



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:03 AM UTC

PDB ID : 6C50 / pdb_00006c50
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

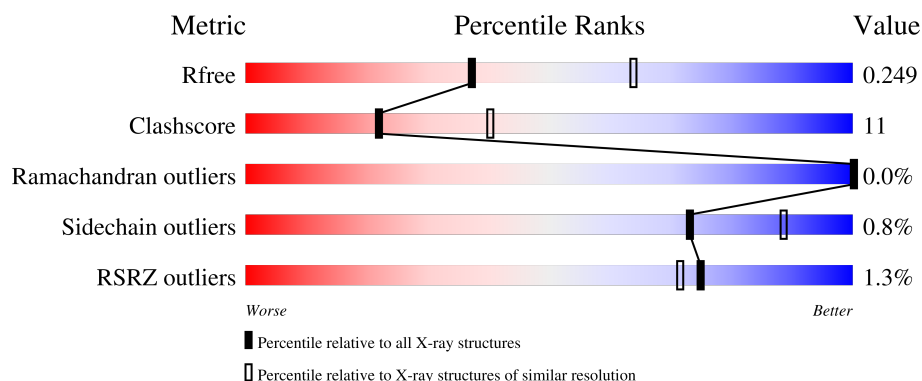
1 Overall quality at a glance

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.



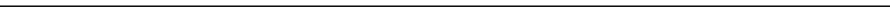
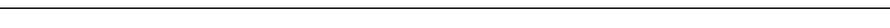
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	11	27	85% 15%
1	12	27	4% 78% 22%
1	13	27	93% 7%
1	14	27	4% 78% 19% .
1	21	27	4% 89% 11%

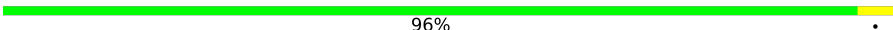
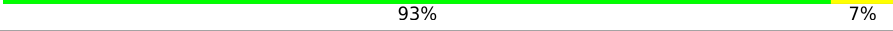
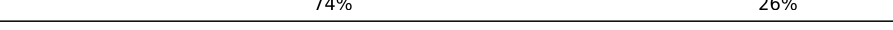
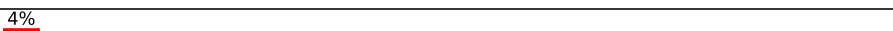
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Mol	Chain	Length	Quality of chain
1	22	27	 85% 15%
1	23	27	 85% 15%
1	24	27	 4% 89% 11%
1	31	27	 4% 67% 33%
1	32	27	 4% 67% 33%
1	33	27	 85% 15%
1	34	27	 78% 22%
1	41	27	 93% 7%
1	42	27	 81% 19%
1	43	27	 81% 15% .
1	44	27	 78% 22%
1	51	27	 4% 78% 22%
1	52	27	 81% 15% .
1	53	27	 85% 15%
1	54	27	 78% 22%
1	61	27	 74% 26%
1	62	27	 81% 19%
1	63	27	 4% 67% 33%
1	64	27	 78% 19% .
1	71	27	 81% 19%
1	72	27	 78% 19% .
1	73	27	 74% 22% .
1	74	27	 74% 26%
1	81	27	 4% 78% 22%
1	82	27	 74% 26%

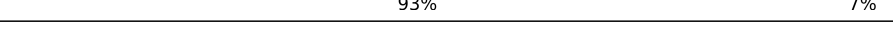
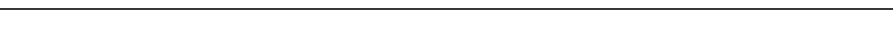
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Mol	Chain	Length	Quality of chain
1	83	27	 96% .
1	84	27	 89% 11%
1	91	27	 70% 30%
1	92	27	 63% 37%
1	93	27	 70% 26% .
1	94	27	 4% 81% 19%
1	A1	27	 85% 11% .
1	A2	27	 93% 7%
1	A3	27	 78% 22%
1	A4	27	 70% 30%
1	B1	27	 70% 30%
1	B2	27	 59% 37% .
1	B3	27	 81% 19%
1	B4	27	 74% 26%
1	C1	27	 67% 33%
1	C2	27	 59% 41%
1	C3	27	 67% 33%
1	C4	27	 78% 22%
1	D1	27	 81% 19%
1	D2	27	 70% 30%
1	D3	27	 89% 11%
1	D4	27	 74% 26%
1	E1	27	 4% 81% 19%
1	E2	27	 81% 19%
1	E3	27	 74% 22% .

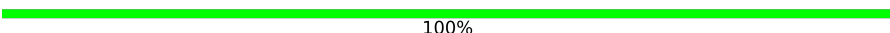
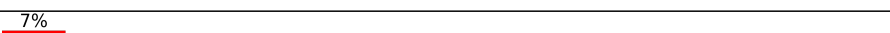
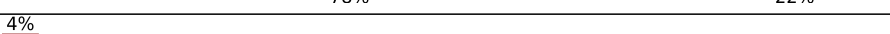
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Mol	Chain	Length	Quality of chain
1	E4	27	 81% 19%
1	F1	27	 85% 15%
1	F2	27	 81% 15% .
1	F3	27	 89% 11%
1	F4	27	 85% 15%
1	G1	27	 4% 70% 30%
1	G2	27	 70% 30%
1	G3	27	 4% 63% 37%
1	G4	27	 67% 33%
1	H1	27	 63% 37%
1	H2	27	 70% 26% .
1	H3	27	 81% 19%
1	H4	27	 63% 37%
1	I1	27	 93% 7%
1	I2	27	 85% 15%
1	I3	27	 89% 11%
1	I4	27	 70% 26% .
1	J1	27	 89% 11%
1	J2	27	 85% 11% .
1	J3	27	 96% .
1	J4	27	 89% 11%
1	K1	27	 4% 96% .
1	K2	27	 96% .
1	K3	27	 81% 19%
1	K4	27	 85% 15%

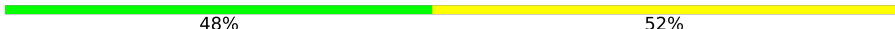
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Mol	Chain	Length	Quality of chain
1	L1	27	 85% 15%
1	L2	27	 85% 15%
1	L3	27	 100%
1	L4	27	 78% 22%
1	M1	27	 4% 89% 11%
1	M2	27	 74% 26%
1	M3	27	 89% 11%
1	M4	27	 78% 22%
1	N1	27	 4% 67% 33%
1	N2	27	 81% 19%
1	N3	27	 78% 22%
1	N4	27	 85% 15%
1	O1	27	 67% 33%
1	O2	27	 78% 22%
1	O3	27	 7% 78% 22%
1	O4	27	 4% 70% 30%
1	P1	27	 70% 30%
1	P2	27	 4% 52% 48%
1	P3	27	 63% 37%
1	P4	27	 74% 26%
1	Q1	27	 89% 11%
1	Q2	27	 78% 22%
1	Q3	27	 85% 15%
1	Q4	27	 70% 30%
1	R1	27	 89% 11%

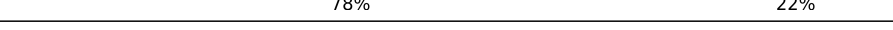
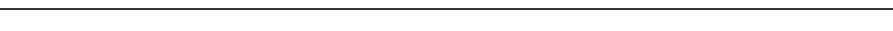
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Mol	Chain	Length	Quality of chain
1	R2	27	
1	R3	27	
1	R4	27	
1	S1	27	
1	S2	27	
1	S3	27	
1	S4	27	
1	T1	27	
1	T2	27	
1	T3	27	
1	T4	27	
1	U1	27	
1	U2	27	
1	U3	27	
1	U4	27	
1	V1	27	
1	V2	27	
1	V3	27	
1	V4	27	
1	W1	27	
1	W2	27	
1	W3	27	
1	W4	27	
1	X1	27	
1	X2	27	

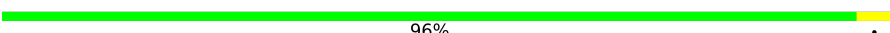
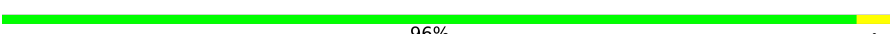
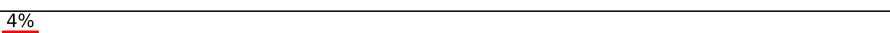
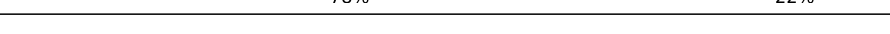
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Mol	Chain	Length	Quality of chain
1	X3	27	 63% 37%
1	X4	27	 81% 19%
1	Y1	27	 67% 33%
1	Y2	27	 89% 11%
1	Y3	27	 81% 19%
1	Y4	27	 81% 19%
1	Z1	27	 89% 11%
1	Z2	27	 4% 81% 19%
1	Z3	27	 4% 85% 15%
1	Z4	27	 81% 19%
1	a1	27	 89% 11%
1	a2	27	 85% 15%
1	a3	27	 89% 11%
1	a4	27	 4% 78% 22%
1	b1	27	 70% 30%
1	b2	27	 78% 22%
1	b3	27	 89% 11%
1	b4	27	 67% 33%
1	c1	27	 81% 19%
1	c2	27	 67% 33%
1	c3	27	 67% 33%
1	c4	27	 7% 85% 15%
1	d1	27	 85% 15%
1	d2	27	 81% 19%
1	d3	27	 78% 22%

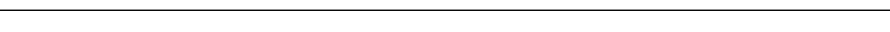
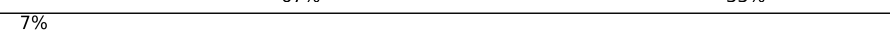
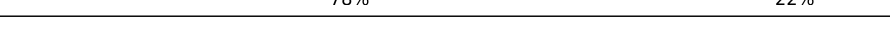
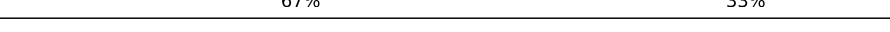
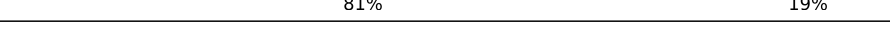
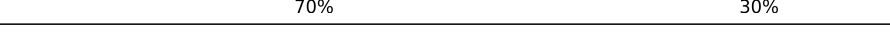
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Mol	Chain	Length	Quality of chain
1	d4	27	 89%11%
1	e1	27	 78%22%
1	e2	27	 89%11%
1	e3	27	 96%.
1	e4	27	 96%.
1	f1	27	 81%19%
1	f2	27	 85%15%
1	f3	27	 78%22%
1	f4	27	 74%26%
1	g1	27	 81%19%
1	g2	27	 81%19%
1	g3	27	 4%74%22%
1	g4	27	 4%78%22%
1	h1	27	 78%22%
1	h2	27	 4%78%22%
1	h3	27	 81%19%
1	h4	27	 81%19%
1	i1	27	 85%15%
1	i2	27	 78%22%
1	i3	27	 85%15%
1	i4	27	 4%81%19%
1	j1	27	 78%22%
1	j2	27	 7%78%22%
1	j3	27	 81%19%
1	j4	27	 7%74%22%.

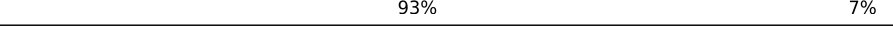
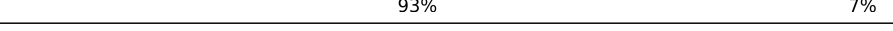
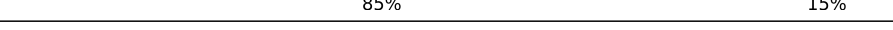
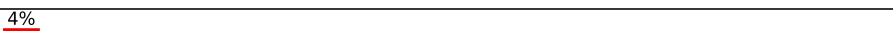
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Mol	Chain	Length	Quality of chain
1	k1	27	 78%22%
1	k2	27	 7%74%26%
1	k3	27	 11%78%22%
1	k4	27	 4%67%30%.
1	l1	27	 4%89%11%
1	l2	27	 4%74%26%
1	l3	27	 4%74%26%
1	l4	27	 74%26%
1	m1	27	 15%70%30%
1	m2	27	 7%74%26%
1	m3	27	 67%33%
1	m4	27	 7%78%22%
1	n1	27	 67%33%
1	n2	27	 81%19%
1	n3	27	 70%30%
1	n4	27	 81%19%
1	o1	27	 7%70%30%
1	o2	27	 78%22%
1	o3	27	 81%19%
1	o4	27	 4%81%19%
1	p1	27	 4%78%22%
1	p2	27	 81%19%
1	p3	27	 15%59%41%
1	p4	27	 70%30%
1	q1	27	 63%33%.

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Mol	Chain	Length	Quality of chain
1	q2	27	 70%30%
1	q3	27	 74%26%
1	q4	27	 74%26%
1	r1	27	 81%19%
1	r2	27	 4%63%37%
1	r3	27	 4%74%26%
1	r4	27	 67%33%
1	s1	27	 4%85%15%
1	s2	27	 70%30%
1	s3	27	 4%85%15%
1	s4	27	 4%85%15%
1	t1	27	 93%7%
1	t2	27	 93%7%
1	t3	27	 85%15%
1	t4	27	 81%19%
1	u1	27	 81%15%4%
1	u2	27	 74%26%
1	u3	27	 67%33%
1	u4	27	 4%70%30%
1	v1	27	 4%78%22%
1	v2	27	 78%22%
1	v3	27	 78%22%
1	v4	27	 4%89%11%
1	w1	27	 78%22%
1	w2	27	 78%22%

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Mol	Chain	Length	Quality of chain
1	w3	27	 4% 78% 22%
1	w4	27	 78% 22%
1	x1	27	 7% 63% 37%
1	x2	27	 74% 26%
1	x3	27	 4% 96%
1	x4	27	 74% 26%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MPD	74	101	-	-	X	-
3	MPD	R3	101	-	-	X	-
3	MPD	W2	101	-	-	X	-

2 Entry composition

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	C	N	O	0	0	1
			209	137	36	36			
1	O4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	P1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	P2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	P3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	P4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	Q1	27	Total	C	N	O	0	0	1
			209	137	36	36			
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	0	1
			209	137	36	36			
1	R1	27	Total	C	N	O	0	0	1
			209	137	36	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	1	1
			217	142	39	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			

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

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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 209	C 137	N 36	O 36	0	0	1
1	a4	27	Total 209	C 137	N 36	O 36	0	0	1
1	b1	27	Total 209	C 137	N 36	O 36	0	0	1
1	b2	27	Total 209	C 137	N 36	O 36	0	0	1
1	b3	27	Total 209	C 137	N 36	O 36	0	0	1
1	b4	27	Total 209	C 137	N 36	O 36	0	0	1
1	c1	27	Total 209	C 137	N 36	O 36	0	0	1
1	c2	27	Total 209	C 137	N 36	O 36	0	0	1
1	c3	27	Total 209	C 137	N 36	O 36	0	0	1
1	c4	27	Total 209	C 137	N 36	O 36	0	0	1
1	d1	27	Total 209	C 137	N 36	O 36	0	0	1
1	d2	27	Total 209	C 137	N 36	O 36	0	0	1
1	d3	27	Total 209	C 137	N 36	O 36	0	0	1
1	d4	27	Total 209	C 137	N 36	O 36	0	0	1
1	e1	27	Total 209	C 137	N 36	O 36	0	0	1
1	e2	27	Total 209	C 137	N 36	O 36	0	0	1
1	e3	27	Total 209	C 137	N 36	O 36	0	0	1
1	e4	27	Total 209	C 137	N 36	O 36	0	0	1
1	f1	27	Total 209	C 137	N 36	O 36	0	0	1
1	f2	27	Total 209	C 137	N 36	O 36	0	0	1
1	f3	27	Total 209	C 137	N 36	O 36	0	0	1

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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	C	N	O	0	0	1
			209	137	36	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
			205	134	35	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			
1	o3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	o4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	p1	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	p2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	p3	27	Total	C	N	O	0	0	1
			205	134	35	36			
1	p4	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	q1	27	Total	C	N	O	0	0	1
			209	137	36	36			

