



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 10:17 AM BST

PDB ID : 6C50
Title : Cross-alpha Amyloid-like Structure alphaAmS
Authors : Liu, L.; Zhang, S.Q.
Deposited on : 2018-01-13
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

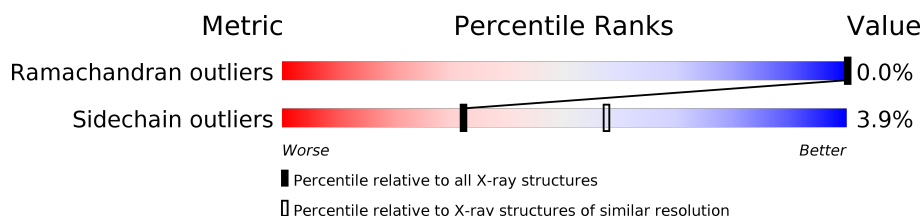
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

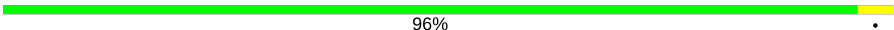

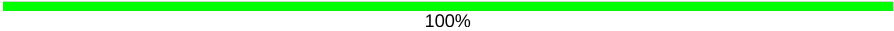
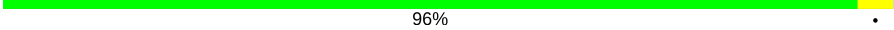
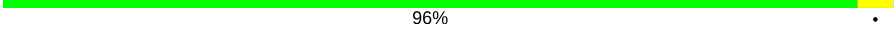
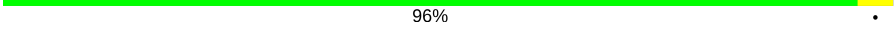
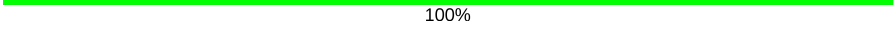
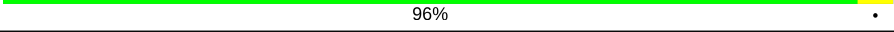
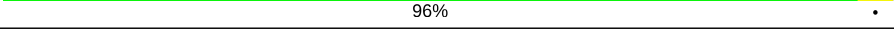
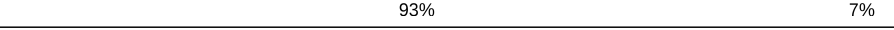
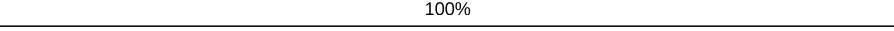
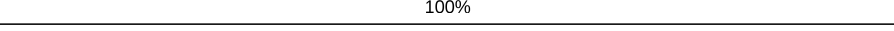
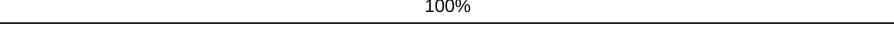
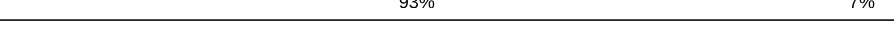
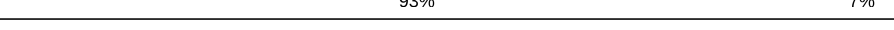
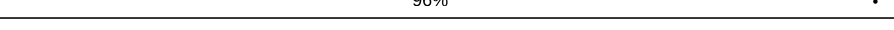
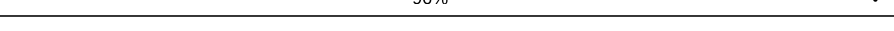
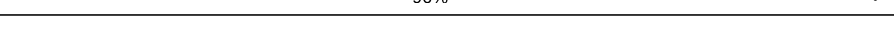
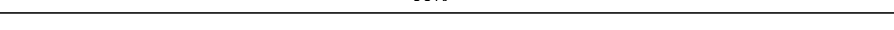
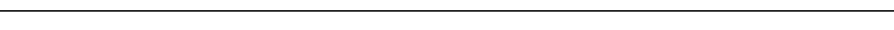
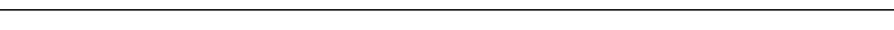
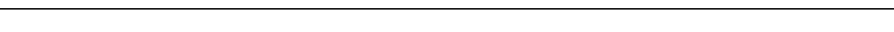
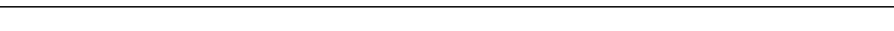
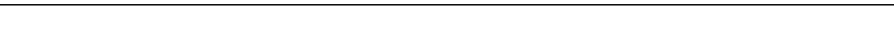

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	11	27	96% .
1	12	27	93% 7%
1	13	27	89% 11%
1	14	27	93% 7%
1	21	27	96% .
1	22	27	96% .
1	23	27	96% .
1	24	27	96% .
1	31	27	96% .



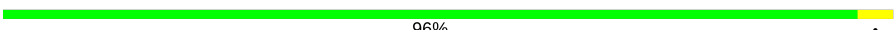
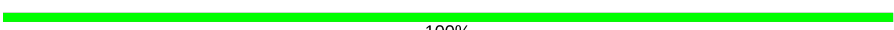











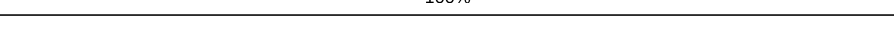
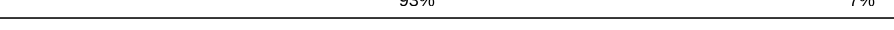
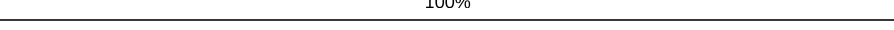
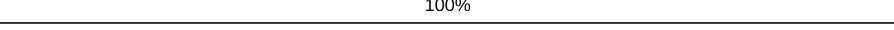
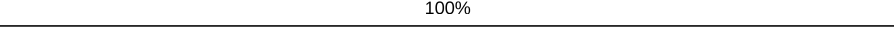
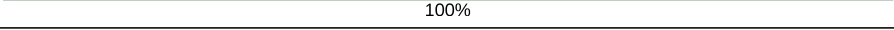

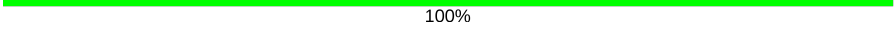

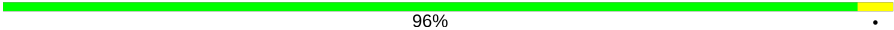
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Mol	Chain	Length	Quality of chain
1	32	27	 96% .
1	33	27	 81% 19%
1	34	27	 100%
1	41	27	 96% .
1	42	27	 96% .
1	43	27	 96% .
1	44	27	 100%
1	51	27	 96% .
1	52	27	 96% .
1	53	27	 93% 7%
1	54	27	 100%
1	61	27	 100%
1	62	27	 100%
1	63	27	 93% 7%
1	64	27	 93% 7%
1	71	27	 96% .
1	72	27	 96% .
1	73	27	 96% .
1	74	27	 96% .
1	81	27	 100%
1	82	27	 96% .
1	83	27	 100%
1	84	27	 100%
1	91	27	 96% .
1	92	27	 96% .

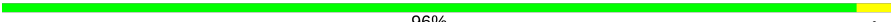















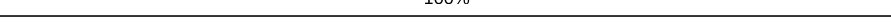
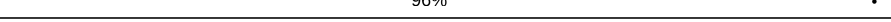

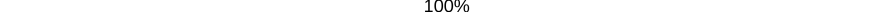
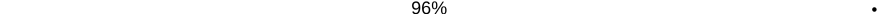
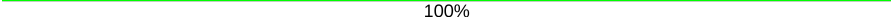
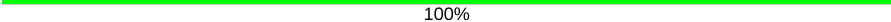

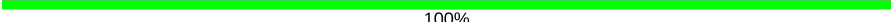
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Mol	Chain	Length	Quality of chain
1	93	27	 93% 7%
1	94	27	 96% .
1	A1	27	 96% .
1	A2	27	 100%
1	A3	27	 100%
1	A4	27	 100%
1	B1	27	 100%
1	B2	27	 89% 11%
1	B3	27	 93% 7%
1	B4	27	 100%
1	C1	27	 100%
1	C2	27	 96% .
1	C3	27	 93% 7%
1	C4	27	 96% .
1	D1	27	 100%
1	D2	27	 93% 7%
1	D3	27	 100%
1	D4	27	 100%
1	E1	27	 100%
1	E2	27	 100%
1	E3	27	 89% 11%
1	E4	27	 100%
1	F1	27	 100%
1	F2	27	 96% .
1	F3	27	 100%





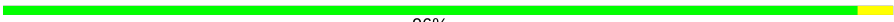




















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Mol	Chain	Length	Quality of chain
1	F4	27	 96% .
1	G1	27	 89% 11%
1	G2	27	 100%
1	G3	27	 96% .
1	G4	27	 96% .
1	H1	27	 100%
1	H2	27	 93% 7%
1	H3	27	 96% .
1	H4	27	 100%
1	I1	27	 100%
1	I2	27	 96% .
1	I3	27	 100%
1	I4	27	 93% 7%
1	J1	27	 96% .
1	J2	27	 93% 7%
1	J3	27	 100%
1	J4	27	 96% .
1	K1	27	 93% 7%
1	K2	27	 100%
1	K3	27	 96% .
1	K4	27	 100%
1	L1	27	 100%
1	L2	27	 100%
1	L3	27	 100%
1	L4	27	 93% 7%


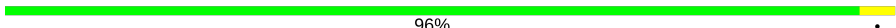
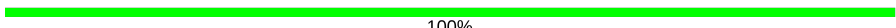












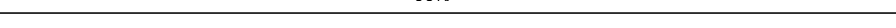
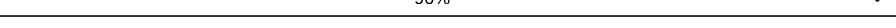
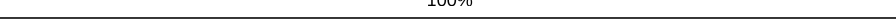
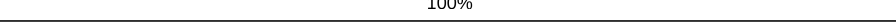
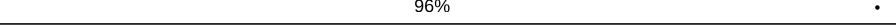
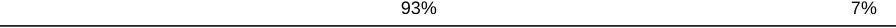
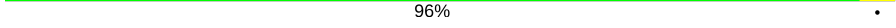
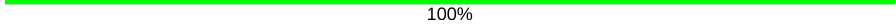
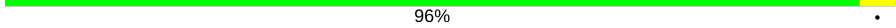
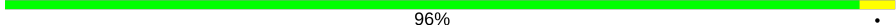
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Mol	Chain	Length	Quality of chain
1	M1	27	 100%
1	M2	27	 100%
1	M3	27	 100%
1	M4	27	 100%
1	N1	27	 96%
1	N2	27	 100%
1	N3	27	 100%
1	N4	27	 100%
1	O1	27	 100%
1	O2	27	 100%
1	O3	27	 100%
1	O4	27	 93% 7%
1	P1	27	 96%
1	P2	27	 100%
1	P3	27	 100%
1	P4	27	 100%
1	Q1	27	 100%
1	Q2	27	 100%
1	Q3	27	 100%
1	Q4	27	 100%
1	R1	27	 100%
1	R2	27	 100%
1	R3	27	 100%
1	R4	27	 85% 15%
1	S1	27	 93% 7%





