



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 9, 2026 – 12:46 AM JST

PDB ID : 9VHC / pdb_00009vhc
Title : ATP-dependent Clp endopeptidase proteolytic subunit ClpP
Authors : Li, X.Y.; Luo, X.
Deposited on : 2025-06-16
Resolution : 3.03 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

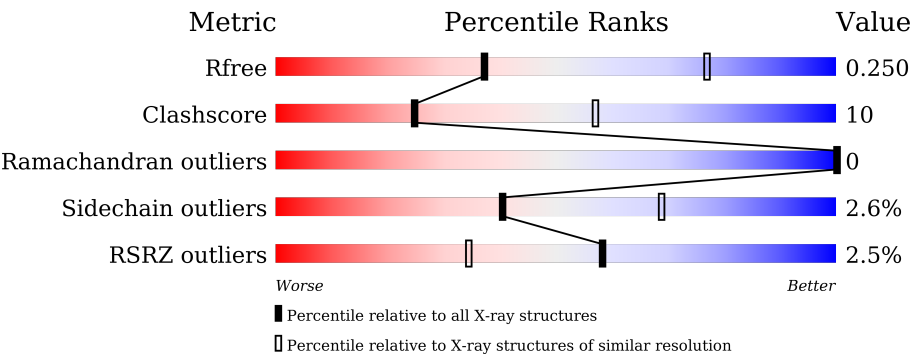
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	A	213	2% 71% 15% • 13%
1	B	213	0% 69% 16% • 14%
1	C	213	2% 69% 15% • 14%
1	D	213	2% 66% 19% • 12%
1	E	213	2% 67% 19% • 14%
1	F	213	3% 68% 18% • 13%

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Mol	Chain	Length	Quality of chain
1	G	213	
1	H	213	
1	I	213	
1	J	213	
1	K	213	
1	L	213	
1	M	213	
1	N	213	
1	O	213	
1	P	213	
1	Q	213	
1	R	213	
1	S	213	
1	T	213	
1	U	213	
1	V	213	
1	W	213	
1	X	213	
1	Y	213	
1	Z	213	
1	a	213	
1	b	213	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	b	302	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 40761 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	185	Total	C	N	O	S	0	0	0
			1440	905	254	269	12			
1	B	183	Total	C	N	O	S	0	0	0
			1425	895	250	268	12			
1	C	184	Total	C	N	O	S	0	0	0
			1429	899	250	268	12			
1	D	187	Total	C	N	O	S	0	0	0
			1457	915	257	272	13			
1	E	184	Total	C	N	O	S	0	0	0
			1429	899	250	268	12			
1	F	185	Total	C	N	O	S	0	0	0
			1440	905	254	269	12			
1	G	181	Total	C	N	O	S	0	0	0
			1407	885	247	263	12			
1	H	183	Total	C	N	O	S	0	0	0
			1424	896	249	267	12			
1	I	184	Total	C	N	O	S	0	0	0
			1429	899	250	268	12			
1	J	182	Total	C	N	O	S	0	0	0
			1415	891	248	264	12			
1	K	184	Total	C	N	O	S	0	0	0
			1429	899	250	268	12			
1	L	184	Total	C	N	O	S	0	0	0
			1429	899	250	268	12			
1	M	180	Total	C	N	O	S	0	0	0
			1400	880	246	262	12			
1	N	181	Total	C	N	O	S	0	0	0
			1401	882	244	263	12			
1	O	184	Total	C	N	O	S	0	0	0
			1433	901	251	269	12			
1	P	182	Total	C	N	O	S	0	0	0
			1415	891	248	264	12			

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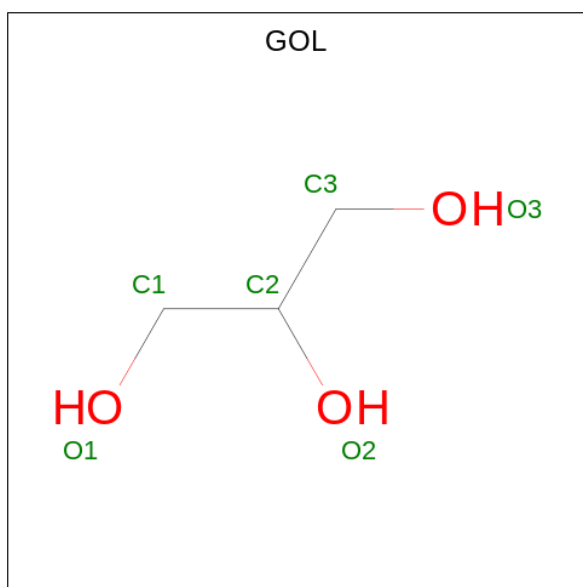
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	183	Total	C	N	O	S	0	0	0
			1424	896	249	267	12			
1	R	180	Total	C	N	O	S	0	0	0
			1400	880	246	262	12			
1	S	183	Total	C	N	O	S	0	0	0
			1424	896	249	267	12			
1	T	181	Total	C	N	O	S	0	0	0
			1407	885	247	263	12			
1	U	183	Total	C	N	O	S	0	0	0
			1424	896	249	267	12			
1	V	183	Total	C	N	O	S	0	0	0
			1424	896	249	267	12			
1	W	185	Total	C	N	O	S	0	0	0
			1440	905	254	269	12			
1	X	183	Total	C	N	O	S	0	0	0
			1424	896	249	267	12			
1	Y	184	Total	C	N	O	S	0	0	0
			1429	899	250	268	12			
1	Z	184	Total	C	N	O	S	0	0	0
			1429	899	250	268	12			
1	a	181	Total	C	N	O	S	0	0	0
			1407	885	247	263	12			
1	b	185	Total	C	N	O	S	0	0	0
			1440	905	254	269	12			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	I	1	Total	Cl	0	0
			1	1		
2	K	1	Total	Cl	0	0
			1	1		
2	O	1	Total	Cl	0	0
			1	1		
2	P	1	Total	Cl	0	0
			1	1		
2	Y	1	Total	Cl	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		
3	T	1	Total	C	O	0	0
			6	3	3		
3	U	1	Total	C	O	0	0
			6	3	3		
3	U	1	Total	C	O	0	0
			6	3	3		
3	V	1	Total	C	O	0	0
			6	3	3		
3	V	1	Total	C	O	0	0
			6	3	3		
3	V	1	Total	C	O	0	0
			6	3	3		
3	W	1	Total	C	O	0	0
			6	3	3		
3	W	1	Total	C	O	0	0
			6	3	3		
3	X	1	Total	C	O	0	0
			6	3	3		
3	X	1	Total	C	O	0	0
			6	3	3		
3	X	1	Total	C	O	0	0
			6	3	3		
3	Y	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	Y	1	Total	C	O	0	0
			6	3	3		
3	Y	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		
3	b	1	Total	C	O	0	0
			6	3	3		
3	b	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	20	Total	O	0	0
			20	20		
4	C	33	Total	O	0	0
			33	33		
4	D	33	Total	O	0	0
			33	33		
4	E	36	Total	O	0	0
			36	36		
4	F	28	Total	O	0	0
			28	28		
4	G	25	Total	O	0	0
			25	25		
4	H	12	Total	O	0	0
			12	12		
4	I	30	Total	O	0	0
			30	30		
4	J	31	Total	O	0	0
			31	31		
4	K	16	Total	O	0	0
			16	16		
4	L	6	Total	O	0	0
			6	6		
4	M	9	Total	O	0	0
			9	9		

