wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 01:13 PM EDT

PDB ID	:	3MT6
Title	:	Structure of ClpP from Escherichia coli in complex with ADEP1
Authors	:	Chung, Y.S.
Deposited on	:	2010-04-30
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

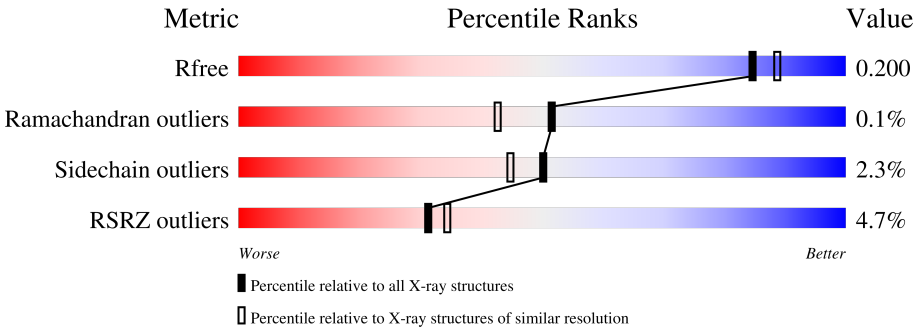
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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}	130704	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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 <=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	207	2% 91% · 7%
1	B	207	3% 89% · 9%
1	C	207	4% 88% · 9%
1	D	207	4% 90% · 9%
1	E	207	3% 89% · 9%
1	F	207	5% 90% · 8%

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Mol	Chain	Length	Quality of chain
1	G	207	4% 91% 8%
1	H	207	3% 88% 10%
1	I	207	2% 89% 8%
1	J	207	3% 90% 8%
1	K	207	4% 89% 9%
1	L	207	3% 89% 10%
1	M	207	6% 91% 8%
1	N	207	4% 89% 10%
1	O	207	3% 90% 9%
1	P	207	4% 90% 8%
1	Q	207	6% 89% 10%
1	R	207	3% 87% 13%
1	S	207	4% 89% 11%
1	T	207	4% 89% 10%
1	U	207	4% 89% 10%
1	V	207	5% 87% 12%
1	W	207	3% 87% 12%
1	X	207	6% 90% 8%
1	Y	207	3% 88% 10%
1	Z	207	4% 88% 12%
1	a	207	5% 86% 12%
1	b	207	3% 86% 13%
2	1	7	14% 14% 57% 29%
2	2	7	14% 14% 71% 14%
2	3	7	14% 14% 71% 14%

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Mol	Chain	Length	Quality of chain
2	4	7	29% 14% 71% 14%
2	c	7	14% 14% 71% 14%
2	d	7	14% 14% 71% 14%
2	e	7	14% 71% 14%
2	f	7	14% 29% 57% 14%
2	g	7	14% 14% 57% 29%
2	h	7	14% 29% 57% 14%
2	i	7	14% 29% 57% 14%
2	j	7	14% 29% 57% 14%
2	k	7	14% 14% 71% 14%
2	l	7	14% 14% 71% 14%
2	m	7	29% 14% 71% 14%
2	n	7	14% 71% 14%
2	o	7	14% 71% 14%
2	p	7	14% 29% 57% 14%
2	q	7	14% 29% 57% 14%
2	r	7	14% 29% 57% 14%
2	s	7	14% 14% 71% 14%
2	t	7	14% 14% 71% 14%
2	u	7	14% 14% 57% 29%
2	v	7	14% 14% 71% 14%
2	w	7	14% 14% 57% 29%
2	x	7	57% 14% 57% 29%
2	y	7	14% 14% 71% 14%
2	z	7	14% 14% 71% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 46463 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	R	180	Total	C	N	O	S	0	1	0
			1408	893	238	265	12			
1	S	184	Total	C	N	O	S	0	1	0
			1440	914	245	269	12			
1	T	186	Total	C	N	O	S	0	4	0
			1481	938	253	278	12			
1	U	186	Total	C	N	O	S	0	2	0
			1466	929	251	274	12			
1	O	189	Total	C	N	O	S	0	2	0
			1487	939	256	280	12			
1	P	190	Total	C	N	O	S	0	0	0
			1484	937	255	280	12			
1	Q	187	Total	C	N	O	S	0	1	0
			1459	923	247	277	12			
1	Y	186	Total	C	N	O	S	0	2	0
			1468	930	251	275	12			
1	Z	183	Total	C	N	O	S	0	1	0
			1432	909	242	269	12			
1	a	183	Total	C	N	O	S	0	1	0
			1435	909	245	269	12			
1	b	180	Total	C	N	O	S	0	0	0
			1404	892	238	262	12			
1	V	183	Total	C	N	O	S	0	2	0
			1438	912	244	270	12			
1	W	183	Total	C	N	O	S	0	1	0
			1429	908	241	268	12			
1	X	190	Total	C	N	O	S	0	1	0
			1478	935	250	281	12			
1	M	190	Total	C	N	O	S	0	1	0
			1484	938	253	281	12			
1	L	187	Total	C	N	O	S	0	0	0
			1454	921	246	275	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	188	Total	C	N	O	S	0	1	0
			1464	927	248	277	12			
1	J	190	Total	C	N	O	S	0	1	0
			1492	942	258	280	12			
1	I	190	Total	C	N	O	S	0	2	0
			1498	946	258	282	12			
1	H	186	Total	C	N	O	S	0	2	0
			1462	927	250	273	12			
1	N	187	Total	C	N	O	S	0	0	0
			1456	922	249	273	12			
1	F	190	Total	C	N	O	S	0	0	0
			1484	937	255	280	12			
1	E	188	Total	C	N	O	S	0	0	0
			1467	928	250	277	12			
1	D	188	Total	C	N	O	S	0	1	0
			1473	932	251	278	12			
1	C	188	Total	C	N	O	S	0	0	0
			1467	928	250	277	12			
1	B	188	Total	C	N	O	S	0	0	0
			1468	929	250	277	12			
1	A	192	Total	C	N	O	S	0	1	0
			1508	951	261	283	13			
1	G	190	Total	C	N	O	S	0	1	0
			1490	941	255	282	12			

- Molecule 2 is a protein called ACYLDEPSIPEPTIDE 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	1	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	2	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	c	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	d	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	e	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	f	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	g	7	Total	C	N	O	0	0	0
			52	38	6	8			

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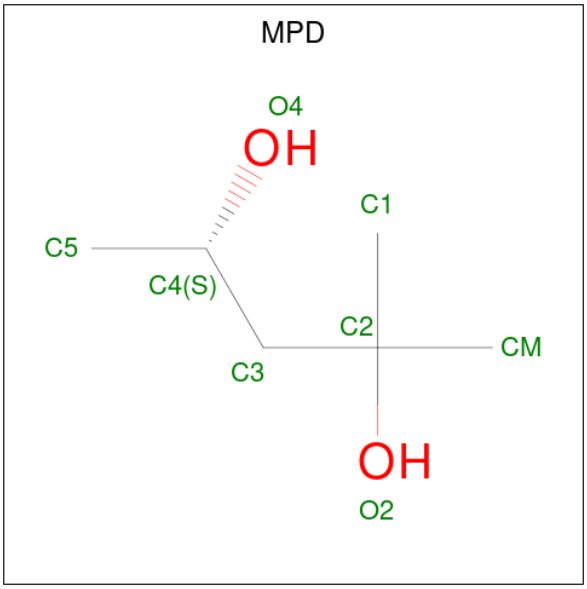
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	h	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	i	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	j	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	k	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	l	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	m	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	n	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	o	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	p	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	q	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	r	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	s	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	t	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	v	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	w	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	x	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	y	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	z	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	3	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	4	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	u	7	Total	C	N	O	0	0	0
			52	38	6	8			

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	R	1	Total C O 8 6 2	0	0
3	R	1	Total C O 8 6 2	0	0
3	R	1	Total C O 8 6 2	0	0
3	S	1	Total C O 8 6 2	0	0
3	T	1	Total C O 8 6 2	0	0
3	T	1	Total C O 8 6 2	0	0
3	U	1	Total C O 8 6 2	0	0
3	U	1	Total C O 8 6 2	0	0
3	O	1	Total C O 8 6 2	0	0
3	O	1	Total C O 8 6 2	0	0
3	P	1	Total C O 8 6 2	0	0
3	P	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Q	1	Total C O 8 6 2	0	0
3	Q	1	Total C O 8 6 2	0	0
3	Y	1	Total C O 8 6 2	0	0
3	Z	1	Total C O 8 6 2	0	0
3	Z	1	Total C O 8 6 2	0	0
3	Z	1	Total C O 8 6 2	0	0
3	a	1	Total C O 8 6 2	0	0
3	b	1	Total C O 8 6 2	0	0
3	b	1	Total C O 8 6 2	0	0
3	V	1	Total C O 8 6 2	0	0
3	V	1	Total C O 8 6 2	0	0
3	W	1	Total C O 8 6 2	0	0
3	W	1	Total C O 8 6 2	0	0
3	X	1	Total C O 8 6 2	0	0
3	X	1	Total C O 8 6 2	0	0
3	M	1	Total C O 8 6 2	0	0
3	M	1	Total C O 8 6 2	0	0
3	M	1	Total C O 8 6 2	0	0
3	L	1	Total C O 8 6 2	0	0
3	L	1	Total C O 8 6 2	0	0
3	K	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total C O 8 6 2	0	0
3	J	1	Total C O 8 6 2	0	0
3	J	1	Total C O 8 6 2	0	0
3	I	1	Total C O 8 6 2	0	0
3	I	1	Total C O 8 6 2	0	0
3	H	1	Total C O 8 6 2	0	0
3	N	1	Total C O 8 6 2	0	0
3	N	1	Total C O 8 6 2	0	0
3	F	1	Total C O 8 6 2	0	0
3	E	1	Total C O 8 6 2	0	0
3	E	1	Total C O 8 6 2	0	0
3	E	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	G	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	R	130	Total O 130 130	0	0
4	S	105	Total O 105 105	0	0
4	T	141	Total O 141 141	0	0
4	U	136	Total O 136 136	0	0
4	O	123	Total O 123 123	0	0
4	P	120	Total O 120 120	0	0
4	Q	125	Total O 125 125	0	0
4	Y	142	Total O 142 142	0	0
4	Z	124	Total O 124 124	0	0
4	a	129	Total O 129 129	0	0
4	b	114	Total O 114 114	0	0
4	V	108	Total O 108 108	0	0
4	W	102	Total O 102 102	0	0
4	X	118	Total O 118 118	0	0
4	M	133	Total O 133 133	0	0
4	L	132	Total O 132 132	0	0
4	K	130	Total O 130 130	0	0
4	J	137	Total O 137 137	0	0

