



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 04:19 PM BST

PDB ID : 4V6B  
Title : Crystal structure of human ferritin Phe167SerfsX26 mutant.  
Authors : Hurley, T.D.; Vidal, R.  
Deposited on : 2009-06-19  
Resolution : 2.85 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

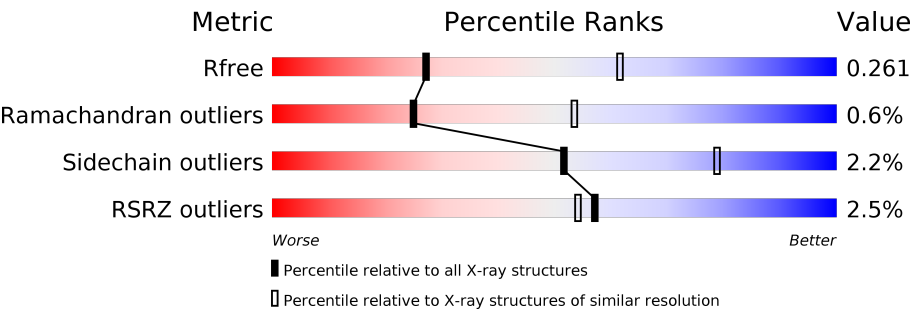
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
<i>R<sub>free</sub></i>	130704	3168 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AA	192	<div><div>3%</div><div><div></div><div>79%</div><div></div><div>18%</div></div><div></div></div>
1	AB	192	<div><div>4%</div><div><div></div><div>82%</div><div></div><div>14%</div></div><div></div></div>
1	AC	192	<div><div>2%</div><div><div></div><div>80%</div><div></div><div>16%</div></div><div></div></div>
1	AD	192	<div><div>2%</div><div><div></div><div>82%</div><div></div><div>17%</div></div><div></div></div>
1	AE	192	<div><div>5%</div><div><div></div><div>83%</div><div></div><div>14%</div></div><div></div></div>
1	AF	192	<div><div>%</div><div><div></div><div>80%</div><div></div><div>18%</div></div><div></div></div>
1	AG	192	<div><div>2%</div><div><div></div><div>81%</div><div></div><div>17%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	AH	192	
1	AI	192	
1	AJ	192	
1	AK	192	
1	AL	192	
1	AM	192	
1	AN	192	
1	AO	192	
1	AP	192	
1	AQ	192	
1	AR	192	
1	AS	192	
1	AT	192	
1	AU	192	
1	AV	192	
1	AW	192	
1	AX	192	
1	Aa	192	
1	Ab	192	
1	Ac	192	
1	Ad	192	
1	Ae	192	
1	Af	192	
1	Ag	192	
1	Ah	192	

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Mol	Chain	Length	Quality of chain
1	Ai	192	
1	Aj	192	
1	Ak	192	
1	Al	192	
1	Am	192	
1	An	192	
1	Ao	192	
1	Ap	192	
1	Aq	192	
1	Ar	192	
1	As	192	
1	At	192	
1	Au	192	
1	Av	192	
1	Aw	192	
1	Ax	192	
1	BA	192	
1	BB	192	
1	BC	192	
1	BD	192	
1	BE	192	
1	BF	192	
1	BG	192	
1	BH	192	
1	BI	192	

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Mol	Chain	Length	Quality of chain
1	BJ	192	 % 80% 18%
1	BK	192	 4% 79% 19%
1	BL	192	 80% 19%
1	BM	192	 % 81% 18%
1	BN	192	 81% 17%
1	BO	192	 2% 81% 17%
1	BP	192	 3% 81% 17%
1	BQ	192	 % 81% 17%
1	BR	192	 2% 82% 16%
1	BS	192	 82% 17%
1	BT	192	 3% 81% 18%
1	BU	192	 % 83% 16%
1	BV	192	 4% 79% 19%
1	BW	192	 2% 83% 16%
1	BX	192	 3% 82% 15%
1	Ba	192	 2% 81% 18%
1	Bb	192	 2% 81% 17%
1	Bc	192	 % 81% 16%
1	Bd	192	 2% 82% 16%
1	Be	192	 % 82% 15%
1	Bf	192	 3% 80% 6% 14%
1	Bg	192	 2% 80% 19%
1	Bh	192	 2% 81% 17%
1	Bi	192	 % 80% 18%
1	Bj	192	 79% 20%

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Mol	Chain	Length	Quality of chain
1	Bk	192	
1	Bl	192	
1	Bm	192	
1	Bn	192	
1	Bo	192	
1	Bp	192	
1	Bq	192	
1	Br	192	
1	Bs	192	
1	Bt	192	
1	Bu	192	
1	Bv	192	
1	Bw	192	
1	Bx	192	
1	CA	192	
1	CB	192	
1	CC	192	
1	CD	192	
1	CE	192	
1	CF	192	
1	CG	192	
1	CH	192	
1	CI	192	
1	CJ	192	
1	CK	192	

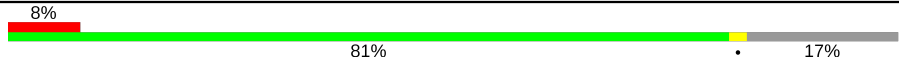
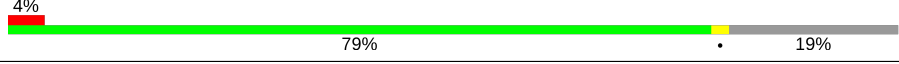



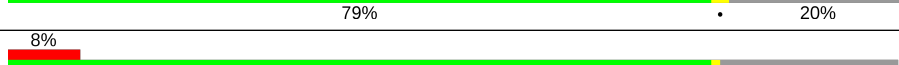
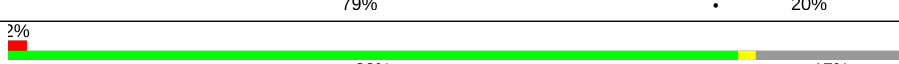
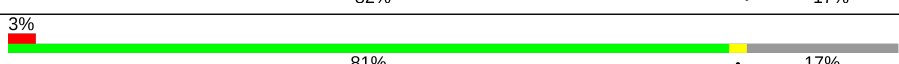
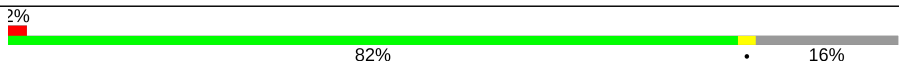



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Mol	Chain	Length	Quality of chain
1	CL	192	
1	CM	192	
1	CN	192	
1	CO	192	
1	CP	192	
1	CQ	192	
1	CR	192	
1	CS	192	
1	CT	192	
1	CU	192	
1	CV	192	
1	CW	192	
1	CX	192	
1	Ca	192	
1	Cb	192	
1	Cc	192	
1	Cd	192	
1	Ce	192	
1	Cf	192	
1	Cg	192	
1	Ch	192	
1	Ci	192	
1	Cj	192	
1	Ck	192	
1	Cl	192	

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Mol	Chain	Length	Quality of chain
1	Cm	192	
1	Cn	192	
1	Co	192	
1	Cp	192	
1	Cq	192	
1	Cr	192	
1	Cs	192	
1	Ct	192	
1	Cu	192	
1	Cv	192	
1	Cw	192	
1	Cx	192	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	Cl	201	-	-	-	X



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 187090 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 Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	158	Total	C	N	O	S	0	0	0
			1270	800	222	243	5			
1	Aa	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	AB	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	Ab	161	Total	C	N	O	S	0	0	0
			1287	810	225	246	6			
1	AC	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	Ac	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	AD	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			
1	Ad	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	AE	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	Ae	162	Total	C	N	O	S	0	0	0
			1298	816	229	247	6			
1	AF	158	Total	C	N	O	S	0	0	0
			1269	800	222	241	6			
1	Af	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	AG	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			
1	Ag	155	Total	C	N	O	S	0	0	0
			1254	791	219	238	6			
1	AH	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	Ah	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AI	158	Total	C	N	O	S	0	0	0
			1269	800	222	241	6			
1	Ai	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			
1	AJ	157	Total	C	N	O	S	0	0	0
			1262	795	221	240	6			
1	Aj	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	AK	157	Total	C	N	O	S	0	0	0
			1269	799	224	240	6			
1	Ak	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	AL	157	Total	C	N	O	S	0	0	0
			1261	795	221	240	5			
1	Al	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	AM	162	Total	C	N	O	S	0	0	0
			1298	816	229	247	6			
1	Am	162	Total	C	N	O	S	0	0	0
			1298	816	229	247	6			
1	AN	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	An	161	Total	C	N	O	S	0	0	0
			1287	810	225	246	6			
1	AO	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	Ao	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	AP	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			
1	Ap	162	Total	C	N	O	S	0	0	0
			1298	816	229	247	6			
1	AQ	165	Total	C	N	O	S	0	0	0
			1319	829	232	252	6			
1	Aq	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	AR	164	Total	C	N	O	S	0	0	0
			1308	823	228	251	6			
1	Ar	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	AS	160	Total	C	N	O	S	0	0	0
			1279	805	224	245	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	As	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	AT	158	Total	C	N	O	S	0	0	0
			1270	800	222	243	5			
1	At	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	AU	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	Au	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	AV	160	Total	C	N	O	S	0	0	0
			1279	805	224	245	5			
1	Av	165	Total	C	N	O	S	0	0	0
			1319	829	232	252	6			
1	AW	158	Total	C	N	O	S	0	0	0
			1270	800	222	243	5			
1	Aw	161	Total	C	N	O	S	0	0	0
			1287	810	225	246	6			
1	AX	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	Ax	155	Total	C	N	O	S	0	0	0
			1254	791	219	238	6			
1	BA	166	Total	C	N	O	S	0	0	0
			1331	838	233	254	6			
1	Ba	158	Total	C	N	O	S	0	0	0
			1269	800	222	241	6			
1	BB	157	Total	C	N	O	S	0	0	0
			1269	799	224	240	6			
1	Bb	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			
1	BC	155	Total	C	N	O	S	0	0	0
			1250	788	219	238	5			
1	Bc	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	BD	160	Total	C	N	O	S	0	0	0
			1289	811	227	245	6			
1	Bd	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	BE	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			
1	Be	163	Total	C	N	O	S	0	0	0
			1300	818	227	250	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BF	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			
1	Bf	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	BG	156	Total	C	N	O	S	0	0	0
			1258	793	220	239	6			
1	Bg	156	Total	C	N	O	S	0	0	0
			1258	793	220	239	6			
1	BH	154	Total	C	N	O	S	0	0	0
			1246	786	218	237	5			
1	Bh	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			
1	BI	155	Total	C	N	O	S	0	0	0
			1254	791	219	238	6			
1	Bi	157	Total	C	N	O	S	0	0	0
			1269	799	224	240	6			
1	BJ	157	Total	C	N	O	S	0	0	0
			1261	795	221	240	5			
1	Bj	154	Total	C	N	O	S	0	0	0
			1244	785	218	236	5			
1	BK	156	Total	C	N	O	S	0	0	0
			1258	793	220	239	6			
1	Bk	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			
1	BL	155	Total	C	N	O	S	0	0	0
			1254	791	219	238	6			
1	Bl	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			
1	BM	158	Total	C	N	O	S	0	0	0
			1270	800	222	243	5			
1	Bm	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			
1	BN	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			
1	Bn	165	Total	C	N	O	S	0	0	0
			1319	829	232	252	6			
1	BO	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	Bo	156	Total	C	N	O	S	0	0	0
			1258	793	220	239	6			
1	BP	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Bp	162	Total	C	N	O	S	0	0	0
			1298	816	229	247	6			
1	BQ	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	Bq	160	Total	C	N	O	S	0	0	0
			1289	811	227	245	6			
1	BR	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	Br	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	BS	159	Total	C	N	O	S	0	0	0
			1280	806	226	242	6			
1	Bs	155	Total	C	N	O	S	0	0	0
			1254	791	219	238	6			
1	BT	157	Total	C	N	O	S	0	0	0
			1261	795	221	240	5			
1	Bt	158	Total	C	N	O	S	0	0	0
			1269	800	222	241	6			
1	BU	162	Total	C	N	O	S	0	0	0
			1298	816	229	247	6			
1	Bu	165	Total	C	N	O	S	0	0	0
			1320	832	229	253	6			
1	BV	156	Total	C	N	O	S	0	0	0
			1254	790	220	239	5			
1	Bv	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	BW	161	Total	C	N	O	S	0	0	0
			1287	810	225	246	6			
1	Bw	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			
1	BX	163	Total	C	N	O	S	0	0	0
			1300	818	227	250	5			
1	Bx	157	Total	C	N	O	S	0	0	0
			1261	795	221	240	5			
1	CA	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	Ca	158	Total	C	N	O	S	0	0	0
			1269	800	222	242	5			
1	CB	161	Total	C	N	O	S	0	0	0
			1287	810	225	246	6			
1	Cb	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CC	157	Total	C	N	O	S	0	0	0
			1261	795	221	240	5			
1	Cc	157	Total	C	N	O	S	0	0	0
			1264	797	221	241	5			
1	CD	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	Cd	153	Total	C	N	O	S	0	0	0
			1240	783	217	235	5			
1	CE	160	Total	C	N	O	S	0	0	0
			1289	811	227	245	6			
1	Ce	154	Total	C	N	O	S	0	0	0
			1246	786	218	237	5			
1	CF	160	Total	C	N	O	S	0	0	0
			1279	805	224	245	5			
1	Cf	153	Total	C	N	O	S	0	0	0
			1238	780	217	236	5			
1	CG	160	Total	C	N	O	S	0	0	0
			1289	811	227	245	6			
1	Cg	160	Total	C	N	O	S	0	0	0
			1279	805	224	245	5			
1	CH	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			
1	Ch	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			
1	CI	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	Ci	153	Total	C	N	O	S	0	0	0
			1240	783	217	235	5			
1	CJ	165	Total	C	N	O	S	0	0	0
			1319	829	232	252	6			
1	Cj	156	Total	C	N	O	S	0	0	0
			1265	797	223	239	6			
1	CK	160	Total	C	N	O	S	0	0	0
			1283	808	224	245	6			
1	Ck	154	Total	C	N	O	S	0	0	0
			1246	786	218	237	5			
1	CL	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			
1	Cl	155	Total	C	N	O	S	0	0	0
			1250	788	219	238	5			
1	CM	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Cm	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			
1	CN	161	Total	C	N	O	S	0	0	0
			1287	810	225	246	6			
1	Cn	155	Total	C	N	O	S	0	0	0
			1254	791	219	238	6			
1	CO	159	Total	C	N	O	S	0	0	0
			1280	806	226	242	6			
1	Co	155	Total	C	N	O	S	0	0	0
			1250	788	219	238	5			
1	CP	158	Total	C	N	O	S	0	0	0
			1269	800	222	241	6			
1	Cp	158	Total	C	N	O	S	0	0	0
			1269	800	222	241	6			
1	CQ	162	Total	C	N	O	S	0	0	0
			1298	816	229	247	6			
1	Cq	155	Total	C	N	O	S	0	0	0
			1250	788	219	238	5			
1	CR	166	Total	C	N	O	S	0	0	0
			1331	838	233	254	6			
1	Cr	154	Total	C	N	O	S	0	0	0
			1246	786	218	237	5			
1	CS	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	Cs	154	Total	C	N	O	S	0	0	0
			1244	785	218	236	5			
1	CT	158	Total	C	N	O	S	0	0	0
			1269	800	222	241	6			
1	Ct	160	Total	C	N	O	S	0	0	0
			1279	805	224	245	5			
1	CU	159	Total	C	N	O	S	0	0	0
			1278	805	223	244	6			
1	Cu	159	Total	C	N	O	S	0	0	0
			1275	803	223	244	5			
1	CV	158	Total	C	N	O	S	0	0	0
			1270	800	222	243	5			
1	Cv	161	Total	C	N	O	S	0	0	0
			1287	810	225	246	6			
1	CW	155	Total	C	N	O	S	0	0	0
			1254	791	219	238	6			
1	Cw	155	Total	C	N	O	S	0	0	0
			1250	788	219	238	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CX	161	Total	C	N	O	S	0	0	0
			1294	814	228	246	6			
1	Cx	156	Total	C	N	O	S	0	0	0
			1265	797	223	239	6			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Aa	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AB	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ab	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AC	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ac	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AD	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ad	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AE	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ae	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AF	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Af	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AG	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ag	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AH	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ah	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AI	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ai	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AJ	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Aj	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AK	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ak	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AL	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Al	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AM	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Am	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AN	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
An	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AO	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ao	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AP	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ap	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AQ	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Aq	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3

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Chain	Residue	Modelled	Actual	Comment	Reference
AR	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ar	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AS	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
As	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AT	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
At	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AU	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Au	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AV	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Av	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AW	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Aw	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
AX	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ax	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BA	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ba	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BB	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bb	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BC	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bc	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BD	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bd	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BE	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Be	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BF	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bf	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BG	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bg	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BH	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bh	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BI	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bi	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BJ	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bj	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BK	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bk	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BL	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bl	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BM	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bm	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BN	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bn	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3

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Chain	Residue	Modelled	Actual	Comment	Reference
BO	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bo	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BP	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bp	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BQ	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bq	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BR	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Br	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BS	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bs	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BT	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bt	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BU	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bu	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BV	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bv	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BW	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bw	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
BX	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Bx	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CA	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ca	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CB	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cb	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CC	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cc	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CD	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cd	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CE	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ce	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CF	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cf	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CG	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cg	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CH	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ch	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CI	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ci	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CJ	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cj	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CK	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ck	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3

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Chain	Residue	Modelled	Actual	Comment	Reference
CL	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cl	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CM	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cm	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CN	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cn	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CO	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Co	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CP	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cp	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CQ	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cq	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CR	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cr	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CS	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cs	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CT	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Ct	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CU	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cu	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CV	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cv	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CW	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cw	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
CX	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3
Cx	0	ARG	-	EXPRESSION TAG	UNP Q6S4P3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Ag	1	Total Ca 1 1	0	0
2	BA	1	Total Ca 1 1	0	0
2	CA	1	Total Ca 1 1	0	0
2	Ah	1	Total Ca 1 1	0	0
2	AB	1	Total Ca 1 1	0	0
2	Ac	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Bd	1	Total 1	Ca 1	0	0
2	CD	1	Total 1	Ca 1	0	0
2	Ce	1	Total 1	Ca 1	0	0
2	Cl	1	Total 1	Ca 1	0	0
2	BB	1	Total 1	Ca 1	0	0
2	Ba	1	Total 1	Ca 1	0	0
2	Ca	1	Total 1	Ca 1	0	0
2	CO	1	Total 1	Ca 1	0	0
2	CF	1	Total 1	Ca 1	0	0
2	Be	1	Total 1	Ca 1	0	0
2	Cb	1	Total 1	Ca 1	0	0
2	AA	1	Total 1	Ca 1	0	0
2	An	1	Total 1	Ca 1	0	0
2	CH	1	Total 1	Ca 1	0	0
2	BC	1	Total 1	Ca 1	0	0
2	AM	1	Total 1	Ca 1	0	0
2	Bb	1	Total 1	Ca 1	0	0
2	Aj	1	Total 1	Ca 1	0	0
2	BN	1	Total 1	Ca 1	0	0
2	Ae	1	Total 1	Ca 1	0	0
2	BG	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	CC	1	Total 1	Ca 1	0	0
2	Bf	1	Total 1	Ca 1	0	0
2	BR	1	Total 1	Ca 1	0	0
2	Aa	1	Total 1	Ca 1	0	0
2	CE	1	Total 1	Ca 1	0	0
2	Cn	1	Total 1	Ca 1	0	0
2	Ck	1	Total 1	Ca 1	0	0
2	AL	1	Total 1	Ca 1	0	0
2	Bc	1	Total 1	Ca 1	0	0
2	Cg	1	Total 1	Ca 1	0	0
2	Bu	1	Total 1	Ca 1	0	0
2	Ad	1	Total 1	Ca 1	0	0
2	AH	1	Total 1	Ca 1	0	0
2	Bg	1	Total 1	Ca 1	0	0
2	AC	1	Total 1	Ca 1	0	0
2	CB	1	Total 1	Ca 1	0	0
2	Cp	1	Total 1	Ca 1	0	0
2	BD	1	Total 1	Ca 1	0	0
2	AO	1	Total 1	Ca 1	0	0
2	AF	1	Total 1	Ca 1	0	0
2	BH	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AA	10	Total O 10 10	0	0
3	Aa	47	Total O 47 47	0	0
3	AB	14	Total O 14 14	0	0
3	Ab	30	Total O 30 30	0	0
3	AC	15	Total O 15 15	0	0
3	Ac	32	Total O 32 32	0	0
3	AD	8	Total O 8 8	0	0
3	Ad	37	Total O 37 37	0	0
3	AE	27	Total O 27 27	0	0
3	Ae	26	Total O 26 26	0	0
3	AF	16	Total O 16 16	0	0
3	Af	48	Total O 48 48	0	0
3	AG	27	Total O 27 27	0	0
3	Ag	37	Total O 37 37	0	0
3	AH	28	Total O 28 28	0	0
3	Ah	28	Total O 28 28	0	0
3	AI	6	Total O 6 6	0	0
3	Ai	40	Total O 40 40	0	0
3	AJ	9	Total O 9 9	0	0
3	Aj	28	Total O 28 28	0	0
3	AK	15	Total O 15 15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Ak	37	Total 37	O 37	0	0
3	AL	11	Total 11	O 11	0	0
3	Al	25	Total 25	O 25	0	0
3	AM	26	Total 26	O 26	0	0
3	Am	45	Total 45	O 45	0	0
3	AN	17	Total 17	O 17	0	0
3	An	41	Total 41	O 41	0	0
3	AO	20	Total 20	O 20	0	0
3	Ao	39	Total 39	O 39	0	0
3	AP	25	Total 25	O 25	0	0
3	Ap	32	Total 32	O 32	0	0
3	AQ	21	Total 21	O 21	0	0
3	Aq	33	Total 33	O 33	0	0
3	AR	18	Total 18	O 18	0	0
3	Ar	40	Total 40	O 40	0	0
3	AS	20	Total 20	O 20	0	0
3	As	44	Total 44	O 44	0	0
3	AT	22	Total 22	O 22	0	0
3	At	31	Total 31	O 31	0	0
3	AU	20	Total 20	O 20	0	0
3	Au	31	Total 31	O 31	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AV	17	Total O 17 17	0	0
3	Av	19	Total O 19 19	0	0
3	AW	19	Total O 19 19	0	0
3	Aw	34	Total O 34 34	0	0
3	AX	33	Total O 33 33	0	0
3	Ax	31	Total O 31 31	0	0
3	BA	15	Total O 15 15	0	0
3	Ba	10	Total O 10 10	0	0
3	BB	5	Total O 5 5	0	0
3	Bb	4	Total O 4 4	0	0
3	BC	2	Total O 2 2	0	0
3	Bc	32	Total O 32 32	0	0
3	BD	10	Total O 10 10	0	0
3	Bd	27	Total O 27 27	0	0
3	BE	15	Total O 15 15	0	0
3	Be	26	Total O 26 26	0	0
3	BF	32	Total O 32 32	0	0
3	Bf	26	Total O 26 26	0	0
3	BG	7	Total O 7 7	0	0
3	Bg	7	Total O 7 7	0	0
3	BH	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Bh	19	Total O 19 19	0	0
3	BI	20	Total O 20 20	0	0
3	Bi	7	Total O 7 7	0	0
3	BJ	8	Total O 8 8	0	0
3	Bj	6	Total O 6 6	0	0
3	BK	6	Total O 6 6	0	0
3	Bk	6	Total O 6 6	0	0
3	BL	10	Total O 10 10	0	0
3	Bl	23	Total O 23 23	0	0
3	BM	25	Total O 25 25	0	0
3	Bm	25	Total O 25 25	0	0
3	BN	18	Total O 18 18	0	0
3	Bn	11	Total O 11 11	0	0
3	BO	13	Total O 13 13	0	0
3	Bo	9	Total O 9 9	0	0
3	BP	10	Total O 10 10	0	0
3	Bp	31	Total O 31 31	0	0
3	BQ	30	Total O 30 30	0	0
3	Bq	18	Total O 18 18	0	0
3	BR	21	Total O 21 21	0	0
3	Br	35	Total O 35 35	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BS	37	Total O 37 37	0	0
3	Bs	15	Total O 15 15	0	0
3	BT	12	Total O 12 12	0	0
3	Bt	11	Total O 11 11	0	0
3	BU	5	Total O 5 5	0	0
3	Bu	28	Total O 28 28	0	0
3	BV	5	Total O 5 5	0	0
3	Bv	25	Total O 25 25	0	0
3	BW	25	Total O 25 25	0	0
3	Bw	39	Total O 39 39	0	0
3	BX	3	Total O 3 3	0	0
3	Bx	7	Total O 7 7	0	0
3	CA	29	Total O 29 29	0	0
3	Ca	11	Total O 11 11	0	0
3	CB	16	Total O 16 16	0	0
3	Cb	6	Total O 6 6	0	0
3	CC	7	Total O 7 7	0	0
3	Cc	7	Total O 7 7	0	0
3	CD	28	Total O 28 28	0	0
3	Cd	6	Total O 6 6	0	0
3	CE	15	Total O 15 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Ce	6	Total O 6 6	0	0
3	CF	25	Total O 25 25	0	0
3	Cf	8	Total O 8 8	0	0
3	CG	19	Total O 19 19	0	0
3	Cg	16	Total O 16 16	0	0
3	CH	10	Total O 10 10	0	0
3	Ch	18	Total O 18 18	0	0
3	CI	30	Total O 30 30	0	0
3	Ci	9	Total O 9 9	0	0
3	CJ	18	Total O 18 18	0	0
3	Cj	9	Total O 9 9	0	0
3	CK	12	Total O 12 12	0	0
3	Ck	11	Total O 11 11	0	0
3	CL	7	Total O 7 7	0	0
3	Cl	2	Total O 2 2	0	0
3	CM	23	Total O 23 23	0	0
3	Cm	2	Total O 2 2	0	0
3	CN	25	Total O 25 25	0	0
3	Cn	4	Total O 4 4	0	0
3	CO	14	Total O 14 14	0	0
3	Co	12	Total O 12 12	0	0

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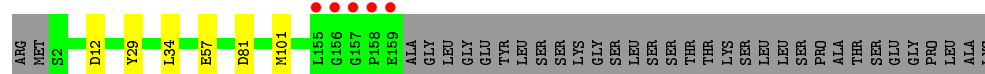
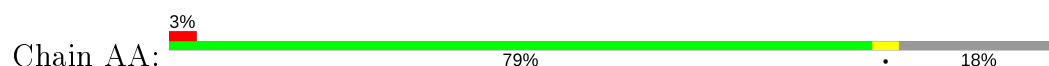
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	CP	14	Total 14	O 14	0	0
3	Cp	10	Total 10	O 10	0	0
3	CQ	41	Total 41	O 41	0	0
3	Cq	2	Total 2	O 2	0	0
3	CR	20	Total 20	O 20	0	0
3	Cr	4	Total 4	O 4	0	0
3	CS	28	Total 28	O 28	0	0
3	CT	15	Total 15	O 15	0	0
3	Ct	17	Total 17	O 17	0	0
3	CU	3	Total 3	O 3	0	0
3	Cu	12	Total 12	O 12	0	0
3	CV	8	Total 8	O 8	0	0
3	Cv	4	Total 4	O 4	0	0
3	CW	15	Total 15	O 15	0	0
3	Cw	10	Total 10	O 10	0	0
3	CX	21	Total 21	O 21	0	0
3	Cx	12	Total 12	O 12	0	0

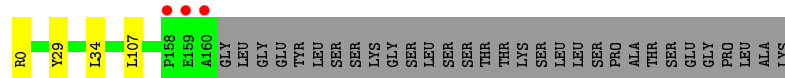
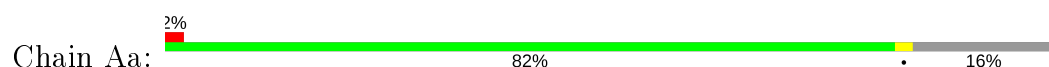
### 3 Residue-property plots [i](#)

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.