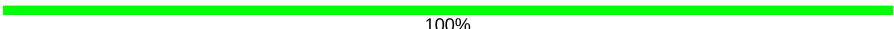

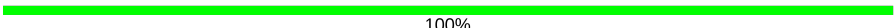
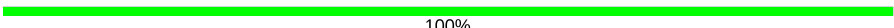
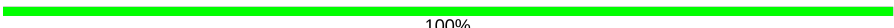
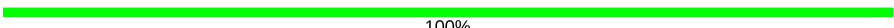


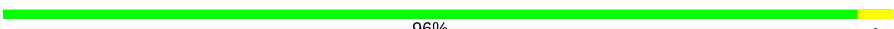




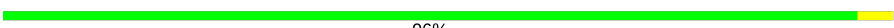
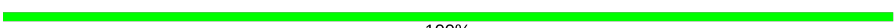
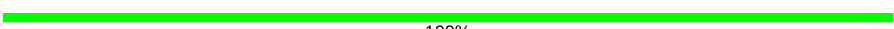
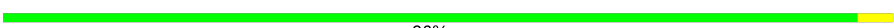

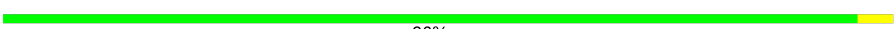


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Mol	Chain	Length	Quality of chain
1	S2	27	 93% 7%
1	S3	27	 96% .
1	S4	27	 100%
1	T1	27	 93% 7%
1	T2	27	 100%
1	T3	27	 100%
1	T4	27	 93% 7%
1	U1	27	 100%
1	U2	27	 100%
1	U3	27	 100%
1	U4	27	 100%
1	V1	27	 100%
1	V2	27	 96% .
1	V3	27	 89% 11%
1	V4	27	 96% .
1	W1	27	 96% .
1	W2	27	 100%
1	W3	27	 100%
1	W4	27	 96% .
1	X1	27	 93% 7%
1	X2	27	 96% .
1	X3	27	 100%
1	X4	27	 96% .
1	Y1	27	 96% .
1	Y2	27	 93% 7%






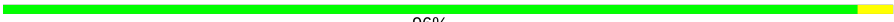
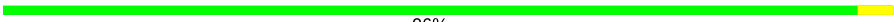


















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Mol	Chain	Length	Quality of chain
1	Y3	27	 93% 7%
1	Y4	27	 85% 15%
1	Z1	27	 100%
1	Z2	27	 100%
1	Z3	27	 100%
1	Z4	27	 96% .
1	a1	27	 100%
1	a2	27	 100%
1	a3	27	 100%
1	a4	27	 100%
1	b1	27	 93% 7%
1	b2	27	 96% .
1	b3	27	 96% .
1	b4	27	 93% 7%
1	c1	27	 93% 7%
1	c2	27	 100%
1	c3	27	 93% 7%
1	c4	27	 96% .
1	d1	27	 100%
1	d2	27	 100%
1	d3	27	 96% .
1	d4	27	 100%
1	e1	27	 96% .
1	e2	27	 100%
1	e3	27	 100%

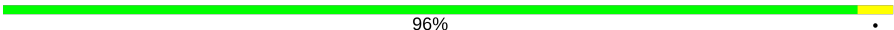
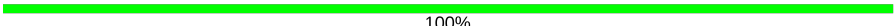



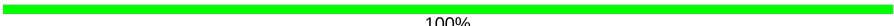
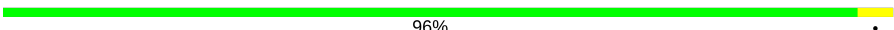
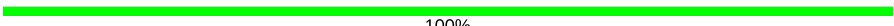


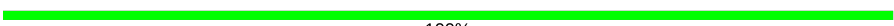
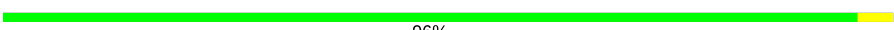




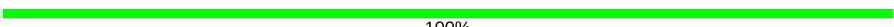




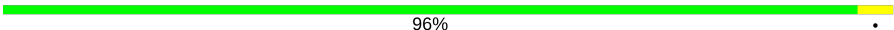

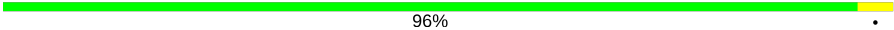

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Mol	Chain	Length	Quality of chain
1	e4	27	 100%
1	f1	27	 100%
1	f2	27	 100%
1	f3	27	 100%
1	f4	27	 93% 7%
1	g1	27	 96% .
1	g2	27	 96% .
1	g3	27	 100%
1	g4	27	 93% 7%
1	h1	27	 93% 7%
1	h2	27	 100%
1	h3	27	 100%
1	h4	27	 96% .
1	i1	27	 100%
1	i2	27	 100%
1	i3	27	 100%
1	i4	27	 89% 11%
1	j1	27	 100%
1	j2	27	 89% 11%
1	j3	27	 96% .
1	j4	27	 96% .
1	k1	27	 96% .
1	k2	27	 93% 7%
1	k3	27	 93% 7%
1	k4	27	 89% 11%
















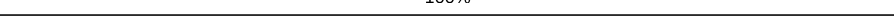
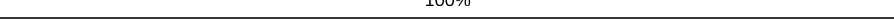

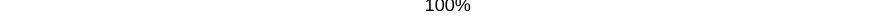
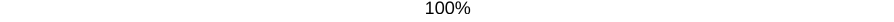
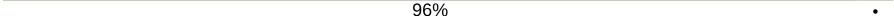
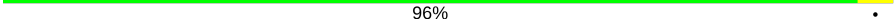
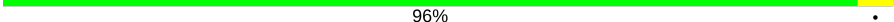
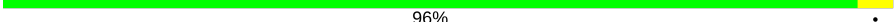

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Mol	Chain	Length	Quality of chain
1	l1	27	 96% .
1	l2	27	 100%
1	l3	27	 100%
1	l4	27	 93% 7%
1	m1	27	 93% 7%
1	m2	27	 100%
1	m3	27	 96% .
1	m4	27	 100%
1	n1	27	 93% 7%
1	n2	27	 100%
1	n3	27	 100%
1	n4	27	 96% .
1	o1	27	 93% 7%
1	o2	27	 100%
1	o3	27	 96% .
1	o4	27	 93% 7%
1	p1	27	 100%
1	p2	27	 93% 7%
1	p3	27	 93% 7%
1	p4	27	 96% .
1	q1	27	 93% 7%
1	q2	27	 96% .
1	q3	27	 93% 7%
1	q4	27	 96% .
1	r1	27	 93% 7%

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Mol	Chain	Length	Quality of chain
1	r2	27	 100%
1	r3	27	 89% 11%
1	r4	27	 96% .
1	s1	27	 96% .
1	s2	27	 100%
1	s3	27	 93% 7%
1	s4	27	 100%
1	t1	27	 100%
1	t2	27	 96% .
1	t3	27	 100%
1	t4	27	 96% .
1	u1	27	 100%
1	u2	27	 100%
1	u3	27	 96% .
1	u4	27	 100%
1	v1	27	 100%
1	v2	27	 93% 7%
1	v3	27	 100%
1	v4	27	 100%
1	w1	27	 96% .
1	w2	27	 96% .
1	w3	27	 96% .
1	w4	27	 96% .
1	x1	27	 96% .
1	x2	27	 96% .

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Mol	Chain	Length	Quality of chain
1	x3	27	<div><div></div><div>93%</div><div>7%</div></div>
1	x4	27	<div><div></div><div>96%</div><div></div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 50163 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 Cross-alpha Amyloid-like Structure alphaAmS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	A2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	A3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	A4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	B1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	B2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	B3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	B4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	C1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	C2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	C3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	C4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	D1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	D2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	D3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	D4	27	Total	C	N	O	0	0	1
			209	137	36	36			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	E1	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	E2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	E3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	E4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	F1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	F2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	F3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	F4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	G1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	G2	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	G3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	G4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	H1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	H2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	H3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	H4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	I1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	I2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	I3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	I4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	J1	27	Total	C	N	O	0	0	1
			209	137	36	36			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	J2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	J3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	J4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	K1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	K2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	K3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	K4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	L1	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	L2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	L3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	L4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	M1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	M2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	M3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	M4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	N1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	N2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	N3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	N4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	O1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	O2	27	Total	C	N	O	0	0	1
			209	137	36	36			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	O3	27	Total 209	C 137	N 36	O 36	0	0	1
1	O4	27	Total 209	C 137	N 36	O 36	0	0	1
1	P1	27	Total 209	C 137	N 36	O 36	0	0	1
1	P2	27	Total 209	C 137	N 36	O 36	0	0	1
1	P3	27	Total 209	C 137	N 36	O 36	0	0	1
1	P4	27	Total 209	C 137	N 36	O 36	0	0	1
1	Q1	27	Total 209	C 137	N 36	O 36	0	0	1
1	Q2	27	Total 209	C 137	N 36	O 36	0	0	1
1	Q3	27	Total 209	C 137	N 36	O 36	0	0	1
1	Q4	27	Total 209	C 137	N 36	O 36	0	0	1
1	R1	27	Total 209	C 137	N 36	O 36	0	0	1
1	R2	27	Total 209	C 137	N 36	O 36	0	0	1
1	R3	27	Total 209	C 137	N 36	O 36	0	0	1
1	R4	27	Total 209	C 137	N 36	O 36	0	0	1
1	S1	27	Total 209	C 137	N 36	O 36	0	0	1
1	S2	27	Total 209	C 137	N 36	O 36	0	0	1
1	S3	27	Total 217	C 142	N 39	O 36	0	1	1
1	S4	27	Total 209	C 137	N 36	O 36	0	0	1
1	T1	27	Total 209	C 137	N 36	O 36	0	0	1
1	T2	27	Total 209	C 137	N 36	O 36	0	0	1
1	T3	27	Total 209	C 137	N 36	O 36	0	0	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	T4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	U1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	U2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	U3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	U4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	V1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	V2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	V3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	V4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	W1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	W2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	W3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	W4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	X1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	X2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	X3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	X4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	Y1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	Y2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	Y3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	Y4	27	Total	C	N	O	0	0	1
			209	137	36	36			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Z1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	Z2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	Z3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	Z4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	11	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	12	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	13	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	14	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	21	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	22	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	23	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	24	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	31	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	32	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	33	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	34	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	41	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	42	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	43	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	44	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	51	27	Total	C	N	O	0	0	1
			209	137	36	36			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	52	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	53	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	54	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	61	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	62	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	63	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	64	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	71	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	72	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	73	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	74	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	81	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	82	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	83	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	84	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	91	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	92	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	93	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	94	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	a1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	a2	27	Total	C	N	O	0	0	1
			209	137	36	36			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	a3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	a4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	b1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	b2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	b3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	b4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	c1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	c2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	c3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	c4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	d1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	d2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	d3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	d4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	e1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	e2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	e3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	e4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	f1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	f2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	f3	27	Total	C	N	O	0	0	1
			209	137	36	36			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	f4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	g1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	g2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	g3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	g4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	h1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	h2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	h3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	h4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	i1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	i2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	i3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	i4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	j1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	j2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	j3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	j4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	k1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	k2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	k3	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	k4	27	Total	C	N	O	0	0	1
			209	137	36	36			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	l1	27	Total 209	C 137	N 36	O 36	0	0	1
1	l2	27	Total 209	C 137	N 36	O 36	0	0	1
1	l3	27	Total 209	C 137	N 36	O 36	0	0	1
1	l4	27	Total 209	C 137	N 36	O 36	0	0	1
1	m1	27	Total 209	C 137	N 36	O 36	0	0	1
1	m2	27	Total 209	C 137	N 36	O 36	0	0	1
1	m3	27	Total 209	C 137	N 36	O 36	0	0	1
1	m4	27	Total 209	C 137	N 36	O 36	0	0	1
1	n1	27	Total 209	C 137	N 36	O 36	0	0	1
1	n2	27	Total 209	C 137	N 36	O 36	0	0	1
1	n3	27	Total 209	C 137	N 36	O 36	0	0	1
1	n4	27	Total 205	C 134	N 35	O 36	0	0	1
1	o1	27	Total 209	C 137	N 36	O 36	0	0	1
1	o2	27	Total 209	C 137	N 36	O 36	0	0	1
1	o3	27	Total 209	C 137	N 36	O 36	0	0	1
1	o4	27	Total 209	C 137	N 36	O 36	0	0	1
1	p1	27	Total 209	C 137	N 36	O 36	0	0	1
1	p2	27	Total 209	C 137	N 36	O 36	0	0	1
1	p3	27	Total 205	C 134	N 35	O 36	0	0	1
1	p4	27	Total 209	C 137	N 36	O 36	0	0	1
1	q1	27	Total 209	C 137	N 36	O 36	0	0	1