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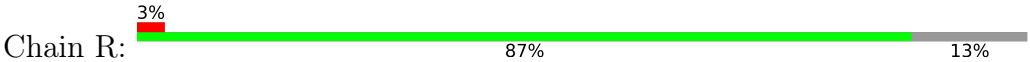
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	147	Total O 147 147	0	0
4	H	123	Total O 123 123	0	0
4	N	137	Total O 137 137	0	0
4	F	123	Total O 123 123	0	0
4	E	125	Total O 125 125	0	0
4	D	147	Total O 147 147	0	0
4	C	137	Total O 137 137	0	0
4	B	134	Total O 134 134	0	0
4	A	125	Total O 125 125	0	0
4	G	143	Total O 143 143	0	0
4	f	1	Total O 1 1	0	0

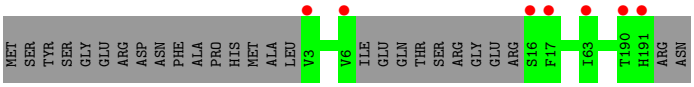
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

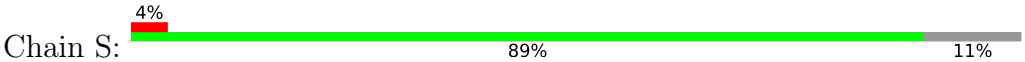
Chain R:

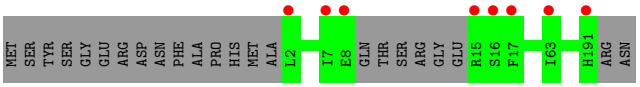




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

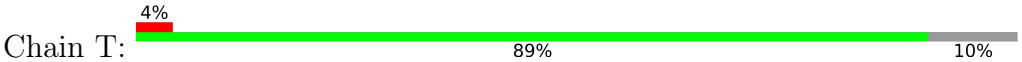
Chain S:

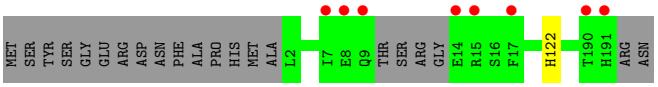




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

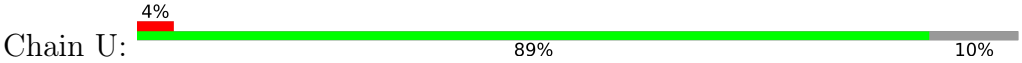
Chain T:

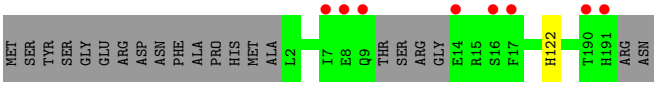




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

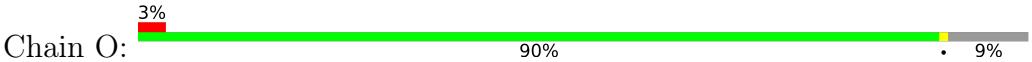
Chain U:

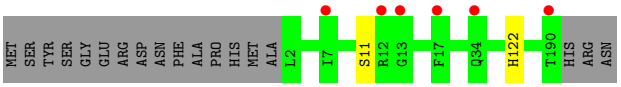




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

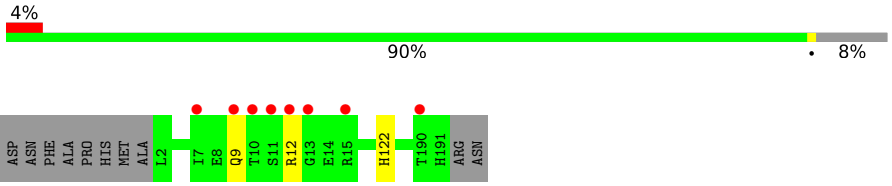
Chain O:





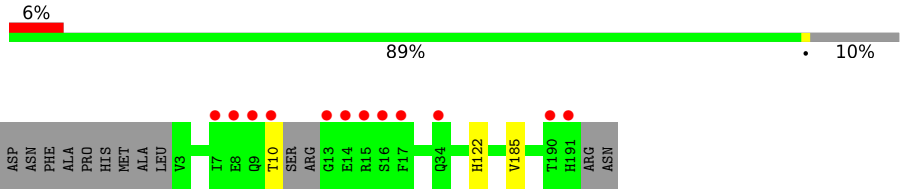
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain P:



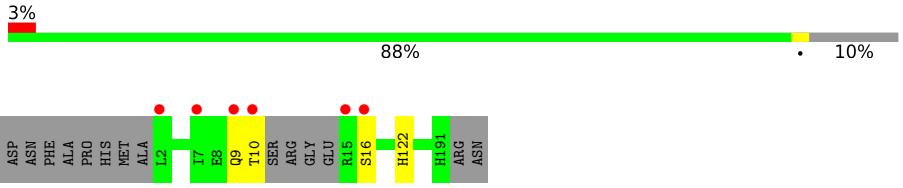
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q:



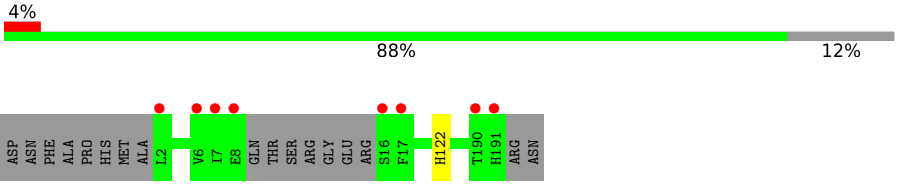
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y:



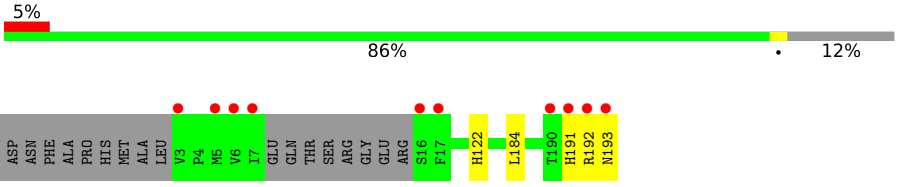
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:



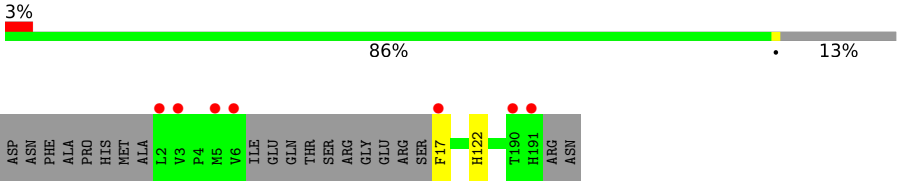
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a:



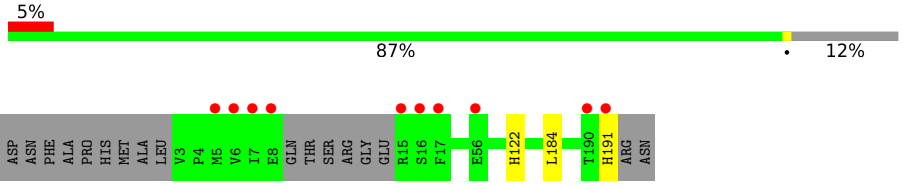
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b:



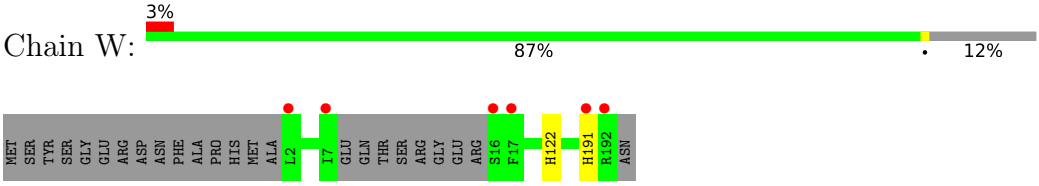
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:



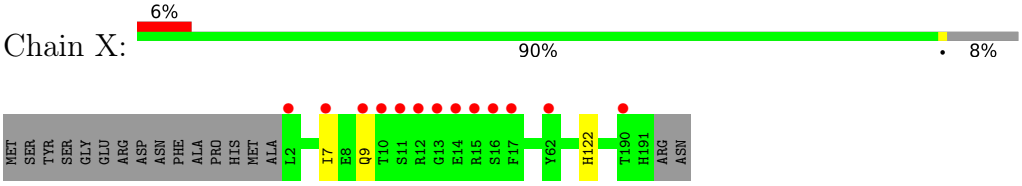
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain W:



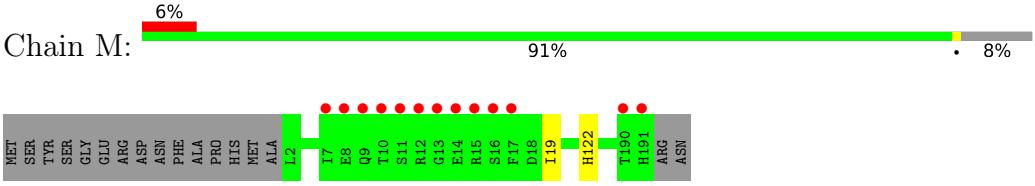
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X:



