wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:14 AM GMT

PDB ID	:	2FZS
Title	:	Crystal structure of E. coli ClpP with a Peptide Chloromethyl Ketone Covalently Bound at the Active Site
Authors	:	Szyk, A.; Maurizi, M.R.
Deposited on	:	2006-02-10
Resolution	:	1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

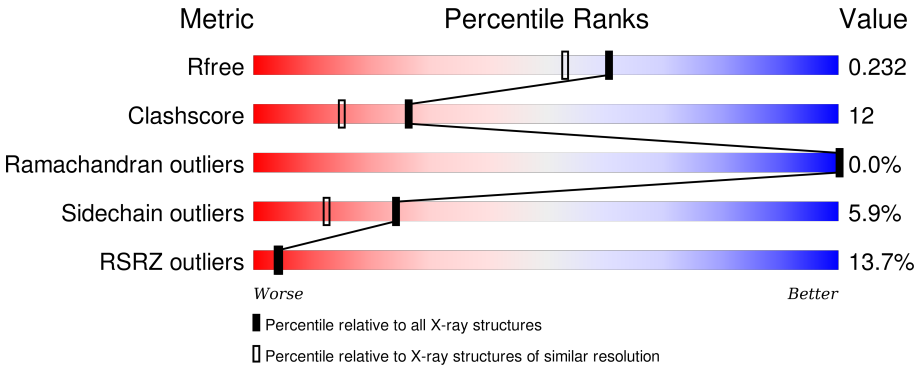
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	193	11% 77% 13% 6%
1	B	193	17% 79% 17%
1	C	193	13% 75% 15% 5% 5%
1	D	193	14% 75% 17%
1	E	193	16% 80% 16%

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Mol	Chain	Length	Quality of chain
1	F	193	9% 79% 15%
1	G	193	12% 74% 18% 5%
1	H	193	12% 78% 13% 5%
1	I	193	13% 72% 21% 5%
1	J	193	13% 76% 18%
1	K	193	13% 76% 18%
1	L	193	12% 75% 17% 5%
1	M	193	13% 76% 18%
1	N	193	15% 83% 10% 5%

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	PGE	E	4005	-	-	-	X
4	GOL	B	3002	-	-	-	X
4	GOL	C	3005	-	-	-	X
4	GOL	C	3006	-	-	X	X
4	GOL	F	3004	-	-	-	X
4	GOL	H	3008	-	-	-	X
4	GOL	K	3010	-	-	-	X

2 Entry composition

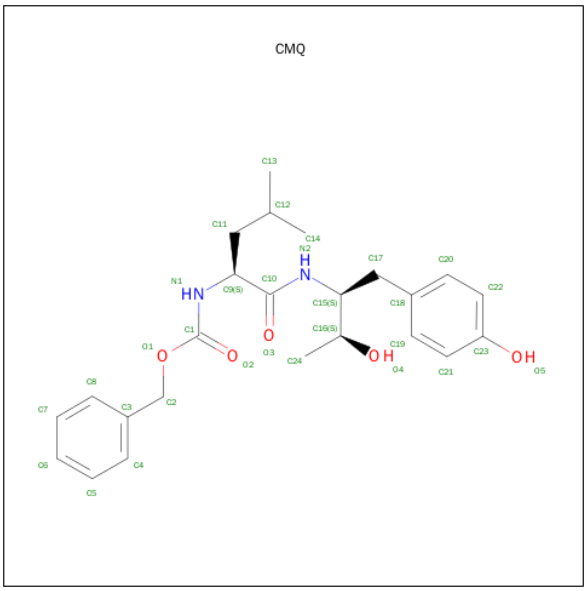
There are 5 unique types of molecules in this entry. The entry contains 24125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

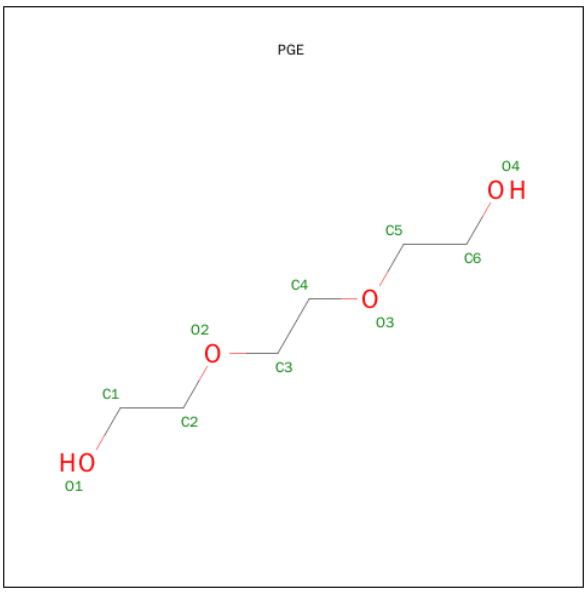
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	7	0
			1487	946	252	274	15			
1	B	192	Total	C	N	O	S	0	10	0
			1554	981	268	290	15			
1	C	183	Total	C	N	O	S	0	7	0
			1467	931	254	270	12			
1	D	185	Total	C	N	O	S	0	3	0
			1462	926	249	275	12			
1	E	188	Total	C	N	O	S	0	2	0
			1479	936	252	278	13			
1	F	185	Total	C	N	O	S	0	2	0
			1453	920	247	274	12			
1	G	183	Total	C	N	O	S	0	4	0
			1448	917	246	271	14			
1	H	183	Total	C	N	O	S	0	2	0
			1439	912	245	270	12			
1	I	183	Total	C	N	O	S	0	7	0
			1461	928	248	270	15			
1	J	185	Total	C	N	O	S	0	2	0
			1456	922	247	274	13			
1	K	186	Total	C	N	O	S	0	1	0
			1462	926	251	273	12			
1	L	183	Total	C	N	O	S	0	11	0
			1478	939	246	278	15			
1	M	186	Total	C	N	O	S	0	11	0
			1505	958	256	276	15			
1	N	183	Total	C	N	O	S	0	10	0
			1469	938	245	271	15			