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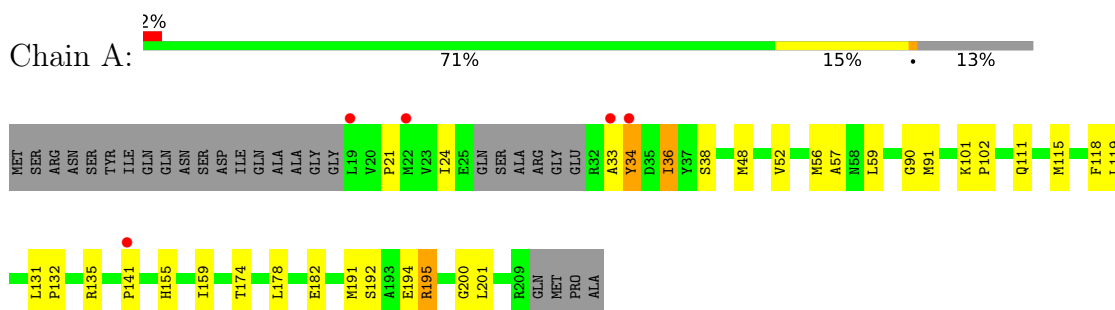
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	N	7	Total 7	O 7	0	0
4	O	26	Total 26	O 26	0	0
4	P	22	Total 22	O 22	0	0
4	Q	18	Total 18	O 18	0	0
4	R	14	Total 14	O 14	0	0
4	S	10	Total 10	O 10	0	0
4	T	9	Total 9	O 9	0	0
4	U	21	Total 21	O 21	0	0
4	V	31	Total 31	O 31	0	0
4	W	24	Total 24	O 24	0	0
4	X	35	Total 35	O 35	0	0
4	Y	31	Total 31	O 31	0	0
4	Z	27	Total 27	O 27	0	0
4	a	34	Total 34	O 34	0	0
4	b	27	Total 27	O 27	0	0

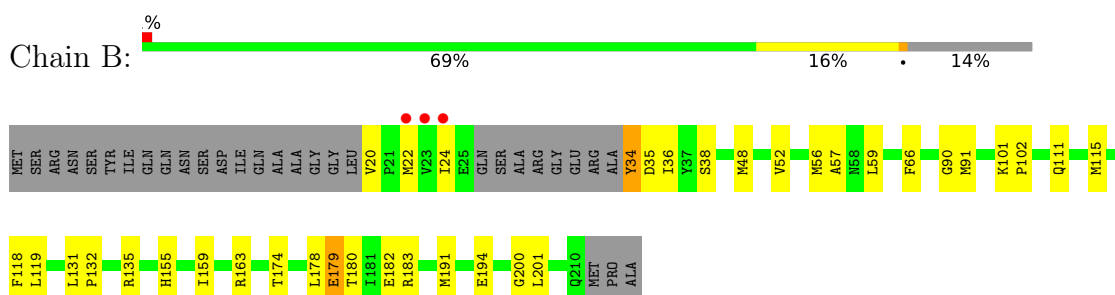
3 Residue-property plots [i](#)

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.

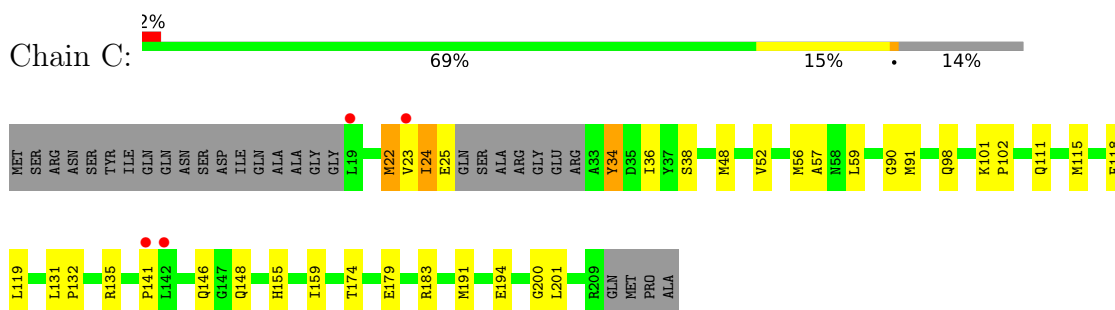
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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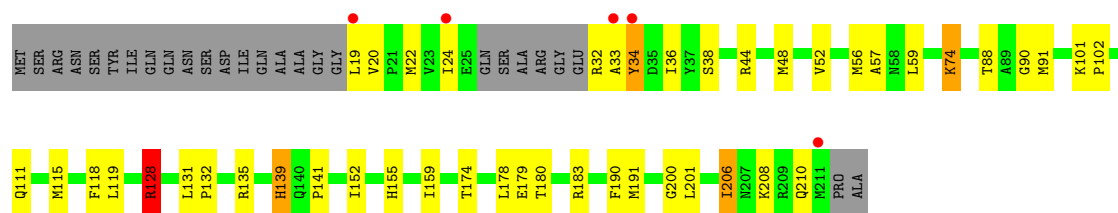


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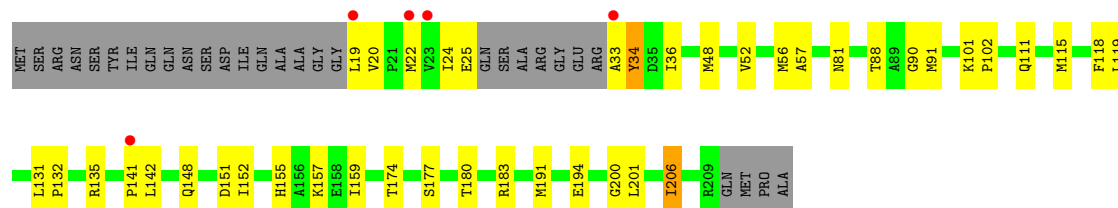