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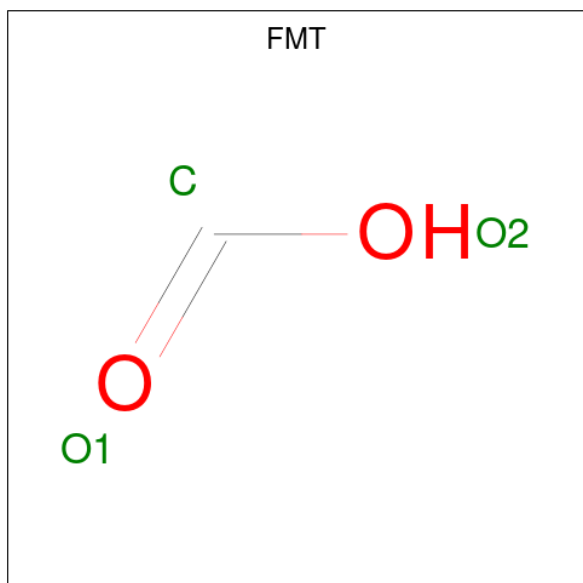
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	q2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	q3	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	q4	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	r1	27	Total	C	N	O	0	1	1
			217	142	39	36			
1	r2	27	Total	C	N	O	0	0	1
			209	137	36	36			
1	r3	27	Total	C	N	O	0	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 (CCD ID: 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	C	O	0	0
			3	1	2		
2	L2	1	Total	C	O	0	0
			3	1	2		
2	L3	1	Total	C	O	0	0
			3	1	2		
2	L4	1	Total	C	O	0	0
			3	1	2		
2	M2	1	Total	C	O	0	0
			3	1	2		
2	N1	1	Total	C	O	0	0
			3	1	2		
2	O1	1	Total	C	O	0	0
			3	1	2		
2	O2	1	Total	C	O	0	0
			3	1	2		
2	O3	1	Total	C	O	0	0
			3	1	2		
2	P2	1	Total	C	O	0	0
			3	1	2		
2	P3	1	Total	C	O	0	0
			3	1	2		
2	Q2	1	Total	C	O	0	0
			3	1	2		
2	Q3	1	Total	C	O	0	0
			3	1	2		
2	R4	1	Total	C	O	0	0
			3	1	2		
2	S1	1	Total	C	O	0	0
			3	1	2		
2	S2	1	Total	C	O	0	0
			3	1	2		
2	T2	1	Total	C	O	0	0
			3	1	2		
2	T3	1	Total	C	O	0	0
			3	1	2		
2	U1	1	Total	C	O	0	0
			3	1	2		
2	U2	1	Total	C	O	0	0
			3	1	2		
2	W4	1	Total	C	O	0	0
			3	1	2		

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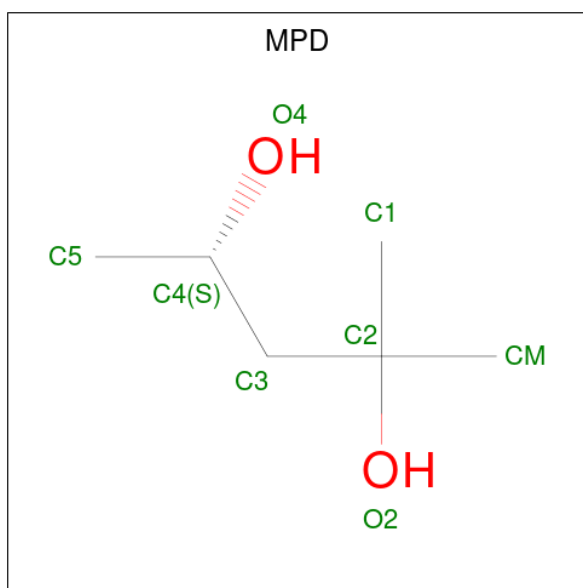
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			3	1	2		
2	c4	1	Total	C	O	0	0
			3	1	2		
2	d1	1	Total	C	O	0	0
			3	1	2		
2	d2	1	Total	C	O	0	0
			3	1	2		
2	e1	1	Total	C	O	0	0
			3	1	2		
2	e4	1	Total	C	O	0	0
			3	1	2		
2	e4	1	Total	C	O	0	0
			3	1	2		
2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

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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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 4 is water.

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E1	3	Total O 3 3	0	0
4	E2	1	Total O 1 1	0	0
4	E3	3	Total O 3 3	0	0
4	E4	3	Total O 3 3	0	0
4	F1	2	Total O 2 2	0	0
4	F2	5	Total O 5 5	0	0
4	F3	2	Total O 2 2	0	0
4	F4	2	Total O 2 2	0	0
4	G1	1	Total O 1 1	0	0
4	G2	3	Total O 3 3	0	0
4	G3	2	Total O 2 2	0	0
4	G4	2	Total O 2 2	0	0
4	H2	4	Total O 4 4	0	0
4	H3	4	Total O 4 4	0	0
4	H4	2	Total O 2 2	0	0
4	I1	1	Total O 1 1	0	0
4	I2	2	Total O 2 2	0	0
4	I3	4	Total O 4 4	0	0
4	I4	3	Total O 3 3	0	0
4	J1	6	Total O 6 6	0	0
4	J2	7	Total O 7 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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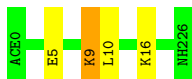
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4	s2	2	Total O 2 2	0	0
4	s3	3	Total O 3 3	0	0
4	s4	6	Total O 6 6	0	0
4	t1	2	Total O 2 2	0	0
4	t2	1	Total O 1 1	0	0
4	t3	1	Total O 1 1	0	0
4	t4	1	Total O 1 1	0	0
4	u1	4	Total O 4 4	0	0
4	u3	1	Total O 1 1	0	0
4	u4	1	Total O 1 1	0	0
4	v1	3	Total O 3 3	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 [i](#)

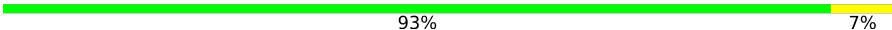
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

Chain A1:  85% 11% .



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

Chain A2:  93% 7%



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

Chain A3:  78% 22%



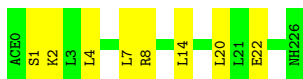
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain A4:  70% 30%



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

Chain B1:  70% 30%



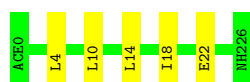
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain B2:  59% 37% .



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

Chain B3:  81% 19%



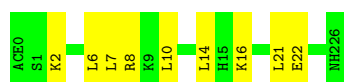
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain B4:  74% 26%



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

Chain C1:  67% 33%



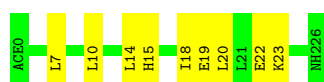
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain C2:  59% 41%



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

Chain C3:  67% 33%



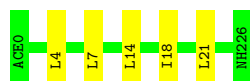
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain C4:  78% 22%



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

Chain D1:  81% 19%



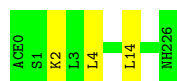
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain D2:  70% 30%



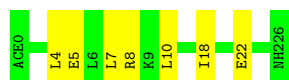
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain D3:  89% 11%



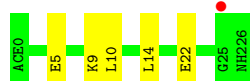
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain D4:  74% 26%



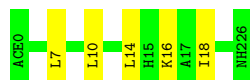
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain E1:  4% 81% 19%



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

Chain E2:  81% 19%



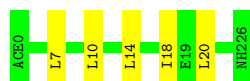
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain E3:  74% 22% •



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

Chain E4:  81% 19%



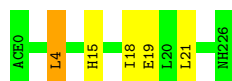
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain F1:  85% 15%



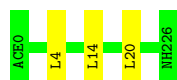
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain F2:  81% 15% .



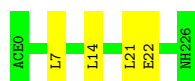
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain F3:  89% 11%



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

Chain F4:  85% 15%



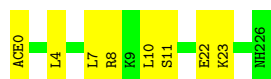
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain G1:  4% 70% 30%



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

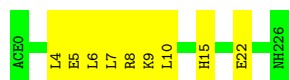
Chain G2:  70% 30%



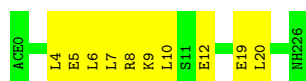
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



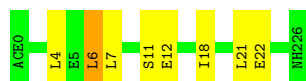
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



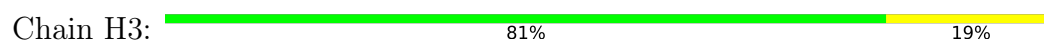
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



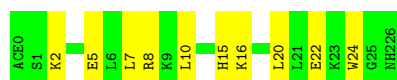
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



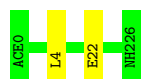
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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

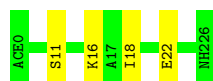


- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



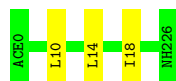
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain I2:  85% 15%



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

Chain I3:  89% 11%



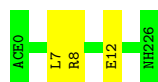
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain I4:  70% 26% .



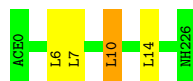
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain J1:  89% 11%



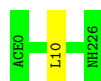
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain J2:  85% 11% .



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

Chain J3:  96% .



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

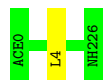
Chain J4:  89% 11%



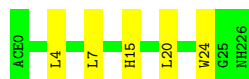
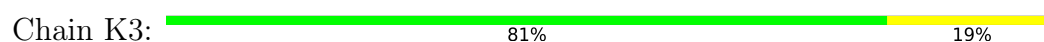
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



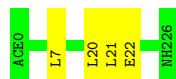
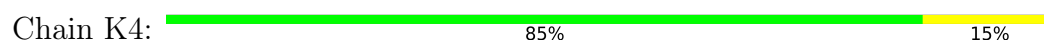
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



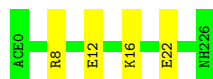
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



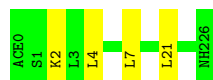
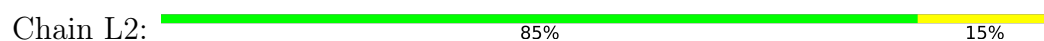
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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



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



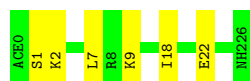
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



There are no outlier residues recorded for this chain.

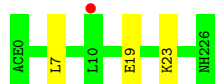
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain L4:  78% 22%



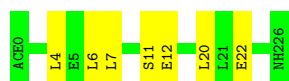
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain M1:  4% 89% 11%



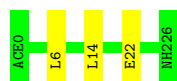
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain M2:  74% 26%



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

Chain M3:  89% 11%



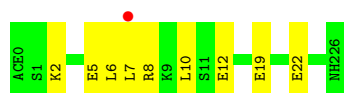
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain M4:  78% 22%



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

Chain N1:  4% 67% 33%



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

Chain N2:  81% 19%



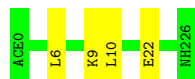
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain N3:  78% 22%



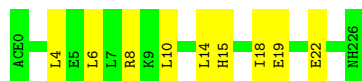
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain N4:  85% 15%



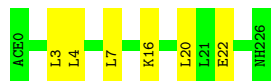
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain O1:  67% 33%



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

Chain O2:  78% 22%



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

Chain O3:  7% 78% 22%



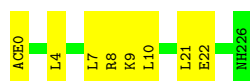
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain O4:  4% 70% 30%



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

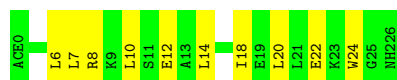
Chain P1:  70% 30%



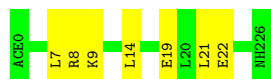
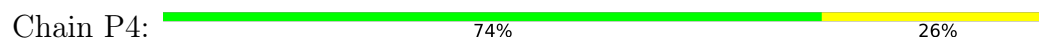
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



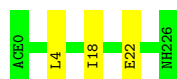
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



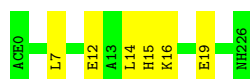
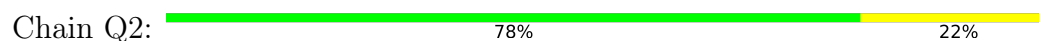
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



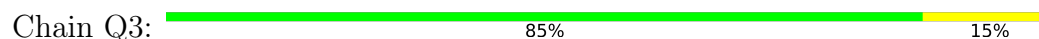
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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



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



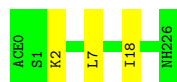
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Q4:  70% 30%



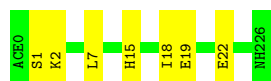
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain R1:  89% 11%



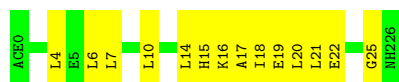
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain R2:  74% 26%



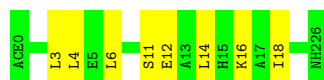
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain R3:  48% 52%



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

Chain R4:  70% 30%



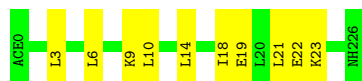
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain S1:  59% 37% .

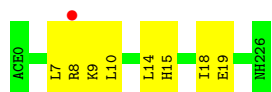
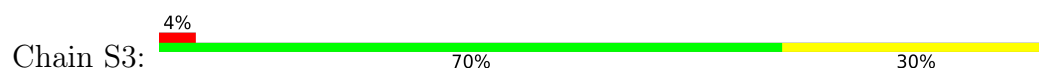


- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

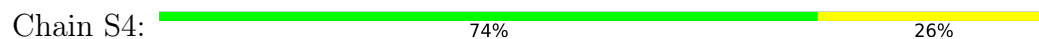
Chain S2:  63% 37%



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



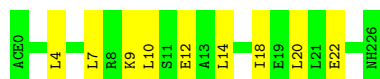
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



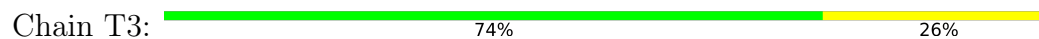
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



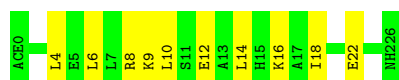
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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



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

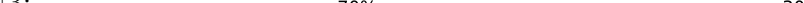


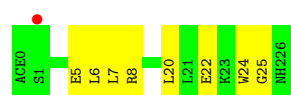
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

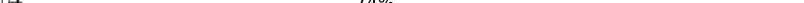


- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

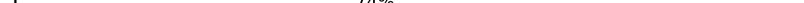
ACE0
S1
K2
L3
L4
L7
L14
I18
E19
L20
W24
G25
NH226

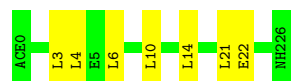
- Chain U3: 

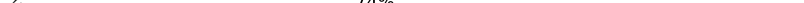


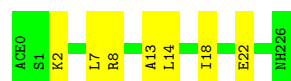
- Chain U4:  74% 26%

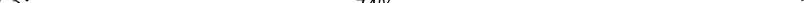


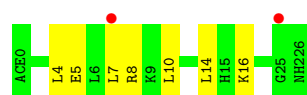
- Chain V1:  74% 26%

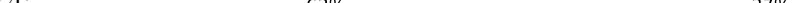


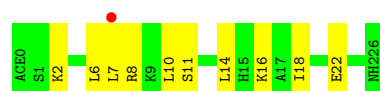
- Chain V2:  74% 26%



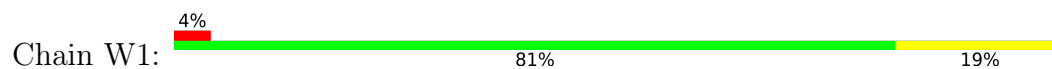
- Chain V3: 



- Chain V4: 



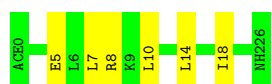
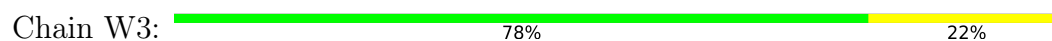
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



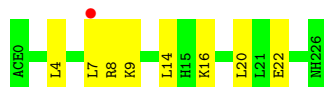
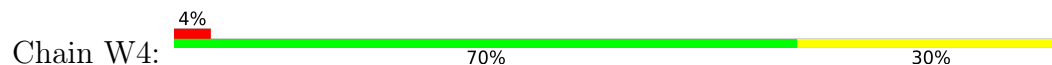
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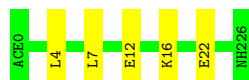
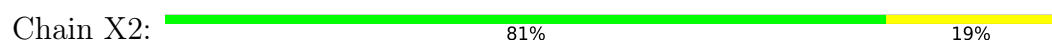
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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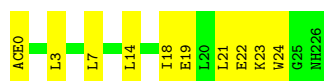


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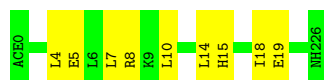
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain X4: 81% 19%



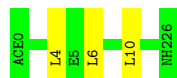
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Y1: 67% 33%



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

Chain Y2: 89% 11%



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

Chain Y3: 81% 19%



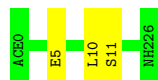
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain Y4: 81% 19%



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

Chain Z1: 89% 11%

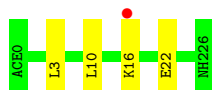
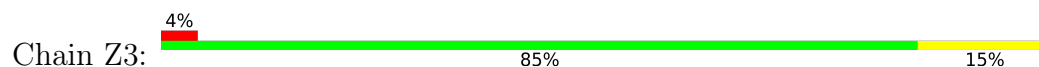


- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

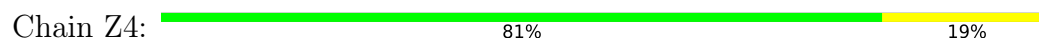
Chain Z2: 4% 81% 19%



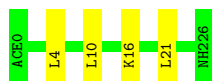
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



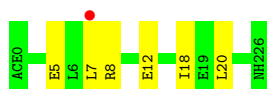
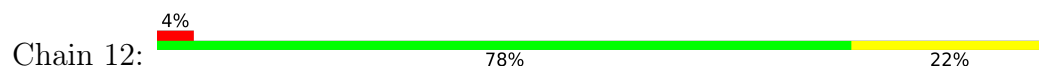
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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



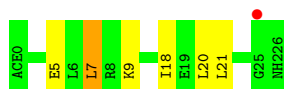
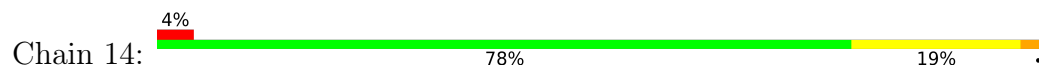
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



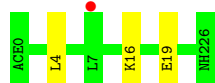
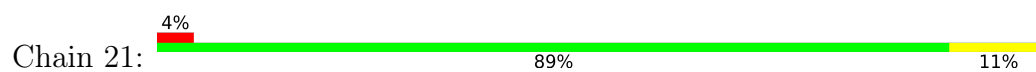
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



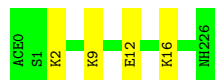
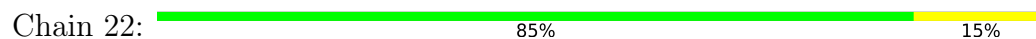
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



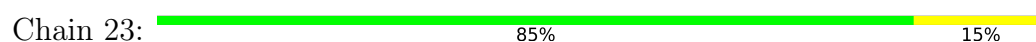
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



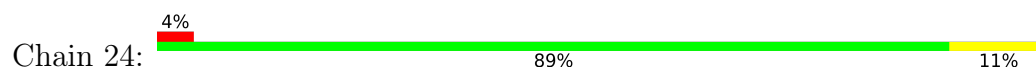
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



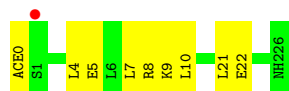
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



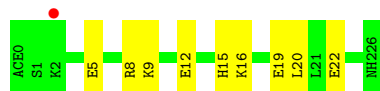
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



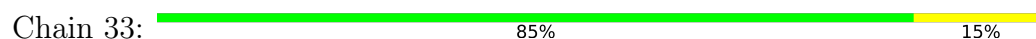
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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

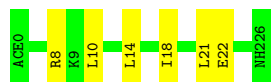


- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



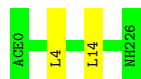
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 34:  78% 22%



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

Chain 41:  93% 7%



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

Chain 42:  81% 19%



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

Chain 43:  81% 15% .



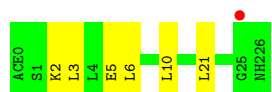
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 44:  78% 22%



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

Chain 51:  4% 78% 22%



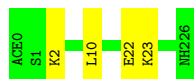
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 52:  81% 15% .



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

Chain 53: 85% 15%



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

Chain 54: 78% 22%



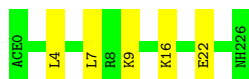
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 61: 74% 26%



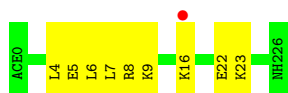
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 62: 81% 19%



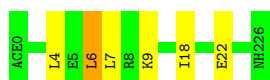
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 63: 4% 67% 33%



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

Chain 64: 78% 19% .



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

Chain 71:  81% 19%



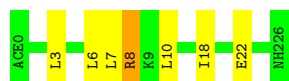
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 72:  78% 19% .



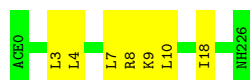
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 73:  74% 22% .



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

Chain 74:  74% 26%



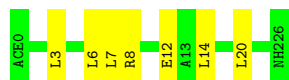
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 81:  4% 78% 22%



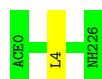
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 82:  74% 26%



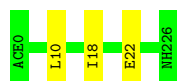
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 83:  96% .



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

Chain 84:  89% 11%



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

Chain 91:  70% 30%



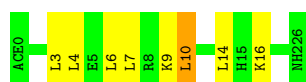
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 92:  63% 37%



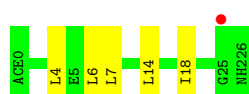
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 93:  70% 26% .



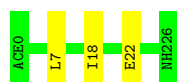
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain 94:  4% 81% 19%



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

Chain a1:  89% 11%



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

Chain a2:  85% 15%



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

Chain a3:  89% 11%



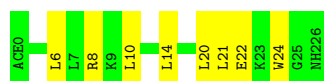
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain a4:  4% 78% 22%



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

Chain b1:  70% 30%



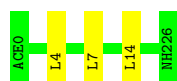
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain b2:  78% 22%



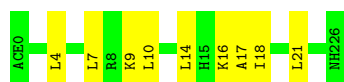
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain b3:  89% 11%



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

Chain b4:  67% 33%



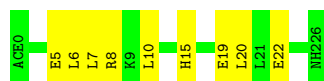
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain c1:  81% 19%



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

Chain c2:  67% 33%



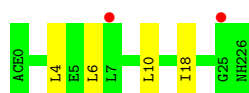
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain c3:  67% 33%



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

Chain c4:  7% 85% 15%



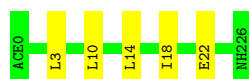
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain d1:  85% 15%



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

Chain d2:  81% 19%



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

Chain d3:  78% 22%



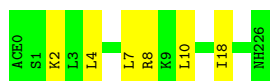
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain d4:  89% 11%



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

Chain e1:  78% 22%



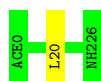
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain e2:  89% 11%



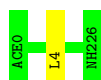
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain e3:  96% .



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

Chain e4:  96% .



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

Chain f1:  81% 19%



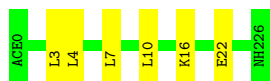
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain f2:  85% 15%



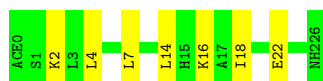
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain f3:  78% 22%



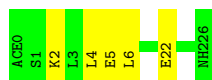
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain f4:  74% 26%



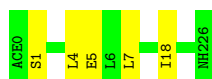
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain g1:  81% 19%



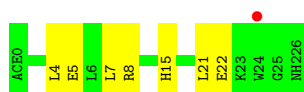
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain g2:  81% 19%



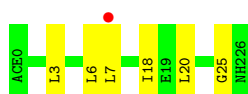
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain g3:  4% 74% 26%



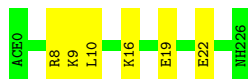
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain g4:  4% 78% 22%



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

Chain h1:  78% 22%



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

Chain h2:  4% 78% 22%



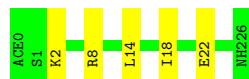
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain h3:  81% 19%



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

Chain h4:  81% 19%



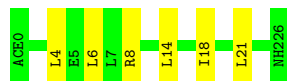
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain i1:  85% 15%



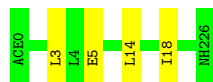
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain i2:  78% 22%



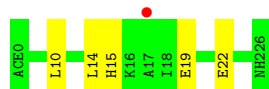
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain i3:  85% 15%



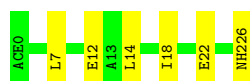
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain i4:  4% 81% 19%

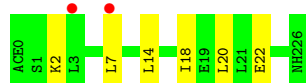
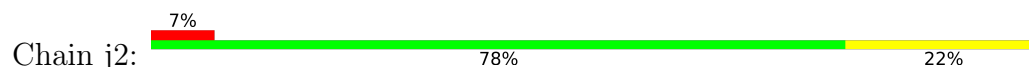


- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

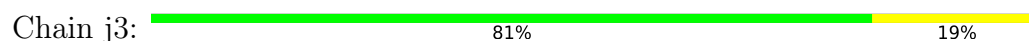
Chain j1:  78% 22%



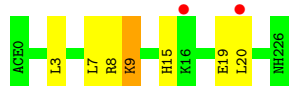
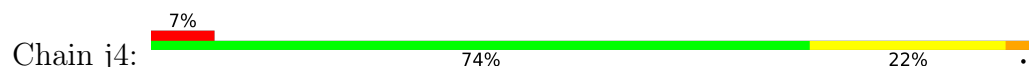
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



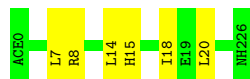
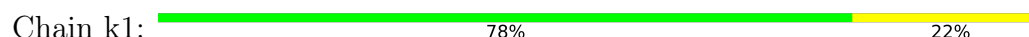
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



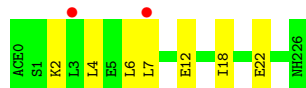
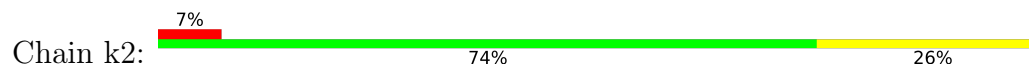
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



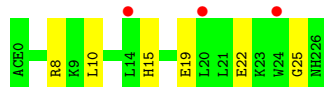
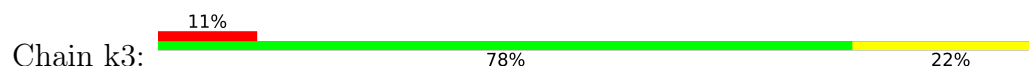
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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



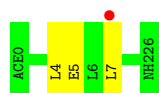
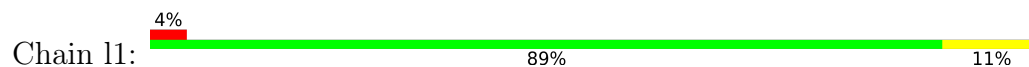
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



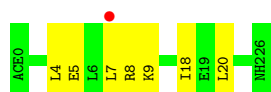
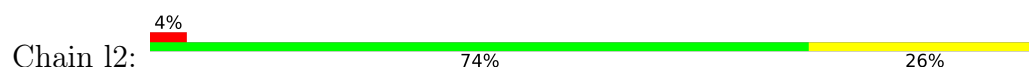
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



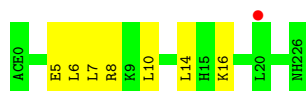
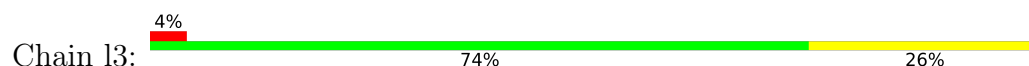
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



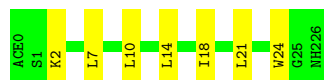
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



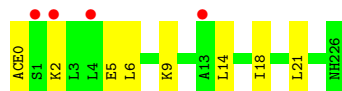
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



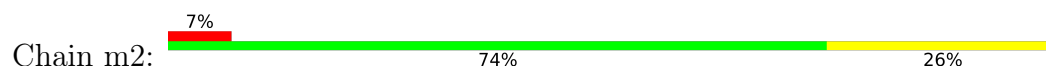
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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



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





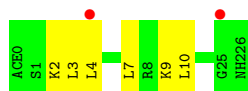
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain m3: 67% 33%



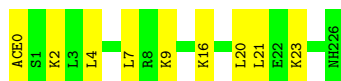
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain m4: 7% 78% 22%



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

Chain n1: 67% 33%



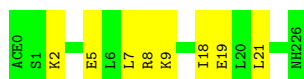
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain n2: 81% 19%



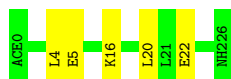
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain n3: 70% 30%

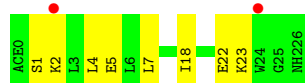


- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

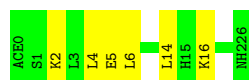
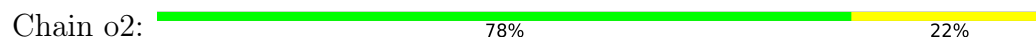
Chain n4: 81% 19%



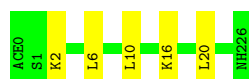
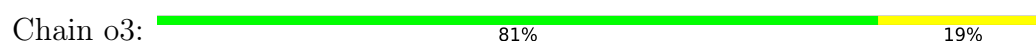
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



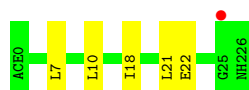
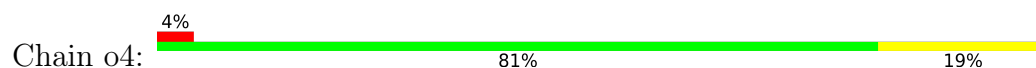
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



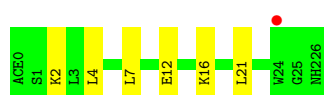
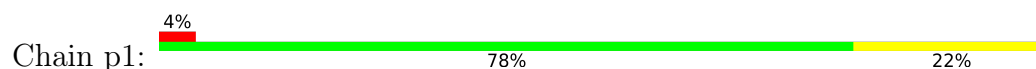
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



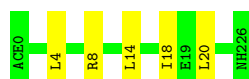
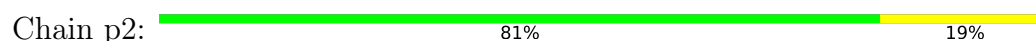
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



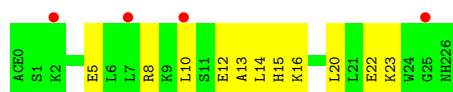
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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



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



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

Chain p4:  70% 30%



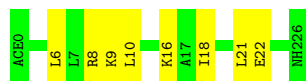
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain q1:  63% 33% .



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

Chain q2:  70% 30%



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

Chain q3:  74% 26%



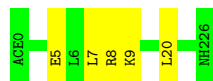
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain q4:  74% 26%



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

Chain r1:  81% 19%

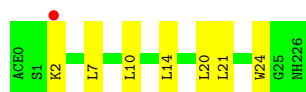
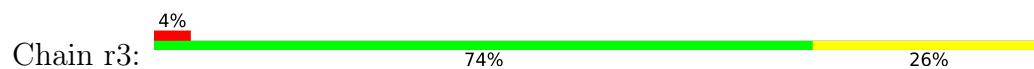


- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

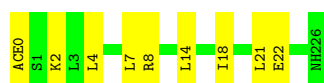
Chain r2:  4% 63% 37%



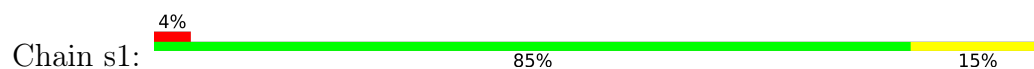
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



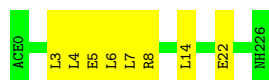
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



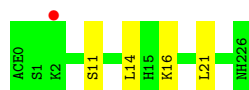
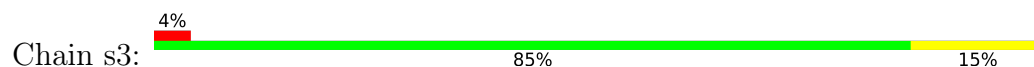
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



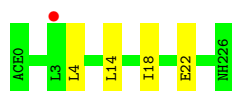
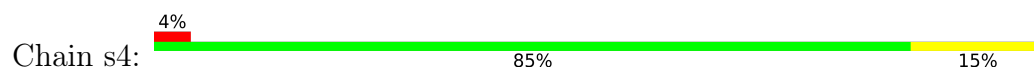
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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



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

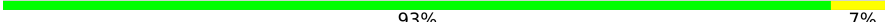


- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain t1:  93% 7%



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

Chain t2:  93% 7%



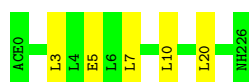
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS

Chain t3:  85% 15%



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

Chain t4:  81% 19%



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

Chain u1:  81% 15% .



