Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 04:04 AM EST

PDB ID	:	6PBS
Title	:	Structure of ClpC1-NTD in complex with Ecumicin
Authors	:	Abad-Zapatero, C.; Wolf, N.M.
Deposited on	:	2019-06-14
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

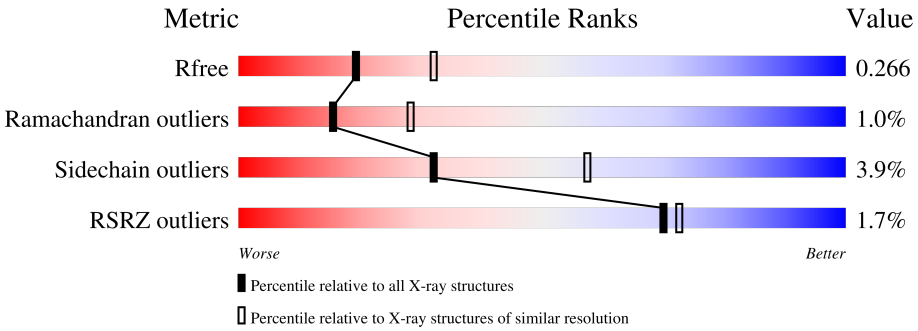
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	158	88% · 9%
1	B	158	89% · 8%
1	C	158	87% · · 8%
1	G	158	89% · 7%
1	I	158	91% · 8%
1	K	158	90% · 8%

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Mol	Chain	Length	Quality of chain
1	M	158	4% 86% 5% 9%
1	O	158	% 91% 7%
1	T	158	% 89% 8%
1	W	158	2% 91% 7%
1	Y	158	% 91% 7%
1	e	158	% 91% 7%
2	D	13	38% 54% 8%
2	E	13	8% 46% 54%
2	F	13	46% 54%
2	H	13	8% 54% 46%
2	J	13	38% 62%
2	L	13	31% 69%
2	N	13	31% 69%
2	P	13	8% 23% 77%
2	Q	13	8% 8% 92%
2	R	13	46% 54%
2	S	13	23% 77%
2	U	13	46% 54%
2	V	13	31% 69%
2	X	13	8% 46% 54%
2	Z	13	31% 69%
2	a	13	8% 23% 77%
2	b	13	46% 54%
2	c	13	8% 46% 54%
2	d	13	54% 46%

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Mol	Chain	Length	Quality of chain
2	f	13	23% 77%
2	g	13	8% 62% 38%
2	h	13	54% 46%
2	i	13	8% 38% 62%
2	j	13	54% 46%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	O7G	E	1	-	-	-	X
2	O7G	H	1	-	-	-	X
2	O7G	P	1	-	-	-	X
2	O7G	Q	1	-	-	-	X
2	MVA	V	9	-	X	-	-
2	O7G	a	1	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16993 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 ATP-binding subunit ClpC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1113	700	206	205	2			
1	I	146	Total	C	N	O	S	0	1	0
			1143	720	211	210	2			
1	C	145	Total	C	N	O	S	0	0	0
			1125	709	207	207	2			
1	W	147	Total	C	N	O	S	0	0	0
			1142	721	210	209	2			
1	Y	147	Total	C	N	O	S	0	0	0
			1142	721	210	209	2			
1	e	147	Total	C	N	O	S	0	0	0
			1142	721	210	209	2			
1	B	145	Total	C	N	O	S	0	0	0
			1125	709	207	207	2			
1	G	147	Total	C	N	O	S	0	0	0
			1142	721	210	209	2			
1	K	146	Total	C	N	O	S	0	0	0
			1134	715	209	208	2			
1	M	144	Total	C	N	O	S	0	0	0
			1113	700	206	205	2			
1	O	147	Total	C	N	O	S	0	0	0
			1142	721	210	209	2			
1	T	146	Total	C	N	O	S	0	0	0
			1134	715	209	208	2			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	LYS	-	expression tag	UNP P9WPC9
A	147	LEU	-	expression tag	UNP P9WPC9
A	148	ALA	-	expression tag	UNP P9WPC9
A	149	ALA	-	expression tag	UNP P9WPC9
A	150	ALA	-	expression tag	UNP P9WPC9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	151	LEU	-	expression tag	UNP P9WPC9
A	152	GLU	-	expression tag	UNP P9WPC9
A	153	HIS	-	expression tag	UNP P9WPC9
A	154	HIS	-	expression tag	UNP P9WPC9
A	155	HIS	-	expression tag	UNP P9WPC9
A	156	HIS	-	expression tag	UNP P9WPC9
A	157	HIS	-	expression tag	UNP P9WPC9
A	158	HIS	-	expression tag	UNP P9WPC9
I	146	LYS	-	expression tag	UNP P9WPC9
I	147	LEU	-	expression tag	UNP P9WPC9
I	148	ALA	-	expression tag	UNP P9WPC9
I	149	ALA	-	expression tag	UNP P9WPC9
I	150	ALA	-	expression tag	UNP P9WPC9
I	151	LEU	-	expression tag	UNP P9WPC9
I	152	GLU	-	expression tag	UNP P9WPC9
I	153	HIS	-	expression tag	UNP P9WPC9
I	154	HIS	-	expression tag	UNP P9WPC9
I	155	HIS	-	expression tag	UNP P9WPC9
I	156	HIS	-	expression tag	UNP P9WPC9
I	157	HIS	-	expression tag	UNP P9WPC9
I	158	HIS	-	expression tag	UNP P9WPC9
C	146	LYS	-	expression tag	UNP P9WPC9
C	147	LEU	-	expression tag	UNP P9WPC9
C	148	ALA	-	expression tag	UNP P9WPC9
C	149	ALA	-	expression tag	UNP P9WPC9
C	150	ALA	-	expression tag	UNP P9WPC9
C	151	LEU	-	expression tag	UNP P9WPC9
C	152	GLU	-	expression tag	UNP P9WPC9
C	153	HIS	-	expression tag	UNP P9WPC9
C	154	HIS	-	expression tag	UNP P9WPC9
C	155	HIS	-	expression tag	UNP P9WPC9
C	156	HIS	-	expression tag	UNP P9WPC9
C	157	HIS	-	expression tag	UNP P9WPC9
C	158	HIS	-	expression tag	UNP P9WPC9
W	146	LYS	-	expression tag	UNP P9WPC9
W	147	LEU	-	expression tag	UNP P9WPC9
W	148	ALA	-	expression tag	UNP P9WPC9
W	149	ALA	-	expression tag	UNP P9WPC9
W	150	ALA	-	expression tag	UNP P9WPC9
W	151	LEU	-	expression tag	UNP P9WPC9
W	152	GLU	-	expression tag	UNP P9WPC9
W	153	HIS	-	expression tag	UNP P9WPC9

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Chain	Residue	Modelled	Actual	Comment	Reference
W	154	HIS	-	expression tag	UNP P9WPC9
W	155	HIS	-	expression tag	UNP P9WPC9
W	156	HIS	-	expression tag	UNP P9WPC9
W	157	HIS	-	expression tag	UNP P9WPC9
W	158	HIS	-	expression tag	UNP P9WPC9
Y	146	LYS	-	expression tag	UNP P9WPC9
Y	147	LEU	-	expression tag	UNP P9WPC9
Y	148	ALA	-	expression tag	UNP P9WPC9
Y	149	ALA	-	expression tag	UNP P9WPC9
Y	150	ALA	-	expression tag	UNP P9WPC9
Y	151	LEU	-	expression tag	UNP P9WPC9
Y	152	GLU	-	expression tag	UNP P9WPC9
Y	153	HIS	-	expression tag	UNP P9WPC9
Y	154	HIS	-	expression tag	UNP P9WPC9
Y	155	HIS	-	expression tag	UNP P9WPC9
Y	156	HIS	-	expression tag	UNP P9WPC9
Y	157	HIS	-	expression tag	UNP P9WPC9
Y	158	HIS	-	expression tag	UNP P9WPC9
e	146	LYS	-	expression tag	UNP P9WPC9
e	147	LEU	-	expression tag	UNP P9WPC9
e	148	ALA	-	expression tag	UNP P9WPC9
e	149	ALA	-	expression tag	UNP P9WPC9
e	150	ALA	-	expression tag	UNP P9WPC9
e	151	LEU	-	expression tag	UNP P9WPC9
e	152	GLU	-	expression tag	UNP P9WPC9
e	153	HIS	-	expression tag	UNP P9WPC9
e	154	HIS	-	expression tag	UNP P9WPC9
e	155	HIS	-	expression tag	UNP P9WPC9
e	156	HIS	-	expression tag	UNP P9WPC9
e	157	HIS	-	expression tag	UNP P9WPC9
e	158	HIS	-	expression tag	UNP P9WPC9
B	146	LYS	-	expression tag	UNP P9WPC9
B	147	LEU	-	expression tag	UNP P9WPC9
B	148	ALA	-	expression tag	UNP P9WPC9
B	149	ALA	-	expression tag	UNP P9WPC9
B	150	ALA	-	expression tag	UNP P9WPC9
B	151	LEU	-	expression tag	UNP P9WPC9
B	152	GLU	-	expression tag	UNP P9WPC9
B	153	HIS	-	expression tag	UNP P9WPC9
B	154	HIS	-	expression tag	UNP P9WPC9
B	155	HIS	-	expression tag	UNP P9WPC9
B	156	HIS	-	expression tag	UNP P9WPC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	157	HIS	-	expression tag	UNP P9WPC9
B	158	HIS	-	expression tag	UNP P9WPC9
G	146	LYS	-	expression tag	UNP P9WPC9
G	147	LEU	-	expression tag	UNP P9WPC9
G	148	ALA	-	expression tag	UNP P9WPC9
G	149	ALA	-	expression tag	UNP P9WPC9
G	150	ALA	-	expression tag	UNP P9WPC9
G	151	LEU	-	expression tag	UNP P9WPC9
G	152	GLU	-	expression tag	UNP P9WPC9
G	153	HIS	-	expression tag	UNP P9WPC9
G	154	HIS	-	expression tag	UNP P9WPC9
G	155	HIS	-	expression tag	UNP P9WPC9
G	156	HIS	-	expression tag	UNP P9WPC9
G	157	HIS	-	expression tag	UNP P9WPC9
G	158	HIS	-	expression tag	UNP P9WPC9
K	146	LYS	-	expression tag	UNP P9WPC9
K	147	LEU	-	expression tag	UNP P9WPC9
K	148	ALA	-	expression tag	UNP P9WPC9
K	149	ALA	-	expression tag	UNP P9WPC9
K	150	ALA	-	expression tag	UNP P9WPC9
K	151	LEU	-	expression tag	UNP P9WPC9
K	152	GLU	-	expression tag	UNP P9WPC9
K	153	HIS	-	expression tag	UNP P9WPC9
K	154	HIS	-	expression tag	UNP P9WPC9
K	155	HIS	-	expression tag	UNP P9WPC9
K	156	HIS	-	expression tag	UNP P9WPC9
K	157	HIS	-	expression tag	UNP P9WPC9
K	158	HIS	-	expression tag	UNP P9WPC9
M	146	LYS	-	expression tag	UNP P9WPC9
M	147	LEU	-	expression tag	UNP P9WPC9
M	148	ALA	-	expression tag	UNP P9WPC9
M	149	ALA	-	expression tag	UNP P9WPC9
M	150	ALA	-	expression tag	UNP P9WPC9
M	151	LEU	-	expression tag	UNP P9WPC9
M	152	GLU	-	expression tag	UNP P9WPC9
M	153	HIS	-	expression tag	UNP P9WPC9
M	154	HIS	-	expression tag	UNP P9WPC9
M	155	HIS	-	expression tag	UNP P9WPC9
M	156	HIS	-	expression tag	UNP P9WPC9
M	157	HIS	-	expression tag	UNP P9WPC9
M	158	HIS	-	expression tag	UNP P9WPC9
O	146	LYS	-	expression tag	UNP P9WPC9

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Chain	Residue	Modelled	Actual	Comment	Reference
O	147	LEU	-	expression tag	UNP P9WPC9
O	148	ALA	-	expression tag	UNP P9WPC9
O	149	ALA	-	expression tag	UNP P9WPC9
O	150	ALA	-	expression tag	UNP P9WPC9
O	151	LEU	-	expression tag	UNP P9WPC9
O	152	GLU	-	expression tag	UNP P9WPC9
O	153	HIS	-	expression tag	UNP P9WPC9
O	154	HIS	-	expression tag	UNP P9WPC9
O	155	HIS	-	expression tag	UNP P9WPC9
O	156	HIS	-	expression tag	UNP P9WPC9
O	157	HIS	-	expression tag	UNP P9WPC9
O	158	HIS	-	expression tag	UNP P9WPC9
T	146	LYS	-	expression tag	UNP P9WPC9
T	147	LEU	-	expression tag	UNP P9WPC9
T	148	ALA	-	expression tag	UNP P9WPC9
T	149	ALA	-	expression tag	UNP P9WPC9
T	150	ALA	-	expression tag	UNP P9WPC9
T	151	LEU	-	expression tag	UNP P9WPC9
T	152	GLU	-	expression tag	UNP P9WPC9
T	153	HIS	-	expression tag	UNP P9WPC9
T	154	HIS	-	expression tag	UNP P9WPC9
T	155	HIS	-	expression tag	UNP P9WPC9
T	156	HIS	-	expression tag	UNP P9WPC9
T	157	HIS	-	expression tag	UNP P9WPC9
T	158	HIS	-	expression tag	UNP P9WPC9

- Molecule 2 is a protein called ecumicin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	E	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	F	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	H	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	J	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	L	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	N	13	Total	C	N	O	0	0	0
			114	83	14	17			

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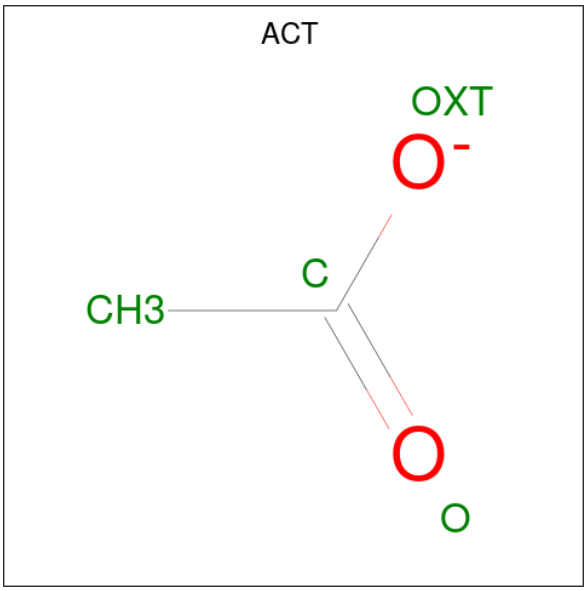
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	Q	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	R	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	S	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	U	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	V	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	X	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	Z	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	a	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	b	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	c	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	d	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	f	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	g	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	h	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	i	13	Total	C	N	O	0	0	0
			114	83	14	17			
2	j	13	Total	C	N	O	0	0	0
			114	83	14	17			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	W	1	Total C O 4 2 2	0	0
3	W	1	Total C O 4 2 2	0	0
3	W	1	Total C O 4 2 2	0	0
3	W	1	Total C O 4 2 2	0	0
3	Y	1	Total C O 4 2 2	0	0
3	Y	1	Total C O 4 2 2	0	0
3	Y	1	Total C O 4 2 2	0	0
3	e	1	Total C O 4 2 2	0	0
3	e	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	O	1	Total C O 4 2 2	0	0
3	T	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	39	Total O 40 40	0	1
4	I	53	Total O 53 53	0	0
4	C	26	Total O 26 26	0	0
4	W	30	Total O 30 30	0	0
4	Y	48	Total O 48 48	0	0
4	e	41	Total O 43 43	0	2
4	B	36	Total O 36 36	0	0
4	G	53	Total O 53 53	0	0
4	K	36	Total O 36 36	0	0
4	M	31	Total O 32 32	0	1
4	O	35	Total O 36 36	0	1
4	T	44	Total O 44 44	0	0
4	D	6	Total O 6 6	0	0

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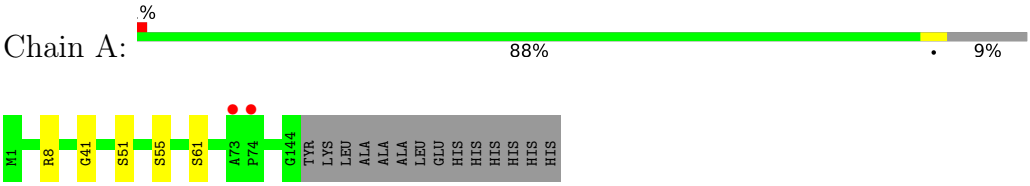
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	4	Total O 4 4	0	0
4	F	5	Total O 5 5	0	0
4	H	4	Total O 4 4	0	0
4	J	6	Total O 6 6	0	0
4	N	2	Total O 2 2	0	0
4	P	3	Total O 3 3	0	0
4	Q	2	Total O 2 2	0	0
4	R	9	Total O 9 9	0	0
4	U	7	Total O 7 7	0	0
4	V	7	Total O 7 7	0	0
4	X	3	Total O 3 3	0	0
4	Z	10	Total O 10 10	0	0
4	a	2	Total O 2 2	0	0
4	b	4	Total O 4 4	0	0
4	c	1	Total O 1 1	0	0
4	d	2	Total O 2 2	0	0
4	f	6	Total O 6 6	0	0
4	g	2	Total O 2 2	0	0
4	h	9	Total O 9 9	0	0
4	i	2	Total O 2 2	0	0
4	j	7	Total O 7 7	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.

