



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 06:10 AM EDT

PDB ID : 3Q7H
Title : Structure of the ClpP subunit of the ATP-dependent Clp Protease from *Coxiella burnetii*
Authors : Anderson, S.M.; Wawrzak, Z.; Gordon, E.; Hasseman, J.; Anderson, W.F.; Savchenko, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-01-04
Resolution : 2.50 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

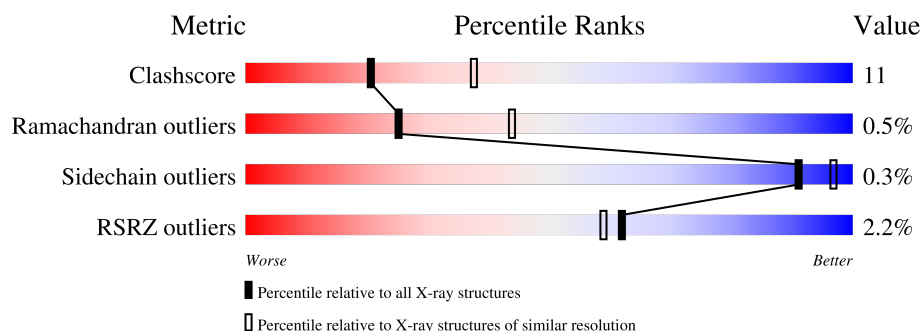
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	195	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>5%</div> </div> </div>
1	B	195	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>
1	C	195	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>.</div> </div> </div>
1	D	195	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
1	E	195	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>.</div> </div> </div>
1	F	195	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	195	
1	H	195	
1	I	195	
1	J	195	
1	K	195	
1	L	195	
1	M	195	
1	N	195	

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
2	PEG	A	197	-	-	X	-
2	PEG	C	197	-	-	X	-
2	PEG	C	198	-	-	X	-
2	PEG	G	196	-	-	X	-
2	PEG	G	197	-	-	X	-
2	PEG	H	199	-	-	X	-
2	PEG	I	196	-	-	X	-
2	PEG	I	197	-	-	X	-
2	PEG	I	198	-	-	X	-
2	PEG	N	197	-	-	X	-