- Molecule 2 is N 2 -[(BENZYLOXY)CARBONYL]-N-[(1S,2S)-2-HYDROXY-1-(4-HYDROXYBENZYL)PROPYL]-L-LEUCINAMIDE (three-letter code: CMQ) (formula: $C_{24}H_{32}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	24	2	5		
2	B	1	Total	C	N	O	0	0
			31	24	2	5		
2	C	1	Total	C	N	O	0	0
			31	24	2	5		
2	D	1	Total	C	N	O	0	0
			31	24	2	5		
2	E	1	Total	C	N	O	0	0
			31	24	2	5		
2	F	1	Total	C	N	O	0	0
			31	24	2	5		
2	G	1	Total	C	N	O	0	0
			31	24	2	5		
2	H	1	Total	C	N	O	0	0
			31	24	2	5		
2	I	1	Total	C	N	O	0	0
			31	24	2	5		
2	J	1	Total	C	N	O	0	0
			31	24	2	5		
2	K	1	Total	C	N	O	0	0
			31	24	2	5		
2	L	1	Total	C	N	O	0	0
			31	24	2	5		
2	M	1	Total	C	N	O	0	0
			31	24	2	5		
2	N	1	Total	C	N	O	0	0
			31	24	2	5		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	B	1	Total C O 10 6 4	0	0
3	C	1	Total C O 10 6 4	0	0
3	D	1	Total C O 10 6 4	0	0
3	E	1	Total C O 10 6 4	0	0
3	F	1	Total C O 10 6 4	0	0
3	G	1	Total C O 10 6 4	0	0
3	H	1	Total C O 10 6 4	0	0
3	I	1	Total C O 10 6 4	0	0
3	J	1	Total C O 10 6 4	0	0
3	K	1	Total C O 10 6 4	0	0
3	L	1	Total C O 10 6 4	0	0
3	M	1	Total C O 10 6 4	0	0

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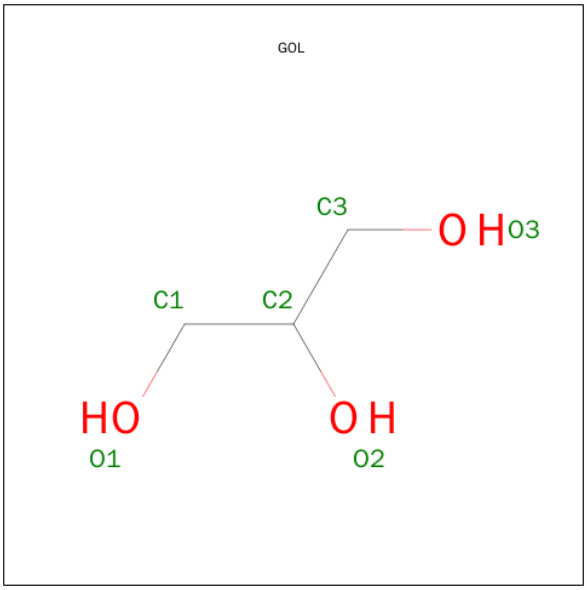
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	1	Total C O 10 6 4	0	0
3	K	1	Total C O 10 6 4	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

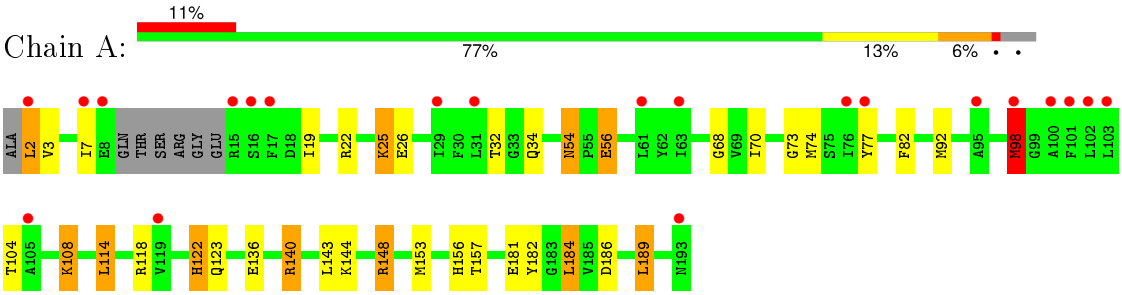
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	234	Total O 234 234	0	0
5	B	188	Total O 188 188	0	0
5	C	189	Total O 189 189	0	0
5	D	165	Total O 165 165	0	0
5	E	199	Total O 199 199	0	0
5	F	218	Total O 218 218	0	0
5	G	232	Total O 232 232	0	0
5	H	176	Total O 176 176	0	0
5	I	171	Total O 171 171	0	0
5	J	176	Total O 176 176	0	0
5	K	192	Total O 192 192	0	0
5	L	247	Total O 247 247	0	0
5	M	251	Total O 251 251	0	0
5	N	217	Total O 217 217	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

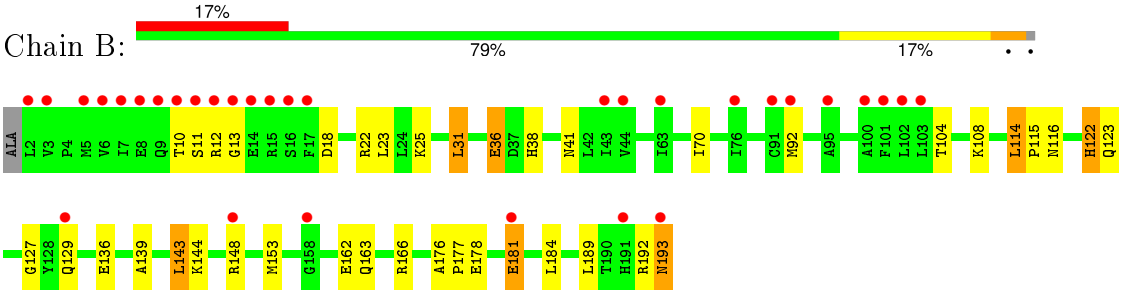
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