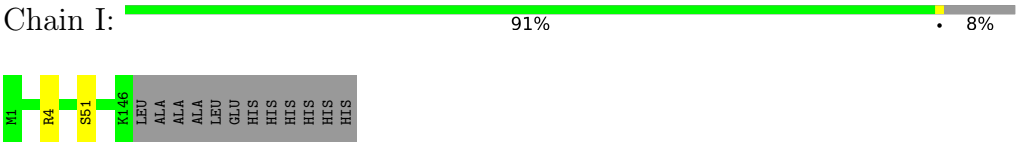
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain A:



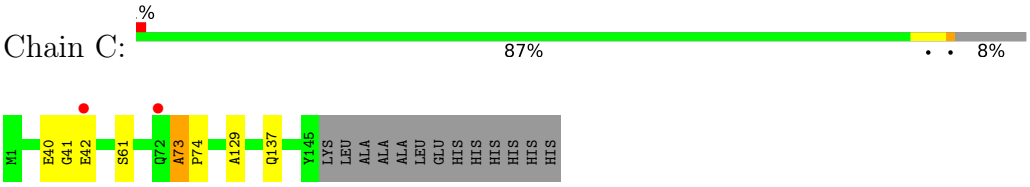
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain I:



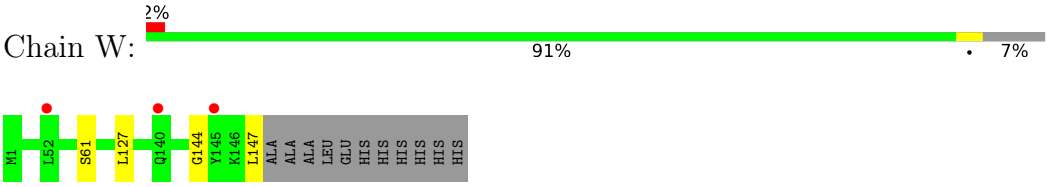
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain C:



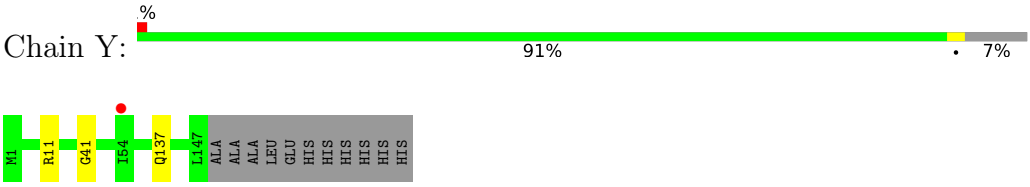
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain W:



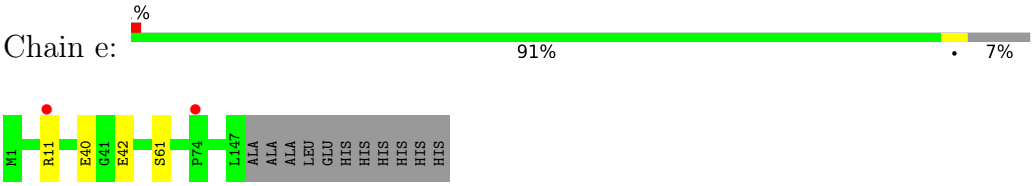
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain Y:



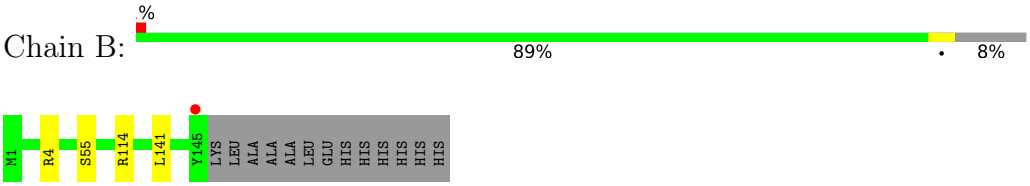
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain e:



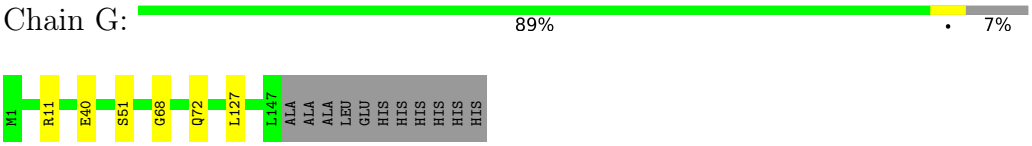
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain B:



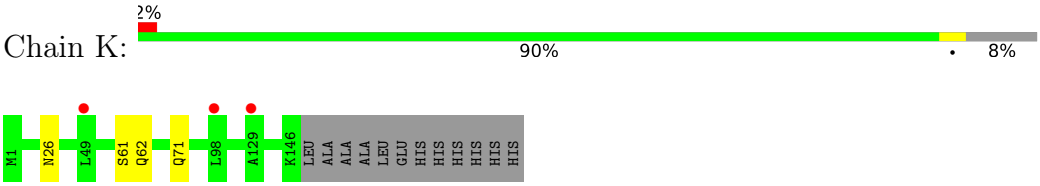
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain G:



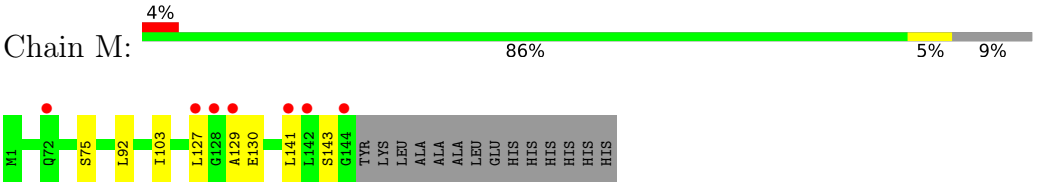
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain K:



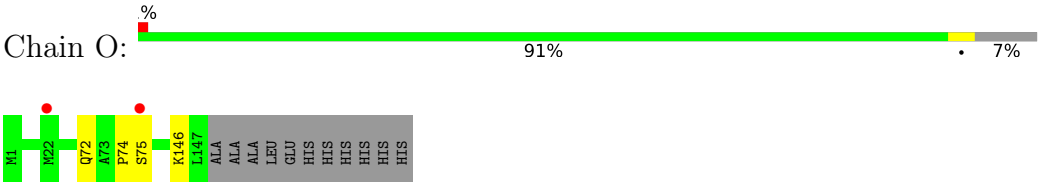
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain M:



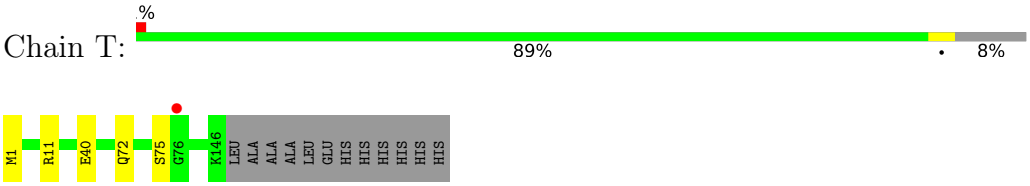
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain O:



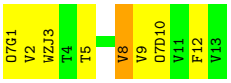
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain T:



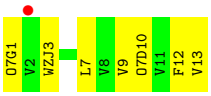
• Molecule 2: ecumicin

Chain D:



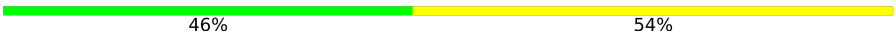
• Molecule 2: ecumicin

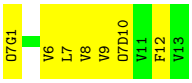
Chain E:



• Molecule 2: ecumicin

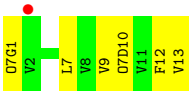
Chain F:





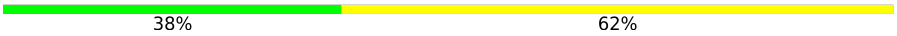
• Molecule 2: ecumicin

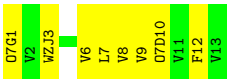
Chain H:



• Molecule 2: ecumicin

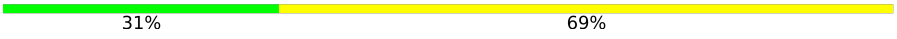
Chain J:

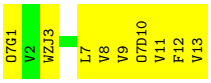




• Molecule 2: ecumicin

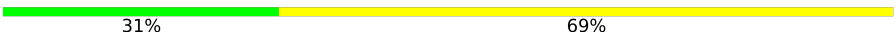
Chain L:





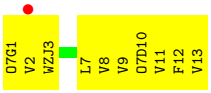
• Molecule 2: ecumicin

Chain N:



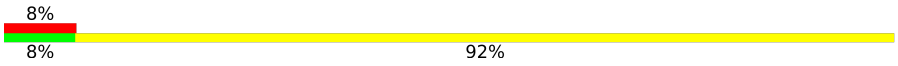
• Molecule 2: ecumicin

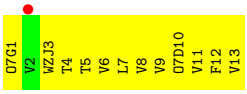
Chain P:



• Molecule 2: ecumicin

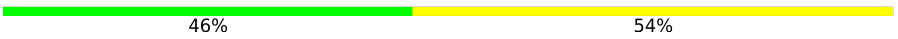
Chain Q:

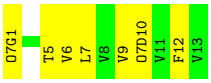




• Molecule 2: ecumicin

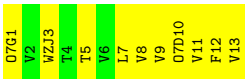
Chain R:





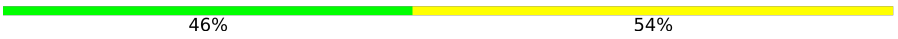
• Molecule 2: ecumicin

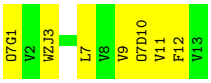
Chain S:



• Molecule 2: ecumicin

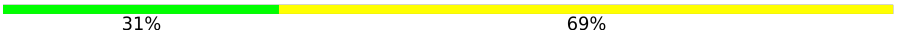
Chain U:

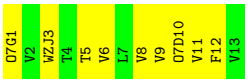




• Molecule 2: ecumicin

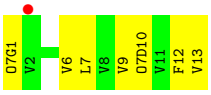
Chain V:





• Molecule 2: ecumicin

Chain X:

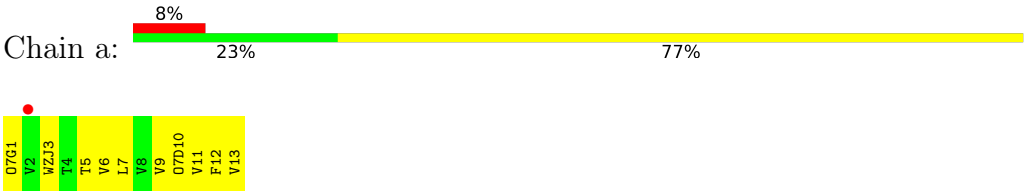


• Molecule 2: ecumicin

Chain Z:

• Molecule 2: ecumicin

Chain a:

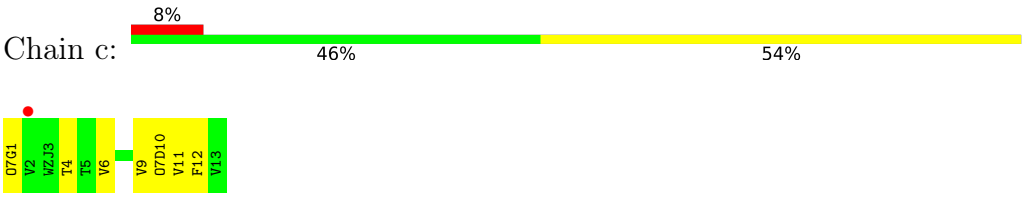


• Molecule 2: ecumicin

Chain b:

• Molecule 2: ecumicin

Chain c:



• Molecule 2: ecumicin

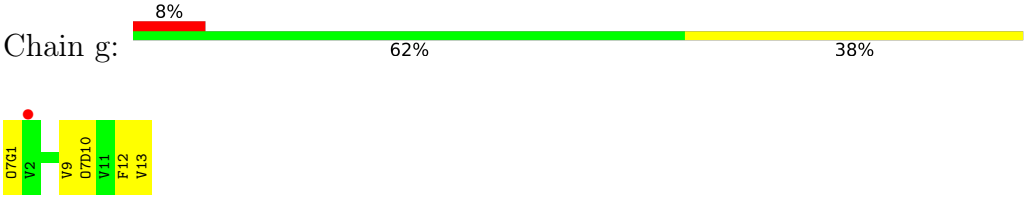
Chain d:

• Molecule 2: ecumicin

Chain f:

• Molecule 2: ecumicin

Chain g:

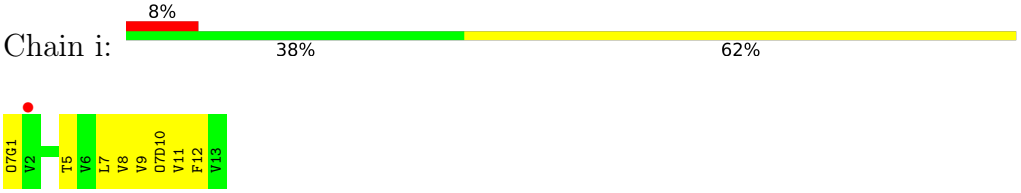


• Molecule 2: ecumicin

Chain h:

• Molecule 2: ecumicin

Chain i:



• Molecule 2: ecumicin

Chain j:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.06Å 130.34Å 112.56Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 19.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (40.00-2.50) 97.8 (19.49-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.180 , 0.257 0.195 , 0.266	Depositor DCC
R_{free} test set	3796 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16993	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.45% 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: O7D, O7G, MLE, WZJ, MVA, NZC, ACT, H14

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	0.51	0/1126	0.62	0/1516
1	B	0.48	0/1139	0.61	0/1534
1	C	0.43	0/1139	0.59	0/1534
1	G	0.50	0/1156	0.60	0/1556
1	I	0.50	0/1157	0.65	1/1557 (0.1%)
1	K	0.44	0/1148	0.59	0/1545
1	M	0.45	0/1126	0.60	0/1516
1	O	0.47	0/1156	0.61	0/1556
1	T	0.50	0/1148	0.64	0/1545
1	W	0.46	0/1156	0.60	0/1556
1	Y	0.48	0/1156	0.64	0/1556
1	e	0.48	0/1156	0.61	0/1556
2	D	1.89	1/36 (2.8%)	1.61	0/42
2	E	1.83	1/36 (2.8%)	1.21	0/42
2	F	1.79	1/36 (2.8%)	1.39	0/42
2	H	1.86	1/36 (2.8%)	1.22	0/42
2	J	1.74	1/36 (2.8%)	1.42	0/42
2	L	2.04	3/36 (8.3%)	1.22	0/42
2	N	1.80	0/36	1.35	0/42
2	P	2.05	2/36 (5.6%)	2.99	4/42 (9.5%)
2	Q	2.20	3/36 (8.3%)	1.69	0/42
2	R	1.79	0/36	1.40	0/42
2	S	1.92	2/36 (5.6%)	1.32	0/42
2	U	1.72	0/36	1.30	0/42
2	V	2.02	1/36 (2.8%)	2.51	3/42 (7.1%)
2	X	1.97	2/36 (5.6%)	1.28	0/42
2	Z	1.84	1/36 (2.8%)	1.67	0/42
2	a	1.93	1/36 (2.8%)	1.31	0/42
2	b	1.65	0/36	1.67	0/42
2	c	1.86	1/36 (2.8%)	1.29	0/42
2	d	2.01	2/36 (5.6%)	1.36	0/42
2	f	1.77	1/36 (2.8%)	1.40	1/42 (2.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	g	1.87	1/36 (2.8%)	1.50	0/42
2	h	1.83	0/36	1.41	0/42
2	i	1.85	1/36 (2.8%)	1.21	0/42
2	j	1.67	0/36	1.46	0/42
All	All	0.65	26/14627 (0.2%)	0.69	9/19535 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	4	THR	CA-C	-7.15	1.34	1.52
2	V	8	VAL	CA-C	-6.50	1.36	1.52
2	Q	13	VAL	CA-C	-6.27	1.36	1.52
2	d	8	VAL	CA-C	-5.99	1.37	1.52
2	d	13	VAL	CA-C	-5.66	1.38	1.52
2	a	13	VAL	CA-C	-5.62	1.38	1.52
2	X	13	VAL	CA-C	-5.54	1.38	1.52
2	L	11	VAL	CA-C	-5.52	1.38	1.52
2	P	13	VAL	CA-C	-5.46	1.38	1.52
2	g	13	VAL	CA-C	-5.45	1.38	1.52
2	L	13	VAL	CA-C	-5.35	1.39	1.52
2	L	8	VAL	CA-C	-5.34	1.39	1.52
2	S	13	VAL	CA-C	-5.33	1.39	1.52
2	E	13	VAL	CA-C	-5.29	1.39	1.52
2	Q	8	VAL	CA-C	-5.17	1.39	1.52
2	F	8	VAL	CA-C	-5.15	1.39	1.52
2	P	8	VAL	CA-C	-5.09	1.39	1.52
2	i	8	VAL	CA-C	-5.09	1.39	1.52
2	f	8	VAL	CA-C	-5.08	1.39	1.52
2	H	13	VAL	CA-C	-5.08	1.39	1.52
2	c	4	THR	CA-C	-5.06	1.39	1.52
2	S	8	VAL	CA-C	-5.06	1.39	1.52
2	X	6	VAL	CA-C	-5.06	1.39	1.52
2	Z	8	VAL	CA-C	-5.03	1.39	1.52
2	D	8	VAL	CA-C	-5.02	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	8	VAL	CA-C	-5.01	1.40	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	2	VAL	CA-CB-CG2	10.24	126.26	110.90
1	I	4	ARG	NE-CZ-NH2	9.87	125.23	120.30
2	P	2	VAL	CB-CA-C	8.74	128.00	111.40
2	P	2	VAL	CA-CB-CG1	-8.07	98.80	110.90
2	V	8	VAL	CB-CA-C	7.02	124.74	111.40
2	P	2	VAL	CG1-CB-CG2	-6.00	101.30	110.90
2	V	11	VAL	CA-CB-CG1	5.44	119.06	110.90
2	f	4	THR	CA-CB-CG2	-5.22	105.09	112.40
2	V	6	VAL	CG1-CB-CG2	-5.07	102.80	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	73	ALA	Peptide