2 Entry composition

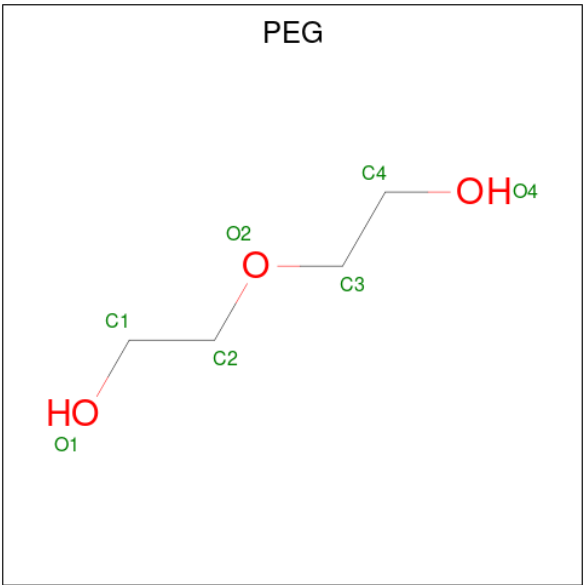
There are 4 unique types of molecules in this entry. The entry contains 22217 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	186	Total	C	N	O	S	Se	0	0	0
			1443	908	252	275	2	6			
1	B	193	Total	C	N	O	S	Se	0	0	0
			1490	937	261	284	2	6			
1	C	191	Total	C	N	O	S	Se	0	0	0
			1486	931	263	284	2	6			
1	D	193	Total	C	N	O	S	Se	0	1	0
			1492	936	262	286	2	6			
1	E	187	Total	C	N	O	S	Se	0	0	0
			1453	915	253	277	2	6			
1	F	185	Total	C	N	O	S	Se	0	0	0
			1434	903	250	273	2	6			
1	G	193	Total	C	N	O	S	Se	0	1	0
			1500	940	268	284	2	6			
1	H	191	Total	C	N	O	S	Se	0	0	0
			1476	926	260	282	2	6			
1	I	189	Total	C	N	O	S	Se	0	0	0
			1464	920	255	281	2	6			
1	J	184	Total	C	N	O	S	Se	0	0	0
			1429	900	249	272	2	6			
1	K	189	Total	C	N	O	S	Se	0	0	0
			1463	921	255	279	2	6			
1	L	192	Total	C	N	O	S	Se	0	0	0
			1494	937	264	285	2	6			
1	M	192	Total	C	N	O	S	Se	0	0	0
			1494	937	264	285	2	6			
1	N	192	Total	C	N	O	S	Se	0	0	0
			1483	932	261	282	2	6			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			7	4	3		
2	H	1	Total	C	O	0	0
			7	4	3		
2	H	1	Total	C	O	0	0
			7	4	3		
2	H	1	Total	C	O	0	0
			7	4	3		
2	I	1	Total	C	O	0	0
			7	4	3		
2	I	1	Total	C	O	0	0
			7	4	3		
2	I	1	Total	C	O	0	0
			7	4	3		
2	I	1	Total	C	O	0	0
			7	4	3		
2	J	1	Total	C	O	0	0
			7	4	3		
2	J	1	Total	C	O	0	0
			7	4	3		
2	J	1	Total	C	O	0	0
			7	4	3		
2	K	1	Total	C	O	0	0
			7	4	3		
2	K	1	Total	C	O	0	0
			7	4	3		
2	L	1	Total	C	O	0	0
			7	4	3		
2	L	1	Total	C	O	0	0
			7	4	3		
2	M	1	Total	C	O	0	0
			7	4	3		
2	M	1	Total	C	O	0	0
			7	4	3		
2	N	1	Total	C	O	0	0
			7	4	3		
2	N	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0
3	E	3	Total Ca 3 3	0	0
3	F	2	Total Ca 2 2	0	0
3	G	2	Total Ca 2 2	0	0
3	H	2	Total Ca 2 2	0	0
3	I	2	Total Ca 2 2	0	0
3	J	2	Total Ca 2 2	0	0
3	K	2	Total Ca 2 2	0	0
3	L	2	Total Ca 2 2	0	0
3	M	2	Total Ca 2 2	0	0
3	N	2	Total Ca 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	88	Total O 88 88	0	0
4	B	88	Total O 88 88	0	0
4	C	99	Total O 99 99	0	0
4	D	112	Total O 113 113	0	1
4	E	74	Total O 74 74	0	0
4	F	88	Total O 88 88	0	0

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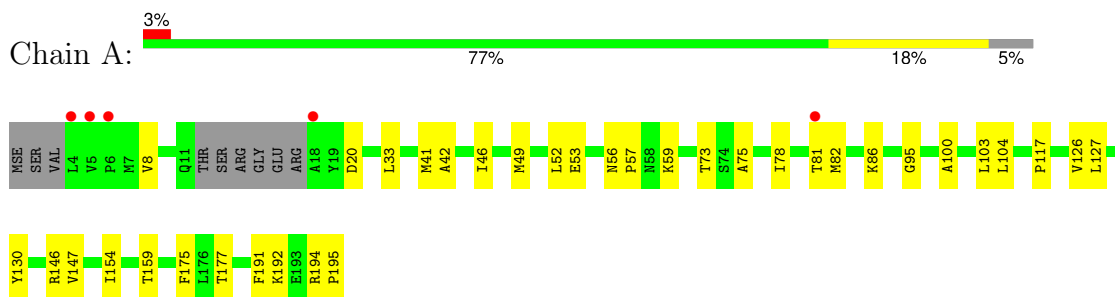
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	102	Total 102	O 102	0	0
4	H	96	Total 96	O 96	0	0
4	I	84	Total 85	O 85	0	1
4	J	87	Total 87	O 87	0	0
4	K	94	Total 94	O 94	0	0
4	L	125	Total 125	O 125	0	0
4	M	100	Total 100	O 100	0	0
4	N	118	Total 118	O 118	0	0