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

Chain u2:  74% 26%



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

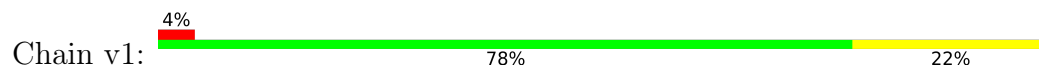
Chain u3:  67% 33%



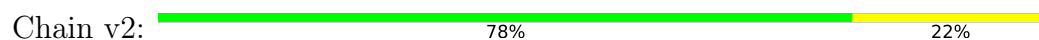
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



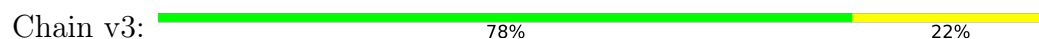
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



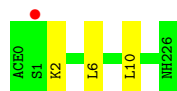
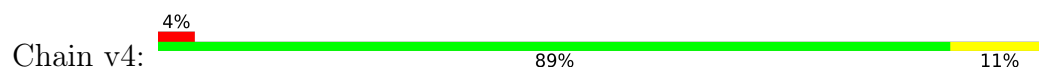
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



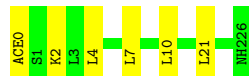
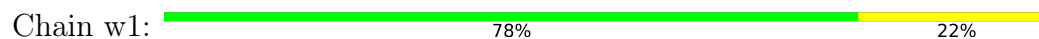
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



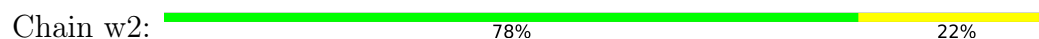
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



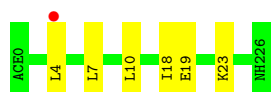
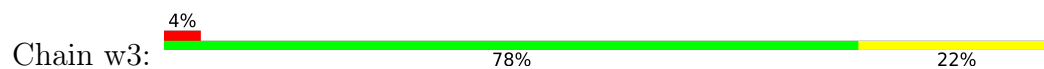
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



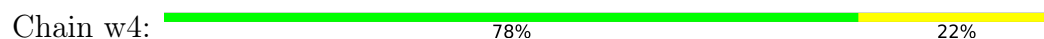
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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



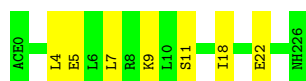
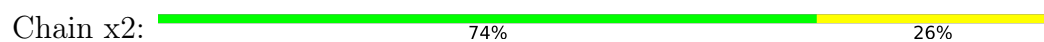
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



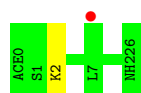
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



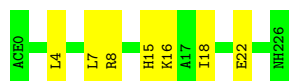
- Molecule 1: Cross-alpha Amyloid-like Structure alphaAmS



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



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



4 Data and refinement statistics

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 – 2.50 151.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (151.47-2.50) 98.7 (151.47-2.50)	Depositor EDS
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 0.202 , 0.249	Depositor DCC
R_{free} test set	16184 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 76.2	EDS
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
F_o, F_c correlation	0.96	EDS
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