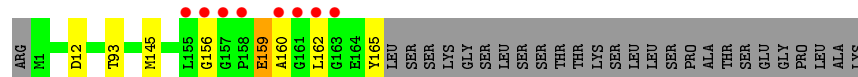
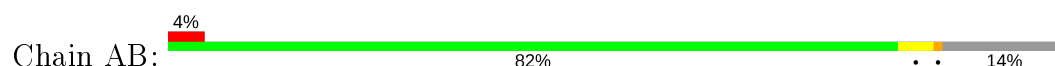
- Molecule 1: Ferritin



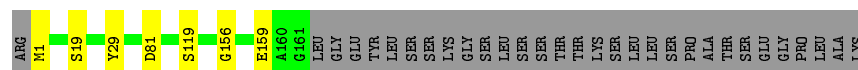
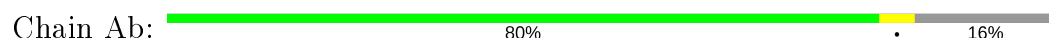
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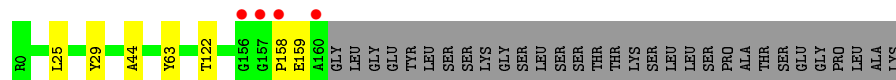
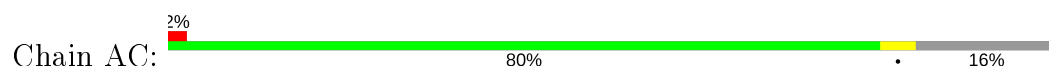
- Molecule 1: Ferritin




- Molecule 1: Ferritin

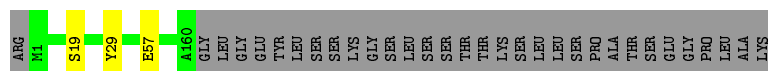


- Molecule 1: Ferritin




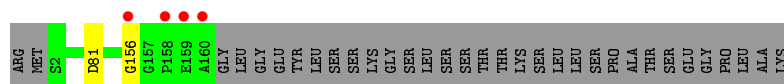
- Molecule 1: Ferritin

Chain Ac:  82% 17%




• Molecule 1: Ferritin

Chain AD:  82% 17%




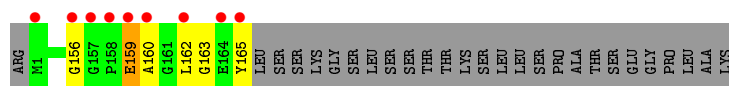
• Molecule 1: Ferritin

Chain Ad:  81% 14% 5% 2%




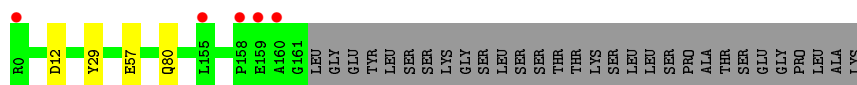
• Molecule 1: Ferritin

Chain AE:  83% 14% 5% 5%




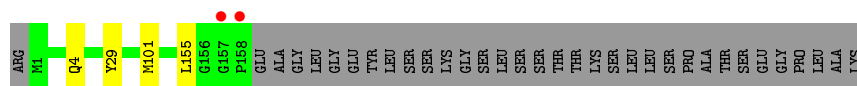
• Molecule 1: Ferritin

Chain Ae:  82% 16% 3% 3%




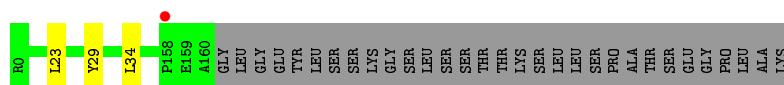
• Molecule 1: Ferritin

Chain AF:  80% 18% 2% 0%

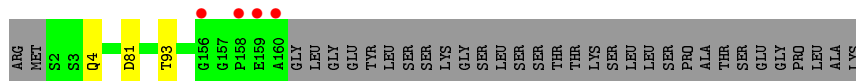
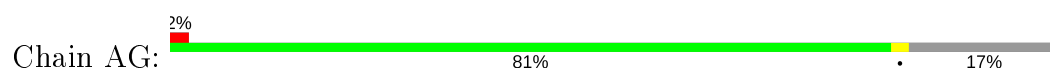


• Molecule 1: Ferritin

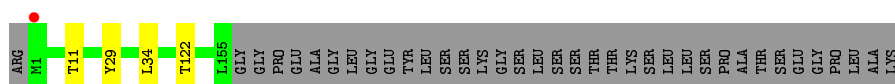
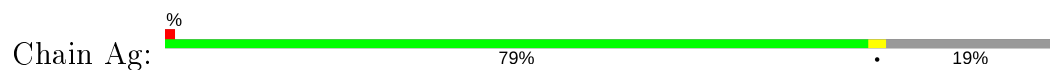
Chain Af:  82% 16% 2% 0%



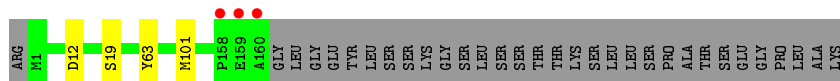
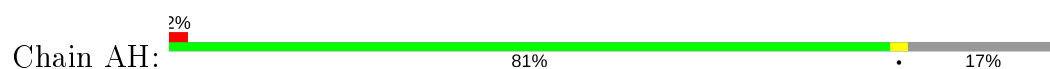
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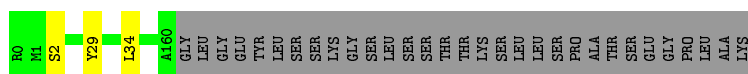
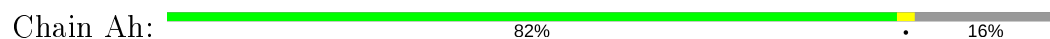
- Molecule 1: Ferritin



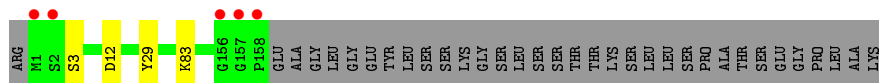
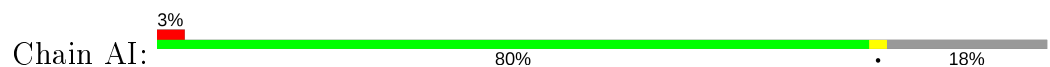
- Molecule 1: Ferritin



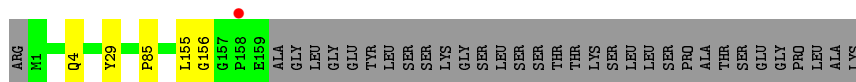
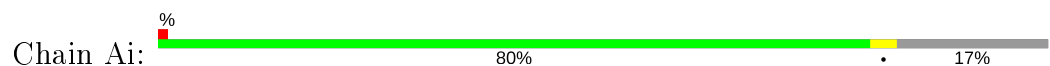
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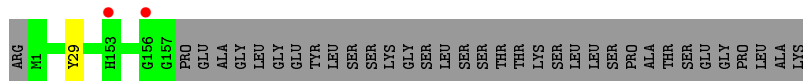
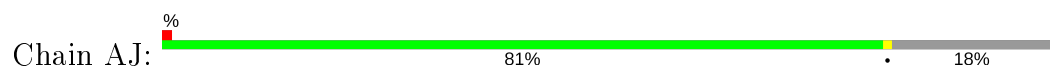
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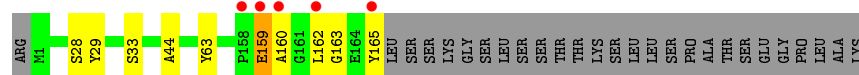
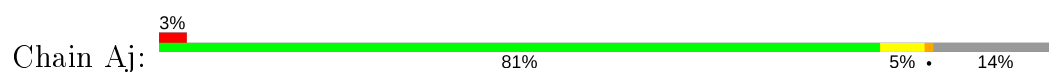
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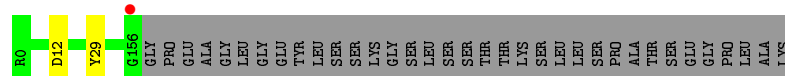
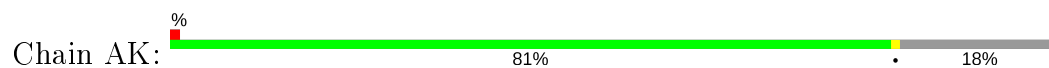
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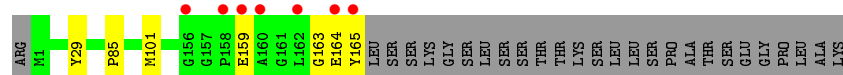
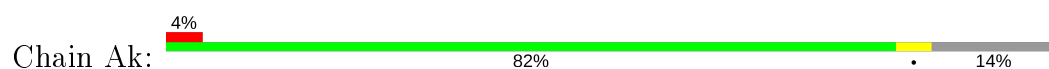
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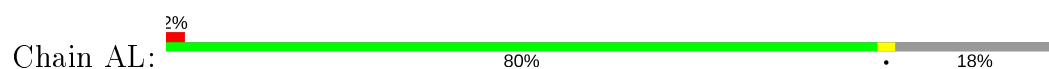
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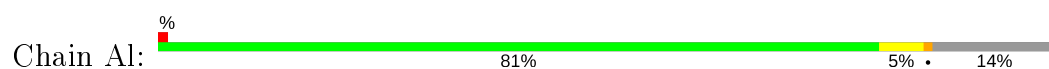
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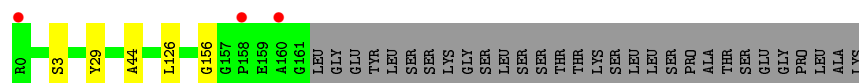
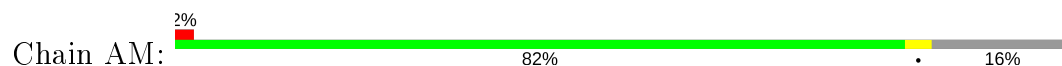
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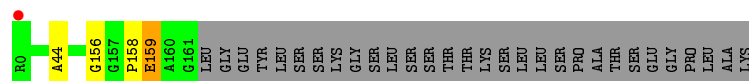
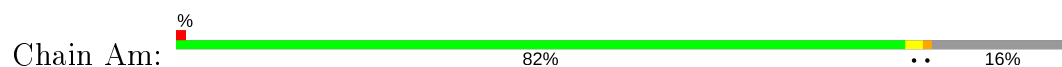
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- Molecule 1: Ferritin

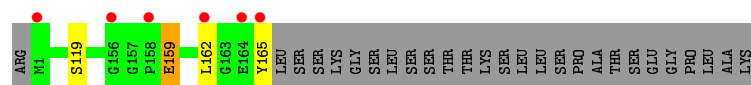
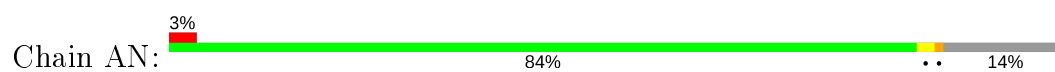


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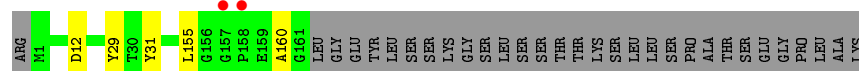
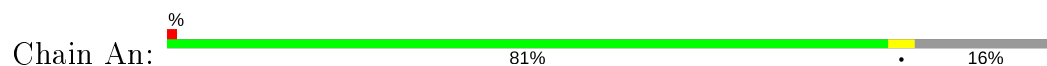


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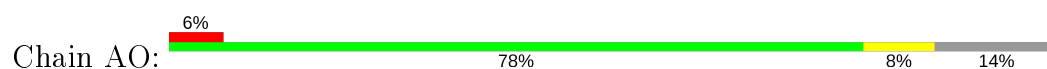




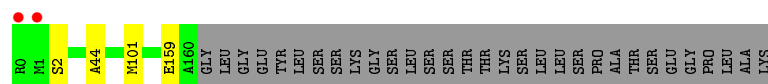
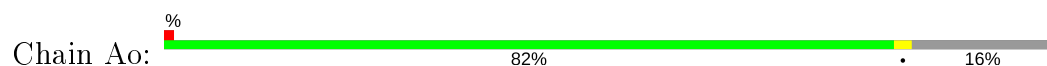
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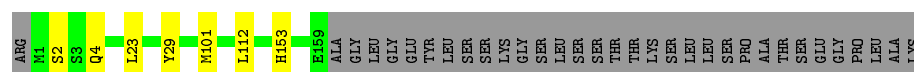
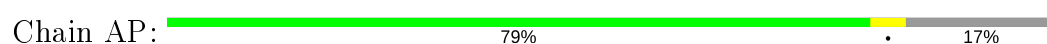
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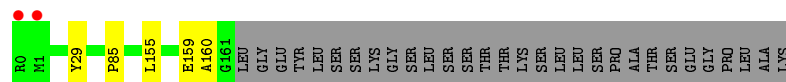
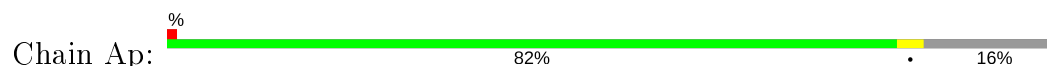
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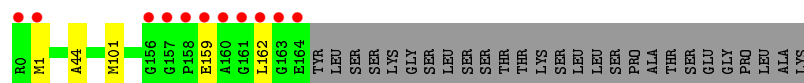
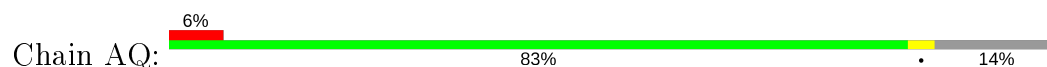
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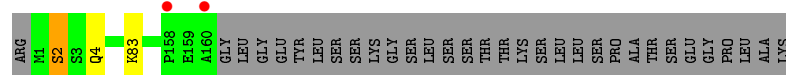
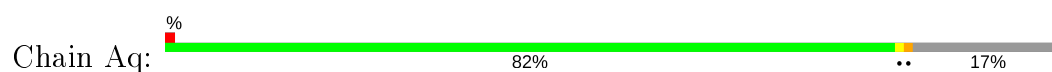
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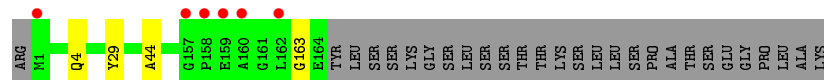
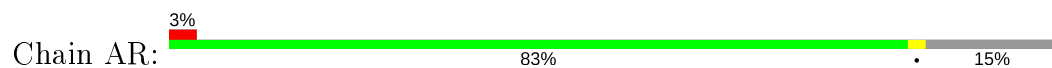
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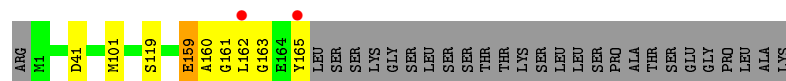
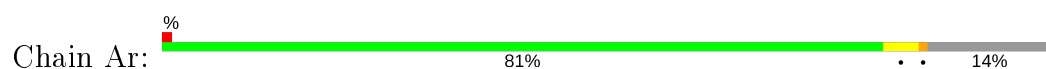
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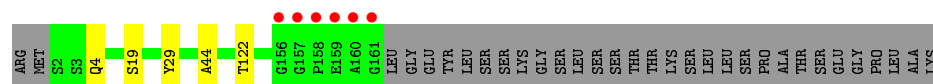
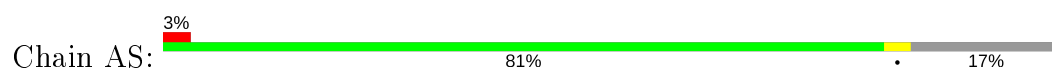
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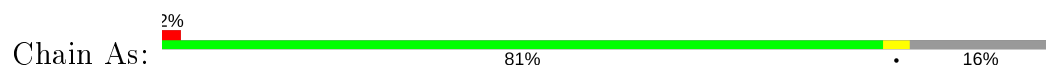
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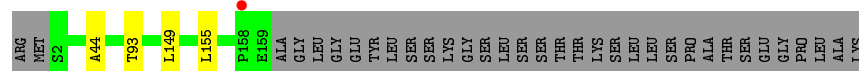
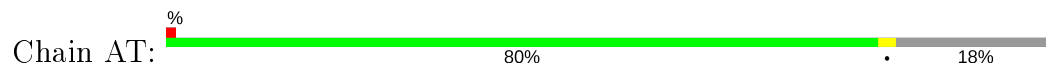
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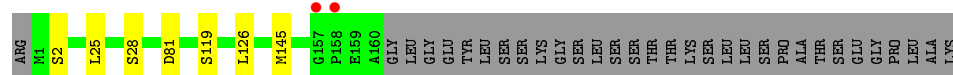
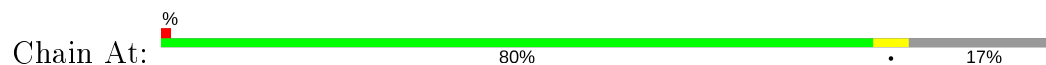
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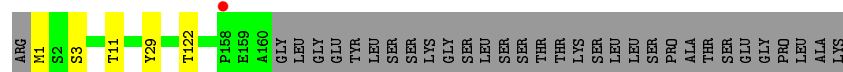
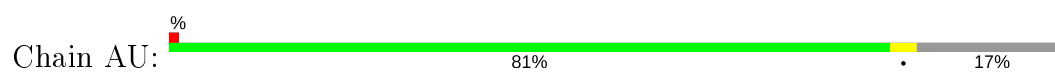
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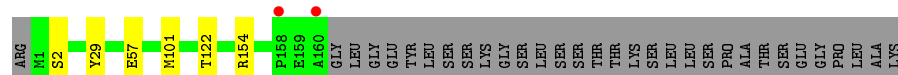
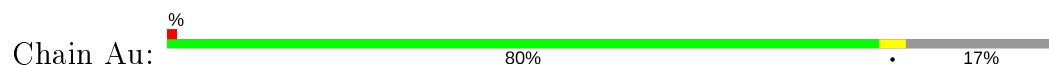
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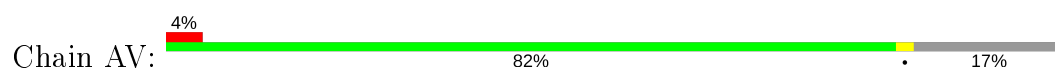
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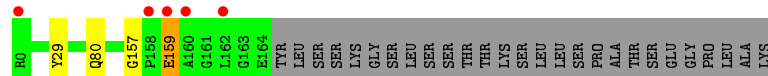
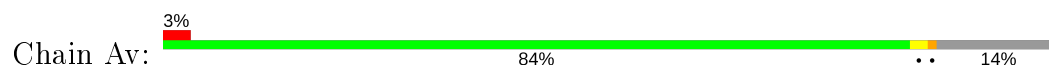
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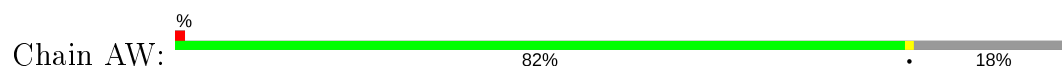
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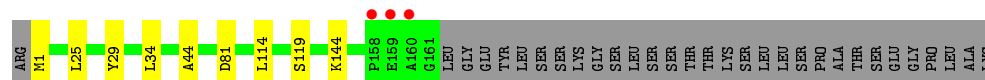
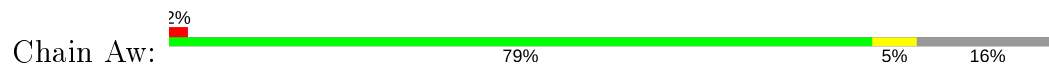
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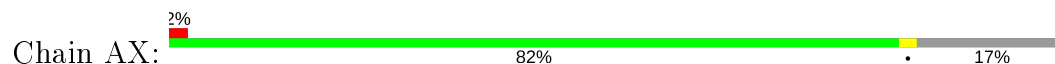
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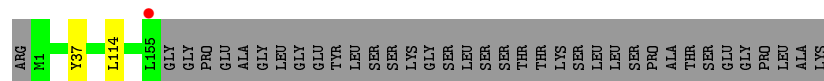
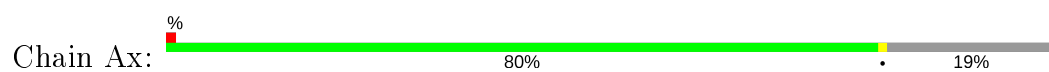
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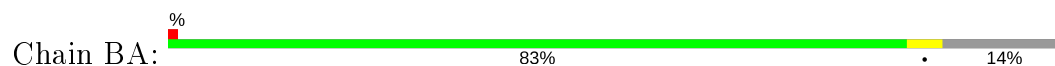
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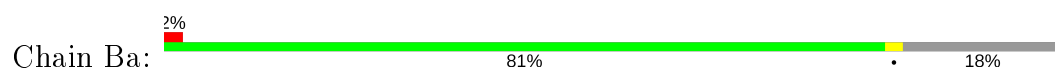
- Molecule 1: Ferritin