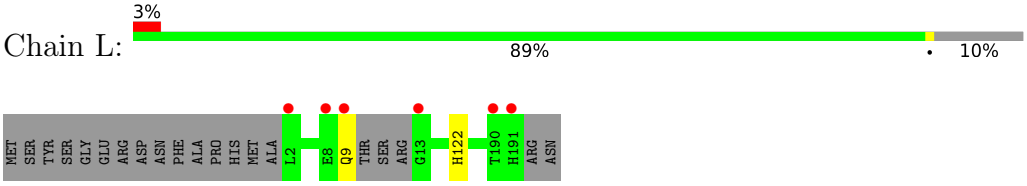
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



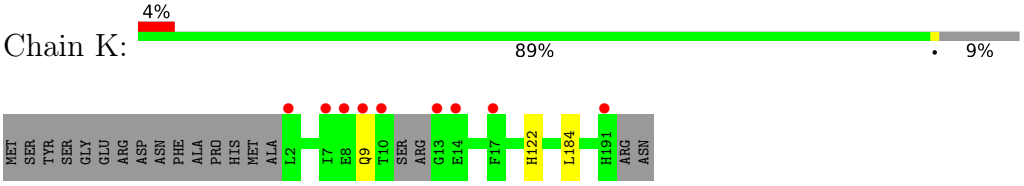
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



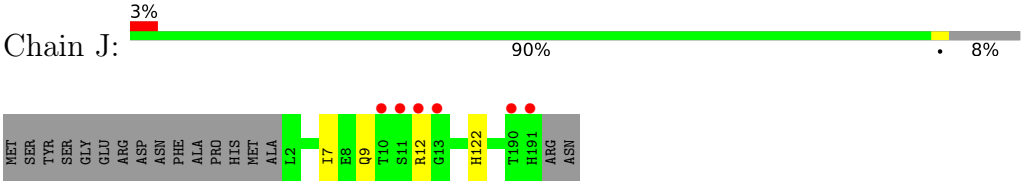
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



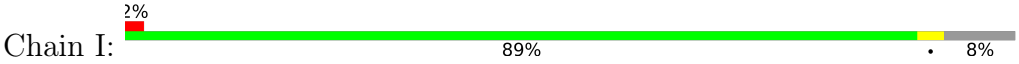
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

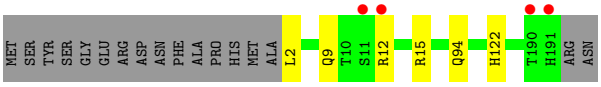
Chain J:



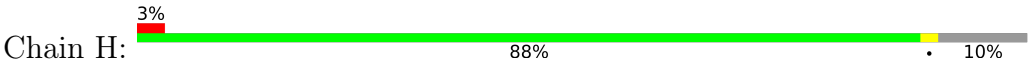
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

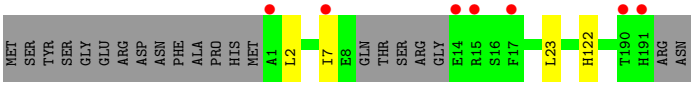
Chain I:



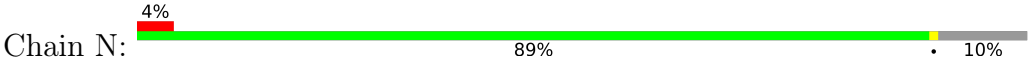


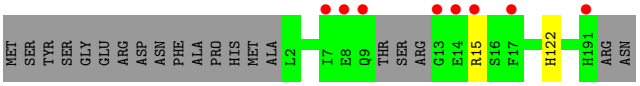
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



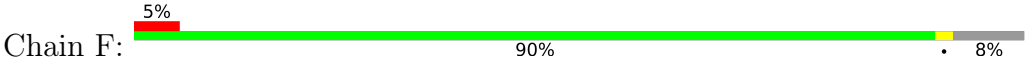


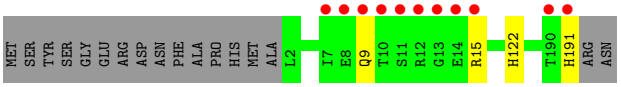
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



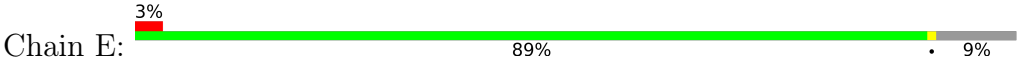


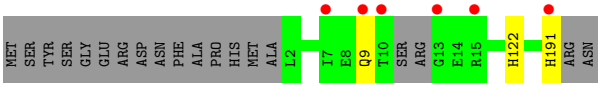
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



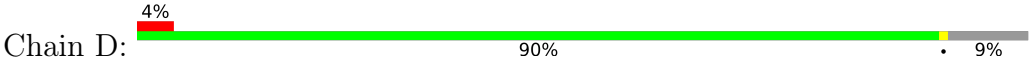


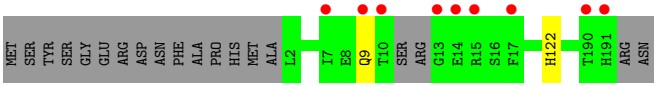
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



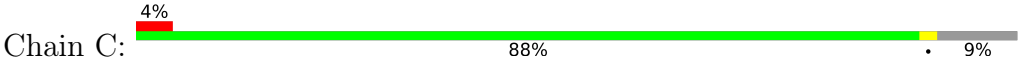


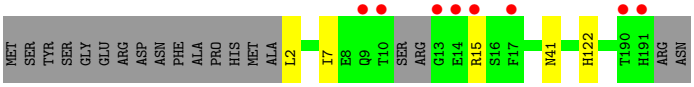
• Molecule 1: ATP-dependent Clp protease proteolytic subunit





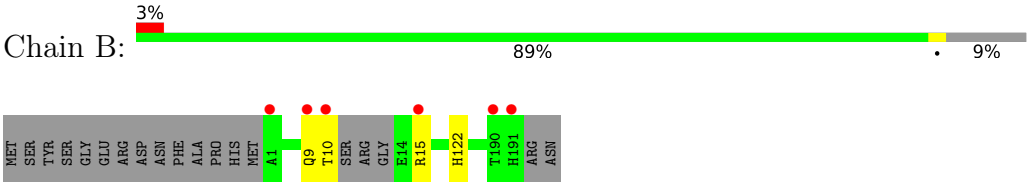
• Molecule 1: ATP-dependent Clp protease proteolytic subunit





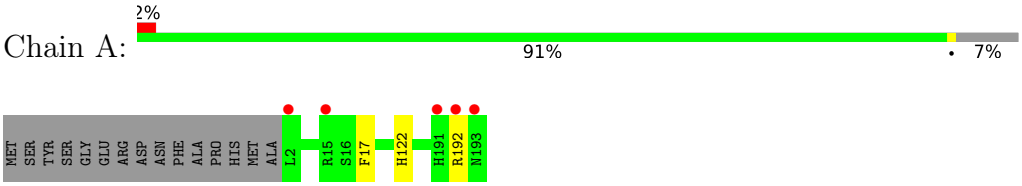
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



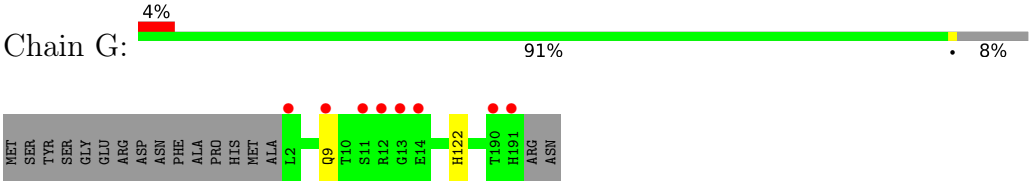
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



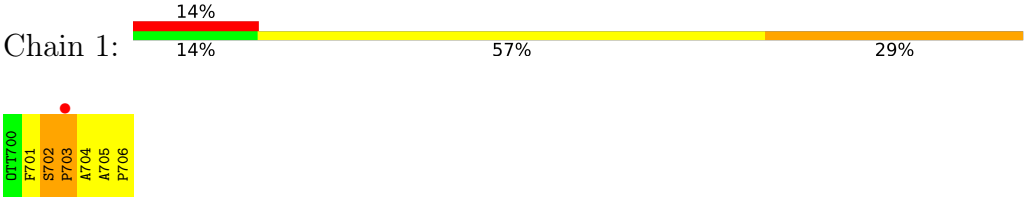
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



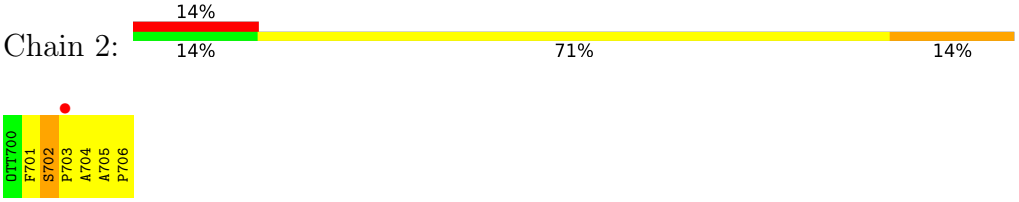
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain 1:



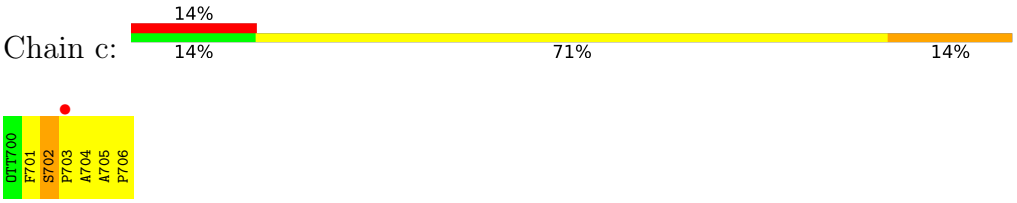
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain 2:



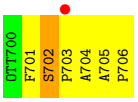
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain c:



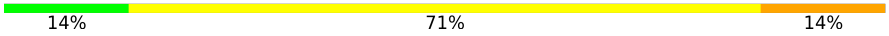
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain d:



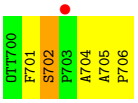
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain e:



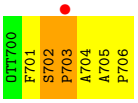
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain f:



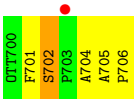
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain g:



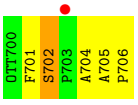
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain h:



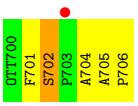
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain i:



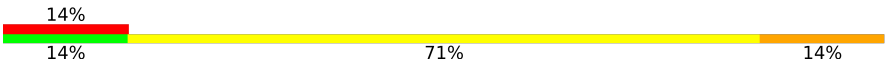
• Molecule 2: ACYLDEPSIPEPTIDE 1

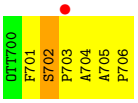
Chain j:



• Molecule 2: ACYLDEPSIPEPTIDE 1

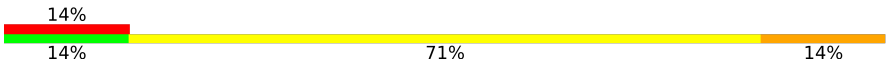
Chain k:

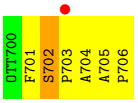




• Molecule 2: ACYLDEPSIPEPTIDE 1

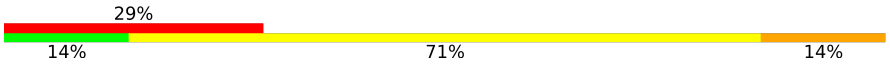
Chain l:

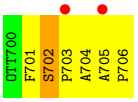




• Molecule 2: ACYLDEPSIPEPTIDE 1

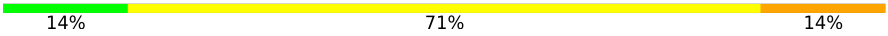
Chain m:





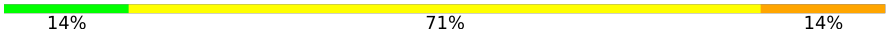
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain n:



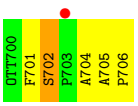
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain o:



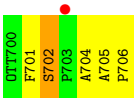
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain p:



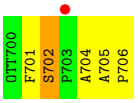
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain q:



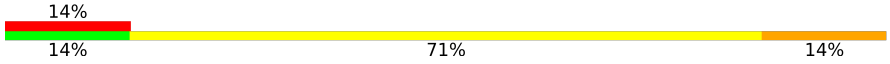
• Molecule 2: ACYLDEPSIPEPTIDE 1

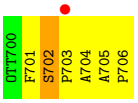
Chain r:



• Molecule 2: ACYLDEPSIPEPTIDE 1

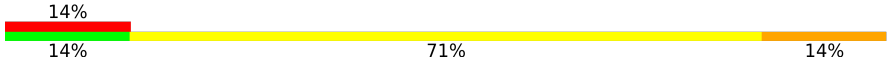
Chain s:

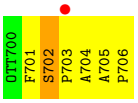




• Molecule 2: ACYLDEPSIPEPTIDE 1

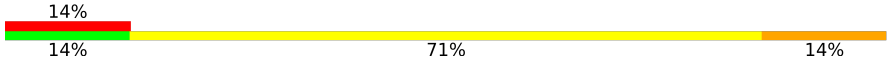
Chain t:

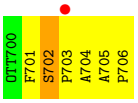




• Molecule 2: ACYLDEPSIPEPTIDE 1

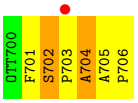
Chain v:





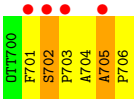
• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain w:



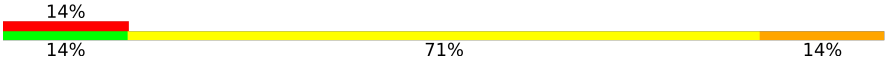
• Molecule 2: ACYLDEPSIPEPTIDE 1

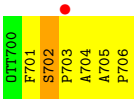
Chain x:



• Molecule 2: ACYLDEPSIPEPTIDE 1

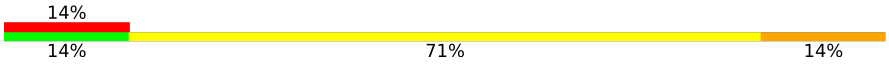
Chain y:

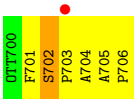




• Molecule 2: ACYLDEPSIPEPTIDE 1

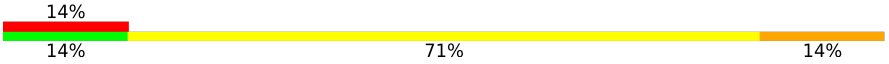
Chain z:

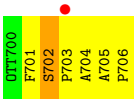




• Molecule 2: ACYLDEPSIPEPTIDE 1

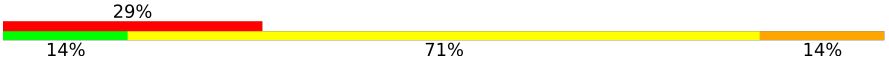
Chain 3:

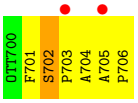




• Molecule 2: ACYLDEPSIPEPTIDE 1

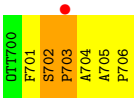
Chain 4:





• Molecule 2: ACYLDEPSIPEPTIDE 1

Chain u:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.25Å 121.15Å 276.17Å 90.00° 91.38° 90.00°	Depositor
Resolution (Å)	29.90 – 1.90 29.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.90-1.90) 98.1 (29.99-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_159)	Depositor
R, R_{free}	0.178 , 0.204 0.175 , 0.200	Depositor DCC
R_{free} test set	5212 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	46463	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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, 0.333 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: MP8, MAA, MPD, OTT

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	0.23	0/1535	0.42	0/2068
1	B	0.24	0/1491	0.42	0/2010
1	C	0.24	0/1490	0.42	0/2008
1	D	0.24	0/1499	0.42	0/2020
1	E	0.24	0/1490	0.42	0/2008
1	F	0.23	0/1508	0.41	0/2033
1	G	0.23	0/1517	0.42	0/2045
1	H	0.23	0/1491	0.41	0/2009
1	I	0.25	0/1528	0.43	0/2059
1	J	0.24	0/1519	0.43	0/2047
1	K	0.23	0/1490	0.41	0/2009
1	L	0.24	0/1477	0.41	0/1991
1	M	0.23	0/1511	0.41	0/2038
1	N	0.23	0/1479	0.41	0/1993
1	O	0.23	0/1516	0.42	0/2043
1	P	0.23	0/1508	0.41	0/2033
1	Q	0.23	0/1485	0.42	0/2002
1	R	0.23	0/1434	0.42	0/1933
1	S	0.23	0/1466	0.42	0/1976
1	T	0.23	0/1516	0.42	0/2042
1	U	0.24	0/1495	0.43	0/2014
1	V	0.23	0/1467	0.41	0/1977
1	W	0.23	0/1455	0.41	0/1962
1	X	0.25	0/1505	0.43	0/2031
1	Y	0.23	0/1497	0.42	0/2017
1	Z	0.23	0/1458	0.41	0/1966
1	a	0.23	0/1461	0.41	0/1969
1	b	0.23	0/1427	0.41	0/1924
2	1	2.88	4/29 (13.8%)	3.44	7/37 (18.9%)
2	2	2.89	4/29 (13.8%)	3.43	6/37 (16.2%)
2	3	2.92	4/29 (13.8%)	3.39	6/37 (16.2%)
2	4	2.92	4/29 (13.8%)	3.51	8/37 (21.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	c	2.90	4/29 (13.8%)	3.44	7/37 (18.9%)
2	d	2.88	4/29 (13.8%)	3.43	6/37 (16.2%)
2	e	2.90	4/29 (13.8%)	3.46	7/37 (18.9%)
2	f	2.91	4/29 (13.8%)	3.42	6/37 (16.2%)
2	g	2.93	4/29 (13.8%)	3.45	7/37 (18.9%)
2	h	2.93	4/29 (13.8%)	3.45	5/37 (13.5%)
2	i	2.89	4/29 (13.8%)	3.45	5/37 (13.5%)
2	j	2.89	4/29 (13.8%)	3.42	6/37 (16.2%)
2	k	2.91	4/29 (13.8%)	3.45	7/37 (18.9%)
2	l	2.92	4/29 (13.8%)	3.46	7/37 (18.9%)
2	m	2.88	4/29 (13.8%)	3.47	8/37 (21.6%)
2	n	2.92	4/29 (13.8%)	3.44	6/37 (16.2%)
2	o	2.84	4/29 (13.8%)	3.39	6/37 (16.2%)
2	p	2.91	4/29 (13.8%)	3.46	6/37 (16.2%)
2	q	2.91	4/29 (13.8%)	3.47	5/37 (13.5%)
2	r	2.91	4/29 (13.8%)	3.47	6/37 (16.2%)
2	s	2.88	4/29 (13.8%)	3.47	7/37 (18.9%)
2	t	2.91	4/29 (13.8%)	3.45	6/37 (16.2%)
2	u	2.92	4/29 (13.8%)	3.45	6/37 (16.2%)
2	v	2.92	4/29 (13.8%)	3.52	7/37 (18.9%)
2	w	2.89	4/29 (13.8%)	3.43	6/37 (16.2%)
2	x	2.96	4/29 (13.8%)	3.51	8/37 (21.6%)
2	y	2.89	4/29 (13.8%)	3.45	6/37 (16.2%)
2	z	2.91	4/29 (13.8%)	3.45	7/37 (18.9%)
All	All	0.46	112/42527 (0.3%)	0.62	180/57263 (0.3%)

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
2	g	0	1
2	w	0	1
2	x	0	1
All	All	0	3