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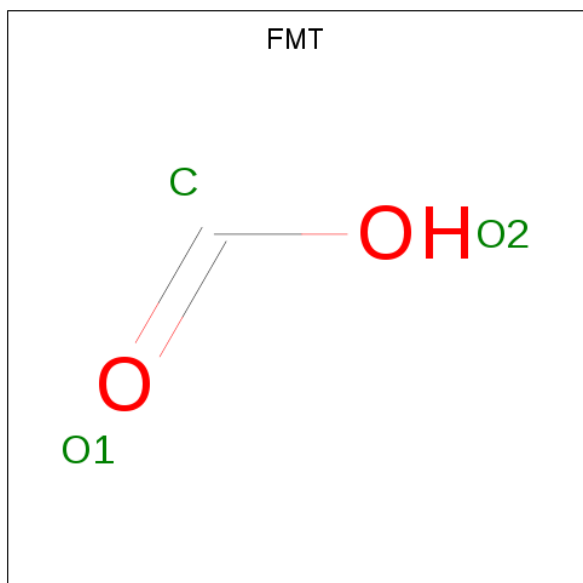
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	q2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	q3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	q4	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	r1	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	r2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	r3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	r4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	s1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	s2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	s3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	s4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	t1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	t2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	t3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	t4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	u1	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	u2	27	Total	C	N	O	0	1	1
			220	143	40	37			
1	u3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	u4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	v1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	v2	27	Total	C	N	O	0	0	1
			209	137	36	36			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	v3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	v4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	w1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	w2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	w3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	w4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	x1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	x2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	x3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	x4	27	Total	C	N	O	0	0	1
			209	137	36	36			

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A1	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A1	1	Total	C	O	0	0
			3	1	2		
2	A3	1	Total	C	O	0	0
			3	1	2		
2	A4	1	Total	C	O	0	0
			3	1	2		
2	B3	1	Total	C	O	0	0
			3	1	2		
2	B4	1	Total	C	O	0	0
			3	1	2		
2	C2	1	Total	C	O	0	0
			3	1	2		
2	D1	1	Total	C	O	0	0
			3	1	2		
2	D2	1	Total	C	O	0	0
			3	1	2		
2	E1	1	Total	C	O	0	0
			3	1	2		
2	E3	1	Total	C	O	0	0
			3	1	2		
2	E4	1	Total	C	O	0	0
			3	1	2		
2	F3	1	Total	C	O	0	0
			3	1	2		
2	F4	1	Total	C	O	0	0
			3	1	2		
2	G2	1	Total	C	O	0	0
			3	1	2		
2	G3	1	Total	C	O	0	0
			3	1	2		
2	H1	1	Total	C	O	0	0
			3	1	2		
2	H2	1	Total	C	O	0	0
			3	1	2		
2	H3	1	Total	C	O	0	0
			3	1	2		
2	I3	1	Total	C	O	0	0
			3	1	2		
2	I4	1	Total	C	O	0	0
			3	1	2		
2	J2	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K2	1	Total 3	C 1	O 2	0	0
2	L2	1	Total 3	C 1	O 2	0	0
2	L3	1	Total 3	C 1	O 2	0	0
2	L4	1	Total 3	C 1	O 2	0	0
2	M2	1	Total 3	C 1	O 2	0	0
2	N1	1	Total 3	C 1	O 2	0	0
2	O1	1	Total 3	C 1	O 2	0	0
2	O2	1	Total 3	C 1	O 2	0	0
2	O3	1	Total 3	C 1	O 2	0	0
2	P2	1	Total 3	C 1	O 2	0	0
2	P3	1	Total 3	C 1	O 2	0	0
2	Q2	1	Total 3	C 1	O 2	0	0
2	Q3	1	Total 3	C 1	O 2	0	0
2	R4	1	Total 3	C 1	O 2	0	0
2	S1	1	Total 3	C 1	O 2	0	0
2	S2	1	Total 3	C 1	O 2	0	0
2	T2	1	Total 3	C 1	O 2	0	0
2	T3	1	Total 3	C 1	O 2	0	0
2	U1	1	Total 3	C 1	O 2	0	0
2	U2	1	Total 3	C 1	O 2	0	0
2	W4	1	Total 3	C 1	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	X4	1	Total 3	C 1	O 2	0	0
2	Y4	1	Total 3	C 1	O 2	0	0
2	Z1	1	Total 3	C 1	O 2	0	0
2	Z3	1	Total 3	C 1	O 2	0	0
2	Z4	1	Total 3	C 1	O 2	0	0
2	13	1	Total 3	C 1	O 2	0	0
2	14	1	Total 3	C 1	O 2	0	0
2	24	1	Total 3	C 1	O 2	0	0
2	32	1	Total 3	C 1	O 2	0	0
2	42	1	Total 3	C 1	O 2	0	0
2	43	1	Total 3	C 1	O 2	0	0
2	44	1	Total 3	C 1	O 2	0	0
2	62	1	Total 3	C 1	O 2	0	0
2	72	1	Total 3	C 1	O 2	0	0
2	81	1	Total 3	C 1	O 2	0	0
2	82	1	Total 3	C 1	O 2	0	0
2	83	1	Total 3	C 1	O 2	0	0
2	92	1	Total 3	C 1	O 2	0	0
2	93	1	Total 3	C 1	O 2	0	0
2	a4	1	Total 3	C 1	O 2	0	0
2	b1	1	Total 3	C 1	O 2	0	0