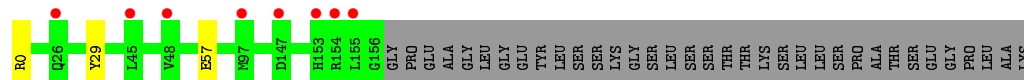
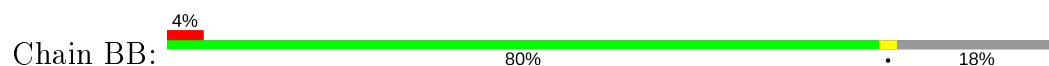
- Molecule 1: Ferritin



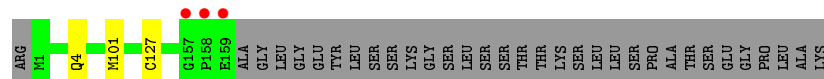
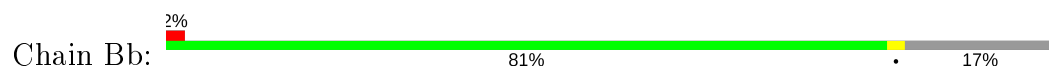
- Molecule 1: Ferritin



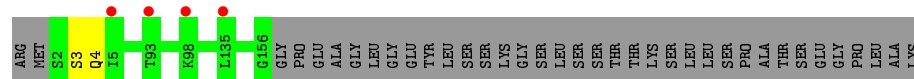
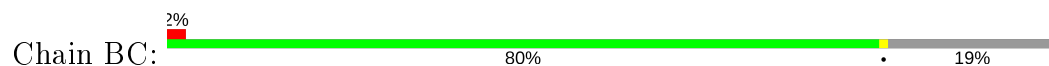
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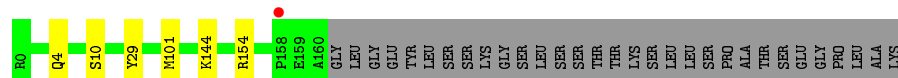
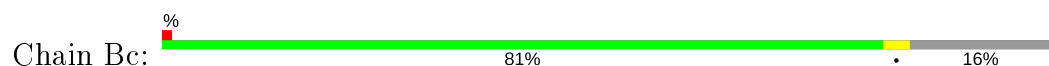
- Molecule 1: Ferritin



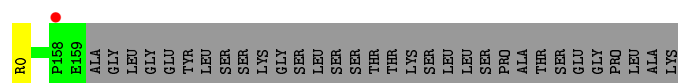
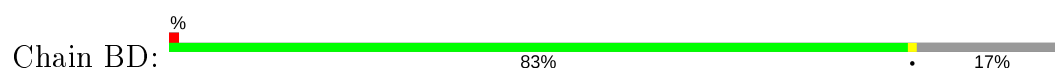
- Molecule 1: Ferritin



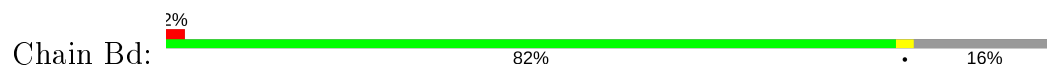
- Molecule 1: Ferritin



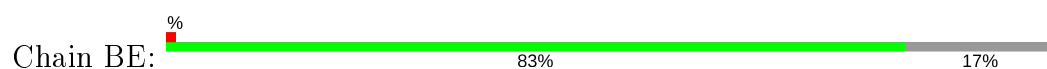
- Molecule 1: Ferritin



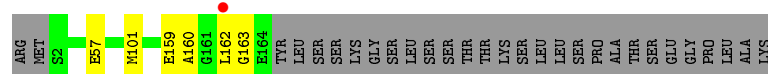
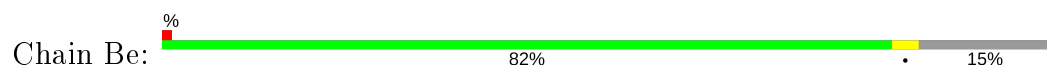
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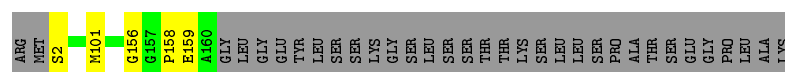
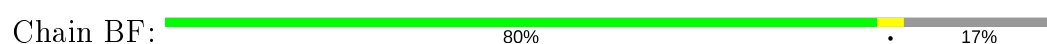
- Molecule 1: Ferritin



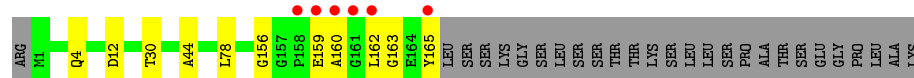
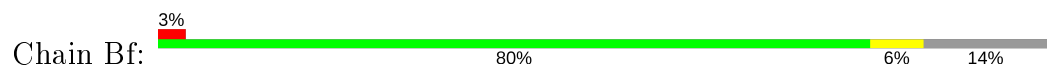
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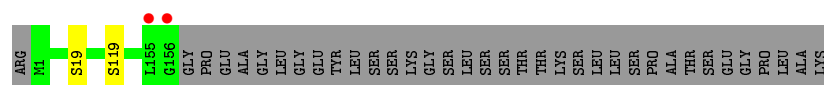
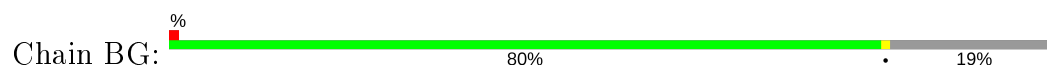
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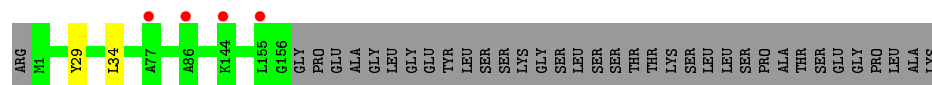
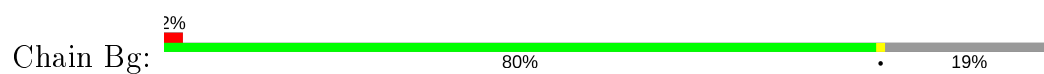
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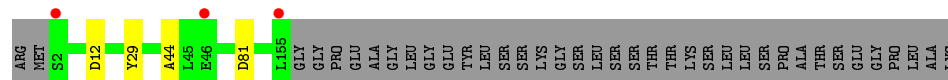
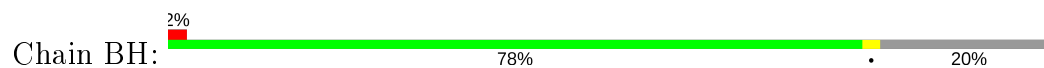
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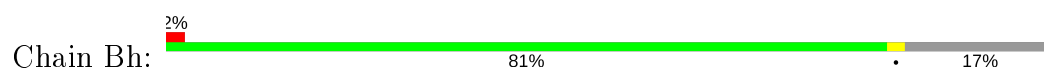
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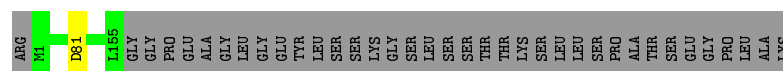
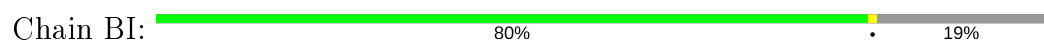
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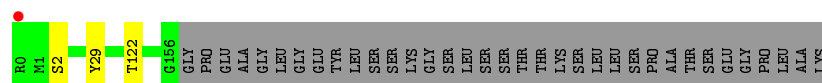
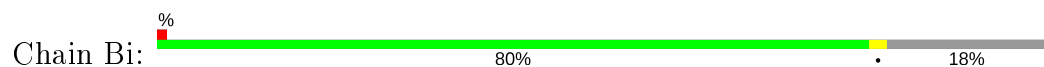
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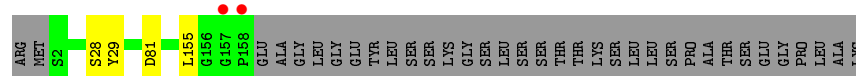
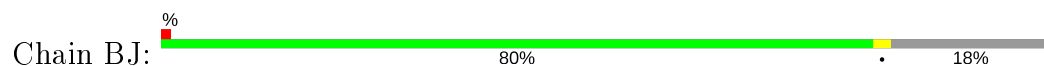
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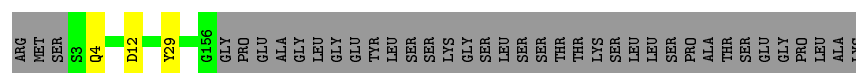
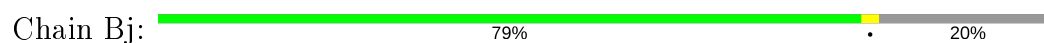
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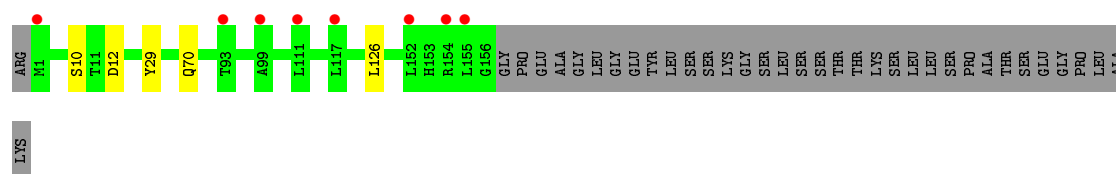
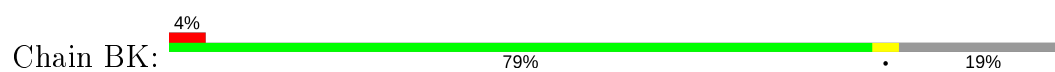
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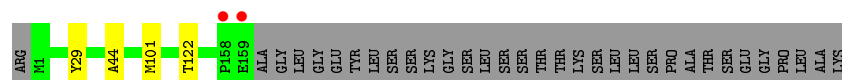
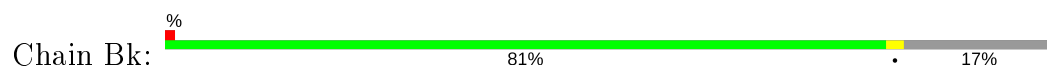
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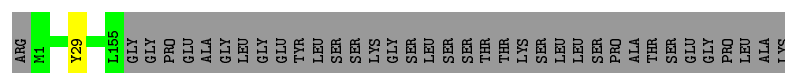
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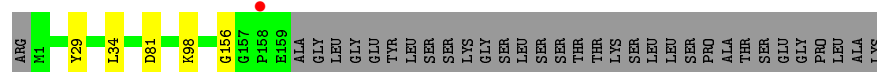
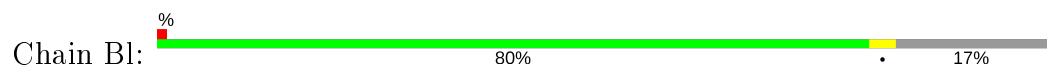
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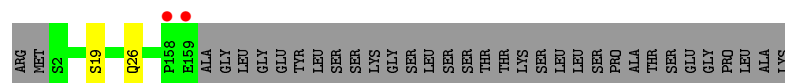
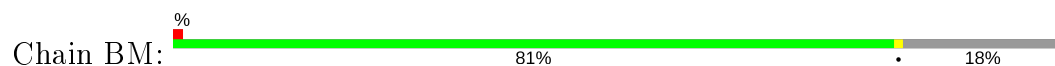
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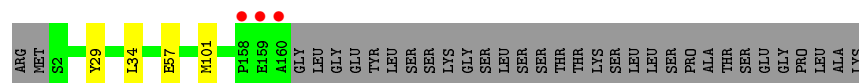
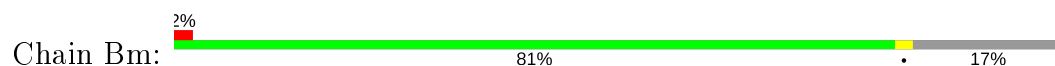
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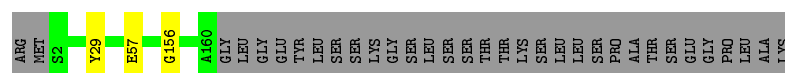
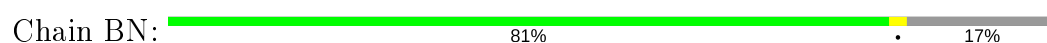
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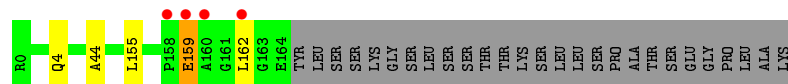
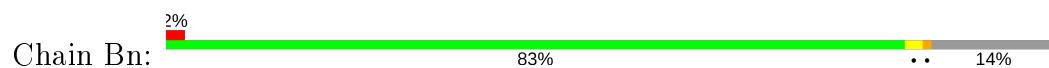
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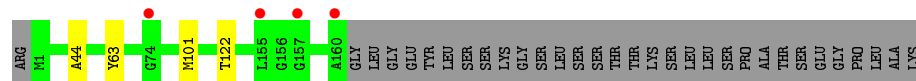
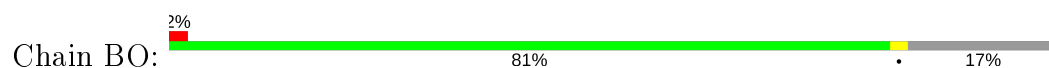
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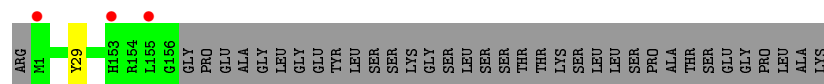
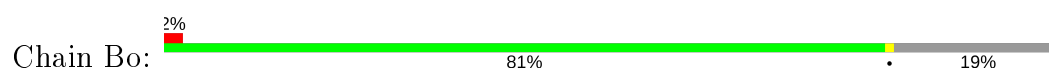
## • Molecule 1: Ferritin



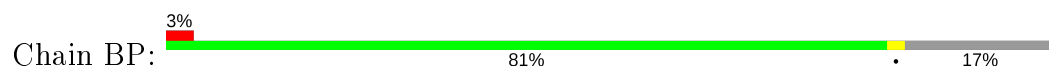
## • Molecule 1: Ferritin



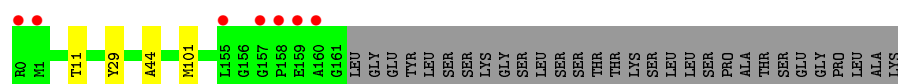
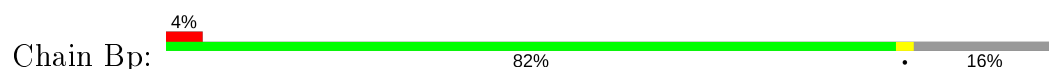
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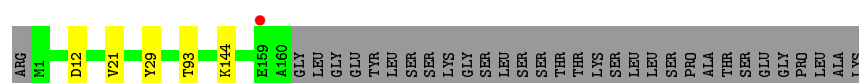
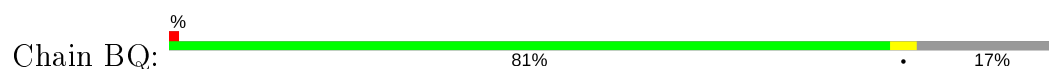
## • Molecule 1: Ferritin



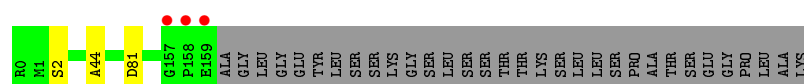
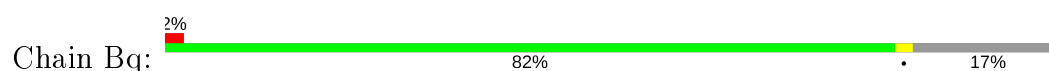
## • Molecule 1: Ferritin



## • Molecule 1: Ferritin

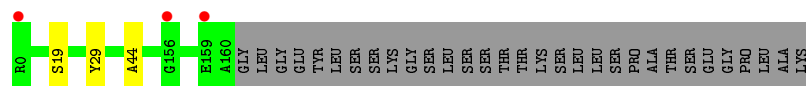
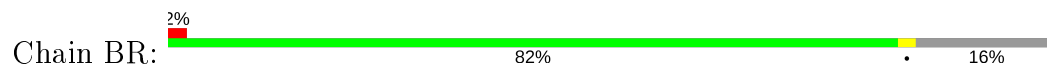


## • Molecule 1: Ferritin

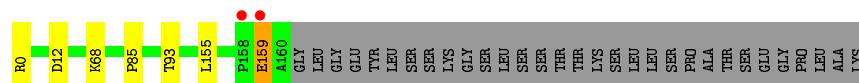
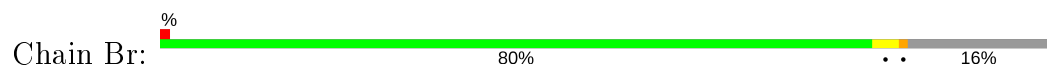




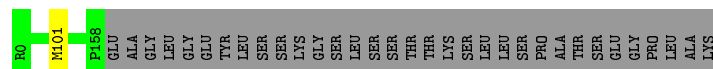
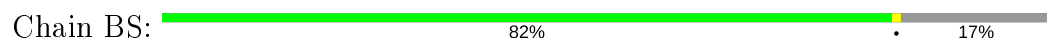
## ● Molecule 1: Ferritin



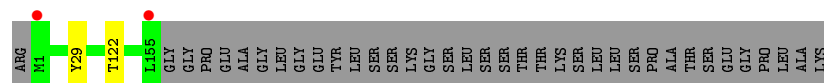
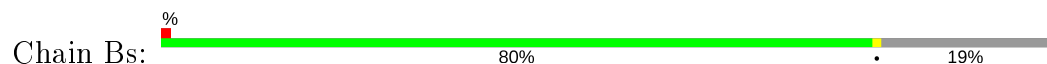
## ● Molecule 1: Ferritin



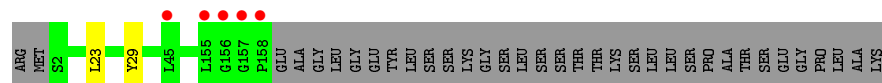
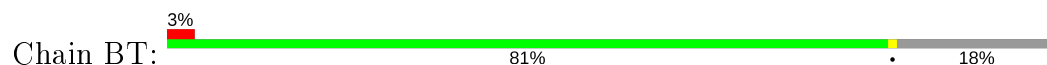
## ● Molecule 1: Ferritin



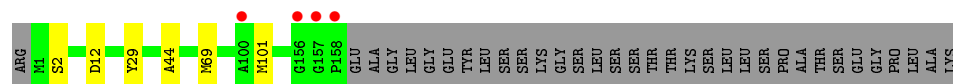
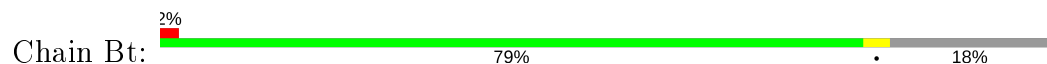
## ● Molecule 1: Ferritin



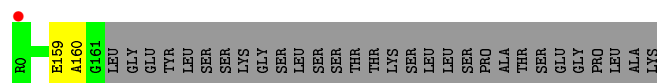
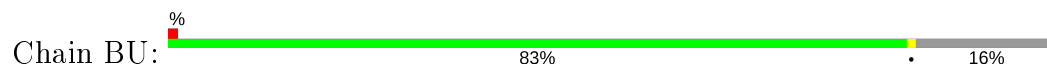
## ● Molecule 1: Ferritin



## ● Molecule 1: Ferritin



## ● Molecule 1: Ferritin



ARG	M1		S28	Y29	E57	T122	G157	P158	E159	A160	G161	L162	G163	A164	Y165	LEU	SER	SER	SER	LYS	GLY	SER	SER	LEU	SER	SER	SER	THR	THR	LYS	SER	LEU	LEU	SER	PRO	ALA	ALA	THR	THR	SER	GLU	GLY	PRO	PHO	LEU	ALA	LYS
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ARG	SET	S3	Y29	D81	K144	M145	L152	H153	R154	L155	G156	P157	GLU	ALA	GLY	LEU	GLY	GLU	TYR	LEU	SER	SER	LYS	GLY	SER	LEU	SER	SER	THR	THR	LYS	SER	LEU	LEU	SER	PRO	PRO	ALA	THR	SER	GLY	GLY	PRO	PRO	LEU	LEU	ALA	LYS
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ARG M1 D12 Y29 G156 G157 P158 E159 A160 GLY LEU LEU GLY GLU TYR SER SER LYS GLY SER SER SER THR THR LYS SER SER LEU LEU SER PRO PRO ALA THR THR SER GLU GLY PRO LEU LEU LYS

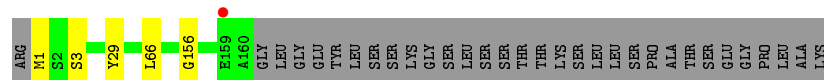
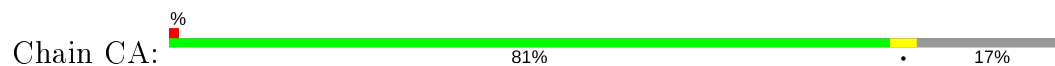
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ARG  
MET  
S2  
Y29  
L34  
G156  
G157  
P158  
E159  
A160  
GLY  
LEU  
GLY  
GLU  
TYR  
LEU  
LEU  
SER  
SER  
LYS  
GLY  
SER  
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SER  
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LEU  
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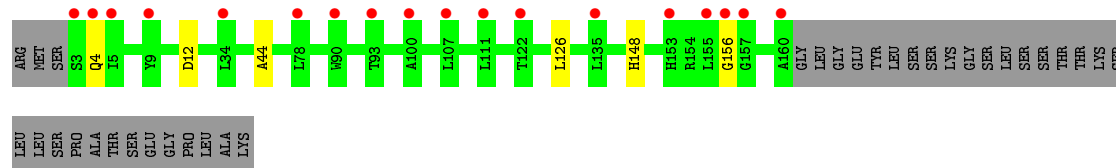
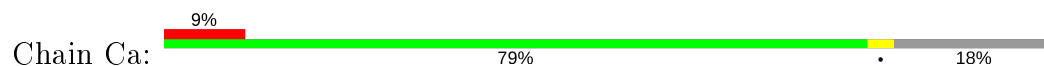
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ARG  
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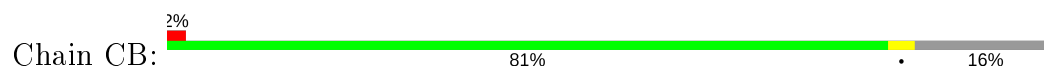
## ● Molecule 1: Ferritin



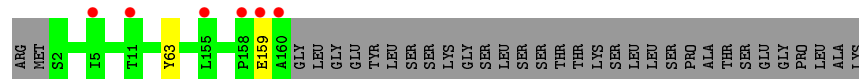
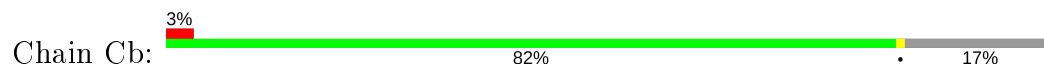
## ● Molecule 1: Ferritin



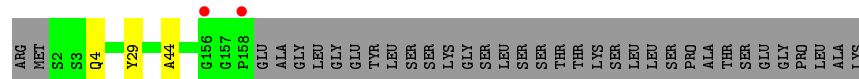
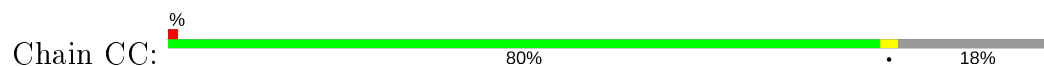
## ● Molecule 1: Ferritin