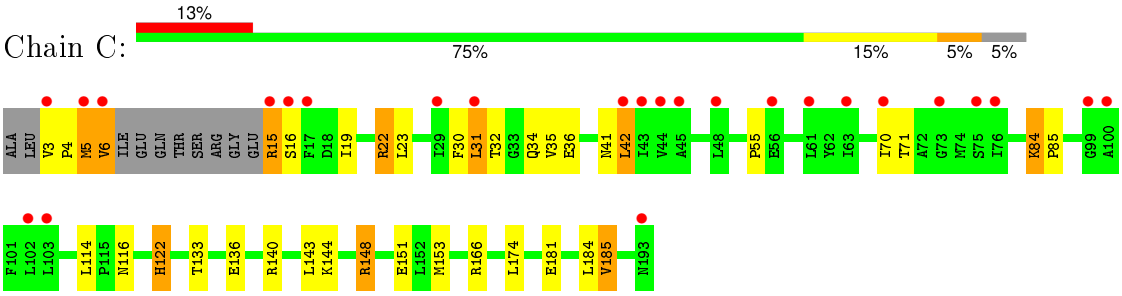
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



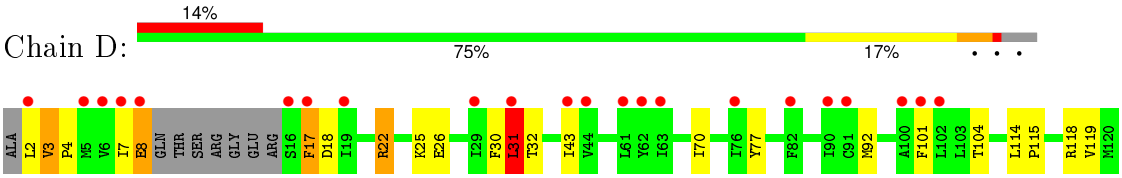
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:

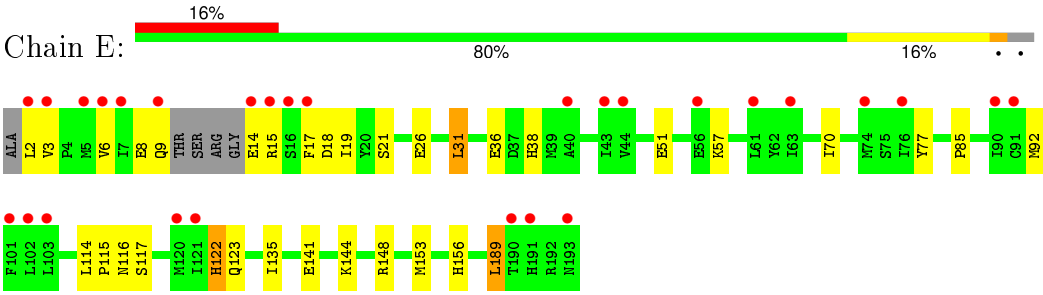


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

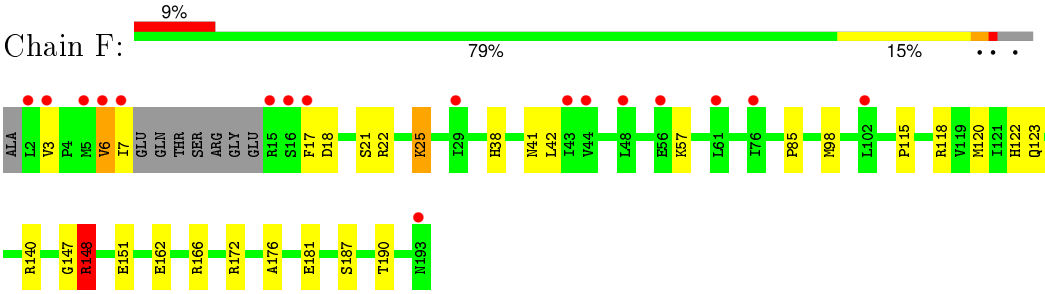
Chain D:



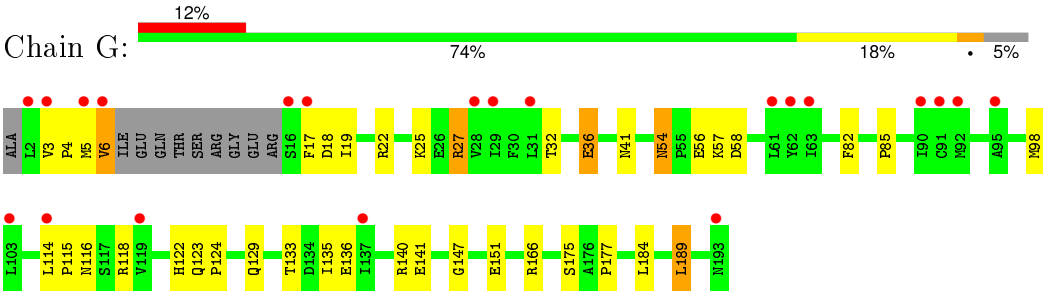
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



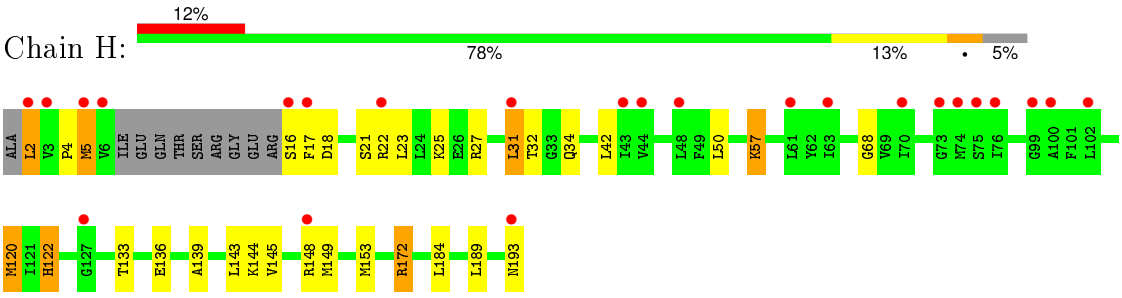
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