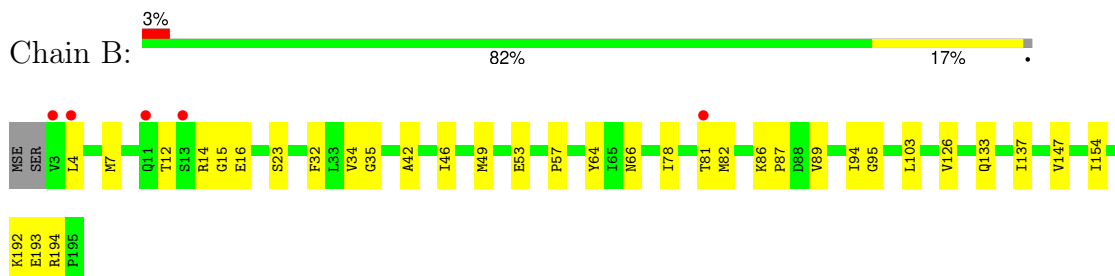
3 Residue-property plots [i](#)

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.

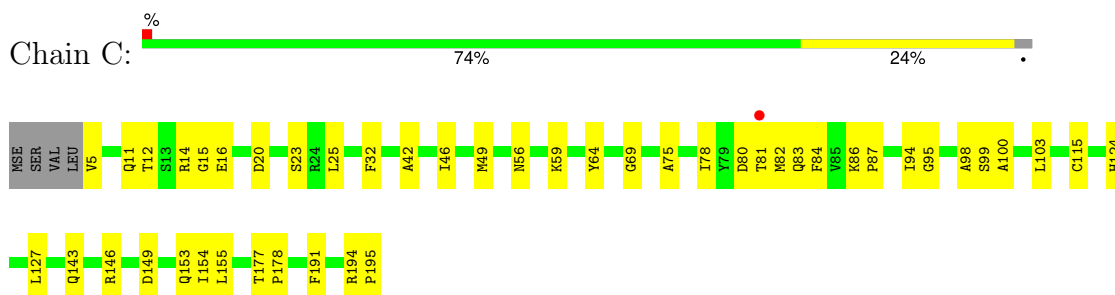
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



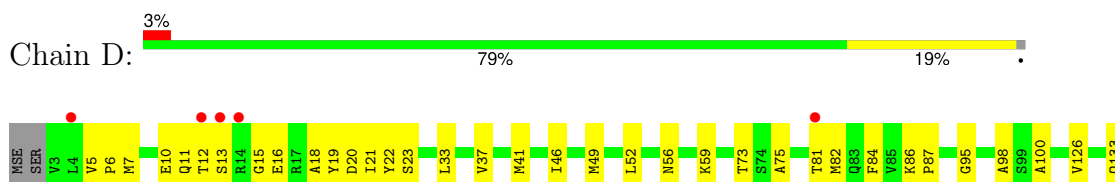
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

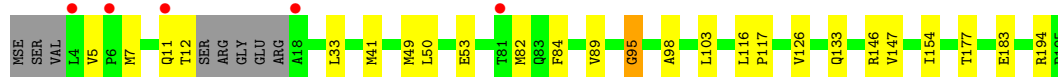
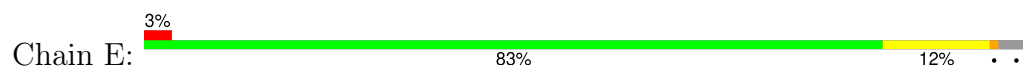


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

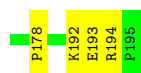
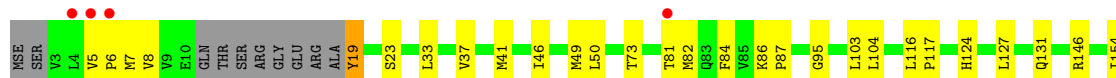




- Molecule 1: ATP-dependent Clp protease proteolytic subunit



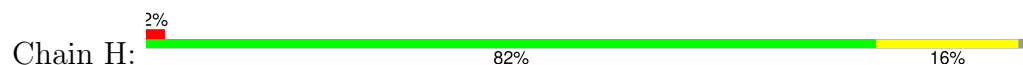
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