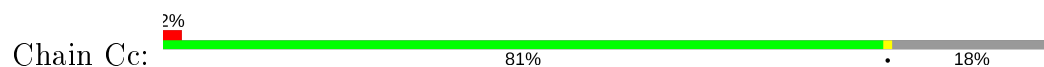
## ● Molecule 1: Ferritin



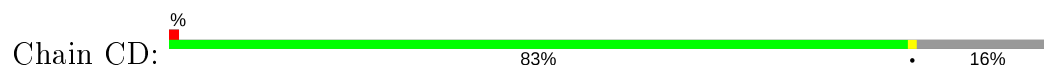
## ● Molecule 1: Ferritin

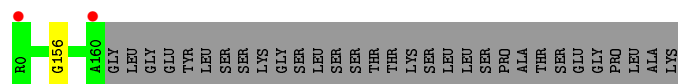


## ● Molecule 1: Ferritin

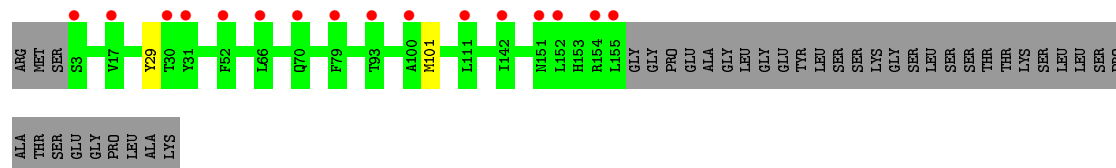
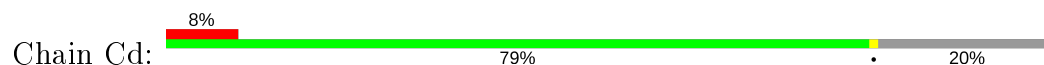


## ● Molecule 1: Ferritin

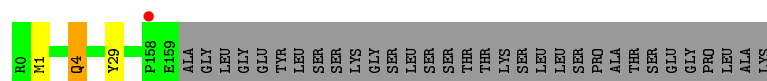
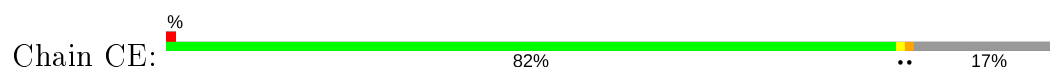




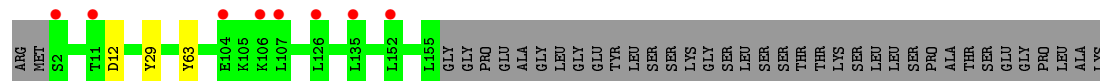
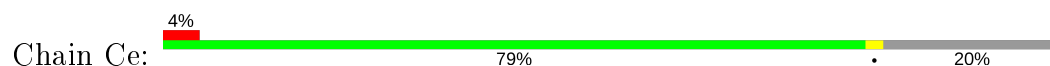
- Molecule 1: Ferritin



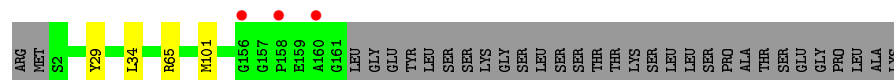
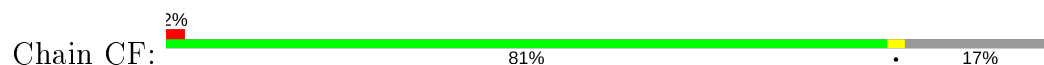
- Molecule 1: Ferritin



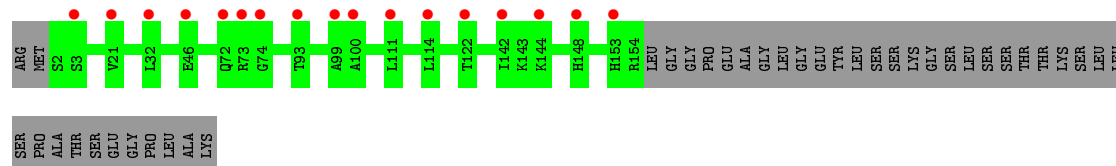
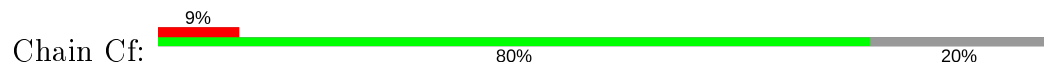
- Molecule 1: Ferritin



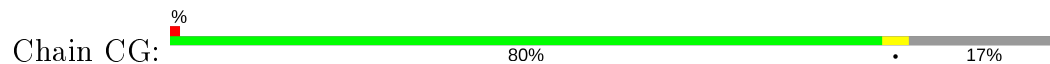
- Molecule 1: Ferritin

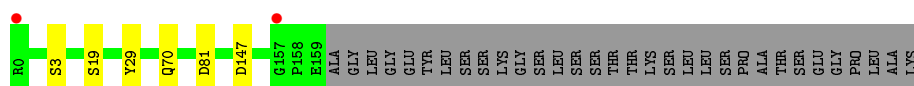


- Molecule 1: Ferritin

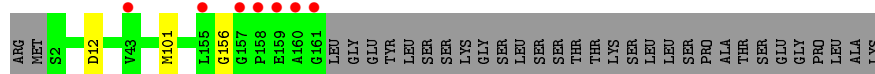
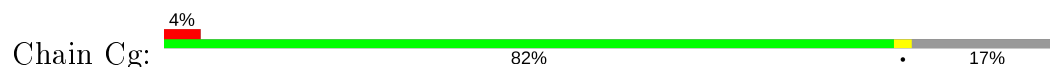


- Molecule 1: Ferritin

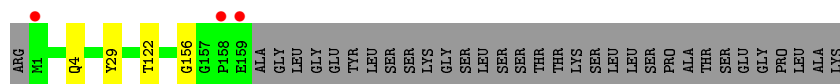
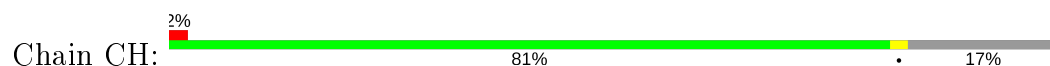




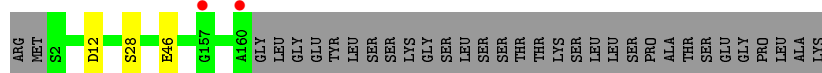
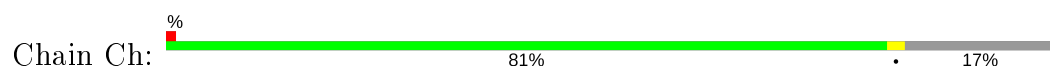
• Molecule 1: Ferritin



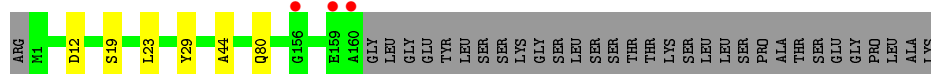
• Molecule 1: Ferritin



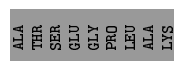
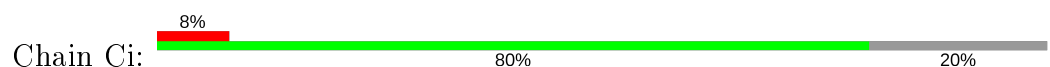
• Molecule 1: Ferritin



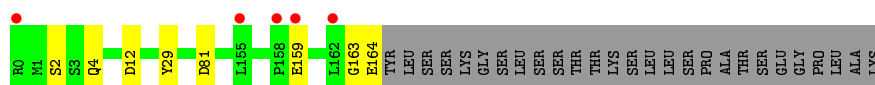
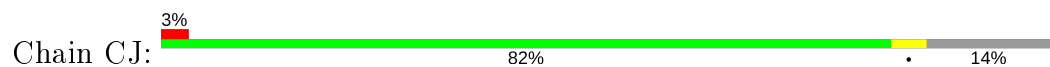
• Molecule 1: Ferritin



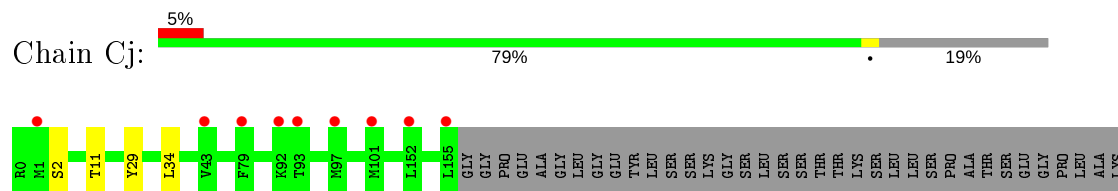
• Molecule 1: Ferritin



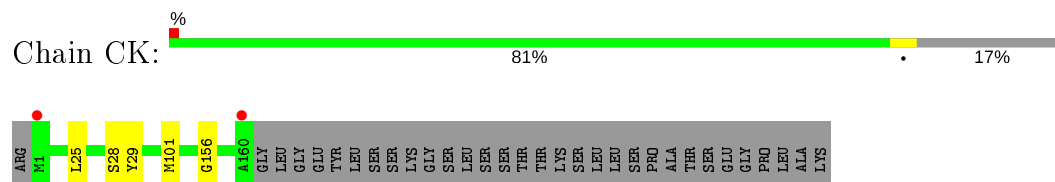
• Molecule 1: Ferritin



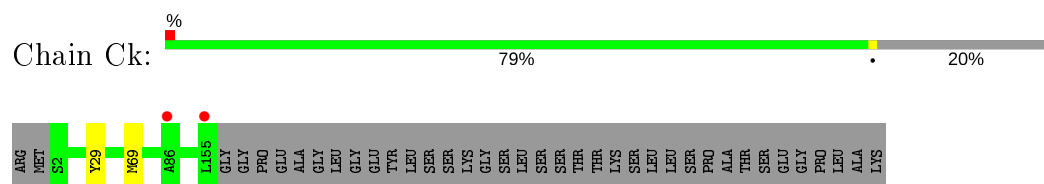
## • Molecule 1: Ferritin



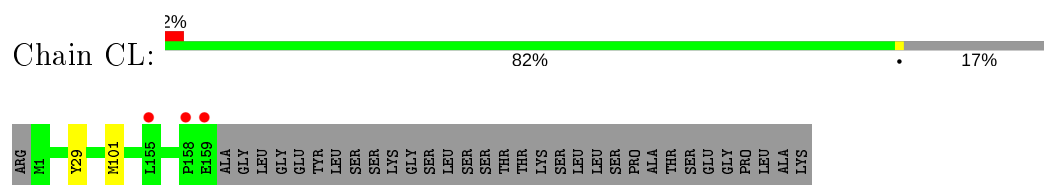
## • Molecule 1: Ferritin



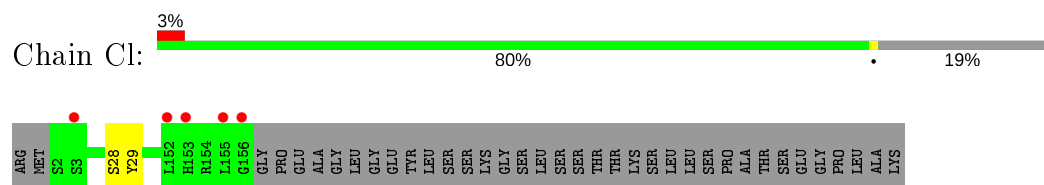
## • Molecule 1: Ferritin



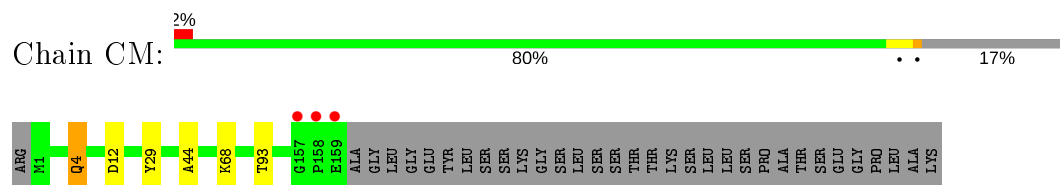
## • Molecule 1: Ferritin



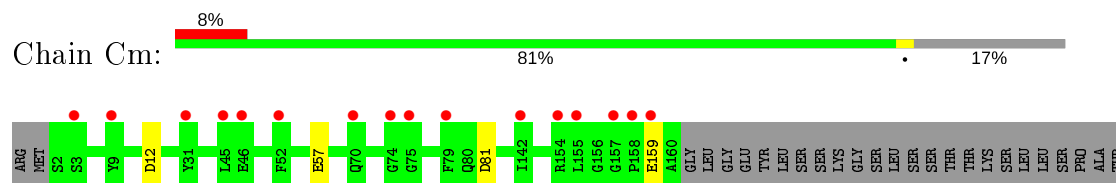
## • Molecule 1: Ferritin



## • Molecule 1: Ferritin

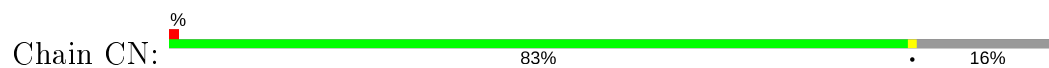


## • Molecule 1: Ferritin



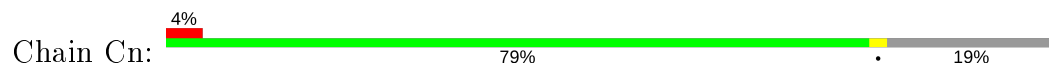
SER  
GLU  
GLY  
PRO  
LEU  
ALA  
LYS

## ● Molecule 1: Ferritin



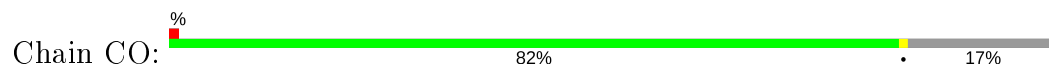
ARG HI Y29 P85 P158  
GLU LEU161  
GLY GLY  
TTR LEU  
SER SER  
LYS LYS  
SER SER  
GLY LEU  
SER SER  
THR THR  
LYS LYS  
SER SER  
LEU LEU  
GLY GLY  
SER SER  
PRO PRO  
ALA ALA  
THR THR  
SER SER  
GLY GLY  
PRO PRO  
LEU LEU  
ALA ALA  
LYS LYS

## ● Molecule 1: Ferritin



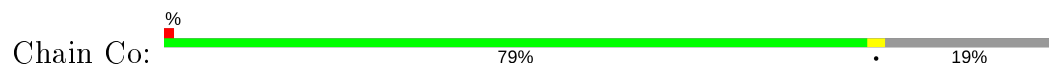
ARG HI S2 S3 Q4 Y29  
H115 L117  
M123 P124  
H125 L126  
L152 H153  
R154 R155  
GLY GLY  
PRO PRO  
GLU GLY  
LEU LEU  
GLY GLY  
TYR TYR  
LEU LEU  
SER SER  
PRO PRO  
ALA ALA  
THR THR  
LYS LYS  
SER SER  
LEU LEU  
SER SER  
SER SER  
THR THR  
THR THR  
SER SER  
GLY GLY  
PRO PRO  
LEU LEU  
ALA ALA  
LYS LYS

## ● Molecule 1: Ferritin



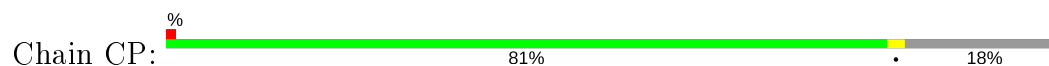
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GLU ALA  
GLY GLY  
GLY GLY  
GLY TYR  
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SER SER  
LYS LYS  
GLY GLY  
SER SER  
LEU LEU  
SER SER  
THR THR  
THR THR  
LYS LYS  
LEU LEU  
LEU LEU  
SER SER  
PRO PRO  
ALA ALA  
THR THR  
SER SER  
GLY GLY  
PRO PRO  
LEU LEU  
ALA ALA  
LYS LYS

## ● Molecule 1: Ferritin



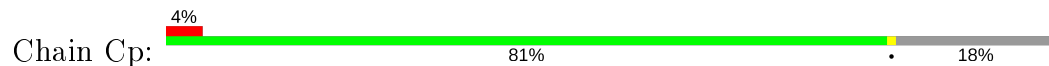
ARG MET S2 Y29 S119 E137  
H153 R154  
R155 G156  
GLY PRO  
GLU GLY  
ALA GLY  
LEU LEU  
GLY GLY  
TYR TYR  
LEU LEU  
SER SER  
SER SER  
LYS LYS  
THR THR  
THR THR  
SER SER  
LEU LEU  
SER SER  
PRO PRO  
ALA ALA  
THR THR  
SER SER  
GLY GLY  
PRO PRO  
LEU LEU  
ALA ALA  
LYS LYS

## ● Molecule 1: Ferritin



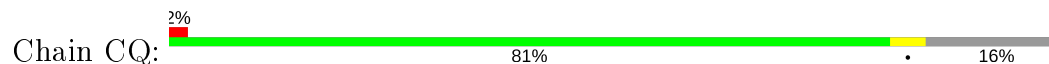
ARG HI Y29 T93 M101  
G157 P158  
GLU ALA  
GLY GLY  
GLY GLY  
GLY GLY  
TYR TYR  
LEU LEU  
SER SER  
SER SER  
LYS LYS  
THR THR  
THR THR  
SER SER  
LEU LEU  
SER SER  
PRO PRO  
ALA ALA  
THR THR  
SER SER  
GLY GLY  
PRO PRO  
LEU LEU  
ALA ALA  
LYS LYS

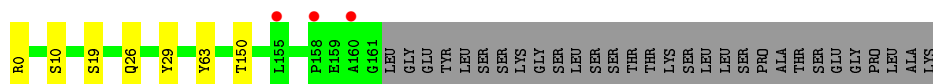
## ● Molecule 1: Ferritin



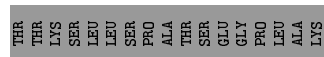
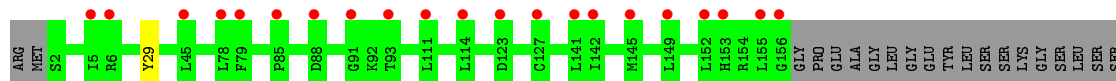
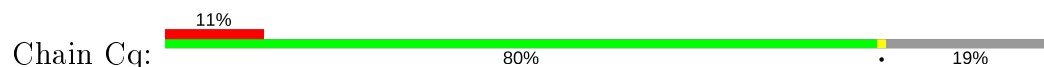
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V48  
G156 G157  
P158  
GLU GLY  
GLY GLY  
GLY GLY  
GLY GLY  
TYR TYR  
LEU LEU  
SER SER  
SER SER  
LYS LYS  
GLY GLY  
SER SER  
LEU LEU  
THR THR  
THR THR  
LYS LYS  
SER SER  
LEU LEU  
SER SER  
PRO PRO  
ALA ALA  
THR THR  
SER SER  
GLY GLY  
PRO PRO  
LEU LEU  
ALA ALA  
LYS LYS

## ● Molecule 1: Ferritin

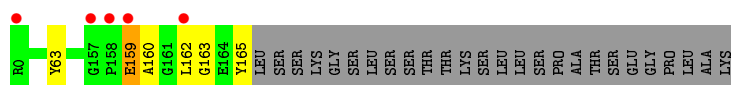
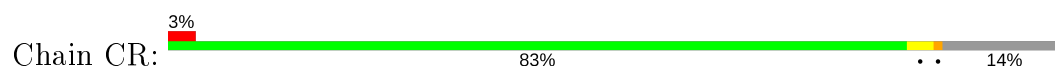




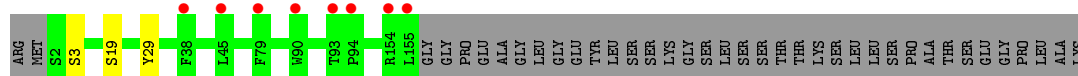
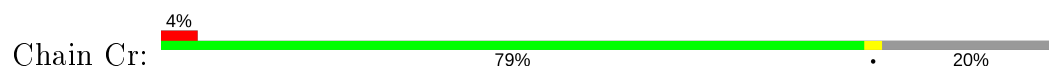
• Molecule 1: Ferritin



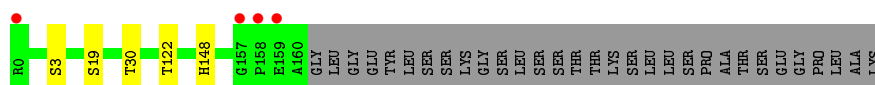
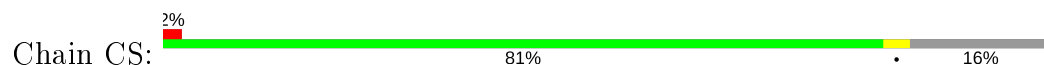
• Molecule 1: Ferritin



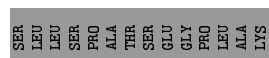
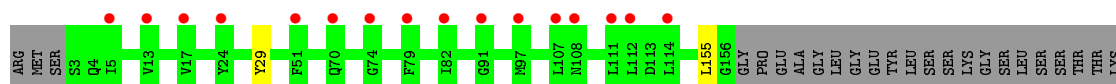
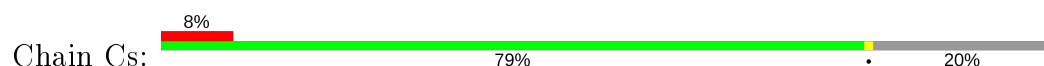
• Molecule 1: Ferritin



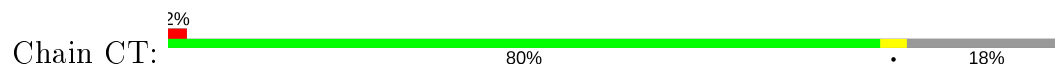
• Molecule 1: Ferritin



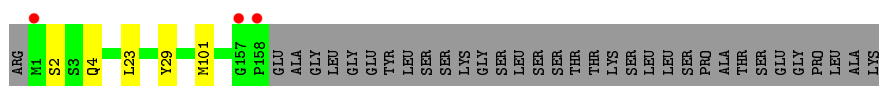
• Molecule 1: Ferritin



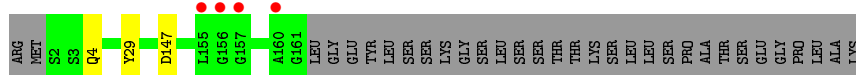
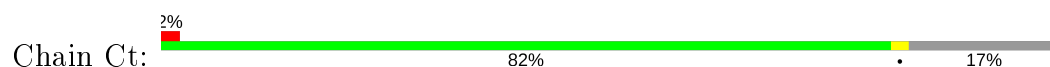
• Molecule 1: Ferritin



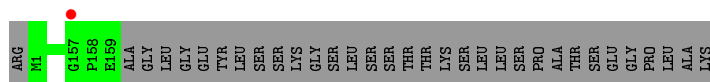
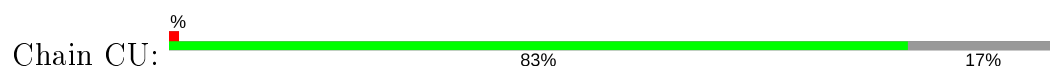




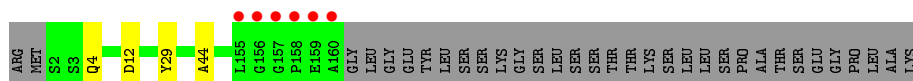
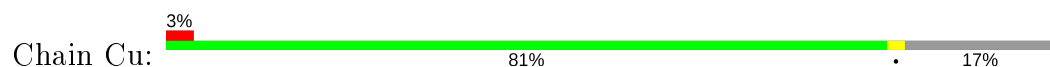
## ● Molecule 1: Ferritin



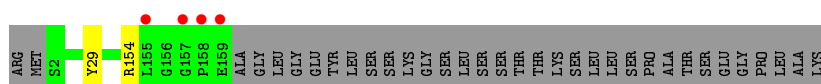
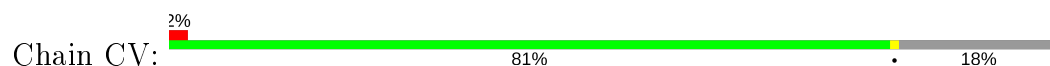
## ● Molecule 1: Ferritin



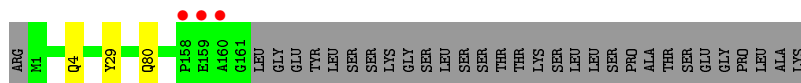
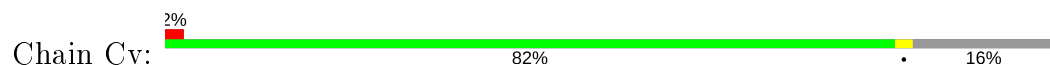
## ● Molecule 1: Ferritin



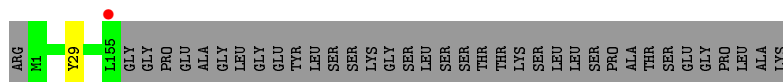
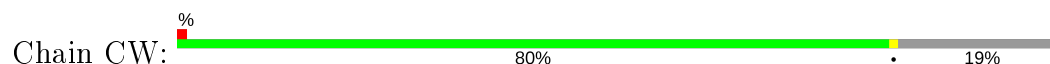
## ● Molecule 1: Ferritin