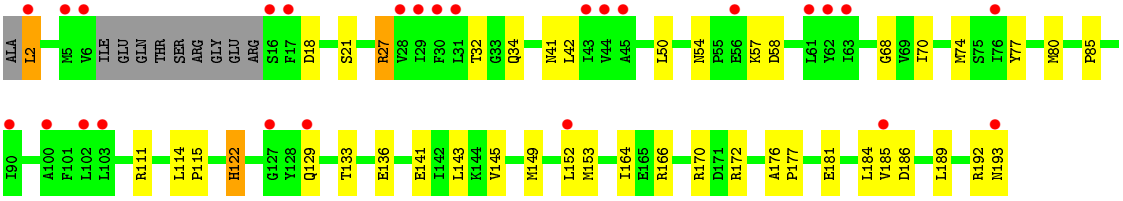
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

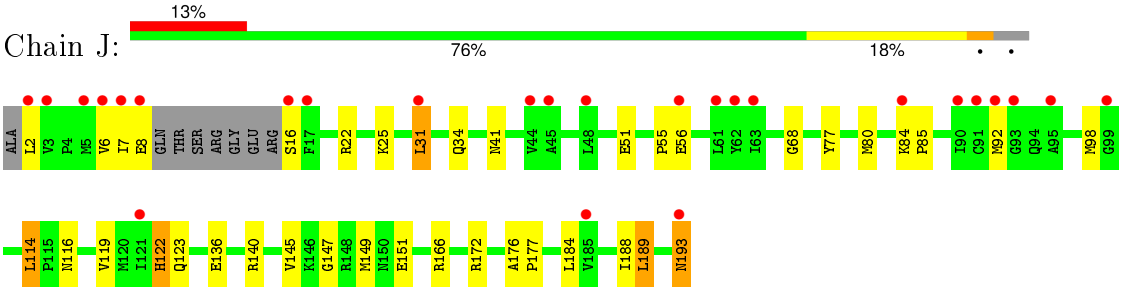


• Molecule 1: ATP-dependent Clp protease proteolytic subunit



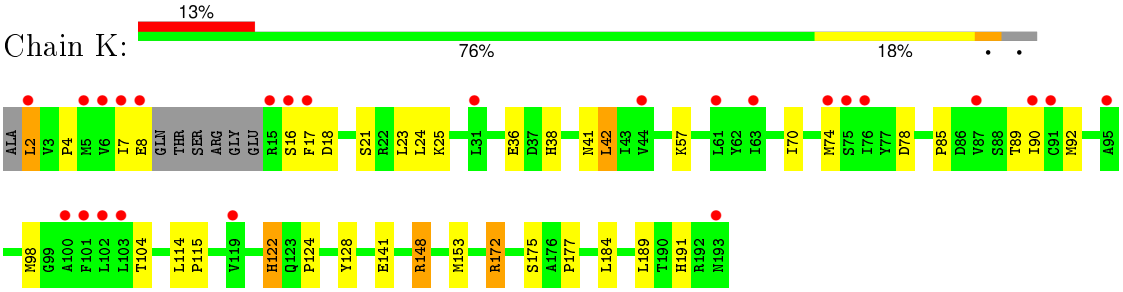
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



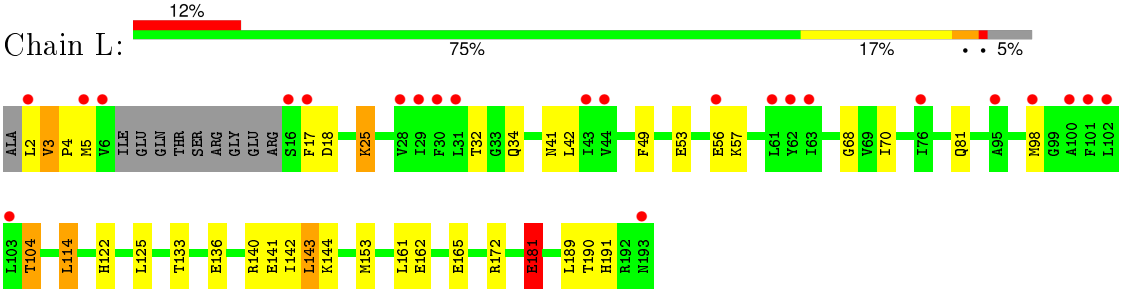
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



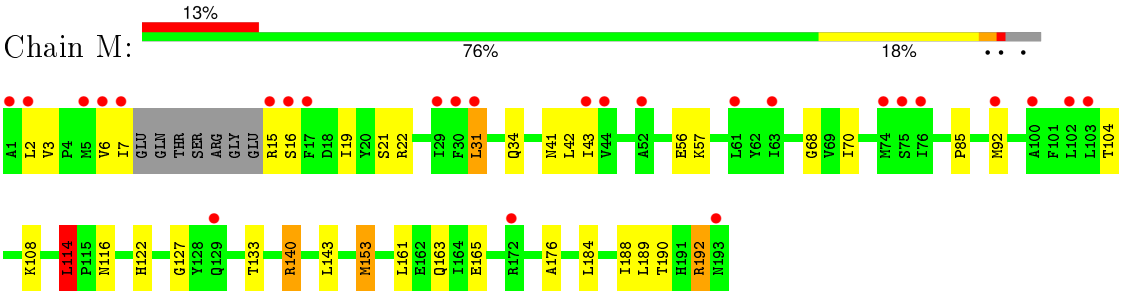
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