5.1 Standard geometry

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

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	0.53	0/208	0.45	0/277
1	12	0.25	0/208	0.38	0/277
1	13	0.25	0/208	0.38	0/277
1	14	0.24	0/208	0.46	0/277
1	21	0.24	0/208	0.41	0/277
1	22	0.24	0/208	0.42	0/277
1	23	0.23	0/208	0.41	0/277
1	24	0.26	0/208	0.41	0/277
1	31	0.25	0/208	0.41	0/277
1	32	0.26	0/219	0.42	0/291
1	33	0.44	0/208	0.60	0/277
1	34	0.25	0/208	0.40	0/277
1	41	0.25	0/208	0.38	0/277
1	42	0.29	0/208	0.41	0/277
1	43	0.22	0/208	0.45	0/277
1	44	0.32	0/208	0.53	0/277
1	51	0.25	0/208	0.51	0/277
1	52	0.52	0/219	0.59	0/291
1	53	0.27	0/208	0.42	0/277
1	54	0.23	0/208	0.44	0/277
1	61	0.28	0/208	0.51	0/277
1	62	0.22	0/208	0.43	0/277
1	63	0.31	0/208	0.44	0/277
1	64	0.23	0/208	0.37	0/277
1	71	0.27	0/208	0.41	0/277
1	72	0.26	0/208	0.45	0/277
1	73	0.85	2/219 (0.9%)	1.01	2/291 (0.7%)
1	74	0.26	0/208	0.41	0/277
1	81	0.25	0/208	0.37	0/277
1	82	0.26	0/208	0.40	0/277
1	83	0.23	0/208	0.39	0/277
1	84	0.26	0/208	0.41	0/277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	91	0.28	0/208	0.41	0/277
1	92	0.27	0/208	0.41	0/277
1	93	0.29	0/208	0.40	0/277
1	94	0.25	0/208	0.38	0/277
1	A1	0.74	2/208 (1.0%)	0.48	0/277
1	A2	0.33	0/208	0.52	0/277
1	A3	0.28	0/208	0.43	0/277
1	A4	0.31	0/208	0.49	0/277
1	B1	0.31	0/208	0.49	0/277
1	B2	0.55	0/208	0.49	0/277
1	B3	0.25	0/208	0.42	0/277
1	B4	0.48	0/208	0.47	0/277
1	C1	0.27	0/208	0.47	0/277
1	C2	0.26	0/208	0.42	0/277
1	C3	0.21	0/208	0.35	0/277
1	C4	0.23	0/208	0.41	0/277
1	D1	0.24	0/208	0.43	0/277
1	D2	0.23	0/208	0.38	0/277
1	D3	0.51	0/208	0.50	0/277
1	D4	0.30	0/208	0.43	0/277
1	E1	0.50	0/219	0.62	0/291
1	E2	0.25	0/208	0.44	0/277
1	E3	0.54	0/208	0.46	0/277
1	E4	0.26	0/208	0.36	0/277
1	F1	0.29	0/208	0.37	0/277
1	F2	0.28	0/208	0.42	0/277
1	F3	0.27	0/208	0.39	0/277
1	F4	0.28	0/208	0.41	0/277
1	G1	0.28	0/208	0.47	0/277
1	G2	0.28	0/219	0.45	0/291
1	G3	0.25	0/208	0.41	0/277
1	G4	0.26	0/208	0.38	0/277
1	H1	0.22	0/208	0.39	0/277
1	H2	0.66	0/208	0.53	0/277
1	H3	0.34	0/208	0.38	0/277
1	H4	0.30	0/208	0.44	0/277
1	I1	0.50	0/208	0.53	0/277
1	I2	0.75	0/208	0.53	0/277
1	I3	0.56	0/208	0.41	0/277
1	I4	0.30	0/208	0.45	0/277
1	J1	0.31	0/208	0.45	0/277
1	J2	0.58	0/208	0.45	0/277
1	J3	0.35	0/208	0.50	0/277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	J4	0.30	0/208	0.48	0/277
1	K1	0.23	0/208	0.42	0/277
1	K2	0.23	0/208	0.35	0/277
1	K3	0.29	0/208	0.45	0/277
1	K4	0.25	0/208	0.46	0/277
1	L1	0.91	2/219 (0.9%)	0.87	2/291 (0.7%)
1	L2	0.27	0/208	0.43	0/277
1	L3	0.23	0/208	0.37	0/277
1	L4	0.27	0/208	0.35	0/277
1	M1	0.25	0/208	0.44	0/277
1	M2	0.25	0/208	0.36	0/277
1	M3	0.22	0/208	0.38	0/277
1	M4	0.20	0/208	0.36	0/277
1	N1	0.26	0/208	0.41	0/277
1	N2	0.27	0/208	0.39	0/277
1	N3	0.24	0/208	0.40	0/277
1	N4	0.25	0/208	0.43	0/277
1	O1	0.20	0/208	0.41	0/277
1	O2	0.46	0/208	0.45	0/277
1	O3	0.20	0/208	0.34	0/277
1	O4	0.21	0/208	0.39	0/277
1	P1	0.22	0/208	0.38	0/277
1	P2	0.24	0/208	0.38	0/277
1	P3	0.25	0/208	0.43	0/277
1	P4	0.23	0/208	0.32	0/277
1	Q1	0.26	0/208	0.45	0/277
1	Q2	0.23	0/208	0.45	0/277
1	Q3	0.23	0/208	0.36	0/277
1	Q4	0.23	0/208	0.45	0/277
1	R1	0.23	0/208	0.35	0/277
1	R2	0.26	0/208	0.40	0/277
1	R3	0.27	0/208	0.44	0/277
1	R4	0.49	0/208	0.39	0/277
1	S1	0.32	0/208	0.44	0/277
1	S2	0.25	0/208	0.43	0/277
1	S3	0.29	0/219	0.46	0/291
1	S4	0.22	0/208	0.39	0/277
1	T1	0.23	0/208	0.50	0/277
1	T2	0.27	0/208	0.41	0/277
1	T3	0.28	0/208	0.51	0/277
1	T4	0.26	0/208	0.40	0/277
1	U1	0.22	0/208	0.36	0/277
1	U2	0.25	0/208	0.37	0/277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	U3	0.26	0/208	0.43	0/277
1	U4	0.44	0/208	0.49	0/277
1	V1	0.25	0/208	0.31	0/277
1	V2	0.25	0/208	0.43	0/277
1	V3	0.53	0/208	0.58	0/277
1	V4	0.24	0/208	0.38	0/277
1	W1	0.24	0/208	0.42	0/277
1	W2	0.26	0/208	0.40	0/277
1	W3	0.22	0/208	0.40	0/277
1	W4	0.23	0/208	0.38	0/277
1	X1	0.25	0/208	0.41	0/277
1	X2	0.47	0/208	0.40	0/277
1	X3	0.29	0/208	0.47	0/277
1	X4	0.28	0/208	0.43	0/277
1	Y1	0.28	0/208	0.41	0/277
1	Y2	0.28	0/208	0.39	0/277
1	Y3	0.23	0/208	0.34	0/277
1	Y4	0.29	0/208	0.51	0/277
1	Z1	0.25	0/208	0.36	0/277
1	Z2	0.27	0/208	0.43	0/277
1	Z3	0.54	0/208	0.53	0/277
1	Z4	0.28	0/208	0.43	0/277
1	a1	0.26	0/208	0.44	0/277
1	a2	0.28	0/208	0.39	0/277
1	a3	0.27	0/208	0.43	0/277
1	a4	0.24	0/208	0.41	0/277
1	b1	0.23	0/208	0.47	0/277
1	b2	0.24	0/208	0.40	0/277
1	b3	0.19	0/208	0.41	0/277
1	b4	0.28	0/208	0.44	0/277
1	c1	0.24	0/208	0.39	0/277
1	c2	0.23	0/208	0.41	0/277
1	c3	0.24	0/208	0.37	0/277
1	c4	0.48	0/208	0.38	0/277
1	d1	0.20	0/208	0.38	0/277
1	d2	0.25	0/208	0.35	0/277
1	d3	0.25	0/208	0.41	0/277
1	d4	0.22	0/208	0.35	0/277
1	e1	0.26	0/208	0.44	0/277
1	e2	0.28	0/208	0.39	0/277
1	e3	0.23	0/208	0.35	0/277
1	e4	0.28	0/208	0.39	0/277
1	f1	0.20	0/208	0.33	0/277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	f2	0.27	0/208	0.34	0/277
1	f3	0.24	0/208	0.40	0/277
1	f4	0.21	0/208	0.36	0/277
1	g1	0.23	0/208	0.35	0/277
1	g2	0.26	0/208	0.46	0/277
1	g3	0.25	0/208	0.43	0/277
1	g4	0.18	0/208	0.33	0/277
1	h1	0.23	0/208	0.37	0/277
1	h2	0.23	0/208	0.35	0/277
1	h3	0.24	0/208	0.35	0/277
1	h4	0.26	0/208	0.36	0/277
1	i1	0.24	0/208	0.42	0/277
1	i2	0.24	0/208	0.40	0/277
1	i3	0.23	0/208	0.33	0/277
1	i4	0.24	0/208	0.42	0/277
1	j1	0.20	0/208	0.35	0/277
1	j2	0.25	0/208	0.43	0/277
1	j3	0.22	0/208	0.35	0/277
1	j4	0.42	0/208	0.46	0/277
1	k1	0.21	0/208	0.38	0/277
1	k2	0.27	0/208	0.48	0/277
1	k3	0.23	0/219	0.44	0/291
1	k4	0.23	0/208	0.42	0/277
1	l1	0.20	0/208	0.37	0/277
1	l2	0.22	0/208	0.38	0/277
1	l3	0.21	0/208	0.44	0/277
1	l4	0.23	0/208	0.40	0/277
1	m1	0.21	0/208	0.33	0/277
1	m2	0.22	0/208	0.37	0/277
1	m3	0.19	0/208	0.35	0/277
1	m4	0.23	0/208	0.35	0/277
1	n1	0.21	0/208	0.36	0/277
1	n2	0.19	0/208	0.35	0/277
1	n3	0.20	0/208	0.38	0/277
1	n4	0.21	0/204	0.40	0/273
1	o1	0.41	0/208	0.50	0/277
1	o2	0.27	0/208	0.39	0/277
1	o3	0.22	0/208	0.37	0/277
1	o4	0.21	0/208	0.43	0/277
1	p1	0.24	0/208	0.44	0/277
1	p2	0.23	0/208	0.41	0/277
1	p3	0.26	0/204	0.41	0/273
1	p4	0.20	0/208	0.37	0/277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	q1	0.29	0/208	0.48	0/277
1	q2	0.20	0/208	0.34	0/277
1	q3	0.27	0/208	0.38	0/277
1	q4	0.23	0/219	0.40	0/291
1	r1	0.23	0/219	0.43	0/291
1	r2	0.21	0/208	0.37	0/277
1	r3	0.26	0/208	0.38	0/277
1	r4	0.20	0/208	0.29	0/277
1	s1	0.26	0/208	0.41	0/277
1	s2	0.20	0/208	0.29	0/277
1	s3	0.24	0/208	0.38	0/277
1	s4	0.26	0/208	0.38	0/277
1	t1	0.25	0/208	0.46	0/277
1	t2	0.22	0/208	0.31	0/277
1	t3	0.23	0/208	0.41	0/277
1	t4	0.28	0/208	0.38	0/277
1	u1	0.76	2/219 (0.9%)	0.67	0/291
1	u2	0.23	0/219	0.43	0/291
1	u3	0.27	0/208	0.44	0/277
1	u4	0.28	0/208	0.44	0/277
1	v1	0.27	0/208	0.39	0/277
1	v2	0.23	0/208	0.42	0/277
1	v3	0.23	0/208	0.35	0/277
1	v4	0.21	0/208	0.37	0/277
1	w1	0.24	0/208	0.47	0/277
1	w2	0.24	0/208	0.41	0/277
1	w3	0.23	0/208	0.37	0/277
1	w4	0.28	0/208	0.38	0/277
1	x1	0.26	0/208	0.43	0/277
1	x2	0.27	0/208	0.44	0/277
1	x3	0.21	0/208	0.33	0/277
1	x4	0.48	0/208	0.57	0/277
All	All	0.31	8/49212 (0.0%)	0.43	4/65532 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	73	8[A]	ARG	CA-C	7.76	1.62	1.52
1	73	8[B]	ARG	CA-C	7.76	1.62	1.52
1	L1	8[A]	ARG	CA-C	-6.75	1.44	1.52
1	L1	8[B]	ARG	CA-C	-6.75	1.44	1.52
1	u1	8[A]	ARG	C-O	5.74	1.30	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	73	8[A]	ARG	CA-C-O	8.37	129.43	120.55
1	73	8[B]	ARG	CA-C-O	8.37	129.43	120.55
1	L1	8[A]	ARG	O-C-N	-6.45	115.42	122.07
1	L1	8[B]	ARG	O-C-N	-6.45	115.42	122.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	11	209	0	231	3	0
1	12	209	0	231	8	0
1	13	209	0	231	2	0
1	14	209	0	231	8	0
1	21	209	0	231	2	0
1	22	209	0	231	5	0
1	23	209	0	231	4	0
1	24	209	0	231	4	0
1	31	209	0	231	8	0
1	32	217	0	244	13	0
1	33	209	0	231	4	0
1	34	209	0	231	9	0
1	41	209	0	231	3	0
1	42	209	0	231	5	0
1	43	209	0	231	5	0
1	44	209	0	231	5	0
1	51	209	0	231	14	0
1	52	217	0	244	13	0
1	53	209	0	231	7	0
1	54	209	0	231	10	0
1	61	209	0	231	14	0
1	62	209	0	231	6	0
1	63	209	0	231	13	0
1	64	209	0	231	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	71	209	0	231	11	0
1	72	209	0	231	18	0
1	73	217	0	244	9	0
1	74	209	0	231	12	0
1	81	209	0	231	10	0
1	82	209	0	231	7	0
1	83	209	0	231	1	0
1	84	209	0	231	4	0
1	91	209	0	231	13	0
1	92	209	0	231	15	0
1	93	209	0	231	14	0
1	94	209	0	231	8	0
1	A1	209	0	231	2	0
1	A2	209	0	231	2	0
1	A3	209	0	231	10	0
1	A4	209	0	231	10	0
1	B1	209	0	231	12	0
1	B2	209	0	231	13	0
1	B3	209	0	231	7	0
1	B4	209	0	231	7	0
1	C1	209	0	231	11	0
1	C2	209	0	231	11	0
1	C3	209	0	231	11	0
1	C4	209	0	231	6	0
1	D1	209	0	231	6	0
1	D2	209	0	231	6	0
1	D3	209	0	231	3	0
1	D4	209	0	231	7	0
1	E1	217	0	244	5	0
1	E2	209	0	231	6	0
1	E3	209	0	231	5	0
1	E4	209	0	231	4	0
1	F1	209	0	231	4	0
1	F2	209	0	231	5	0
1	F3	209	0	231	5	0
1	F4	209	0	231	5	0
1	G1	209	0	231	12	0
1	G2	217	0	244	12	0
1	G3	209	0	231	13	0
1	G4	209	0	231	10	0
1	H1	209	0	231	12	0
1	H2	209	0	231	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H3	209	0	231	4	0
1	H4	209	0	231	12	0
1	I1	209	0	231	2	0
1	I2	209	0	231	5	0
1	I3	209	0	231	4	0
1	I4	209	0	231	8	0
1	J1	209	0	231	4	0
1	J2	209	0	231	9	0
1	J3	209	0	231	2	0
1	J4	209	0	231	2	0
1	K1	209	0	231	0	0
1	K2	209	0	231	1	0
1	K3	209	0	231	6	0
1	K4	209	0	231	5	0
1	L1	217	0	244	4	0
1	L2	209	0	231	4	0
1	L3	209	0	231	0	0
1	L4	209	0	231	6	0
1	M1	209	0	231	2	0
1	M2	209	0	231	7	0
1	M3	209	0	231	3	0
1	M4	209	0	231	6	0
1	N1	209	0	231	7	0
1	N2	209	0	231	7	0
1	N3	209	0	231	9	0
1	N4	209	0	231	3	0
1	O1	209	0	231	11	0
1	O2	209	0	231	9	0
1	O3	209	0	231	9	0
1	O4	209	0	231	13	0
1	P1	209	0	231	9	0
1	P2	209	0	231	14	0
1	P3	209	0	231	16	0
1	P4	209	0	231	10	0
1	Q1	209	0	231	3	0
1	Q2	209	0	231	5	0
1	Q3	209	0	231	5	0
1	Q4	209	0	231	8	0
1	R1	209	0	231	3	0
1	R2	209	0	231	8	0
1	R3	209	0	231	17	0
1	R4	209	0	231	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S1	209	0	231	19	0
1	S2	209	0	231	10	0
1	S3	217	0	244	13	0
1	S4	209	0	231	6	0
1	T1	209	0	231	10	0
1	T2	209	0	231	13	0
1	T3	209	0	231	8	0
1	T4	209	0	231	12	0
1	U1	209	0	231	3	0
1	U2	209	0	231	6	0
1	U3	209	0	231	9	0
1	U4	209	0	231	9	0
1	V1	209	0	231	8	0
1	V2	209	0	231	12	0
1	V3	209	0	231	9	0
1	V4	209	0	231	13	0
1	W1	209	0	231	4	0
1	W2	209	0	231	16	0
1	W3	209	0	231	9	0
1	W4	209	0	231	10	0
1	X1	209	0	231	6	0
1	X2	209	0	231	6	0
1	X3	209	0	231	11	0
1	X4	209	0	231	7	0
1	Y1	209	0	231	10	0
1	Y2	209	0	231	3	0
1	Y3	209	0	231	3	0
1	Y4	209	0	231	8	0
1	Z1	209	0	231	3	0
1	Z2	209	0	231	9	0
1	Z3	209	0	231	4	0
1	Z4	209	0	231	8	0
1	a1	209	0	231	9	0
1	a2	209	0	231	7	0
1	a3	209	0	231	4	0
1	a4	209	0	231	13	0
1	b1	209	0	231	10	0
1	b2	209	0	231	17	0
1	b3	209	0	231	4	0
1	b4	209	0	231	11	0
1	c1	209	0	231	6	0
1	c2	209	0	231	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	c3	209	0	231	6	0
1	c4	209	0	231	5	0
1	d1	209	0	231	4	0
1	d2	209	0	231	5	0
1	d3	209	0	231	8	0
1	d4	209	0	231	3	0
1	e1	209	0	231	6	0
1	e2	209	0	231	4	0
1	e3	209	0	231	1	0
1	e4	209	0	231	1	0
1	f1	209	0	231	7	0
1	f2	209	0	231	4	0
1	f3	209	0	231	10	0
1	f4	209	0	231	7	0
1	g1	209	0	231	5	0
1	g2	209	0	231	9	0
1	g3	209	0	231	12	0
1	g4	209	0	231	11	0
1	h1	209	0	231	8	0
1	h2	209	0	231	9	0
1	h3	209	0	231	4	0
1	h4	209	0	231	7	0
1	i1	209	0	231	6	0
1	i2	209	0	231	7	0
1	i3	209	0	231	4	0
1	i4	209	0	231	6	0
1	j1	209	0	231	6	0
1	j2	209	0	231	6	0
1	j3	209	0	231	5	0
1	j4	209	0	231	7	0
1	k1	209	0	231	5	0
1	k2	209	0	231	12	0
1	k3	217	0	244	4	0
1	k4	209	0	231	16	0
1	l1	209	0	231	3	0
1	l2	209	0	231	11	0
1	l3	209	0	231	6	0
1	l4	209	0	231	9	0
1	m1	209	0	231	11	0
1	m2	209	0	231	9	0
1	m3	209	0	231	12	0
1	m4	209	0	231	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	n1	209	0	231	11	0
1	n2	209	0	231	5	0
1	n3	209	0	231	17	0
1	n4	205	0	220	15	0
1	o1	209	0	231	14	0
1	o2	209	0	231	9	0
1	o3	209	0	231	14	0
1	o4	209	0	231	9	0
1	p1	209	0	231	6	0
1	p2	209	0	231	6	0
1	p3	205	0	220	18	0
1	p4	209	0	231	11	0
1	q1	209	0	231	13	0
1	q2	209	0	231	11	0
1	q3	209	0	231	7	0
1	q4	217	0	244	10	0
1	r1	217	0	244	4	0
1	r2	209	0	231	11	0
1	r3	209	0	231	8	0
1	r4	209	0	231	11	0
1	s1	209	0	231	5	0
1	s2	209	0	231	7	0
1	s3	209	0	231	4	0
1	s4	209	0	231	5	0
1	t1	209	0	231	2	0
1	t2	209	0	231	2	0
1	t3	209	0	231	5	0
1	t4	209	0	231	5	0
1	u1	217	0	244	5	0
1	u2	220	0	243	13	0
1	u3	209	0	231	17	0
1	u4	209	0	231	17	0
1	v1	209	0	231	10	0
1	v2	209	0	231	5	0
1	v3	209	0	231	10	0
1	v4	209	0	231	3	0
1	w1	209	0	231	11	0
1	w2	209	0	231	7	0
1	w3	209	0	231	14	0
1	w4	209	0	231	9	0
1	x1	209	0	231	13	0
1	x2	209	0	231	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	x3	209	0	231	1	0
1	x4	209	0	231	7	0
2	13	3	0	1	0	0
2	14	3	0	1	0	0
2	24	3	0	1	0	0
2	32	3	0	1	0	0
2	42	3	0	1	0	0
2	43	3	0	1	0	0
2	44	3	0	1	0	0
2	62	3	0	1	0	0
2	72	3	0	1	0	0
2	81	3	0	1	0	0
2	82	3	0	1	0	0
2	83	3	0	1	0	0
2	92	3	0	1	0	0
2	93	3	0	1	0	0
2	A1	6	0	2	0	0
2	A3	3	0	1	0	0
2	A4	3	0	1	0	0
2	B3	3	0	1	0	0
2	B4	3	0	1	0	0
2	C2	3	0	1	0	0
2	D1	3	0	1	0	0
2	D2	3	0	1	0	0
2	E1	3	0	1	0	0
2	E3	3	0	1	0	0
2	E4	3	0	1	0	0
2	F3	3	0	1	0	0
2	F4	3	0	1	0	0
2	G2	3	0	1	0	0
2	G3	3	0	1	0	0
2	H1	3	0	1	1	0
2	H2	3	0	1	0	0
2	H3	3	0	1	0	0
2	I3	3	0	1	0	0
2	I4	3	0	1	0	0
2	J2	3	0	1	0	0
2	K2	3	0	1	0	0
2	L2	3	0	1	1	0
2	L3	3	0	1	0	0
2	L4	3	0	1	0	0
2	M2	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N1	3	0	1	0	0
2	O1	3	0	1	0	0
2	O2	3	0	1	0	0
2	O3	3	0	1	0	0
2	P2	3	0	1	0	0
2	P3	3	0	1	0	0
2	Q2	3	0	1	0	0
2	Q3	3	0	1	0	0
2	R4	3	0	1	0	0
2	S1	3	0	1	0	0
2	S2	3	0	1	0	0
2	T2	3	0	1	0	0
2	T3	3	0	1	0	0
2	U1	3	0	1	0	0
2	U2	3	0	1	0	0
2	W4	3	0	1	0	0
2	X4	3	0	1	0	0
2	Y4	3	0	1	0	0
2	Z1	3	0	1	0	0
2	Z3	3	0	1	0	0
2	Z4	3	0	1	0	0
2	a4	3	0	1	0	0
2	b1	3	0	1	0	0
2	b4	3	0	1	0	0
2	c4	3	0	1	0	0
2	d1	3	0	1	0	0
2	d2	3	0	1	0	0
2	e1	3	0	1	0	0
2	e4	6	0	2	0	0
2	f4	3	0	1	0	0
2	g1	3	0	1	0	0
2	g4	3	0	1	0	0
2	h2	3	0	1	0	0
2	i1	3	0	1	0	0
2	i2	3	0	1	0	0
2	j1	3	0	1	0	0
2	j3	3	0	1	0	0
2	k4	3	0	1	0	0
2	m2	3	0	1	0	0
2	m3	3	0	1	0	0
2	m4	3	0	1	0	0
2	n2	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	o4	3	0	1	0	0
2	q1	3	0	1	0	0
2	r2	3	0	1	0	0
2	r3	3	0	1	0	0
2	s2	3	0	1	0	0
2	t1	3	0	1	0	0
2	t3	3	0	1	0	0
2	u2	3	0	1	0	0
2	u3	3	0	1	0	0
2	v3	3	0	1	0	0
2	w4	3	0	1	0	0
2	x1	3	0	1	0	0
2	x4	3	0	1	0	0
3	74	8	0	14	15	0
3	G2	8	0	14	4	0
3	R3	8	0	14	8	0
3	W2	8	0	14	9	0
3	X3	8	0	14	2	0
3	q3	8	0	14	0	0
4	11	1	0	0	0	0
4	13	3	0	0	0	0
4	14	1	0	0	0	0
4	21	2	0	0	0	0
4	22	2	0	0	0	0
4	23	3	0	0	0	0
4	31	1	0	0	0	0
4	32	4	0	0	0	0
4	33	1	0	0	0	0
4	34	1	0	0	0	0
4	41	5	0	0	0	0
4	42	3	0	0	0	0
4	43	3	0	0	0	0
4	44	2	0	0	0	0
4	51	1	0	0	3	0
4	52	1	0	0	0	0
4	53	2	0	0	0	0
4	54	2	0	0	0	0
4	61	1	0	0	0	0
4	62	2	0	0	0	0
4	63	5	0	0	0	0
4	64	1	0	0	0	0
4	71	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	72	2	0	0	0	0
4	73	2	0	0	0	0
4	74	1	0	0	0	0
4	81	2	0	0	0	0
4	82	3	0	0	1	0
4	83	1	0	0	0	0
4	84	1	0	0	0	0
4	92	3	0	0	0	0
4	93	3	0	0	0	0
4	94	3	0	0	0	0
4	A1	4	0	0	0	0
4	A2	6	0	0	0	0
4	A3	2	0	0	0	0
4	A4	3	0	0	0	0
4	B1	1	0	0	0	0
4	B2	1	0	0	1	0
4	B3	3	0	0	0	0
4	B4	2	0	0	1	0
4	C2	1	0	0	0	0
4	C4	2	0	0	0	0
4	D1	1	0	0	0	0
4	D2	1	0	0	0	0
4	D3	3	0	0	0	0
4	D4	1	0	0	0	0
4	E1	3	0	0	0	0
4	E2	1	0	0	0	0
4	E3	3	0	0	0	0
4	E4	3	0	0	0	0
4	F1	2	0	0	0	0
4	F2	5	0	0	0	0
4	F3	2	0	0	0	0
4	F4	2	0	0	0	0
4	G1	1	0	0	0	0
4	G2	3	0	0	0	0
4	G3	2	0	0	0	0
4	G4	2	0	0	0	0
4	H2	4	0	0	0	0
4	H3	4	0	0	0	0
4	H4	2	0	0	0	0
4	I1	1	0	0	0	0
4	I2	2	0	0	0	0
4	I3	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I4	3	0	0	0	0
4	J1	6	0	0	0	0
4	J2	7	0	0	0	0
4	J3	3	0	0	0	0
4	K1	2	0	0	0	0
4	K2	3	0	0	0	0
4	K3	2	0	0	0	0
4	K4	4	0	0	0	0
4	L1	2	0	0	0	0
4	L2	1	0	0	0	0
4	L3	3	0	0	0	0
4	M2	1	0	0	0	0
4	M3	2	0	0	0	0
4	M4	3	0	0	0	0
4	N1	1	0	0	0	0
4	N2	2	0	0	0	0
4	N3	3	0	0	0	0
4	N4	2	0	0	0	0
4	O1	1	0	0	0	0
4	O2	1	0	0	0	0
4	O3	2	0	0	0	0
4	O4	2	0	0	1	0
4	P1	1	0	0	0	0
4	P2	1	0	0	0	0
4	P3	2	0	0	0	0
4	P4	3	0	0	0	0
4	Q1	4	0	0	0	0
4	Q2	1	0	0	0	0
4	Q3	1	0	0	0	0
4	Q4	1	0	0	0	0
4	R1	1	0	0	0	0
4	R2	4	0	0	0	0
4	R3	3	0	0	1	0
4	S1	2	0	0	0	0
4	S2	2	0	0	0	0
4	S3	2	0	0	0	0
4	S4	3	0	0	0	0
4	T2	1	0	0	0	0
4	T4	1	0	0	0	0
4	U1	2	0	0	0	0
4	U2	1	0	0	0	0
4	U4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V1	1	0	0	0	0
4	V2	3	0	0	0	0
4	V3	2	0	0	0	0
4	V4	1	0	0	0	0
4	W1	2	0	0	0	0
4	W3	1	0	0	0	0
4	X1	1	0	0	1	0
4	X2	4	0	0	1	0
4	X3	3	0	0	0	0
4	Y1	2	0	0	0	0
4	Y2	4	0	0	0	0
4	Y3	2	0	0	0	0
4	Y4	2	0	0	1	0
4	Z1	1	0	0	0	0
4	Z2	1	0	0	0	0
4	Z3	4	0	0	0	0
4	Z4	3	0	0	0	0
4	a1	3	0	0	0	0
4	a2	5	0	0	0	0
4	a3	3	0	0	0	0
4	a4	1	0	0	0	0
4	b1	1	0	0	0	0
4	b2	1	0	0	0	0
4	b3	1	0	0	0	0
4	c2	1	0	0	0	0
4	c3	2	0	0	0	0
4	c4	1	0	0	0	0
4	d1	2	0	0	0	0
4	d3	2	0	0	0	0
4	d4	2	0	0	0	0
4	e1	1	0	0	0	0
4	e2	2	0	0	0	0
4	e3	1	0	0	0	0
4	e4	3	0	0	0	0
4	f1	1	0	0	0	0
4	f2	3	0	0	0	0
4	f3	2	0	0	0	0
4	f4	2	0	0	0	0
4	g1	3	0	0	0	0
4	g2	1	0	0	0	0
4	g3	1	0	0	0	0
4	g4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	h1	2	0	0	0	0
4	h2	1	0	0	0	0
4	h3	4	0	0	0	0
4	h4	1	0	0	0	0
4	i1	2	0	0	0	0
4	i2	1	0	0	0	0
4	i4	2	0	0	0	0
4	j3	2	0	0	0	0
4	j4	1	0	0	1	0
4	k3	1	0	0	0	0
4	l2	1	0	0	0	0
4	l3	1	0	0	0	0
4	l4	1	0	0	0	0
4	m1	1	0	0	0	0
4	m3	1	0	0	0	0
4	m4	1	0	0	0	0
4	n2	1	0	0	0	0
4	n3	1	0	0	0	0
4	n4	2	0	0	0	0
4	o1	1	0	0	0	0
4	o2	1	0	0	0	0
4	o3	2	0	0	0	0
4	o4	2	0	0	0	0
4	p1	1	0	0	0	0
4	p2	1	0	0	0	0
4	p4	1	0	0	0	0
4	q1	2	0	0	0	0
4	q2	1	0	0	0	0
4	q3	1	0	0	0	0
4	q4	2	0	0	0	0
4	r1	1	0	0	0	0
4	r2	1	0	0	0	0
4	r3	1	0	0	0	0
4	s1	2	0	0	0	0
4	s2	2	0	0	0	0
4	s3	3	0	0	0	0
4	s4	6	0	0	0	0
4	t1	2	0	0	0	0
4	t2	1	0	0	0	0
4	t3	1	0	0	0	0
4	t4	1	0	0	0	0
4	u1	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	u3	1	0	0	0	0
4	u4	1	0	0	0	0
4	v1	3	0	0	0	0
4	v2	2	0	0	0	0
4	v3	1	0	0	0	0
4	w3	3	0	0	0	0
4	w4	1	0	0	0	0
4	x1	3	0	0	0	0
4	x2	1	0	0	0	0
4	x3	2	0	0	0	0
4	x4	1	0	0	0	0
All	All	50163	0	54830	1122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1122 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a4:16:LYS:NZ	1:b2:9:LYS:HG3	1.48	1.27
1:o3:20:LEU:CD2	1:o4:21:LEU:HD12	1.68	1.23
3:R3:101:MPD:H31	1:S1:0:ACE:CH3	1.73	1.19
3:R3:101:MPD:H31	1:S1:0:ACE:H2	1.30	1.13
1:a4:16:LYS:HZ3	1:b2:9:LYS:CG	1.66	1.08