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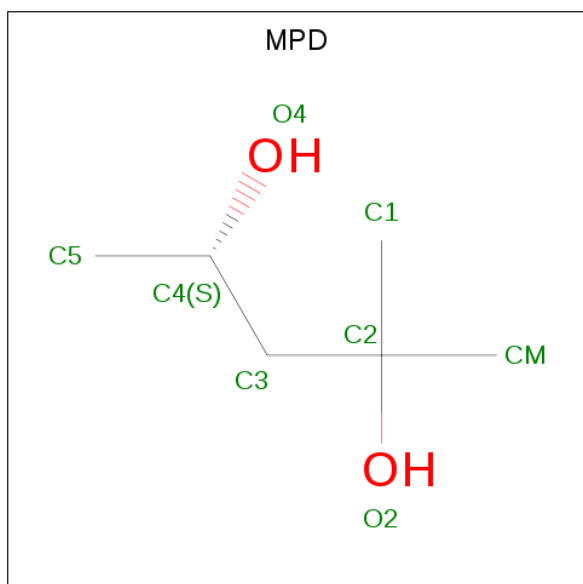
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	b4	1	Total 3	C 1	O 2	0	0
2	c4	1	Total 3	C 1	O 2	0	0
2	d1	1	Total 3	C 1	O 2	0	0
2	d2	1	Total 3	C 1	O 2	0	0
2	e1	1	Total 3	C 1	O 2	0	0
2	e4	1	Total 3	C 1	O 2	0	0
2	e4	1	Total 3	C 1	O 2	0	0
2	f4	1	Total 3	C 1	O 2	0	0
2	g1	1	Total 3	C 1	O 2	0	0
2	g4	1	Total 3	C 1	O 2	0	0
2	h2	1	Total 3	C 1	O 2	0	0
2	i1	1	Total 3	C 1	O 2	0	0
2	i2	1	Total 3	C 1	O 2	0	0
2	j1	1	Total 3	C 1	O 2	0	0
2	j3	1	Total 3	C 1	O 2	0	0
2	k4	1	Total 3	C 1	O 2	0	0
2	m2	1	Total 3	C 1	O 2	0	0
2	m3	1	Total 3	C 1	O 2	0	0
2	m4	1	Total 3	C 1	O 2	0	0
2	n2	1	Total 3	C 1	O 2	0	0
2	o4	1	Total 3	C 1	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	q1	1	Total	C	O	0	0
			3	1	2		
2	r2	1	Total	C	O	0	0
			3	1	2		
2	r3	1	Total	C	O	0	0
			3	1	2		
2	s2	1	Total	C	O	0	0
			3	1	2		
2	t1	1	Total	C	O	0	0
			3	1	2		
2	t3	1	Total	C	O	0	0
			3	1	2		
2	u2	1	Total	C	O	0	0
			3	1	2		
2	u3	1	Total	C	O	0	0
			3	1	2		
2	v3	1	Total	C	O	0	0
			3	1	2		
2	w4	1	Total	C	O	0	0
			3	1	2		
2	x1	1	Total	C	O	0	0
			3	1	2		
2	x4	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G2	1	Total	C	O	0	0
			8	6	2		
3	R3	1	Total	C	O	0	0
			8	6	2		
3	W2	1	Total	C	O	0	0
			8	6	2		
3	X3	1	Total	C	O	0	0
			8	6	2		
3	74	1	Total	C	O	0	0
			8	6	2		
3	q3	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A1	4	Total	O	0	0
			4	4		
4	A2	6	Total	O	0	0
			6	6		
4	A3	2	Total	O	0	0
			2	2		
4	A4	3	Total	O	0	0
			3	3		
4	B1	1	Total	O	0	0
			1	1		
4	B2	1	Total	O	0	0
			1	1		
4	B3	3	Total	O	0	0
			3	3		
4	B4	2	Total	O	0	0
			2	2		
4	C2	1	Total	O	0	0
			1	1		
4	C4	2	Total	O	0	0
			2	2		
4	D1	1	Total	O	0	0
			1	1		
4	D2	1	Total	O	0	0
			1	1		
4	D3	3	Total	O	0	0
			3	3		
4	D4	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E1	3	Total 3	O 3	0	0
4	E2	1	Total 1	O 1	0	0
4	E3	3	Total 3	O 3	0	0
4	E4	3	Total 3	O 3	0	0
4	F1	2	Total 2	O 2	0	0
4	F2	5	Total 5	O 5	0	0
4	F3	2	Total 2	O 2	0	0
4	F4	2	Total 2	O 2	0	0
4	G1	1	Total 1	O 1	0	0
4	G2	3	Total 3	O 3	0	0
4	G3	2	Total 2	O 2	0	0
4	G4	2	Total 2	O 2	0	0
4	H2	4	Total 4	O 4	0	0
4	H3	4	Total 4	O 4	0	0
4	H4	2	Total 2	O 2	0	0
4	I1	1	Total 1	O 1	0	0
4	I2	2	Total 2	O 2	0	0
4	I3	4	Total 4	O 4	0	0
4	I4	3	Total 3	O 3	0	0
4	J1	6	Total 6	O 6	0	0
4	J2	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J3	3	Total O 3 3	0	0
4	K1	2	Total O 2 2	0	0
4	K2	3	Total O 3 3	0	0
4	K3	2	Total O 2 2	0	0
4	K4	4	Total O 4 4	0	0
4	L1	2	Total O 2 2	0	0
4	L2	1	Total O 1 1	0	0
4	L3	3	Total O 3 3	0	0
4	M2	1	Total O 1 1	0	0
4	M3	2	Total O 2 2	0	0
4	M4	3	Total O 3 3	0	0
4	N1	1	Total O 1 1	0	0
4	N2	2	Total O 2 2	0	0
4	N3	3	Total O 3 3	0	0
4	N4	2	Total O 2 2	0	0
4	O1	1	Total O 1 1	0	0
4	O2	1	Total O 1 1	0	0
4	O3	2	Total O 2 2	0	0
4	O4	2	Total O 2 2	0	0
4	P1	1	Total O 1 1	0	0
4	P2	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P3	2	Total O 2 2	0	0
4	P4	3	Total O 3 3	0	0
4	Q1	4	Total O 4 4	0	0
4	Q2	1	Total O 1 1	0	0
4	Q3	1	Total O 1 1	0	0
4	Q4	1	Total O 1 1	0	0
4	R1	1	Total O 1 1	0	0
4	R2	4	Total O 4 4	0	0
4	R3	3	Total O 3 3	0	0
4	S1	2	Total O 2 2	0	0
4	S2	2	Total O 2 2	0	0
4	S3	2	Total O 2 2	0	0
4	S4	3	Total O 3 3	0	0
4	T2	1	Total O 1 1	0	0
4	T4	1	Total O 1 1	0	0
4	U1	2	Total O 2 2	0	0
4	U2	1	Total O 1 1	0	0
4	U4	1	Total O 1 1	0	0
4	V1	1	Total O 1 1	0	0
4	V2	3	Total O 3 3	0	0
4	V3	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	V4	1	Total O 1 1	0	0
4	W1	2	Total O 2 2	0	0
4	W3	1	Total O 1 1	0	0
4	X1	1	Total O 1 1	0	0
4	X2	4	Total O 4 4	0	0
4	X3	3	Total O 3 3	0	0
4	Y1	2	Total O 2 2	0	0
4	Y2	4	Total O 4 4	0	0
4	Y3	2	Total O 2 2	0	0
4	Y4	2	Total O 2 2	0	0
4	Z1	1	Total O 1 1	0	0
4	Z2	1	Total O 1 1	0	0
4	Z3	4	Total O 4 4	0	0
4	Z4	3	Total O 3 3	0	0
4	11	1	Total O 1 1	0	0
4	13	3	Total O 3 3	0	0
4	14	1	Total O 1 1	0	0
4	21	2	Total O 2 2	0	0
4	22	2	Total O 2 2	0	0
4	23	3	Total O 3 3	0	0
4	31	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	32	4	Total O 4 4	0	0
4	33	1	Total O 1 1	0	0
4	34	1	Total O 1 1	0	0
4	41	5	Total O 5 5	0	0
4	42	3	Total O 3 3	0	0
4	43	3	Total O 3 3	0	0
4	44	2	Total O 2 2	0	0
4	51	1	Total O 1 1	0	0
4	52	1	Total O 1 1	0	0
4	53	2	Total O 2 2	0	0
4	54	2	Total O 2 2	0	0
4	61	1	Total O 1 1	0	0
4	62	2	Total O 2 2	0	0
4	63	5	Total O 5 5	0	0
4	64	1	Total O 1 1	0	0
4	71	2	Total O 2 2	0	0
4	72	2	Total O 2 2	0	0
4	73	2	Total O 2 2	0	0
4	74	1	Total O 1 1	0	0
4	81	2	Total O 2 2	0	0
4	82	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	83	1	Total O 1 1	0	0
4	84	1	Total O 1 1	0	0
4	92	3	Total O 3 3	0	0
4	93	3	Total O 3 3	0	0
4	94	3	Total O 3 3	0	0
4	a1	3	Total O 3 3	0	0
4	a2	5	Total O 5 5	0	0
4	a3	3	Total O 3 3	0	0
4	a4	1	Total O 1 1	0	0
4	b1	1	Total O 1 1	0	0
4	b2	1	Total O 1 1	0	0
4	b3	1	Total O 1 1	0	0
4	c2	1	Total O 1 1	0	0
4	c3	2	Total O 2 2	0	0
4	c4	1	Total O 1 1	0	0
4	d1	2	Total O 2 2	0	0
4	d3	2	Total O 2 2	0	0
4	d4	2	Total O 2 2	0	0
4	e1	1	Total O 1 1	0	0
4	e2	2	Total O 2 2	0	0
4	e3	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	e4	3	Total O 3 3	0	0
4	f1	1	Total O 1 1	0	0
4	f2	3	Total O 3 3	0	0
4	f3	2	Total O 2 2	0	0
4	f4	2	Total O 2 2	0	0
4	g1	3	Total O 3 3	0	0
4	g2	1	Total O 1 1	0	0
4	g3	1	Total O 1 1	0	0
4	g4	1	Total O 1 1	0	0
4	h1	2	Total O 2 2	0	0
4	h2	1	Total O 1 1	0	0
4	h3	4	Total O 4 4	0	0
4	h4	1	Total O 1 1	0	0
4	i1	2	Total O 2 2	0	0
4	i2	1	Total O 1 1	0	0
4	i4	2	Total O 2 2	0	0
4	j3	2	Total O 2 2	0	0
4	j4	1	Total O 1 1	0	0
4	k3	1	Total O 1 1	0	0
4	l2	1	Total O 1 1	0	0
4	l3	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	l4	1	Total O 1 1	0	0
4	m1	1	Total O 1 1	0	0
4	m3	1	Total O 1 1	0	0
4	m4	1	Total O 1 1	0	0
4	n2	1	Total O 1 1	0	0
4	n3	1	Total O 1 1	0	0
4	n4	2	Total O 2 2	0	0
4	o1	1	Total O 1 1	0	0
4	o2	1	Total O 1 1	0	0
4	o3	2	Total O 2 2	0	0
4	o4	2	Total O 2 2	0	0
4	p1	1	Total O 1 1	0	0
4	p2	1	Total O 1 1	0	0
4	p4	1	Total O 1 1	0	0
4	q1	2	Total O 2 2	0	0
4	q2	1	Total O 1 1	0	0
4	q3	1	Total O 1 1	0	0
4	q4	2	Total O 2 2	0	0
4	r1	1	Total O 1 1	0	0
4	r2	1	Total O 1 1	0	0
4	r3	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	s1	2	Total O 2 2	0	0
4	s2	2	Total O 2 2	0	0
4	s3	3	Total O 3 3	0	0
4	s4	6	Total O 6 6	0	0
4	t1	2	Total O 2 2	0	0
4	t2	1	Total O 1 1	0	0
4	t3	1	Total O 1 1	0	0
4	t4	1	Total O 1 1	0	0
4	u1	4	Total O 4 4	0	0
4	u3	1	Total O 1 1	0	0
4	u4	1	Total O 1 1	0	0
4	v1	3	Total O 3 3	0	0
4	v2	2	Total O 2 2	0	0
4	v3	1	Total O 1 1	0	0
4	w3	3	Total O 3 3	0	0
4	w4	1	Total O 1 1	0	0
4	x1	3	Total O 3 3	0	0
4	x2	1	Total O 1 1	0	0
4	x3	2	Total O 2 2	0	0
4	x4	1	Total O 1 1	0	0

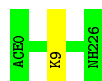
3 Residue-property plots

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain A1:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain A2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain A3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain A4:  100%

There are no outlier residues recorded for this chain.

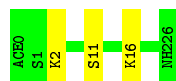
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain B1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain B2:  89% 11%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain B3:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain B4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain C1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain C2:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain C3:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain C4:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain D1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain D2:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain D3: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain D4: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain E1: 100%

There are no outlier residues recorded for this chain.

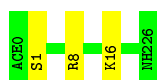
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain E2: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain E3: 89% 11%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain E4: 100%

There are no outlier residues recorded for this chain.

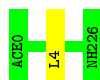
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain F1: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain F2: 96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain F3:  100%

There are no outlier residues recorded for this chain.

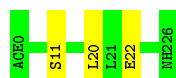
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain F4:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain G1:  89% 11%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain G2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain G3:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain G4:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain H1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain H2:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain H3: 96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain H4: 100%

There are no outlier residues recorded for this chain.

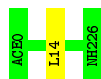
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain I1: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain I2: 96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain I3: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain I4: 93% 7%



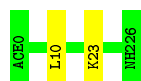
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain J1: 96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain J2:  93% 7%



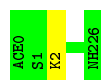
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain J3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain J4:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain K1:  93% 7%



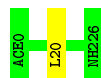
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain K2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain K3:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain K4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain L1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain L2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain L3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain L4:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain M1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain M2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain M3:  100%

There are no outlier residues recorded for this chain.

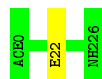
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain M4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain N1:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain N2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain N3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain N4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain O1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain O2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain O3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain O4:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain P1:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain P2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain P3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain P4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Q1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Q2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Q3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Q4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain R1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain R2:  100%


There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain R3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain R4:  85% 15%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain S1:  93% 7%



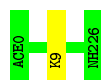
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain S2:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain S3:  96% .



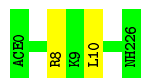
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain S4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain T1:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain T2:  100%

There are no outlier residues recorded for this chain.

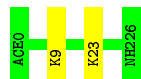
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain T3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain T4:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain U1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain U2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain U3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain U4:  100%

There are no outlier residues recorded for this chain.

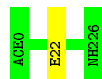
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain V1:  100%

There are no outlier residues recorded for this chain.

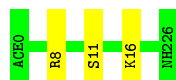
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain V2:  96%



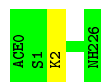
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain V3:  89% 11%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain V4:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain W1:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain W2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain W3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain W4:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain X1:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain X2:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain X3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain X4:  96%



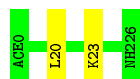
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Y1:  96%



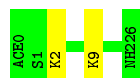
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Y2:  93% 7%




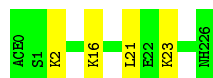
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Y3:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Y4:  85% 15%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Z1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Z2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Z3:  100%

There are no outlier residues recorded for this chain.

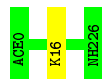
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Z4:  96%



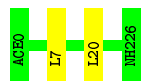
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 11:  96%



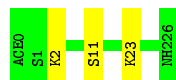
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 12:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 13:  89% 11%



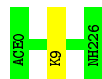
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 14:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 21:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 22:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 23:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 24:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 31:  96% .