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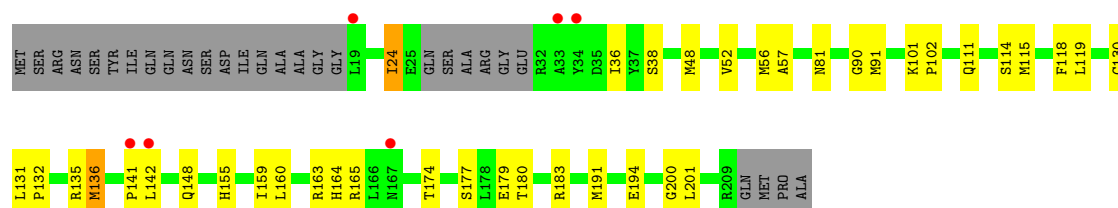




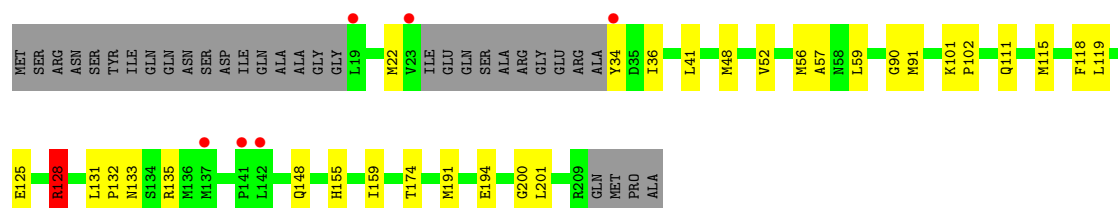
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



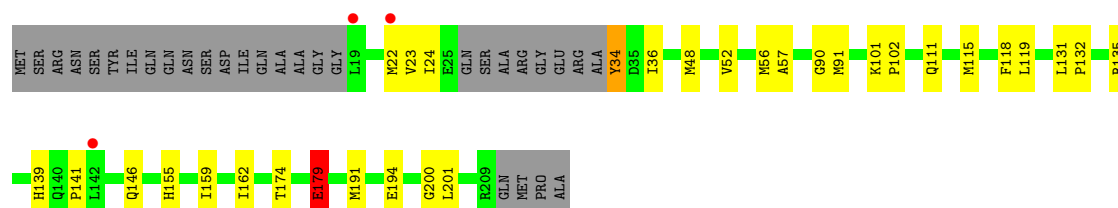
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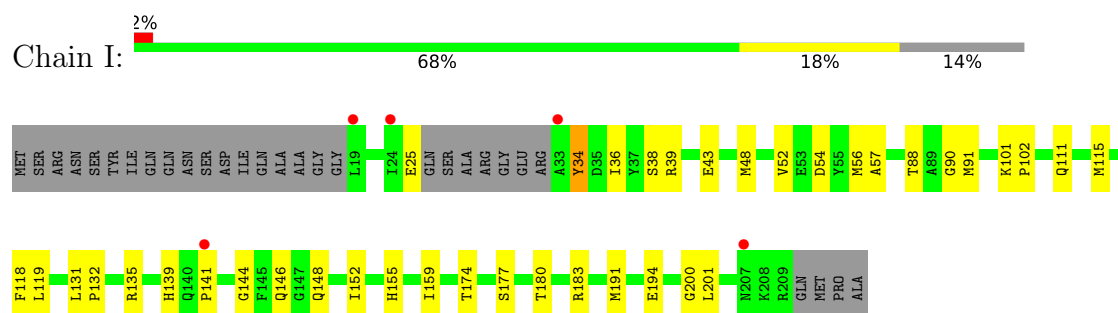
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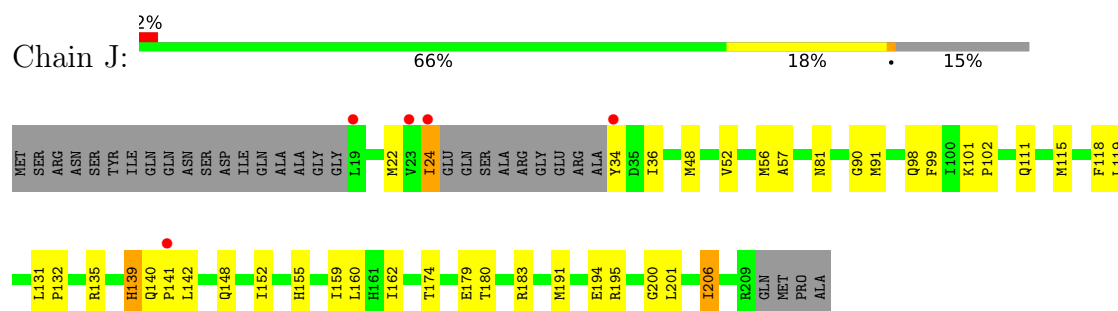
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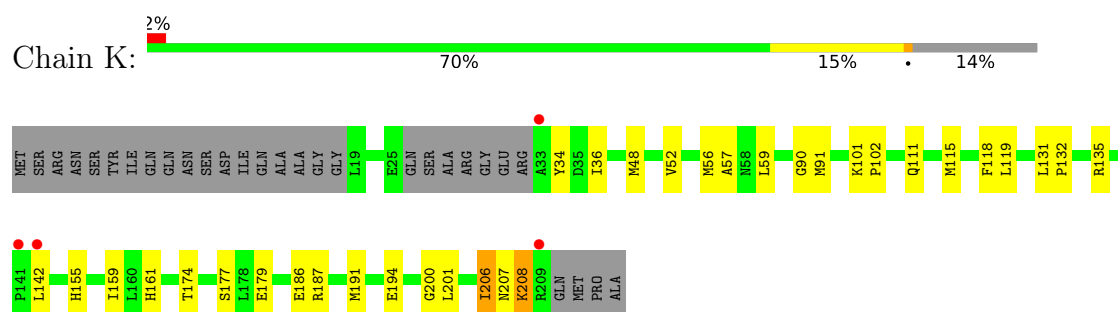
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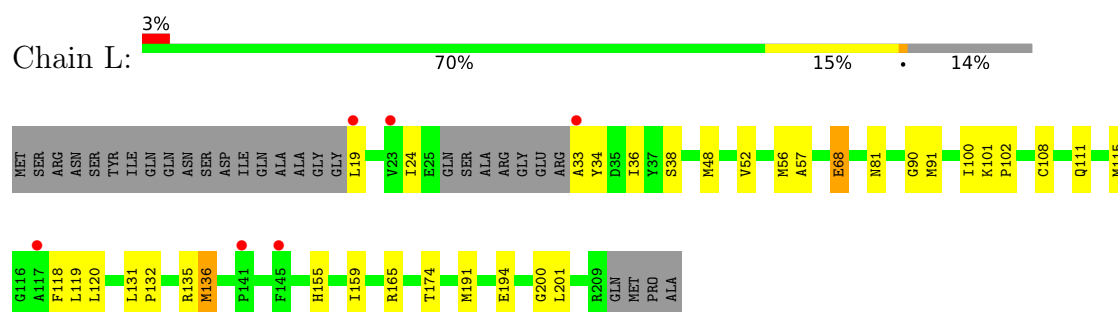
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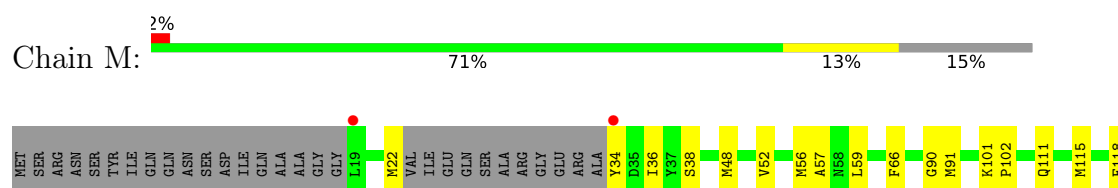
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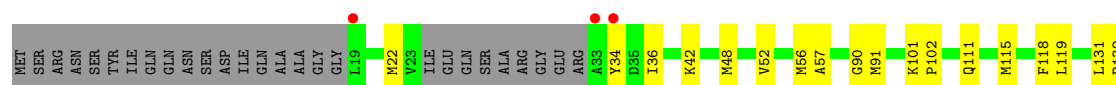