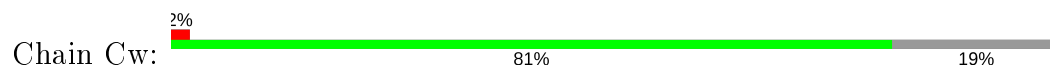
## ● Molecule 1: Ferritin

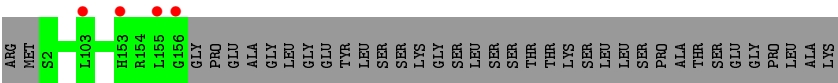


## ● Molecule 1: Ferritin

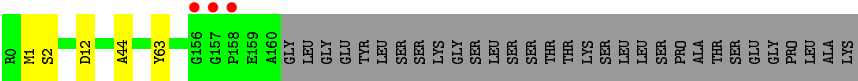
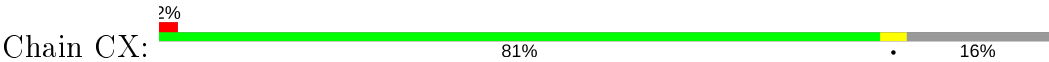


## ● Molecule 1: Ferritin

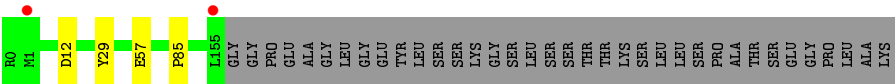
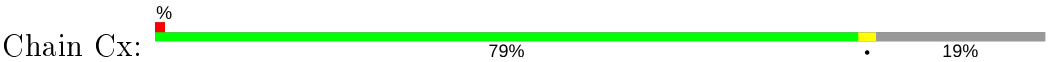




● Molecule 1: Ferritin



● Molecule 1: Ferritin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.34Å 236.94Å 249.71Å 94.69° 115.06° 114.96°	Depositor
Resolution (Å)	50.00 – 2.85 49.77 – 2.84	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.85) 94.7 (49.77-2.84)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.291 0.224 , 0.261	Depositor DCC
$R_{free}$ test set	42321 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	187090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA

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	AA	0.37	0/1294	0.54	0/1741
1	AB	0.42	0/1345	0.63	0/1809
1	AC	0.36	0/1318	0.56	0/1772
1	AD	0.33	0/1299	0.52	0/1748
1	AE	0.47	0/1345	0.64	0/1809
1	AF	0.41	0/1293	0.56	0/1739
1	AG	0.41	0/1299	0.61	0/1748
1	AH	0.45	0/1307	0.60	0/1758
1	AI	0.35	0/1293	0.55	0/1739
1	AJ	0.38	0/1285	0.56	0/1727
1	AK	0.39	0/1292	0.56	0/1736
1	AL	0.32	0/1285	0.55	0/1729
1	AM	0.44	0/1322	0.59	0/1777
1	AN	0.43	0/1345	0.62	0/1809
1	AO	0.43	0/1345	0.63	0/1809
1	AP	0.51	0/1302	0.67	0/1751
1	AQ	0.36	0/1343	0.57	0/1805
1	AR	0.42	0/1332	0.58	0/1791
1	AS	0.35	0/1303	0.54	0/1753
1	AT	0.46	0/1294	0.62	0/1741
1	AU	0.43	0/1307	0.59	0/1758
1	AV	0.41	0/1303	0.58	0/1753
1	AW	0.37	0/1294	0.55	0/1741
1	AX	0.44	0/1307	0.61	0/1758
1	Aa	0.47	0/1318	0.65	1/1772 (0.1%)
1	Ab	0.47	0/1311	0.60	0/1763
1	Ac	0.45	0/1307	0.62	0/1758
1	Ad	0.57	0/1345	0.70	1/1809 (0.1%)
1	Ae	0.51	0/1322	0.67	0/1777
1	Af	0.47	0/1318	0.64	0/1772
1	Ag	0.52	0/1277	0.63	0/1717
1	Ah	0.51	0/1318	0.63	0/1772

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Ai	0.54	0/1302	0.69	0/1751
1	Aj	0.47	0/1345	0.66	0/1809
1	Ak	0.44	0/1345	0.62	0/1809
1	Al	0.48	0/1345	0.66	0/1809
1	Am	0.49	0/1322	0.64	0/1777
1	An	0.49	0/1311	0.63	0/1763
1	Ao	0.48	0/1318	0.64	0/1772
1	Ap	0.49	0/1322	0.65	0/1777
1	Aq	0.49	0/1307	0.65	0/1758
1	Ar	0.59	0/1345	0.69	1/1809 (0.1%)
1	As	0.47	0/1318	0.62	0/1772
1	At	0.50	0/1307	0.62	0/1758
1	Au	0.46	0/1307	0.61	0/1758
1	Av	0.45	0/1343	0.61	0/1805
1	Aw	0.57	2/1311 (0.2%)	0.69	1/1763 (0.1%)
1	Ax	0.53	0/1277	0.63	0/1717
1	BA	0.40	0/1356	0.60	0/1823
1	BB	0.37	0/1292	0.60	1/1736 (0.1%)
1	BC	0.32	0/1273	0.53	0/1712
1	BD	0.37	0/1313	0.58	0/1765
1	BE	0.38	0/1302	0.59	0/1751
1	BF	0.47	0/1299	0.62	0/1748
1	BG	0.37	0/1281	0.57	0/1722
1	BH	0.36	0/1269	0.54	0/1707
1	BI	0.38	0/1277	0.56	0/1717
1	BJ	0.37	0/1285	0.56	0/1729
1	BK	0.35	0/1281	0.52	0/1722
1	BL	0.34	0/1277	0.53	0/1717
1	BM	0.45	0/1294	0.60	0/1741
1	BN	0.42	0/1299	0.62	0/1748
1	BO	0.35	0/1307	0.54	0/1758
1	BP	0.38	0/1299	0.56	0/1748
1	BQ	0.43	0/1307	0.59	0/1758
1	BR	0.40	0/1318	0.57	0/1772
1	BS	0.45	0/1304	0.59	0/1753
1	BT	0.34	0/1285	0.57	0/1729
1	BU	0.34	0/1322	0.53	0/1777
1	BV	0.36	0/1277	0.57	0/1717
1	BW	0.36	0/1311	0.55	0/1763
1	BX	0.37	0/1324	0.59	0/1781
1	Ba	0.33	0/1293	0.53	0/1739
1	Bb	0.35	0/1302	0.52	0/1751
1	Bc	0.43	0/1318	0.60	0/1772

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Bd	0.44	0/1318	0.59	0/1772
1	Be	0.46	0/1324	0.62	0/1781
1	Bf	0.43	0/1345	0.63	0/1809
1	Bg	0.35	0/1281	0.53	0/1722
1	Bh	0.39	0/1302	0.57	0/1751
1	Bi	0.37	0/1292	0.57	0/1736
1	Bj	0.34	0/1267	0.54	0/1704
1	Bk	0.35	0/1302	0.54	0/1751
1	Bl	0.43	0/1302	0.59	0/1751
1	Bm	0.44	0/1299	0.61	0/1748
1	Bn	0.41	0/1343	0.59	0/1805
1	Bo	0.36	0/1281	0.57	0/1722
1	Bp	0.42	0/1322	0.60	0/1777
1	Bq	0.36	0/1313	0.55	0/1765
1	Br	0.55	0/1318	0.69	0/1772
1	Bs	0.37	0/1277	0.56	0/1717
1	Bt	0.34	0/1293	0.55	0/1739
1	Bu	0.48	0/1345	0.64	1/1809 (0.1%)
1	Bv	0.41	0/1307	0.56	0/1758
1	Bw	0.51	0/1299	0.67	0/1748
1	Bx	0.34	0/1285	0.55	0/1729
1	CA	0.47	0/1307	0.61	0/1758
1	CB	0.40	0/1311	0.58	0/1763
1	CC	0.33	0/1285	0.53	0/1729
1	CD	0.43	0/1318	0.60	0/1772
1	CE	0.40	0/1313	0.56	0/1765
1	CF	0.48	0/1303	0.61	0/1753
1	CG	0.42	0/1313	0.58	0/1765
1	CH	0.34	0/1302	0.53	0/1751
1	CI	0.46	0/1307	0.63	0/1758
1	CJ	0.52	1/1343 (0.1%)	0.66	0/1805
1	CK	0.36	0/1307	0.56	0/1758
1	CL	0.35	0/1302	0.54	0/1751
1	CM	0.46	0/1302	0.60	0/1751
1	CN	0.45	0/1311	0.61	0/1763
1	CO	0.36	0/1304	0.55	0/1753
1	CP	0.38	0/1293	0.55	0/1739
1	CQ	0.49	0/1322	0.61	0/1777
1	CR	0.50	0/1356	0.65	0/1823
1	CS	0.48	0/1318	0.61	0/1772
1	CT	0.41	0/1293	0.55	0/1739
1	CU	0.32	0/1302	0.52	0/1751
1	CV	0.33	0/1294	0.55	0/1741

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	CW	0.37	0/1277	0.55	0/1717
1	CX	0.43	0/1318	0.62	0/1772
1	Ca	0.36	0/1293	0.59	0/1740
1	Cb	0.34	0/1299	0.54	0/1748
1	Cc	0.35	0/1288	0.55	0/1733
1	Cd	0.34	0/1263	0.54	0/1699
1	Ce	0.34	0/1269	0.53	0/1707
1	Cf	0.34	0/1261	0.51	0/1696
1	Cg	0.35	0/1303	0.53	0/1753
1	Ch	0.39	0/1299	0.58	0/1748
1	Ci	0.37	0/1263	0.54	0/1699
1	Cj	0.35	0/1288	0.57	0/1731
1	Ck	0.34	0/1269	0.54	0/1707
1	Cl	0.35	0/1273	0.56	0/1712
1	Cm	0.33	0/1299	0.53	0/1748
1	Cn	0.33	0/1277	0.52	0/1717
1	Co	0.41	0/1273	0.59	0/1712
1	Cp	0.34	0/1293	0.55	0/1739
1	Cq	0.36	0/1273	0.53	0/1712
1	Cr	0.35	0/1269	0.52	0/1707
1	Cs	0.34	0/1267	0.55	0/1704
1	Ct	0.39	0/1303	0.58	0/1753
1	Cu	0.36	0/1299	0.55	0/1748
1	Cv	0.36	0/1311	0.54	0/1763
1	Cw	0.35	0/1273	0.53	0/1712
1	Cx	0.38	0/1288	0.58	0/1731
All	All	0.41	3/187767 (0.0%)	0.59	6/252515 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AX	0	1
1	An	0	1
1	Ar	0	1
1	Ax	0	1
1	CR	0	1
1	CX	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aw	1	MET	CG-SD	-8.22	1.59	1.81
1	Aw	1	MET	SD-CE	-5.27	1.48	1.77
1	CJ	159	GLU	CB-CG	5.21	1.62	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aw	1	MET	CG-SD-CE	7.72	112.55	100.20
1	BB	0	ARG	N-CA-C	6.15	127.60	111.00
1	Bu	161	GLY	N-CA-C	-5.78	98.66	113.10
1	Aa	107	LEU	CA-CB-CG	5.20	127.26	115.30
1	Ad	161	GLY	N-CA-C	-5.16	100.19	113.10
1	Ar	161	GLY	N-CA-C	-5.07	100.43	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AX	63	TYR	Sidechain
1	An	31	TYR	Sidechain
1	Ar	163	GLY	Mainchain
1	Ax	37	TYR	Sidechain
1	CR	163	GLY	Mainchain
1	CX	63	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	156/192 (81%)	151 (97%)	5 (3%)	0	100	100
1	AB	163/192 (85%)	149 (91%)	10 (6%)	4 (2%)	5	18
1	AC	159/192 (83%)	146 (92%)	10 (6%)	3 (2%)	8	24
1	AD	157/192 (82%)	151 (96%)	5 (3%)	1 (1%)	25	53
1	AE	163/192 (85%)	147 (90%)	11 (7%)	5 (3%)	4	14
1	AF	156/192 (81%)	151 (97%)	4 (3%)	1 (1%)	25	53
1	AG	157/192 (82%)	150 (96%)	7 (4%)	0	100	100
1	AH	158/192 (82%)	148 (94%)	10 (6%)	0	100	100
1	AI	156/192 (81%)	147 (94%)	8 (5%)	1 (1%)	25	53
1	AJ	155/192 (81%)	149 (96%)	6 (4%)	0	100	100
1	AK	155/192 (81%)	152 (98%)	3 (2%)	0	100	100
1	AL	155/192 (81%)	147 (95%)	8 (5%)	0	100	100
1	AM	160/192 (83%)	151 (94%)	7 (4%)	2 (1%)	12	33
1	AN	163/192 (85%)	154 (94%)	7 (4%)	2 (1%)	13	35
1	AO	163/192 (85%)	148 (91%)	11 (7%)	4 (2%)	5	18
1	AP	157/192 (82%)	152 (97%)	5 (3%)	0	100	100
1	AQ	163/192 (85%)	150 (92%)	10 (6%)	3 (2%)	8	25
1	AR	162/192 (84%)	152 (94%)	8 (5%)	2 (1%)	13	35
1	AS	158/192 (82%)	149 (94%)	8 (5%)	1 (1%)	25	53
1	AT	156/192 (81%)	144 (92%)	10 (6%)	2 (1%)	12	33
1	AU	158/192 (82%)	152 (96%)	5 (3%)	1 (1%)	25	53
1	AV	158/192 (82%)	148 (94%)	8 (5%)	2 (1%)	12	33
1	AW	156/192 (81%)	150 (96%)	6 (4%)	0	100	100
1	AX	158/192 (82%)	149 (94%)	8 (5%)	1 (1%)	25	53
1	Aa	159/192 (83%)	153 (96%)	6 (4%)	0	100	100
1	Ab	159/192 (83%)	151 (95%)	6 (4%)	2 (1%)	12	33
1	Ac	158/192 (82%)	155 (98%)	3 (2%)	0	100	100
1	Ad	163/192 (85%)	152 (93%)	8 (5%)	3 (2%)	8	25
1	Ae	160/192 (83%)	157 (98%)	3 (2%)	0	100	100
1	Af	159/192 (83%)	152 (96%)	7 (4%)	0	100	100
1	Ag	153/192 (80%)	148 (97%)	5 (3%)	0	100	100
1	Ah	159/192 (83%)	153 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ai	157/192 (82%)	150 (96%)	5 (3%)	2 (1%)	12	33
1	Aj	163/192 (85%)	147 (90%)	11 (7%)	5 (3%)	4	14
1	Ak	163/192 (85%)	153 (94%)	8 (5%)	2 (1%)	13	35
1	Al	163/192 (85%)	149 (91%)	10 (6%)	4 (2%)	5	18
1	Am	160/192 (83%)	149 (93%)	7 (4%)	4 (2%)	5	18
1	An	159/192 (83%)	149 (94%)	8 (5%)	2 (1%)	12	33
1	Ao	159/192 (83%)	150 (94%)	7 (4%)	2 (1%)	12	33
1	Ap	160/192 (83%)	150 (94%)	7 (4%)	3 (2%)	8	24
1	Aq	158/192 (82%)	146 (92%)	11 (7%)	1 (1%)	25	53
1	Ar	163/192 (85%)	152 (93%)	8 (5%)	3 (2%)	8	25
1	As	159/192 (83%)	153 (96%)	6 (4%)	0	100	100
1	At	158/192 (82%)	151 (96%)	7 (4%)	0	100	100
1	Au	158/192 (82%)	153 (97%)	4 (2%)	1 (1%)	25	53
1	Av	163/192 (85%)	148 (91%)	13 (8%)	2 (1%)	13	35
1	Aw	159/192 (83%)	149 (94%)	9 (6%)	1 (1%)	25	53
1	Ax	153/192 (80%)	150 (98%)	3 (2%)	0	100	100
1	BA	164/192 (85%)	150 (92%)	12 (7%)	2 (1%)	13	35
1	BB	155/192 (81%)	146 (94%)	9 (6%)	0	100	100
1	BC	153/192 (80%)	148 (97%)	5 (3%)	0	100	100
1	BD	158/192 (82%)	151 (96%)	7 (4%)	0	100	100
1	BE	157/192 (82%)	150 (96%)	7 (4%)	0	100	100
1	BF	157/192 (82%)	147 (94%)	7 (4%)	3 (2%)	8	24
1	BG	154/192 (80%)	145 (94%)	9 (6%)	0	100	100
1	BH	152/192 (79%)	146 (96%)	5 (3%)	1 (1%)	22	50
1	BI	153/192 (80%)	150 (98%)	3 (2%)	0	100	100
1	BJ	155/192 (81%)	147 (95%)	7 (4%)	1 (1%)	25	53
1	BK	154/192 (80%)	147 (96%)	7 (4%)	0	100	100
1	BL	153/192 (80%)	149 (97%)	4 (3%)	0	100	100
1	BM	156/192 (81%)	151 (97%)	5 (3%)	0	100	100
1	BN	157/192 (82%)	150 (96%)	6 (4%)	1 (1%)	25	53
1	BO	158/192 (82%)	146 (92%)	11 (7%)	1 (1%)	25	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BP	157/192 (82%)	150 (96%)	7 (4%)	0	100	100
1	BQ	158/192 (82%)	152 (96%)	6 (4%)	0	100	100
1	BR	159/192 (83%)	150 (94%)	8 (5%)	1 (1%)	25	53
1	BS	157/192 (82%)	152 (97%)	5 (3%)	0	100	100
1	BT	155/192 (81%)	150 (97%)	5 (3%)	0	100	100
1	BU	160/192 (83%)	152 (95%)	7 (4%)	1 (1%)	25	53
1	BV	154/192 (80%)	149 (97%)	3 (2%)	2 (1%)	12	33
1	BW	159/192 (83%)	154 (97%)	5 (3%)	0	100	100
1	BX	161/192 (84%)	150 (93%)	7 (4%)	4 (2%)	5	18
1	Ba	156/192 (81%)	149 (96%)	7 (4%)	0	100	100
1	Bb	157/192 (82%)	148 (94%)	9 (6%)	0	100	100
1	Bc	159/192 (83%)	147 (92%)	12 (8%)	0	100	100
1	Bd	159/192 (83%)	152 (96%)	4 (2%)	3 (2%)	8	24
1	Be	161/192 (84%)	146 (91%)	12 (8%)	3 (2%)	8	24
1	Bf	163/192 (85%)	147 (90%)	11 (7%)	5 (3%)	4	14
1	Bg	154/192 (80%)	150 (97%)	4 (3%)	0	100	100
1	Bh	157/192 (82%)	151 (96%)	5 (3%)	1 (1%)	25	53
1	Bi	155/192 (81%)	148 (96%)	6 (4%)	1 (1%)	25	53
1	Bj	152/192 (79%)	147 (97%)	5 (3%)	0	100	100
1	Bk	157/192 (82%)	148 (94%)	8 (5%)	1 (1%)	25	53
1	Bl	157/192 (82%)	150 (96%)	6 (4%)	1 (1%)	25	53
1	Bm	157/192 (82%)	151 (96%)	6 (4%)	0	100	100
1	Bn	163/192 (85%)	153 (94%)	7 (4%)	3 (2%)	8	25
1	Bo	154/192 (80%)	149 (97%)	5 (3%)	0	100	100
1	Bp	160/192 (83%)	148 (92%)	11 (7%)	1 (1%)	25	53
1	Bq	158/192 (82%)	150 (95%)	6 (4%)	2 (1%)	12	33
1	Br	159/192 (83%)	148 (93%)	9 (6%)	2 (1%)	12	33
1	Bs	153/192 (80%)	148 (97%)	5 (3%)	0	100	100
1	Bt	156/192 (81%)	147 (94%)	7 (4%)	2 (1%)	12	33
1	Bu	163/192 (85%)	152 (93%)	9 (6%)	2 (1%)	13	35
1	Bv	158/192 (82%)	149 (94%)	8 (5%)	1 (1%)	25	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bw	157/192 (82%)	150 (96%)	6 (4%)	1 (1%)	25	53
1	Bx	155/192 (81%)	147 (95%)	8 (5%)	0	100	100
1	CA	158/192 (82%)	153 (97%)	4 (2%)	1 (1%)	25	53
1	CB	159/192 (83%)	154 (97%)	5 (3%)	0	100	100
1	CC	155/192 (81%)	149 (96%)	5 (3%)	1 (1%)	25	53
1	CD	159/192 (83%)	152 (96%)	6 (4%)	1 (1%)	25	53
1	CE	158/192 (82%)	149 (94%)	7 (4%)	2 (1%)	12	33
1	CF	158/192 (82%)	150 (95%)	8 (5%)	0	100	100
1	CG	158/192 (82%)	153 (97%)	4 (2%)	1 (1%)	25	53
1	CH	157/192 (82%)	146 (93%)	10 (6%)	1 (1%)	25	53
1	CI	158/192 (82%)	147 (93%)	10 (6%)	1 (1%)	25	53
1	CJ	163/192 (85%)	153 (94%)	8 (5%)	2 (1%)	13	35
1	CK	158/192 (82%)	152 (96%)	5 (3%)	1 (1%)	25	53
1	CL	157/192 (82%)	150 (96%)	7 (4%)	0	100	100
1	CM	157/192 (82%)	148 (94%)	7 (4%)	2 (1%)	12	33
1	CN	159/192 (83%)	152 (96%)	7 (4%)	0	100	100
1	CO	157/192 (82%)	146 (93%)	11 (7%)	0	100	100
1	CP	156/192 (81%)	152 (97%)	4 (3%)	0	100	100
1	CQ	160/192 (83%)	150 (94%)	10 (6%)	0	100	100
1	CR	164/192 (85%)	150 (92%)	11 (7%)	3 (2%)	8	25
1	CS	159/192 (83%)	150 (94%)	9 (6%)	0	100	100
1	CT	156/192 (81%)	147 (94%)	8 (5%)	1 (1%)	25	53
1	CU	157/192 (82%)	152 (97%)	5 (3%)	0	100	100
1	CV	156/192 (81%)	149 (96%)	7 (4%)	0	100	100
1	CW	153/192 (80%)	151 (99%)	2 (1%)	0	100	100
1	CX	159/192 (83%)	147 (92%)	10 (6%)	2 (1%)	12	33
1	Ca	156/192 (81%)	148 (95%)	5 (3%)	3 (2%)	8	24
1	Cb	157/192 (82%)	148 (94%)	9 (6%)	0	100	100
1	Cc	155/192 (81%)	148 (96%)	7 (4%)	0	100	100
1	Cd	151/192 (79%)	146 (97%)	5 (3%)	0	100	100
1	Ce	152/192 (79%)	148 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Cf	151/192 (79%)	146 (97%)	5 (3%)	0	100	100
1	Cg	158/192 (82%)	150 (95%)	7 (4%)	1 (1%)	25	53
1	Ch	157/192 (82%)	149 (95%)	8 (5%)	0	100	100
1	Ci	151/192 (79%)	147 (97%)	4 (3%)	0	100	100
1	Cj	154/192 (80%)	146 (95%)	7 (4%)	1 (1%)	25	53
1	Ck	152/192 (79%)	147 (97%)	5 (3%)	0	100	100
1	Cl	153/192 (80%)	150 (98%)	3 (2%)	0	100	100
1	Cm	157/192 (82%)	148 (94%)	9 (6%)	0	100	100
1	Cn	153/192 (80%)	149 (97%)	4 (3%)	0	100	100
1	Co	153/192 (80%)	151 (99%)	2 (1%)	0	100	100
1	Cp	156/192 (81%)	149 (96%)	6 (4%)	1 (1%)	25	53
1	Cq	153/192 (80%)	146 (95%)	7 (5%)	0	100	100
1	Cr	152/192 (79%)	147 (97%)	4 (3%)	1 (1%)	22	50
1	Cs	152/192 (79%)	147 (97%)	4 (3%)	1 (1%)	22	50
1	Ct	158/192 (82%)	154 (98%)	4 (2%)	0	100	100
1	Cu	157/192 (82%)	149 (95%)	7 (4%)	1 (1%)	25	53
1	Cv	159/192 (83%)	151 (95%)	8 (5%)	0	100	100
1	Cw	153/192 (80%)	149 (97%)	4 (3%)	0	100	100
1	Cx	154/192 (80%)	151 (98%)	3 (2%)	0	100	100
All	All	22658/27648 (82%)	21530 (95%)	982 (4%)	146 (1%)	25	53

All (146) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AE	162	LEU
1	AO	4	GLN
1	Aq	2	SER
1	Au	2	SER
1	Bi	2	SER
1	Bt	2	SER
1	BU	160	ALA
1	Ca	4	GLN
1	CJ	163	GLY
1	Cj	2	SER
1	CR	160	ALA