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	142/158 (90%)	137 (96%)	4 (3%)	1 (1%)	22 39
1	B	143/158 (90%)	136 (95%)	7 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	143/158 (90%)	126 (88%)	12 (8%)	5 (4%)	3	4
1	G	145/158 (92%)	140 (97%)	4 (3%)	1 (1%)	22	39
1	I	145/158 (92%)	141 (97%)	4 (3%)	0	100	100
1	K	144/158 (91%)	136 (94%)	8 (6%)	0	100	100
1	M	142/158 (90%)	132 (93%)	8 (6%)	2 (1%)	11	20
1	O	145/158 (92%)	135 (93%)	6 (4%)	4 (3%)	5	7
1	T	144/158 (91%)	132 (92%)	10 (7%)	2 (1%)	11	20
1	W	145/158 (92%)	141 (97%)	3 (2%)	1 (1%)	22	39
1	Y	145/158 (92%)	135 (93%)	9 (6%)	1 (1%)	22	39
1	e	145/158 (92%)	137 (94%)	7 (5%)	1 (1%)	22	39
2	D	5/13 (38%)	5 (100%)	0	0	100	100
2	E	5/13 (38%)	4 (80%)	1 (20%)	0	100	100
2	F	5/13 (38%)	5 (100%)	0	0	100	100
2	H	5/13 (38%)	5 (100%)	0	0	100	100
2	J	5/13 (38%)	5 (100%)	0	0	100	100
2	L	5/13 (38%)	5 (100%)	0	0	100	100
2	N	5/13 (38%)	5 (100%)	0	0	100	100
2	P	5/13 (38%)	5 (100%)	0	0	100	100
2	Q	5/13 (38%)	4 (80%)	1 (20%)	0	100	100
2	R	5/13 (38%)	5 (100%)	0	0	100	100
2	S	5/13 (38%)	5 (100%)	0	0	100	100
2	U	5/13 (38%)	5 (100%)	0	0	100	100
2	V	5/13 (38%)	5 (100%)	0	0	100	100
2	X	5/13 (38%)	5 (100%)	0	0	100	100
2	Z	5/13 (38%)	5 (100%)	0	0	100	100
2	a	5/13 (38%)	5 (100%)	0	0	100	100
2	b	5/13 (38%)	5 (100%)	0	0	100	100
2	c	5/13 (38%)	5 (100%)	0	0	100	100
2	d	5/13 (38%)	5 (100%)	0	0	100	100
2	f	5/13 (38%)	5 (100%)	0	0	100	100
2	g	5/13 (38%)	5 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	h	5/13 (38%)	5 (100%)	0	0	100 100
2	i	5/13 (38%)	5 (100%)	0	0	100 100
2	j	5/13 (38%)	5 (100%)	0	0	100 100
All	All	1848/2208 (84%)	1746 (94%)	84 (4%)	18 (1%)	15 28

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	41	GLY
1	e	40	GLU
1	M	129	ALA
1	A	41	GLY
1	C	41	GLY
1	M	130	GLU
1	T	40	GLU
1	C	42	GLU
1	G	68	GLY
1	O	72	GLN
1	O	146	LYS
1	T	75	SER
1	C	74	PRO
1	C	129	ALA
1	W	144	GLY
1	O	75	SER
1	C	73	ALA
1	O	74	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	117/128 (91%)	113 (97%)	4 (3%)	37 63
1	B	118/128 (92%)	114 (97%)	4 (3%)	37 63
1	C	118/128 (92%)	115 (98%)	3 (2%)	47 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	120/128 (94%)	115 (96%)	5 (4%)	30 54
1	I	120/128 (94%)	119 (99%)	1 (1%)	81 93
1	K	119/128 (93%)	115 (97%)	4 (3%)	37 63
1	M	117/128 (91%)	111 (95%)	6 (5%)	24 45
1	O	120/128 (94%)	120 (100%)	0	100 100
1	T	119/128 (93%)	116 (98%)	3 (2%)	47 73
1	W	120/128 (94%)	117 (98%)	3 (2%)	47 73
1	Y	120/128 (94%)	118 (98%)	2 (2%)	60 82
1	e	120/128 (94%)	117 (98%)	3 (2%)	47 73
2	D	6/6 (100%)	4 (67%)	2 (33%)	0 0
2	E	6/6 (100%)	6 (100%)	0	100 100
2	F	6/6 (100%)	5 (83%)	1 (17%)	2 4
2	H	6/6 (100%)	6 (100%)	0	100 100
2	J	6/6 (100%)	5 (83%)	1 (17%)	2 4
2	L	6/6 (100%)	6 (100%)	0	100 100
2	N	6/6 (100%)	3 (50%)	3 (50%)	0 0
2	P	6/6 (100%)	5 (83%)	1 (17%)	2 4
2	Q	6/6 (100%)	4 (67%)	2 (33%)	0 0
2	R	6/6 (100%)	5 (83%)	1 (17%)	2 4
2	S	6/6 (100%)	5 (83%)	1 (17%)	2 4
2	U	6/6 (100%)	5 (83%)	1 (17%)	2 4
2	V	6/6 (100%)	6 (100%)	0	100 100
2	X	6/6 (100%)	6 (100%)	0	100 100
2	Z	6/6 (100%)	4 (67%)	2 (33%)	0 0
2	a	6/6 (100%)	4 (67%)	2 (33%)	0 0
2	b	6/6 (100%)	5 (83%)	1 (17%)	2 4
2	c	6/6 (100%)	4 (67%)	2 (33%)	0 0
2	d	6/6 (100%)	6 (100%)	0	100 100
2	f	6/6 (100%)	4 (67%)	2 (33%)	0 0
2	g	6/6 (100%)	6 (100%)	0	100 100
2	h	6/6 (100%)	5 (83%)	1 (17%)	2 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	i	6/6 (100%)	5 (83%)	1 (17%)	2 4
2	j	6/6 (100%)	6 (100%)	0	100 100
All	All	1572/1680 (94%)	1510 (96%)	62 (4%)	32 57

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	51	SER
1	A	55	SER
1	A	61	SER
1	I	51	SER
1	C	40	GLU
1	C	61	SER
1	C	137	GLN
1	W	61	SER
1	W	127	LEU
1	W	147	LEU
1	Y	11	ARG
1	Y	137	GLN
1	e	11	ARG
1	e	42	GLU
1	e	61	SER
1	B	4	ARG
1	B	55	SER
1	B	114	ARG
1	B	141	LEU
1	G	11	ARG
1	G	40	GLU
1	G	51	SER
1	G	72	GLN
1	G	127	LEU
1	K	26	ASN
1	K	61	SER
1	K	62	GLN
1	K	71	GLN
1	M	75	SER
1	M	92	LEU
1	M	103	ILE
1	M	127	LEU
1	M	141	LEU

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Mol	Chain	Res	Type
1	M	143	SER
1	T	1	MET
1	T	11	ARG
1	T	72	GLN
2	D	2	VAL
2	D	8	VAL
2	F	6	VAL
2	J	6	VAL
2	N	6	VAL
2	N	8	VAL
2	N	11	VAL
2	P	11	VAL
2	Q	6	VAL
2	Q	11	VAL
2	R	6	VAL
2	S	11	VAL
2	U	11	VAL
2	Z	6	VAL
2	Z	11	VAL
2	a	6	VAL
2	a	11	VAL
2	b	6	VAL
2	c	6	VAL
2	c	11	VAL
2	f	6	VAL
2	f	11	VAL
2	h	11	VAL
2	i	11	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	72	GLN
1	W	72	GLN
1	Y	137	GLN
1	M	122	GLN
1	O	69	GLN
1	T	72	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

168 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	O7G	h	1	2	7,8,9	0.72	0	7,10,12	2.14	3 (42%)
2	O7D	V	10	2	16,18,19	2.00	3 (18%)	16,24,26	2.63	5 (31%)
2	MLE	g	7	2	7,8,9	0.76	0	6,9,11	1.19	0
2	MLE	j	7	2	7,8,9	1.06	0	6,9,11	1.09	0
2	O7G	Q	1	2	7,8,9	0.79	0	7,10,12	2.41	2 (28%)
2	O7G	D	1	2	7,8,9	1.03	0	7,10,12	2.11	2 (28%)
2	NZC	H	5	2	6,7,8	1.05	0	6,8,10	0.99	0
2	O7G	H	1	2	7,8,9	0.61	0	7,10,12	1.40	1 (14%)
2	H14	D	12	2	12,12,13	3.23	3 (25%)	14,15,17	1.74	2 (14%)
2	WZJ	J	3	2	7,8,9	0.51	0	7,9,11	1.53	1 (14%)
2	MVA	b	9	2	6,7,8	1.24	1 (16%)	7,8,10	1.61	2 (28%)
2	NZC	U	5	2	6,7,8	1.13	0	6,8,10	0.87	0
2	NZC	S	5	2	6,7,8	0.92	0	6,8,10	1.53	1 (16%)
2	O7G	X	1	2	7,8,9	2.59	2 (28%)	7,10,12	3.92	5 (71%)
2	MLE	P	7	2	7,8,9	0.73	0	6,9,11	1.22	1 (16%)
2	MLE	L	7	2	7,8,9	0.87	0	6,9,11	1.18	1 (16%)
2	WZJ	S	3	2	7,8,9	0.43	0	7,9,11	1.59	1 (14%)
2	O7D	F	10	2	16,18,19	1.96	3 (18%)	16,24,26	1.95	3 (18%)
2	O7G	N	1	2	7,8,9	0.65	0	7,10,12	2.18	3 (42%)
2	MLE	E	7	2	7,8,9	0.83	0	6,9,11	1.46	1 (16%)
2	NZC	N	5	2	6,7,8	1.02	1 (16%)	6,8,10	2.05	1 (16%)
2	MLE	f	7	2	7,8,9	0.87	0	6,9,11	1.35	0
2	MLE	H	7	2	7,8,9	0.79	0	6,9,11	1.40	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	H14	P	12	2	12,12,13	3.46	3 (25%)	14,15,17	1.72	2 (14%)
2	MLE	U	7	2	7,8,9	1.08	1 (14%)	6,9,11	1.04	0
2	WZJ	D	3	2	7,8,9	0.47	0	7,9,11	1.14	1 (14%)
2	H14	V	12	2	12,12,13	3.29	4 (33%)	14,15,17	1.79	3 (21%)
2	O7G	E	1	2	7,8,9	0.72	0	7,10,12	1.69	1 (14%)
2	O7D	g	10	2	16,18,19	2.04	4 (25%)	16,24,26	1.69	1 (6%)
2	MVA	j	9	2	6,7,8	1.08	1 (16%)	7,8,10	2.48	1 (14%)
2	MVA	h	9	2	6,7,8	0.85	0	7,8,10	1.18	0
2	O7D	h	10	2	16,18,19	2.07	3 (18%)	16,24,26	1.69	3 (18%)
2	O7G	i	1	2	7,8,9	1.21	1 (14%)	7,10,12	2.29	2 (28%)
2	WZJ	i	3	2	7,8,9	0.82	0	7,9,11	1.02	0
2	H14	R	12	2	12,12,13	2.99	3 (25%)	14,15,17	1.55	2 (14%)
2	NZC	h	5	2	6,7,8	0.90	0	6,8,10	1.58	2 (33%)
2	MVA	S	9	2	6,7,8	1.87	1 (16%)	7,8,10	1.11	0
2	WZJ	h	3	2	7,8,9	0.70	0	7,9,11	1.39	2 (28%)
2	O7D	R	10	2	16,18,19	1.94	3 (18%)	16,24,26	2.32	4 (25%)
2	H14	g	12	2	12,12,13	3.35	3 (25%)	14,15,17	1.97	3 (21%)
2	MLE	J	7	2	7,8,9	1.37	1 (14%)	6,9,11	0.94	0
2	MVA	g	9	2	6,7,8	1.23	1 (16%)	7,8,10	2.06	1 (14%)
2	H14	E	12	2	12,12,13	3.14	3 (25%)	14,15,17	1.70	1 (7%)
2	NZC	X	5	2	6,7,8	1.05	0	6,8,10	1.12	0
2	MVA	X	9	2	6,7,8	0.97	0	7,8,10	1.50	1 (14%)
2	MVA	a	9	2	6,7,8	1.47	1 (16%)	7,8,10	1.38	0
2	NZC	f	5	2	6,7,8	1.11	0	6,8,10	1.45	1 (16%)
2	WZJ	f	3	2	7,8,9	0.67	0	7,9,11	1.76	2 (28%)
2	MVA	U	9	2	6,7,8	0.71	0	7,8,10	1.34	1 (14%)
2	MLE	Q	7	2	7,8,9	0.68	0	6,9,11	1.56	1 (16%)
2	O7D	D	10	2	16,18,19	1.95	3 (18%)	16,24,26	1.56	1 (6%)
2	O7G	V	1	2	7,8,9	0.68	0	7,10,12	1.74	3 (42%)
2	H14	U	12	2	12,12,13	3.23	3 (25%)	14,15,17	1.71	2 (14%)
2	MLE	S	7	2	7,8,9	0.75	0	6,9,11	1.27	1 (16%)
2	MVA	N	9	2	6,7,8	0.90	0	7,8,10	2.91	1 (14%)
2	H14	X	12	2	12,12,13	3.59	3 (25%)	14,15,17	1.81	2 (14%)
2	H14	a	12	2	12,12,13	3.66	3 (25%)	14,15,17	1.76	3 (21%)
2	MVA	d	9	2	6,7,8	0.98	0	7,8,10	1.64	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	WZJ	E	3	2	7,8,9	0.51	0	7,9,11	1.29	1 (14%)
2	NZC	a	5	2	6,7,8	0.66	0	6,8,10	1.12	1 (16%)
2	MVA	Z	9	2	6,7,8	1.15	1 (16%)	7,8,10	1.21	1 (14%)
2	O7D	H	10	2	16,18,19	2.04	3 (18%)	16,24,26	1.20	3 (18%)
2	H14	L	12	2	12,12,13	3.47	3 (25%)	14,15,17	1.48	1 (7%)
2	MLE	X	7	2	7,8,9	0.76	0	6,9,11	1.12	1 (16%)
2	WZJ	a	3	2	7,8,9	0.48	0	7,9,11	2.01	1 (14%)
2	MLE	i	7	2	7,8,9	0.73	0	6,9,11	1.39	1 (16%)
2	O7D	L	10	2	16,18,19	1.98	4 (25%)	16,24,26	1.53	1 (6%)
2	H14	Z	12	2	12,12,13	3.27	4 (33%)	14,15,17	2.03	2 (14%)
2	MVA	P	9	2	6,7,8	1.08	1 (16%)	7,8,10	1.91	1 (14%)
2	O7D	j	10	2	16,18,19	2.11	3 (18%)	16,24,26	1.58	2 (12%)
2	WZJ	L	3	2	7,8,9	0.70	0	7,9,11	2.31	1 (14%)
2	WZJ	c	3	2	7,8,9	0.81	0	7,9,11	0.80	0
2	H14	J	12	2	12,12,13	3.39	3 (25%)	14,15,17	1.50	2 (14%)
2	H14	d	12	2	12,12,13	3.42	3 (25%)	14,15,17	1.80	2 (14%)
2	O7D	i	10	2	16,18,19	1.80	3 (18%)	16,24,26	1.75	2 (12%)
2	O7G	f	1	2	7,8,9	0.56	0	7,10,12	1.81	2 (28%)
2	NZC	Z	5	2	6,7,8	0.79	0	6,8,10	1.77	1 (16%)
2	MLE	c	7	2	7,8,9	0.62	0	6,9,11	1.15	0
2	O7G	U	1	2	7,8,9	0.88	0	7,10,12	1.70	1 (14%)
2	O7G	b	1	2	7,8,9	0.64	0	7,10,12	1.75	1 (14%)
2	WZJ	j	3	2	7,8,9	0.61	0	7,9,11	1.19	1 (14%)
2	O7G	d	1	2	7,8,9	0.79	0	7,10,12	2.09	1 (14%)
2	O7D	Q	10	2	16,18,19	2.11	3 (18%)	16,24,26	1.54	3 (18%)
2	H14	S	12	2	12,12,13	3.61	3 (25%)	14,15,17	1.53	2 (14%)
2	H14	h	12	2	12,12,13	2.99	4 (33%)	14,15,17	1.94	2 (14%)
2	MVA	D	9	2	6,7,8	1.30	1 (16%)	7,8,10	2.15	3 (42%)
2	NZC	P	5	2	6,7,8	1.04	0	6,8,10	1.07	0
2	H14	c	12	2	12,12,13	3.47	3 (25%)	14,15,17	1.86	3 (21%)
2	NZC	Q	5	2	6,7,8	0.99	0	6,8,10	1.40	1 (16%)
2	NZC	F	5	2	6,7,8	0.98	0	6,8,10	0.86	0
2	O7G	L	1	2	7,8,9	2.62	2 (28%)	7,10,12	4.28	4 (57%)
2	WZJ	Q	3	2	7,8,9	1.07	1 (14%)	7,9,11	1.53	1 (14%)
2	MVA	H	9	2	6,7,8	1.10	1 (16%)	7,8,10	1.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	O7D	E	10	2	16,18,19	2.18	3 (18%)	16,24,26	1.50	4 (25%)
2	O7D	f	10	2	16,18,19	1.94	3 (18%)	16,24,26	1.93	3 (18%)
2	O7G	c	1	2	7,8,9	0.56	0	7,10,12	1.27	1 (14%)
2	H14	i	12	2	12,12,13	3.22	3 (25%)	14,15,17	1.74	2 (14%)
2	MVA	c	9	2	6,7,8	1.20	1 (16%)	7,8,10	1.29	1 (14%)
2	MVA	i	9	2	6,7,8	1.21	1 (16%)	7,8,10	1.02	0
2	O7D	U	10	2	16,18,19	2.20	3 (18%)	16,24,26	1.52	2 (12%)
2	WZJ	V	3	2	7,8,9	0.48	0	7,9,11	1.50	1 (14%)
2	WZJ	g	3	2	7,8,9	0.51	0	7,9,11	1.07	0
2	H14	H	12	2	12,12,13	3.09	3 (25%)	14,15,17	1.73	3 (21%)
2	H14	f	12	2	12,12,13	2.96	3 (25%)	14,15,17	1.70	2 (14%)
2	NZC	J	5	2	6,7,8	0.68	0	6,8,10	0.89	0
2	O7G	J	1	2	7,8,9	0.77	0	7,10,12	2.15	2 (28%)
2	MLE	N	7	2	7,8,9	0.74	0	6,9,11	1.31	0
2	MLE	V	7	2	7,8,9	0.45	0	6,9,11	1.03	0
2	O7D	b	10	2	16,18,19	2.01	3 (18%)	16,24,26	1.64	2 (12%)
2	NZC	i	5	2	6,7,8	1.21	1 (16%)	6,8,10	1.45	2 (33%)
2	WZJ	U	3	2	7,8,9	0.46	0	7,9,11	1.30	1 (14%)
2	WZJ	X	3	2	7,8,9	0.50	0	7,9,11	0.95	0
2	O7D	d	10	2	16,18,19	2.21	3 (18%)	16,24,26	1.55	4 (25%)
2	MVA	F	9	2	6,7,8	1.28	1 (16%)	7,8,10	0.96	0
2	NZC	D	5	2	6,7,8	1.20	1 (16%)	6,8,10	0.99	0
2	O7D	c	10	2	16,18,19	2.03	3 (18%)	16,24,26	1.59	3 (18%)
2	WZJ	b	3	2	7,8,9	0.91	0	7,9,11	1.62	1 (14%)
2	H14	F	12	2	12,12,13	3.14	3 (25%)	14,15,17	1.65	2 (14%)
2	O7G	P	1	2	7,8,9	0.87	0	7,10,12	2.33	2 (28%)
2	MVA	f	9	2	6,7,8	0.96	0	7,8,10	1.42	2 (28%)
2	O7G	R	1	2	7,8,9	0.80	0	7,10,12	2.28	2 (28%)
2	NZC	R	5	2	6,7,8	0.64	0	6,8,10	2.35	1 (16%)
2	MVA	E	9	2	6,7,8	1.10	1 (16%)	7,8,10	1.07	0
2	MLE	a	7	2	7,8,9	0.68	0	6,9,11	1.22	1 (16%)
2	O7D	J	10	2	16,18,19	2.17	3 (18%)	16,24,26	1.54	4 (25%)
2	H14	b	12	2	12,12,13	2.89	3 (25%)	14,15,17	1.48	2 (14%)
2	H14	N	12	2	12,12,13	3.36	3 (25%)	14,15,17	1.46	2 (14%)
2	NZC	d	5	2	6,7,8	0.88	0	6,8,10	0.98	0
2	MVA	L	9	2	6,7,8	1.45	1 (16%)	7,8,10	1.32	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	O7D	S	10	2	16,18,19	1.89	3 (18%)	16,24,26	1.55	1 (6%)
2	WZJ	Z	3	2	7,8,9	0.75	0	7,9,11	1.06	0
2	MVA	R	9	2	6,7,8	0.95	0	7,8,10	1.24	2 (28%)
2	H14	j	12	2	12,12,13	2.73	4 (33%)	14,15,17	1.61	2 (14%)
2	WZJ	R	3	2	7,8,9	0.41	0	7,9,11	0.84	0
2	WZJ	N	3	2	7,8,9	0.47	0	7,9,11	1.45	1 (14%)
2	NZC	j	5	2	6,7,8	0.91	0	6,8,10	1.97	3 (50%)
2	O7D	X	10	2	16,18,19	2.27	3 (18%)	16,24,26	1.27	2 (12%)
2	MLE	Z	7	2	7,8,9	0.88	0	6,9,11	1.09	1 (16%)
2	O7G	a	1	2	7,8,9	0.80	0	7,10,12	2.11	1 (14%)
2	MLE	d	7	2	7,8,9	1.05	0	6,9,11	0.91	0
2	WZJ	P	3	2	7,8,9	0.68	0	7,9,11	1.20	1 (14%)
2	NZC	L	5	2	6,7,8	0.67	0	6,8,10	0.98	0
2	NZC	g	5	2	6,7,8	0.77	0	6,8,10	0.84	0
2	MLE	h	7	2	7,8,9	0.89	0	6,9,11	0.97	0
2	NZC	E	5	2	6,7,8	0.54	0	6,8,10	0.65	0
2	MLE	F	7	2	7,8,9	1.09	1 (14%)	6,9,11	1.26	1 (16%)
2	MVA	Q	9	2	6,7,8	0.88	0	7,8,10	1.80	3 (42%)
2	NZC	b	5	2	6,7,8	0.80	0	6,8,10	1.52	2 (33%)
2	MVA	J	9	2	6,7,8	0.92	0	7,8,10	2.87	1 (14%)
2	MLE	R	7	2	7,8,9	0.94	0	6,9,11	1.45	2 (33%)
2	O7G	Z	1	2	7,8,9	0.40	0	7,10,12	1.89	3 (42%)
2	H14	Q	12	2	12,12,13	3.12	3 (25%)	14,15,17	1.66	1 (7%)
2	MVA	V	9	2	6,7,8	1.36	2 (33%)	7,8,10	3.30	4 (57%)
2	O7G	j	1	2	7,8,9	0.77	0	7,10,12	1.88	2 (28%)
2	WZJ	F	3	2	7,8,9	0.61	0	7,9,11	0.86	0
2	MLE	b	7	2	7,8,9	0.81	0	6,9,11	0.93	0
2	O7D	Z	10	2	16,18,19	2.10	3 (18%)	16,24,26	1.63	5 (31%)
2	O7G	F	1	2	7,8,9	0.87	0	7,10,12	1.98	2 (28%)
2	NZC	V	5	2	6,7,8	1.15	0	6,8,10	1.82	2 (33%)
2	NZC	c	5	2	6,7,8	0.83	0	6,8,10	0.53	0
2	MLE	D	7	2	7,8,9	1.05	0	6,9,11	1.27	0
2	WZJ	H	3	2	7,8,9	0.48	0	7,9,11	1.08	0
2	O7D	a	10	2	16,18,19	2.00	3 (18%)	16,24,26	1.41	1 (6%)
2	O7G	g	1	2	7,8,9	0.73	0	7,10,12	1.83	1 (14%)
2	O7D	P	10	2	16,18,19	2.20	3 (18%)	16,24,26	1.28	3 (18%)
2	O7G	S	1	2	7,8,9	0.57	0	7,10,12	2.18	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	WZJ	d	3	2	7,8,9	0.49	0	7,9,11	1.16	0
2	O7D	N	10	2	16,18,19	2.16	4 (25%)	16,24,26	1.86	3 (18%)