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

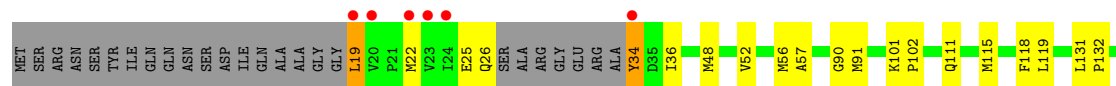




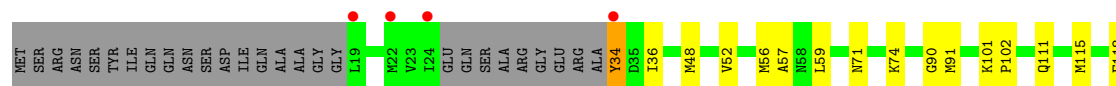
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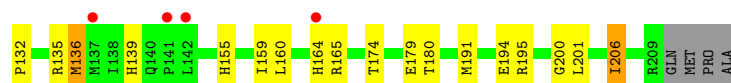
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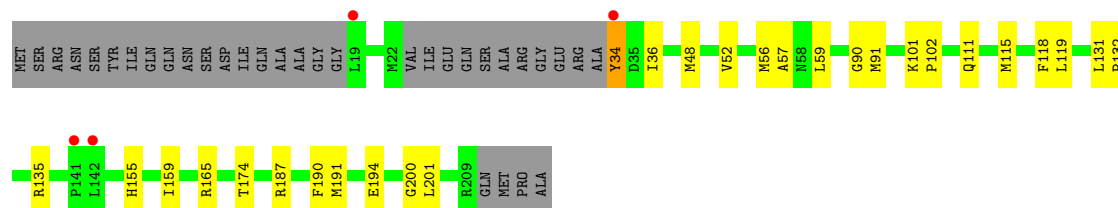
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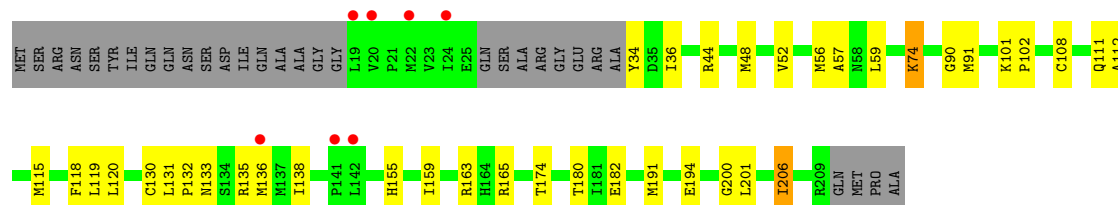
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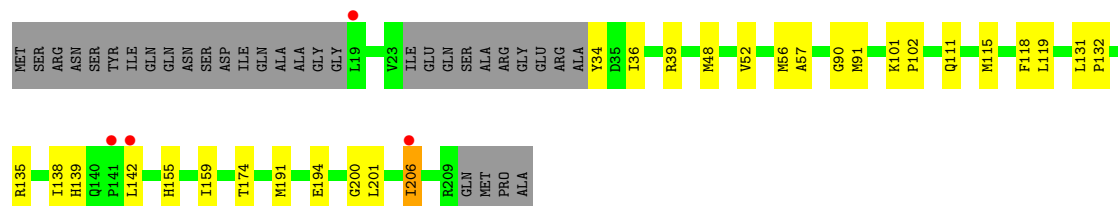
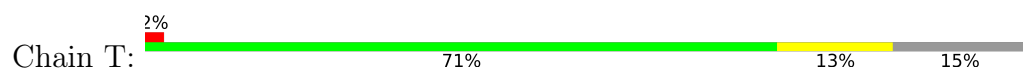
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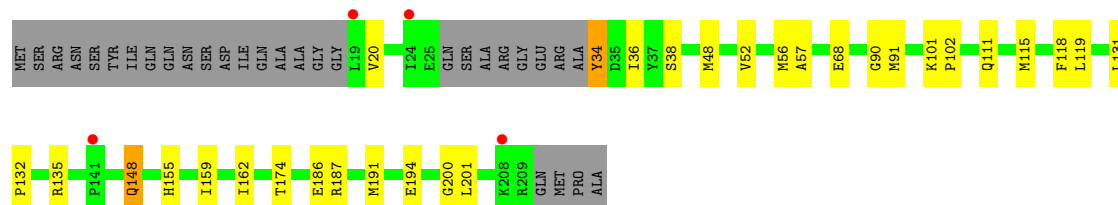
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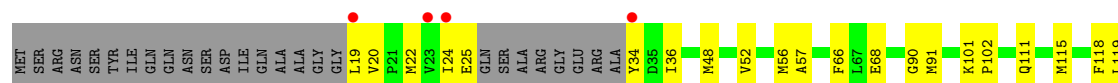
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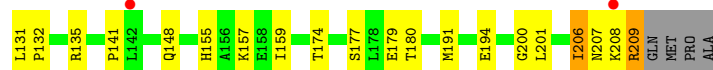
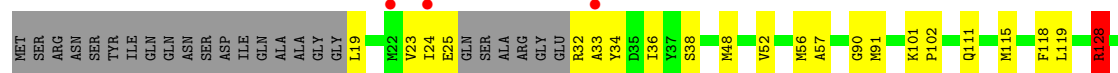