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	x	702	SER	CA-CB	7.23	1.63	1.52
2	n	702	SER	CA-CB	7.20	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	702	SER	CA-CB	7.18	1.63	1.52
2	p	702	SER	CA-CB	7.17	1.63	1.52
2	z	702	SER	CA-CB	7.15	1.63	1.52

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	q	701	PHE	O-C-N	10.39	139.32	122.70
2	y	701	PHE	O-C-N	10.32	139.21	122.70
2	g	701	PHE	O-C-N	10.24	139.09	122.70
2	2	701	PHE	O-C-N	10.18	138.99	122.70
2	u	701	PHE	O-C-N	10.18	138.98	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	g	703	PRO	Mainchain
2	w	704	MAA	Mainchain
2	x	705	ALA	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	191/207 (92%)	187 (98%)	4 (2%)	0	100	100
1	B	184/207 (89%)	180 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	184/207 (89%)	182 (99%)	2 (1%)	0	100	100
1	D	185/207 (89%)	182 (98%)	3 (2%)	0	100	100
1	E	184/207 (89%)	182 (99%)	2 (1%)	0	100	100
1	F	188/207 (91%)	186 (99%)	2 (1%)	0	100	100
1	G	189/207 (91%)	187 (99%)	2 (1%)	0	100	100
1	H	184/207 (89%)	182 (99%)	2 (1%)	0	100	100
1	I	190/207 (92%)	186 (98%)	4 (2%)	0	100	100
1	J	189/207 (91%)	186 (98%)	3 (2%)	0	100	100
1	K	185/207 (89%)	181 (98%)	4 (2%)	0	100	100
1	L	183/207 (88%)	180 (98%)	3 (2%)	0	100	100
1	M	189/207 (91%)	185 (98%)	4 (2%)	0	100	100
1	N	183/207 (88%)	180 (98%)	3 (2%)	0	100	100
1	O	189/207 (91%)	187 (99%)	2 (1%)	0	100	100
1	P	188/207 (91%)	185 (98%)	3 (2%)	0	100	100
1	Q	184/207 (89%)	181 (98%)	3 (2%)	0	100	100
1	R	177/207 (86%)	175 (99%)	2 (1%)	0	100	100
1	S	181/207 (87%)	179 (99%)	2 (1%)	0	100	100
1	T	186/207 (90%)	183 (98%)	3 (2%)	0	100	100
1	U	184/207 (89%)	181 (98%)	3 (2%)	0	100	100
1	V	181/207 (87%)	179 (99%)	2 (1%)	0	100	100
1	W	180/207 (87%)	177 (98%)	3 (2%)	0	100	100
1	X	189/207 (91%)	187 (99%)	2 (1%)	0	100	100
1	Y	184/207 (89%)	181 (98%)	3 (2%)	0	100	100
1	Z	180/207 (87%)	178 (99%)	2 (1%)	0	100	100
1	a	180/207 (87%)	176 (98%)	2 (1%)	2 (1%)	14	5
1	b	176/207 (85%)	173 (98%)	3 (2%)	0	100	100
2	1	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	2	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	3	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	4	3/7 (43%)	3 (100%)	0	0	100	100
2	c	3/7 (43%)	2 (67%)	1 (33%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	d	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	e	3/7 (43%)	3 (100%)	0	0	100	100
2	f	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	g	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	h	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	i	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	j	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	k	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	l	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	m	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	n	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	o	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	p	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	q	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	r	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	s	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	t	3/7 (43%)	3 (100%)	0	0	100	100
2	u	3/7 (43%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	v	3/7 (43%)	3 (100%)	0	0	100	100
2	w	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	x	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	y	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	z	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
All	All	5251/5992 (88%)	5133 (98%)	115 (2%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	191	HIS
1	a	192	ARG
2	u	703	PRO

5.3.2 Protein sidechains (i)

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	164/175 (94%)	161 (98%)	3 (2%)	59	55
1	B	159/175 (91%)	155 (98%)	4 (2%)	47	41
1	C	159/175 (91%)	154 (97%)	5 (3%)	40	32
1	D	160/175 (91%)	158 (99%)	2 (1%)	69	68
1	E	159/175 (91%)	156 (98%)	3 (2%)	57	53
1	F	161/175 (92%)	157 (98%)	4 (2%)	47	41
1	G	162/175 (93%)	160 (99%)	2 (1%)	71	70
1	H	158/175 (90%)	154 (98%)	4 (2%)	47	41
1	I	163/175 (93%)	157 (96%)	6 (4%)	34	25
1	J	162/175 (93%)	158 (98%)	4 (2%)	47	41
1	K	158/175 (90%)	155 (98%)	3 (2%)	57	53
1	L	157/175 (90%)	155 (99%)	2 (1%)	69	68
1	M	161/175 (92%)	159 (99%)	2 (1%)	71	70
1	N	157/175 (90%)	155 (99%)	2 (1%)	69	68
1	O	162/175 (93%)	160 (99%)	2 (1%)	71	70
1	P	161/175 (92%)	158 (98%)	3 (2%)	57	53
1	Q	158/175 (90%)	155 (98%)	3 (2%)	57	53
1	R	153/175 (87%)	153 (100%)	0	100	100
1	S	156/175 (89%)	156 (100%)	0	100	100
1	T	162/175 (93%)	161 (99%)	1 (1%)	86	87
1	U	159/175 (91%)	158 (99%)	1 (1%)	86	87
1	V	156/175 (89%)	153 (98%)	3 (2%)	57	53
1	W	155/175 (89%)	153 (99%)	2 (1%)	69	68
1	X	160/175 (91%)	157 (98%)	3 (2%)	57	53
1	Y	160/175 (91%)	156 (98%)	4 (2%)	47	41
1	Z	156/175 (89%)	155 (99%)	1 (1%)	86	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	156/175 (89%)	153 (98%)	3 (2%)	57	53
1	b	152/175 (87%)	150 (99%)	2 (1%)	69	68
2	1	3/3 (100%)	1 (33%)	2 (67%)	0	0
2	2	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	3	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	4	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	c	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	d	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	e	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	f	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	g	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	h	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	i	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	j	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	k	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	l	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	m	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	n	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	o	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	p	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	q	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	r	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	s	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	t	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	u	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	v	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	w	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	x	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	y	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	z	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	4530/4984 (91%)	4427 (98%)	103 (2%)	50	45

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	191	HIS
1	A	192	ARG
2	z	702	SER
1	D	122	HIS
1	B	9	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	94	GLN
1	B	34	GLN
1	b	116	ASN
1	a	116	ASN
1	B	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)

56 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	MAA	1	704	2	4,5,6	0.67	0	1,5,7	2.40	1 (100%)
2	MAA	d	704	2	4,5,6	0.67	0	1,5,7	2.48	1 (100%)
2	MAA	i	704	2	4,5,6	0.67	0	1,5,7	2.42	1 (100%)
2	MP8	n	706	2	5,8,9	1.67	1 (20%)	3,10,12	3.91	1 (33%)
2	MAA	2	704	2	4,5,6	0.69	0	1,5,7	2.45	1 (100%)
2	MP8	w	706	2	5,8,9	1.69	1 (20%)	3,10,12	4.01	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MP8	f	706	2	5,8,9	1.68	1 (20%)	3,10,12	3.89	1 (33%)
2	MAA	e	704	2	4,5,6	0.68	0	1,5,7	2.46	1 (100%)
2	MP8	e	706	2	5,8,9	1.69	1 (20%)	3,10,12	4.01	1 (33%)
2	MP8	z	706	2	5,8,9	1.71	1 (20%)	3,10,12	4.03	1 (33%)
2	MP8	4	706	2	5,8,9	1.67	1 (20%)	3,10,12	3.96	1 (33%)
2	MAA	g	704	2	4,5,6	0.67	0	1,5,7	2.55	1 (100%)
2	MAA	y	704	2	4,5,6	0.66	0	1,5,7	2.56	1 (100%)
2	MP8	q	706	2	5,8,9	1.67	1 (20%)	3,10,12	4.05	1 (33%)
2	MP8	3	706	2	5,8,9	1.64	1 (20%)	3,10,12	3.94	1 (33%)
2	MAA	t	704	2	4,5,6	0.68	0	1,5,7	2.46	1 (100%)
2	MP8	y	706	2	5,8,9	1.73	1 (20%)	3,10,12	3.99	1 (33%)
2	MAA	v	704	2	4,5,6	0.71	0	1,5,7	2.19	1 (100%)
2	MAA	o	704	2	4,5,6	0.66	0	1,5,7	2.31	1 (100%)
2	MP8	g	706	2	5,8,9	1.65	1 (20%)	3,10,12	3.99	1 (33%)
2	MP8	1	706	2	5,8,9	1.69	1 (20%)	3,10,12	3.88	1 (33%)
2	MP8	o	706	2	5,8,9	1.67	1 (20%)	3,10,12	3.95	1 (33%)
2	MAA	s	704	2	4,5,6	0.69	0	1,5,7	2.41	1 (100%)
2	MP8	i	706	2	5,8,9	1.67	1 (20%)	3,10,12	3.99	1 (33%)
2	MP8	2	706	2	5,8,9	1.69	1 (20%)	3,10,12	4.07	1 (33%)
2	MAA	f	704	2	4,5,6	0.67	0	1,5,7	2.29	1 (100%)
2	MAA	p	704	2	4,5,6	0.67	0	1,5,7	2.33	1 (100%)
2	MAA	q	704	2	4,5,6	0.69	0	1,5,7	2.23	1 (100%)
2	MAA	r	704	2	4,5,6	0.64	0	1,5,7	2.44	1 (100%)
2	MAA	x	704	2	4,5,6	0.71	0	1,5,7	2.37	1 (100%)
2	MP8	m	706	2	5,8,9	1.67	1 (20%)	3,10,12	3.96	1 (33%)
2	MAA	l	704	2	4,5,6	0.69	0	1,5,7	2.41	1 (100%)
2	MP8	v	706	2	5,8,9	1.64	1 (20%)	3,10,12	3.99	1 (33%)
2	MAA	h	704	2	4,5,6	0.65	0	1,5,7	2.33	1 (100%)
2	MAA	w	704	2	4,5,6	0.68	0	1,5,7	2.34	1 (100%)
2	MAA	3	704	2	4,5,6	0.64	0	1,5,7	2.25	1 (100%)
2	MAA	4	704	2	4,5,6	0.67	0	1,5,7	2.43	1 (100%)
2	MP8	c	706	2	5,8,9	1.62	1 (20%)	3,10,12	4.01	1 (33%)
2	MP8	j	706	2	5,8,9	1.68	1 (20%)	3,10,12	3.89	1 (33%)
2	MP8	u	706	2	5,8,9	1.67	1 (20%)	3,10,12	3.91	1 (33%)
2	MAA	k	704	2	4,5,6	0.66	0	1,5,7	2.37	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MP8	s	706	2	5,8,9	1.66	1 (20%)	3,10,12	3.94	1 (33%)
2	MP8	l	706	2	5,8,9	1.66	1 (20%)	3,10,12	4.05	1 (33%)
2	MAA	z	704	2	4,5,6	0.68	0	1,5,7	2.21	1 (100%)
2	MP8	x	706	2	5,8,9	1.67	1 (20%)	3,10,12	3.95	1 (33%)
2	MP8	d	706	2	5,8,9	1.68	1 (20%)	3,10,12	4.06	1 (33%)
2	MAA	c	704	2	4,5,6	0.67	0	1,5,7	2.50	1 (100%)
2	MAA	m	704	2	4,5,6	0.67	0	1,5,7	2.41	1 (100%)
2	MAA	u	704	2	4,5,6	0.68	0	1,5,7	2.15	1 (100%)
2	MP8	t	706	2	5,8,9	1.70	1 (20%)	3,10,12	3.91	1 (33%)
2	MP8	h	706	2	5,8,9	1.66	1 (20%)	3,10,12	3.97	1 (33%)
2	MP8	r	706	2	5,8,9	1.69	1 (20%)	3,10,12	3.96	1 (33%)
2	MAA	n	704	2	4,5,6	0.67	0	1,5,7	2.29	1 (100%)
2	MP8	p	706	2	5,8,9	1.66	1 (20%)	3,10,12	3.89	1 (33%)
2	MAA	j	704	2	4,5,6	0.68	0	1,5,7	2.58	1 (100%)
2	MP8	k	706	2	5,8,9	1.64	1 (20%)	3,10,12	4.03	1 (33%)