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	O7G	h	1	2	-	6/7/10/12	-
2	O7D	V	10	2	-	3/6/10/12	0/2/2/2
2	MLE	g	7	2	-	0/5/8/10	-
2	MLE	j	7	2	-	0/5/8/10	-
2	O7G	Q	1	2	-	4/7/10/12	-
2	O7G	D	1	2	-	3/7/10/12	-
2	NZC	H	5	2	-	1/5/8/10	-
2	O7G	H	1	2	-	4/7/10/12	-
2	H14	D	12	2	-	3/10/10/12	0/1/1/1
2	WZJ	J	3	2	-	1/8/10/12	-
2	MVA	b	9	2	-	1/6/8/10	-
2	NZC	U	5	2	-	1/5/8/10	-
2	NZC	S	5	2	-	5/5/8/10	-
2	O7G	X	1	2	-	0/7/10/12	-
2	MLE	P	7	2	-	0/5/8/10	-
2	MLE	L	7	2	-	1/5/8/10	-
2	WZJ	S	3	2	-	6/8/10/12	-
2	O7D	F	10	2	-	2/6/10/12	0/2/2/2
2	O7G	N	1	2	-	0/7/10/12	-
2	MLE	E	7	2	-	1/5/8/10	-
2	NZC	N	5	2	-	1/5/8/10	-
2	MLE	f	7	2	-	0/5/8/10	-
2	MLE	H	7	2	-	0/5/8/10	-
2	H14	P	12	2	-	1/10/10/12	0/1/1/1
2	MLE	U	7	2	-	0/5/8/10	-
2	WZJ	D	3	2	-	2/8/10/12	-
2	H14	V	12	2	-	3/10/10/12	0/1/1/1
2	O7G	E	1	2	-	0/7/10/12	-
2	O7D	g	10	2	-	1/6/10/12	0/2/2/2
2	MVA	j	9	2	-	5/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MVA	h	9	2	-	3/6/8/10	-
2	O7D	h	10	2	-	1/6/10/12	0/2/2/2
2	O7G	i	1	2	-	0/7/10/12	-
2	WZJ	i	3	2	-	3/8/10/12	-
2	H14	R	12	2	-	5/10/10/12	0/1/1/1
2	NZC	h	5	2	-	1/5/8/10	-
2	MVA	S	9	2	-	1/6/8/10	-
2	WZJ	h	3	2	-	7/8/10/12	-
2	O7D	R	10	2	-	0/6/10/12	0/2/2/2
2	H14	g	12	2	-	3/10/10/12	0/1/1/1
2	MLE	J	7	2	-	0/5/8/10	-
2	MVA	g	9	2	-	1/6/8/10	-
2	H14	E	12	2	-	2/10/10/12	0/1/1/1
2	NZC	X	5	2	-	3/5/8/10	-
2	MVA	X	9	2	-	2/6/8/10	-
2	MVA	a	9	2	-	1/6/8/10	-
2	NZC	f	5	2	-	1/5/8/10	-
2	WZJ	f	3	2	-	1/8/10/12	-
2	MVA	U	9	2	-	3/6/8/10	-
2	MLE	Q	7	2	-	0/5/8/10	-
2	O7D	D	10	2	-	4/6/10/12	0/2/2/2
2	O7G	V	1	2	-	1/7/10/12	-
2	H14	U	12	2	-	3/10/10/12	0/1/1/1
2	MLE	S	7	2	-	0/5/8/10	-
2	MVA	N	9	2	-	3/6/8/10	-
2	H14	X	12	2	-	2/10/10/12	0/1/1/1
2	H14	a	12	2	-	2/10/10/12	0/1/1/1
2	MVA	d	9	2	-	5/6/8/10	-
2	WZJ	E	3	2	-	5/8/10/12	-
2	NZC	a	5	2	-	1/5/8/10	-
2	MVA	Z	9	2	-	2/6/8/10	-
2	O7D	H	10	2	-	1/6/10/12	0/2/2/2
2	H14	L	12	2	-	0/10/10/12	0/1/1/1
2	MLE	X	7	2	-	0/5/8/10	-
2	WZJ	a	3	2	-	4/8/10/12	-
2	MLE	i	7	2	-	0/5/8/10	-
2	O7D	L	10	2	-	1/6/10/12	0/2/2/2
2	H14	Z	12	2	-	2/10/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MVA	P	9	2	-	1/6/8/10	-
2	O7D	j	10	2	-	0/6/10/12	0/2/2/2
2	WZJ	L	3	2	-	7/8/10/12	-
2	WZJ	c	3	2	-	3/8/10/12	-
2	H14	J	12	2	-	3/10/10/12	0/1/1/1
2	H14	d	12	2	-	2/10/10/12	0/1/1/1
2	O7D	i	10	2	-	1/6/10/12	0/2/2/2
2	O7G	f	1	2	-	0/7/10/12	-
2	NZC	Z	5	2	-	5/5/8/10	-
2	MLE	c	7	2	-	2/5/8/10	-
2	O7G	U	1	2	-	0/7/10/12	-
2	O7G	b	1	2	-	0/7/10/12	-
2	WZJ	j	3	2	-	1/8/10/12	-
2	O7G	d	1	2	-	3/7/10/12	-
2	O7D	Q	10	2	-	2/6/10/12	0/2/2/2
2	H14	S	12	2	-	0/10/10/12	0/1/1/1
2	H14	h	12	2	-	3/10/10/12	0/1/1/1
2	MVA	D	9	2	-	3/6/8/10	-
2	NZC	P	5	2	-	1/5/8/10	-
2	H14	c	12	2	-	2/10/10/12	0/1/1/1
2	NZC	Q	5	2	-	5/5/8/10	-
2	NZC	F	5	2	-	1/5/8/10	-
2	O7G	L	1	2	-	0/7/10/12	-
2	WZJ	Q	3	2	-	3/8/10/12	-
2	MVA	H	9	2	-	3/6/8/10	-
2	O7D	E	10	2	-	1/6/10/12	0/2/2/2
2	O7D	f	10	2	-	1/6/10/12	0/2/2/2
2	O7G	c	1	2	-	4/7/10/12	-
2	H14	i	12	2	-	0/10/10/12	0/1/1/1
2	MVA	c	9	2	-	3/6/8/10	-
2	MVA	i	9	2	-	1/6/8/10	-
2	O7D	U	10	2	-	2/6/10/12	0/2/2/2
2	WZJ	V	3	2	-	2/8/10/12	-
2	WZJ	g	3	2	-	3/8/10/12	-
2	H14	H	12	2	-	2/10/10/12	0/1/1/1
2	H14	f	12	2	-	3/10/10/12	0/1/1/1
2	NZC	J	5	2	-	5/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	O7G	J	1	2	-	1/7/10/12	-
2	MLE	N	7	2	-	0/5/8/10	-
2	MLE	V	7	2	-	3/5/8/10	-
2	O7D	b	10	2	-	0/6/10/12	0/2/2/2
2	NZC	i	5	2	-	1/5/8/10	-
2	WZJ	U	3	2	-	3/8/10/12	-
2	WZJ	X	3	2	-	4/8/10/12	-
2	O7D	d	10	2	-	1/6/10/12	0/2/2/2
2	MVA	F	9	2	-	3/6/8/10	-
2	NZC	D	5	2	-	2/5/8/10	-
2	O7D	c	10	2	-	1/6/10/12	0/2/2/2
2	WZJ	b	3	2	-	6/8/10/12	-
2	H14	F	12	2	-	3/10/10/12	0/1/1/1
2	O7G	P	1	2	-	1/7/10/12	-
2	MVA	f	9	2	-	4/6/8/10	-
2	O7G	R	1	2	-	5/7/10/12	-
2	NZC	R	5	2	-	5/5/8/10	-
2	MVA	E	9	2	-	1/6/8/10	-
2	MLE	a	7	2	-	0/5/8/10	-
2	O7D	J	10	2	-	2/6/10/12	0/2/2/2
2	H14	b	12	2	-	3/10/10/12	0/1/1/1
2	H14	N	12	2	-	3/10/10/12	0/1/1/1
2	NZC	d	5	2	-	2/5/8/10	-
2	MVA	L	9	2	-	5/6/8/10	-
2	O7D	S	10	2	-	1/6/10/12	0/2/2/2
2	WZJ	Z	3	2	-	4/8/10/12	-
2	MVA	R	9	2	-	1/6/8/10	-
2	H14	j	12	2	-	3/10/10/12	0/1/1/1
2	WZJ	R	3	2	-	3/8/10/12	-
2	WZJ	N	3	2	-	1/8/10/12	-
2	NZC	j	5	2	-	1/5/8/10	-
2	O7D	X	10	2	-	1/6/10/12	0/2/2/2
2	MLE	Z	7	2	-	0/5/8/10	-
2	O7G	a	1	2	-	1/7/10/12	-
2	MLE	d	7	2	-	3/5/8/10	-
2	WZJ	P	3	2	-	1/8/10/12	-
2	NZC	L	5	2	-	1/5/8/10	-
2	NZC	g	5	2	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLE	h	7	2	-	0/5/8/10	-
2	NZC	E	5	2	-	5/5/8/10	-
2	MLE	F	7	2	-	0/5/8/10	-
2	MVA	Q	9	2	-	1/6/8/10	-
2	NZC	b	5	2	-	1/5/8/10	-
2	MVA	J	9	2	-	5/6/8/10	-
2	MLE	R	7	2	-	2/5/8/10	-
2	O7G	Z	1	2	-	1/7/10/12	-
2	H14	Q	12	2	-	2/10/10/12	0/1/1/1
2	MVA	V	9	2	-	5/6/8/10	-
2	O7G	j	1	2	-	0/7/10/12	-
2	WZJ	F	3	2	-	6/8/10/12	-
2	MLE	b	7	2	-	0/5/8/10	-
2	O7D	Z	10	2	-	3/6/10/12	0/2/2/2
2	O7G	F	1	2	-	2/7/10/12	-
2	NZC	V	5	2	-	5/5/8/10	-
2	NZC	c	5	2	-	5/5/8/10	-
2	MLE	D	7	2	-	3/5/8/10	-
2	WZJ	H	3	2	-	3/8/10/12	-
2	O7D	a	10	2	-	1/6/10/12	0/2/2/2
2	O7G	g	1	2	-	2/7/10/12	-
2	O7D	P	10	2	-	1/6/10/12	0/2/2/2
2	O7G	S	1	2	-	4/7/10/12	-
2	WZJ	d	3	2	-	2/8/10/12	-
2	O7D	N	10	2	-	1/6/10/12	0/2/2/2