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Mol	Chain	Res	Type
1	AB	160	ALA
1	AB	162	LEU
1	Ab	156	GLY
1	AC	159	GLU
1	Ai	156	GLY
1	Al	3	SER
1	Al	160	ALA
1	Al	162	LEU
1	Am	44	ALA
1	An	155	LEU
1	Ao	159	GLU
1	AQ	1	MET
1	Ar	160	ALA
1	Ar	162	LEU
1	Bd	1	MET
1	Be	162	LEU
1	Be	163	GLY
1	Bf	44	ALA
1	Bf	162	LEU
1	Bq	2	SER
1	Br	159	GLU
1	BV	3	SER
1	BX	159	GLU
1	CG	3	SER
1	CI	44	ALA
1	CR	159	GLU
1	CT	2	SER
1	CX	1	MET
1	AD	156	GLY
1	Ad	159	GLU
1	AE	160	ALA
1	Aj	44	ALA
1	Aj	160	ALA
1	Ak	163	GLY
1	AM	44	ALA
1	AN	162	LEU
1	AO	160	ALA
1	AO	162	LEU
1	Ap	155	LEU
1	AQ	162	LEU
1	AU	3	SER
1	Av	159	GLU

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Mol	Chain	Res	Type
1	AX	81	ASP
1	BF	159	GLU
1	BH	44	ALA
1	Bh	157	GLY
1	BN	156	GLY
1	Bq	44	ALA
1	BX	155	LEU
1	CA	156	GLY
1	CC	44	ALA
1	CH	156	GLY
1	CM	44	ALA
1	Cr	3	SER
1	Cs	155	LEU
1	Cu	44	ALA
1	CX	44	ALA
1	AB	156	GLY
1	Ab	159	GLU
1	Ad	160	ALA
1	Ai	155	LEU
1	Ak	164	GLU
1	AM	156	GLY
1	Am	156	GLY
1	Am	158	PRO
1	An	160	ALA
1	AO	163	GLY
1	Ao	44	ALA
1	Ap	159	GLU
1	Ar	159	GLU
1	AS	44	ALA
1	AV	44	ALA
1	BA	162	LEU
1	Bf	163	GLY
1	BJ	155	LEU
1	Bk	44	ALA
1	Bl	156	GLY
1	BO	44	ALA
1	Bt	44	ALA
1	BV	156	GLY
1	Bv	159	GLU
1	BX	160	ALA
1	Ca	44	ALA
1	CE	1	MET

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Mol	Chain	Res	Type
1	CE	4	GLN
1	CJ	81	ASP
1	CR	162	LEU
1	AB	159	GLU
1	AC	44	ALA
1	Ad	81	ASP
1	AF	155	LEU
1	AI	3	SER
1	Aj	159	GLU
1	Aj	162	LEU
1	Al	159	GLU
1	Am	159	GLU
1	AQ	44	ALA
1	AR	44	ALA
1	AT	44	ALA
1	AV	155	LEU
1	Aw	44	ALA
1	Bd	44	ALA
1	Bd	155	LEU
1	Be	160	ALA
1	Bf	160	ALA
1	Bn	44	ALA
1	Bn	155	LEU
1	Bp	44	ALA
1	Br	155	LEU
1	Bu	159	GLU
1	Bw	156	GLY
1	BX	162	LEU
1	Ca	156	GLY
1	Cg	156	GLY
1	CM	4	GLN
1	Cp	44	ALA
1	AE	159	GLU
1	Aj	163	GLY
1	AN	159	GLU
1	Ap	160	ALA
1	AT	155	LEU
1	BF	158	PRO
1	Bn	159	GLU
1	BR	44	ALA
1	Bu	162	LEU
1	AR	163	GLY

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Mol	Chain	Res	Type
1	AE	163	GLY
1	Av	157	GLY
1	BA	163	GLY
1	CK	156	GLY
1	AC	158	PRO
1	CD	156	GLY
1	AE	156	GLY
1	BF	156	GLY
1	Bf	156	GLY

### 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	AA	134/161 (83%)	128 (96%)	6 (4%)	27	57
1	AB	138/161 (86%)	133 (96%)	5 (4%)	35	66
1	AC	136/161 (84%)	132 (97%)	4 (3%)	42	72
1	AD	134/161 (83%)	133 (99%)	1 (1%)	84	94
1	AE	138/161 (86%)	136 (99%)	2 (1%)	67	86
1	AF	134/161 (83%)	131 (98%)	3 (2%)	52	79
1	AG	134/161 (83%)	131 (98%)	3 (2%)	52	79
1	AH	135/161 (84%)	131 (97%)	4 (3%)	41	72
1	AI	134/161 (83%)	131 (98%)	3 (2%)	52	79
1	AJ	133/161 (83%)	132 (99%)	1 (1%)	81	93
1	AK	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	AL	133/161 (83%)	130 (98%)	3 (2%)	50	78
1	AM	136/161 (84%)	133 (98%)	3 (2%)	52	79
1	AN	138/161 (86%)	135 (98%)	3 (2%)	52	79
1	AO	138/161 (86%)	127 (92%)	11 (8%)	12	31
1	AP	135/161 (84%)	128 (95%)	7 (5%)	23	51
1	AQ	138/161 (86%)	136 (99%)	2 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AR	137/161 (85%)	135 (98%)	2 (2%)	65	86
1	AS	134/161 (83%)	130 (97%)	4 (3%)	41	72
1	AT	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	AU	135/161 (84%)	131 (97%)	4 (3%)	41	72
1	AV	134/161 (83%)	133 (99%)	1 (1%)	84	94
1	AW	134/161 (83%)	133 (99%)	1 (1%)	84	94
1	AX	135/161 (84%)	134 (99%)	1 (1%)	84	94
1	Aa	136/161 (84%)	133 (98%)	3 (2%)	52	79
1	Ab	135/161 (84%)	130 (96%)	5 (4%)	34	65
1	Ac	135/161 (84%)	132 (98%)	3 (2%)	52	79
1	Ad	138/161 (86%)	131 (95%)	7 (5%)	24	52
1	Ae	136/161 (84%)	132 (97%)	4 (3%)	42	72
1	Af	136/161 (84%)	133 (98%)	3 (2%)	52	79
1	Ag	133/161 (83%)	129 (97%)	4 (3%)	41	72
1	Ah	136/161 (84%)	133 (98%)	3 (2%)	52	79
1	Ai	135/161 (84%)	132 (98%)	3 (2%)	52	79
1	Aj	138/161 (86%)	132 (96%)	6 (4%)	29	59
1	Ak	138/161 (86%)	133 (96%)	5 (4%)	35	66
1	Al	138/161 (86%)	131 (95%)	7 (5%)	24	52
1	Am	136/161 (84%)	135 (99%)	1 (1%)	84	94
1	An	135/161 (84%)	133 (98%)	2 (2%)	65	86
1	Ao	136/161 (84%)	134 (98%)	2 (2%)	65	86
1	Ap	136/161 (84%)	134 (98%)	2 (2%)	65	86
1	Aq	135/161 (84%)	132 (98%)	3 (2%)	52	79
1	Ar	138/161 (86%)	133 (96%)	5 (4%)	35	66
1	As	136/161 (84%)	130 (96%)	6 (4%)	28	58
1	At	135/161 (84%)	128 (95%)	7 (5%)	23	51
1	Au	135/161 (84%)	130 (96%)	5 (4%)	34	65
1	Av	138/161 (86%)	135 (98%)	3 (2%)	52	79
1	Aw	135/161 (84%)	128 (95%)	7 (5%)	23	51
1	Ax	133/161 (83%)	132 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	139/161 (86%)	134 (96%)	5 (4%)	35	66
1	BB	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	BC	132/161 (82%)	130 (98%)	2 (2%)	65	86
1	BD	136/161 (84%)	135 (99%)	1 (1%)	84	94
1	BE	135/161 (84%)	135 (100%)	0	100	100
1	BF	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	BG	133/161 (83%)	131 (98%)	2 (2%)	65	86
1	BH	132/161 (82%)	129 (98%)	3 (2%)	50	78
1	BI	133/161 (83%)	132 (99%)	1 (1%)	81	93
1	BJ	133/161 (83%)	130 (98%)	3 (2%)	50	78
1	BK	133/161 (83%)	128 (96%)	5 (4%)	33	64
1	BL	133/161 (83%)	132 (99%)	1 (1%)	81	93
1	BM	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	BN	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	BO	135/161 (84%)	132 (98%)	3 (2%)	52	79
1	BP	134/161 (83%)	131 (98%)	3 (2%)	52	79
1	BQ	135/161 (84%)	130 (96%)	5 (4%)	34	65
1	BR	136/161 (84%)	134 (98%)	2 (2%)	65	86
1	BS	135/161 (84%)	134 (99%)	1 (1%)	84	94
1	BT	133/161 (83%)	131 (98%)	2 (2%)	65	86
1	BU	136/161 (84%)	135 (99%)	1 (1%)	84	94
1	BV	132/161 (82%)	130 (98%)	2 (2%)	65	86
1	BW	135/161 (84%)	133 (98%)	2 (2%)	65	86
1	BX	136/161 (84%)	133 (98%)	3 (2%)	52	79
1	Ba	134/161 (83%)	131 (98%)	3 (2%)	52	79
1	Bb	135/161 (84%)	132 (98%)	3 (2%)	52	79
1	Bc	136/161 (84%)	130 (96%)	6 (4%)	28	58
1	Bd	136/161 (84%)	136 (100%)	0	100	100
1	Be	136/161 (84%)	133 (98%)	3 (2%)	52	79
1	Bf	138/161 (86%)	132 (96%)	6 (4%)	29	59
1	Bg	133/161 (83%)	131 (98%)	2 (2%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bh	135/161 (84%)	132 (98%)	3 (2%)	52	79
1	Bi	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	Bj	131/161 (81%)	128 (98%)	3 (2%)	50	78
1	Bk	135/161 (84%)	132 (98%)	3 (2%)	52	79
1	Bl	135/161 (84%)	131 (97%)	4 (3%)	41	72
1	Bm	134/161 (83%)	130 (97%)	4 (3%)	41	72
1	Bn	138/161 (86%)	135 (98%)	3 (2%)	52	79
1	Bo	133/161 (83%)	132 (99%)	1 (1%)	81	93
1	Bp	136/161 (84%)	133 (98%)	3 (2%)	52	79
1	Bq	136/161 (84%)	135 (99%)	1 (1%)	84	94
1	Br	136/161 (84%)	130 (96%)	6 (4%)	28	58
1	Bs	133/161 (83%)	131 (98%)	2 (2%)	65	86
1	Bt	134/161 (83%)	130 (97%)	4 (3%)	41	72
1	Bu	138/161 (86%)	133 (96%)	5 (4%)	35	66
1	Bv	135/161 (84%)	133 (98%)	2 (2%)	65	86
1	Bw	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	Bx	133/161 (83%)	131 (98%)	2 (2%)	65	86
1	CA	135/161 (84%)	131 (97%)	4 (3%)	41	72
1	CB	135/161 (84%)	130 (96%)	5 (4%)	34	65
1	CC	133/161 (83%)	131 (98%)	2 (2%)	65	86
1	CD	136/161 (84%)	136 (100%)	0	100	100
1	CE	136/161 (84%)	134 (98%)	2 (2%)	65	86
1	CF	134/161 (83%)	130 (97%)	4 (3%)	41	72
1	CG	136/161 (84%)	131 (96%)	5 (4%)	34	65
1	CH	135/161 (84%)	132 (98%)	3 (2%)	52	79
1	CI	135/161 (84%)	130 (96%)	5 (4%)	34	65
1	CJ	138/161 (86%)	133 (96%)	5 (4%)	35	66
1	CK	135/161 (84%)	131 (97%)	4 (3%)	41	72
1	CL	135/161 (84%)	133 (98%)	2 (2%)	65	86
1	CM	135/161 (84%)	130 (96%)	5 (4%)	34	65
1	CN	135/161 (84%)	133 (98%)	2 (2%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CO	135/161 (84%)	133 (98%)	2 (2%)	65	86
1	CP	134/161 (83%)	131 (98%)	3 (2%)	52	79
1	CQ	136/161 (84%)	129 (95%)	7 (5%)	24	52
1	CR	139/161 (86%)	136 (98%)	3 (2%)	52	79
1	CS	136/161 (84%)	131 (96%)	5 (4%)	34	65
1	CT	134/161 (83%)	130 (97%)	4 (3%)	41	72
1	CU	135/161 (84%)	135 (100%)	0	100	100
1	CV	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	CW	133/161 (83%)	132 (99%)	1 (1%)	81	93
1	CX	136/161 (84%)	134 (98%)	2 (2%)	65	86
1	Ca	133/161 (83%)	130 (98%)	3 (2%)	50	78
1	Cb	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	Cc	133/161 (83%)	131 (98%)	2 (2%)	65	86
1	Cd	131/161 (81%)	129 (98%)	2 (2%)	65	86
1	Ce	132/161 (82%)	129 (98%)	3 (2%)	50	78
1	Cf	131/161 (81%)	131 (100%)	0	100	100
1	Cg	134/161 (83%)	132 (98%)	2 (2%)	65	86
1	Ch	134/161 (83%)	131 (98%)	3 (2%)	52	79
1	Ci	131/161 (81%)	131 (100%)	0	100	100
1	Cj	134/161 (83%)	131 (98%)	3 (2%)	52	79
1	Ck	132/161 (82%)	130 (98%)	2 (2%)	65	86
1	Cl	132/161 (82%)	130 (98%)	2 (2%)	65	86
1	Cm	134/161 (83%)	130 (97%)	4 (3%)	41	72
1	Cn	133/161 (83%)	130 (98%)	3 (2%)	50	78
1	Co	132/161 (82%)	129 (98%)	3 (2%)	50	78
1	Cp	134/161 (83%)	133 (99%)	1 (1%)	84	94
1	Cq	132/161 (82%)	131 (99%)	1 (1%)	81	93
1	Cr	132/161 (82%)	130 (98%)	2 (2%)	65	86
1	Cs	131/161 (81%)	130 (99%)	1 (1%)	81	93
1	Ct	134/161 (83%)	131 (98%)	3 (2%)	52	79
1	Cu	134/161 (83%)	131 (98%)	3 (2%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Cv	135/161 (84%)	132 (98%)	3 (2%)	52	79
1	Cw	132/161 (82%)	132 (100%)	0	100	100
1	Cx	134/161 (83%)	130 (97%)	4 (3%)	41	72
All	All	19400/23184 (84%)	18968 (98%)	432 (2%)	52	79

All (432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	12	ASP
1	AA	29	TYR
1	AA	34	LEU
1	AA	57	GLU
1	AA	81	ASP
1	AA	101	MET
1	Aa	0	ARG
1	Aa	29	TYR
1	Aa	34	LEU
1	AB	12	ASP
1	AB	93	THR
1	AB	145	MET
1	AB	159	GLU
1	AB	165	TYR
1	Ab	1	MET
1	Ab	19	SER
1	Ab	29	TYR
1	Ab	81	ASP
1	Ab	119	SER
1	AC	25	LEU
1	AC	29	TYR
1	AC	63	TYR
1	AC	122	THR
1	Ac	19	SER
1	Ac	29	TYR
1	Ac	57	GLU
1	AD	81	ASP
1	Ad	4	GLN
1	Ad	29	TYR
1	Ad	54	GLU
1	Ad	64	GLU
1	Ad	144	LYS
1	Ad	159	GLU

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Mol	Chain	Res	Type
1	Ad	165	TYR
1	AE	159	GLU
1	AE	165	TYR
1	Ae	12	ASP
1	Ae	29	TYR
1	Ae	57	GLU
1	Ae	80	GLN
1	AF	4	GLN
1	AF	29	TYR
1	AF	101	MET
1	Af	23	LEU
1	Af	29	TYR
1	Af	34	LEU
1	AG	4	GLN
1	AG	81	ASP
1	AG	93	THR
1	Ag	11	THR
1	Ag	29	TYR
1	Ag	34	LEU
1	Ag	122	THR
1	AH	12	ASP
1	AH	19	SER
1	AH	63	TYR
1	AH	101	MET
1	Ah	2	SER
1	Ah	29	TYR
1	Ah	34	LEU
1	AI	12	ASP
1	AI	29	TYR
1	AI	83	LYS
1	Ai	4	GLN
1	Ai	29	TYR
1	Ai	85	PRO
1	AJ	29	TYR
1	Aj	28	SER
1	Aj	29	TYR
1	Aj	33	SER
1	Aj	63	TYR
1	Aj	159	GLU
1	Aj	165	TYR
1	AK	12	ASP
1	AK	29	TYR

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Mol	Chain	Res	Type
1	Ak	29	TYR
1	Ak	85	PRO
1	Ak	101	MET
1	Ak	159	GLU
1	Ak	165	TYR
1	AL	29	TYR
1	AL	122	THR
1	AL	148	HIS
1	Al	12	ASP
1	Al	68	LYS
1	Al	119	SER
1	Al	122	THR
1	Al	148	HIS
1	Al	159	GLU
1	Al	165	TYR
1	AM	3	SER
1	AM	29	TYR
1	AM	126	LEU
1	Am	159	GLU
1	AN	119	SER
1	AN	159	GLU
1	AN	165	TYR
1	An	12	ASP
1	An	29	TYR
1	AO	10	SER
1	AO	19	SER
1	AO	26	GLN
1	AO	29	TYR
1	AO	57	GLU
1	AO	95	ASP
1	AO	122	THR
1	AO	139	VAL
1	AO	150	THR
1	AO	159	GLU
1	AO	165	TYR
1	Ao	2	SER
1	Ao	101	MET
1	AP	2	SER
1	AP	4	GLN
1	AP	23	LEU
1	AP	29	TYR
1	AP	101	MET

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Mol	Chain	Res	Type
1	AP	112	LEU
1	AP	153	HIS
1	Ap	29	TYR
1	Ap	85	PRO
1	AQ	101	MET
1	AQ	159	GLU
1	Aq	2	SER
1	Aq	4	GLN
1	Aq	83	LYS
1	AR	4	GLN
1	AR	29	TYR
1	Ar	41	ASP
1	Ar	101	MET
1	Ar	119	SER
1	Ar	159	GLU
1	Ar	165	TYR
1	AS	4	GLN
1	AS	19	SER
1	AS	29	TYR
1	AS	122	THR
1	As	4	GLN
1	As	19	SER
1	As	29	TYR
1	As	101	MET
1	As	122	THR
1	As	155	LEU
1	AT	93	THR
1	AT	149	LEU
1	At	2	SER
1	At	25	LEU
1	At	28	SER
1	At	81	ASP
1	At	119	SER
1	At	126	LEU
1	At	145	MET
1	AU	1	MET
1	AU	11	THR
1	AU	29	TYR
1	AU	122	THR
1	Au	29	TYR
1	Au	57	GLU
1	Au	101	MET

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Mol	Chain	Res	Type
1	Au	122	THR
1	Au	154	ARG
1	AV	4	GLN
1	Av	29	TYR
1	Av	80	GLN
1	Av	159	GLU
1	AW	29	TYR
1	Aw	25	LEU
1	Aw	29	TYR
1	Aw	34	LEU
1	Aw	81	ASP
1	Aw	114	LEU
1	Aw	119	SER
1	Aw	144	LYS
1	AX	29	TYR
1	Ax	114	LEU
1	BA	2	SER
1	BA	25	LEU
1	BA	29	TYR
1	BA	159	GLU
1	BA	165	TYR
1	Ba	2	SER
1	Ba	29	TYR
1	Ba	81	ASP
1	BB	29	TYR
1	BB	57	GLU
1	Bb	4	GLN
1	Bb	101	MET
1	Bb	127	CYS
1	BC	3	SER
1	BC	4	GLN
1	Bc	4	GLN
1	Bc	10	SER
1	Bc	29	TYR
1	Bc	101	MET
1	Bc	144	LYS
1	Bc	154	ARG
1	BD	0	ARG
1	Be	57	GLU
1	Be	101	MET
1	Be	159	GLU
1	BF	2	SER

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Mol	Chain	Res	Type
1	BF	101	MET
1	Bf	4	GLN
1	Bf	12	ASP
1	Bf	30	THR
1	Bf	78	LEU
1	Bf	159	GLU
1	Bf	165	TYR
1	BG	19	SER
1	BG	119	SER
1	Bg	29	TYR
1	Bg	34	LEU
1	BH	12	ASP
1	BH	29	TYR
1	BH	81	ASP
1	Bh	19	SER
1	Bh	29	TYR
1	Bh	72	GLN
1	BI	81	ASP
1	Bi	29	TYR
1	Bi	122	THR
1	BJ	28	SER
1	BJ	29	TYR
1	BJ	81	ASP
1	Bj	4	GLN
1	Bj	12	ASP
1	Bj	29	TYR
1	BK	10	SER
1	BK	12	ASP
1	BK	29	TYR
1	BK	70	GLN
1	BK	126	LEU
1	Bk	29	TYR
1	Bk	101	MET
1	Bk	122	THR
1	BL	29	TYR
1	Bl	29	TYR
1	Bl	34	LEU
1	Bl	81	ASP
1	Bl	98	LYS
1	BM	19	SER
1	BM	26	GLN
1	Bm	29	TYR

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Mol	Chain	Res	Type
1	Bm	34	LEU
1	Bm	57	GLU
1	Bm	101	MET
1	BN	29	TYR
1	BN	57	GLU
1	Bn	4	GLN
1	Bn	159	GLU
1	Bn	162	LEU
1	BO	63	TYR
1	BO	101	MET
1	BO	122	THR
1	Bo	29	TYR
1	BP	29	TYR
1	BP	83	LYS
1	BP	159	GLU
1	Bp	11	THR
1	Bp	29	TYR
1	Bp	101	MET
1	BQ	12	ASP
1	BQ	21	VAL
1	BQ	29	TYR
1	BQ	93	THR
1	BQ	144	LYS
1	Bq	81	ASP
1	BR	19	SER
1	BR	29	TYR
1	Br	0	ARG
1	Br	12	ASP
1	Br	68	LYS
1	Br	85	PRO
1	Br	93	THR
1	Br	159	GLU
1	BS	101	MET
1	Bs	29	TYR
1	Bs	122	THR
1	BT	23	LEU
1	BT	29	TYR
1	Bt	12	ASP
1	Bt	29	TYR
1	Bt	69	MET
1	Bt	101	MET
1	BU	159	GLU

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Mol	Chain	Res	Type
1	Bu	28	SER
1	Bu	29	TYR
1	Bu	57	GLU
1	Bu	122	THR
1	Bu	159	GLU
1	BV	29	TYR
1	BV	81	ASP
1	Bv	12	ASP
1	Bv	29	TYR
1	BW	12	ASP
1	BW	29	TYR
1	Bw	29	TYR
1	Bw	34	LEU
1	BX	63	TYR
1	BX	72	GLN
1	BX	159	GLU
1	Bx	29	TYR
1	Bx	81	ASP
1	CA	1	MET
1	CA	3	SER
1	CA	29	TYR
1	CA	66	LEU
1	Ca	12	ASP
1	Ca	126	LEU
1	Ca	148	HIS
1	CB	3	SER
1	CB	12	ASP
1	CB	29	TYR
1	CB	101	MET
1	CB	122	THR
1	Cb	63	TYR
1	Cb	159	GLU
1	CC	4	GLN
1	CC	29	TYR
1	Cc	12	ASP
1	Cc	154	ARG
1	Cd	29	TYR
1	Cd	101	MET
1	CE	4	GLN
1	CE	29	TYR
1	Ce	12	ASP
1	Ce	29	TYR

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Mol	Chain	Res	Type
1	Ce	63	TYR
1	CF	29	TYR
1	CF	34	LEU
1	CF	65	ARG
1	CF	101	MET
1	CG	19	SER
1	CG	29	TYR
1	CG	70	GLN
1	CG	81	ASP
1	CG	147	ASP
1	Cg	12	ASP
1	Cg	101	MET
1	CH	4	GLN
1	CH	29	TYR
1	CH	122	THR
1	Ch	12	ASP
1	Ch	28	SER
1	Ch	46	GLU
1	CI	12	ASP
1	CI	19	SER
1	CI	23	LEU
1	CI	29	TYR
1	CI	80	GLN
1	CJ	2	SER
1	CJ	4	GLN
1	CJ	12	ASP
1	CJ	29	TYR
1	CJ	164	GLU
1	Cj	11	THR
1	Cj	29	TYR
1	Cj	34	LEU
1	CK	25	LEU
1	CK	28	SER
1	CK	29	TYR
1	CK	101	MET
1	Ck	29	TYR
1	Ck	69	MET
1	CL	29	TYR
1	CL	101	MET
1	Cl	28	SER
1	Cl	29	TYR
1	CM	4	GLN