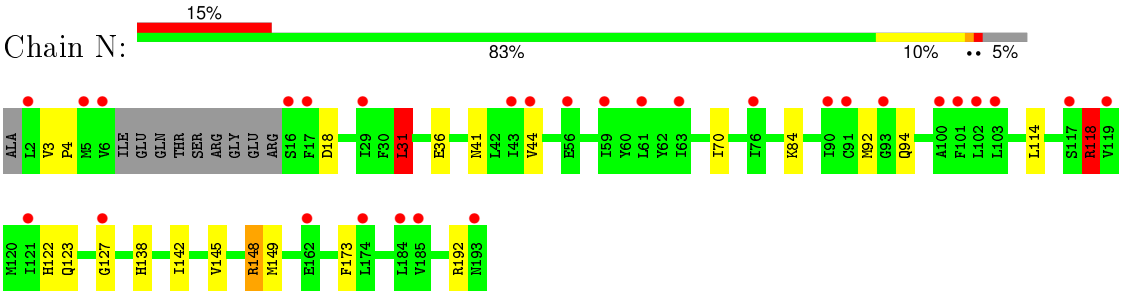
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:


15%
83%
10%
5%
ALA L2 V3 P4 M5 V6 ILE GLU GLN THR SER ARG GLY GLU ARG S16 F17 D18 I29 F30 L31 E36 N41 L42 I43 V44 E56 I59 Y60 L61 Y62 I63 I70 I76 K84 I90 C91 M92 G93 Q94 A100 F101 L102 L103 L114 S117 R118 V119
M120 I121 H122 Q123 G127 H138 I142 V145 R148 M149 E162 F173 L174 L184 V185 R192 N193

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.70Å 101.00Å 155.40Å 90.00° 99.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 29.85 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (15.00-1.90) 93.4 (29.85-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.173 , 0.233 0.172 , 0.232	Depositor DCC
R_{free} test set	10734 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	1 of 215053 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24125	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, CMQ

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	0.90	0/1538	0.85	2/2069 (0.1%)
1	B	0.81	1/1618 (0.1%)	0.87	4/2175 (0.2%)
1	C	0.83	1/1518 (0.1%)	0.88	4/2043 (0.2%)
1	D	0.79	0/1497	0.85	2/2016 (0.1%)
1	E	0.88	0/1510	0.84	2/2032 (0.1%)
1	F	1.03	2/1484 (0.1%)	0.97	5/1999 (0.3%)
1	G	0.99	1/1487 (0.1%)	1.26	10/2001 (0.5%)
1	H	0.83	2/1470 (0.1%)	0.84	3/1980 (0.2%)
1	I	0.74	0/1512	0.85	3/2034 (0.1%)
1	J	0.75	0/1487	0.80	3/2002 (0.1%)
1	K	0.84	0/1489	0.86	3/2006 (0.1%)
1	L	1.00	6/1545 (0.4%)	0.91	4/2079 (0.2%)
1	M	0.96	0/1572	0.94	2/2113 (0.1%)
1	N	0.86	0/1532	0.89	4/2063 (0.2%)
All	All	0.88	13/21259 (0.1%)	0.91	51/28612 (0.2%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	136	GLU	CD-OE1	8.13	1.34	1.25
1	C	181	GLU	CG-CD	6.54	1.61	1.51
1	L	181[A]	GLU	CD-OE1	6.41	1.32	1.25
1	L	181[B]	GLU	CD-OE1	6.41	1.32	1.25
1	H	136	GLU	CG-CD	6.24	1.61	1.51

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	27	ARG	NE-CZ-NH2	-28.69	105.95	120.30
1	G	27	ARG	NE-CZ-NH1	20.06	130.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	27	ARG	CD-NE-CZ	10.11	137.75	123.60
1	I	27	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	K	98	MET	CG-SD-CE	-9.80	84.52	100.20

There are no chirality outliers.

There are no planarity outliers.

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	1487	0	1509	61	0
1	B	1554	0	1567	53	0
1	C	1467	0	1487	44	0
1	D	1462	0	1471	49	0
1	E	1479	0	1486	39	0
1	F	1453	0	1456	20	0
1	G	1448	0	1455	39	0
1	H	1439	0	1448	37	0
1	I	1461	0	1477	47	0
1	J	1456	0	1463	36	0
1	K	1462	0	1476	42	0
1	L	1478	0	1483	43	0
1	M	1505	0	1533	37	0
1	N	1469	0	1492	23	0
2	A	31	0	31	9	0
2	B	31	0	30	7	0
2	C	31	0	30	6	0
2	D	31	0	31	8	0
2	E	31	0	31	8	0
2	F	31	0	28	1	0
2	G	31	0	29	1	0
2	H	31	0	31	6	0
2	I	31	0	31	7	0
2	J	31	0	31	8	0
2	K	31	0	31	9	0
2	L	31	0	29	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	31	0	29	1	0
2	N	31	0	29	2	0
3	A	10	0	14	1	0
3	B	10	0	14	2	0
3	C	10	0	14	0	0
3	D	10	0	14	0	0
3	E	10	0	14	0	0
3	F	10	0	14	1	0
3	G	10	0	14	0	0
3	H	10	0	14	0	0
3	I	10	0	14	0	0
3	J	10	0	14	1	0
3	K	20	0	28	2	0
3	L	10	0	14	0	0
3	M	10	0	14	1	0
3	N	10	0	14	2	0
4	A	6	0	8	2	0
4	B	12	0	16	0	0
4	C	12	0	16	6	0
4	F	6	0	8	2	0
4	G	6	0	8	1	0
4	H	6	0	8	2	0
4	K	6	0	8	1	0
4	L	6	0	8	0	0
4	N	6	0	8	3	0
5	A	234	0	0	12	0
5	B	188	0	0	6	0
5	C	189	0	0	8	0
5	D	165	0	0	5	0
5	E	199	0	0	10	0
5	F	218	0	0	7	0
5	G	232	0	0	8	0
5	H	176	0	0	5	0
5	I	171	0	0	4	0
5	J	176	0	0	6	0
5	K	192	0	0	8	0
5	L	247	0	0	12	0
5	M	251	0	0	5	0
5	N	217	0	0	6	0
All	All	24125	0	21522	514	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 12.