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	c	12	H14	CG-CB	-8.77	1.38	1.51
2	X	12	H14	CG-CB	-8.53	1.39	1.51
2	L	12	H14	CG-CB	-8.49	1.39	1.51
2	S	12	H14	CG-CB	-8.38	1.39	1.51
2	d	12	H14	CG-CB	-8.29	1.39	1.51
2	a	12	H14	CG-CB	-8.28	1.39	1.51
2	i	12	H14	CG-CB	-8.16	1.39	1.51
2	a	12	H14	C-CA	-8.15	1.39	1.52
2	S	12	H14	C-CA	-8.00	1.39	1.52
2	P	12	H14	CG-CB	-7.97	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	12	H14	C-CA	-7.87	1.40	1.52
2	Q	12	H14	CG-CB	-7.85	1.40	1.51
2	h	12	H14	CG-CB	-7.84	1.40	1.51
2	H	12	H14	CG-CB	-7.68	1.40	1.51
2	X	12	H14	C-CA	-7.65	1.40	1.52
2	U	12	H14	CG-CB	-7.63	1.40	1.51
2	N	12	H14	C-CA	-7.61	1.40	1.52
2	g	12	H14	C-CA	-7.59	1.40	1.52
2	D	12	H14	CG-CB	-7.53	1.40	1.51
2	V	12	H14	C-CA	-7.53	1.40	1.52
2	Z	12	H14	CG-CB	-7.49	1.40	1.51
2	E	12	H14	CG-CB	-7.46	1.40	1.51
2	J	12	H14	CG-CB	-7.42	1.40	1.51
2	f	12	H14	CG-CB	-7.39	1.40	1.51
2	g	12	H14	CG-CB	-7.38	1.40	1.51
2	P	12	H14	C-CA	-7.31	1.40	1.52
2	N	12	H14	CG-CB	-7.12	1.41	1.51
2	d	12	H14	C-CA	-7.10	1.41	1.52
2	L	12	H14	C-CA	-7.03	1.41	1.52
2	F	12	H14	CG-CB	-7.01	1.41	1.51
2	R	12	H14	CG-CB	-6.87	1.41	1.51
2	F	12	H14	C-CA	-6.82	1.41	1.52
2	D	12	H14	C-CA	-6.74	1.41	1.52
2	U	12	H14	C-CA	-6.74	1.41	1.52
2	b	12	H14	CG-CB	-6.65	1.42	1.51
2	E	12	H14	C-CA	-6.34	1.42	1.52
2	c	12	H14	C-CA	-6.33	1.42	1.52
2	V	12	H14	CG-CB	-6.33	1.42	1.51
2	Z	12	H14	C-CA	-6.02	1.42	1.52
2	X	1	O7G	CA-N	-5.99	1.42	1.48
2	L	1	O7G	CA-N	-5.86	1.42	1.48
2	R	12	H14	C-CA	-5.81	1.43	1.52
2	H	12	H14	C-CA	-5.79	1.43	1.52
2	i	12	H14	C-CA	-5.75	1.43	1.52
2	j	12	H14	CG-CB	-5.61	1.43	1.51
2	Q	12	H14	C-CA	-5.60	1.43	1.52
2	b	12	H14	C-CA	-5.45	1.43	1.52
2	f	12	H14	C-CA	-5.13	1.44	1.52
2	U	10	O7D	CDF-CDA	-5.07	1.33	1.41
2	X	10	O7D	CCX-CDB	-5.05	1.33	1.41
2	J	10	O7D	CCX-CDB	-5.05	1.33	1.41
2	P	10	O7D	CDF-CDA	-5.04	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	d	10	O7D	CCX-CDB	-4.95	1.33	1.41
2	V	10	O7D	CDF-CDA	-4.91	1.33	1.41
2	E	10	O7D	CCX-CDB	-4.91	1.33	1.41
2	j	12	H14	C-CA	-4.84	1.44	1.52
2	F	10	O7D	CDF-CDA	-4.83	1.33	1.41
2	D	10	O7D	CDF-CDA	-4.80	1.33	1.41
2	N	10	O7D	CCX-CDB	-4.79	1.33	1.41
2	X	10	O7D	CDF-CDA	-4.76	1.33	1.41
2	P	10	O7D	CCX-CDB	-4.74	1.34	1.41
2	E	10	O7D	CDF-CDA	-4.73	1.33	1.41
2	Q	10	O7D	CDF-CDA	-4.70	1.33	1.41
2	d	10	O7D	CDF-CDA	-4.70	1.33	1.41
2	N	12	H14	OXT-C	-4.70	1.22	1.42
2	H	10	O7D	CDF-CDA	-4.66	1.33	1.41
2	Z	10	O7D	CDF-CDA	-4.66	1.33	1.41
2	R	12	H14	OXT-C	-4.65	1.22	1.42
2	P	12	H14	OXT-C	-4.63	1.22	1.42
2	U	12	H14	OXT-C	-4.60	1.23	1.42
2	L	12	H14	OXT-C	-4.60	1.23	1.42
2	h	12	H14	C-CA	-4.56	1.45	1.52
2	V	12	H14	OXT-C	-4.55	1.23	1.42
2	E	12	H14	OXT-C	-4.54	1.23	1.42
2	h	10	O7D	CDF-CDA	-4.52	1.34	1.41
2	J	10	O7D	CDF-CDA	-4.51	1.34	1.41
2	N	10	O7D	CDC-CDB	-4.50	1.33	1.42
2	j	10	O7D	CCX-CDB	-4.50	1.34	1.41
2	L	10	O7D	CCX-CDB	-4.50	1.34	1.41
2	a	12	H14	OXT-C	-4.48	1.23	1.42
2	c	10	O7D	CDF-CDA	-4.48	1.34	1.41
2	Q	12	H14	OXT-C	-4.47	1.23	1.42
2	c	12	H14	OXT-C	-4.46	1.23	1.42
2	d	12	H14	OXT-C	-4.45	1.23	1.42
2	H	10	O7D	CCX-CDB	-4.43	1.34	1.41
2	J	12	H14	OXT-C	-4.43	1.23	1.42
2	F	12	H14	OXT-C	-4.42	1.23	1.42
2	g	10	O7D	CCX-CDB	-4.42	1.34	1.41
2	j	10	O7D	CDF-CDA	-4.42	1.34	1.41
2	X	10	O7D	CDC-CDB	-4.42	1.33	1.42
2	i	12	H14	OXT-C	-4.41	1.23	1.42
2	H	12	H14	OXT-C	-4.41	1.23	1.42
2	S	12	H14	OXT-C	-4.41	1.23	1.42
2	b	10	O7D	CDF-CDA	-4.39	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	12	H14	OXT-C	-4.38	1.23	1.42
2	D	12	H14	OXT-C	-4.37	1.24	1.42
2	U	10	O7D	CCX-CDB	-4.37	1.34	1.41
2	f	12	H14	OXT-C	-4.35	1.24	1.42
2	c	10	O7D	CCX-CDB	-4.34	1.34	1.41
2	g	12	H14	OXT-C	-4.34	1.24	1.42
2	j	12	H14	OXT-C	-4.32	1.24	1.42
2	d	10	O7D	CDC-CDB	-4.32	1.33	1.42
2	h	12	H14	OXT-C	-4.31	1.24	1.42
2	h	10	O7D	CCX-CDB	-4.30	1.34	1.41
2	Q	10	O7D	CCX-CDB	-4.29	1.34	1.41
2	Z	12	H14	OXT-C	-4.28	1.24	1.42
2	U	10	O7D	CDC-CDB	-4.27	1.33	1.42
2	Z	10	O7D	CCX-CDB	-4.25	1.34	1.41
2	b	12	H14	OXT-C	-4.24	1.24	1.42
2	i	10	O7D	CDF-CDA	-4.24	1.34	1.41
2	a	10	O7D	CCX-CDB	-4.22	1.34	1.41
2	b	10	O7D	CCX-CDB	-4.20	1.34	1.41
2	S	9	MVA	CA-N	4.17	1.54	1.47
2	R	10	O7D	CDF-CDA	-4.17	1.34	1.41
2	P	10	O7D	CDC-CDB	-4.17	1.33	1.42
2	J	10	O7D	CDC-CDB	-4.16	1.33	1.42
2	f	10	O7D	CCX-CDB	-4.15	1.34	1.41
2	N	10	O7D	CDF-CDA	-4.12	1.34	1.41
2	E	10	O7D	CDC-CDB	-4.11	1.33	1.42
2	g	10	O7D	CDF-CDA	-4.10	1.34	1.41
2	Z	12	H14	CB-CA	4.03	1.58	1.54
2	V	10	O7D	CCX-CDB	-3.98	1.35	1.41
2	f	10	O7D	CDF-CDA	-3.93	1.35	1.41
2	j	10	O7D	CDC-CDB	-3.92	1.34	1.42
2	Q	10	O7D	CDC-CDB	-3.90	1.34	1.42
2	R	10	O7D	CCX-CDB	-3.86	1.35	1.41
2	S	10	O7D	CDF-CDA	-3.85	1.35	1.41
2	a	10	O7D	CDC-CDB	-3.75	1.34	1.42
2	D	10	O7D	CCX-CDB	-3.75	1.35	1.41
2	L	10	O7D	CDC-CDB	-3.70	1.34	1.42
2	c	10	O7D	CDC-CDB	-3.70	1.34	1.42
2	S	10	O7D	CCX-CDB	-3.69	1.35	1.41
2	g	10	O7D	CDC-CDB	-3.68	1.34	1.42
2	a	10	O7D	CDF-CDA	-3.68	1.35	1.41
2	b	10	O7D	CDC-CDB	-3.67	1.34	1.42
2	S	10	O7D	CDC-CDB	-3.66	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	10	O7D	CDC-CDB	-3.66	1.34	1.42
2	f	10	O7D	CDC-CDB	-3.63	1.34	1.42
2	Z	10	O7D	CDC-CDB	-3.61	1.34	1.42
2	V	10	O7D	CDC-CDB	-3.60	1.34	1.42
2	R	10	O7D	CDC-CDB	-3.50	1.35	1.42
2	H	10	O7D	CDC-CDB	-3.43	1.35	1.42
2	D	10	O7D	CDC-CDB	-3.36	1.35	1.42
2	F	10	O7D	CDC-CDB	-3.33	1.35	1.42
2	i	10	O7D	CDC-CDB	-3.29	1.35	1.42
2	a	9	MVA	CA-N	3.25	1.53	1.47
2	L	10	O7D	CDF-CDA	-3.25	1.36	1.41
2	F	10	O7D	CCX-CDB	-3.20	1.36	1.41
2	i	10	O7D	CCX-CDB	-3.15	1.36	1.41
2	V	12	H14	CB-CA	3.00	1.57	1.54
2	L	9	MVA	CA-N	2.86	1.52	1.47
2	F	9	MVA	CA-N	2.82	1.52	1.47
2	i	1	O7G	CB-CA	2.82	1.57	1.54
2	J	7	MLE	CA-N	2.80	1.52	1.47
2	j	12	H14	OB-CB	2.78	1.48	1.42
2	L	1	O7G	CAA-N	2.74	1.56	1.46
2	X	1	O7G	CAA-N	2.71	1.56	1.46
2	c	9	MVA	CA-N	2.66	1.52	1.47
2	D	5	NZC	CA-N	2.63	1.52	1.47
2	g	9	MVA	CA-N	2.62	1.52	1.47
2	b	9	MVA	CA-N	2.45	1.51	1.47
2	i	9	MVA	CA-N	2.39	1.51	1.47
2	D	9	MVA	CA-N	2.35	1.51	1.47
2	P	9	MVA	CA-N	2.34	1.51	1.47
2	V	9	MVA	CB-CA	2.29	1.58	1.54
2	h	12	H14	CB-CA	2.26	1.56	1.54
2	H	9	MVA	CA-N	2.23	1.51	1.47
2	V	9	MVA	CA-N	2.18	1.51	1.47
2	Z	9	MVA	CA-N	2.16	1.51	1.47
2	F	7	MLE	CA-N	2.14	1.51	1.47
2	L	10	O7D	CCY-NCZ	-2.14	1.32	1.36
2	N	10	O7D	CCY-NCZ	-2.12	1.32	1.36
2	j	9	MVA	CA-N	2.10	1.51	1.47
2	N	5	NZC	CA-N	2.09	1.51	1.47
2	i	5	NZC	CA-N	2.09	1.51	1.47
2	E	9	MVA	CA-N	2.08	1.51	1.47
2	Q	3	WZJ	CA-N	2.08	1.51	1.47
2	g	10	O7D	CCY-CCX	-2.04	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	7	MLE	CA-N	2.02	1.51	1.47