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Mol	Chain	Res	Type
1	CM	12	ASP
1	CM	29	TYR
1	CM	68	LYS
1	CM	93	THR
1	Cm	12	ASP
1	Cm	57	GLU
1	Cm	81	ASP
1	Cm	159	GLU
1	CN	29	TYR
1	CN	85	PRO
1	Cn	2	SER
1	Cn	4	GLN
1	Cn	29	TYR
1	CO	29	TYR
1	CO	101	MET
1	Co	29	TYR
1	Co	119	SER
1	Co	137	GLU
1	CP	29	TYR
1	CP	93	THR
1	CP	101	MET
1	Cp	29	TYR
1	CQ	0	ARG
1	CQ	10	SER
1	CQ	19	SER
1	CQ	26	GLN
1	CQ	29	TYR
1	CQ	63	TYR
1	CQ	150	THR
1	Cq	29	TYR
1	CR	63	TYR
1	CR	159	GLU
1	CR	165	TYR
1	Cr	19	SER
1	Cr	29	TYR
1	CS	3	SER
1	CS	19	SER
1	CS	30	THR
1	CS	122	THR
1	CS	148	HIS
1	Cs	29	TYR
1	CT	4	GLN

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Mol	Chain	Res	Type
1	CT	23	LEU
1	CT	29	TYR
1	CT	101	MET
1	Ct	4	GLN
1	Ct	29	TYR
1	Ct	147	ASP
1	Cu	4	GLN
1	Cu	12	ASP
1	Cu	29	TYR
1	CV	29	TYR
1	CV	154	ARG
1	Cv	4	GLN
1	Cv	29	TYR
1	Cv	80	GLN
1	CW	29	TYR
1	CX	2	SER
1	CX	12	ASP
1	Cx	12	ASP
1	Cx	29	TYR
1	Cx	57	GLU
1	Cx	85	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (253) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	22	ASN
1	AA	71	ASN
1	AB	4	GLN
1	AB	70	GLN
1	AB	72	GLN
1	AC	26	GLN
1	Ac	4	GLN
1	Ac	22	ASN
1	AE	4	GLN
1	AE	50	HIS
1	Ae	4	GLN
1	Ae	22	ASN
1	Ae	80	GLN
1	AF	8	ASN
1	AF	71	ASN
1	AF	72	GLN
1	AF	115	HIS

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Mol	Chain	Res	Type
1	AG	108	ASN
1	AH	26	GLN
1	AH	71	ASN
1	AI	26	GLN
1	Ai	50	HIS
1	AJ	8	ASN
1	AJ	72	GLN
1	Aj	8	ASN
1	Aj	71	ASN
1	Aj	72	GLN
1	Aj	115	HIS
1	AK	71	ASN
1	AK	72	GLN
1	Ak	71	ASN
1	AL	108	ASN
1	Al	8	ASN
1	AM	71	ASN
1	AM	72	GLN
1	Am	8	ASN
1	Am	71	ASN
1	AN	72	GLN
1	AN	148	HIS
1	AO	8	ASN
1	AO	72	GLN
1	AO	148	HIS
1	Ao	71	ASN
1	Ao	72	GLN
1	AP	4	GLN
1	Ap	8	ASN
1	Ap	50	HIS
1	Ap	72	GLN
1	AQ	8	ASN
1	Aq	8	ASN
1	Aq	26	GLN
1	Aq	50	HIS
1	Aq	72	GLN
1	Aq	108	ASN
1	AR	71	ASN
1	AR	72	GLN
1	AS	72	GLN
1	AS	148	HIS
1	As	8	ASN

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Mol	Chain	Res	Type
1	As	148	HIS
1	AT	22	ASN
1	AT	71	ASN
1	AT	108	ASN
1	AT	125	HIS
1	AT	133	HIS
1	At	71	ASN
1	AU	8	ASN
1	AU	72	GLN
1	AV	72	GLN
1	AV	148	HIS
1	AW	8	ASN
1	AW	71	ASN
1	AW	72	GLN
1	AW	115	HIS
1	Aw	50	HIS
1	AX	71	ASN
1	Ax	8	ASN
1	Ax	50	HIS
1	BA	72	GLN
1	Ba	4	GLN
1	Ba	22	ASN
1	BB	71	ASN
1	BB	72	GLN
1	Bb	72	GLN
1	BC	8	ASN
1	BC	72	GLN
1	Bc	8	ASN
1	Bc	70	GLN
1	Bc	108	ASN
1	BD	71	ASN
1	Bd	8	ASN
1	Bd	71	ASN
1	BE	8	ASN
1	Be	108	ASN
1	BF	50	HIS
1	Bf	8	ASN
1	Bf	71	ASN
1	BG	70	GLN
1	BG	72	GLN
1	Bg	8	ASN
1	Bg	22	ASN

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Mol	Chain	Res	Type
1	Bg	71	ASN
1	Bg	72	GLN
1	BH	26	GLN
1	Bi	72	GLN
1	BJ	8	ASN
1	BJ	71	ASN
1	BJ	72	GLN
1	Bj	22	ASN
1	BK	71	ASN
1	BK	72	GLN
1	BK	108	ASN
1	Bk	22	ASN
1	BL	72	GLN
1	BM	8	ASN
1	BM	50	HIS
1	Bn	71	ASN
1	Bo	50	HIS
1	Bo	71	ASN
1	Bo	72	GLN
1	BP	72	GLN
1	Bp	26	GLN
1	Bp	151	ASN
1	Bq	8	ASN
1	Bq	72	GLN
1	BR	72	GLN
1	Br	71	ASN
1	Br	72	GLN
1	Bs	26	GLN
1	Bs	72	GLN
1	BT	72	GLN
1	Bt	8	ASN
1	BU	8	ASN
1	BU	72	GLN
1	Bu	50	HIS
1	Bu	72	GLN
1	BV	4	GLN
1	BV	8	ASN
1	BV	71	ASN
1	BV	72	GLN
1	Bv	71	ASN
1	Bv	72	GLN
1	BW	70	GLN

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Mol	Chain	Res	Type
1	BW	71	ASN
1	BW	72	GLN
1	Bw	8	ASN
1	Bw	22	ASN
1	Bw	71	ASN
1	Bw	72	GLN
1	BX	8	ASN
1	BX	70	GLN
1	BX	72	GLN
1	BX	148	HIS
1	Bx	26	GLN
1	Bx	72	GLN
1	CA	8	ASN
1	CA	50	HIS
1	CA	71	ASN
1	Ca	4	GLN
1	Ca	70	GLN
1	Ca	72	GLN
1	Ca	115	HIS
1	CB	72	GLN
1	Cb	8	ASN
1	Cb	108	ASN
1	Cb	148	HIS
1	Cc	71	ASN
1	Cc	72	GLN
1	CD	50	HIS
1	Cd	8	ASN
1	Cd	22	ASN
1	Cd	71	ASN
1	Cd	72	GLN
1	Cd	108	ASN
1	Cd	115	HIS
1	CE	18	ASN
1	CE	71	ASN
1	Ce	72	GLN
1	CF	50	HIS
1	CF	71	ASN
1	CF	72	GLN
1	Cf	22	ASN
1	Cf	72	GLN
1	CG	8	ASN
1	CG	72	GLN

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Mol	Chain	Res	Type
1	Cg	8	ASN
1	Cg	26	GLN
1	CH	115	HIS
1	Ch	8	ASN
1	Ch	22	ASN
1	Ch	108	ASN
1	Ch	133	HIS
1	Ch	148	HIS
1	CI	8	ASN
1	CI	148	HIS
1	Ci	8	ASN
1	Ci	71	ASN
1	Ci	72	GLN
1	Ci	109	GLN
1	CJ	8	ASN
1	CJ	71	ASN
1	CJ	72	GLN
1	CK	8	ASN
1	CK	71	ASN
1	CK	115	HIS
1	Ck	8	ASN
1	Ck	72	GLN
1	Cl	71	ASN
1	Cl	72	GLN
1	CM	71	ASN
1	CM	115	HIS
1	Cm	26	GLN
1	Cm	72	GLN
1	Cn	22	ASN
1	Cn	72	GLN
1	Co	8	ASN
1	Co	26	GLN
1	Co	72	GLN
1	Co	109	GLN
1	CP	108	ASN
1	Cp	133	HIS
1	CQ	72	GLN
1	Cq	22	ASN
1	Cq	26	GLN
1	Cq	72	GLN
1	CR	8	ASN
1	CR	70	GLN

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Mol	Chain	Res	Type
1	CR	72	GLN
1	CR	148	HIS
1	Cr	72	GLN
1	CS	26	GLN
1	Cs	26	GLN
1	Cs	71	ASN
1	Cs	72	GLN
1	CT	71	ASN
1	CT	108	ASN
1	Ct	4	GLN
1	Ct	72	GLN
1	CU	72	GLN
1	Cu	22	ASN
1	Cu	71	ASN
1	CV	22	ASN
1	CV	71	ASN
1	CV	72	GLN
1	Cv	71	ASN
1	Cv	72	GLN
1	Cv	80	GLN
1	CW	72	GLN
1	Cw	22	ASN
1	Cw	72	GLN
1	CX	8	ASN
1	CX	70	GLN
1	Cx	71	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	158/192 (82%)	-0.35	5 (3%) 47 42	31, 61, 82, 117	0
1	AB	165/192 (85%)	-0.24	8 (4%) 30 26	26, 54, 95, 109	0
1	AC	161/192 (83%)	-0.32	4 (2%) 57 54	38, 58, 77, 111	0
1	AD	159/192 (82%)	-0.24	4 (2%) 57 54	51, 68, 82, 118	0
1	AE	165/192 (85%)	-0.40	9 (5%) 25 20	12, 34, 96, 112	0
1	AF	158/192 (82%)	-0.49	2 (1%) 77 76	19, 47, 66, 104	0
1	AG	159/192 (82%)	-0.45	4 (2%) 57 54	31, 47, 63, 123	0
1	AH	160/192 (83%)	-0.25	3 (1%) 66 64	21, 42, 69, 112	0
1	AI	158/192 (82%)	-0.21	5 (3%) 47 42	54, 70, 84, 114	0
1	AJ	157/192 (81%)	-0.28	2 (1%) 77 76	25, 60, 79, 99	0
1	AK	157/192 (81%)	-0.35	1 (0%) 89 89	33, 59, 75, 101	0
1	AL	157/192 (81%)	-0.18	4 (2%) 57 54	52, 68, 82, 120	0
1	AM	162/192 (84%)	-0.47	3 (1%) 66 64	17, 39, 69, 112	0
1	AN	165/192 (85%)	-0.33	6 (3%) 42 37	31, 48, 89, 107	0
1	AO	165/192 (85%)	-0.21	11 (6%) 17 13	17, 46, 87, 110	0
1	AP	159/192 (82%)	-0.54	0 100 100	7, 30, 51, 102	0
1	AQ	165/192 (85%)	-0.15	11 (6%) 17 13	33, 62, 90, 110	0
1	AR	164/192 (85%)	-0.35	6 (3%) 41 36	20, 46, 89, 111	0
1	AS	160/192 (83%)	-0.21	6 (3%) 40 35	32, 56, 87, 117	0
1	AT	158/192 (82%)	-0.51	1 (0%) 89 89	15, 43, 62, 110	0
1	AU	160/192 (83%)	-0.49	1 (0%) 89 89	24, 42, 68, 107	0
1	AV	160/192 (83%)	-0.20	7 (4%) 34 29	30, 49, 82, 115	0
1	AW	158/192 (82%)	-0.33	2 (1%) 77 76	26, 56, 76, 113	0
1	AX	160/192 (83%)	-0.35	3 (1%) 66 64	23, 45, 78, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Aa	161/192 (83%)	-0.51	3 (1%) 66 64	12, 30, 54, 109	0
1	Ab	161/192 (83%)	-0.58	0 100 100	13, 35, 65, 110	0
1	Ac	160/192 (83%)	-0.56	0 100 100	15, 35, 66, 103	0
1	Ad	165/192 (85%)	-0.58	3 (1%) 68 66	7, 26, 87, 107	0
1	Ae	162/192 (84%)	-0.33	5 (3%) 49 44	8, 29, 65, 113	0
1	Af	161/192 (83%)	-0.45	1 (0%) 89 89	10, 28, 56, 106	0
1	Ag	155/192 (80%)	-0.65	1 (0%) 89 89	8, 28, 45, 70	0
1	Ah	161/192 (83%)	-0.42	0 100 100	12, 32, 55, 109	0
1	Ai	159/192 (82%)	-0.54	1 (0%) 89 89	8, 23, 46, 96	0
1	Aj	165/192 (85%)	-0.20	5 (3%) 50 45	12, 31, 85, 109	0
1	Ak	165/192 (85%)	-0.34	7 (4%) 36 31	18, 37, 86, 107	0
1	Al	165/192 (85%)	-0.39	1 (0%) 89 89	8, 33, 81, 108	0
1	Am	162/192 (84%)	-0.49	1 (0%) 89 89	11, 31, 57, 102	0
1	An	161/192 (83%)	-0.58	2 (1%) 79 78	13, 28, 56, 96	0
1	Ao	161/192 (83%)	-0.50	2 (1%) 79 78	11, 32, 54, 105	0
1	Ap	162/192 (84%)	-0.58	2 (1%) 79 78	11, 30, 63, 101	0
1	Aq	160/192 (83%)	-0.51	2 (1%) 77 76	9, 30, 58, 110	0
1	Ar	165/192 (85%)	-0.49	2 (1%) 79 78	9, 28, 81, 105	0
1	As	161/192 (83%)	-0.51	3 (1%) 66 64	9, 32, 60, 109	0
1	At	160/192 (83%)	-0.60	2 (1%) 77 76	9, 31, 67, 107	0
1	Au	160/192 (83%)	-0.30	2 (1%) 77 76	19, 40, 66, 104	0
1	Av	165/192 (85%)	-0.31	5 (3%) 50 45	16, 39, 85, 110	0
1	Aw	161/192 (83%)	-0.47	3 (1%) 66 64	8, 31, 58, 109	0
1	Ax	155/192 (80%)	-0.71	1 (0%) 89 89	11, 31, 45, 76	0
1	BA	166/192 (86%)	-0.25	2 (1%) 79 78	30, 51, 87, 108	0
1	BB	157/192 (81%)	0.47	8 (5%) 28 23	68, 86, 98, 109	0
1	BC	155/192 (80%)	0.24	4 (2%) 56 52	64, 84, 94, 103	0
1	BD	160/192 (83%)	-0.30	1 (0%) 89 89	22, 52, 76, 105	0
1	BE	159/192 (82%)	-0.38	2 (1%) 77 76	26, 46, 72, 111	0
1	BF	159/192 (82%)	-0.63	0 100 100	13, 32, 53, 102	0
1	BG	156/192 (81%)	-0.22	2 (1%) 77 76	31, 58, 70, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	BH	154/192 (80%)	0.05	3 (1%) 66 64	40, 70, 86, 99	0
1	BI	155/192 (80%)	-0.36	0 100 100	19, 52, 73, 97	0
1	BJ	157/192 (81%)	-0.06	2 (1%) 77 76	50, 69, 91, 111	0
1	BK	156/192 (81%)	0.49	8 (5%) 28 23	71, 87, 98, 105	0
1	BL	155/192 (80%)	0.04	0 100 100	57, 74, 89, 92	0
1	BM	158/192 (82%)	-0.33	2 (1%) 77 76	9, 33, 54, 102	0
1	BN	159/192 (82%)	-0.36	0 100 100	20, 41, 63, 114	0
1	BO	160/192 (83%)	-0.11	4 (2%) 57 54	37, 62, 86, 114	0
1	BP	159/192 (82%)	-0.26	5 (3%) 49 44	29, 55, 83, 114	0
1	BQ	160/192 (83%)	-0.49	1 (0%) 89 89	17, 37, 63, 114	0
1	BR	161/192 (83%)	-0.44	3 (1%) 66 64	18, 42, 68, 103	0
1	BS	159/192 (82%)	-0.41	0 100 100	18, 34, 54, 98	0
1	BT	157/192 (81%)	0.20	5 (3%) 47 42	58, 74, 92, 118	0
1	BU	162/192 (84%)	0.05	1 (0%) 89 89	55, 78, 91, 115	0
1	BV	156/192 (81%)	0.27	7 (4%) 33 28	69, 87, 96, 111	0
1	BW	161/192 (83%)	-0.15	4 (2%) 57 54	38, 60, 81, 117	0
1	BX	163/192 (84%)	0.31	6 (3%) 41 36	61, 78, 91, 110	0
1	Ba	158/192 (82%)	-0.11	4 (2%) 57 54	52, 71, 88, 111	0
1	Bb	159/192 (82%)	-0.01	3 (1%) 66 64	49, 72, 90, 118	0
1	Bc	161/192 (83%)	-0.41	1 (0%) 89 89	15, 38, 69, 109	0
1	Bd	161/192 (83%)	-0.47	3 (1%) 66 64	21, 40, 64, 114	0
1	Be	163/192 (84%)	-0.47	1 (0%) 89 89	13, 36, 77, 107	0
1	Bf	165/192 (85%)	-0.31	6 (3%) 42 37	14, 44, 85, 110	0
1	Bg	156/192 (81%)	0.11	4 (2%) 56 52	54, 76, 89, 108	0
1	Bh	159/192 (82%)	-0.45	3 (1%) 66 64	30, 48, 72, 108	0
1	Bi	157/192 (81%)	-0.22	1 (0%) 89 89	32, 58, 70, 94	0
1	Bj	154/192 (80%)	0.09	0 100 100	55, 76, 85, 96	0
1	Bk	159/192 (82%)	-0.20	2 (1%) 77 76	37, 57, 80, 114	0
1	Bl	159/192 (82%)	-0.53	1 (0%) 89 89	12, 38, 61, 109	0
1	Bm	159/192 (82%)	-0.52	3 (1%) 66 64	18, 36, 59, 113	0
1	Bn	165/192 (85%)	-0.09	4 (2%) 59 56	33, 61, 89, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Bo	156/192 (81%)	-0.19	3 (1%) 66 64	44, 65, 84, 96	0
1	Bp	162/192 (84%)	-0.39	7 (4%) 35 30	17, 41, 79, 116	0
1	Bq	160/192 (83%)	-0.11	3 (1%) 66 64	26, 55, 76, 111	0
1	Br	161/192 (83%)	-0.58	2 (1%) 79 78	8, 28, 57, 105	0
1	Bs	155/192 (80%)	-0.24	2 (1%) 77 76	37, 57, 80, 97	0
1	Bt	158/192 (82%)	0.14	4 (2%) 57 54	61, 79, 93, 110	0
1	Bu	165/192 (85%)	-0.40	6 (3%) 42 37	14, 36, 83, 106	0
1	Bv	160/192 (83%)	-0.43	5 (3%) 49 44	23, 45, 72, 120	0
1	Bw	159/192 (82%)	-0.40	3 (1%) 66 64	11, 29, 55, 112	0
1	Bx	157/192 (81%)	0.23	7 (4%) 33 28	62, 83, 95, 113	0
1	CA	160/192 (83%)	-0.51	1 (0%) 89 89	12, 36, 61, 111	0
1	CB	161/192 (83%)	-0.25	4 (2%) 57 54	19, 52, 79, 108	0
1	CC	157/192 (81%)	-0.24	2 (1%) 77 76	45, 65, 78, 109	0
1	CD	161/192 (83%)	-0.49	2 (1%) 79 78	13, 39, 68, 107	0
1	CE	160/192 (83%)	-0.27	1 (0%) 89 89	29, 52, 80, 112	0
1	CF	160/192 (83%)	-0.48	3 (1%) 66 64	11, 35, 53, 101	0
1	CG	160/192 (83%)	-0.41	2 (1%) 77 76	21, 45, 72, 112	0
1	CH	159/192 (82%)	-0.13	3 (1%) 66 64	33, 62, 79, 119	0
1	CI	160/192 (83%)	-0.21	3 (1%) 66 64	15, 35, 74, 107	0
1	CJ	165/192 (85%)	-0.38	5 (3%) 50 45	24, 44, 85, 105	0
1	CK	160/192 (83%)	-0.28	2 (1%) 77 76	22, 60, 77, 115	0
1	CL	159/192 (82%)	-0.35	3 (1%) 66 64	38, 57, 73, 121	0
1	CM	159/192 (82%)	-0.46	3 (1%) 66 64	16, 42, 63, 112	0
1	CN	161/192 (83%)	-0.51	1 (0%) 89 89	16, 40, 77, 110	0
1	CO	159/192 (82%)	-0.37	2 (1%) 77 76	38, 58, 74, 99	0
1	CP	158/192 (82%)	-0.38	2 (1%) 77 76	25, 57, 76, 110	0
1	CQ	162/192 (84%)	-0.48	3 (1%) 66 64	9, 31, 61, 104	0
1	CR	166/192 (86%)	-0.40	5 (3%) 50 45	24, 42, 82, 107	0
1	CS	161/192 (83%)	-0.34	4 (2%) 57 54	10, 35, 65, 114	0
1	CT	158/192 (82%)	-0.40	3 (1%) 66 64	26, 50, 66, 106	0
1	CU	159/192 (82%)	-0.23	1 (0%) 89 89	51, 67, 82, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	CV	158/192 (82%)	-0.21	4 (2%) 57 54	55, 68, 84, 120	0
1	CW	155/192 (80%)	-0.49	1 (0%) 89 89	27, 47, 69, 87	0
1	CX	161/192 (83%)	-0.47	3 (1%) 66 64	20, 48, 70, 107	0
1	Ca	158/192 (82%)	0.62	18 (11%) 5 3	58, 89, 103, 121	0
1	Cb	159/192 (82%)	0.02	6 (3%) 40 35	37, 69, 87, 109	0
1	Cc	157/192 (81%)	-0.12	4 (2%) 57 54	40, 69, 86, 118	0
1	Cd	153/192 (79%)	0.65	16 (10%) 6 4	76, 91, 104, 109	0
1	Ce	154/192 (80%)	0.26	8 (5%) 27 22	59, 81, 92, 95	0
1	Cf	153/192 (79%)	0.84	17 (11%) 5 3	83, 97, 107, 110	0
1	Cg	160/192 (83%)	0.02	7 (4%) 34 29	48, 68, 93, 126	0
1	Ch	159/192 (82%)	-0.43	2 (1%) 77 76	23, 49, 66, 114	0
1	Ci	153/192 (79%)	0.62	15 (9%) 7 5	69, 89, 104, 111	0
1	Cj	156/192 (81%)	0.31	9 (5%) 23 18	61, 81, 100, 112	0
1	Ck	154/192 (80%)	-0.08	2 (1%) 77 76	45, 74, 92, 104	0
1	Cl	155/192 (80%)	0.18	5 (3%) 47 42	56, 85, 97, 113	0
1	Cm	159/192 (82%)	0.42	16 (10%) 7 5	71, 88, 100, 113	0
1	Cn	155/192 (80%)	0.22	7 (4%) 33 28	65, 86, 101, 104	0
1	Co	155/192 (80%)	-0.34	2 (1%) 77 76	26, 52, 71, 100	0
1	Cp	158/192 (82%)	-0.08	7 (4%) 34 29	46, 67, 89, 109	0
1	Cq	155/192 (80%)	0.75	21 (13%) 3 2	83, 96, 106, 112	0
1	Cr	154/192 (80%)	0.20	8 (5%) 27 22	78, 91, 103, 111	0
1	Cs	154/192 (80%)	0.57	16 (10%) 6 4	83, 98, 106, 107	0
1	Ct	160/192 (83%)	-0.38	4 (2%) 57 54	34, 51, 79, 115	0
1	Cu	159/192 (82%)	-0.23	6 (3%) 40 35	44, 62, 81, 119	0
1	Cv	161/192 (83%)	-0.13	3 (1%) 66 64	39, 59, 81, 119	0
1	Cw	155/192 (80%)	0.19	4 (2%) 56 52	71, 89, 98, 107	0
1	Cx	156/192 (81%)	-0.21	2 (1%) 77 76	39, 59, 78, 99	0
All	All	22946/27648 (82%)	-0.23	578 (2%) 57 54	7, 52, 95, 126	0