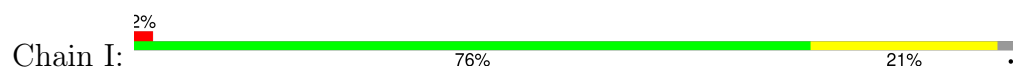
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

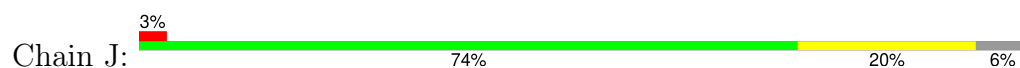


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

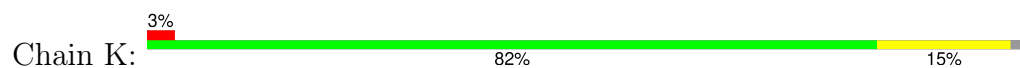




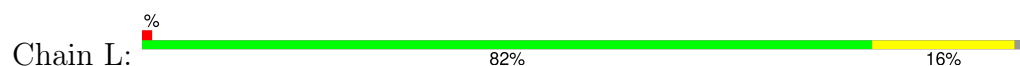
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



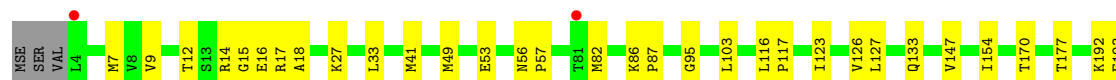
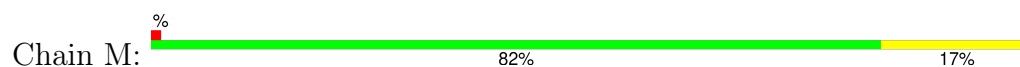
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



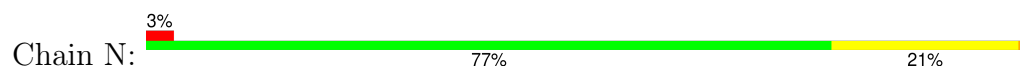
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.91Å 137.47Å 127.78Å 90.00° 109.03° 90.00°	Depositor
Resolution (Å)	37.49 – 2.50 37.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.49-2.50) 95.3 (37.49-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.170 , 0.208 0.168 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22217	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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, PEG

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	0.45	0/1460	0.57	0/1961
1	B	0.42	0/1508	0.55	0/2028
1	C	0.45	0/1504	0.58	0/2020
1	D	0.47	0/1513	0.56	0/2034
1	E	0.45	0/1470	0.57	0/1975
1	F	0.44	0/1451	0.54	0/1949
1	G	0.47	0/1521	0.56	0/2043
1	H	0.52	0/1494	0.57	0/2008
1	I	0.47	0/1481	0.56	0/1990
1	J	0.49	0/1446	0.58	0/1942
1	K	0.50	0/1480	0.57	0/1989
1	L	0.44	0/1512	0.56	0/2031
1	M	0.48	0/1512	0.57	0/2031
1	N	0.51	0/1500	0.59	0/2017
All	All	0.47	0/20852	0.57	0/28018