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	1	O7G	CAB-N-CA	7.50	133.72	114.16
2	R	10	O7D	CCW-CCX-CCY	-7.48	118.72	127.97
2	N	9	MVA	CB-CA-C	-7.39	103.77	113.04
2	J	9	MVA	CB-CA-C	-7.20	104.01	113.04
2	V	10	O7D	CCW-CCX-CCY	-6.69	119.70	127.97
2	Z	12	H14	OXT-C-CA	6.61	125.32	111.43
2	X	1	O7G	CAB-N-CA	6.59	131.33	114.16
2	j	9	MVA	CB-CA-C	-6.34	105.08	113.04
2	F	10	O7D	CCW-CCX-CCY	-6.18	120.33	127.97
2	f	10	O7D	CCW-CCX-CCY	-6.16	120.35	127.97
2	h	12	H14	OXT-C-CA	5.88	123.78	111.43
2	X	1	O7G	CAB-N-CAA	-5.81	93.24	110.38
2	Q	1	O7G	CB-CA-N	-5.76	107.45	112.46
2	P	12	H14	OXT-C-CA	5.56	123.12	111.43
2	L	3	WZJ	CB-CA-C	5.54	120.37	112.82
2	L	1	O7G	CAB-N-CAA	-5.52	94.09	110.38
2	E	12	H14	OXT-C-CA	5.51	123.01	111.43
2	X	12	H14	OXT-C-CA	5.50	122.98	111.43
2	Q	12	H14	OXT-C-CA	5.46	122.91	111.43
2	R	5	NZC	CB-CA-N	-5.45	97.92	111.69
2	V	9	MVA	CB-CA-C	-5.44	106.22	113.04
2	S	1	O7G	CB-CA-N	-5.43	107.74	112.46
2	i	10	O7D	CCW-CCX-CCY	-5.41	121.28	127.97
2	U	12	H14	OXT-C-CA	5.39	122.75	111.43
2	R	1	O7G	CB-CA-C	-5.29	105.81	112.94
2	d	12	H14	OXT-C-CA	5.27	122.50	111.43
2	g	10	O7D	CCW-CCX-CCY	-5.25	121.48	127.97
2	N	10	O7D	CCW-CCX-CCY	-5.23	121.51	127.97
2	f	12	H14	OXT-C-CA	5.18	122.32	111.43
2	j	12	H14	OXT-C-CA	5.18	122.30	111.43
2	H	12	H14	OXT-C-CA	5.12	122.18	111.43
2	c	12	H14	OXT-C-CA	5.00	121.94	111.43
2	a	12	H14	OXT-C-CA	5.00	121.94	111.43
2	L	10	O7D	CCW-CCX-CCY	-5.00	121.79	127.97
2	d	1	O7G	CB-CA-N	-4.97	108.14	112.46
2	F	12	H14	OXT-C-CA	4.96	121.85	111.43
2	a	3	WZJ	CB-CA-C	-4.96	106.06	112.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	1	O7G	CB-CA-N	-4.93	108.17	112.46
2	D	10	O7D	CCW-CCX-CCY	-4.92	121.89	127.97
2	g	12	H14	OXT-C-CA	4.92	121.75	111.43
2	i	12	H14	OXT-C-CA	4.88	121.68	111.43
2	S	10	O7D	CCW-CCX-CCY	-4.81	122.03	127.97
2	J	1	O7G	CB-CA-C	-4.79	106.48	112.94
2	V	9	MVA	CG2-CB-CA	-4.76	103.92	111.21
2	c	10	O7D	CCW-CCX-CCY	-4.75	122.09	127.97
2	b	10	O7D	CCW-CCX-CCY	-4.73	122.13	127.97
2	L	12	H14	OXT-C-CA	4.72	121.34	111.43
2	P	1	O7G	CB-CA-C	-4.71	106.58	112.94
2	D	12	H14	OXT-C-CA	4.69	121.28	111.43
2	g	9	MVA	CB-CA-C	-4.67	107.19	113.04
2	S	12	H14	OXT-C-CA	4.56	121.01	111.43
2	h	10	O7D	CCW-CCX-CCY	-4.54	122.36	127.97
2	b	12	H14	OXT-C-CA	4.52	120.93	111.43
2	a	10	O7D	CCW-CCX-CCY	-4.51	122.39	127.97
2	L	1	O7G	CB-CA-N	4.48	116.35	112.46
2	U	10	O7D	CCW-CCX-CCY	-4.46	122.46	127.97
2	V	10	O7D	CDH-ODG-CDC	-4.42	111.56	117.75
2	V	12	H14	OXT-C-CA	4.40	120.67	111.43
2	J	12	H14	OXT-C-CA	4.37	120.61	111.43
2	R	12	H14	OXT-C-CA	4.36	120.58	111.43
2	P	9	MVA	CB-CA-C	-4.35	107.59	113.04
2	i	1	O7G	CB-CA-N	-4.24	108.78	112.46
2	j	10	O7D	CCW-CCX-CCY	-4.20	122.78	127.97
2	b	1	O7G	CB-CA-C	-4.10	107.41	112.94
2	j	1	O7G	CB-CA-C	-4.05	107.48	112.94
2	F	1	O7G	CB-CA-C	-4.03	107.50	112.94
2	D	1	O7G	CB-CA-C	-4.03	107.50	112.94
2	g	12	H14	CG-CB-CA	4.00	118.61	111.57
2	N	5	NZC	CB-CA-N	-3.96	101.69	111.69
2	i	1	O7G	CB-CA-C	-3.94	107.62	112.94
2	V	10	O7D	ODG-CDC-CDD	-3.94	117.71	124.24
2	N	1	O7G	CB-CA-C	-3.92	107.65	112.94
2	U	1	O7G	CB-CA-C	-3.82	107.78	112.94
2	d	10	O7D	CCW-CCX-CCY	-3.80	123.28	127.97
2	f	3	WZJ	CB-CA-C	-3.77	107.69	112.82
2	D	12	H14	C-CA-CB	-3.75	104.53	113.10
2	J	10	O7D	CCW-CCX-CCY	-3.69	123.40	127.97
2	Q	10	O7D	CCW-CCX-CCY	-3.68	123.42	127.97
2	g	1	O7G	CB-CA-C	-3.67	108.00	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	1	O7G	CB-CA-C	-3.65	108.02	112.94
2	N	12	H14	OXT-C-CA	3.64	119.08	111.43
2	b	3	WZJ	CG2-CB-CA	3.64	119.99	111.03
2	D	9	MVA	CB-CA-N	3.61	115.86	111.17
2	N	12	H14	C-CA-CB	-3.60	104.86	113.10
2	h	1	O7G	CB-CA-C	-3.59	108.09	112.94
2	X	10	O7D	CCW-CCX-CCY	-3.59	123.53	127.97
2	Z	5	NZC	CB-CA-N	-3.56	102.71	111.69
2	V	9	MVA	CG1-CB-CA	-3.53	105.81	111.21
2	L	1	O7G	CAA-N-CA	-3.49	105.08	114.16
2	j	10	O7D	CDH-ODG-CDC	-3.48	112.87	117.75
2	E	1	O7G	CB-CA-N	-3.43	109.48	112.46
2	V	12	H14	CG-CB-CA	3.41	117.57	111.57
2	f	1	O7G	CB-CA-C	-3.39	108.36	112.94
2	d	9	MVA	CB-CA-C	-3.36	108.83	113.04
2	V	12	H14	C-CA-CB	-3.36	105.43	113.10
2	Q	10	O7D	CDH-ODG-CDC	-3.35	113.06	117.75
2	V	1	O7G	CB-CA-C	-3.34	108.43	112.94
2	E	10	O7D	CCW-CCX-CCY	-3.30	123.88	127.97
2	X	1	O7G	CB-CA-N	3.30	115.33	112.46
2	S	3	WZJ	CB-CA-C	-3.28	108.36	112.82
2	Z	10	O7D	CDH-ODG-CDC	-3.26	113.18	117.75
2	b	9	MVA	CB-CA-N	-3.24	106.95	111.17
2	N	1	O7G	CB-CA-N	-3.16	109.71	112.46
2	V	3	WZJ	CB-CA-C	-3.14	108.54	112.82
2	Z	10	O7D	CCW-CCX-CCY	-3.13	124.10	127.97
2	f	12	H14	C-CA-CB	-3.09	106.04	113.10
2	J	3	WZJ	CB-CA-C	-3.08	108.62	112.82
2	D	9	MVA	CB-CA-C	-3.07	109.19	113.04
2	V	10	O7D	ODG-CDC-CDB	3.07	120.40	115.89
2	Q	9	MVA	CG2-CB-CA	-3.06	106.52	111.21
2	R	12	H14	C-CA-CB	-3.05	106.12	113.10
2	Q	3	WZJ	C-CA-N	-3.00	100.84	110.88
2	P	1	O7G	CB-CA-N	-3.00	109.86	112.46
2	N	10	O7D	CDH-ODG-CDC	-2.99	113.56	117.75
2	c	12	H14	C-CA-CB	-2.97	106.32	113.10
2	F	12	H14	C-CA-CB	-2.95	106.36	113.10
2	J	12	H14	C-CA-CB	-2.95	106.36	113.10
2	c	12	H14	CG-CB-CA	2.92	116.71	111.57
2	f	5	NZC	CB-CA-N	-2.92	104.32	111.69
2	j	5	NZC	CB-CA-N	-2.88	104.42	111.69
2	h	12	H14	C-CA-CB	-2.88	106.52	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	10	O7D	CCW-CA-C	-2.87	106.21	111.65
2	N	3	WZJ	CB-CA-C	-2.85	108.94	112.82
2	X	1	O7G	CB-CA-C	-2.83	109.12	112.94
2	E	3	WZJ	CB-CA-C	-2.83	108.97	112.82
2	a	12	H14	CG-CB-CA	2.81	116.51	111.57
2	X	9	MVA	CB-CA-N	-2.80	107.53	111.17
2	h	10	O7D	CDH-ODG-CDC	-2.75	113.90	117.75
2	D	1	O7G	CAB-N-CAA	-2.74	102.29	110.38
2	U	9	MVA	CB-CA-C	-2.74	109.60	113.04
2	b	10	O7D	CDH-ODG-CDC	-2.72	113.94	117.75
2	V	5	NZC	CB-CA-N	-2.72	104.83	111.69
2	Q	7	MLE	O-C-CA	-2.72	117.66	124.78
2	N	10	O7D	CCW-CA-C	-2.70	106.52	111.65
2	R	10	O7D	CCW-CCX-CDB	2.65	130.98	126.42
2	S	12	H14	C-CA-CB	-2.63	107.09	113.10
2	i	12	H14	C-CA-CB	-2.63	107.09	113.10
2	X	1	O7G	CAA-N-CA	-2.62	107.33	114.16
2	E	10	O7D	CCW-CA-C	-2.62	106.69	111.65
2	Q	9	MVA	CB-CA-C	-2.61	109.77	113.04
2	d	12	H14	C-CA-CB	-2.59	107.17	113.10
2	d	10	O7D	CCW-CA-C	-2.58	106.76	111.65
2	P	3	WZJ	CB-CA-C	-2.55	109.34	112.82
2	H	1	O7G	CB-CA-C	-2.54	109.51	112.94
2	N	1	O7G	CAB-N-CA	-2.51	107.61	114.16
2	i	5	NZC	CB-CA-N	-2.51	105.35	111.69
2	P	10	O7D	CCW-CCX-CCY	-2.51	124.87	127.97
2	d	10	O7D	CDH-ODG-CDC	-2.50	114.25	117.75
2	F	7	MLE	CG-CB-CA	-2.49	109.13	115.34
2	h	1	O7G	CB-CA-N	-2.49	110.30	112.46
2	Z	12	H14	C-CA-CB	-2.47	107.45	113.10
2	S	5	NZC	CB-CA-N	-2.41	105.59	111.69
2	a	12	H14	C-CA-CB	-2.39	107.63	113.10
2	j	5	NZC	OG1-CB-CG2	-2.39	102.66	109.74
2	U	3	WZJ	CB-CA-C	-2.39	109.57	112.82
2	E	7	MLE	O-C-CA	-2.39	118.52	124.78
2	j	1	O7G	CAB-N-CA	-2.38	107.95	114.16
2	E	10	O7D	O-C-CA	-2.38	118.53	124.78
2	P	10	O7D	CDH-ODG-CDC	-2.38	114.41	117.75
2	i	10	O7D	CDF-CDE-CDD	-2.38	117.20	120.99
2	V	10	O7D	CCW-CCX-CDB	2.38	130.52	126.42
2	b	5	NZC	CB-CA-N	-2.38	105.69	111.69
2	H	12	H14	C-CA-CB	-2.37	107.68	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1	O7G	CAB-N-CA	-2.37	107.99	114.16
2	D	9	MVA	CG1-CB-CA	-2.37	107.58	111.21
2	f	9	MVA	CB-CA-C	-2.36	110.08	113.04
2	Z	9	MVA	CB-CA-C	-2.36	110.08	113.04
2	c	10	O7D	O-C-CA	-2.35	118.61	124.78
2	F	10	O7D	CDH-ODG-CDC	-2.35	114.46	117.75
2	j	3	WZJ	CB-CA-C	-2.34	109.63	112.82
2	f	1	O7G	CAB-N-CA	-2.33	108.10	114.16
2	E	10	O7D	CDH-ODG-CDC	-2.33	114.49	117.75
2	H	7	MLE	O-C-CA	-2.32	118.69	124.78
2	H	12	H14	CG-CB-CA	2.32	115.65	111.57
2	R	10	O7D	O-C-CA	-2.32	118.70	124.78
2	b	12	H14	C-CA-CB	-2.32	107.80	113.10
2	h	1	O7G	CAB-N-CA	-2.32	108.13	114.16
2	j	5	NZC	CG2-CB-CA	2.31	116.93	112.27
2	Z	1	O7G	CAB-N-CA	-2.31	108.14	114.16
2	g	12	H14	C-CA-CB	-2.31	107.82	113.10
2	R	7	MLE	CN-N-CA	2.31	120.82	113.64
2	c	9	MVA	CB-CA-C	-2.29	110.17	113.04
2	h	10	O7D	CDF-CDE-CDD	-2.29	117.35	120.99
2	Z	10	O7D	CDF-CDE-CDD	-2.29	117.35	120.99
2	V	5	NZC	C-CA-N	2.27	118.48	110.88
2	L	9	MVA	CG1-CB-CA	-2.27	107.73	111.21
2	R	9	MVA	CB-CA-N	-2.26	108.22	111.17
2	D	3	WZJ	CB-CA-C	-2.26	109.74	112.82
2	j	12	H14	OB-CB-CA	2.25	114.37	109.64
2	Q	5	NZC	CB-CA-N	-2.25	106.02	111.69
2	P	10	O7D	O-C-CA	-2.24	118.91	124.78
2	h	5	NZC	CB-CA-N	-2.24	106.04	111.69
2	R	1	O7G	CAB-N-CAA	-2.23	103.79	110.38
2	c	1	O7G	CB-CA-C	-2.23	109.93	112.94
2	P	12	H14	C-CA-CB	-2.23	108.00	113.10
2	U	12	H14	C-CA-CB	-2.23	108.01	113.10
2	a	7	MLE	O-C-CA	-2.22	118.97	124.78
2	L	9	MVA	CB-CA-C	-2.21	110.27	113.04
2	X	10	O7D	O-C-CA	-2.20	119.01	124.78
2	J	10	O7D	CDH-ODG-CDC	-2.20	114.67	117.75
2	S	7	MLE	O-C-CA	-2.20	119.02	124.78
2	R	7	MLE	O-C-CA	-2.19	119.03	124.78
2	J	10	O7D	CCW-CA-N	2.19	114.04	110.65
2	Z	10	O7D	O-C-CA	-2.18	119.06	124.78
2	a	5	NZC	CB-CA-N	-2.18	106.18	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	10	O7D	O-C-CA	-2.18	119.06	124.78
2	Q	1	O7G	CAB-N-CA	-2.18	108.48	114.16
2	h	3	WZJ	CB-CA-C	-2.18	109.86	112.82
2	H	10	O7D	CDH-ODG-CDC	-2.17	114.71	117.75
2	f	10	O7D	O-C-CA	-2.17	119.10	124.78
2	X	7	MLE	CG-CB-CA	-2.16	109.94	115.34
2	Q	10	O7D	O-C-CA	-2.15	119.15	124.78
2	J	10	O7D	CDF-CDE-CDD	-2.15	117.57	120.99
2	P	7	MLE	CG-CB-CA	-2.14	109.99	115.34
2	U	10	O7D	CDF-CDE-CDD	-2.14	117.58	120.99
2	b	9	MVA	CG2-CB-CA	-2.13	107.94	111.21
2	Z	1	O7G	CB-CA-N	-2.13	110.61	112.46
2	V	1	O7G	CAB-N-CA	-2.12	108.65	114.16
2	i	7	MLE	O-C-CA	-2.12	119.23	124.78
2	R	10	O7D	CDF-CDE-CDD	-2.12	117.62	120.99
2	F	1	O7G	CAB-N-CA	-2.11	108.66	114.16
2	V	9	MVA	C-CA-N	2.10	117.92	110.88
2	F	10	O7D	CCW-CCX-CDB	2.10	130.04	126.42
2	X	12	H14	C-CA-CB	-2.10	108.29	113.10
2	Q	9	MVA	CB-CA-N	2.09	113.90	111.17
2	V	1	O7G	CB-CA-N	-2.05	110.68	112.46
2	h	3	WZJ	O-C-CA	-2.05	119.11	124.83
2	c	10	O7D	CDF-CDE-CDD	-2.05	117.73	120.99
2	h	5	NZC	CG2-CB-CA	2.04	116.39	112.27
2	H	10	O7D	CCW-CCX-CCY	-2.04	125.44	127.97
2	i	5	NZC	O-C-CA	-2.04	119.13	124.83
2	f	10	O7D	CCW-CCX-CDB	2.03	129.92	126.42
2	Z	7	MLE	CG-CB-CA	-2.03	110.27	115.34
2	d	10	O7D	CDF-CDE-CDD	-2.02	117.77	120.99
2	f	3	WZJ	O-C-CA	-2.02	119.21	124.83
2	b	5	NZC	OG1-CB-CG2	-2.01	103.78	109.74
2	f	9	MVA	CB-CA-N	-2.01	108.55	111.17
2	R	9	MVA	CG2-CB-CA	-2.01	108.13	111.21
2	L	7	MLE	O-C-CA	-2.01	119.52	124.78

There are no chirality outliers.

All (348) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	O7G	CB-CA-N-CAB
2	D	1	O7G	C-CA-CB-CAG
2	F	1	O7G	CB-CA-N-CAA

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Mol	Chain	Res	Type	Atoms
2	F	1	O7G	CB-CA-N-CAB
2	H	1	O7G	C-CA-CB-CAF
2	H	1	O7G	C-CA-CB-CAG
2	Q	1	O7G	CB-CA-N-CAA
2	Q	1	O7G	C-CA-CB-CAF
2	Q	1	O7G	C-CA-CB-CAG
2	R	1	O7G	CB-CA-N-CAB
2	R	1	O7G	N-CA-CB-CAG
2	R	1	O7G	C-CA-CB-CAF
2	R	1	O7G	C-CA-CB-CAG
2	S	1	O7G	CB-CA-N-CAA
2	S	1	O7G	CB-CA-N-CAB
2	S	1	O7G	C-CA-CB-CAG
2	c	1	O7G	N-CA-CB-CAF
2	c	1	O7G	C-CA-CB-CAF
2	c	1	O7G	C-CA-CB-CAG
2	d	1	O7G	C-CA-CB-CAF
2	d	1	O7G	C-CA-CB-CAG
2	g	1	O7G	CB-CA-N-CAA
2	g	1	O7G	CB-CA-N-CAB
2	h	1	O7G	CB-CA-N-CAB
2	h	1	O7G	O-C-CA-CB
2	h	1	O7G	N-CA-CB-CAF
2	h	1	O7G	N-CA-CB-CAG
2	h	1	O7G	C-CA-CB-CAF
2	h	1	O7G	C-CA-CB-CAG
2	D	3	WZJ	CB-CA-N-CN
2	E	3	WZJ	N-CA-CB-CG2
2	E	3	WZJ	C-CA-CB-CG2
2	E	3	WZJ	C-CA-CB-CG1
2	F	3	WZJ	N-CA-CB-CG1
2	F	3	WZJ	C-CA-CB-CG2
2	F	3	WZJ	C-CA-CB-CG1
2	H	3	WZJ	CB-CA-N-CN
2	J	3	WZJ	CB-CA-N-CN
2	L	3	WZJ	CB-CA-N-CN
2	L	3	WZJ	N-CA-CB-CG2
2	L	3	WZJ	C-CA-CB-CG2
2	N	3	WZJ	CB-CA-N-CN
2	Q	3	WZJ	CB-CA-N-CN
2	R	3	WZJ	CB-CA-N-CN
2	R	3	WZJ	CG2-CB-CG1-CD1

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Mol	Chain	Res	Type	Atoms
2	S	3	WZJ	CB-CA-N-CN
2	V	3	WZJ	CB-CA-N-CN
2	Z	3	WZJ	O-C-CA-CB
2	b	3	WZJ	O-C-CA-CB
2	b	3	WZJ	N-CA-CB-CG2
2	b	3	WZJ	N-CA-CB-CG1
2	b	3	WZJ	C-CA-CB-CG2
2	b	3	WZJ	C-CA-CB-CG1
2	c	3	WZJ	CB-CA-N-CN
2	f	3	WZJ	CB-CA-N-CN
2	g	3	WZJ	CB-CA-N-CN
2	h	3	WZJ	CB-CA-N-CN
2	h	3	WZJ	O-C-CA-CB
2	h	3	WZJ	C-CA-CB-CG2
2	j	3	WZJ	CB-CA-N-CN
2	E	5	NZC	N-CA-CB-OG1
2	E	5	NZC	N-CA-CB-CG2
2	E	5	NZC	C-CA-CB-OG1
2	E	5	NZC	C-CA-CB-CG2
2	H	5	NZC	CB-CA-N-C40
2	J	5	NZC	N-CA-CB-CG2
2	J	5	NZC	C-CA-CB-OG1
2	J	5	NZC	C-CA-CB-CG2
2	Q	5	NZC	N-CA-CB-OG1
2	Q	5	NZC	C-CA-CB-CG2
2	R	5	NZC	N-CA-CB-OG1
2	R	5	NZC	N-CA-CB-CG2
2	R	5	NZC	C-CA-CB-OG1
2	R	5	NZC	C-CA-CB-CG2
2	S	5	NZC	N-CA-CB-OG1
2	S	5	NZC	N-CA-CB-CG2
2	S	5	NZC	C-CA-CB-CG2
2	V	5	NZC	CB-CA-N-C40
2	V	5	NZC	N-CA-CB-OG1
2	V	5	NZC	N-CA-CB-CG2
2	V	5	NZC	C-CA-CB-OG1
2	V	5	NZC	C-CA-CB-CG2
2	Z	5	NZC	N-CA-CB-OG1
2	Z	5	NZC	N-CA-CB-CG2
2	Z	5	NZC	C-CA-CB-CG2
2	a	5	NZC	CB-CA-N-C40
2	c	5	NZC	CB-CA-N-C40