All (578) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ci	155	LEU	6.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	Bn	159	GLU	6.2
1	Ar	162	LEU	6.1
1	Av	159	GLU	5.6
1	Av	162	LEU	5.6
1	AS	160	ALA	5.5
1	AC	158	PRO	5.4
1	AB	162	LEU	5.3
1	AB	160	ALA	5.1
1	Aj	159	GLU	5.1
1	Ca	157	GLY	5.1
1	Cs	5	ILE	5.1
1	Cv	159	GLU	5.1
1	Bq	159	GLU	5.1
1	CK	160	ALA	5.0
1	Cq	85	PRO	5.0
1	Bg	155	LEU	5.0
1	AG	159	GLU	4.9
1	BA	158	PRO	4.9
1	Al	162	LEU	4.9
1	Bc	158	PRO	4.8
1	BW	158	PRO	4.8
1	AI	1	MET	4.8
1	AX	160	ALA	4.7
1	Bd	160	ALA	4.7
1	Cd	93	THR	4.7
1	AS	159	GLU	4.6
1	AL	158	PRO	4.6
1	CT	157	GLY	4.5
1	AD	160	ALA	4.5
1	AE	158	PRO	4.5
1	Bq	158	PRO	4.5
1	AO	159	GLU	4.4
1	Cl	155	LEU	4.4
1	Cm	159	GLU	4.3
1	AQ	162	LEU	4.3
1	Cm	158	PRO	4.3
1	Cd	155	LEU	4.3
1	BK	155	LEU	4.3
1	Cr	155	LEU	4.3
1	AG	158	PRO	4.2
1	Cg	159	GLU	4.2
1	CQ	158	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	BW	159	GLU	4.2
1	Cs	79	PHE	4.2
1	BW	160	ALA	4.1
1	Cf	93	THR	4.1
1	Cs	82	ILE	4.1
1	Bu	157	GLY	4.1
1	CM	159	GLU	4.1
1	At	157	GLY	4.1
1	Cf	99	ALA	4.1
1	Bu	165	TYR	4.1
1	Bp	158	PRO	4.0
1	Cm	155	LEU	4.0
1	BP	158	PRO	4.0
1	Ca	156	GLY	4.0
1	AE	159	GLU	4.0
1	Cc	159	GLU	4.0
1	Ct	160	ALA	4.0
1	AD	159	GLU	4.0
1	As	0	ARG	4.0
1	Bf	158	PRO	4.0
1	AB	157	GLY	4.0
1	CC	158	PRO	4.0
1	Cj	43	VAL	4.0
1	Cc	158	PRO	4.0
1	Be	162	LEU	4.0
1	Bv	157	GLY	4.0
1	CB	160	ALA	4.0
1	Cx	1	MET	3.9
1	CJ	158	PRO	3.9
1	AE	160	ALA	3.9
1	AV	161	GLY	3.9
1	AE	156	GLY	3.9
1	CF	158	PRO	3.9
1	AR	162	LEU	3.9
1	Ca	107	LEU	3.9
1	AQ	158	PRO	3.8
1	BX	164	GLU	3.8
1	AL	157	GLY	3.8
1	BW	157	GLY	3.8
1	BT	158	PRO	3.8
1	Cj	93	THR	3.8
1	Ae	159	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	Cb	159	GLU	3.7
1	Bn	158	PRO	3.7
1	Bh	1	MET	3.7
1	AM	158	PRO	3.7
1	Bm	158	PRO	3.7
1	AG	160	ALA	3.7
1	Ae	158	PRO	3.7
1	CN	158	PRO	3.7
1	Bn	160	ALA	3.7
1	AA	158	PRO	3.7
1	Cb	158	PRO	3.7
1	AO	165	TYR	3.6
1	BX	162	LEU	3.6
1	Cf	114	LEU	3.6
1	CV	158	PRO	3.6
1	Cj	97	MET	3.6
1	AA	159	GLU	3.6
1	Cu	158	PRO	3.6
1	Bi	0	ARG	3.6
1	Aa	159	GLU	3.6
1	Ap	0	ARG	3.6
1	AH	158	PRO	3.6
1	Ci	93	THR	3.6
1	Aj	160	ALA	3.6
1	BX	160	ALA	3.6
1	AO	163	GLY	3.6
1	Bf	160	ALA	3.6
1	AC	157	GLY	3.6
1	AV	159	GLU	3.6
1	Aj	165	TYR	3.6
1	CG	0	ARG	3.6
1	Bo	155	LEU	3.5
1	Cl	153	HIS	3.5
1	Ad	162	LEU	3.5
1	Aw	160	ALA	3.5
1	At	158	PRO	3.5
1	CB	156	GLY	3.5
1	AN	162	LEU	3.5
1	CW	155	LEU	3.5
1	Ar	165	TYR	3.5
1	AV	155	LEU	3.5
1	Ct	155	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	BR	0	ARG	3.5
1	BD	158	PRO	3.5
1	BT	155	LEU	3.5
1	Bu	164	GLU	3.5
1	Cr	90	TRP	3.5
1	Ad	158	PRO	3.5
1	AQ	159	GLU	3.5
1	CV	159	GLU	3.5
1	CJ	159	GLU	3.4
1	CL	159	GLU	3.4
1	An	158	PRO	3.4
1	Bp	159	GLU	3.4
1	Cq	142	ILE	3.4
1	AX	158	PRO	3.4
1	Av	160	ALA	3.4
1	AB	155	LEU	3.4
1	BJ	158	PRO	3.4
1	AO	160	ALA	3.4
1	Cm	9	TYR	3.4
1	Aa	158	PRO	3.4
1	AI	158	PRO	3.4
1	Ba	155	LEU	3.4
1	AR	159	GLU	3.4
1	Aj	162	LEU	3.4
1	Ci	111	LEU	3.4
1	AD	158	PRO	3.4
1	Cg	160	ALA	3.4
1	AE	162	LEU	3.4
1	Cd	154	ARG	3.4
1	Cf	3	SER	3.4
1	Cf	100	ALA	3.3
1	Bf	162	LEU	3.3
1	Br	158	PRO	3.3
1	Bd	159	GLU	3.3
1	Cq	114	LEU	3.3
1	Bu	162	LEU	3.3
1	CI	160	ALA	3.3
1	AE	157	GLY	3.3
1	Cj	1	MET	3.3
1	AJ	156	GLY	3.3
1	Bn	162	LEU	3.3
1	Cl	152	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	Cu	159	GLU	3.2
1	Bm	159	GLU	3.2
1	Cw	156	GLY	3.2
1	Ak	162	LEU	3.2
1	BV	152	LEU	3.2
1	Bu	160	ALA	3.2
1	Ci	108	ASN	3.2
1	Ae	0	ARG	3.2
1	Bh	158	PRO	3.2
1	Bt	158	PRO	3.2
1	Ci	92	LYS	3.2
1	Cq	88	ASP	3.2
1	Cm	154	ARG	3.2
1	AF	158	PRO	3.2
1	Bo	1	MET	3.2
1	Cf	148	HIS	3.2
1	AB	163	GLY	3.2
1	AW	157	GLY	3.2
1	BK	111	LEU	3.1
1	CA	159	GLU	3.1
1	Cd	79	PHE	3.1
1	Ao	0	ARG	3.1
1	BT	156	GLY	3.1
1	CJ	162	LEU	3.1
1	CM	158	PRO	3.1
1	Cv	158	PRO	3.1
1	BB	48	VAL	3.1
1	Cf	46	GLU	3.1
1	Cq	152	LEU	3.1
1	AV	160	ALA	3.1
1	AQ	0	ARG	3.1
1	BE	155	LEU	3.1
1	Cn	117	LEU	3.1
1	Av	158	PRO	3.1
1	Cn	124	PRO	3.1
1	Cu	156	GLY	3.1
1	Cj	79	PHE	3.1
1	AR	1	MET	3.1
1	CX	157	GLY	3.1
1	CR	159	GLU	3.1
1	Cq	145	MET	3.1
1	Cd	151	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	AO	162	LEU	3.0
1	Bu	163	GLY	3.0
1	CR	157	GLY	3.0
1	Cb	11	THR	3.0
1	CK	1	MET	3.0
1	Au	158	PRO	3.0
1	Bp	160	ALA	3.0
1	AR	158	PRO	3.0
1	Ca	160	ALA	3.0
1	CD	160	ALA	3.0
1	Ca	111	LEU	3.0
1	Ad	165	TYR	3.0
1	Bb	159	GLU	3.0
1	BQ	159	GLU	3.0
1	BB	97	MET	3.0
1	Af	158	PRO	3.0
1	BV	155	LEU	3.0
1	Cb	155	LEU	3.0
1	Ck	155	LEU	3.0
1	Cd	3	SER	3.0
1	AN	164	GLU	3.0
1	Bf	159	GLU	3.0
1	Cq	5	ILE	3.0
1	AB	158	PRO	2.9
1	Bm	160	ALA	2.9
1	Cm	45	LEU	2.9
1	Co	155	LEU	2.9
1	AL	156	GLY	2.9
1	BT	157	GLY	2.9
1	Ca	93	THR	2.9
1	Ci	115	HIS	2.9
1	BB	153	HIS	2.9
1	CF	156	GLY	2.9
1	As	159	GLU	2.9
1	AS	157	GLY	2.9
1	BP	156	GLY	2.9
1	Ca	155	LEU	2.9
1	BC	93	THR	2.9
1	Bd	158	PRO	2.9
1	BJ	157	GLY	2.9
1	AA	157	GLY	2.9
1	AH	160	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	CL	158	PRO	2.9
1	Cq	141	LEU	2.9
1	AO	158	PRO	2.9
1	Ak	165	TYR	2.9
1	AO	156	GLY	2.9
1	AV	156	GLY	2.9
1	Cd	17	VAL	2.9
1	Cf	74	GLY	2.9
1	BO	74	GLY	2.8
1	Ci	75	GLY	2.8
1	BG	155	LEU	2.8
1	AV	158	PRO	2.8
1	AE	165	TYR	2.8
1	Ca	5	ILE	2.8
1	Cu	157	GLY	2.8
1	AI	156	GLY	2.8
1	Cm	74	GLY	2.8
1	Ct	157	GLY	2.8
1	Cs	112	LEU	2.8
1	AC	156	GLY	2.8
1	AS	161	GLY	2.8
1	Bg	77	ALA	2.8
1	Cq	45	LEU	2.8
1	Bv	160	ALA	2.8
1	AI	157	GLY	2.8
1	BX	158	PRO	2.8
1	Ci	124	PRO	2.8
1	CS	157	GLY	2.8
1	AR	160	ALA	2.8
1	CQ	160	ALA	2.8
1	Cp	156	GLY	2.8
1	BX	159	GLU	2.8
1	Cf	32	LEU	2.8
1	CR	162	LEU	2.8
1	Ca	4	GLN	2.8
1	Am	0	ARG	2.7
1	Cq	79	PHE	2.7
1	CR	158	PRO	2.7
1	Ae	160	ALA	2.7
1	Bf	165	TYR	2.7
1	AN	1	MET	2.7
1	Ct	156	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	AS	158	PRO	2.7
1	Cg	158	PRO	2.7
1	Cp	1	MET	2.7
1	Ak	160	ALA	2.7
1	AM	0	ARG	2.7
1	Aa	160	ALA	2.7
1	Ci	24	TYR	2.7
1	Cf	122	THR	2.7
1	Cs	24	TYR	2.7
1	CO	0	ARG	2.7
1	Br	159	GLU	2.7
1	CU	157	GLY	2.7
1	Ca	135	LEU	2.7
1	AQ	1	MET	2.7
1	Cf	142	ILE	2.7
1	Cm	142	ILE	2.7
1	CJ	155	LEU	2.7
1	Bv	156	GLY	2.7
1	CS	158	PRO	2.6
1	CT	158	PRO	2.6
1	Au	160	ALA	2.6
1	BK	1	MET	2.6
1	Bx	155	LEU	2.6
1	Cs	70	GLN	2.6
1	AQ	156	GLY	2.6
1	As	160	ALA	2.6
1	Cr	79	PHE	2.6
1	AQ	164	GLU	2.6
1	BV	153	HIS	2.6
1	Cj	101	MET	2.6
1	Cd	111	LEU	2.6
1	Cp	45	LEU	2.6
1	AX	156	GLY	2.6
1	CM	157	GLY	2.6
1	CH	159	GLU	2.6
1	Cn	153	HIS	2.6
1	Cd	70	GLN	2.6
1	AQ	157	GLY	2.6
1	Cg	161	GLY	2.6
1	Cf	144	LYS	2.6
1	CI	159	GLU	2.6
1	Ce	2	SER	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AW	158	PRO	2.6
1	CE	158	PRO	2.6
1	BB	26	GLN	2.6
1	CT	1	MET	2.6
1	Ba	156	GLY	2.6
1	AH	159	GLU	2.6
1	Cm	70	GLN	2.6
1	BC	135	LEU	2.6
1	BV	145	MET	2.6
1	Av	0	ARG	2.6
1	Ba	158	PRO	2.6
1	BK	93	THR	2.6
1	AR	157	GLY	2.6
1	BT	45	LEU	2.6
1	BV	144	LYS	2.6
1	An	157	GLY	2.5
1	Bw	159	GLU	2.5
1	Cq	78	LEU	2.5
1	Cq	149	LEU	2.5
1	Bo	153	HIS	2.5
1	Bw	158	PRO	2.5
1	AL	155	LEU	2.5
1	Cr	45	LEU	2.5
1	BM	158	PRO	2.5
1	Cq	156	GLY	2.5
1	Cp	43	VAL	2.5
1	CQ	155	LEU	2.5
1	Cs	111	LEU	2.5
1	Ca	153	HIS	2.5
1	Bp	0	ARG	2.5
1	BK	117	LEU	2.5
1	Cw	155	LEU	2.5
1	Bp	1	MET	2.5
1	Cn	123	ASP	2.5
1	Co	153	HIS	2.5
1	Cq	153	HIS	2.5
1	AQ	161	GLY	2.5
1	AS	156	GLY	2.5
1	Aj	158	PRO	2.5
1	Aw	158	PRO	2.5
1	Cu	155	LEU	2.5
1	Bq	157	GLY	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	Ai	158	PRO	2.5
1	Ca	78	LEU	2.5
1	Ak	164	GLU	2.5
1	Cc	156	GLY	2.5
1	Cd	100	ALA	2.5
1	CG	157	GLY	2.5
1	CO	1	MET	2.4
1	Bw	160	ALA	2.4
1	Ak	159	GLU	2.4
1	BO	155	LEU	2.4
1	Cd	152	LEU	2.4
1	CI	156	GLY	2.4
1	Bt	100	ALA	2.4
1	Ci	5	ILE	2.4
1	BC	98	LYS	2.4
1	Cr	94	PRO	2.4
1	CX	158	PRO	2.4
1	Ca	3	SER	2.4
1	AF	157	GLY	2.4
1	BK	154	ARG	2.4
1	BU	0	ARG	2.4
1	Ca	100	ALA	2.4
1	Cd	142	ILE	2.4
1	Cs	91	GLY	2.4
1	BB	155	LEU	2.4
1	Ba	1	MET	2.4
1	Bt	156	GLY	2.4
1	Cg	157	GLY	2.4
1	Bx	38	PHE	2.4
1	BR	159	GLU	2.4
1	BA	162	LEU	2.4
1	Cf	153	HIS	2.4
1	Cq	127	CYS	2.4
1	Bv	158	PRO	2.4
1	CP	157	GLY	2.4
1	CP	158	PRO	2.4
1	AO	155	LEU	2.4
1	Bh	156	GLY	2.4
1	Cs	74	GLY	2.4
1	AE	1	MET	2.4
1	BP	155	LEU	2.4
1	Ch	157	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	Cm	46	GLU	2.3
1	Ch	160	ALA	2.3
1	Cu	160	ALA	2.3
1	Cs	114	LEU	2.3
1	Bp	157	GLY	2.3
1	BH	2	SER	2.3
1	AO	157	GLY	2.3
1	Cs	17	VAL	2.3
1	Aw	159	GLU	2.3
1	Bv	159	GLU	2.3
1	Ca	122	THR	2.3
1	Cg	155	LEU	2.3
1	CB	158	PRO	2.3
1	Bp	155	LEU	2.3
1	Ak	156	GLY	2.3
1	BK	99	ALA	2.3
1	CC	156	GLY	2.3
1	AI	2	SER	2.3
1	CS	159	GLU	2.3
1	Cw	153	HIS	2.3
1	Bg	144	LYS	2.3
1	Cq	123	ASP	2.3
1	Cf	111	LEU	2.3
1	CL	155	LEU	2.3
1	Bx	156	GLY	2.3
1	Aq	158	PRO	2.3
1	AA	156	GLY	2.3
1	AO	161	GLY	2.3
1	Cd	52	PHE	2.3
1	Cj	92	LYS	2.3
1	Cm	79	PHE	2.3
1	BV	156	GLY	2.2
1	Ci	97	MET	2.2
1	Ck	86	ALA	2.2
1	Cq	111	LEU	2.2
1	Cv	160	ALA	2.2
1	AN	165	TYR	2.2
1	BX	142	ILE	2.2
1	Cf	73	ARG	2.2
1	Ce	126	LEU	2.2
1	Cj	152	LEU	2.2
1	Ca	9	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	BB	154	ARG	2.2
1	Ce	11	THR	2.2
1	Cm	3	SER	2.2
1	AD	156	GLY	2.2
1	AN	156	GLY	2.2
1	Cq	155	LEU	2.2
1	CX	156	GLY	2.2
1	AN	158	PRO	2.2
1	Bb	158	PRO	2.2
1	BH	46	GLU	2.2
1	Bl	158	PRO	2.2
1	Ag	1	MET	2.2
1	Cg	43	VAL	2.2
1	Cd	66	LEU	2.2
1	CV	157	GLY	2.2
1	Ak	158	PRO	2.2
1	BC	5	ILE	2.2
1	Cp	158	PRO	2.2
1	Ci	106	LYS	2.2
1	BB	147	ASP	2.2
1	Bb	157	GLY	2.2
1	BK	152	LEU	2.2
1	Cl	3	SER	2.2
1	Cx	155	LEU	2.2
1	AC	160	ALA	2.2
1	AQ	160	ALA	2.2
1	Cm	52	PHE	2.2
1	Cn	115	HIS	2.2
1	Cr	38	PHE	2.2
1	Cs	13	VAL	2.2
1	AB	156	GLY	2.2
1	Bt	157	GLY	2.2
1	Cl	156	GLY	2.2
1	Ax	155	LEU	2.2
1	BH	155	LEU	2.2
1	Cd	31	TYR	2.2
1	Cf	21	VAL	2.2
1	Cm	31	TYR	2.2
1	Ca	90	TRP	2.2
1	CR	0	ARG	2.2
1	Cr	154	ARG	2.2
1	Aq	160	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	Bx	158	PRO	2.2
1	Cq	93	THR	2.2
1	Cr	93	THR	2.2
1	Bk	159	GLU	2.2
1	BG	156	GLY	2.2
1	Bs	155	LEU	2.2
1	Ce	135	LEU	2.2
1	BP	157	GLY	2.1
1	BM	159	GLU	2.1
1	CH	158	PRO	2.1
1	Cd	30	THR	2.1
1	CS	0	ARG	2.1
1	BB	45	LEU	2.1
1	CV	155	LEU	2.1
1	BV	157	GLY	2.1
1	Cm	157	GLY	2.1
1	Cp	48	VAL	2.1
1	Bs	1	MET	2.1
1	AB	161	GLY	2.1
1	BO	157	GLY	2.1
1	Cm	75	GLY	2.1
1	CJ	0	ARG	2.1
1	AQ	163	GLY	2.1
1	AT	158	PRO	2.1
1	Bx	97	MET	2.1
1	Cp	157	GLY	2.1
1	Ce	104	GLU	2.1
1	Cn	152	LEU	2.1
1	Ci	7	GLN	2.1
1	Ci	147	ASP	2.1
1	Cs	108	ASN	2.1
1	AV	152	LEU	2.1
1	Cs	107	LEU	2.1
1	BO	160	ALA	2.1
1	Cb	160	ALA	2.1
1	CB	157	GLY	2.1
1	Cj	155	LEU	2.1
1	Cn	126	LEU	2.1
1	Cf	72	GLN	2.1
1	AM	160	ALA	2.1
1	CF	160	ALA	2.1
1	AG	156	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	BR	156	GLY	2.1
1	Bx	157	GLY	2.1
1	Ao	1	MET	2.1
1	Ci	17	VAL	2.1
1	Cb	5	ILE	2.1
1	Cc	74	GLY	2.1
1	Bk	158	PRO	2.1
1	Cs	51	PHE	2.1
1	Cw	103	LEU	2.0
1	Bg	86	ALA	2.0
1	Bf	161	GLY	2.0
1	CH	1	MET	2.0
1	AA	155	LEU	2.0
1	Cq	6	ARG	2.0
1	AO	164	GLU	2.0
1	BE	156	GLY	2.0
1	Ce	106	LYS	2.0
1	Ap	1	MET	2.0
1	CD	0	ARG	2.0
1	Bx	82	ILE	2.0
1	Cq	91	GLY	2.0
1	Cs	97	MET	2.0
1	Ae	155	LEU	2.0
1	AU	158	PRO	2.0
1	Ca	34	LEU	2.0
1	Ce	107	LEU	2.0
1	Ce	152	LEU	2.0
1	AE	164	GLU	2.0
1	AJ	153	HIS	2.0
1	AK	156	GLY	2.0
1	BP	160	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CA	BN	201	1/1	0.55	0.35	73,73,73,73	0
2	CA	An	201	1/1	0.58	0.30	61,61,61,61	0
2	CA	Cl	201	1/1	0.59	0.45	85,85,85,85	1
2	CA	Cn	201	1/1	0.65	0.17	108,108,108,108	0
2	CA	BB	201	1/1	0.71	0.12	86,86,86,86	0
2	CA	AC	201	1/1	0.72	0.32	86,86,86,86	0
2	CA	BG	201	1/1	0.73	0.27	94,94,94,94	0
2	CA	BR	201	1/1	0.76	0.31	72,72,72,72	0
2	CA	Bb	201	1/1	0.76	0.26	98,98,98,98	0
2	CA	Cg	201	1/1	0.78	0.18	85,85,85,85	0
2	CA	Bd	201	1/1	0.79	0.27	61,61,61,61	0
2	CA	Ac	201	1/1	0.79	0.27	70,70,70,70	0
2	CA	Ag	201	1/1	0.79	0.25	55,55,55,55	0
2	CA	CE	201	1/1	0.80	0.31	83,83,83,83	0
2	CA	BA	201	1/1	0.83	0.24	78,78,78,78	0
2	CA	CA	201	1/1	0.83	0.32	67,67,67,67	0
2	CA	Aa	201	1/1	0.84	0.24	58,58,58,58	0
2	CA	AB	201	1/1	0.84	0.21	75,75,75,75	0
2	CA	BC	201	1/1	0.84	0.45	73,73,73,73	1
2	CA	Ck	201	1/1	0.85	0.18	78,78,78,78	0
2	CA	AF	201	1/1	0.85	0.25	68,68,68,68	0
2	CA	CC	201	1/1	0.85	0.20	96,96,96,96	0
2	CA	BD	201	1/1	0.85	0.19	81,81,81,81	0
2	CA	Ba	201	1/1	0.85	0.18	80,80,80,80	0
2	CA	CO	201	1/1	0.86	0.21	68,68,68,68	0
2	CA	AA	201	1/1	0.86	0.18	106,106,106,106	0
2	CA	AL	201	1/1	0.87	0.17	84,84,84,84	0
2	CA	AO	201	1/1	0.88	0.24	67,67,67,67	0
2	CA	Ce	201	1/1	0.88	0.27	106,106,106,106	0
2	CA	Bc	201	1/1	0.88	0.31	73,73,73,73	0
2	CA	Be	201	1/1	0.88	0.31	66,66,66,66	0
2	CA	Bg	201	1/1	0.90	0.24	88,88,88,88	0
2	CA	AM	201	1/1	0.90	0.24	68,68,68,68	0
2	CA	Ae	201	1/1	0.90	0.26	70,70,70,70	0
2	CA	Aj	201	1/1	0.90	0.29	56,56,56,56	0
2	CA	AH	201	1/1	0.91	0.28	62,62,62,62	0
2	CA	Ad	201	1/1	0.91	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	Cb	201	1/1	0.91	0.26	80,80,80,80	0
2	CA	Bf	201	1/1	0.92	0.27	68,68,68,68	0
2	CA	CB	201	1/1	0.92	0.24	60,60,60,60	0
2	CA	CF	201	1/1	0.93	0.33	63,63,63,63	0
2	CA	BH	201	1/1	0.95	0.26	96,96,96,96	0
2	CA	CH	201	1/1	0.96	0.15	69,69,69,69	0
2	CA	Cp	201	1/1	0.96	0.25	69,69,69,69	0
2	CA	Bu	201	1/1	0.97	0.27	61,61,61,61	0
2	CA	Ah	201	1/1	0.97	0.28	56,56,56,56	0
2	CA	Ca	201	1/1	0.97	0.42	87,87,87,87	1
2	CA	CD	201	1/1	0.97	0.17	68,68,68,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.