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	11	25/27 (93%)	25 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	2	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

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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%)	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
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

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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	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%)	24	49
1	12	22/22 (100%)	22 (100%)	0	100	100
1	13	22/22 (100%)	22 (100%)	0	100	100
1	14	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	21	22/22 (100%)	22 (100%)	0	100	100
1	22	22/22 (100%)	22 (100%)	0	100	100
1	23	22/22 (100%)	22 (100%)	0	100	100
1	24	22/22 (100%)	22 (100%)	0	100	100
1	31	22/22 (100%)	22 (100%)	0	100	100
1	32	23/22 (104%)	23 (100%)	0	100	100
1	33	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	34	22/22 (100%)	22 (100%)	0	100	100
1	41	22/22 (100%)	22 (100%)	0	100	100
1	42	22/22 (100%)	22 (100%)	0	100	100
1	43	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	44	22/22 (100%)	22 (100%)	0	100	100
1	51	22/22 (100%)	22 (100%)	0	100	100
1	52	23/22 (104%)	21 (91%)	2 (9%)	9	21
1	53	22/22 (100%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100
1	64	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	71	22/22 (100%)	22 (100%)	0	100	100
1	72	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	73	23/22 (104%)	23 (100%)	0	100	100
1	74	22/22 (100%)	22 (100%)	0	100	100
1	81	22/22 (100%)	22 (100%)	0	100	100
1	82	22/22 (100%)	22 (100%)	0	100	100
1	83	22/22 (100%)	22 (100%)	0	100	100
1	84	22/22 (100%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	91	22/22 (100%)	22 (100%)	0	100	100
1	92	22/22 (100%)	22 (100%)	0	100	100
1	93	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	94	22/22 (100%)	22 (100%)	0	100	100
1	A1	22/22 (100%)	21 (96%)	1 (4%)	24	49
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%)	21 (96%)	1 (4%)	24	49
1	B3	22/22 (100%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100
1	C3	22/22 (100%)	22 (100%)	0	100	100
1	C4	22/22 (100%)	22 (100%)	0	100	100
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%)	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
1	E3	22/22 (100%)	20 (91%)	2 (9%)	9	19
1	E4	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	F1	22/22 (100%)	22 (100%)	0	100	100
1	F2	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	F3	22/22 (100%)	22 (100%)	0	100	100
1	F4	22/22 (100%)	22 (100%)	0	100	100
1	G1	22/22 (100%)	22 (100%)	0	100	100
1	G2	23/22 (104%)	23 (100%)	0	100	100
1	G3	22/22 (100%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G4	22/22 (100%)	22 (100%)	0	100	100
1	H1	22/22 (100%)	22 (100%)	0	100	100
1	H2	22/22 (100%)	19 (86%)	3 (14%)	3	8
1	H3	22/22 (100%)	21 (96%)	1 (4%)	24	49
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%)	22 (100%)	0	100	100
1	I3	22/22 (100%)	22 (100%)	0	100	100
1	I4	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	J1	22/22 (100%)	22 (100%)	0	100	100
1	J2	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	J3	22/22 (100%)	22 (100%)	0	100	100
1	J4	22/22 (100%)	22 (100%)	0	100	100
1	K1	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	K2	22/22 (100%)	22 (100%)	0	100	100
1	K3	22/22 (100%)	22 (100%)	0	100	100
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%)	21 (96%)	1 (4%)	24	49
1	M1	22/22 (100%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O3	22/22 (100%)	22 (100%)	0	100	100
1	O4	22/22 (100%)	22 (100%)	0	100	100
1	P1	22/22 (100%)	22 (100%)	0	100	100
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%)	21 (96%)	1 (4%)	24	49
1	S1	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	S2	22/22 (100%)	22 (100%)	0	100	100
1	S3	23/22 (104%)	23 (100%)	0	100	100
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%)	22 (100%)	0	100	100
1	T3	22/22 (100%)	22 (100%)	0	100	100
1	T4	22/22 (100%)	21 (96%)	1 (4%)	24	49
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%)	22 (100%)	0	100	100
1	V3	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	V4	22/22 (100%)	22 (100%)	0	100	100
1	W1	22/22 (100%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	22 (100%)	0	100	100
1	X1	22/22 (100%)	22 (100%)	0	100	100
1	X2	22/22 (100%)	22 (100%)	0	100	100
1	X3	22/22 (100%)	22 (100%)	0	100	100
1	X4	22/22 (100%)	22 (100%)	0	100	100
1	Y1	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	Y2	22/22 (100%)	22 (100%)	0	100	100
1	Y3	22/22 (100%)	20 (91%)	2 (9%)	9	19
1	Y4	22/22 (100%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100
1	b2	22/22 (100%)	22 (100%)	0	100	100
1	b3	22/22 (100%)	22 (100%)	0	100	100
1	b4	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	c1	22/22 (100%)	22 (100%)	0	100	100
1	c2	22/22 (100%)	22 (100%)	0	100	100
1	c3	22/22 (100%)	20 (91%)	2 (9%)	9	19
1	c4	22/22 (100%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100
1	d4	22/22 (100%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e1	22/22 (100%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100
1	g1	22/22 (100%)	22 (100%)	0	100	100
1	g2	22/22 (100%)	22 (100%)	0	100	100
1	g3	22/22 (100%)	22 (100%)	0	100	100
1	g4	22/22 (100%)	22 (100%)	0	100	100
1	h1	22/22 (100%)	22 (100%)	0	100	100
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%)	24	49
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%)	22 (100%)	0	100	100
1	j1	22/22 (100%)	22 (100%)	0	100	100
1	j2	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	j3	22/22 (100%)	22 (100%)	0	100	100
1	j4	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	k1	22/22 (100%)	22 (100%)	0	100	100
1	k2	22/22 (100%)	22 (100%)	0	100	100
1	k3	23/22 (104%)	21 (91%)	2 (9%)	9	21
1	k4	22/22 (100%)	22 (100%)	0	100	100
1	l1	22/22 (100%)	22 (100%)	0	100	100
1	l2	22/22 (100%)	22 (100%)	0	100	100
1	l3	22/22 (100%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	l4	22/22 (100%)	22 (100%)	0	100	100
1	m1	22/22 (100%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100
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%)	21 (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%)	21 (96%)	1 (4%)	24	49
1	p1	22/22 (100%)	22 (100%)	0	100	100
1	p2	22/22 (100%)	22 (100%)	0	100	100
1	p3	21/22 (96%)	21 (100%)	0	100	100
1	p4	22/22 (100%)	22 (100%)	0	100	100
1	q1	22/22 (100%)	21 (96%)	1 (4%)	24	49
1	q2	22/22 (100%)	22 (100%)	0	100	100
1	q3	22/22 (100%)	22 (100%)	0	100	100
1	q4	23/22 (104%)	23 (100%)	0	100	100
1	r1	23/22 (104%)	23 (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%)	22 (100%)	0	100	100
1	s1	22/22 (100%)	22 (100%)	0	100	100
1	s2	22/22 (100%)	22 (100%)	0	100	100
1	s3	22/22 (100%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	t3	22/22 (100%)	22 (100%)	0	100	100
1	t4	22/22 (100%)	22 (100%)	0	100	100
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%)	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%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100
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%)	22 (100%)	0	100	100
1	x1	22/22 (100%)	22 (100%)	0	100	100
1	x2	22/22 (100%)	22 (100%)	0	100	100
1	x3	22/22 (100%)	22 (100%)	0	100	100
1	x4	22/22 (100%)	21 (96%)	1 (4%)	24	49
All	All	5202/5192 (100%)	5161 (99%)	41 (1%)	73	88

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	72	7	LEU
1	j4	9	LYS
1	93	10	LEU
1	c3	18	ILE
1	k3	8[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	d3	15	HIS
1	x3	15	HIS
1	L2	15	HIS