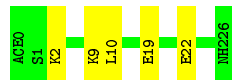
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 32:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 33:  81% 19%



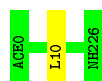
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 34:  100%

There are no outlier residues recorded for this chain.

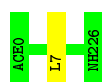
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 41:  96% .



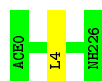
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 42:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 43:  96% .



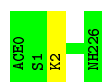
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 44:  100%

There are no outlier residues recorded for this chain.

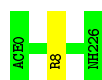
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 51:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 52:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 53:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 54:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 61:  100%

There are no outlier residues recorded for this chain.

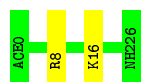
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 62:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 63:  93% 7%



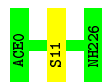
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 64:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 71:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 72:  96% .



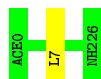
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 73:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 74:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 81:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 82:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 83:  100%

There are no outlier residues recorded for this chain.

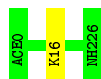
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 84:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 91:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 92:  96%



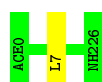
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 93:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 94:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain a1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain a2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain a3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain a4:  100%

There are no outlier residues recorded for this chain.

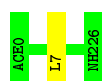
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain b1:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain b2:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain b3:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain b4:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain c1:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain c2:  100%

There are no outlier residues recorded for this chain.

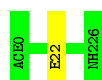
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain c3:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain c4:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain d1:  100%

There are no outlier residues recorded for this chain.

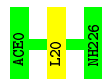
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain d2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain d3:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain d4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain e1:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain e2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain e3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain e4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain f1:  100%


There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain f2:  100%

There are no outlier residues recorded for this chain.

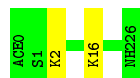
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain f3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain f4:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain g1:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain g2:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain g3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain g4:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain h1:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain h2:  100%

There are no outlier residues recorded for this chain.

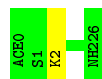
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain h3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain h4:  96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain i1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain i2:  100%


There are no outlier residues recorded for this chain.

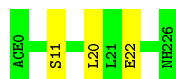
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain i3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain i4:  89% 11%




- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain j1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain j2:  89% 11%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain j3: 96%



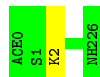
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain j4: 96%



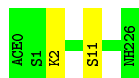
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain k1: 96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain k2: 93% 7%



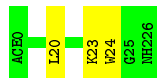
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain k3: 93% 7%



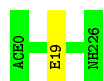
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain k4: 89% 11%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain l1:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain l2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain l3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain l4:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain m1:  93% 7%



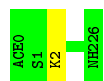
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain m2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain m3:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain m4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain n1:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain n2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain n3:  100%

There are no outlier residues recorded for this chain.

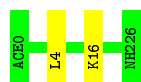
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain n4:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain o1:  93% 7%



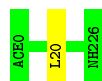
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain o2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain o3:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain o4:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain p2: 93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain p3: 93% 7%



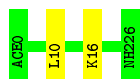
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain p4: 96% .



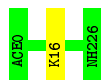
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain q1: 93% 7%



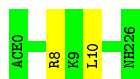
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain q2: 96% .



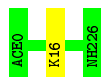
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain q3: 93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain q4: 96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain r1: 93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain r2: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain r3: 89% 11%



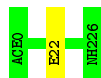
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain r4: 96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain s1: 96%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain s2: 100%

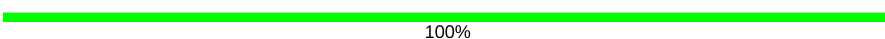
There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain s3:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain s4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain t1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain t2:  96% .



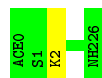
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain t3:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain t4:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain u1:  100%

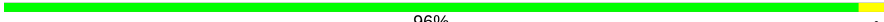
There are no outlier residues recorded for this chain.

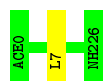
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain u2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain u3:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain u4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain v1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain v2:  93% 7%



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain v3:  100%

There are no outlier residues recorded for this chain.

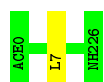
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain v4:  100%

There are no outlier residues recorded for this chain.

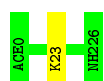
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain w1:  96% .



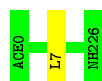
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain w2:  96% .



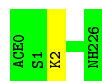
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain w3:  96% .



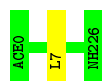
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain w4:  96% .



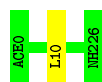
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain x1:  96% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain x2:  96% .



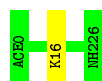
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain x3:  93% 7% .



- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain x4:  96% .



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	161.17Å 160.16Å 198.50Å 90.00° 109.97° 90.00°	Depositor
Resolution (Å)	151.47 – 2.50	Depositor
% Data completeness (in resolution range)	98.5 (151.47-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.52Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.198 , 0.246	Depositor
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.015	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	50163	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6107e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, FMT, ACE, NH2

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	11	0.43	0/208	0.52	0/277
1	12	0.34	0/208	0.48	0/277
1	13	0.31	0/208	0.45	0/277
1	14	0.30	0/208	0.55	0/277
1	21	0.30	0/208	0.45	0/277
1	22	0.31	0/208	0.53	0/277
1	23	0.29	0/208	0.49	0/277
1	24	0.32	0/208	0.48	0/277
1	31	0.29	0/208	0.52	0/277
1	32	0.32	0/219	0.50	0/291
1	33	0.36	0/208	0.60	0/277
1	34	0.29	0/208	0.45	0/277
1	41	0.32	0/208	0.49	0/277
1	42	0.37	0/208	0.48	0/277
1	43	0.30	0/208	0.51	0/277
1	44	0.39	0/208	0.59	0/277
1	51	0.31	0/208	0.57	0/277
1	52	0.46	0/219	0.61	0/291
1	53	0.33	0/208	0.53	0/277
1	54	0.29	0/208	0.47	0/277
1	61	0.31	0/208	0.52	0/277
1	62	0.28	0/208	0.54	0/277
1	63	0.38	0/208	0.49	0/277
1	64	0.30	0/208	0.43	0/277
1	71	0.32	0/208	0.51	0/277
1	72	0.32	0/208	0.56	0/277
1	73	0.65	0/219	0.77	0/291
1	74	0.30	0/208	0.58	0/277
1	81	0.30	0/208	0.52	0/277
1	82	0.34	0/208	0.44	0/277
1	83	0.31	0/208	0.48	0/277
1	84	0.30	0/208	0.54	0/277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	91	0.34	0/208	0.50	0/277
1	92	0.32	0/208	0.45	0/277
1	93	0.33	0/208	0.50	0/277
1	94	0.31	0/208	0.50	0/277
1	A1	0.59	0/208	0.46	0/277
1	A2	0.37	0/208	0.60	0/277
1	A3	0.34	0/208	0.50	0/277
1	A4	0.35	0/208	0.54	0/277
1	B1	0.36	0/208	0.54	0/277
1	B2	0.45	0/208	0.56	0/277
1	B3	0.30	0/208	0.52	0/277
1	B4	0.44	0/208	0.49	0/277
1	C1	0.30	0/208	0.57	0/277
1	C2	0.31	0/208	0.49	0/277
1	C3	0.27	0/208	0.43	0/277
1	C4	0.29	0/208	0.50	0/277
1	D1	0.30	0/208	0.53	0/277
1	D2	0.30	0/208	0.46	0/277
1	D3	0.41	0/208	0.52	0/277
1	D4	0.32	0/208	0.53	0/277
1	E1	0.41	0/219	0.61	0/291
1	E2	0.31	0/208	0.48	0/277
1	E3	0.41	0/208	0.43	0/277
1	E4	0.30	0/208	0.40	0/277
1	F1	0.35	0/208	0.45	0/277
1	F2	0.34	0/208	0.49	0/277
1	F3	0.37	0/208	0.50	0/277
1	F4	0.34	0/208	0.46	0/277
1	G1	0.31	0/208	0.55	0/277
1	G2	0.35	0/219	0.53	0/291
1	G3	0.32	0/208	0.47	0/277
1	G4	0.32	0/208	0.51	0/277
1	H1	0.27	0/208	0.43	0/277
1	H2	0.48	0/208	0.53	0/277
1	H3	0.39	0/208	0.42	0/277
1	H4	0.36	0/208	0.54	0/277
1	I1	0.40	0/208	0.55	0/277
1	I2	0.50	0/208	0.49	0/277
1	I3	0.44	0/208	0.44	0/277
1	I4	0.31	0/208	0.47	0/277
1	J1	0.36	0/208	0.48	0/277
1	J2	0.45	0/208	0.57	0/277
1	J3	0.38	0/208	0.56	0/277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	J4	0.37	0/208	0.55	0/277
1	K1	0.29	0/208	0.49	0/277
1	K2	0.30	0/208	0.46	0/277
1	K3	0.34	0/208	0.51	0/277
1	K4	0.32	0/208	0.52	0/277
1	L1	0.58	0/219	0.68	0/291
1	L2	0.34	0/208	0.55	0/277
1	L3	0.28	0/208	0.45	0/277
1	L4	0.33	0/208	0.45	0/277
1	M1	0.32	0/208	0.50	0/277
1	M2	0.31	0/208	0.42	0/277
1	M3	0.28	0/208	0.46	0/277
1	M4	0.28	0/208	0.43	0/277
1	N1	0.33	0/208	0.42	0/277
1	N2	0.34	0/208	0.52	0/277
1	N3	0.31	0/208	0.49	0/277
1	N4	0.30	0/208	0.48	0/277
1	O1	0.27	0/208	0.52	0/277
1	O2	0.38	0/208	0.55	0/277
1	O3	0.27	0/208	0.43	0/277
1	O4	0.30	0/208	0.43	0/277
1	P1	0.31	0/208	0.48	0/277
1	P2	0.30	0/208	0.46	0/277
1	P3	0.30	0/208	0.48	0/277
1	P4	0.28	0/208	0.47	0/277
1	Q1	0.33	0/208	0.54	0/277
1	Q2	0.30	0/208	0.48	0/277
1	Q3	0.30	0/208	0.41	0/277
1	Q4	0.32	0/208	0.53	0/277
1	R1	0.31	0/208	0.40	0/277
1	R2	0.32	0/208	0.49	0/277
1	R3	0.32	0/208	0.49	0/277
1	R4	0.41	0/208	0.46	0/277
1	S1	0.31	0/208	0.52	0/277
1	S2	0.29	0/208	0.48	0/277
1	S3	0.33	0/219	0.52	0/291
1	S4	0.29	0/208	0.45	0/277
1	T1	0.30	0/208	0.56	0/277
1	T2	0.31	0/208	0.48	0/277
1	T3	0.35	0/208	0.57	0/277
1	T4	0.33	0/208	0.50	0/277
1	U1	0.28	0/208	0.46	0/277
1	U2	0.31	0/208	0.41	0/277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	U3	0.34	0/208	0.52	0/277
1	U4	0.37	0/208	0.53	0/277
1	V1	0.30	0/208	0.41	0/277
1	V2	0.31	0/208	0.53	0/277
1	V3	0.45	0/208	0.58	0/277
1	V4	0.30	0/208	0.47	0/277
1	W1	0.32	0/208	0.50	0/277
1	W2	0.30	0/208	0.53	0/277
1	W3	0.28	0/208	0.46	0/277
1	W4	0.30	0/208	0.52	0/277
1	X1	0.33	0/208	0.52	0/277
1	X2	0.38	0/208	0.43	0/277
1	X3	0.33	0/208	0.56	0/277
1	X4	0.35	0/208	0.50	0/277
1	Y1	0.33	0/208	0.55	0/277
1	Y2	0.34	0/208	0.44	0/277
1	Y3	0.30	0/208	0.42	0/277
1	Y4	0.32	0/208	0.59	0/277
1	Z1	0.28	0/208	0.44	0/277
1	Z2	0.32	0/208	0.54	0/277
1	Z3	0.48	0/208	0.60	0/277
1	Z4	0.34	0/208	0.54	0/277
1	a1	0.32	0/208	0.45	0/277
1	a2	0.34	0/208	0.48	0/277
1	a3	0.33	0/208	0.52	0/277
1	a4	0.33	0/208	0.49	0/277
1	b1	0.30	0/208	0.52	0/277
1	b2	0.30	0/208	0.48	0/277
1	b3	0.28	0/208	0.49	0/277
1	b4	0.33	0/208	0.48	0/277
1	c1	0.30	0/208	0.48	0/277
1	c2	0.30	0/208	0.50	0/277
1	c3	0.31	0/208	0.43	0/277
1	c4	0.39	0/208	0.43	0/277
1	d1	0.28	0/208	0.47	0/277
1	d2	0.30	0/208	0.42	0/277
1	d3	0.30	0/208	0.47	0/277
1	d4	0.29	0/208	0.42	0/277
1	e1	0.32	0/208	0.54	0/277
1	e2	0.35	0/208	0.42	0/277
1	e3	0.30	0/208	0.41	0/277
1	e4	0.34	0/208	0.47	0/277
1	f1	0.25	0/208	0.38	0/277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	f2	0.33	0/208	0.47	0/277
1	f3	0.31	0/208	0.54	0/277
1	f4	0.28	0/208	0.48	0/277
1	g1	0.30	0/208	0.40	0/277
1	g2	0.29	0/208	0.56	0/277
1	g3	0.31	0/208	0.55	0/277
1	g4	0.26	0/208	0.39	0/277
1	h1	0.29	0/208	0.43	0/277
1	h2	0.31	0/208	0.42	0/277
1	h3	0.29	0/208	0.43	0/277
1	h4	0.31	0/208	0.44	0/277
1	i1	0.31	0/208	0.50	0/277
1	i2	0.32	0/208	0.42	0/277
1	i3	0.31	0/208	0.41	0/277
1	i4	0.32	0/208	0.50	0/277
1	j1	0.27	0/208	0.42	0/277
1	j2	0.34	0/208	0.46	0/277
1	j3	0.30	0/208	0.42	0/277
1	j4	0.38	0/208	0.54	0/277
1	k1	0.29	0/208	0.46	0/277
1	k2	0.30	0/208	0.63	0/277
1	k3	0.29	0/219	0.53	0/291
1	k4	0.30	0/208	0.43	0/277
1	l1	0.27	0/208	0.41	0/277
1	l2	0.30	0/208	0.47	0/277
1	l3	0.27	0/208	0.47	0/277
1	l4	0.28	0/208	0.49	0/277
1	m1	0.28	0/208	0.44	0/277
1	m2	0.27	0/208	0.52	0/277
1	m3	0.27	0/208	0.45	0/277
1	m4	0.27	0/208	0.47	0/277
1	n1	0.27	0/208	0.48	0/277
1	n2	0.28	0/208	0.42	0/277
1	n3	0.27	0/208	0.39	0/277
1	n4	0.27	0/204	0.45	0/273
1	o1	0.37	0/208	0.55	0/277
1	o2	0.33	0/208	0.44	0/277
1	o3	0.29	0/208	0.40	0/277
1	o4	0.26	0/208	0.51	0/277
1	p1	0.32	0/208	0.51	0/277
1	p2	0.29	0/208	0.46	0/277
1	p3	0.30	0/204	0.50	0/273
1	p4	0.26	0/208	0.46	0/277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	q1	0.37	0/208	0.51	0/277
1	q2	0.26	0/208	0.41	0/277
1	q3	0.32	0/208	0.49	0/277
1	q4	0.29	0/219	0.51	0/291
1	r1	0.30	0/219	0.48	0/291
1	r2	0.27	0/208	0.42	0/277
1	r3	0.30	0/208	0.45	0/277
1	r4	0.28	0/208	0.40	0/277
1	s1	0.33	0/208	0.51	0/277
1	s2	0.29	0/208	0.38	0/277
1	s3	0.31	0/208	0.42	0/277
1	s4	0.32	0/208	0.44	0/277
1	t1	0.31	0/208	0.59	0/277
1	t2	0.29	0/208	0.39	0/277
1	t3	0.31	0/208	0.46	0/277
1	t4	0.34	0/208	0.48	0/277
1	u1	0.56	0/219	0.55	0/291
1	u2	0.29	0/219	0.51	0/291
1	u3	0.33	0/208	0.56	0/277
1	u4	0.33	0/208	0.52	0/277
1	v1	0.33	0/208	0.46	0/277
1	v2	0.27	0/208	0.48	0/277
1	v3	0.30	0/208	0.47	0/277
1	v4	0.29	0/208	0.45	0/277
1	w1	0.28	0/208	0.63	0/277
1	w2	0.30	0/208	0.55	0/277
1	w3	0.32	0/208	0.49	0/277
1	w4	0.36	0/208	0.50	0/277
1	x1	0.29	0/208	0.56	0/277
1	x2	0.28	0/208	0.52	0/277
1	x3	0.26	0/208	0.41	0/277
1	x4	0.37	0/208	0.53	0/277
All	All	0.33	0/49212	0.49	0/65532