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Mol	Chain	Res	Type	Atoms
2	c	5	NZC	N-CA-CB-OG1
2	c	5	NZC	N-CA-CB-CG2
2	c	5	NZC	C-CA-CB-OG1
2	c	5	NZC	C-CA-CB-CG2
2	d	5	NZC	CB-CA-N-C40
2	D	7	MLE	C-CA-CB-CG
2	L	7	MLE	O-C-CA-CB
2	R	7	MLE	C-CA-CB-CG
2	V	7	MLE	C-CA-CB-CG
2	D	9	MVA	C-CA-CB-CG2
2	J	9	MVA	CB-CA-N-CN
2	J	9	MVA	N-CA-CB-CG1
2	J	9	MVA	N-CA-CB-CG2
2	J	9	MVA	C-CA-CB-CG1
2	L	9	MVA	N-CA-CB-CG1
2	L	9	MVA	N-CA-CB-CG2
2	L	9	MVA	C-CA-CB-CG1
2	L	9	MVA	C-CA-CB-CG2
2	N	9	MVA	CB-CA-N-CN
2	U	9	MVA	N-CA-CB-CG2
2	V	9	MVA	CB-CA-N-CN
2	V	9	MVA	N-CA-CB-CG1
2	V	9	MVA	N-CA-CB-CG2
2	V	9	MVA	C-CA-CB-CG1
2	V	9	MVA	C-CA-CB-CG2
2	d	9	MVA	N-CA-CB-CG1
2	d	9	MVA	N-CA-CB-CG2
2	d	9	MVA	C-CA-CB-CG1
2	d	9	MVA	C-CA-CB-CG2
2	f	9	MVA	N-CA-CB-CG1
2	f	9	MVA	N-CA-CB-CG2
2	h	9	MVA	N-CA-CB-CG1
2	h	9	MVA	N-CA-CB-CG2
2	j	9	MVA	N-CA-CB-CG1
2	j	9	MVA	N-CA-CB-CG2
2	j	9	MVA	C-CA-CB-CG1
2	j	9	MVA	C-CA-CB-CG2
2	D	10	O7D	O-C-CA-CCW
2	E	10	O7D	O-C-CA-CCW
2	F	10	O7D	O-C-CA-CCW
2	H	10	O7D	O-C-CA-CCW
2	J	10	O7D	O-C-CA-CCW

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Mol	Chain	Res	Type	Atoms
2	L	10	O7D	O-C-CA-CCW
2	N	10	O7D	O-C-CA-CCW
2	P	10	O7D	O-C-CA-CCW
2	S	10	O7D	O-C-CA-CCW
2	U	10	O7D	O-C-CA-CCW
2	V	10	O7D	O-C-CA-CCW
2	X	10	O7D	O-C-CA-CCW
2	Z	10	O7D	O-C-CA-CCW
2	a	10	O7D	O-C-CA-CCW
2	c	10	O7D	O-C-CA-CCW
2	d	10	O7D	O-C-CA-CCW
2	f	10	O7D	O-C-CA-CCW
2	g	10	O7D	O-C-CA-CCW
2	h	10	O7D	O-C-CA-CCW
2	i	10	O7D	O-C-CA-CCW
2	E	12	H14	OXT-C-CA-N
2	H	12	H14	OXT-C-CA-N
2	Q	12	H14	OXT-C-CA-N
2	R	12	H14	OXT-C-CA-N
2	d	12	H14	OXT-C-CA-CB
2	L	3	WZJ	CG2-CB-CG1-CD1
2	Z	3	WZJ	CG2-CB-CG1-CD1
2	a	3	WZJ	CG2-CB-CG1-CD1
2	R	7	MLE	N-CA-CB-CG
2	V	10	O7D	CDD-CDC-ODG-CDH
2	F	3	WZJ	N-CA-CB-CG2
2	i	3	WZJ	CG2-CB-CG1-CD1
2	V	10	O7D	CDB-CDC-ODG-CDH
2	Z	3	WZJ	CA-CB-CG1-CD1
2	a	3	WZJ	CA-CB-CG1-CD1
2	i	3	WZJ	CA-CB-CG1-CD1
2	D	7	MLE	N-CA-CB-CG
2	D	3	WZJ	CG2-CB-CG1-CD1
2	X	3	WZJ	CG2-CB-CG1-CD1
2	U	3	WZJ	CG2-CB-CG1-CD1
2	L	3	WZJ	N-CA-CB-CG1
2	R	3	WZJ	CA-CB-CG1-CD1
2	H	3	WZJ	N-CA-CB-CG2
2	S	3	WZJ	N-CA-CB-CG2
2	Q	3	WZJ	CG2-CB-CG1-CD1
2	Q	5	NZC	N-CA-CB-CG2
2	S	3	WZJ	CG2-CB-CG1-CD1

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Mol	Chain	Res	Type	Atoms
2	L	3	WZJ	CA-CB-CG1-CD1
2	Q	3	WZJ	CA-CB-CG1-CD1
2	S	3	WZJ	CA-CB-CG1-CD1
2	E	3	WZJ	N-CA-CB-CG1
2	D	7	MLE	CA-CB-CG-CD2
2	V	7	MLE	N-CA-CB-CG
2	h	3	WZJ	N-CA-CB-CG2
2	S	1	O7G	C-CA-CB-CAF
2	c	7	MLE	CA-CB-CG-CD1
2	a	3	WZJ	N-CA-CB-CG2
2	c	3	WZJ	CG2-CB-CG1-CD1
2	E	12	H14	OXT-C-CA-CB
2	H	12	H14	OXT-C-CA-CB
2	Q	12	H14	OXT-C-CA-CB
2	R	12	H14	OXT-C-CA-CB
2	X	12	H14	OXT-C-CA-CB
2	d	3	WZJ	CG2-CB-CG1-CD1
2	S	3	WZJ	C-CA-CB-CG2
2	g	3	WZJ	CG2-CB-CG1-CD1
2	D	9	MVA	C-CA-CB-CG1
2	J	9	MVA	C-CA-CB-CG2
2	h	3	WZJ	CG2-CB-CG1-CD1
2	H	9	MVA	N-CA-CB-CG1
2	H	9	MVA	N-CA-CB-CG2
2	U	9	MVA	N-CA-CB-CG1
2	c	9	MVA	N-CA-CB-CG1
2	c	9	MVA	N-CA-CB-CG2
2	J	5	NZC	N-CA-CB-OG1
2	X	5	NZC	N-CA-CB-CG2
2	D	10	O7D	N-CA-CCW-CCX
2	F	10	O7D	N-CA-CCW-CCX
2	J	10	O7D	N-CA-CCW-CCX
2	U	10	O7D	N-CA-CCW-CCX
2	Z	10	O7D	N-CA-CCW-CCX
2	Q	5	NZC	C-CA-CB-OG1
2	S	5	NZC	C-CA-CB-OG1
2	Z	5	NZC	C-CA-CB-OG1
2	Q	1	O7G	N-CA-CB-CAG
2	L	3	WZJ	C-CA-CB-CG1
2	D	12	H14	C-CA-CB-CG
2	F	12	H14	C-CA-CB-OB
2	F	12	H14	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	J	12	H14	C-CA-CB-OB
2	J	12	H14	C-CA-CB-CG
2	N	12	H14	C-CA-CB-OB
2	N	12	H14	C-CA-CB-CG
2	R	12	H14	C-CA-CB-CG
2	U	12	H14	C-CA-CB-OB
2	U	12	H14	C-CA-CB-CG
2	V	12	H14	C-CA-CB-OB
2	V	12	H14	C-CA-CB-CG
2	Z	12	H14	C-CA-CB-OB
2	Z	12	H14	C-CA-CB-CG
2	b	12	H14	C-CA-CB-OB
2	b	12	H14	C-CA-CB-CG
2	c	12	H14	C-CA-CB-OB
2	c	12	H14	C-CA-CB-CG
2	f	12	H14	C-CA-CB-CG
2	g	12	H14	C-CA-CB-OB
2	g	12	H14	C-CA-CB-CG
2	h	12	H14	C-CA-CB-OB
2	h	12	H14	C-CA-CB-CG
2	j	12	H14	C-CA-CB-OB
2	j	12	H14	C-CA-CB-CG
2	P	1	O7G	CB-CA-N-CAA
2	X	12	H14	OXT-C-CA-N
2	d	12	H14	OXT-C-CA-N
2	Q	10	O7D	CDB-CDC-ODG-CDH
2	d	7	MLE	CA-CB-CG-CD1
2	Q	10	O7D	CDD-CDC-ODG-CDH
2	E	7	MLE	N-CA-CB-CG
2	D	5	NZC	CB-CA-N-C40
2	E	5	NZC	CB-CA-N-C40
2	F	5	NZC	CB-CA-N-C40
2	J	5	NZC	CB-CA-N-C40
2	L	5	NZC	CB-CA-N-C40
2	N	5	NZC	CB-CA-N-C40
2	P	5	NZC	CB-CA-N-C40
2	Q	5	NZC	CB-CA-N-C40
2	R	5	NZC	CB-CA-N-C40
2	S	5	NZC	CB-CA-N-C40
2	U	5	NZC	CB-CA-N-C40
2	X	5	NZC	CB-CA-N-C40
2	Z	5	NZC	CB-CA-N-C40

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Mol	Chain	Res	Type	Atoms
2	b	5	NZC	CB-CA-N-C40
2	f	5	NZC	CB-CA-N-C40
2	g	5	NZC	CB-CA-N-C40
2	h	5	NZC	CB-CA-N-C40
2	i	5	NZC	CB-CA-N-C40
2	j	5	NZC	CB-CA-N-C40
2	X	3	WZJ	CA-CB-CG1-CD1
2	E	3	WZJ	CB-CA-N-CN
2	F	3	WZJ	CB-CA-N-CN
2	P	3	WZJ	CB-CA-N-CN
2	U	3	WZJ	CB-CA-N-CN
2	X	3	WZJ	CB-CA-N-CN
2	Z	3	WZJ	CB-CA-N-CN
2	a	3	WZJ	CB-CA-N-CN
2	b	3	WZJ	CB-CA-N-CN
2	d	3	WZJ	CB-CA-N-CN
2	i	3	WZJ	CB-CA-N-CN
2	D	9	MVA	CB-CA-N-CN
2	E	9	MVA	CB-CA-N-CN
2	F	9	MVA	CB-CA-N-CN
2	H	9	MVA	CB-CA-N-CN
2	L	9	MVA	CB-CA-N-CN
2	P	9	MVA	CB-CA-N-CN
2	Q	9	MVA	CB-CA-N-CN
2	R	9	MVA	CB-CA-N-CN
2	S	9	MVA	CB-CA-N-CN
2	U	9	MVA	CB-CA-N-CN
2	X	9	MVA	CB-CA-N-CN
2	Z	9	MVA	CB-CA-N-CN
2	a	9	MVA	CB-CA-N-CN
2	b	9	MVA	CB-CA-N-CN
2	c	9	MVA	CB-CA-N-CN
2	d	9	MVA	CB-CA-N-CN
2	f	9	MVA	CB-CA-N-CN
2	g	9	MVA	CB-CA-N-CN
2	h	9	MVA	CB-CA-N-CN
2	i	9	MVA	CB-CA-N-CN
2	j	9	MVA	CB-CA-N-CN
2	D	1	O7G	C-CA-CB-CAF
2	D	10	O7D	CDB-CDC-ODG-CDH
2	d	5	NZC	N-CA-CB-CG2
2	H	1	O7G	N-CA-CB-CAG

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Mol	Chain	Res	Type	Atoms
2	d	1	O7G	N-CA-CB-CAG
2	c	7	MLE	CA-CB-CG-CD2
2	H	1	O7G	O-C-CA-CB
2	J	1	O7G	O-C-CA-CB
2	V	1	O7G	O-C-CA-CB
2	Z	1	O7G	O-C-CA-CB
2	a	1	O7G	O-C-CA-CB
2	H	3	WZJ	C-CA-CB-CG2
2	c	3	WZJ	C-CA-CB-CG2
2	X	5	NZC	C-CA-CB-CG2
2	D	10	O7D	CDD-CDC-ODG-CDH
2	D	12	H14	N-CA-CB-CG
2	F	12	H14	N-CA-CB-CG
2	J	12	H14	N-CA-CB-CG
2	N	12	H14	N-CA-CB-CG
2	R	12	H14	N-CA-CB-CG
2	U	12	H14	N-CA-CB-CG
2	V	12	H14	N-CA-CB-CG
2	a	12	H14	N-CA-CB-CG
2	b	12	H14	N-CA-CB-CG
2	f	12	H14	N-CA-CB-CG
2	g	12	H14	N-CA-CB-CG
2	h	12	H14	N-CA-CB-CG
2	j	12	H14	N-CA-CB-CG
2	F	3	WZJ	O-C-CA-CB
2	U	3	WZJ	O-C-CA-CB
2	X	3	WZJ	O-C-CA-CB
2	g	3	WZJ	O-C-CA-CB
2	f	9	MVA	C-CA-CB-CG1
2	V	7	MLE	CA-CB-CG-CD2
2	F	9	MVA	N-CA-CB-CG1
2	F	9	MVA	N-CA-CB-CG2
2	N	9	MVA	N-CA-CB-CG1
2	N	9	MVA	N-CA-CB-CG2
2	X	9	MVA	N-CA-CB-CG1
2	Z	9	MVA	N-CA-CB-CG1
2	D	5	NZC	N-CA-CB-CG2
2	Z	10	O7D	CDB-CDC-ODG-CDH
2	V	3	WZJ	CG2-CB-CG1-CD1
2	d	7	MLE	N-CA-CB-CG
2	h	3	WZJ	N-CA-CB-CG1
2	R	1	O7G	N-CA-CB-CAF

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Mol	Chain	Res	Type	Atoms
2	c	1	O7G	N-CA-CB-CAG
2	S	3	WZJ	C-CA-CB-CG1
2	h	3	WZJ	C-CA-CB-CG1
2	D	12	H14	C-CA-CB-OB
2	P	12	H14	C-CA-CB-CG
2	R	12	H14	C-CA-CB-OB
2	a	12	H14	C-CA-CB-CG
2	f	12	H14	C-CA-CB-OB
2	d	7	MLE	CA-CB-CG-CD2

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)

20 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	ACT	Y	503	-	3,3,3	0.64	0	3,3,3	1.91	2 (66%)
3	ACT	A	501	-	3,3,3	1.69	1 (33%)	3,3,3	1.64	1 (33%)
3	ACT	e	401	-	3,3,3	1.48	1 (33%)	3,3,3	1.60	1 (33%)
3	ACT	e	402	-	3,3,3	1.26	0	3,3,3	1.48	0
3	ACT	I	502	-	3,3,3	1.35	0	3,3,3	1.64	1 (33%)
3	ACT	I	501	-	3,3,3	1.54	1 (33%)	3,3,3	1.43	0
3	ACT	A	502	-	3,3,3	0.93	0	3,3,3	1.92	1 (33%)
3	ACT	B	501	-	3,3,3	1.58	1 (33%)	3,3,3	1.62	1 (33%)
3	ACT	M	501	-	3,3,3	1.39	0	3,3,3	1.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ACT	C	501	-	3,3,3	1.47	0	3,3,3	1.58	1 (33%)
3	ACT	Y	502	-	3,3,3	2.13	2 (66%)	3,3,3	1.32	0
3	ACT	T	501	-	3,3,3	1.64	1 (33%)	3,3,3	1.61	1 (33%)
3	ACT	W	402	-	3,3,3	1.31	0	3,3,3	1.31	0
3	ACT	W	401	-	3,3,3	1.51	1 (33%)	3,3,3	1.36	0
3	ACT	G	501	-	3,3,3	1.37	0	3,3,3	1.47	0
3	ACT	K	501	-	3,3,3	1.56	1 (33%)	3,3,3	1.45	0
3	ACT	W	404	-	3,3,3	1.26	0	3,3,3	1.30	0
3	ACT	O	501	-	3,3,3	1.26	0	3,3,3	1.48	1 (33%)
3	ACT	Y	501	-	3,3,3	1.12	0	3,3,3	1.59	0
3	ACT	W	403	-	3,3,3	1.71	1 (33%)	3,3,3	1.28	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	502	ACT	CH3-C	2.90	1.61	1.49
3	W	403	ACT	CH3-C	2.62	1.60	1.49
3	A	501	ACT	CH3-C	2.49	1.59	1.49
3	K	501	ACT	CH3-C	2.28	1.58	1.49
3	B	501	ACT	CH3-C	2.25	1.58	1.49
3	Y	502	ACT	O-C	2.25	1.32	1.22
3	W	401	ACT	CH3-C	2.24	1.58	1.49
3	I	501	ACT	CH3-C	2.23	1.58	1.49
3	e	401	ACT	CH3-C	2.17	1.58	1.49
3	T	501	ACT	CH3-C	2.11	1.58	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	ACT	OXT-C-O	2.64	131.78	122.05
3	Y	503	ACT	OXT-C-O	2.34	130.67	122.05
3	Y	503	ACT	O-C-CH3	-2.33	113.25	122.33
3	T	501	ACT	OXT-C-O	2.23	130.27	122.05
3	B	501	ACT	OXT-C-O	2.19	130.13	122.05
3	I	502	ACT	OXT-C-O	2.17	130.04	122.05
3	C	501	ACT	OXT-C-O	2.15	129.97	122.05
3	e	401	ACT	O-C-CH3	-2.06	114.32	122.33
3	A	501	ACT	OXT-C-O	2.05	129.59	122.05
3	O	501	ACT	OXT-C-O	2.00	129.44	122.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	144/158 (91%)	-0.20	2 (1%) 75 77	42, 58, 88, 110	0
1	B	145/158 (91%)	-0.20	1 (0%) 87 89	41, 60, 96, 115	0
1	C	145/158 (91%)	-0.03	2 (1%) 75 77	49, 72, 97, 123	0
1	G	147/158 (93%)	-0.30	0 100 100	42, 55, 78, 100	0
1	I	146/158 (92%)	-0.31	0 100 100	41, 55, 80, 104	0
1	K	146/158 (92%)	0.08	3 (2%) 63 66	50, 72, 93, 109	0
1	M	144/158 (91%)	0.03	7 (4%) 29 31	49, 70, 94, 112	0
1	O	147/158 (93%)	-0.15	2 (1%) 75 77	43, 58, 85, 107	0
1	T	146/158 (92%)	-0.24	1 (0%) 87 89	43, 58, 89, 108	0
1	W	147/158 (93%)	0.02	3 (2%) 65 68	49, 69, 101, 114	0
1	Y	147/158 (93%)	-0.26	1 (0%) 87 89	41, 59, 81, 136	0
1	e	147/158 (93%)	-0.30	2 (1%) 75 77	40, 56, 85, 111	0
2	D	6/13 (46%)	-0.26	0 100 100	48, 50, 51, 54	0
2	E	6/13 (46%)	0.84	1 (16%) 1 1	52, 64, 86, 134	0
2	F	6/13 (46%)	-0.51	0 100 100	48, 49, 52, 54	0
2	H	6/13 (46%)	0.58	1 (16%) 1 1	52, 62, 82, 141	0
2	J	6/13 (46%)	-0.49	0 100 100	52, 56, 56, 58	0
2	L	6/13 (46%)	-0.43	0 100 100	56, 59, 72, 97	0
2	N	6/13 (46%)	-0.42	0 100 100	45, 49, 54, 56	0
2	P	6/13 (46%)	0.43	1 (16%) 1 1	55, 64, 90, 135	0
2	Q	6/13 (46%)	0.42	1 (16%) 1 1	52, 65, 96, 132	0
2	R	6/13 (46%)	-0.60	0 100 100	48, 52, 53, 54	0
2	S	6/13 (46%)	-0.20	0 100 100	60, 61, 70, 105	0
2	U	6/13 (46%)	-0.41	0 100 100	49, 52, 55, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	V	6/13 (46%)	-0.07	0 100 100	51, 55, 57, 63	0
2	X	6/13 (46%)	0.56	1 (16%) 1 1	53, 63, 82, 140	0
2	Z	6/13 (46%)	-0.37	0 100 100	42, 46, 49, 54	0
2	a	6/13 (46%)	1.42	1 (16%) 1 1	62, 75, 99, 137	0
2	b	6/13 (46%)	-0.37	0 100 100	47, 48, 52, 54	0
2	c	6/13 (46%)	-0.02	1 (16%) 1 1	56, 64, 86, 124	0
2	d	6/13 (46%)	0.02	0 100 100	52, 62, 82, 116	0
2	f	6/13 (46%)	-0.56	0 100 100	48, 50, 51, 53	0
2	g	6/13 (46%)	0.50	1 (16%) 1 1	62, 72, 95, 131	0
2	h	6/13 (46%)	-0.68	0 100 100	44, 48, 49, 54	0
2	i	6/13 (46%)	0.84	1 (16%) 1 1	56, 69, 87, 137	0
2	j	6/13 (46%)	-0.42	0 100 100	49, 50, 52, 54	0
All	All	1895/2208 (85%)	-0.14	33 (1%) 70 72	40, 61, 94, 141	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2	VAL	7.6
2	a	2	VAL	7.6
2	i	2	VAL	6.8
1	M	141	LEU	6.3
2	H	2	VAL	5.3
1	W	145	TYR	5.2
1	B	145	TYR	5.2
2	P	2	VAL	4.7
2	X	2	VAL	4.5
1	C	42	GLU	4.1
1	M	127	LEU	3.6
2	c	2	VAL	3.5
1	A	74	PRO	3.4
2	Q	2	VAL	3.4
2	g	2	VAL	3.3
1	K	49	LEU	3.0
1	A	73	ALA	2.8
1	K	98	LEU	2.7
1	e	11	ARG	2.7
1	Y	54	ILE	2.5
1	M	142	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	144	GLY	2.4
1	W	52	LEU	2.4
1	O	75	SER	2.4
1	M	129	ALA	2.4
1	T	76	GLY	2.3
1	K	129	ALA	2.2
1	O	22	MET	2.2
1	M	128	GLY	2.2
1	C	72	GLN	2.1
1	M	72	GLN	2.1
1	e	74	PRO	2.0
1	W	140	GLN	2.0