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	MAA	1	704	2	-	0/1/4/6	-
2	MAA	d	704	2	-	0/1/4/6	-
2	MAA	i	704	2	-	0/1/4/6	-
2	MP8	n	706	2	-	0/0/11/13	0/1/1/1
2	MAA	2	704	2	-	0/1/4/6	-
2	MP8	w	706	2	-	0/0/11/13	0/1/1/1
2	MP8	f	706	2	-	0/0/11/13	0/1/1/1
2	MAA	e	704	2	-	0/1/4/6	-
2	MP8	e	706	2	-	0/0/11/13	0/1/1/1
2	MP8	z	706	2	-	0/0/11/13	0/1/1/1
2	MP8	4	706	2	-	0/0/11/13	0/1/1/1
2	MAA	g	704	2	-	0/1/4/6	-
2	MAA	y	704	2	-	0/1/4/6	-
2	MP8	q	706	2	-	0/0/11/13	0/1/1/1
2	MP8	3	706	2	-	0/0/11/13	0/1/1/1
2	MAA	t	704	2	-	0/1/4/6	-
2	MP8	y	706	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAA	v	704	2	-	0/1/4/6	-
2	MAA	o	704	2	-	0/1/4/6	-
2	MP8	g	706	2	-	0/0/11/13	0/1/1/1
2	MP8	1	706	2	-	0/0/11/13	0/1/1/1
2	MP8	o	706	2	-	0/0/11/13	0/1/1/1
2	MAA	s	704	2	-	0/1/4/6	-
2	MP8	i	706	2	-	0/0/11/13	0/1/1/1
2	MP8	2	706	2	-	0/0/11/13	0/1/1/1
2	MAA	f	704	2	-	0/1/4/6	-
2	MAA	p	704	2	-	0/1/4/6	-
2	MAA	q	704	2	-	0/1/4/6	-
2	MAA	r	704	2	-	0/1/4/6	-
2	MAA	x	704	2	-	0/1/4/6	-
2	MP8	m	706	2	-	0/0/11/13	0/1/1/1
2	MAA	l	704	2	-	0/1/4/6	-
2	MP8	v	706	2	-	0/0/11/13	0/1/1/1
2	MAA	h	704	2	-	0/1/4/6	-
2	MAA	w	704	2	-	0/1/4/6	-
2	MAA	3	704	2	-	0/1/4/6	-
2	MAA	4	704	2	-	0/1/4/6	-
2	MP8	c	706	2	-	0/0/11/13	0/1/1/1
2	MP8	j	706	2	-	0/0/11/13	0/1/1/1
2	MP8	u	706	2	-	0/0/11/13	0/1/1/1
2	MAA	k	704	2	-	0/1/4/6	-
2	MP8	s	706	2	-	0/0/11/13	0/1/1/1
2	MP8	l	706	2	-	0/0/11/13	0/1/1/1
2	MAA	z	704	2	-	0/1/4/6	-
2	MP8	x	706	2	-	0/0/11/13	0/1/1/1
2	MP8	d	706	2	-	0/0/11/13	0/1/1/1
2	MAA	c	704	2	-	0/1/4/6	-
2	MAA	m	704	2	-	0/1/4/6	-
2	MAA	u	704	2	-	0/1/4/6	-
2	MP8	t	706	2	-	0/0/11/13	0/1/1/1
2	MP8	h	706	2	-	0/0/11/13	0/1/1/1
2	MP8	r	706	2	-	0/0/11/13	0/1/1/1
2	MAA	n	704	2	-	0/1/4/6	-
2	MP8	p	706	2	-	0/0/11/13	0/1/1/1
2	MAA	j	704	2	-	0/1/4/6	-
2	MP8	k	706	2	-	0/0/11/13	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	y	706	MP8	CB-CA	-3.41	1.46	1.54
2	z	706	MP8	CB-CA	-3.37	1.47	1.54
2	t	706	MP8	CB-CA	-3.32	1.47	1.54
2	1	706	MP8	CB-CA	-3.31	1.47	1.54
2	e	706	MP8	CB-CA	-3.30	1.47	1.54

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	706	MP8	O-C-CA	-6.62	107.43	124.78
2	2	706	MP8	O-C-CA	-6.57	107.55	124.78
2	l	706	MP8	O-C-CA	-6.57	107.56	124.78
2	g	706	MP8	O-C-CA	-6.54	107.63	124.78
2	k	706	MP8	O-C-CA	-6.54	107.63	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