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	11	25/27 (93%)	25 (100%)	0	0	100	100
1	12	25/27 (93%)	25 (100%)	0	0	100	100
1	13	25/27 (93%)	25 (100%)	0	0	100	100
1	14	25/27 (93%)	25 (100%)	0	0	100	100
1	21	25/27 (93%)	25 (100%)	0	0	100	100
1	22	25/27 (93%)	25 (100%)	0	0	100	100
1	23	25/27 (93%)	25 (100%)	0	0	100	100
1	24	25/27 (93%)	25 (100%)	0	0	100	100
1	31	25/27 (93%)	25 (100%)	0	0	100	100
1	32	26/27 (96%)	25 (96%)	1 (4%)	0	100	100
1	33	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	34	25/27 (93%)	25 (100%)	0	0	100	100
1	41	25/27 (93%)	25 (100%)	0	0	100	100
1	42	25/27 (93%)	25 (100%)	0	0	100	100
1	43	25/27 (93%)	25 (100%)	0	0	100	100
1	44	25/27 (93%)	25 (100%)	0	0	100	100
1	51	25/27 (93%)	25 (100%)	0	0	100	100
1	52	26/27 (96%)	26 (100%)	0	0	100	100
1	53	25/27 (93%)	25 (100%)	0	0	100	100
1	54	25/27 (93%)	25 (100%)	0	0	100	100
1	61	25/27 (93%)	25 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	62	25/27 (93%)	25 (100%)	0	0	100	100
1	63	25/27 (93%)	25 (100%)	0	0	100	100
1	64	25/27 (93%)	25 (100%)	0	0	100	100
1	71	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	72	25/27 (93%)	25 (100%)	0	0	100	100
1	73	26/27 (96%)	26 (100%)	0	0	100	100
1	74	25/27 (93%)	25 (100%)	0	0	100	100
1	81	25/27 (93%)	25 (100%)	0	0	100	100
1	82	25/27 (93%)	25 (100%)	0	0	100	100
1	83	25/27 (93%)	25 (100%)	0	0	100	100
1	84	25/27 (93%)	25 (100%)	0	0	100	100
1	91	25/27 (93%)	25 (100%)	0	0	100	100
1	92	25/27 (93%)	25 (100%)	0	0	100	100
1	93	25/27 (93%)	25 (100%)	0	0	100	100
1	94	25/27 (93%)	25 (100%)	0	0	100	100
1	A1	25/27 (93%)	25 (100%)	0	0	100	100
1	A2	25/27 (93%)	25 (100%)	0	0	100	100
1	A3	25/27 (93%)	25 (100%)	0	0	100	100
1	A4	25/27 (93%)	25 (100%)	0	0	100	100
1	B1	25/27 (93%)	25 (100%)	0	0	100	100
1	B2	25/27 (93%)	25 (100%)	0	0	100	100
1	B3	25/27 (93%)	25 (100%)	0	0	100	100
1	B4	25/27 (93%)	25 (100%)	0	0	100	100
1	C1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	C2	25/27 (93%)	25 (100%)	0	0	100	100
1	C3	25/27 (93%)	25 (100%)	0	0	100	100
1	C4	25/27 (93%)	25 (100%)	0	0	100	100
1	D1	25/27 (93%)	25 (100%)	0	0	100	100
1	D2	25/27 (93%)	25 (100%)	0	0	100	100
1	D3	25/27 (93%)	25 (100%)	0	0	100	100
1	D4	25/27 (93%)	25 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E1	26/27 (96%)	26 (100%)	0	0	100	100
1	E2	25/27 (93%)	25 (100%)	0	0	100	100
1	E3	25/27 (93%)	25 (100%)	0	0	100	100
1	E4	25/27 (93%)	25 (100%)	0	0	100	100
1	F1	25/27 (93%)	25 (100%)	0	0	100	100
1	F2	25/27 (93%)	25 (100%)	0	0	100	100
1	F3	25/27 (93%)	25 (100%)	0	0	100	100
1	F4	25/27 (93%)	25 (100%)	0	0	100	100
1	G1	25/27 (93%)	25 (100%)	0	0	100	100
1	G2	26/27 (96%)	26 (100%)	0	0	100	100
1	G3	25/27 (93%)	25 (100%)	0	0	100	100
1	G4	25/27 (93%)	25 (100%)	0	0	100	100
1	H1	25/27 (93%)	25 (100%)	0	0	100	100
1	H2	25/27 (93%)	25 (100%)	0	0	100	100
1	H3	25/27 (93%)	25 (100%)	0	0	100	100
1	H4	25/27 (93%)	25 (100%)	0	0	100	100
1	I1	25/27 (93%)	25 (100%)	0	0	100	100
1	I2	25/27 (93%)	25 (100%)	0	0	100	100
1	I3	25/27 (93%)	25 (100%)	0	0	100	100
1	I4	25/27 (93%)	25 (100%)	0	0	100	100
1	J1	25/27 (93%)	25 (100%)	0	0	100	100
1	J2	25/27 (93%)	25 (100%)	0	0	100	100
1	J3	25/27 (93%)	25 (100%)	0	0	100	100
1	J4	25/27 (93%)	25 (100%)	0	0	100	100
1	K1	25/27 (93%)	25 (100%)	0	0	100	100
1	K2	25/27 (93%)	25 (100%)	0	0	100	100
1	K3	25/27 (93%)	25 (100%)	0	0	100	100
1	K4	25/27 (93%)	25 (100%)	0	0	100	100
1	L1	26/27 (96%)	26 (100%)	0	0	100	100
1	L2	25/27 (93%)	25 (100%)	0	0	100	100
1	L3	25/27 (93%)	25 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L4	25/27 (93%)	25 (100%)	0	0	100	100
1	M1	25/27 (93%)	25 (100%)	0	0	100	100
1	M2	25/27 (93%)	25 (100%)	0	0	100	100
1	M3	25/27 (93%)	25 (100%)	0	0	100	100
1	M4	25/27 (93%)	25 (100%)	0	0	100	100
1	N1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	N2	25/27 (93%)	25 (100%)	0	0	100	100
1	N3	25/27 (93%)	25 (100%)	0	0	100	100
1	N4	25/27 (93%)	25 (100%)	0	0	100	100
1	O1	25/27 (93%)	25 (100%)	0	0	100	100
1	O2	25/27 (93%)	25 (100%)	0	0	100	100
1	O3	25/27 (93%)	25 (100%)	0	0	100	100
1	O4	25/27 (93%)	25 (100%)	0	0	100	100
1	P1	25/27 (93%)	25 (100%)	0	0	100	100
1	P2	25/27 (93%)	25 (100%)	0	0	100	100
1	P3	25/27 (93%)	25 (100%)	0	0	100	100
1	P4	25/27 (93%)	25 (100%)	0	0	100	100
1	Q1	25/27 (93%)	25 (100%)	0	0	100	100
1	Q2	25/27 (93%)	25 (100%)	0	0	100	100
1	Q3	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	Q4	25/27 (93%)	25 (100%)	0	0	100	100
1	R1	25/27 (93%)	25 (100%)	0	0	100	100
1	R2	25/27 (93%)	25 (100%)	0	0	100	100
1	R3	25/27 (93%)	25 (100%)	0	0	100	100
1	R4	25/27 (93%)	25 (100%)	0	0	100	100
1	S1	25/27 (93%)	25 (100%)	0	0	100	100
1	S2	25/27 (93%)	25 (100%)	0	0	100	100
1	S3	26/27 (96%)	26 (100%)	0	0	100	100
1	S4	25/27 (93%)	25 (100%)	0	0	100	100
1	T1	25/27 (93%)	25 (100%)	0	0	100	100
1	T2	25/27 (93%)	25 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T3	25/27 (93%)	25 (100%)	0	0	100	100
1	T4	25/27 (93%)	25 (100%)	0	0	100	100
1	U1	25/27 (93%)	25 (100%)	0	0	100	100
1	U2	25/27 (93%)	25 (100%)	0	0	100	100
1	U3	25/27 (93%)	25 (100%)	0	0	100	100
1	U4	25/27 (93%)	25 (100%)	0	0	100	100
1	V1	25/27 (93%)	25 (100%)	0	0	100	100
1	V2	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	V3	25/27 (93%)	25 (100%)	0	0	100	100
1	V4	25/27 (93%)	25 (100%)	0	0	100	100
1	W1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	W2	25/27 (93%)	25 (100%)	0	0	100	100
1	W3	25/27 (93%)	25 (100%)	0	0	100	100
1	W4	25/27 (93%)	25 (100%)	0	0	100	100
1	X1	25/27 (93%)	25 (100%)	0	0	100	100
1	X2	25/27 (93%)	25 (100%)	0	0	100	100
1	X3	25/27 (93%)	25 (100%)	0	0	100	100
1	X4	25/27 (93%)	25 (100%)	0	0	100	100
1	Y1	25/27 (93%)	25 (100%)	0	0	100	100
1	Y2	25/27 (93%)	25 (100%)	0	0	100	100
1	Y3	25/27 (93%)	25 (100%)	0	0	100	100
1	Y4	25/27 (93%)	25 (100%)	0	0	100	100
1	Z1	25/27 (93%)	25 (100%)	0	0	100	100
1	Z2	25/27 (93%)	25 (100%)	0	0	100	100
1	Z3	25/27 (93%)	25 (100%)	0	0	100	100
1	Z4	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	a1	25/27 (93%)	25 (100%)	0	0	100	100
1	a2	25/27 (93%)	25 (100%)	0	0	100	100
1	a3	25/27 (93%)	25 (100%)	0	0	100	100
1	a4	25/27 (93%)	25 (100%)	0	0	100	100
1	b1	25/27 (93%)	25 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b2	25/27 (93%)	25 (100%)	0	0	100	100
1	b3	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	b4	25/27 (93%)	25 (100%)	0	0	100	100
1	c1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	c2	25/27 (93%)	25 (100%)	0	0	100	100
1	c3	25/27 (93%)	25 (100%)	0	0	100	100
1	c4	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	d1	25/27 (93%)	25 (100%)	0	0	100	100
1	d2	25/27 (93%)	25 (100%)	0	0	100	100
1	d3	25/27 (93%)	25 (100%)	0	0	100	100
1	d4	25/27 (93%)	25 (100%)	0	0	100	100
1	e1	25/27 (93%)	25 (100%)	0	0	100	100
1	e2	25/27 (93%)	25 (100%)	0	0	100	100
1	e3	25/27 (93%)	25 (100%)	0	0	100	100
1	e4	25/27 (93%)	25 (100%)	0	0	100	100
1	f1	25/27 (93%)	25 (100%)	0	0	100	100
1	f2	25/27 (93%)	25 (100%)	0	0	100	100
1	f3	25/27 (93%)	25 (100%)	0	0	100	100
1	f4	25/27 (93%)	25 (100%)	0	0	100	100
1	g1	25/27 (93%)	25 (100%)	0	0	100	100
1	g2	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	g3	25/27 (93%)	25 (100%)	0	0	100	100
1	g4	25/27 (93%)	25 (100%)	0	0	100	100
1	h1	25/27 (93%)	25 (100%)	0	0	100	100
1	h2	25/27 (93%)	25 (100%)	0	0	100	100
1	h3	25/27 (93%)	25 (100%)	0	0	100	100
1	h4	25/27 (93%)	25 (100%)	0	0	100	100
1	i1	25/27 (93%)	25 (100%)	0	0	100	100
1	i2	25/27 (93%)	25 (100%)	0	0	100	100
1	i3	25/27 (93%)	25 (100%)	0	0	100	100
1	i4	25/27 (93%)	23 (92%)	2 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j1	25/27 (93%)	25 (100%)	0	0	100	100
1	j2	25/27 (93%)	25 (100%)	0	0	100	100
1	j3	25/27 (93%)	25 (100%)	0	0	100	100
1	j4	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	k1	25/27 (93%)	25 (100%)	0	0	100	100
1	k2	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	k3	26/27 (96%)	26 (100%)	0	0	100	100
1	k4	25/27 (93%)	24 (96%)	0	1 (4%)	3	3
1	l1	25/27 (93%)	25 (100%)	0	0	100	100
1	l2	25/27 (93%)	25 (100%)	0	0	100	100
1	l3	25/27 (93%)	25 (100%)	0	0	100	100
1	l4	25/27 (93%)	25 (100%)	0	0	100	100
1	m1	25/27 (93%)	25 (100%)	0	0	100	100
1	m2	25/27 (93%)	25 (100%)	0	0	100	100
1	m3	25/27 (93%)	25 (100%)	0	0	100	100
1	m4	25/27 (93%)	25 (100%)	0	0	100	100
1	n1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	n2	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	n3	25/27 (93%)	25 (100%)	0	0	100	100
1	n4	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	o1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	o2	25/27 (93%)	25 (100%)	0	0	100	100
1	o3	25/27 (93%)	25 (100%)	0	0	100	100
1	o4	25/27 (93%)	25 (100%)	0	0	100	100
1	p1	25/27 (93%)	25 (100%)	0	0	100	100
1	p2	25/27 (93%)	25 (100%)	0	0	100	100
1	p3	25/27 (93%)	25 (100%)	0	0	100	100
1	p4	25/27 (93%)	25 (100%)	0	0	100	100
1	q1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	q2	25/27 (93%)	25 (100%)	0	0	100	100
1	q3	25/27 (93%)	24 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	q4	26/27 (96%)	26 (100%)	0	0	100	100
1	r1	26/27 (96%)	26 (100%)	0	0	100	100
1	r2	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	r3	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
1	r4	25/27 (93%)	25 (100%)	0	0	100	100
1	s1	25/27 (93%)	25 (100%)	0	0	100	100
1	s2	25/27 (93%)	25 (100%)	0	0	100	100
1	s3	25/27 (93%)	25 (100%)	0	0	100	100
1	s4	25/27 (93%)	25 (100%)	0	0	100	100
1	t1	25/27 (93%)	25 (100%)	0	0	100	100
1	t2	25/27 (93%)	25 (100%)	0	0	100	100
1	t3	25/27 (93%)	25 (100%)	0	0	100	100
1	t4	25/27 (93%)	25 (100%)	0	0	100	100
1	u1	26/27 (96%)	26 (100%)	0	0	100	100
1	u2	26/27 (96%)	26 (100%)	0	0	100	100
1	u3	25/27 (93%)	25 (100%)	0	0	100	100
1	u4	25/27 (93%)	25 (100%)	0	0	100	100
1	v1	25/27 (93%)	25 (100%)	0	0	100	100
1	v2	25/27 (93%)	25 (100%)	0	0	100	100
1	v3	25/27 (93%)	25 (100%)	0	0	100	100
1	v4	25/27 (93%)	25 (100%)	0	0	100	100
1	w1	25/27 (93%)	25 (100%)	0	0	100	100
1	w2	25/27 (93%)	25 (100%)	0	0	100	100
1	w3	25/27 (93%)	25 (100%)	0	0	100	100
1	w4	25/27 (93%)	25 (100%)	0	0	100	100
1	x1	25/27 (93%)	25 (100%)	0	0	100	100
1	x2	25/27 (93%)	25 (100%)	0	0	100	100
1	x3	25/27 (93%)	25 (100%)	0	0	100	100
1	x4	25/27 (93%)	25 (100%)	0	0	100	100
All	All	5912/6372 (93%)	5886 (100%)	25 (0%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	k4	24	TRP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	11	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	12	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	13	22/22 (100%)	19 (86%)	3 (14%)	3	7
1	14	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	21	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	22	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	23	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	24	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	31	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	32	23/22 (104%)	21 (91%)	2 (9%)	10	20
1	33	22/22 (100%)	17 (77%)	5 (23%)	1	1
1	34	22/22 (100%)	22 (100%)	0	100	100