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Mol	Chain	Res	Type
1	M1	15	HIS
1	O1	15	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	u3	101	-	2,2,2	0.71	0	1,1,1	0.21	0
2	FMT	Y4	101	-	2,2,2	0.71	0	1,1,1	0.20	0
2	FMT	m4	101	-	2,2,2	0.65	0	1,1,1	0.04	0
2	FMT	b4	101	-	2,2,2	0.73	0	1,1,1	0.23	0
2	FMT	u2	101	-	2,2,2	0.69	0	1,1,1	0.13	0
2	FMT	42	101	-	2,2,2	0.55	0	1,1,1	0.60	0
2	FMT	e1	101	-	2,2,2	0.69	0	1,1,1	0.21	0
2	FMT	j1	101	-	2,2,2	0.73	0	1,1,1	0.21	0
2	FMT	A1	102	-	2,2,2	0.61	0	1,1,1	0.07	0
2	FMT	f4	101	-	2,2,2	0.72	0	1,1,1	0.21	0
2	FMT	93	101	-	2,2,2	0.71	0	1,1,1	0.26	0
2	FMT	h2	101	-	2,2,2	0.71	0	1,1,1	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMT	k4	101	-	2,2,2	0.73	0	1,1,1	0.25	0
2	FMT	A3	101	-	2,2,2	0.68	0	1,1,1	0.15	0
2	FMT	w4	101	-	2,2,2	0.72	0	1,1,1	0.18	0
2	FMT	A4	101	-	2,2,2	0.67	0	1,1,1	0.23	0
2	FMT	o4	101	-	2,2,2	0.71	0	1,1,1	0.23	0
2	FMT	s2	101	-	2,2,2	0.70	0	1,1,1	0.20	0
2	FMT	P2	101	-	2,2,2	0.72	0	1,1,1	0.18	0
2	FMT	g4	101	-	2,2,2	0.71	0	1,1,1	0.19	0
2	FMT	H2	101	-	2,2,2	0.67	0	1,1,1	0.15	0
2	FMT	A1	101	-	2,2,2	0.69	0	1,1,1	0.16	0
2	FMT	F4	101	-	2,2,2	0.69	0	1,1,1	0.20	0
2	FMT	e4	101	-	2,2,2	0.71	0	1,1,1	0.21	0
2	FMT	24	101	-	2,2,2	0.70	0	1,1,1	0.18	0
2	FMT	X4	101	-	2,2,2	0.69	0	1,1,1	0.19	0
2	FMT	83	101	-	2,2,2	0.69	0	1,1,1	0.18	0
2	FMT	r3	101	-	2,2,2	0.70	0	1,1,1	0.21	0
2	FMT	a4	101	-	2,2,2	0.70	0	1,1,1	0.17	0
3	MPD	W2	101	-	7,7,7	0.30	0	9,10,10	0.22	0
2	FMT	13	101	-	2,2,2	0.72	0	1,1,1	0.20	0
2	FMT	K2	101	-	2,2,2	0.70	0	1,1,1	0.16	0
2	FMT	q1	101	-	2,2,2	0.73	0	1,1,1	0.24	0
2	FMT	i1	101	-	2,2,2	0.70	0	1,1,1	0.21	0
2	FMT	D2	101	-	2,2,2	0.70	0	1,1,1	0.19	0
2	FMT	t3	101	-	2,2,2	0.74	0	1,1,1	0.24	0
2	FMT	32	101	-	2,2,2	0.72	0	1,1,1	0.18	0
3	MPD	74	101	-	7,7,7	0.29	0	9,10,10	0.22	0
2	FMT	Q2	101	-	2,2,2	0.71	0	1,1,1	0.23	0
2	FMT	62	101	-	2,2,2	0.69	0	1,1,1	0.17	0
3	MPD	X3	101	-	7,7,7	0.33	0	9,10,10	0.33	0
3	MPD	R3	101	-	7,7,7	0.37	0	9,10,10	0.47	0
2	FMT	C2	101	-	2,2,2	0.73	0	1,1,1	0.22	0
2	FMT	43	101	-	2,2,2	0.45	0	1,1,1	0.79	0
2	FMT	b1	101	-	2,2,2	0.72	0	1,1,1	0.20	0
2	FMT	t1	101	-	2,2,2	0.71	0	1,1,1	0.18	0
2	FMT	H1	101	-	2,2,2	0.46	0	1,1,1	0.74	0
3	MPD	G2	102	-	7,7,7	0.34	0	9,10,10	0.55	0
2	FMT	U1	101	-	2,2,2	0.71	0	1,1,1	0.21	0
2	FMT	Z1	101	-	2,2,2	0.71	0	1,1,1	0.22	0
2	FMT	e4	102	-	2,2,2	0.64	0	1,1,1	0.02	0
2	FMT	O3	101	-	2,2,2	0.69	0	1,1,1	0.17	0
2	FMT	Z4	101	-	2,2,2	0.70	0	1,1,1	0.17	0
2	FMT	H3	101	-	2,2,2	0.71	0	1,1,1	0.21	0
2	FMT	D1	101	-	2,2,2	0.74	0	1,1,1	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMT	I3	101	-	2,2,2	0.71	0	1,1,1	0.23	0
2	FMT	S2	101	-	2,2,2	0.70	0	1,1,1	0.17	0
2	FMT	82	101	-	2,2,2	0.68	0	1,1,1	0.17	0
2	FMT	L3	101	-	2,2,2	0.69	0	1,1,1	0.16	0
2	FMT	U2	101	-	2,2,2	0.72	0	1,1,1	0.25	0
2	FMT	d1	101	-	2,2,2	0.72	0	1,1,1	0.20	0
2	FMT	G2	101	-	2,2,2	0.71	0	1,1,1	0.22	0
3	MPD	q3	101	-	7,7,7	0.28	0	9,10,10	0.97	0
2	FMT	O1	101	-	2,2,2	0.71	0	1,1,1	0.18	0
2	FMT	T2	101	-	2,2,2	0.73	0	1,1,1	0.24	0
2	FMT	m3	101	-	2,2,2	0.72	0	1,1,1	0.24	0
2	FMT	S1	101	-	2,2,2	0.73	0	1,1,1	0.21	0
2	FMT	Z3	101	-	2,2,2	0.70	0	1,1,1	0.18	0
2	FMT	d2	101	-	2,2,2	0.71	0	1,1,1	0.19	0
2	FMT	N1	101	-	2,2,2	0.72	0	1,1,1	0.19	0
2	FMT	81	101	-	2,2,2	0.71	0	1,1,1	0.25	0
2	FMT	44	101	-	2,2,2	0.70	0	1,1,1	0.20	0
2	FMT	L4	101	-	2,2,2	0.67	0	1,1,1	0.11	0
2	FMT	Q3	101	-	2,2,2	0.70	0	1,1,1	0.23	0
2	FMT	j3	101	-	2,2,2	0.71	0	1,1,1	0.21	0
2	FMT	L2	101	-	2,2,2	0.68	0	1,1,1	0.03	0
2	FMT	14	101	-	2,2,2	0.75	0	1,1,1	0.27	0
2	FMT	c4	101	-	2,2,2	0.69	0	1,1,1	0.13	0
2	FMT	M2	101	-	2,2,2	0.70	0	1,1,1	0.20	0
2	FMT	O2	101	-	2,2,2	0.70	0	1,1,1	0.19	0
2	FMT	T3	101	-	2,2,2	0.72	0	1,1,1	0.20	0
2	FMT	P3	101	-	2,2,2	0.67	0	1,1,1	0.09	0
2	FMT	m2	101	-	2,2,2	0.73	0	1,1,1	0.25	0
2	FMT	I4	101	-	2,2,2	0.70	0	1,1,1	0.20	0
2	FMT	J2	101	-	2,2,2	0.69	0	1,1,1	0.20	0
2	FMT	B4	101	-	2,2,2	0.70	0	1,1,1	0.16	0
2	FMT	W4	101	-	2,2,2	0.69	0	1,1,1	0.19	0
2	FMT	B3	101	-	2,2,2	0.71	0	1,1,1	0.20	0
2	FMT	E4	101	-	2,2,2	0.73	0	1,1,1	0.24	0
2	FMT	v3	101	-	2,2,2	0.71	0	1,1,1	0.18	0
2	FMT	i2	101	-	2,2,2	0.71	0	1,1,1	0.20	0
2	FMT	x4	101	-	2,2,2	0.69	0	1,1,1	0.16	0
2	FMT	x1	101	-	2,2,2	0.70	0	1,1,1	0.15	0
2	FMT	72	101	-	2,2,2	0.70	0	1,1,1	0.21	0
2	FMT	E1	101	-	2,2,2	0.70	0	1,1,1	0.16	0
2	FMT	g1	101	-	2,2,2	0.62	0	1,1,1	0.05	0
2	FMT	n2	101	-	2,2,2	0.74	0	1,1,1	0.23	0
2	FMT	G3	101	-	2,2,2	0.69	0	1,1,1	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMT	92	101	-	2,2,2	0.70	0	1,1,1	0.18	0
2	FMT	R4	101	-	2,2,2	0.69	0	1,1,1	0.21	0
2	FMT	E3	101	-	2,2,2	0.71	0	1,1,1	0.21	0
2	FMT	r2	101	-	2,2,2	0.73	0	1,1,1	0.24	0
2	FMT	F3	101	-	2,2,2	0.71	0	1,1,1	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	R3	101	-	-	4/5/5/5	-
3	MPD	W2	101	-	-	2/5/5/5	-
3	MPD	q3	101	-	-	3/5/5/5	-
3	MPD	74	101	-	-	2/5/5/5	-
3	MPD	G2	102	-	-	4/5/5/5	-
3	MPD	X3	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	R3	101	MPD	C2-C3-C4-O4
3	R3	101	MPD	C2-C3-C4-C5
3	W2	101	MPD	C2-C3-C4-O4
3	q3	101	MPD	C2-C3-C4-C5
3	q3	101	MPD	O2-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	W2	101	MPD	9	0
3	74	101	MPD	15	0
3	X3	101	MPD	2	0
3	R3	101	MPD	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H1	101	FMT	1	0
3	G2	102	MPD	4	0
2	L2	101	FMT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	11	25/27 (92%)	-0.00	0 100 100	58, 70, 90, 104	0
1	12	25/27 (92%)	0.17	1 (4%) 42 38	68, 87, 102, 134	0
1	13	25/27 (92%)	0.14	0 100 100	64, 75, 118, 122	0
1	14	25/27 (92%)	0.51	1 (4%) 42 38	71, 94, 129, 139	0
1	21	25/27 (92%)	0.45	1 (4%) 42 38	60, 77, 102, 116	0
1	22	25/27 (92%)	0.32	0 100 100	63, 80, 105, 142	0
1	23	25/27 (92%)	0.62	0 100 100	74, 89, 114, 135	0
1	24	25/27 (92%)	0.57	1 (4%) 42 38	68, 89, 114, 126	0
1	31	25/27 (92%)	0.49	1 (4%) 42 38	67, 85, 109, 135	0
1	32	25/27 (92%)	0.24	1 (4%) 42 38	49, 81, 100, 121	1 (4%)
1	33	25/27 (92%)	0.24	0 100 100	73, 86, 105, 118	0
1	34	25/27 (92%)	0.13	0 100 100	69, 77, 106, 116	0
1	41	25/27 (92%)	0.04	0 100 100	63, 76, 91, 100	0
1	42	25/27 (92%)	-0.04	0 100 100	58, 67, 81, 103	0
1	43	25/27 (92%)	-0.03	0 100 100	62, 78, 105, 108	0
1	44	25/27 (92%)	-0.19	0 100 100	58, 68, 88, 96	0
1	51	25/27 (92%)	0.41	1 (4%) 42 38	60, 76, 111, 138	0
1	52	25/27 (92%)	0.26	0 100 100	44, 71, 96, 105	1 (4%)
1	53	25/27 (92%)	0.08	0 100 100	63, 74, 103, 111	0
1	54	25/27 (92%)	0.26	0 100 100	66, 83, 109, 122	0
1	61	25/27 (92%)	0.17	0 100 100	63, 78, 104, 111	0
1	62	25/27 (92%)	0.18	0 100 100	66, 82, 107, 120	0
1	63	25/27 (92%)	0.19	1 (4%) 42 38	61, 76, 91, 100	0
1	64	25/27 (92%)	0.09	0 100 100	62, 78, 97, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	71	25/27 (92%)	0.09	0	100	100	65, 72, 96, 129	0
1	72	25/27 (92%)	-0.09	0	100	100	66, 79, 111, 115	0
1	73	25/27 (92%)	0.19	0	100	100	42, 71, 94, 99	1 (4%)
1	74	25/27 (92%)	0.09	0	100	100	61, 78, 90, 110	0
1	81	25/27 (92%)	0.12	1 (4%)	42	38	61, 75, 105, 122	0
1	82	25/27 (92%)	0.04	0	100	100	66, 76, 90, 105	0
1	83	25/27 (92%)	0.08	0	100	100	64, 78, 100, 118	0
1	84	25/27 (92%)	0.09	0	100	100	67, 81, 101, 106	0
1	91	25/27 (92%)	0.20	0	100	100	64, 78, 98, 106	0
1	92	25/27 (92%)	0.06	0	100	100	61, 75, 94, 108	0
1	93	25/27 (92%)	0.05	0	100	100	61, 70, 89, 99	0
1	94	25/27 (92%)	0.07	1 (4%)	42	38	57, 69, 87, 93	0
1	A1	25/27 (92%)	-0.21	0	100	100	55, 70, 91, 99	0
1	A2	25/27 (92%)	0.02	0	100	100	57, 71, 87, 96	0
1	A3	25/27 (92%)	0.01	0	100	100	60, 76, 102, 105	0
1	A4	25/27 (92%)	-0.08	0	100	100	54, 67, 91, 103	0
1	B1	25/27 (92%)	0.00	0	100	100	59, 74, 91, 112	0
1	B2	25/27 (92%)	0.05	0	100	100	59, 71, 86, 111	0
1	B3	25/27 (92%)	0.11	0	100	100	72, 88, 121, 132	0
1	B4	25/27 (92%)	0.34	0	100	100	69, 84, 104, 111	0
1	C1	25/27 (92%)	0.30	0	100	100	75, 94, 113, 134	0
1	C2	25/27 (92%)	0.35	0	100	100	75, 88, 109, 123	0
1	C3	25/27 (92%)	0.18	0	100	100	79, 87, 122, 128	0
1	C4	25/27 (92%)	0.61	0	100	100	75, 87, 126, 153	0
1	D1	25/27 (92%)	0.31	0	100	100	67, 88, 105, 128	0
1	D2	25/27 (92%)	0.24	0	100	100	65, 83, 94, 126	0
1	D3	25/27 (92%)	0.10	0	100	100	61, 75, 101, 110	0
1	D4	25/27 (92%)	0.24	0	100	100	59, 74, 95, 103	0
1	E1	25/27 (92%)	0.47	1 (4%)	42	38	42, 74, 102, 111	1 (4%)
1	E2	25/27 (92%)	-0.05	0	100	100	56, 71, 86, 104	0
1	E3	25/27 (92%)	0.22	0	100	100	61, 73, 94, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E4	25/27 (92%)	0.06	0 100 100	63, 74, 100, 107	0
1	F1	25/27 (92%)	0.11	0 100 100	65, 78, 96, 108	0
1	F2	25/27 (92%)	0.19	0 100 100	61, 73, 91, 94	0
1	F3	25/27 (92%)	-0.11	0 100 100	62, 77, 87, 96	0
1	F4	25/27 (92%)	0.09	0 100 100	61, 74, 92, 103	0
1	G1	25/27 (92%)	0.15	1 (4%) 42 38	63, 73, 99, 108	0
1	G2	25/27 (92%)	0.28	0 100 100	43, 74, 109, 129	1 (4%)
1	G3	25/27 (92%)	0.46	1 (4%) 42 38	65, 81, 103, 125	0
1	G4	25/27 (92%)	0.27	0 100 100	64, 80, 97, 130	0
1	H1	25/27 (92%)	0.47	0 100 100	70, 85, 110, 113	0
1	H2	25/27 (92%)	0.24	0 100 100	62, 78, 113, 115	0
1	H3	25/27 (92%)	0.18	0 100 100	62, 76, 100, 139	0
1	H4	25/27 (92%)	0.04	0 100 100	59, 81, 100, 123	0
1	I1	25/27 (92%)	0.16	0 100 100	64, 75, 109, 121	0
1	I2	25/27 (92%)	0.23	0 100 100	64, 85, 120, 128	0
1	I3	25/27 (92%)	0.04	0 100 100	52, 67, 85, 112	0
1	I4	25/27 (92%)	0.49	0 100 100	58, 76, 93, 129	0
1	J1	25/27 (92%)	-0.15	0 100 100	52, 61, 85, 90	0
1	J2	25/27 (92%)	0.02	0 100 100	56, 66, 89, 96	0
1	J3	25/27 (92%)	-0.39	0 100 100	54, 64, 82, 100	0
1	J4	25/27 (92%)	0.06	0 100 100	57, 68, 82, 90	0
1	K1	25/27 (92%)	0.32	1 (4%) 42 38	65, 80, 94, 115	0
1	K2	25/27 (92%)	-0.04	0 100 100	60, 77, 93, 118	0
1	K3	25/27 (92%)	0.28	0 100 100	66, 76, 93, 109	0
1	K4	25/27 (92%)	-0.05	0 100 100	60, 70, 92, 97	0
1	L1	25/27 (92%)	0.21	0 100 100	43, 73, 91, 94	1 (4%)
1	L2	25/27 (92%)	0.10	0 100 100	55, 68, 86, 96	0
1	L3	25/27 (92%)	-0.03	0 100 100	61, 74, 94, 98	0
1	L4	25/27 (92%)	0.10	0 100 100	62, 68, 92, 97	0
1	M1	25/27 (92%)	0.18	1 (4%) 42 38	63, 78, 97, 112	0
1	M2	25/27 (92%)	0.22	0 100 100	68, 81, 92, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	M3	25/27 (92%)	0.20	0 100 100	67, 80, 110, 120	0
1	M4	25/27 (92%)	0.02	0 100 100	67, 82, 107, 114	0
1	N1	25/27 (92%)	0.29	1 (4%) 42 38	63, 79, 107, 121	0
1	N2	25/27 (92%)	0.01	0 100 100	61, 80, 99, 117	0
1	N3	25/27 (92%)	0.37	0 100 100	69, 84, 133, 146	0
1	N4	25/27 (92%)	0.27	0 100 100	73, 87, 121, 137	0
1	O1	25/27 (92%)	0.59	0 100 100	70, 93, 115, 139	0
1	O2	25/27 (92%)	0.30	0 100 100	74, 90, 115, 135	0
1	O3	25/27 (92%)	0.42	2 (8%) 18 16	74, 88, 119, 125	0
1	O4	25/27 (92%)	0.49	1 (4%) 42 38	72, 91, 115, 165	0
1	P1	25/27 (92%)	0.33	0 100 100	68, 83, 111, 121	0
1	P2	25/27 (92%)	0.44	1 (4%) 42 38	71, 84, 104, 131	0
1	P3	25/27 (92%)	0.20	0 100 100	69, 80, 106, 119	0
1	P4	25/27 (92%)	0.39	0 100 100	69, 85, 105, 117	0
1	Q1	25/27 (92%)	0.28	0 100 100	61, 77, 97, 110	0
1	Q2	25/27 (92%)	0.28	0 100 100	64, 82, 94, 122	0
1	Q3	25/27 (92%)	0.39	0 100 100	70, 81, 117, 119	0
1	Q4	25/27 (92%)	0.22	0 100 100	72, 82, 109, 126	0
1	R1	25/27 (92%)	0.25	0 100 100	68, 83, 99, 114	0
1	R2	25/27 (92%)	0.25	0 100 100	68, 78, 102, 115	0
1	R3	25/27 (92%)	0.36	0 100 100	73, 87, 96, 107	0
1	R4	25/27 (92%)	0.12	0 100 100	68, 81, 93, 108	0
1	S1	25/27 (92%)	0.02	0 100 100	73, 85, 108, 110	0
1	S2	25/27 (92%)	0.00	0 100 100	71, 80, 112, 126	0
1	S3	25/27 (92%)	0.37	1 (4%) 42 38	58, 86, 101, 124	1 (4%)
1	S4	25/27 (92%)	0.25	0 100 100	68, 82, 102, 123	0
1	T1	25/27 (92%)	0.38	0 100 100	75, 90, 107, 113	0
1	T2	25/27 (92%)	0.52	0 100 100	75, 92, 113, 129	0
1	T3	25/27 (92%)	0.15	0 100 100	69, 81, 99, 107	0
1	T4	25/27 (92%)	0.20	0 100 100	67, 85, 105, 144	0
1	U1	25/27 (92%)	0.52	0 100 100	77, 90, 108, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	U2	25/27 (92%)	0.31	0 100 100	73, 85, 107, 117	0
1	U3	25/27 (92%)	0.44	1 (4%) 42 38	73, 89, 111, 125	0
1	U4	25/27 (92%)	0.23	0 100 100	72, 84, 103, 115	0
1	V1	25/27 (92%)	0.39	0 100 100	74, 89, 115, 138	0
1	V2	25/27 (92%)	0.49	0 100 100	79, 91, 123, 133	0
1	V3	25/27 (92%)	0.59	2 (8%) 18 16	74, 89, 113, 136	0
1	V4	25/27 (92%)	0.32	1 (4%) 42 38	76, 87, 106, 136	0
1	W1	25/27 (92%)	0.30	1 (4%) 42 38	74, 88, 108, 130	0
1	W2	25/27 (92%)	0.18	0 100 100	76, 91, 119, 125	0
1	W3	25/27 (92%)	0.26	0 100 100	72, 85, 106, 106	0
1	W4	25/27 (92%)	0.30	1 (4%) 42 38	78, 88, 102, 112	0
1	X1	25/27 (92%)	0.32	0 100 100	67, 85, 109, 125	0
1	X2	25/27 (92%)	-0.05	0 100 100	67, 79, 94, 118	0
1	X3	25/27 (92%)	0.27	0 100 100	72, 87, 121, 130	0
1	X4	25/27 (92%)	0.13	0 100 100	64, 77, 105, 117	0
1	Y1	25/27 (92%)	0.01	0 100 100	65, 80, 94, 104	0
1	Y2	25/27 (92%)	0.05	0 100 100	61, 72, 84, 100	0
1	Y3	25/27 (92%)	0.22	0 100 100	68, 81, 103, 114	0
1	Y4	25/27 (92%)	0.26	0 100 100	66, 76, 92, 97	0
1	Z1	25/27 (92%)	0.02	0 100 100	66, 76, 95, 113	0
1	Z2	25/27 (92%)	0.07	1 (4%) 42 38	64, 75, 101, 122	0
1	Z3	25/27 (92%)	0.19	1 (4%) 42 38	64, 75, 95, 99	0
1	Z4	25/27 (92%)	0.12	0 100 100	65, 76, 91, 104	0
1	a1	25/27 (92%)	-0.02	0 100 100	56, 66, 87, 116	0
1	a2	25/27 (92%)	0.01	0 100 100	61, 71, 87, 105	0
1	a3	25/27 (92%)	0.13	0 100 100	61, 71, 92, 99	0
1	a4	25/27 (92%)	0.16	1 (4%) 42 38	61, 77, 91, 104	0
1	b1	25/27 (92%)	0.11	0 100 100	63, 80, 105, 114	0
1	b2	25/27 (92%)	0.20	0 100 100	68, 84, 105, 116	0
1	b3	25/27 (92%)	0.24	0 100 100	72, 85, 119, 133	0
1	b4	25/27 (92%)	0.47	0 100 100	73, 88, 109, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	c1	25/27 (92%)	0.36	0 100 100	75, 91, 111, 122	0
1	c2	25/27 (92%)	0.26	0 100 100	72, 86, 107, 118	0
1	c3	25/27 (92%)	0.18	0 100 100	70, 83, 98, 109	0
1	c4	25/27 (92%)	0.47	2 (8%) 18 16	70, 85, 114, 135	0
1	d1	25/27 (92%)	0.15	0 100 100	70, 83, 106, 120	0
1	d2	25/27 (92%)	-0.05	0 100 100	69, 77, 98, 110	0
1	d3	25/27 (92%)	0.11	0 100 100	73, 85, 103, 118	0
1	d4	25/27 (92%)	0.12	0 100 100	69, 81, 105, 110	0
1	e1	25/27 (92%)	0.23	0 100 100	66, 83, 107, 130	0
1	e2	25/27 (92%)	0.16	0 100 100	61, 73, 88, 106	0
1	e3	25/27 (92%)	0.37	0 100 100	73, 88, 111, 124	0
1	e4	25/27 (92%)	-0.03	0 100 100	64, 71, 99, 107	0
1	f1	25/27 (92%)	0.25	0 100 100	66, 81, 106, 110	0
1	f2	25/27 (92%)	0.17	0 100 100	62, 74, 103, 121	0
1	f3	25/27 (92%)	0.21	0 100 100	67, 82, 105, 121	0
1	f4	25/27 (92%)	0.10	0 100 100	68, 81, 113, 126	0
1	g1	25/27 (92%)	0.16	0 100 100	70, 86, 108, 131	0
1	g2	25/27 (92%)	0.20	0 100 100	76, 89, 112, 119	0
1	g3	25/27 (92%)	0.55	1 (4%) 42 38	73, 87, 114, 137	0
1	g4	25/27 (92%)	0.34	1 (4%) 42 38	78, 95, 113, 118	0
1	h1	25/27 (92%)	0.35	0 100 100	75, 89, 112, 122	0
1	h2	25/27 (92%)	0.62	1 (4%) 42 38	74, 90, 105, 120	0
1	h3	25/27 (92%)	0.26	0 100 100	71, 86, 110, 120	0
1	h4	25/27 (92%)	0.22	0 100 100	65, 80, 110, 114	0
1	i1	25/27 (92%)	0.01	0 100 100	59, 81, 95, 121	0
1	i2	25/27 (92%)	0.10	0 100 100	64, 75, 87, 107	0
1	i3	25/27 (92%)	0.09	0 100 100	68, 80, 98, 117	0
1	i4	25/27 (92%)	0.34	1 (4%) 42 38	68, 84, 108, 114	0
1	j1	25/27 (92%)	0.08	0 100 100	74, 82, 120, 134	0
1	j2	25/27 (92%)	0.39	2 (8%) 18 16	73, 93, 114, 125	0
1	j3	25/27 (92%)	0.36	0 100 100	75, 90, 112, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	j4	25/27 (92%)	0.42	2 (8%) 18 16	85, 103, 117, 133	0
1	k1	25/27 (92%)	0.40	0 100 100	80, 93, 113, 152	0
1	k2	25/27 (92%)	0.47	2 (8%) 18 16	90, 107, 125, 152	0
1	k3	25/27 (92%)	0.61	3 (12%) 9 7	50, 103, 137, 141	1 (4%)
1	k4	25/27 (92%)	0.58	1 (4%) 42 38	83, 116, 145, 172	0
1	l1	25/27 (92%)	0.34	1 (4%) 42 38	73, 88, 113, 133	0
1	l2	25/27 (92%)	0.58	1 (4%) 42 38	81, 103, 140, 175	0
1	l3	25/27 (92%)	0.58	1 (4%) 42 38	81, 96, 140, 152	0
1	l4	25/27 (92%)	0.70	0 100 100	88, 114, 159, 174	0
1	m1	25/27 (92%)	0.83	4 (16%) 5 4	84, 105, 119, 152	0
1	m2	25/27 (92%)	0.65	2 (8%) 18 16	79, 105, 133, 155	0
1	m3	25/27 (92%)	0.63	0 100 100	83, 101, 126, 142	0
1	m4	25/27 (92%)	0.55	2 (8%) 18 16	83, 103, 130, 141	0
1	n1	25/27 (92%)	0.31	0 100 100	82, 100, 122, 132	0
1	n2	25/27 (92%)	0.31	0 100 100	75, 92, 116, 124	0
1	n3	25/27 (92%)	0.28	0 100 100	83, 110, 147, 174	0
1	n4	25/27 (92%)	0.27	0 100 100	73, 92, 124, 153	0
1	o1	25/27 (92%)	0.95	2 (8%) 18 16	85, 108, 133, 172	0
1	o2	25/27 (92%)	0.43	0 100 100	72, 90, 114, 161	0
1	o3	25/27 (92%)	0.43	0 100 100	77, 96, 119, 134	0
1	o4	25/27 (92%)	0.29	1 (4%) 42 38	75, 84, 115, 130	0
1	p1	25/27 (92%)	0.72	1 (4%) 42 38	77, 95, 115, 129	0
1	p2	25/27 (92%)	0.47	0 100 100	74, 88, 117, 138	0
1	p3	25/27 (92%)	0.80	4 (16%) 5 4	62, 93, 112, 128	0
1	p4	25/27 (92%)	0.47	0 100 100	76, 98, 131, 141	0
1	q1	25/27 (92%)	0.19	0 100 100	66, 82, 125, 132	0
1	q2	25/27 (92%)	0.30	0 100 100	71, 90, 139, 155	0
1	q3	25/27 (92%)	0.32	0 100 100	56, 80, 115, 145	0
1	q4	25/27 (92%)	0.12	0 100 100	58, 82, 117, 155	1 (4%)
1	r1	25/27 (92%)	0.40	0 100 100	47, 89, 122, 129	1 (4%)
1	r2	25/27 (92%)	0.25	1 (4%) 42 38	73, 91, 121, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	r3	25/27 (92%)	0.43	1 (4%) 42 38	74, 91, 112, 139	0
1	r4	25/27 (92%)	0.10	0 100 100	69, 88, 110, 126	0
1	s1	25/27 (92%)	0.39	1 (4%) 42 38	74, 88, 116, 133	0
1	s2	25/27 (92%)	0.08	0 100 100	75, 86, 102, 105	0
1	s3	25/27 (92%)	0.15	1 (4%) 42 38	66, 83, 102, 111	0
1	s4	25/27 (92%)	0.18	1 (4%) 42 38	67, 81, 97, 105	0
1	t1	25/27 (92%)	0.04	0 100 100	71, 76, 104, 109	0
1	t2	25/27 (92%)	0.09	0 100 100	67, 78, 96, 108	0
1	t3	25/27 (92%)	0.17	0 100 100	66, 79, 99, 103	0
1	t4	25/27 (92%)	0.61	0 100 100	66, 82, 102, 116	0
1	u1	25/27 (92%)	0.33	0 100 100	46, 78, 100, 115	1 (4%)
1	u2	25/27 (92%)	0.23	0 100 100	43, 83, 101, 107	1 (4%)
1	u3	25/27 (92%)	0.25	0 100 100	71, 80, 100, 106	0
1	u4	25/27 (92%)	0.32	1 (4%) 42 38	67, 77, 105, 115	0
1	v1	25/27 (92%)	0.34	1 (4%) 42 38	69, 80, 89, 115	0
1	v2	25/27 (92%)	0.40	0 100 100	73, 85, 103, 109	0
1	v3	25/27 (92%)	0.20	0 100 100	67, 84, 97, 107	0
1	v4	25/27 (92%)	0.34	1 (4%) 42 38	66, 80, 105, 124	0
1	w1	25/27 (92%)	0.18	0 100 100	65, 84, 112, 120	0
1	w2	25/27 (92%)	0.12	0 100 100	67, 80, 111, 118	0
1	w3	25/27 (92%)	0.31	1 (4%) 42 38	68, 81, 97, 117	0
1	w4	25/27 (92%)	0.21	0 100 100	66, 82, 105, 118	0
1	x1	25/27 (92%)	0.58	2 (8%) 18 16	78, 85, 106, 116	0
1	x2	25/27 (92%)	0.32	0 100 100	77, 87, 116, 119	0
1	x3	25/27 (92%)	0.39	1 (4%) 42 38	74, 95, 112, 116	0
1	x4	25/27 (92%)	0.44	0 100 100	80, 91, 105, 132	0
All	All	5900/6372 (92%)	0.25	77 (1%) 75 71	42, 84, 117, 175	12 (0%)

