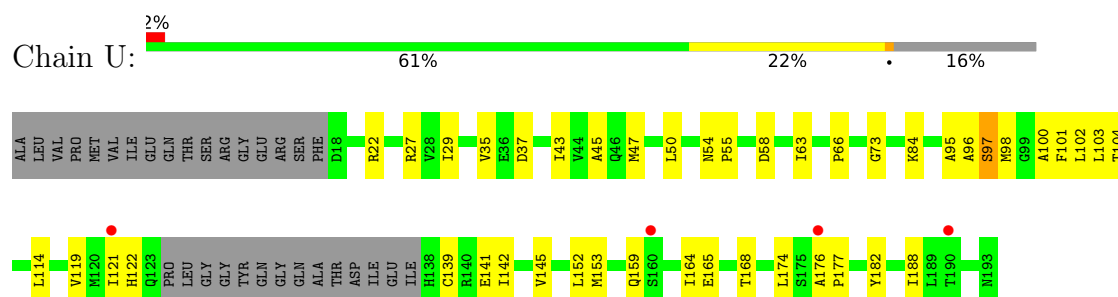
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



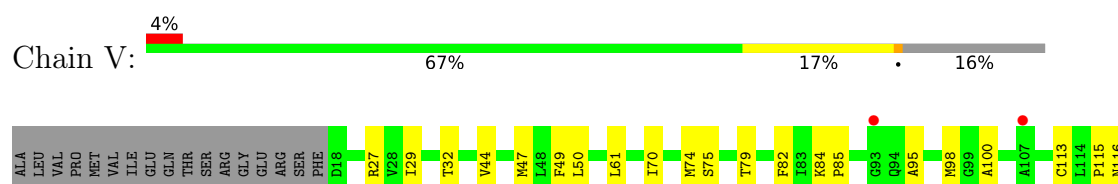
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

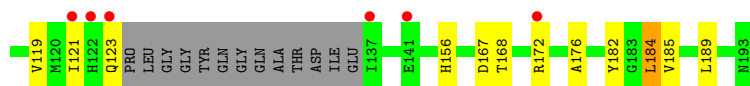


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

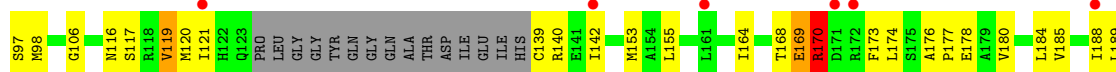


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

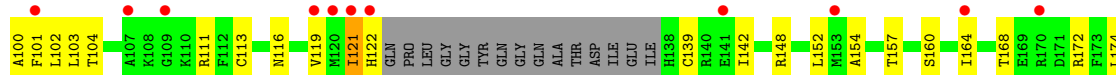




- Molecule 1: ATP-dependent Clp protease proteolytic subunit



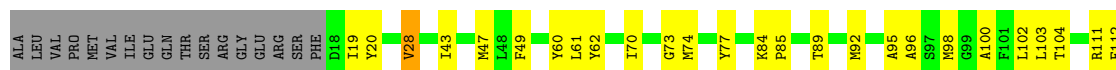
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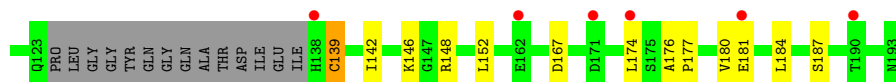
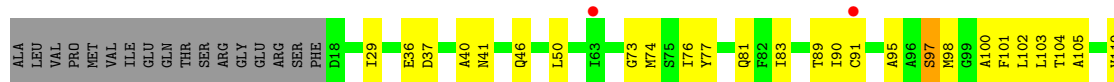




- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.30Å 182.30Å 476.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.22 – 3.20 42.22 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (42.22-3.20) 97.5 (42.22-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.253 0.270 , 0.281	Depositor DCC
R_{free} test set	7454 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	105.3	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.49	0/1302	0.75	0/1750
1	2	0.50	0/1294	0.81	0/1739
1	A	0.51	0/1294	0.75	0/1739
1	B	0.51	0/1294	0.81	1/1739 (0.1%)
1	C	0.48	0/1294	0.78	0/1739
1	D	0.54	0/1314	0.83	1/1767 (0.1%)
1	E	0.50	0/1294	0.80	0/1739
1	F	0.49	0/1327	0.77	0/1784
1	G	0.48	0/1294	0.80	0/1739
1	H	0.45	0/1311	0.74	0/1762
1	I	0.47	0/1302	0.77	0/1751
1	J	0.49	0/1302	0.79	1/1751 (0.1%)
1	K	0.45	0/1283	0.77	0/1724
1	L	0.47	0/1294	0.79	0/1739
1	M	0.47	0/1294	0.76	0/1739
1	N	0.47	0/1294	0.77	0/1739
1	O	0.54	0/1327	0.81	0/1785
1	P	0.48	0/1302	0.75	0/1751
1	Q	0.48	0/1294	0.77	0/1739
1	R	0.46	0/1294	0.75	2/1739 (0.1%)
1	S	0.49	0/1294	0.76	0/1739
1	T	0.45	0/1283	0.76	2/1724 (0.1%)
1	U	0.49	0/1294	0.76	1/1739 (0.1%)
1	V	0.47	0/1302	0.75	0/1750
1	W	0.50	0/1283	0.76	1/1724 (0.1%)
1	X	0.49	0/1285	0.76	0/1727
1	Y	0.51	0/1302	0.80	0/1750
1	Z	0.52	0/1319	0.78	1/1774 (0.1%)
All	All	0.49	0/36366	0.78	10/48881 (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	J	0	1
1	W	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	170	ARG	N-CA-C	6.61	118.18	108.86
1	U	37	ASP	N-CA-C	5.98	118.29	111.11
1	D	161	LEU	N-CA-C	-5.85	104.59	110.97
1	B	170	ARG	N-CA-C	5.59	117.61	108.55
1	W	170	ARG	N-CA-C	5.53	115.58	108.34

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	26	0
1	2	1275	0	1284	34	0
1	A	1275	0	1284	46	0
1	B	1275	0	1284	32	0
1	C	1275	0	1284	37	0
1	D	1294	0	1305	38	0
1	E	1275	0	1284	32	0
1	F	1308	0	1316	38	0
1	G	1275	0	1284	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1292	0	1301	52	0
1	I	1282	0	1291	40	0
1	J	1282	0	1291	26	0
1	K	1265	0	1277	36	0
1	L	1275	0	1284	43	0
1	M	1275	0	1284	40	0
1	N	1275	0	1284	45	0
1	O	1307	0	1320	46	0
1	P	1282	0	1291	47	0
1	Q	1275	0	1284	37	0
1	R	1275	0	1285	35	0
1	S	1275	0	1284	42	0
1	T	1265	0	1277	38	0
1	U	1275	0	1285	33	0
1	V	1283	0	1295	32	0
1	W	1265	0	1278	48	0
1	X	1266	0	1276	46	0
1	Y	1283	0	1295	39	0
1	Z	1299	0	1309	45	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	953	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 13.

The worst 5 of 953 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:O:44:VAL:HG11	1:P:92:MET:HE1	1.26	1.08
1:K:44:VAL:HG11	1:L:92:MET:HE1	1.40	1.02
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