The worst 5 of 514 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:HIS:NE2	2:I:509:CMQ:H242	1.24	1.45
1:D:122:HIS:NE2	2:D:504:CMQ:H242	1.14	1.45
1:B:122:HIS:NE2	2:B:502:CMQ:H242	1.20	1.43
1:H:122:HIS:NE2	2:H:508:CMQ:H242	1.14	1.43
1:A:122:HIS:NE2	2:A:501:CMQ:H242	1.20	1.41

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	189/193 (98%)	184 (97%)	5 (3%)	0	100	100
1	B	200/193 (104%)	195 (98%)	5 (2%)	0	100	100
1	C	186/193 (96%)	182 (98%)	4 (2%)	0	100	100
1	D	184/193 (95%)	180 (98%)	3 (2%)	1 (0%)	34	21
1	E	186/193 (96%)	180 (97%)	6 (3%)	0	100	100
1	F	183/193 (95%)	180 (98%)	3 (2%)	0	100	100
1	G	183/193 (95%)	179 (98%)	4 (2%)	0	100	100
1	H	181/193 (94%)	178 (98%)	3 (2%)	0	100	100
1	I	186/193 (96%)	183 (98%)	3 (2%)	0	100	100
1	J	183/193 (95%)	179 (98%)	4 (2%)	0	100	100
1	K	183/193 (95%)	178 (97%)	5 (3%)	0	100	100
1	L	190/193 (98%)	187 (98%)	3 (2%)	0	100	100
1	M	193/193 (100%)	188 (97%)	5 (3%)	0	100	100
1	N	189/193 (98%)	186 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2616/2702 (97%)	2559 (98%)	56 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	17	PHE

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	165/163 (101%)	150 (91%)	15 (9%)	12 4
1	B	173/163 (106%)	163 (94%)	10 (6%)	25 13
1	C	162/163 (99%)	145 (90%)	17 (10%)	8 3
1	D	160/163 (98%)	146 (91%)	14 (9%)	12 5
1	E	161/163 (99%)	154 (96%)	7 (4%)	35 23
1	F	158/163 (97%)	148 (94%)	10 (6%)	22 10
1	G	159/163 (98%)	151 (95%)	8 (5%)	30 18
1	H	157/163 (96%)	146 (93%)	11 (7%)	19 8
1	I	162/163 (99%)	156 (96%)	6 (4%)	41 29
1	J	159/163 (98%)	151 (95%)	8 (5%)	30 18
1	K	159/163 (98%)	152 (96%)	7 (4%)	35 22
1	L	166/163 (102%)	156 (94%)	10 (6%)	24 12
1	M	168/163 (103%)	156 (93%)	12 (7%)	18 8
1	N	165/163 (101%)	154 (93%)	11 (7%)	20 9
All	All	2274/2282 (100%)	2128 (94%)	146 (6%)	24 10

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	21	SER

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Mol	Chain	Res	Type
1	H	2	LEU
1	M	192	ARG
1	F	25	LYS
1	G	22	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	34	GLN
1	G	54	ASN
1	M	123	GLN
1	F	41	ASN
1	G	191	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

40 ligands are modelled in this entry.

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	$\#\|Z\|>2$
4	GOL	A	3001	-	5,5,5	0.29	0	5,5,5	0.49	0
3	PGE	A	4001	-	9,9,9	0.50	0	8,8,8	0.32	0
2	CMQ	A	501	1	31,32,32	1.22	1 (3%)	41,42,42	1.67	9 (21%)
4	GOL	B	3002	-	5,5,5	0.20	0	5,5,5	0.61	0
4	GOL	B	3003	-	5,5,5	0.41	0	5,5,5	0.33	0
3	PGE	B	4002	-	9,9,9	0.51	0	8,8,8	0.18	0
2	CMQ	B	502	1	31,32,32	1.08	1 (3%)	41,42,42	1.42	5 (12%)
4	GOL	C	3005	-	5,5,5	0.23	0	5,5,5	0.64	0
4	GOL	C	3006	-	5,5,5	0.33	0	5,5,5	0.50	0
3	PGE	C	4003	-	9,9,9	0.51	0	8,8,8	0.31	0
2	CMQ	C	503	1	31,32,32	1.21	2 (6%)	41,42,42	1.50	6 (14%)
3	PGE	D	4004	-	9,9,9	0.48	0	8,8,8	0.34	0
2	CMQ	D	504	1	31,32,32	1.17	1 (3%)	41,42,42	1.59	7 (17%)
3	PGE	E	4005	-	9,9,9	0.49	0	8,8,8	0.36	0
2	CMQ	E	505	1	31,32,32	1.28	1 (3%)	41,42,42	1.75	13 (31%)
4	GOL	F	3004	-	5,5,5	0.61	0	5,5,5	0.70	0
3	PGE	F	4006	-	9,9,9	0.38	0	8,8,8	0.51	0
2	CMQ	F	506	1	31,32,32	1.13	1 (3%)	41,42,42	1.43	6 (14%)
4	GOL	G	3009	-	5,5,5	0.47	0	5,5,5	0.39	0
3	PGE	G	4007	-	9,9,9	0.50	0	8,8,8	0.49	0
2	CMQ	G	507	1	31,32,32	1.39	2 (6%)	41,42,42	1.32	7 (17%)
4	GOL	H	3008	-	5,5,5	0.39	0	5,5,5	0.86	0
3	PGE	H	4008	-	9,9,9	0.43	0	8,8,8	0.55	0
2	CMQ	H	508	1	31,32,32	1.17	1 (3%)	41,42,42	1.69	10 (24%)
3	PGE	I	4009	-	9,9,9	0.45	0	8,8,8	0.47	0
2	CMQ	I	509	1	31,32,32	1.16	1 (3%)	41,42,42	1.66	6 (14%)
3	PGE	J	4010	-	9,9,9	0.60	0	8,8,8	0.46	0
2	CMQ	J	510	1	31,32,32	1.17	1 (3%)	41,42,42	1.57	7 (17%)
4	GOL	K	3010	-	5,5,5	0.33	0	5,5,5	0.78	0
3	PGE	K	4011	-	9,9,9	0.52	0	8,8,8	0.45	0
3	PGE	K	4015	-	9,9,9	0.23	0	8,8,8	0.89	0
2	CMQ	K	511	1	31,32,32	1.11	1 (3%)	41,42,42	1.32	7 (17%)
4	GOL	L	3011	-	5,5,5	0.44	0	5,5,5	0.69	0
3	PGE	L	4012	-	9,9,9	0.59	0	8,8,8	0.30	0
2	CMQ	L	512	1	31,32,32	1.21	3 (9%)	41,42,42	1.41	6 (14%)
3	PGE	M	4013	-	9,9,9	0.43	0	8,8,8	0.50	0
2	CMQ	M	513	1	31,32,32	1.16	3 (9%)	41,42,42	1.35	3 (7%)
4	GOL	N	3007	-	5,5,5	0.32	0	5,5,5	0.70	0
3	PGE	N	4014	-	9,9,9	0.44	0	8,8,8	0.46	0
2	CMQ	N	514	1	31,32,32	1.19	1 (3%)	41,42,42	1.18	3 (7%)