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, 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
2	O7G	a	1	9/10	0.47	0.79	156,161,174,176	0
2	O7G	Q	1	9/10	0.69	0.58	101,114,141,142	0
2	O7G	P	1	9/10	0.73	0.46	112,124,141,144	0
2	WZJ	c	3	9/10	0.74	0.27	90,96,110,121	0
2	O7G	H	1	9/10	0.75	0.60	158,169,173,174	0
2	O7G	E	1	9/10	0.77	0.59	139,148,154,155	0
2	O7G	X	1	9/10	0.77	0.33	137,142,147,149	0
2	WZJ	a	3	9/10	0.78	0.30	105,115,129,129	0
2	WZJ	i	3	9/10	0.79	0.26	93,106,125,132	0
2	WZJ	P	3	9/10	0.80	0.22	100,116,123,131	0
2	O7G	d	1	9/10	0.80	0.32	120,131,140,141	0
2	WZJ	Q	3	9/10	0.83	0.22	92,119,127,129	0
2	O7G	i	1	9/10	0.83	0.43	133,139,146,148	0
2	WZJ	E	3	9/10	0.84	0.30	96,107,118,120	0
2	O7G	c	1	9/10	0.84	0.36	135,140,145,148	0
2	WZJ	d	3	9/10	0.86	0.20	89,103,110,114	0
2	NZC	P	5	8/9	0.87	0.20	69,82,91,94	0
2	WZJ	g	3	9/10	0.88	0.20	91,110,115,117	0
2	O7G	g	1	9/10	0.89	0.22	126,130,141,142	0
2	O7G	L	1	9/10	0.90	0.20	73,88,96,98	0
2	NZC	g	5	8/9	0.90	0.15	69,74,85,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NZC	a	5	8/9	0.91	0.18	72,84,91,91	0
2	NZC	i	5	8/9	0.91	0.15	71,76,87,88	0
2	WZJ	X	3	9/10	0.92	0.28	100,105,123,128	0
2	WZJ	L	3	9/10	0.92	0.19	79,86,94,98	0
2	WZJ	H	3	9/10	0.92	0.18	87,102,119,120	0
2	NZC	c	5	8/9	0.92	0.15	63,74,84,87	0
2	WZJ	J	3	9/10	0.92	0.13	45,50,54,55	0
2	WZJ	S	3	9/10	0.92	0.18	74,82,92,93	0
2	MVA	F	9	8/9	0.92	0.14	51,53,57,60	0
2	O7G	b	1	9/10	0.93	0.16	45,54,62,65	0
2	MLE	L	7	9/10	0.93	0.19	53,56,59,61	0
2	MLE	g	7	9/10	0.93	0.15	52,62,64,65	0
2	O7G	U	1	9/10	0.93	0.20	48,58,68,76	0
2	MVA	N	9	8/9	0.93	0.23	59,67,76,79	0
2	MVA	V	9	8/9	0.93	0.16	65,72,80,80	0
2	O7D	Z	10	17/18	0.93	0.16	43,48,59,62	0
2	H14	Q	12	12/13	0.93	0.14	52,60,64,65	0
2	MLE	X	7	9/10	0.94	0.16	49,51,53,57	0
2	WZJ	h	3	9/10	0.94	0.12	53,54,61,64	0
2	WZJ	U	3	9/10	0.94	0.15	48,49,55,58	0
2	NZC	N	5	8/9	0.94	0.18	39,43,54,68	0
2	O7G	f	1	9/10	0.94	0.15	54,57,65,65	0
2	O7D	L	10	17/18	0.94	0.14	46,53,57,64	0
2	NZC	Q	5	8/9	0.94	0.19	66,85,89,91	0
2	H14	D	12	12/13	0.94	0.14	42,48,52,52	0
2	H14	F	12	12/13	0.94	0.12	44,47,52,52	0
2	H14	J	12	12/13	0.94	0.12	52,55,58,62	0
2	MLE	Q	7	9/10	0.94	0.14	51,52,60,61	0
2	NZC	H	5	8/9	0.95	0.21	58,74,79,83	0
2	MVA	J	9	8/9	0.95	0.14	54,61,73,78	0
2	NZC	S	5	8/9	0.95	0.13	60,66,79,79	0
2	NZC	j	5	8/9	0.95	0.13	43,48,57,61	0
2	MVA	i	9	8/9	0.95	0.15	44,51,58,61	0
2	MVA	j	9	8/9	0.95	0.17	50,55,66,69	0
2	O7D	F	10	17/18	0.95	0.14	45,55,60,61	0
2	MLE	H	7	9/10	0.95	0.11	50,57,62,63	0
2	O7D	U	10	17/18	0.95	0.17	51,56,61,65	0
2	NZC	V	5	8/9	0.95	0.11	48,54,58,67	0
2	O7D	h	10	17/18	0.95	0.14	47,52,60,61	0
2	WZJ	b	3	9/10	0.95	0.16	35,46,52,69	0
2	WZJ	Z	3	9/10	0.95	0.14	40,49,55,57	0
2	H14	H	12	12/13	0.95	0.19	43,54,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NZC	d	5	8/9	0.95	0.14	58,70,74,75	0
2	H14	N	12	12/13	0.95	0.14	40,44,47,53	0
2	MLE	i	7	9/10	0.95	0.17	51,57,61,62	0
2	H14	R	12	12/13	0.95	0.11	42,48,50,52	0
2	H14	j	12	12/13	0.95	0.15	43,46,53,54	0
2	MLE	b	7	9/10	0.96	0.18	45,53,56,57	0
2	MLE	c	7	9/10	0.96	0.15	49,58,61,61	0
2	MLE	d	7	9/10	0.96	0.12	49,54,56,58	0
2	MLE	f	7	9/10	0.96	0.11	44,49,52,53	0
2	NZC	R	5	8/9	0.96	0.15	43,54,56,59	0
2	MLE	h	7	9/10	0.96	0.15	44,47,52,55	0
2	O7G	R	1	9/10	0.96	0.15	46,52,67,73	0
2	MVA	D	9	8/9	0.96	0.12	49,55,57,59	0
2	O7G	S	1	9/10	0.96	0.13	72,86,91,93	0
2	NZC	X	5	8/9	0.96	0.20	56,65,72,74	0
2	NZC	Z	5	8/9	0.96	0.14	40,43,51,55	0
2	O7G	F	1	9/10	0.96	0.16	53,60,71,77	0
2	MVA	c	9	8/9	0.96	0.12	43,50,57,58	0
2	MVA	f	9	8/9	0.96	0.13	50,55,57,58	0
2	MVA	g	9	8/9	0.96	0.25	52,60,63,72	0
2	NZC	b	5	8/9	0.96	0.15	41,45,63,63	0
2	WZJ	N	3	9/10	0.96	0.14	38,46,49,52	0
2	O7D	D	10	17/18	0.96	0.10	44,57,62,63	0
2	O7G	V	1	9/10	0.96	0.17	62,66,70,76	0
2	O7D	H	10	17/18	0.96	0.15	43,47,53,56	0
2	O7G	D	1	9/10	0.96	0.14	56,60,70,80	0
2	O7D	N	10	17/18	0.96	0.12	46,52,57,58	0
2	O7D	P	10	17/18	0.96	0.12	45,53,56,57	0
2	O7G	Z	1	9/10	0.96	0.10	52,56,63,70	0
2	O7G	j	1	9/10	0.96	0.11	48,51,63,66	0
2	O7D	a	10	17/18	0.96	0.11	42,53,61,61	0
2	O7D	b	10	17/18	0.96	0.14	48,53,57,59	0
2	O7D	d	10	17/18	0.96	0.11	46,52,57,61	0
2	O7D	g	10	17/18	0.96	0.15	45,55,57,59	0
2	MLE	D	7	9/10	0.96	0.15	48,50,51,52	0
2	O7D	j	10	17/18	0.96	0.14	43,53,55,56	0
2	MLE	E	7	9/10	0.96	0.14	52,57,59,62	0
2	H14	E	12	12/13	0.96	0.15	47,53,62,62	0
2	MLE	F	7	9/10	0.96	0.15	48,50,55,55	0
2	NZC	L	5	8/9	0.96	0.14	59,64,75,84	0
2	WZJ	V	3	9/10	0.96	0.14	43,49,57,57	0
2	H14	L	12	12/13	0.96	0.14	57,61,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MLE	P	7	9/10	0.96	0.15	50,55,59,60	0
2	H14	P	12	12/13	0.96	0.11	57,60,63,66	0
2	WZJ	D	3	9/10	0.96	0.13	43,47,54,55	0
2	O7G	J	1	9/10	0.96	0.23	51,56,68,70	0
2	H14	V	12	12/13	0.96	0.13	51,52,56,57	0
2	H14	a	12	12/13	0.96	0.12	57,66,73,73	0
2	MLE	a	7	9/10	0.96	0.13	59,64,66,67	0
2	O7G	h	1	9/10	0.97	0.09	52,57,64,68	0
2	MVA	L	9	8/9	0.97	0.14	55,60,68,70	0
2	O7D	Q	10	17/18	0.97	0.10	39,49,56,56	0
2	O7D	R	10	17/18	0.97	0.14	44,49,56,56	0
2	O7D	S	10	17/18	0.97	0.11	46,52,58,59	0
2	NZC	U	5	8/9	0.97	0.10	42,48,52,56	0
2	O7D	V	10	17/18	0.97	0.12	55,58,64,73	0
2	MVA	Q	9	8/9	0.97	0.14	44,51,60,62	0
2	MVA	S	9	8/9	0.97	0.13	56,59,62,63	0
2	MVA	U	9	8/9	0.97	0.17	54,56,60,61	0
2	O7D	c	10	17/18	0.97	0.12	45,49,55,55	0
2	WZJ	f	3	9/10	0.97	0.16	43,47,56,57	0
2	O7D	f	10	17/18	0.97	0.10	45,54,56,57	0
2	MVA	X	9	8/9	0.97	0.12	45,53,57,62	0
2	MVA	a	9	8/9	0.97	0.11	48,57,62,72	0
2	O7D	i	10	17/18	0.97	0.11	44,49,53,57	0
2	MVA	b	9	8/9	0.97	0.16	52,60,66,68	0
2	NZC	f	5	8/9	0.97	0.13	43,54,56,66	0
2	MVA	d	9	8/9	0.97	0.10	40,51,54,56	0
2	MLE	J	7	9/10	0.97	0.13	51,54,59,60	0
2	WZJ	j	3	9/10	0.97	0.13	40,44,51,54	0
2	MVA	h	9	8/9	0.97	0.13	48,52,60,63	0
2	NZC	h	5	8/9	0.97	0.13	41,47,58,59	0
2	NZC	E	5	8/9	0.97	0.16	65,74,82,84	0
2	MLE	j	7	9/10	0.97	0.12	48,51,54,55	0
2	O7D	E	10	17/18	0.97	0.11	41,47,53,56	0
2	MLE	V	7	9/10	0.97	0.12	45,54,59,64	0
2	H14	S	12	12/13	0.97	0.11	58,62,64,65	0
2	H14	U	12	12/13	0.97	0.14	42,48,51,52	0
2	WZJ	F	3	9/10	0.97	0.16	43,49,54,65	0
2	O7D	J	10	17/18	0.97	0.13	52,57,62,65	0
2	H14	b	12	12/13	0.97	0.15	41,46,51,53	0
2	H14	c	12	12/13	0.97	0.12	48,58,65,73	0
2	H14	d	12	12/13	0.97	0.14	46,51,56,57	0
2	H14	f	12	12/13	0.97	0.11	47,52,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	H14	g	12	12/13	0.97	0.09	56,64,67,67	0
2	H14	h	12	12/13	0.97	0.13	41,45,48,48	0
2	H14	i	12	12/13	0.97	0.14	51,55,70,74	0
2	MVA	H	9	8/9	0.97	0.12	44,52,55,63	0
2	NZC	F	5	8/9	0.98	0.11	42,46,52,57	0
2	WZJ	R	3	9/10	0.98	0.12	39,49,52,55	0
2	MLE	Z	7	9/10	0.98	0.14	39,44,50,53	0
2	MVA	Z	9	8/9	0.98	0.11	43,47,55,58	0
2	MVA	E	9	8/9	0.98	0.11	51,55,60,62	0
2	NZC	J	5	8/9	0.98	0.13	47,53,59,64	0
2	H14	X	12	12/13	0.98	0.13	47,54,58,60	0
2	H14	Z	12	12/13	0.98	0.12	34,39,42,43	0
2	MLE	N	7	9/10	0.98	0.14	40,50,54,58	0
2	NZC	D	5	8/9	0.98	0.10	41,47,55,63	0
2	O7G	N	1	9/10	0.98	0.12	54,56,67,69	0
2	MLE	R	7	9/10	0.98	0.13	44,48,51,53	0
2	MVA	P	9	8/9	0.98	0.11	50,54,66,68	0
2	MLE	S	7	9/10	0.98	0.14	53,54,61,61	0
2	O7D	X	10	17/18	0.98	0.12	48,52,55,58	0
2	MVA	R	9	8/9	0.98	0.13	50,54,57,57	0
2	MLE	U	7	9/10	0.98	0.15	45,48,54,54	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	A	502	4/4	0.70	0.17	67,74,77,78	0
3	ACT	Y	502	4/4	0.72	0.24	54,64,64,73	0
3	ACT	Y	503	4/4	0.73	0.23	51,63,64,64	0
3	ACT	W	403	4/4	0.81	0.39	87,91,92,93	0
3	ACT	I	502	4/4	0.84	0.21	63,74,75,77	0
3	ACT	T	501	4/4	0.85	0.14	45,46,50,54	0
3	ACT	W	404	4/4	0.88	0.19	86,89,94,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	W	401	4/4	0.88	0.23	68,75,85,86	0
3	ACT	M	501	4/4	0.90	0.38	54,57,61,61	4
3	ACT	A	501	4/4	0.91	0.18	37,45,55,56	0
3	ACT	W	402	4/4	0.91	0.23	57,58,58,62	4
3	ACT	e	401	4/4	0.92	0.30	74,77,81,87	0
3	ACT	B	501	4/4	0.93	0.12	39,43,53,54	0
3	ACT	O	501	4/4	0.94	0.20	43,48,49,54	4
3	ACT	K	501	4/4	0.94	0.42	59,61,65,65	4
3	ACT	I	501	4/4	0.95	0.18	41,42,51,51	4
3	ACT	C	501	4/4	0.95	0.13	53,57,64,67	0
3	ACT	Y	501	4/4	0.96	0.14	42,44,45,47	4
3	ACT	G	501	4/4	0.96	0.14	40,49,51,54	0
3	ACT	e	402	4/4	0.96	0.15	41,44,47,49	0

6.5 Other polymers (i)

There are no such residues in this entry.