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	1	159/193 (82%)	155 (98%)	4 (2%)	0	100	100
1	2	158/193 (82%)	154 (98%)	3 (2%)	1 (1%)	21	56
1	A	158/193 (82%)	151 (96%)	5 (3%)	2 (1%)	9	40
1	B	158/193 (82%)	148 (94%)	8 (5%)	2 (1%)	9	40
1	C	158/193 (82%)	152 (96%)	5 (3%)	1 (1%)	21	56
1	D	161/193 (83%)	150 (93%)	8 (5%)	3 (2%)	6	33
1	E	158/193 (82%)	149 (94%)	8 (5%)	1 (1%)	21	56
1	F	162/193 (84%)	155 (96%)	6 (4%)	1 (1%)	21	56
1	G	158/193 (82%)	149 (94%)	8 (5%)	1 (1%)	21	56
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%)	21	56
1	L	158/193 (82%)	148 (94%)	9 (6%)	1 (1%)	21	56
1	M	158/193 (82%)	146 (92%)	11 (7%)	1 (1%)	21	56
1	N	158/193 (82%)	147 (93%)	11 (7%)	0	100	100
1	O	162/193 (84%)	151 (93%)	9 (6%)	2 (1%)	10	42
1	P	159/193 (82%)	151 (95%)	8 (5%)	0	100	100
1	Q	158/193 (82%)	151 (96%)	6 (4%)	1 (1%)	21	56
1	R	158/193 (82%)	147 (93%)	11 (7%)	0	100	100
1	S	158/193 (82%)	144 (91%)	12 (8%)	2 (1%)	9	40
1	T	157/193 (81%)	150 (96%)	5 (3%)	2 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	158/193 (82%)	146 (92%)	11 (7%)	1 (1%)	21	56
1	V	159/193 (82%)	150 (94%)	9 (6%)	0	100	100
1	W	157/193 (81%)	148 (94%)	8 (5%)	1 (1%)	21	56
1	X	157/193 (81%)	144 (92%)	13 (8%)	0	100	100
1	Y	159/193 (82%)	147 (92%)	11 (7%)	1 (1%)	21	56
1	Z	161/193 (83%)	147 (91%)	14 (9%)	0	100	100
All	All	4442/5404 (82%)	4174 (94%)	243 (6%)	25 (1%)	21	56

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%)	137 (98%)	3 (2%)	47	71
1	2	139/164 (85%)	135 (97%)	4 (3%)	37	67
1	A	139/164 (85%)	137 (99%)	2 (1%)	59	77
1	B	139/164 (85%)	133 (96%)	6 (4%)	26	59
1	C	139/164 (85%)	135 (97%)	4 (3%)	37	67
1	D	141/164 (86%)	134 (95%)	7 (5%)	22	55
1	E	139/164 (85%)	132 (95%)	7 (5%)	22	55
1	F	143/164 (87%)	140 (98%)	3 (2%)	47	71
1	G	139/164 (85%)	135 (97%)	4 (3%)	37	67
1	H	141/164 (86%)	139 (99%)	2 (1%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	140/164 (85%)	137 (98%)	3 (2%)	47	71
1	J	140/164 (85%)	135 (96%)	5 (4%)	31	63
1	K	138/164 (84%)	135 (98%)	3 (2%)	45	71
1	L	139/164 (85%)	138 (99%)	1 (1%)	76	83
1	M	139/164 (85%)	135 (97%)	4 (3%)	37	67
1	N	139/164 (85%)	135 (97%)	4 (3%)	37	67
1	O	143/164 (87%)	139 (97%)	4 (3%)	38	68
1	P	140/164 (85%)	137 (98%)	3 (2%)	47	71
1	Q	139/164 (85%)	133 (96%)	6 (4%)	26	59
1	R	139/164 (85%)	138 (99%)	1 (1%)	76	83
1	S	139/164 (85%)	136 (98%)	3 (2%)	45	71
1	T	138/164 (84%)	135 (98%)	3 (2%)	45	71
1	U	139/164 (85%)	137 (99%)	2 (1%)	59	77
1	V	140/164 (85%)	138 (99%)	2 (1%)	59	77
1	W	138/164 (84%)	136 (99%)	2 (1%)	59	77
1	X	138/164 (84%)	135 (98%)	3 (2%)	45	71
1	Y	140/164 (85%)	136 (97%)	4 (3%)	37	67
1	Z	142/164 (87%)	139 (98%)	3 (2%)	47	71
All	All	3909/4592 (85%)	3811 (98%)	98 (2%)	42	69

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	76	ILE
1	S	139	CYS
1	P	39	MET
1	Q	139	CYS
1	U	22	ARG

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

Mol	Chain	Res	Type
1	K	41	ASN
1	Z	123	GLN
1	O	116	ASN

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Mol	Chain	Res	Type
1	Z	122	HIS
1	Y	38	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 oligosaccharides 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 ⓘ