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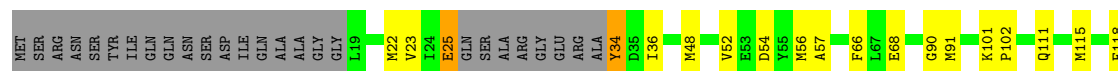




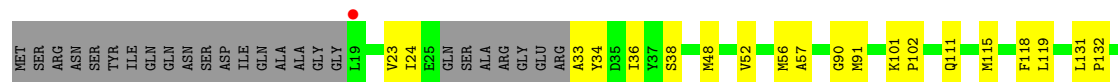
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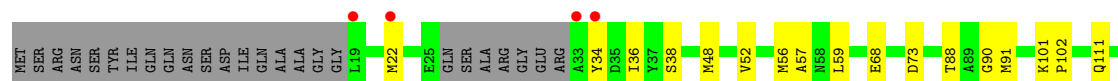
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● Molecule 1: ATP-dependent Clp protease proteolytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	252.98Å 273.58Å 249.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.73 – 3.03 32.73 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.73-3.03) 99.5 (32.73-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.215 , 0.248 0.217 , 0.250	Depositor DCC
R_{free} test set	8375 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	40761	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.34% 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: GOL, CL

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	0.97	0/1465	1.43	1/1974 (0.1%)
1	B	0.99	0/1450	1.44	2/1954 (0.1%)
1	C	0.97	0/1454	1.45	2/1960 (0.1%)
1	D	1.03	1/1482 (0.1%)	1.49	4/1996 (0.2%)
1	E	0.99	0/1454	1.45	1/1960 (0.1%)
1	F	0.99	0/1465	1.47	1/1974 (0.1%)
1	G	0.97	0/1432	1.46	2/1930 (0.1%)
1	H	0.97	0/1449	1.43	1/1953 (0.1%)
1	I	0.96	0/1454	1.42	0/1960
1	J	1.01	1/1440 (0.1%)	1.46	2/1941 (0.1%)
1	K	1.02	1/1454 (0.1%)	1.46	4/1960 (0.2%)
1	L	0.99	1/1454 (0.1%)	1.43	0/1960
1	M	0.95	0/1425	1.41	0/1920
1	N	0.96	0/1426	1.42	0/1923
1	O	0.99	1/1458 (0.1%)	1.47	2/1965 (0.1%)
1	P	0.97	0/1440	1.43	0/1941
1	Q	0.99	0/1449	1.46	2/1953 (0.1%)
1	R	0.96	0/1425	1.42	0/1920
1	S	0.98	1/1449 (0.1%)	1.43	1/1953 (0.1%)
1	T	0.97	0/1432	1.44	1/1930 (0.1%)
1	U	0.97	0/1449	1.43	0/1953
1	V	1.04	1/1449 (0.1%)	1.45	1/1953 (0.1%)
1	W	0.99	0/1465	1.51	4/1974 (0.2%)
1	X	1.00	1/1449 (0.1%)	1.45	2/1953 (0.1%)
1	Y	0.97	0/1454	1.43	0/1960
1	Z	0.98	0/1454	1.44	0/1960
1	a	0.96	0/1432	1.43	0/1930
1	b	1.00	0/1465	1.44	0/1974
All	All	0.98	8/40574 (0.0%)	1.45	33/54684 (0.1%)

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	D	0	1
1	G	0	1
1	O	0	1
1	W	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	139	HIS	CE1-NE2	9.90	1.42	1.32
1	K	207	ASN	C-O	8.82	1.34	1.24
1	J	139	HIS	CE1-NE2	8.36	1.41	1.32
1	D	139	HIS	CE1-NE2	8.32	1.40	1.32
1	X	139	HIS	CE1-NE2	7.25	1.39	1.32

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	128	ARG	NH1-CZ-NH2	-13.02	102.38	119.30
1	O	179	GLU	CB-CG-CD	11.20	131.65	112.60
1	D	179	GLU	CB-CG-CD	10.79	130.94	112.60
1	G	128	ARG	NE-CZ-NH1	-9.65	111.85	121.50
1	Q	179	GLU	CB-CG-CD	9.57	128.87	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	128	ARG	Sidechain
1	G	128	ARG	Sidechain
1	O	19	LEU	Mainchain
1	W	128	ARG	Sidechain

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	1440	0	1430	31	0
1	B	1425	0	1409	29	0
1	C	1429	0	1417	27	0
1	D	1457	0	1447	41	0
1	E	1429	0	1417	41	0
1	F	1440	0	1430	35	0
1	G	1407	0	1395	25	0
1	H	1424	0	1412	37	0
1	I	1429	0	1417	28	0
1	J	1415	0	1406	34	0
1	K	1429	0	1417	29	0
1	L	1429	0	1417	30	0
1	M	1400	0	1386	21	0
1	N	1401	0	1387	33	0
1	O	1433	0	1420	36	0
1	P	1415	0	1406	29	0
1	Q	1424	0	1412	40	0
1	R	1400	0	1386	22	0
1	S	1424	0	1412	32	0
1	T	1407	0	1395	25	0
1	U	1424	0	1412	25	0
1	V	1424	0	1412	27	0
1	W	1440	0	1430	37	0
1	X	1424	0	1412	30	0
1	Y	1429	0	1417	29	0
1	Z	1429	0	1417	34	0
1	a	1407	0	1395	27	0
1	b	1440	0	1430	31	0
2	A	1	0	0	0	0
2	I	1	0	0	1	0
2	K	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Y	1	0	0	0	0
3	B	12	0	16	0	0
3	C	6	0	8	0	0
3	D	24	0	32	4	0
3	E	12	0	16	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	3	0
3	I	18	0	24	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	18	0	24	3	0
3	K	6	0	8	2	0
3	O	18	0	24	4	0
3	P	6	0	8	3	0
3	T	6	0	8	3	0
3	U	12	0	16	1	0
3	V	18	0	24	2	0
3	W	12	0	16	1	0
3	X	18	0	24	7	0
3	Y	18	0	24	2	0
3	Z	12	0	16	6	0
3	b	12	0	16	4	0
4	A	20	0	0	1	0
4	B	20	0	0	2	0
4	C	33	0	0	1	0
4	D	33	0	0	3	0
4	E	36	0	0	4	0
4	F	28	0	0	10	0
4	G	25	0	0	2	0
4	H	12	0	0	1	0
4	I	30	0	0	1	0
4	J	31	0	0	2	0
4	K	16	0	0	1	0
4	L	6	0	0	1	0
4	M	9	0	0	1	0
4	N	7	0	0	3	0
4	O	26	0	0	2	0
4	P	22	0	0	0	0
4	Q	18	0	0	3	0
4	R	14	0	0	1	0
4	S	10	0	0	2	0
4	T	9	0	0	0	0
4	U	21	0	0	0	0
4	V	31	0	0	1	0
4	W	24	0	0	4	0
4	X	35	0	0	1	0
4	Y	31	0	0	1	0
4	Z	27	0	0	2	0
4	a	34	0	0	4	0
4	b	27	0	0	0	0
All	All	40761	0	39871	782	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 10.