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1443	0	1441	39	0
1	B	1490	0	1487	38	0
1	C	1486	0	1487	47	0
1	D	1492	0	1482	38	0
1	E	1453	0	1457	26	0
1	F	1434	0	1430	32	0
1	G	1500	0	1500	50	0
1	H	1476	0	1472	27	0
1	I	1464	0	1456	43	0
1	J	1429	0	1428	39	0
1	K	1463	0	1461	29	0
1	L	1494	0	1498	28	0
1	M	1494	0	1498	33	0
1	N	1483	0	1485	51	0
2	A	21	0	30	6	0
2	B	21	0	30	2	0
2	C	21	0	30	18	0
2	D	7	0	10	0	0
2	E	7	0	10	1	0
2	F	7	0	10	0	0
2	G	14	0	20	11	0
2	H	28	0	40	12	0
2	I	28	0	40	24	0
2	J	21	0	30	5	0
2	K	14	0	20	0	0
2	L	14	0	20	1	0
2	M	14	0	20	0	0
2	N	14	0	20	12	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
4	A	88	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	88	0	0	0	0
4	C	99	0	0	1	0
4	D	113	0	0	4	0
4	E	74	0	0	3	0
4	F	88	0	0	3	0
4	G	102	0	0	7	0
4	H	96	0	0	1	0
4	I	85	0	0	0	0
4	J	87	0	0	8	0
4	K	94	0	0	3	0
4	L	125	0	0	1	0
4	M	100	0	0	2	0
4	N	118	0	0	1	0
All	All	22217	0	20912	458	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 458 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:C:83:GLN:HB2	2:C:197:PEG:H12	1.16	1.12
1:M:49:MSE:HE1	1:M:82:MSE:HA	1.29	1.11
1:H:49:MSE:HE1	1:H:82:MSE:HA	1.31	1.07
1:N:40:HIS:HA	2:N:197:PEG:H32	1.32	1.07
1:I:68:PRO:HB3	1:I:96:GLN:OE1	1.52	1.07

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	182/195 (93%)	174 (96%)	7 (4%)	1 (0%)	25	44
1	B	191/195 (98%)	189 (99%)	1 (0%)	1 (0%)	25	44
1	C	189/195 (97%)	186 (98%)	2 (1%)	1 (0%)	25	44
1	D	192/195 (98%)	190 (99%)	1 (0%)	1 (0%)	25	44
1	E	183/195 (94%)	180 (98%)	2 (1%)	1 (0%)	25	44
1	F	181/195 (93%)	177 (98%)	3 (2%)	1 (1%)	22	39
1	G	192/195 (98%)	190 (99%)	1 (0%)	1 (0%)	25	44
1	H	189/195 (97%)	186 (98%)	2 (1%)	1 (0%)	25	44
1	I	185/195 (95%)	181 (98%)	3 (2%)	1 (0%)	25	44
1	J	180/195 (92%)	177 (98%)	2 (1%)	1 (1%)	22	39
1	K	185/195 (95%)	179 (97%)	5 (3%)	1 (0%)	25	44
1	L	190/195 (97%)	187 (98%)	2 (1%)	1 (0%)	25	44
1	M	190/195 (97%)	185 (97%)	4 (2%)	1 (0%)	25	44
1	N	190/195 (97%)	188 (99%)	1 (0%)	1 (0%)	25	44
All	All	2619/2730 (96%)	2569 (98%)	36 (1%)	14 (0%)	25	44