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	1	163/193 (84%)	0.57	3 (1%) 67 48	111, 117, 125, 128	0
1	2	162/193 (83%)	0.67	8 (4%) 35 22	107, 115, 122, 126	0
1	A	162/193 (83%)	0.69	3 (1%) 66 46	104, 112, 122, 125	0
1	B	162/193 (83%)	0.74	9 (5%) 30 19	103, 112, 122, 124	0
1	C	162/193 (83%)	0.69	8 (4%) 35 22	100, 110, 121, 127	0
1	D	165/193 (85%)	0.67	8 (4%) 35 22	102, 111, 123, 132	0
1	E	162/193 (83%)	0.66	4 (2%) 58 39	107, 114, 124, 128	0
1	F	166/193 (86%)	0.47	1 (0%) 85 73	106, 112, 124, 129	0
1	G	162/193 (83%)	0.67	4 (2%) 58 39	110, 117, 125, 129	0
1	H	164/193 (84%)	0.51	4 (2%) 59 40	118, 123, 129, 134	0
1	I	163/193 (84%)	0.47	3 (1%) 67 48	112, 118, 125, 131	0
1	J	163/193 (84%)	0.29	2 (1%) 76 58	109, 113, 120, 123	0
1	K	161/193 (83%)	0.42	3 (1%) 66 46	112, 117, 125, 128	0
1	L	162/193 (83%)	0.48	1 (0%) 85 73	113, 120, 129, 135	0
1	M	162/193 (83%)	0.50	3 (1%) 66 46	117, 122, 128, 132	0
1	N	162/193 (83%)	0.58	11 (6%) 23 15	116, 124, 130, 134	0
1	O	166/193 (86%)	0.44	4 (2%) 59 40	104, 112, 126, 135	0
1	P	163/193 (84%)	0.32	4 (2%) 58 39	112, 117, 124, 130	0
1	Q	162/193 (83%)	0.43	2 (1%) 76 58	118, 123, 130, 132	0
1	R	162/193 (83%)	0.78	5 (3%) 51 32	121, 125, 132, 135	0
1	S	162/193 (83%)	0.68	5 (3%) 51 32	117, 122, 127, 130	0
1	T	161/193 (83%)	0.59	4 (2%) 58 39	116, 122, 129, 134	0
1	U	162/193 (83%)	0.48	4 (2%) 58 39	108, 118, 127, 132	0
1	V	163/193 (84%)	0.53	8 (4%) 35 22	105, 115, 125, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	W	161/193 (83%)	0.67	7 (4%)	40 24	111, 116, 122, 126	0
1	X	161/193 (83%)	0.88	14 (8%)	16 11	106, 116, 124, 126	0
1	Y	163/193 (84%)	0.80	10 (6%)	27 17	101, 109, 117, 124	0
1	Z	165/193 (85%)	0.49	5 (3%)	52 33	107, 117, 130, 136	0
All	All	4554/5404 (84%)	0.58	147 (3%)	50 31	100, 117, 127, 136	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	PRO	5.3
1	R	121	ILE	4.7
1	H	137	ILE	4.6
1	Y	123	GLN	3.7
1	2	190	THR	3.6

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	2	216	1/1	0.19	0.22	186,186,186,186	0
2	CA	J	219	1/1	0.57	0.17	173,173,173,173	0
2	CA	T	201	1/1	0.60	0.33	162,162,162,162	0
2	CA	V	221	1/1	0.60	0.12	177,177,177,177	0
2	CA	J	202	1/1	0.60	0.23	176,176,176,176	0
2	CA	Z	215	1/1	0.65	0.28	182,182,182,182	0
2	CA	E	217	1/1	0.75	0.20	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	I	203	1/1	0.79	0.10	125,125,125,125	0
2	CA	M	220	1/1	0.80	0.14	176,176,176,176	0
2	CA	E	218	1/1	0.81	0.18	155,155,155,155	0
2	CA	1	205	1/1	0.82	0.16	154,154,154,154	0
2	CA	J	206	1/1	0.92	0.12	109,109,109,109	0
2	CA	I	204	1/1	0.93	0.10	129,129,129,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.