1	41	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	42	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	43	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	44	22/22 (100%)	22 (100%)	0	100	100
1	51	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	52	23/22 (104%)	21 (91%)	2 (9%)	10	20
1	53	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	54	22/22 (100%)	22 (100%)	0	100	100
1	61	22/22 (100%)	22 (100%)	0	100	100
1	62	22/22 (100%)	22 (100%)	0	100	100
1	63	22/22 (100%)	20 (91%)	2 (9%)	9	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	64	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	71	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	72	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	73	23/22 (104%)	21 (91%)	2 (9%)	10	20
1	74	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	81	22/22 (100%)	22 (100%)	0	100	100
1	82	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	83	22/22 (100%)	22 (100%)	0	100	100
1	84	22/22 (100%)	22 (100%)	0	100	100
1	91	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	92	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	93	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	94	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	A1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	A2	22/22 (100%)	22 (100%)	0	100	100
1	A3	22/22 (100%)	22 (100%)	0	100	100
1	A4	22/22 (100%)	22 (100%)	0	100	100
1	B1	22/22 (100%)	22 (100%)	0	100	100
1	B2	22/22 (100%)	19 (86%)	3 (14%)	3	7
1	B3	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	B4	22/22 (100%)	22 (100%)	0	100	100
1	C1	22/22 (100%)	22 (100%)	0	100	100
1	C2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	C3	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	C4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	D1	22/22 (100%)	22 (100%)	0	100	100
1	D2	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	D3	22/22 (100%)	22 (100%)	0	100	100
1	D4	22/22 (100%)	22 (100%)	0	100	100
1	E1	23/22 (104%)	23 (100%)	0	100	100
1	E2	22/22 (100%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E3	22/22 (100%)	19 (86%)	3 (14%)	3	7
1	E4	22/22 (100%)	22 (100%)	0	100	100
1	F1	22/22 (100%)	22 (100%)	0	100	100
1	F2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	F3	22/22 (100%)	22 (100%)	0	100	100
1	F4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	G1	22/22 (100%)	19 (86%)	3 (14%)	3	7
1	G2	23/22 (104%)	23 (100%)	0	100	100
1	G3	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	G4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	H1	22/22 (100%)	22 (100%)	0	100	100
1	H2	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	H3	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	H4	22/22 (100%)	22 (100%)	0	100	100
1	I1	22/22 (100%)	22 (100%)	0	100	100
1	I2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	I3	22/22 (100%)	22 (100%)	0	100	100
1	I4	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	J1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	J2	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	J3	22/22 (100%)	22 (100%)	0	100	100
1	J4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	K1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	K2	22/22 (100%)	22 (100%)	0	100	100
1	K3	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	K4	22/22 (100%)	22 (100%)	0	100	100
1	L1	23/22 (104%)	23 (100%)	0	100	100
1	L2	22/22 (100%)	22 (100%)	0	100	100
1	L3	22/22 (100%)	22 (100%)	0	100	100
1	L4	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	M1	22/22 (100%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M2	22/22 (100%)	22 (100%)	0	100	100
1	M3	22/22 (100%)	22 (100%)	0	100	100
1	M4	22/22 (100%)	22 (100%)	0	100	100
1	N1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	N2	22/22 (100%)	22 (100%)	0	100	100
1	N3	22/22 (100%)	22 (100%)	0	100	100
1	N4	22/22 (100%)	22 (100%)	0	100	100
1	O1	22/22 (100%)	22 (100%)	0	100	100
1	O2	22/22 (100%)	22 (100%)	0	100	100
1	O3	22/22 (100%)	22 (100%)	0	100	100
1	O4	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	P1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	P2	22/22 (100%)	22 (100%)	0	100	100
1	P3	22/22 (100%)	22 (100%)	0	100	100
1	P4	22/22 (100%)	22 (100%)	0	100	100
1	Q1	22/22 (100%)	22 (100%)	0	100	100
1	Q2	22/22 (100%)	22 (100%)	0	100	100
1	Q3	22/22 (100%)	22 (100%)	0	100	100
1	Q4	22/22 (100%)	22 (100%)	0	100	100
1	R1	22/22 (100%)	22 (100%)	0	100	100
1	R2	22/22 (100%)	22 (100%)	0	100	100
1	R3	22/22 (100%)	22 (100%)	0	100	100
1	R4	22/22 (100%)	18 (82%)	4 (18%)	1	3
1	S1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	S2	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	S3	23/22 (104%)	22 (96%)	1 (4%)	29	53
1	S4	22/22 (100%)	22 (100%)	0	100	100
1	T1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	T2	22/22 (100%)	22 (100%)	0	100	100
1	T3	22/22 (100%)	22 (100%)	0	100	100
1	T4	22/22 (100%)	20 (91%)	2 (9%)	9	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U1	22/22 (100%)	22 (100%)	0	100	100
1	U2	22/22 (100%)	22 (100%)	0	100	100
1	U3	22/22 (100%)	22 (100%)	0	100	100
1	U4	22/22 (100%)	22 (100%)	0	100	100
1	V1	22/22 (100%)	22 (100%)	0	100	100
1	V2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	V3	22/22 (100%)	19 (86%)	3 (14%)	3	7
1	V4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	W1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	W2	22/22 (100%)	22 (100%)	0	100	100
1	W3	22/22 (100%)	22 (100%)	0	100	100
1	W4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	X1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	X2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	X3	22/22 (100%)	22 (100%)	0	100	100
1	X4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	Y1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	Y2	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	Y3	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	Y4	22/22 (100%)	18 (82%)	4 (18%)	1	3
1	Z1	22/22 (100%)	22 (100%)	0	100	100
1	Z2	22/22 (100%)	22 (100%)	0	100	100
1	Z3	22/22 (100%)	22 (100%)	0	100	100
1	Z4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	a1	22/22 (100%)	22 (100%)	0	100	100
1	a2	22/22 (100%)	22 (100%)	0	100	100
1	a3	22/22 (100%)	22 (100%)	0	100	100
1	a4	22/22 (100%)	22 (100%)	0	100	100
1	b1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	b2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	b3	22/22 (100%)	21 (96%)	1 (4%)	27	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b4	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	c1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	c2	22/22 (100%)	22 (100%)	0	100	100
1	c3	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	c4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	d1	22/22 (100%)	22 (100%)	0	100	100
1	d2	22/22 (100%)	22 (100%)	0	100	100
1	d3	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	d4	22/22 (100%)	22 (100%)	0	100	100
1	e1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	e2	22/22 (100%)	22 (100%)	0	100	100
1	e3	22/22 (100%)	22 (100%)	0	100	100
1	e4	22/22 (100%)	22 (100%)	0	100	100
1	f1	22/22 (100%)	22 (100%)	0	100	100
1	f2	22/22 (100%)	22 (100%)	0	100	100
1	f3	22/22 (100%)	22 (100%)	0	100	100
1	f4	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	g1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	g2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	g3	22/22 (100%)	22 (100%)	0	100	100
1	g4	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	h1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	h2	22/22 (100%)	22 (100%)	0	100	100
1	h3	22/22 (100%)	22 (100%)	0	100	100
1	h4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	i1	22/22 (100%)	22 (100%)	0	100	100
1	i2	22/22 (100%)	22 (100%)	0	100	100
1	i3	22/22 (100%)	22 (100%)	0	100	100
1	i4	22/22 (100%)	19 (86%)	3 (14%)	3	7
1	j1	22/22 (100%)	22 (100%)	0	100	100
1	j2	22/22 (100%)	19 (86%)	3 (14%)	3	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j3	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	j4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	k1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	k2	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	k3	23/22 (104%)	20 (87%)	3 (13%)	4	7
1	k4	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	l1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	l2	22/22 (100%)	22 (100%)	0	100	100
1	l3	22/22 (100%)	22 (100%)	0	100	100
1	l4	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	m1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	m2	22/22 (100%)	22 (100%)	0	100	100
1	m3	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	m4	22/22 (100%)	22 (100%)	0	100	100
1	n1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	n2	22/22 (100%)	22 (100%)	0	100	100
1	n3	22/22 (100%)	22 (100%)	0	100	100
1	n4	21/22 (96%)	20 (95%)	1 (5%)	25	48
1	o1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	o2	22/22 (100%)	22 (100%)	0	100	100
1	o3	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	o4	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	p1	22/22 (100%)	22 (100%)	0	100	100
1	p2	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	p3	21/22 (96%)	19 (90%)	2 (10%)	8	17
1	p4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	q1	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	q2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	q3	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	q4	23/22 (104%)	22 (96%)	1 (4%)	29	53
1	r1	23/22 (104%)	21 (91%)	2 (9%)	10	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	r2	22/22 (100%)	22 (100%)	0	100	100
1	r3	22/22 (100%)	19 (86%)	3 (14%)	3	7
1	r4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	s1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	s2	22/22 (100%)	22 (100%)	0	100	100
1	s3	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	s4	22/22 (100%)	22 (100%)	0	100	100
1	t1	22/22 (100%)	22 (100%)	0	100	100
1	t2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	t3	22/22 (100%)	22 (100%)	0	100	100
1	t4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	u1	23/22 (104%)	23 (100%)	0	100	100
1	u2	23/22 (104%)	23 (100%)	0	100	100
1	u3	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	u4	22/22 (100%)	22 (100%)	0	100	100
1	v1	22/22 (100%)	22 (100%)	0	100	100
1	v2	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	v3	22/22 (100%)	22 (100%)	0	100	100
1	v4	22/22 (100%)	22 (100%)	0	100	100
1	w1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	w2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	w3	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	w4	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	x1	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	x2	22/22 (100%)	21 (96%)	1 (4%)	27	51
1	x3	22/22 (100%)	20 (91%)	2 (9%)	9	18
1	x4	22/22 (100%)	21 (96%)	1 (4%)	27	51
All	All	5202/5192 (100%)	4998 (96%)	204 (4%)	32	57