55 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	$\#\|Z\| > 2$
3	MPD	Z	802	-	7,7,7	0.27	0	9,10,10	0.20	0
3	MPD	V	202	-	7,7,7	0.27	0	9,10,10	0.21	0
3	MPD	J	801	-	7,7,7	0.28	0	9,10,10	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MPD	L	800	-	7,7,7	0.27	0	9,10,10	0.20	0
3	MPD	C	800	-	7,7,7	0.27	0	9,10,10	0.20	0
3	MPD	E	801	-	7,7,7	0.28	0	9,10,10	0.20	0
3	MPD	W	800	-	7,7,7	0.28	0	9,10,10	0.19	0
3	MPD	K	800	-	7,7,7	0.26	0	9,10,10	0.20	0
3	MPD	Z	801	-	7,7,7	0.25	0	9,10,10	0.17	0
3	MPD	a	800	-	7,7,7	0.26	0	9,10,10	0.19	0
3	MPD	X	202	-	7,7,7	0.25	0	9,10,10	0.21	0
3	MPD	L	801	-	7,7,7	0.26	0	9,10,10	0.24	0
3	MPD	E	802	-	7,7,7	0.27	0	9,10,10	0.18	0
3	MPD	X	201	-	7,7,7	0.27	0	9,10,10	0.18	0
3	MPD	D	801	-	7,7,7	0.27	0	9,10,10	0.19	0
3	MPD	b	801	-	7,7,7	0.26	0	9,10,10	0.23	0
3	MPD	D	800	-	7,7,7	0.26	0	9,10,10	0.19	0
3	MPD	A	801	-	7,7,7	0.26	0	9,10,10	0.19	0
3	MPD	R	202	-	7,7,7	0.27	0	9,10,10	0.20	0
3	MPD	P	801	-	7,7,7	0.27	0	9,10,10	0.22	0
3	MPD	N	801	-	7,7,7	0.25	0	9,10,10	0.17	0
3	MPD	U	201	-	7,7,7	0.28	0	9,10,10	0.21	0
3	MPD	V	201	-	7,7,7	0.25	0	9,10,10	0.18	0
3	MPD	I	800	-	7,7,7	0.25	0	9,10,10	0.18	0
3	MPD	H	800	-	7,7,7	0.25	0	9,10,10	0.19	0
3	MPD	B	800	-	7,7,7	0.26	0	9,10,10	0.20	0
3	MPD	O	801	-	7,7,7	0.25	0	9,10,10	0.18	0
3	MPD	E	803	-	7,7,7	0.26	0	9,10,10	0.21	0
3	MPD	R	203	-	7,7,7	0.27	0	9,10,10	0.20	0
3	MPD	M	202	-	7,7,7	0.27	0	9,10,10	0.24	0
3	MPD	A	800	-	7,7,7	0.27	0	9,10,10	0.19	0
3	MPD	Q	801	-	7,7,7	0.26	0	9,10,10	0.19	0
3	MPD	Q	800	-	7,7,7	0.28	0	9,10,10	0.18	0
3	MPD	R	201	-	7,7,7	0.26	0	9,10,10	0.21	0
3	MPD	Y	800	-	7,7,7	0.27	0	9,10,10	0.15	0
3	MPD	M	201	-	7,7,7	0.26	0	9,10,10	0.18	0
3	MPD	Z	803	-	7,7,7	0.27	0	9,10,10	0.24	0
3	MPD	B	801	-	7,7,7	0.29	0	9,10,10	0.23	0
3	MPD	G	800	-	7,7,7	0.27	0	9,10,10	0.16	0
3	MPD	O	800	-	7,7,7	0.25	0	9,10,10	0.19	0
3	MPD	N	800	-	7,7,7	0.29	0	9,10,10	0.18	0
3	MPD	T	801	-	7,7,7	0.28	0	9,10,10	0.25	0
3	MPD	T	800	-	7,7,7	0.27	0	9,10,10	0.17	0
3	MPD	b	800	-	7,7,7	0.27	0	9,10,10	0.18	0
3	MPD	W	801	-	7,7,7	0.28	0	9,10,10	0.21	0
3	MPD	K	801	-	7,7,7	0.25	0	9,10,10	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MPD	P	800	-	7,7,7	0.27	0	9,10,10	0.23	0
3	MPD	G	801	-	7,7,7	0.27	0	9,10,10	0.21	0
3	MPD	M	203	-	7,7,7	0.28	0	9,10,10	0.16	0
3	MPD	J	800	-	7,7,7	0.26	0	9,10,10	0.19	0
3	MPD	C	801	-	7,7,7	0.26	0	9,10,10	0.20	0
3	MPD	S	800	-	7,7,7	0.29	0	9,10,10	0.15	0
3	MPD	I	801	-	7,7,7	0.26	0	9,10,10	0.24	0
3	MPD	F	800	-	7,7,7	0.27	0	9,10,10	0.20	0
3	MPD	U	202	-	7,7,7	0.28	0	9,10,10	0.17	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	MPD	Z	802	-	-	1/5/5/5	-
3	MPD	V	202	-	-	2/5/5/5	-
3	MPD	J	801	-	-	1/5/5/5	-
3	MPD	L	800	-	-	3/5/5/5	-
3	MPD	C	800	-	-	2/5/5/5	-
3	MPD	E	801	-	-	1/5/5/5	-
3	MPD	W	800	-	-	1/5/5/5	-
3	MPD	K	800	-	-	3/5/5/5	-
3	MPD	Z	801	-	-	3/5/5/5	-
3	MPD	a	800	-	-	3/5/5/5	-
3	MPD	X	202	-	-	2/5/5/5	-
3	MPD	L	801	-	-	2/5/5/5	-
3	MPD	E	802	-	-	3/5/5/5	-
3	MPD	X	201	-	-	3/5/5/5	-
3	MPD	D	801	-	-	1/5/5/5	-
3	MPD	b	801	-	-	2/5/5/5	-
3	MPD	D	800	-	-	3/5/5/5	-
3	MPD	A	801	-	-	2/5/5/5	-
3	MPD	R	202	-	-	3/5/5/5	-
3	MPD	P	801	-	-	0/5/5/5	-
3	MPD	N	801	-	-	3/5/5/5	-
3	MPD	U	201	-	-	1/5/5/5	-
3	MPD	V	201	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	I	800	-	-	3/5/5/5	-
3	MPD	H	800	-	-	3/5/5/5	-
3	MPD	B	800	-	-	3/5/5/5	-
3	MPD	O	801	-	-	3/5/5/5	-
3	MPD	E	803	-	-	1/5/5/5	-
3	MPD	R	203	-	-	2/5/5/5	-
3	MPD	M	202	-	-	0/5/5/5	-
3	MPD	A	800	-	-	2/5/5/5	-
3	MPD	Q	801	-	-	1/5/5/5	-
3	MPD	Q	800	-	-	2/5/5/5	-
3	MPD	R	201	-	-	0/5/5/5	-
3	MPD	Y	800	-	-	3/5/5/5	-
3	MPD	M	201	-	-	3/5/5/5	-
3	MPD	Z	803	-	-	1/5/5/5	-
3	MPD	B	801	-	-	2/5/5/5	-
3	MPD	G	800	-	-	3/5/5/5	-
3	MPD	O	800	-	-	3/5/5/5	-
3	MPD	N	800	-	-	3/5/5/5	-
3	MPD	T	801	-	-	0/5/5/5	-
3	MPD	T	800	-	-	3/5/5/5	-
3	MPD	b	800	-	-	3/5/5/5	-
3	MPD	W	801	-	-	1/5/5/5	-
3	MPD	K	801	-	-	2/5/5/5	-
3	MPD	P	800	-	-	0/5/5/5	-
3	MPD	G	801	-	-	2/5/5/5	-
3	MPD	M	203	-	-	3/5/5/5	-
3	MPD	J	800	-	-	3/5/5/5	-
3	MPD	C	801	-	-	0/5/5/5	-
3	MPD	S	800	-	-	3/5/5/5	-
3	MPD	I	801	-	-	1/5/5/5	-
3	MPD	F	800	-	-	2/5/5/5	-
3	MPD	U	202	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 110 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	800	MPD	O2-C2-C3-C4
3	b	800	MPD	O2-C2-C3-C4
3	J	800	MPD	O2-C2-C3-C4
3	E	802	MPD	O2-C2-C3-C4
3	D	800	MPD	O2-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	192/207 (92%)	-0.13	5 (2%)	56	58	14, 20, 36, 48	0
1	B	188/207 (90%)	-0.18	6 (3%)	47	50	13, 18, 40, 71	0
1	C	188/207 (90%)	-0.06	8 (4%)	35	38	12, 19, 42, 78	0
1	D	188/207 (90%)	-0.11	9 (4%)	30	33	13, 18, 40, 68	0
1	E	188/207 (90%)	-0.13	6 (3%)	47	50	15, 20, 40, 62	0
1	F	190/207 (91%)	-0.04	11 (5%)	23	25	16, 21, 45, 79	0
1	G	190/207 (91%)	-0.03	8 (4%)	36	39	16, 22, 44, 62	0
1	H	186/207 (89%)	-0.20	7 (3%)	40	43	13, 19, 40, 61	0
1	I	190/207 (91%)	-0.22	4 (2%)	63	66	12, 18, 37, 54	0
1	J	190/207 (91%)	-0.14	6 (3%)	47	50	12, 18, 45, 63	0
1	K	188/207 (90%)	-0.09	9 (4%)	30	33	13, 19, 45, 70	0
1	L	187/207 (90%)	-0.08	6 (3%)	47	50	15, 21, 44, 72	0
1	M	190/207 (91%)	0.04	13 (6%)	17	19	16, 22, 45, 68	0
1	N	187/207 (90%)	-0.07	8 (4%)	35	38	15, 20, 45, 66	0
1	O	189/207 (91%)	-0.09	6 (3%)	47	50	16, 21, 38, 65	0
1	P	190/207 (91%)	-0.04	8 (4%)	36	39	17, 22, 42, 62	0
1	Q	187/207 (90%)	0.07	12 (6%)	19	22	14, 21, 49, 75	0
1	R	180/207 (86%)	0.00	7 (3%)	39	42	15, 20, 37, 59	0
1	S	184/207 (88%)	0.04	8 (4%)	35	38	14, 20, 38, 60	0
1	T	186/207 (89%)	-0.05	8 (4%)	35	38	13, 19, 40, 71	0
1	U	186/207 (89%)	-0.11	8 (4%)	35	38	14, 19, 37, 68	0
1	V	183/207 (88%)	0.19	10 (5%)	25	28	17, 25, 47, 71	0
1	W	183/207 (88%)	0.10	6 (3%)	46	49	17, 25, 44, 66	0
1	X	190/207 (91%)	0.11	13 (6%)	17	19	15, 22, 50, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Y	186/207 (89%)	-0.16	6 (3%) 47 50	13, 19, 35, 66	0
1	Z	183/207 (88%)	-0.11	8 (4%) 34 37	14, 20, 39, 60	0
1	a	183/207 (88%)	0.18	10 (5%) 25 28	15, 21, 41, 73	0
1	b	180/207 (86%)	0.09	7 (3%) 39 42	15, 24, 43, 63	0
2	1	4/7 (57%)	1.13	1 (25%) 0 0	24, 31, 35, 40	0
2	2	4/7 (57%)	1.24	1 (25%) 0 0	22, 27, 31, 43	0
2	3	4/7 (57%)	1.77	1 (25%) 0 0	27, 32, 33, 44	0
2	4	4/7 (57%)	1.64	2 (50%) 0 0	34, 41, 44, 52	0
2	c	4/7 (57%)	1.35	1 (25%) 0 0	22, 30, 32, 43	0
2	d	4/7 (57%)	0.91	1 (25%) 0 0	20, 28, 31, 40	0
2	e	4/7 (57%)	0.90	0 100 100	23, 33, 33, 39	0
2	f	4/7 (57%)	0.91	1 (25%) 0 0	24, 31, 34, 46	0
2	g	4/7 (57%)	1.54	1 (25%) 0 0	26, 32, 36, 48	0
2	h	4/7 (57%)	0.91	1 (25%) 0 0	23, 30, 35, 44	0
2	i	4/7 (57%)	1.20	1 (25%) 0 0	21, 29, 32, 44	0
2	j	4/7 (57%)	1.23	1 (25%) 0 0	22, 29, 32, 44	0
2	k	4/7 (57%)	1.33	1 (25%) 0 0	24, 31, 33, 45	0
2	l	4/7 (57%)	1.28	1 (25%) 0 0	24, 31, 35, 44	0
2	m	4/7 (57%)	1.60	2 (50%) 0 0	27, 31, 34, 41	0
2	n	4/7 (57%)	0.66	0 100 100	24, 33, 36, 46	0
2	o	4/7 (57%)	0.45	0 100 100	20, 26, 27, 36	0
2	p	4/7 (57%)	0.93	1 (25%) 0 0	25, 32, 33, 43	0
2	q	4/7 (57%)	1.12	1 (25%) 0 0	25, 33, 37, 45	0
2	r	4/7 (57%)	1.20	1 (25%) 0 0	22, 27, 29, 41	0
2	s	4/7 (57%)	1.07	1 (25%) 0 0	24, 32, 34, 44	0
2	t	4/7 (57%)	1.45	1 (25%) 0 0	23, 31, 33, 48	0
2	u	4/7 (57%)	0.83	1 (25%) 0 0	22, 27, 30, 43	0
2	v	4/7 (57%)	1.43	1 (25%) 0 0	33, 41, 43, 54	0
2	w	4/7 (57%)	0.85	1 (25%) 0 0	28, 34, 34, 42	0
2	x	4/7 (57%)	3.48	4 (100%) 0 0	28, 34, 35, 39	4 (100%)
2	y	4/7 (57%)	1.10	1 (25%) 0 0	22, 28, 29, 42	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
2	z	4/7 (57%)	1.69	1 (25%)	0	0	26, 34, 34, 45	0
All	All	5344/5992 (89%)	-0.02	253 (4%)	31	34	12, 21, 44, 79	4 (0%)