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	95	GLY
1	G	95	GLY
1	L	95	GLY
1	N	95	GLY
1	A	95	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	155/157 (99%)	155 (100%)	0	100	100
1	B	159/157 (101%)	159 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	160/157 (102%)	160 (100%)	0	100	100
1	D	159/157 (101%)	159 (100%)	0	100	100
1	E	157/157 (100%)	157 (100%)	0	100	100
1	F	154/157 (98%)	153 (99%)	1 (1%)	84	94
1	G	160/157 (102%)	159 (99%)	1 (1%)	84	94
1	H	158/157 (101%)	158 (100%)	0	100	100
1	I	157/157 (100%)	157 (100%)	0	100	100
1	J	154/157 (98%)	154 (100%)	0	100	100
1	K	157/157 (100%)	155 (99%)	2 (1%)	65	85
1	L	161/157 (102%)	161 (100%)	0	100	100
1	M	161/157 (102%)	161 (100%)	0	100	100
1	N	159/157 (101%)	157 (99%)	2 (1%)	65	85
All	All	2211/2198 (101%)	2205 (100%)	6 (0%)	91	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	54	SER
1	N	19	TYR
1	N	194	ARG
1	G	7	MSE
1	F	19	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	124	HIS
1	L	145	GLN
1	N	96	GLN
1	M	145	GLN
1	C	124	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 61 ligands modelled in this entry, 28 are monoatomic - leaving 33 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	$\# Z > 2$
2	PEG	B	196	-	6,6,6	0.53	0	5,5,5	0.19	0
2	PEG	C	197	-	6,6,6	0.54	0	5,5,5	0.28	0
2	PEG	N	197	-	6,6,6	0.50	0	5,5,5	0.33	0
2	PEG	I	198	-	6,6,6	0.56	0	5,5,5	0.29	0
2	PEG	H	197	-	6,6,6	0.37	0	5,5,5	0.39	0
2	PEG	I	199	-	6,6,6	0.48	0	5,5,5	0.15	0
2	PEG	N	196	-	6,6,6	0.41	0	5,5,5	0.36	0
2	PEG	A	197	-	6,6,6	0.53	0	5,5,5	0.26	0
2	PEG	H	196	-	6,6,6	0.45	0	5,5,5	0.28	0
2	PEG	J	197	-	6,6,6	0.43	0	5,5,5	0.37	0
2	PEG	K	196	-	6,6,6	0.41	0	5,5,5	0.38	0
2	PEG	G	196	-	6,6,6	0.44	0	5,5,5	0.37	0
2	PEG	D	196	-	6,6,6	0.48	0	5,5,5	0.22	0
2	PEG	L	197	-	6,6,6	0.48	0	5,5,5	0.23	0
2	PEG	M	196	-	6,6,6	0.40	0	5,5,5	0.42	0
2	PEG	J	198	-	6,6,6	0.46	0	5,5,5	0.25	0
2	PEG	A	196	-	6,6,6	0.43	0	5,5,5	0.36	0
2	PEG	B	197	-	6,6,6	0.42	0	5,5,5	0.37	0
2	PEG	M	197	-	6,6,6	0.59	0	5,5,5	0.31	0
2	PEG	E	196	-	6,6,6	0.47	0	5,5,5	0.18	0
2	PEG	H	198	-	6,6,6	0.37	0	5,5,5	0.52	0
2	PEG	G	197	-	6,6,6	0.47	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	J	196	-	6,6,6	0.40	0	5,5,5	0.30	0
2	PEG	H	199	-	6,6,6	0.45	0	5,5,5	0.37	0
2	PEG	L	196	-	6,6,6	0.38	0	5,5,5	0.55	0
2	PEG	K	197	-	6,6,6	0.45	0	5,5,5	0.27	0
2	PEG	I	197	-	6,6,6	0.44	0	5,5,5	0.16	0
2	PEG	C	198	-	6,6,6	0.49	0	5,5,5	0.18	0
2	PEG	I	196	-	6,6,6	0.46	0	5,5,5	0.24	0
2	PEG	B	198	-	6,6,6	0.51	0	5,5,5	0.24	0
2	PEG	A	198	-	6,6,6	0.43	0	5,5,5	0.30	0
2	PEG	C	196	-	6,6,6	0.47	0	5,5,5	0.26	0
2	PEG	F	196	-	6,6,6	0.48	0	5,5,5	0.14	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
2	PEG	B	196	-	-	3/4/4/4	-
2	PEG	C	197	-	-	3/4/4/4	-
2	PEG	N	197	-	-	4/4/4/4	-
2	PEG	I	198	-	-	2/4/4/4	-
2	PEG	H	197	-	-	3/4/4/4	-
2	PEG	I	199	-	-	4/4/4/4	-
2	PEG	N	196	-	-	3/4/4/4	-
2	PEG	A	197	-	-	4/4/4/4	-
2	PEG	H	196	-	-	2/4/4/4	-
2	PEG	J	197	-	-	1/4/4/4	-
2	PEG	K	196	-	-	2/4/4/4	-
2	PEG	G	196	-	-	3/4/4/4	-
2	PEG	D	196	-	-	3/4/4/4	-
2	PEG	L	197	-	-	3/4/4/4	-
2	PEG	M	196	-	-	4/4/4/4	-
2	PEG	J	198	-	-	4/4/4/4	-
2	PEG	A	196	-	-	2/4/4/4	-
2	PEG	B	197	-	-	2/4/4/4	-
2	PEG	M	197	-	-	3/4/4/4	-
2	PEG	E	196	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	H	198	-	-	3/4/4/4	-
2	PEG	G	197	-	-	3/4/4/4	-
2	PEG	J	196	-	-	4/4/4/4	-
2	PEG	H	199	-	-	4/4/4/4	-
2	PEG	L	196	-	-	4/4/4/4	-
2	PEG	K	197	-	-	2/4/4/4	-
2	PEG	I	197	-	-	4/4/4/4	-
2	PEG	C	198	-	-	3/4/4/4	-
2	PEG	I	196	-	-	2/4/4/4	-
2	PEG	B	198	-	-	2/4/4/4	-
2	PEG	A	198	-	-	2/4/4/4	-
2	PEG	C	196	-	-	2/4/4/4	-
2	PEG	F	196	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	198	PEG	C4-C3-O2-C2
2	C	196	PEG	C4-C3-O2-C2
2	G	196	PEG	C4-C3-O2-C2
2	B	197	PEG	O2-C3-C4-O4
2	J	198	PEG	O1-C1-C2-O2