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O4	25	GLY	4.4
1	G3	1	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	V4	7	LEU	3.7
1	g3	24	TRP	3.2
1	v4	1	SER	3.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMT	32	101	3/3	0.68	0.24	117,117,117,118	0
2	FMT	T3	101	3/3	0.72	0.21	116,116,116,117	0
2	FMT	82	101	3/3	0.73	0.14	108,108,108,108	0
2	FMT	m2	101	3/3	0.73	0.11	119,119,119,119	0
2	FMT	42	101	3/3	0.74	0.28	116,116,116,117	0
2	FMT	14	101	3/3	0.74	0.12	124,124,124,124	0
2	FMT	H1	101	3/3	0.74	0.21	104,104,105,105	0
2	FMT	X4	101	3/3	0.75	0.17	108,108,109,109	0
2	FMT	D1	101	3/3	0.75	0.14	126,126,126,126	0
2	FMT	r2	101	3/3	0.75	0.15	110,110,110,110	0
2	FMT	u2	101	3/3	0.75	0.18	108,108,108,109	0
2	FMT	u3	101	3/3	0.75	0.15	115,115,115,115	0
2	FMT	P3	101	3/3	0.76	0.18	111,111,111,111	0
2	FMT	e1	101	3/3	0.76	0.15	113,113,113,113	0
2	FMT	r3	101	3/3	0.77	0.22	113,113,114,114	0
2	FMT	v3	101	3/3	0.77	0.14	109,109,110,110	0
2	FMT	81	101	3/3	0.78	0.20	113,113,113,113	0
2	FMT	k4	101	3/3	0.78	0.14	123,123,123,123	0
2	FMT	A1	102	3/3	0.78	0.17	101,101,102,102	0
2	FMT	b4	101	3/3	0.78	0.13	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMT	B4	101	3/3	0.79	0.17	109,109,109,110	0
2	FMT	e4	102	3/3	0.79	0.17	114,114,115,115	0
2	FMT	H2	101	3/3	0.79	0.19	94,94,94,94	0
2	FMT	L3	101	3/3	0.79	0.20	108,108,109,109	0
2	FMT	O1	101	3/3	0.79	0.20	115,115,115,115	0
2	FMT	O2	101	3/3	0.79	0.21	113,113,114,114	0
2	FMT	D2	101	3/3	0.79	0.22	113,113,113,113	0
2	FMT	93	101	3/3	0.79	0.26	106,106,106,106	0
2	FMT	F4	101	3/3	0.79	0.14	115,115,115,115	0
2	FMT	M2	101	3/3	0.80	0.21	106,106,106,106	0
2	FMT	A1	101	3/3	0.80	0.17	112,112,112,112	0
2	FMT	s2	101	3/3	0.80	0.16	106,106,106,106	0
2	FMT	g4	101	3/3	0.80	0.13	110,110,110,110	0
2	FMT	a4	101	3/3	0.80	0.23	112,112,112,113	0
2	FMT	S2	101	3/3	0.80	0.16	102,102,102,102	0
2	FMT	P2	101	3/3	0.81	0.16	108,108,108,108	0
2	FMT	G3	101	3/3	0.81	0.13	109,109,109,110	0
2	FMT	U1	101	3/3	0.81	0.12	110,110,110,110	0
2	FMT	U2	101	3/3	0.81	0.14	111,111,112,112	0
2	FMT	Z4	101	3/3	0.82	0.17	109,109,109,109	0
2	FMT	B3	101	3/3	0.82	0.17	126,126,126,126	0
2	FMT	24	101	3/3	0.82	0.17	106,106,107,107	0
2	FMT	E4	101	3/3	0.82	0.22	111,111,112,112	0
2	FMT	c4	101	3/3	0.82	0.13	104,104,104,105	0
2	FMT	O3	101	3/3	0.82	0.19	110,110,110,110	0
2	FMT	62	101	3/3	0.82	0.15	115,115,115,115	0
2	FMT	T2	101	3/3	0.82	0.13	110,110,110,110	0
2	FMT	x1	101	3/3	0.82	0.17	110,110,111,111	0
2	FMT	83	101	3/3	0.83	0.17	101,101,101,101	0
2	FMT	92	101	3/3	0.83	0.18	105,105,105,105	0
2	FMT	Y4	101	3/3	0.83	0.15	102,102,102,102	0
2	FMT	d2	101	3/3	0.83	0.19	107,107,107,107	0
2	FMT	72	101	3/3	0.84	0.18	100,100,100,101	0
2	FMT	Q3	101	3/3	0.84	0.23	106,106,106,106	0
2	FMT	K2	101	3/3	0.84	0.18	110,110,110,110	0
2	FMT	m4	101	3/3	0.84	0.19	123,123,123,123	0
2	FMT	o4	101	3/3	0.84	0.16	116,116,116,116	0
2	FMT	w4	101	3/3	0.84	0.15	112,112,112,112	0
2	FMT	g1	101	3/3	0.84	0.18	110,110,111,111	0
2	FMT	L2	101	3/3	0.85	0.11	97,97,98,98	0
2	FMT	S1	101	3/3	0.85	0.15	116,116,116,116	0
2	FMT	n2	101	3/3	0.85	0.09	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMT	I4	101	3/3	0.85	0.15	100,100,100,100	0
2	FMT	x4	101	3/3	0.85	0.18	113,113,113,113	0
2	FMT	W4	101	3/3	0.86	0.16	111,111,111,111	0
2	FMT	f4	101	3/3	0.86	0.21	106,106,106,106	0
2	FMT	H3	101	3/3	0.86	0.17	100,100,100,100	0
2	FMT	E1	101	3/3	0.86	0.15	119,119,119,119	0
2	FMT	i1	101	3/3	0.86	0.16	114,114,114,114	0
2	FMT	i2	101	3/3	0.86	0.11	124,124,124,124	0
2	FMT	F3	101	3/3	0.86	0.20	101,101,102,102	0
2	FMT	43	101	3/3	0.86	0.28	122,122,122,122	0
2	FMT	44	101	3/3	0.86	0.15	100,100,100,100	0
2	FMT	e4	101	3/3	0.86	0.17	105,105,105,105	0
2	FMT	L4	101	3/3	0.87	0.21	102,102,102,103	0
2	FMT	b1	101	3/3	0.87	0.15	109,109,109,109	0
2	FMT	Z1	101	3/3	0.87	0.11	95,95,95,95	0
2	FMT	t3	101	3/3	0.87	0.18	105,105,105,105	0
2	FMT	I3	101	3/3	0.87	0.20	102,102,102,102	0
2	FMT	N1	101	3/3	0.87	0.19	107,107,108,108	0
2	FMT	Q2	101	3/3	0.87	0.10	103,103,103,103	0
2	FMT	C2	101	3/3	0.87	0.10	119,119,119,119	0
2	FMT	R4	101	3/3	0.87	0.16	103,103,104,104	0
2	FMT	J2	101	3/3	0.87	0.24	102,102,103,103	0
2	FMT	A3	101	3/3	0.88	0.20	108,108,108,108	0
2	FMT	Z3	101	3/3	0.88	0.14	110,110,110,111	0
2	FMT	m3	101	3/3	0.88	0.15	121,121,121,121	0
2	FMT	d1	101	3/3	0.88	0.12	126,126,127,127	0
2	FMT	t1	101	3/3	0.88	0.16	99,99,99,99	0
2	FMT	j3	101	3/3	0.88	0.17	121,121,121,122	0
2	FMT	A4	101	3/3	0.89	0.13	92,92,93,93	0
2	FMT	E3	101	3/3	0.90	0.15	101,101,101,101	0
2	FMT	j1	101	3/3	0.90	0.13	119,119,120,120	0
3	MPD	W2	101	8/8	0.90	0.17	87,90,91,92	0
3	MPD	X3	101	8/8	0.90	0.19	88,89,92,93	0
3	MPD	q3	101	8/8	0.90	0.19	99,101,103,104	0
2	FMT	l3	101	3/3	0.91	0.11	117,117,117,117	0
2	FMT	h2	101	3/3	0.92	0.15	120,120,120,120	0
2	FMT	G2	101	3/3	0.92	0.17	120,120,120,120	0
3	MPD	G2	102	8/8	0.92	0.17	86,87,91,91	0
3	MPD	R3	101	8/8	0.93	0.13	98,99,101,101	0
2	FMT	q1	101	3/3	0.93	0.10	120,120,120,120	0
3	MPD	74	101	8/8	0.94	0.13	94,95,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.