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
4	GOL	A	3001	-	-	0/4/4/4	0/0/0/0
3	PGE	A	4001	-	-	0/7/7/7	0/0/0/0
2	CMQ	A	501	1	-	0/29/29/29	0/2/2/2
4	GOL	B	3002	-	-	0/4/4/4	0/0/0/0
4	GOL	B	3003	-	-	0/4/4/4	0/0/0/0
3	PGE	B	4002	-	-	0/7/7/7	0/0/0/0
2	CMQ	B	502	1	-	0/29/29/29	0/2/2/2
4	GOL	C	3005	-	-	0/4/4/4	0/0/0/0
4	GOL	C	3006	-	-	0/4/4/4	0/0/0/0
3	PGE	C	4003	-	-	0/7/7/7	0/0/0/0
2	CMQ	C	503	1	-	0/29/29/29	0/2/2/2
3	PGE	D	4004	-	-	0/7/7/7	0/0/0/0
2	CMQ	D	504	1	-	0/29/29/29	0/2/2/2
3	PGE	E	4005	-	-	0/7/7/7	0/0/0/0
2	CMQ	E	505	1	-	0/29/29/29	0/2/2/2
4	GOL	F	3004	-	-	0/4/4/4	0/0/0/0
3	PGE	F	4006	-	-	0/7/7/7	0/0/0/0
2	CMQ	F	506	1	-	0/29/29/29	0/2/2/2
4	GOL	G	3009	-	-	0/4/4/4	0/0/0/0
3	PGE	G	4007	-	-	0/7/7/7	0/0/0/0
2	CMQ	G	507	1	-	0/29/29/29	0/2/2/2
4	GOL	H	3008	-	-	0/4/4/4	0/0/0/0
3	PGE	H	4008	-	-	0/7/7/7	0/0/0/0
2	CMQ	H	508	1	-	0/29/29/29	0/2/2/2
3	PGE	I	4009	-	-	0/7/7/7	0/0/0/0
2	CMQ	I	509	1	-	0/29/29/29	0/2/2/2
3	PGE	J	4010	-	-	0/7/7/7	0/0/0/0
2	CMQ	J	510	1	-	0/29/29/29	0/2/2/2
4	GOL	K	3010	-	-	0/4/4/4	0/0/0/0
3	PGE	K	4011	-	-	0/7/7/7	0/0/0/0
3	PGE	K	4015	-	-	0/7/7/7	0/0/0/0
2	CMQ	K	511	1	-	0/29/29/29	0/2/2/2
4	GOL	L	3011	-	-	0/4/4/4	0/0/0/0
3	PGE	L	4012	-	-	0/7/7/7	0/0/0/0
2	CMQ	L	512	1	-	0/29/29/29	0/2/2/2
3	PGE	M	4013	-	-	0/7/7/7	0/0/0/0
2	CMQ	M	513	1	-	0/29/29/29	0/2/2/2
4	GOL	N	3007	-	-	0/4/4/4	0/0/0/0
3	PGE	N	4014	-	-	0/7/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CMQ	N	514	1	-	0/29/29/29	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	512	CMQ	C20-C22	2.03	1.42	1.38
2	C	503	CMQ	C21-C19	2.12	1.42	1.38
2	M	513	CMQ	C24-C16	2.15	1.57	1.51
2	L	512	CMQ	C24-C16	2.26	1.57	1.51
2	G	507	CMQ	C24-C16	2.34	1.57	1.51