The worst 5 of 782 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:22:MET:HG3	4:a:302:HOH:O	1.30	1.24
1:L:108:CYS:SG	1:L:136:MET:HE1	1.83	1.19
1:F:163:ARG:NH1	1:H:179:GLU:OE1	1.81	1.12
1:I:39:ARG:NH2	1:I:43:GLU:OE2	1.82	1.12
1:Q:130:CYS:HB3	1:Q:136:MET:HE1	1.33	1.10

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	181/213 (85%)	177 (98%)	4 (2%)	0	100	100
1	B	179/213 (84%)	174 (97%)	5 (3%)	0	100	100
1	C	180/213 (84%)	176 (98%)	4 (2%)	0	100	100
1	D	183/213 (86%)	179 (98%)	4 (2%)	0	100	100
1	E	180/213 (84%)	175 (97%)	5 (3%)	0	100	100
1	F	181/213 (85%)	176 (97%)	5 (3%)	0	100	100
1	G	177/213 (83%)	172 (97%)	5 (3%)	0	100	100
1	H	179/213 (84%)	174 (97%)	5 (3%)	0	100	100
1	I	180/213 (84%)	176 (98%)	4 (2%)	0	100	100
1	J	178/213 (84%)	174 (98%)	4 (2%)	0	100	100
1	K	180/213 (84%)	174 (97%)	6 (3%)	0	100	100
1	L	180/213 (84%)	175 (97%)	5 (3%)	0	100	100
1	M	176/213 (83%)	171 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	177/213 (83%)	172 (97%)	5 (3%)	0	100	100
1	O	180/213 (84%)	176 (98%)	4 (2%)	0	100	100
1	P	178/213 (84%)	173 (97%)	5 (3%)	0	100	100
1	Q	179/213 (84%)	174 (97%)	5 (3%)	0	100	100
1	R	176/213 (83%)	171 (97%)	5 (3%)	0	100	100
1	S	179/213 (84%)	175 (98%)	4 (2%)	0	100	100
1	T	177/213 (83%)	172 (97%)	5 (3%)	0	100	100
1	U	179/213 (84%)	175 (98%)	4 (2%)	0	100	100
1	V	179/213 (84%)	175 (98%)	4 (2%)	0	100	100
1	W	181/213 (85%)	176 (97%)	5 (3%)	0	100	100
1	X	179/213 (84%)	175 (98%)	4 (2%)	0	100	100
1	Y	180/213 (84%)	176 (98%)	4 (2%)	0	100	100
1	Z	180/213 (84%)	176 (98%)	4 (2%)	0	100	100
1	a	177/213 (83%)	173 (98%)	4 (2%)	0	100	100
1	b	181/213 (85%)	177 (98%)	4 (2%)	0	100	100
All	All	5016/5964 (84%)	4889 (98%)	127 (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	155/176 (88%)	153 (99%)	2 (1%)	61	79
1	B	154/176 (88%)	151 (98%)	3 (2%)	50	73
1	C	154/176 (88%)	150 (97%)	4 (3%)	40	69
1	D	157/176 (89%)	150 (96%)	7 (4%)	24	56
1	E	154/176 (88%)	148 (96%)	6 (4%)	28	59
1	F	155/176 (88%)	151 (97%)	4 (3%)	40	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	152/176 (86%)	148 (97%)	4 (3%)	40	69
1	H	154/176 (88%)	151 (98%)	3 (2%)	50	73
1	I	154/176 (88%)	148 (96%)	6 (4%)	28	59
1	J	153/176 (87%)	147 (96%)	6 (4%)	28	59
1	K	154/176 (88%)	152 (99%)	2 (1%)	61	79
1	L	154/176 (88%)	151 (98%)	3 (2%)	50	73
1	M	151/176 (86%)	149 (99%)	2 (1%)	61	79
1	N	151/176 (86%)	151 (100%)	0	100	100
1	O	155/176 (88%)	150 (97%)	5 (3%)	34	64
1	P	153/176 (87%)	147 (96%)	6 (4%)	28	59
1	Q	154/176 (88%)	150 (97%)	4 (3%)	40	69
1	R	151/176 (86%)	149 (99%)	2 (1%)	61	79
1	S	154/176 (88%)	149 (97%)	5 (3%)	34	64
1	T	152/176 (86%)	148 (97%)	4 (3%)	40	69
1	U	154/176 (88%)	151 (98%)	3 (2%)	50	73
1	V	154/176 (88%)	150 (97%)	4 (3%)	40	69
1	W	155/176 (88%)	150 (97%)	5 (3%)	34	64
1	X	154/176 (88%)	149 (97%)	5 (3%)	34	64
1	Y	154/176 (88%)	150 (97%)	4 (3%)	40	69
1	Z	154/176 (88%)	151 (98%)	3 (2%)	50	73
1	a	152/176 (86%)	148 (97%)	4 (3%)	40	69
1	b	155/176 (88%)	148 (96%)	7 (4%)	24	56
All	All	4303/4928 (87%)	4190 (97%)	113 (3%)	40	69

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	34	TYR
1	b	138	ILE
1	S	74	LYS
1	b	36	ILE
1	Z	34	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 199 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	63	GLN
1	U	63	GLN
1	Q	176	GLN
1	S	81	ASN
1	V	63	GLN