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	33	10	LEU

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Mol	Chain	Res	Type
1	92	9	LYS
1	s3	3	LEU
1	33	22	GLU
1	63	8	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	M1	15	HIS
1	O1	15	HIS
1	54	15	HIS
1	L2	15	HIS
1	a2	15	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

103 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
2	FMT	U2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	b1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	Z1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	D2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	Z4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	j3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	P2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	I4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	e1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	e4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	d1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	G2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
3	MPD	X3	101	-	7,7,7	0.30	0	9,10,10	0.33	0
2	FMT	l3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	j1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	A1	102	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	b4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	Y4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	C2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	D1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	a4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	A4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	24	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	d2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	93	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	c4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	T2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	S2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	44	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	o4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	Q2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	g1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	R4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	J2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	W4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	42	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	H3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	t1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	O3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	81	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	L2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	x1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	F3	101	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMT	43	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	P3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	m4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	X4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	E1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	E4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	t3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	m3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	B3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	n2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	i2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	L4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	I3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	Z3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	G3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	Q3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	H2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	k4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	A1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	O2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	x4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
3	MPD	W2	101	-	7,7,7	0.26	0	9,10,10	0.22	0
2	FMT	f4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	U1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	i1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	72	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	62	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	E3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	g4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
3	MPD	R3	101	-	7,7,7	0.33	0	9,10,10	0.51	0
2	FMT	H1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	F4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	u3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	s2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	u2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	92	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	e4	102	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	14	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	T3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	w4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	h2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	S1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	L3	101	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMT	A3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	m2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	N1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	82	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	q1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	v3	101	-	0,2,2	0.00	-	0,1,1	0.00	-
3	MPD	74	101	-	7,7,7	0.25	0	9,10,10	0.22	0
2	FMT	M2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	32	101	-	0,2,2	0.00	-	0,1,1	0.00	-
3	MPD	q3	101	-	7,7,7	0.28	0	9,10,10	0.97	0
2	FMT	K2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
3	MPD	G2	102	-	7,7,7	0.32	0	9,10,10	0.52	0
2	FMT	B4	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	O1	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	83	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	r2	101	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	r3	101	-	0,2,2	0.00	-	0,1,1	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	q3	101	-	-	2/5/5/5	-
3	MPD	G2	102	-	-	4/5/5/5	-
3	MPD	74	101	-	-	2/5/5/5	-
3	MPD	R3	101	-	-	4/5/5/5	-
3	MPD	X3	101	-	-	3/5/5/5	-
3	MPD	W2	101	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	W2	101	MPD	C2-C3-C4-O4
3	R3	101	MPD	C2-C3-C4-O4
3	X3	101	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	G2	102	MPD	O2-C2-C3-C4
3	W2	101	MPD	C2-C3-C4-C5

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 ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.