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	503	CMQ	C17-C15-N2	-5.48	104.14	110.14
2	F	506	CMQ	C17-C15-N2	-5.33	104.31	110.14
2	M	513	CMQ	C17-C15-N2	-5.21	104.44	110.14
2	E	505	CMQ	C16-C15-N2	-5.07	100.61	110.11
2	I	509	CMQ	O1-C1-O2	-5.04	113.85	124.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	GOL	2	0
3	A	4001	PGE	1	0
2	A	501	CMQ	9	0
3	B	4002	PGE	2	0
2	B	502	CMQ	7	0
4	C	3006	GOL	6	0
2	C	503	CMQ	6	0
2	D	504	CMQ	8	0
2	E	505	CMQ	8	0
4	F	3004	GOL	2	0
3	F	4006	PGE	1	0
2	F	506	CMQ	1	0
4	G	3009	GOL	1	0
2	G	507	CMQ	1	0
4	H	3008	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	508	CMQ	6	0
2	I	509	CMQ	7	0
3	J	4010	PGE	1	0
2	J	510	CMQ	8	0
4	K	3010	GOL	1	0
3	K	4015	PGE	2	0
2	K	511	CMQ	9	0
2	L	512	CMQ	7	0
3	M	4013	PGE	1	0
2	M	513	CMQ	1	0
4	N	3007	GOL	3	0
3	N	4014	PGE	2	0
2	N	514	CMQ	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	186/193 (96%)	0.87	21 (11%)	7	7	24, 32, 50, 69	0
1	B	192/193 (99%)	0.96	32 (16%)	2	2	26, 33, 53, 69	0
1	C	183/193 (94%)	0.88	25 (13%)	4	4	26, 33, 43, 66	0
1	D	185/193 (95%)	0.97	27 (14%)	3	3	26, 33, 52, 72	0
1	E	188/193 (97%)	1.02	30 (15%)	3	3	26, 32, 50, 66	0
1	F	185/193 (95%)	0.80	17 (9%)	11	12	26, 32, 46, 59	0
1	G	183/193 (94%)	0.86	23 (12%)	5	5	26, 32, 46, 68	0
1	H	183/193 (94%)	0.87	24 (13%)	5	5	24, 32, 46, 78	0
1	I	183/193 (94%)	0.87	26 (14%)	4	4	27, 33, 43, 64	0
1	J	185/193 (95%)	0.82	26 (14%)	4	4	26, 32, 48, 79	0
1	K	186/193 (96%)	0.89	25 (13%)	4	5	26, 33, 53, 70	0
1	L	183/193 (94%)	0.84	23 (12%)	5	5	25, 32, 45, 69	0
1	M	186/193 (96%)	0.91	26 (13%)	4	4	27, 33, 52, 70	0
1	N	183/193 (94%)	0.88	29 (15%)	3	3	25, 33, 44, 73	0
All	All	2591/2702 (95%)	0.89	354 (13%)	4	4	24, 33, 51, 79	0

The worst 5 of 354 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	1	ALA	15.7
1	L	17	PHE	11.3
1	D	2	LEU	9.8
1	F	7	ILE	9.5
1	J	7	ILE	9.3

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	H	3008	6/6	0.83	0.27	11.39	53,55,57,58	0
4	GOL	C	3005	6/6	0.82	0.27	9.85	53,55,56,56	0
4	GOL	C	3006	6/6	0.81	0.34	8.02	60,62,63,64	0
4	GOL	B	3002	6/6	0.85	0.24	3.26	52,54,56,56	0
4	GOL	F	3004	6/6	0.91	0.19	2.86	30,33,34,40	0
4	GOL	K	3010	6/6	0.81	0.24	2.74	43,46,46,46	0
3	PGE	E	4005	10/10	0.80	0.26	2.19	59,60,63,63	0
4	GOL	L	3011	6/6	0.89	0.18	1.78	30,36,38,42	0
4	GOL	A	3001	6/6	0.94	0.19	1.73	32,35,37,42	0
3	PGE	K	4015	10/10	0.86	0.18	1.66	37,40,42,45	0
4	GOL	N	3007	6/6	0.86	0.20	1.27	44,48,50,50	0
3	PGE	D	4004	10/10	0.82	0.21	1.24	55,57,58,60	0
4	GOL	G	3009	6/6	0.92	0.20	1.23	42,46,48,49	0
3	PGE	M	4013	10/10	0.92	0.17	1.17	43,45,49,54	0
3	PGE	H	4008	10/10	0.89	0.17	1.01	52,55,58,59	0
4	GOL	B	3003	6/6	0.89	0.21	0.89	56,58,58,60	0
3	PGE	K	4011	10/10	0.78	0.17	0.74	48,51,57,59	0
2	CMQ	J	510	31/31	0.91	0.13	0.63	36,41,53,54	0
2	CMQ	B	502	31/31	0.89	0.15	0.52	33,42,58,59	0
2	CMQ	H	508	31/31	0.92	0.15	0.42	33,39,62,63	0
3	PGE	N	4014	10/10	0.75	0.19	0.24	59,65,69,70	0
2	CMQ	L	512	31/31	0.89	0.16	0.17	35,40,62,64	0
2	CMQ	F	506	31/31	0.92	0.12	0.16	34,40,58,59	0
2	CMQ	C	503	31/31	0.89	0.13	0.16	34,40,56,58	0
2	CMQ	E	505	31/31	0.89	0.15	0.12	33,39,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CMQ	A	501	31/31	0.87	0.15	0.10	36,41,56,58	0
2	CMQ	I	509	31/31	0.91	0.12	0.09	35,41,55,58	0
3	PGE	J	4010	10/10	0.81	0.18	-0.03	41,46,51,52	0
3	PGE	B	4002	10/10	0.80	0.18	-0.14	61,62,63,64	0
2	CMQ	K	511	31/31	0.92	0.12	-0.21	36,40,56,57	0
2	CMQ	D	504	31/31	0.93	0.12	-0.25	34,38,55,56	0
2	CMQ	N	514	31/31	0.91	0.13	-0.25	34,41,59,60	0
2	CMQ	G	507	31/31	0.92	0.12	-0.29	32,41,56,57	0
3	PGE	F	4006	10/10	0.91	0.13	-0.38	41,43,49,50	0
3	PGE	I	4009	10/10	0.88	0.14	-0.39	48,52,60,60	0
2	CMQ	M	513	31/31	0.92	0.11	-0.46	33,39,54,55	0
3	PGE	C	4003	10/10	0.78	0.14	-0.49	63,64,66,66	0
3	PGE	L	4012	10/10	0.91	0.11	-0.83	45,46,49,50	0
3	PGE	G	4007	10/10	0.90	0.11	-1.01	36,39,44,44	0
3	PGE	A	4001	10/10	0.88	0.11	-1.04	43,46,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.