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 47 ligands modelled in this entry, 6 are monoatomic - leaving 41 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	V	302	-	5,5,5	0.34	0	5,5,5	0.56	0
3	GOL	B	301	-	5,5,5	0.24	0	5,5,5	0.54	0
3	GOL	J	302	-	5,5,5	0.34	0	5,5,5	0.71	0
3	GOL	O	304	-	5,5,5	0.27	0	5,5,5	0.53	0
3	GOL	D	302	-	5,5,5	0.21	0	5,5,5	0.51	0
3	GOL	B	302	-	5,5,5	0.25	0	5,5,5	0.72	0
3	GOL	U	302	-	5,5,5	0.16	0	5,5,5	0.43	0
3	GOL	I	304	-	5,5,5	0.21	0	5,5,5	0.60	0
3	GOL	W	302	-	5,5,5	0.13	0	5,5,5	0.54	0
3	GOL	C	301	-	5,5,5	0.29	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	J	303	-	5,5,5	0.32	0	5,5,5	0.86	0
3	GOL	P	302	-	5,5,5	0.21	0	5,5,5	0.50	0
3	GOL	Y	304	-	5,5,5	0.16	0	5,5,5	0.36	0
3	GOL	Z	302	-	5,5,5	0.21	0	5,5,5	0.53	0
3	GOL	G	301	-	5,5,5	0.12	0	5,5,5	0.31	0
3	GOL	D	304	-	5,5,5	0.16	0	5,5,5	0.49	0
3	GOL	D	301	-	5,5,5	0.27	0	5,5,5	0.71	0
3	GOL	E	302	-	5,5,5	0.15	0	5,5,5	0.48	0
3	GOL	V	301	-	5,5,5	0.31	0	5,5,5	0.91	0
3	GOL	X	302	-	5,5,5	0.17	0	5,5,5	0.61	0
3	GOL	X	303	-	5,5,5	0.26	0	5,5,5	0.54	0
3	GOL	Y	302	-	5,5,5	0.30	0	5,5,5	0.70	0
3	GOL	O	303	-	5,5,5	0.14	0	5,5,5	0.36	0
3	GOL	U	301	-	5,5,5	0.21	0	5,5,5	0.48	0
3	GOL	X	301	-	5,5,5	0.28	0	5,5,5	0.56	0
3	GOL	Y	303	-	5,5,5	0.15	0	5,5,5	0.43	0
3	GOL	V	303	-	5,5,5	0.24	0	5,5,5	0.58	0
3	GOL	Z	301	-	5,5,5	0.25	0	5,5,5	0.84	0
3	GOL	F	301	-	5,5,5	0.17	0	5,5,5	0.36	0
3	GOL	b	302	-	5,5,5	0.23	0	5,5,5	0.68	0
3	GOL	D	303	-	5,5,5	0.21	0	5,5,5	0.57	0
3	GOL	K	302	-	5,5,5	0.27	0	5,5,5	0.55	0
3	GOL	I	303	-	5,5,5	0.23	0	5,5,5	0.61	0
3	GOL	I	302	-	5,5,5	0.26	0	5,5,5	0.61	0
3	GOL	J	301	-	5,5,5	0.31	0	5,5,5	0.63	0
3	GOL	b	301	-	5,5,5	0.16	0	5,5,5	0.37	0
3	GOL	O	302	-	5,5,5	0.33	0	5,5,5	1.09	0
3	GOL	T	301	-	5,5,5	0.09	0	5,5,5	0.60	0
3	GOL	W	301	-	5,5,5	0.35	0	5,5,5	0.85	0
3	GOL	H	301	-	5,5,5	0.24	0	5,5,5	0.66	0
3	GOL	E	301	-	5,5,5	0.22	0	5,5,5	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	V	302	-	-	4/4/4/4	-
3	GOL	B	301	-	-	4/4/4/4	-
3	GOL	J	302	-	-	4/4/4/4	-
3	GOL	O	304	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	302	-	-	2/4/4/4	-
3	GOL	B	302	-	-	2/4/4/4	-
3	GOL	U	302	-	-	4/4/4/4	-
3	GOL	I	304	-	-	1/4/4/4	-
3	GOL	W	302	-	-	2/4/4/4	-
3	GOL	C	301	-	-	0/4/4/4	-
3	GOL	J	303	-	-	0/4/4/4	-
3	GOL	P	302	-	-	0/4/4/4	-
3	GOL	Y	304	-	-	4/4/4/4	-
3	GOL	Z	302	-	-	2/4/4/4	-
3	GOL	G	301	-	-	1/4/4/4	-
3	GOL	D	304	-	-	4/4/4/4	-
3	GOL	D	301	-	-	3/4/4/4	-
3	GOL	E	302	-	-	3/4/4/4	-
3	GOL	V	301	-	-	3/4/4/4	-
3	GOL	X	302	-	-	0/4/4/4	-
3	GOL	X	303	-	-	0/4/4/4	-
3	GOL	Y	302	-	-	0/4/4/4	-
3	GOL	O	303	-	-	2/4/4/4	-
3	GOL	U	301	-	-	2/4/4/4	-
3	GOL	X	301	-	-	4/4/4/4	-
3	GOL	Y	303	-	-	3/4/4/4	-
3	GOL	V	303	-	-	2/4/4/4	-
3	GOL	Z	301	-	-	0/4/4/4	-
3	GOL	F	301	-	-	4/4/4/4	-
3	GOL	b	302	-	-	4/4/4/4	-
3	GOL	D	303	-	-	4/4/4/4	-
3	GOL	K	302	-	-	2/4/4/4	-
3	GOL	I	303	-	-	2/4/4/4	-
3	GOL	I	302	-	-	3/4/4/4	-
3	GOL	J	301	-	-	3/4/4/4	-
3	GOL	b	301	-	-	2/4/4/4	-
3	GOL	O	302	-	-	4/4/4/4	-
3	GOL	T	301	-	-	0/4/4/4	-
3	GOL	W	301	-	-	2/4/4/4	-
3	GOL	H	301	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	GOL	O1-C1-C2-C3
3	B	302	GOL	O1-C1-C2-C3
3	D	303	GOL	O1-C1-C2-C3
3	D	303	GOL	C1-C2-C3-O3
3	D	304	GOL	O1-C1-C2-C3

There are no ring outliers.

25 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	302	GOL	2	0
3	O	304	GOL	1	0
3	D	302	GOL	2	0
3	I	304	GOL	3	0
3	J	303	GOL	1	0
3	P	302	GOL	3	0
3	Y	304	GOL	1	0
3	Z	302	GOL	3	0
3	V	301	GOL	1	0
3	X	302	GOL	3	0
3	X	303	GOL	3	0
3	Y	302	GOL	1	0
3	U	301	GOL	1	0
3	X	301	GOL	1	0
3	V	303	GOL	1	0
3	Z	301	GOL	3	0
3	b	302	GOL	4	0
3	D	303	GOL	2	0
3	K	302	GOL	2	0
3	I	303	GOL	1	0
3	I	302	GOL	1	0
3	O	302	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	301	GOL	3	0
3	W	301	GOL	1	0
3	H	301	GOL	3	0