There are no ring outliers.

22 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	196	PEG	1	0
2	C	197	PEG	12	0
2	N	197	PEG	12	0
2	I	198	PEG	8	0
2	I	199	PEG	1	0
2	A	197	PEG	5	0
2	H	196	PEG	1	0
2	G	196	PEG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	198	PEG	2	0
2	B	197	PEG	1	0
2	E	196	PEG	1	0
2	H	198	PEG	2	0
2	G	197	PEG	4	0
2	J	196	PEG	3	0
2	H	199	PEG	9	0
2	L	196	PEG	1	0
2	I	197	PEG	9	0
2	C	198	PEG	5	0
2	I	196	PEG	6	0
2	B	198	PEG	1	0
2	A	198	PEG	1	0
2	C	196	PEG	1	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	180/195 (92%)	-0.40	5 (2%) 55 51	26, 34, 65, 98	0
1	B	187/195 (95%)	-0.42	5 (2%) 56 52	25, 33, 69, 115	0
1	C	185/195 (94%)	-0.42	1 (0%) 87 85	24, 33, 66, 118	0
1	D	187/195 (95%)	-0.40	5 (2%) 56 52	19, 33, 71, 143	1 (0%)
1	E	181/195 (92%)	-0.35	5 (2%) 55 51	26, 35, 66, 108	0
1	F	179/195 (91%)	-0.38	4 (2%) 62 59	26, 35, 62, 102	0
1	G	187/195 (95%)	-0.40	5 (2%) 56 52	17, 32, 79, 146	1 (0%)
1	H	185/195 (94%)	-0.46	3 (1%) 70 67	25, 33, 64, 131	0
1	I	183/195 (93%)	-0.52	4 (2%) 62 59	25, 33, 63, 91	0
1	J	178/195 (91%)	-0.40	6 (3%) 48 45	26, 34, 61, 99	0
1	K	183/195 (93%)	-0.46	5 (2%) 56 52	25, 33, 61, 115	0
1	L	186/195 (95%)	-0.55	2 (1%) 77 74	23, 31, 57, 80	0
1	M	186/195 (95%)	-0.53	2 (1%) 77 74	24, 32, 57, 81	0
1	N	186/195 (95%)	-0.47	5 (2%) 56 52	24, 32, 67, 162	0
All	All	2573/2730 (94%)	-0.44	57 (2%) 62 59	17, 33, 66, 162	2 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	17	ARG	5.1
1	J	5	VAL	4.1
1	N	14	ARG	4.1
1	K	3	VAL	4.0
1	E	4	LEU	3.9