The worst 5 of 253 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	7	ILE	10.4
1	b	17	PHE	10.1
1	b	2	LEU	9.1
1	a	7	ILE	8.5
1	a	16	SER	8.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAA	x	704	6/7	0.61	0.36	36,38,39,39	6
2	MAA	4	704	6/7	0.74	0.39	45,50,54,54	0
2	MAA	z	704	6/7	0.77	0.22	38,39,42,50	0
2	MAA	h	704	6/7	0.77	0.22	33,37,40,41	0
2	MAA	v	704	6/7	0.79	0.33	45,52,55,55	0
2	MAA	l	704	6/7	0.79	0.25	31,37,44,47	0
2	MAA	m	704	6/7	0.80	0.18	33,35,38,38	0
2	MAA	d	704	6/7	0.80	0.23	32,38,40,41	0
2	MAA	3	704	6/7	0.80	0.27	32,37,43,43	0
2	MAA	w	704	6/7	0.80	0.16	34,38,39,41	0
2	MAA	n	704	6/7	0.81	0.21	32,42,44,48	0
2	MAA	j	704	6/7	0.82	0.22	27,33,39,41	0
2	MAA	e	704	6/7	0.82	0.20	30,39,41,44	0
2	MAA	r	704	6/7	0.82	0.22	30,32,39,41	0
2	MP8	x	706	8/9	0.82	0.21	28,30,34,37	8
2	MAA	k	704	6/7	0.83	0.19	30,35,40,43	0
2	MAA	y	704	6/7	0.83	0.24	31,35,41,42	0
2	MAA	u	704	6/7	0.84	0.23	31,36,39,41	0
2	MAA	o	704	6/7	0.84	0.17	25,32,35,35	0
2	MAA	t	704	6/7	0.85	0.19	35,40,41,42	0
2	MAA	1	704	6/7	0.85	0.19	30,32,36,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAA	p	704	6/7	0.86	0.19	35,36,42,46	0
2	MAA	i	704	6/7	0.87	0.20	29,33,36,41	0
2	MP8	4	706	8/9	0.87	0.16	35,38,44,47	0
2	MAA	s	704	6/7	0.88	0.20	31,38,40,46	0
2	MP8	f	706	8/9	0.88	0.13	23,26,31,32	0
2	MAA	c	704	6/7	0.88	0.20	30,35,42,43	0
2	MP8	3	706	8/9	0.88	0.14	24,27,30,30	0
2	MAA	f	704	6/7	0.88	0.18	32,35,41,42	0
2	MP8	v	706	8/9	0.89	0.11	34,39,41,42	0
2	MAA	g	704	6/7	0.89	0.21	30,35,41,42	0
2	MAA	2	704	6/7	0.89	0.15	31,33,36,38	0
2	MAA	q	704	6/7	0.89	0.24	35,39,40,42	0
2	MP8	y	706	8/9	0.90	0.10	21,22,28,31	0
2	MP8	1	706	8/9	0.90	0.13	24,27,30,33	0
2	MP8	s	706	8/9	0.90	0.12	24,25,30,31	0
2	MP8	e	706	8/9	0.91	0.10	24,26,33,34	0
2	MP8	j	706	8/9	0.91	0.12	21,22,27,27	0
2	MP8	n	706	8/9	0.92	0.09	27,28,31,41	0
2	MP8	o	706	8/9	0.92	0.09	18,22,25,25	0
2	MP8	g	706	8/9	0.92	0.11	26,28,32,35	0
2	MP8	2	706	8/9	0.92	0.10	19,23,27,28	0
2	MP8	w	706	8/9	0.93	0.10	31,33,34,34	0
2	MP8	p	706	8/9	0.93	0.10	26,29,32,33	0
2	MP8	r	706	8/9	0.93	0.10	20,25,28,28	0
2	MP8	z	706	8/9	0.93	0.11	24,28,34,34	0
2	MP8	i	706	8/9	0.93	0.08	21,23,26,30	0
2	MP8	c	706	8/9	0.93	0.10	23,25,31,33	0
2	MP8	m	706	8/9	0.94	0.11	26,28,32,32	0
2	MP8	d	706	8/9	0.94	0.10	20,24,30,30	0
2	MP8	t	706	8/9	0.94	0.09	22,25,28,30	0
2	MP8	h	706	8/9	0.94	0.08	24,27,30,32	0
2	MP8	k	706	8/9	0.94	0.08	23,27,29,30	0
2	MP8	u	706	8/9	0.94	0.08	19,23,28,30	0
2	MP8	q	706	8/9	0.95	0.10	21,24,30,31	0
2	MP8	l	706	8/9	0.95	0.09	24,28,31,35	0

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, 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	B-factors(Å^2)	Q<0.9
3	MPD	V	202	8/8	0.81	0.21	30,37,39,41	0
3	MPD	A	801	8/8	0.82	0.22	33,39,42,43	0
3	MPD	R	202	8/8	0.84	0.19	30,34,39,40	0
3	MPD	Y	800	8/8	0.85	0.18	19,23,27,27	0
3	MPD	X	202	8/8	0.86	0.16	29,33,35,38	0
3	MPD	Z	801	8/8	0.86	0.17	29,32,36,36	0
3	MPD	Z	803	8/8	0.88	0.16	30,36,38,40	0
3	MPD	S	800	8/8	0.88	0.17	19,22,27,29	0
3	MPD	M	203	8/8	0.89	0.14	29,34,36,39	0
3	MPD	B	800	8/8	0.89	0.16	16,21,23,31	0
3	MPD	R	203	8/8	0.89	0.19	32,35,38,40	0
3	MPD	K	801	8/8	0.90	0.13	26,30,37,40	0
3	MPD	I	801	8/8	0.90	0.17	26,32,34,35	0
3	MPD	R	201	8/8	0.90	0.13	24,28,31,35	0
3	MPD	B	801	8/8	0.90	0.12	24,29,33,34	0
3	MPD	W	801	8/8	0.90	0.16	29,34,35,40	0
3	MPD	M	202	8/8	0.91	0.14	24,35,39,40	0
3	MPD	P	800	8/8	0.91	0.17	21,27,35,38	0
3	MPD	L	801	8/8	0.91	0.12	28,32,34,36	0
3	MPD	K	800	8/8	0.91	0.14	18,22,26,27	0
3	MPD	b	801	8/8	0.91	0.14	30,34,40,42	0
3	MPD	J	801	8/8	0.91	0.10	26,30,32,35	0
3	MPD	P	801	8/8	0.91	0.15	30,39,43,43	0
3	MPD	E	801	8/8	0.91	0.13	28,35,36,36	0
3	MPD	E	803	8/8	0.91	0.15	25,30,32,34	0
3	MPD	C	801	8/8	0.91	0.12	25,30,32,35	0
3	MPD	W	800	8/8	0.91	0.16	24,31,33,34	0
3	MPD	T	801	8/8	0.91	0.18	26,34,36,38	0
3	MPD	O	800	8/8	0.91	0.16	22,24,28,30	0
3	MPD	D	801	8/8	0.92	0.12	25,29,31,33	0
3	MPD	b	800	8/8	0.92	0.13	22,26,29,32	0
3	MPD	N	800	8/8	0.92	0.15	20,26,27,27	0
3	MPD	Q	801	8/8	0.92	0.11	26,36,40,41	0
3	MPD	A	800	8/8	0.92	0.13	17,25,28,31	0
3	MPD	a	800	8/8	0.92	0.18	21,24,28,29	0
3	MPD	G	800	8/8	0.92	0.12	22,25,28,30	0
3	MPD	Q	800	8/8	0.93	0.13	22,27,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MPD	D	800	8/8	0.93	0.17	17,20,23,26	0
3	MPD	M	201	8/8	0.93	0.15	18,26,27,28	0
3	MPD	C	800	8/8	0.93	0.14	16,21,25,26	0
3	MPD	U	202	8/8	0.93	0.14	19,24,29,30	0
3	MPD	V	201	8/8	0.93	0.12	23,29,33,33	0
3	MPD	H	800	8/8	0.93	0.13	16,21,23,26	0
3	MPD	L	800	8/8	0.93	0.13	21,24,28,29	0
3	MPD	N	801	8/8	0.93	0.13	32,34,36,42	0
3	MPD	X	201	8/8	0.93	0.18	23,27,29,31	0
3	MPD	Z	802	8/8	0.94	0.14	24,31,32,32	0
3	MPD	T	800	8/8	0.94	0.11	18,22,24,28	0
3	MPD	U	201	8/8	0.94	0.11	27,30,32,35	0
3	MPD	J	800	8/8	0.94	0.12	16,21,24,28	0
3	MPD	G	801	8/8	0.94	0.12	28,33,35,36	0
3	MPD	O	801	8/8	0.95	0.12	28,30,34,35	0
3	MPD	I	800	8/8	0.95	0.11	16,20,21,25	0
3	MPD	F	800	8/8	0.95	0.11	22,25,26,31	0
3	MPD	E	802	8/8	0.96	0.11	19,24,26,28	0

6.5 Other polymers (i)

There are no such residues in this entry.