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	185/213 (86%)	0.11	5 (2%) 56 32	58, 77, 116, 161	0
1	B	183/213 (85%)	-0.11	3 (1%) 70 47	51, 70, 103, 146	0
1	C	184/213 (86%)	-0.15	4 (2%) 62 38	49, 65, 111, 143	0
1	D	187/213 (87%)	-0.14	5 (2%) 56 32	48, 60, 116, 175	0
1	E	184/213 (86%)	-0.16	5 (2%) 56 32	47, 64, 112, 167	0
1	F	185/213 (86%)	0.04	6 (3%) 50 28	50, 71, 116, 145	0
1	G	181/213 (84%)	0.07	6 (3%) 49 27	61, 76, 108, 142	0
1	H	183/213 (85%)	0.03	3 (1%) 70 47	57, 76, 114, 169	0
1	I	184/213 (86%)	-0.06	5 (2%) 56 32	55, 69, 109, 186	0
1	J	182/213 (85%)	-0.09	5 (2%) 56 32	53, 67, 98, 151	0
1	K	184/213 (86%)	0.10	4 (2%) 62 38	59, 83, 127, 167	0
1	L	184/213 (86%)	0.40	6 (3%) 49 27	71, 98, 132, 161	0
1	M	180/213 (84%)	0.40	4 (2%) 62 38	77, 103, 135, 160	0
1	N	181/213 (84%)	0.24	5 (2%) 55 31	67, 92, 122, 220	0
1	O	184/213 (86%)	-0.07	7 (3%) 44 24	53, 68, 115, 166	0
1	P	182/213 (85%)	0.05	6 (3%) 49 27	56, 76, 111, 153	0
1	Q	183/213 (85%)	0.23	5 (2%) 56 32	56, 84, 124, 157	0
1	R	180/213 (84%)	0.40	4 (2%) 62 38	71, 98, 128, 154	0
1	S	183/213 (85%)	0.48	7 (3%) 44 24	76, 102, 140, 175	0
1	T	181/213 (84%)	0.21	4 (2%) 62 38	59, 88, 123, 144	0
1	U	183/213 (85%)	-0.00	4 (2%) 62 38	46, 77, 116, 152	0
1	V	183/213 (85%)	-0.07	4 (2%) 62 38	46, 64, 103, 167	0
1	W	185/213 (86%)	-0.05	5 (2%) 56 32	49, 64, 114, 169	0
1	X	183/213 (85%)	-0.26	0 100 100	45, 59, 99, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	184/213 (86%)	-0.16	3 (1%) 70 47	47, 62, 109, 175	0
1	Z	184/213 (86%)	-0.10	5 (2%) 56 32	48, 64, 100, 144	0
1	a	181/213 (84%)	-0.08	4 (2%) 62 38	53, 70, 107, 143	0
1	b	185/213 (86%)	-0.08	2 (1%) 78 56	52, 69, 103, 147	0
All	All	5128/5964 (85%)	0.04	126 (2%) 58 34	45, 75, 122, 220	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	33	ALA	4.8
1	D	33	ALA	4.7
1	R	141	PRO	4.2
1	Q	141	PRO	4.0
1	I	19	LEU	4.0

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
3	GOL	G	301	6/6	0.76	0.14	76,86,88,90	0
3	GOL	D	304	6/6	0.77	0.25	99,103,107,109	0
3	GOL	W	302	6/6	0.79	0.14	91,102,107,108	0
3	GOL	C	301	6/6	0.84	0.20	65,73,75,77	0
3	GOL	I	304	6/6	0.85	0.25	69,74,83,91	0
3	GOL	P	302	6/6	0.85	0.25	71,89,98,105	0
3	GOL	T	301	6/6	0.85	0.24	82,89,95,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	W	301	6/6	0.85	0.21	66,74,81,91	0
3	GOL	D	301	6/6	0.85	0.19	50,59,67,75	0
3	GOL	B	302	6/6	0.87	0.21	69,80,91,95	0
3	GOL	b	302	6/6	0.87	0.25	81,89,94,94	0
3	GOL	Z	301	6/6	0.88	0.15	54,66,68,69	0
3	GOL	V	301	6/6	0.88	0.17	50,60,63,71	0
3	GOL	V	303	6/6	0.89	0.17	47,67,71,74	0
3	GOL	O	302	6/6	0.89	0.17	48,60,63,66	0
2	CL	A	301	1/1	0.89	0.08	75,75,75,75	0
3	GOL	Y	302	6/6	0.89	0.14	49,63,64,74	0
2	CL	O	301	1/1	0.89	0.12	76,76,76,76	0
3	GOL	J	303	6/6	0.89	0.16	46,52,58,70	0
3	GOL	Y	303	6/6	0.90	0.10	73,84,86,88	0
3	GOL	J	301	6/6	0.91	0.16	52,58,63,69	0
3	GOL	I	303	6/6	0.91	0.15	76,80,86,91	0
3	GOL	I	302	6/6	0.91	0.13	59,63,71,77	0
3	GOL	O	303	6/6	0.91	0.09	64,77,79,82	0
3	GOL	O	304	6/6	0.91	0.16	55,67,69,70	0
3	GOL	X	301	6/6	0.92	0.15	54,62,65,70	0
3	GOL	K	302	6/6	0.92	0.15	59,74,75,75	0
3	GOL	H	301	6/6	0.92	0.14	64,72,81,82	0
3	GOL	E	301	6/6	0.92	0.13	49,57,61,62	0
3	GOL	b	301	6/6	0.92	0.09	76,80,83,84	0
3	GOL	U	301	6/6	0.92	0.18	69,84,86,87	0
3	GOL	X	303	6/6	0.93	0.12	44,58,68,87	0
3	GOL	V	302	6/6	0.94	0.12	52,58,61,64	0
3	GOL	E	302	6/6	0.94	0.13	47,58,70,81	0
3	GOL	F	301	6/6	0.94	0.15	59,75,78,86	0
3	GOL	J	302	6/6	0.94	0.10	50,59,61,65	0
2	CL	K	301	1/1	0.94	0.12	76,76,76,76	0
3	GOL	X	302	6/6	0.94	0.12	45,55,58,58	0
3	GOL	Y	304	6/6	0.95	0.11	59,60,61,62	0
2	CL	Y	301	1/1	0.95	0.14	66,66,66,66	0
3	GOL	Z	302	6/6	0.95	0.10	38,48,54,56	0
3	GOL	U	302	6/6	0.95	0.13	76,80,85,85	0
3	GOL	D	303	6/6	0.95	0.10	47,53,56,58	0
3	GOL	B	301	6/6	0.96	0.12	53,62,68,69	0
3	GOL	D	302	6/6	0.96	0.11	48,59,63,72	0
2	CL	I	301	1/1	0.98	0.08	73,73,73,73	0
2	CL	P	301	1/1	0.98	0.05	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.