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 monosaccharides 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(\AA^2)	Q<0.9
2	PEG	G	196	7/7	0.73	0.15	54,59,67,69	0
2	PEG	B	196	7/7	0.75	0.17	58,63,67,76	0
2	PEG	I	199	7/7	0.75	0.20	57,64,68,72	0
2	PEG	J	198	7/7	0.75	0.16	63,69,74,75	0
2	PEG	N	197	7/7	0.75	0.31	49,53,58,60	0
2	PEG	B	197	7/7	0.77	0.16	51,63,69,77	0
2	PEG	D	196	7/7	0.78	0.18	65,66,78,81	0
2	PEG	I	198	7/7	0.79	0.24	43,52,57,62	0
2	PEG	M	196	7/7	0.80	0.15	54,60,69,76	0
3	CA	E	198	1/1	0.80	0.16	74,74,74,74	0
2	PEG	E	196	7/7	0.81	0.21	57,62,70,80	0
2	PEG	C	196	7/7	0.81	0.16	46,50,71,71	0
2	PEG	H	196	7/7	0.82	0.15	53,56,64,71	0
2	PEG	N	196	7/7	0.82	0.16	44,52,60,81	0
2	PEG	B	198	7/7	0.82	0.15	43,55,62,72	0
2	PEG	L	197	7/7	0.82	0.14	45,56,69,74	0
2	PEG	C	197	7/7	0.83	0.28	34,47,59,59	0
2	PEG	J	196	7/7	0.83	0.24	45,50,76,86	0
2	PEG	J	197	7/7	0.83	0.15	52,57,69,69	0
2	PEG	G	197	7/7	0.83	0.20	48,52,60,61	0
2	PEG	K	196	7/7	0.83	0.16	59,62,70,71	0
2	PEG	H	198	7/7	0.84	0.22	31,44,63,66	0
2	PEG	K	197	7/7	0.86	0.14	51,54,65,67	0
2	PEG	C	198	7/7	0.86	0.20	46,52,58,60	0
2	PEG	F	196	7/7	0.86	0.14	56,57,67,70	0
2	PEG	L	196	7/7	0.87	0.13	35,39,54,56	0
2	PEG	H	197	7/7	0.88	0.11	48,53,62,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEG	H	199	7/7	0.88	0.21	38,41,52,52	0
2	PEG	M	197	7/7	0.88	0.13	36,43,60,61	0
2	PEG	A	197	7/7	0.89	0.19	36,39,45,48	0
2	PEG	A	196	7/7	0.89	0.13	51,57,65,66	0
2	PEG	A	198	7/7	0.90	0.12	49,53,62,65	0
2	PEG	I	196	7/7	0.90	0.26	38,44,50,51	0
2	PEG	I	197	7/7	0.91	0.29	40,41,49,50	0
3	CA	J	200	1/1	0.95	0.09	44,44,44,44	0
3	CA	E	197	1/1	0.96	0.04	41,41,41,41	0
3	CA	K	198	1/1	0.96	0.05	38,38,38,38	0
3	CA	C	200	1/1	0.97	0.11	55,55,55,55	0
3	CA	H	201	1/1	0.97	0.09	53,53,53,53	0
3	CA	K	199	1/1	0.97	0.05	45,45,45,45	0
3	CA	L	198	1/1	0.97	0.06	34,34,34,34	0
3	CA	L	199	1/1	0.97	0.08	44,44,44,44	0
3	CA	N	198	1/1	0.97	0.06	32,32,32,32	0
3	CA	I	201	1/1	0.98	0.09	52,52,52,52	0
3	CA	A	199	1/1	0.98	0.04	37,37,37,37	0
3	CA	F	197	1/1	0.98	0.06	39,39,39,39	0
3	CA	F	198	1/1	0.98	0.07	58,58,58,58	0
3	CA	G	198	1/1	0.98	0.05	38,38,38,38	0
3	CA	G	199	1/1	0.98	0.04	47,47,47,47	0
3	CA	M	198	1/1	0.98	0.03	34,34,34,34	0
3	CA	M	199	1/1	0.98	0.06	48,48,48,48	0
3	CA	B	200	1/1	0.98	0.10	48,48,48,48	0
3	CA	N	199	1/1	0.98	0.06	51,51,51,51	0
3	CA	C	199	1/1	0.99	0.06	35,35,35,35	0
3	CA	B	199	1/1	0.99	0.02	32,32,32,32	0
3	CA	H	200	1/1	0.99	0.04	40,40,40,40	0
3	CA	E	199	1/1	0.99	0.05	54,54,54,54	0
3	CA	I	200	1/1	0.99	0.04	38,38,38,38	0
3	CA	D	197	1/1	0.99	0.04	32,32,32,32	0
3	CA	J	199	1/1	0.99	0.03	34,34,34,34	0
3	CA	D	198	1/1	0.99	0.05	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.