



# wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 06:10 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 wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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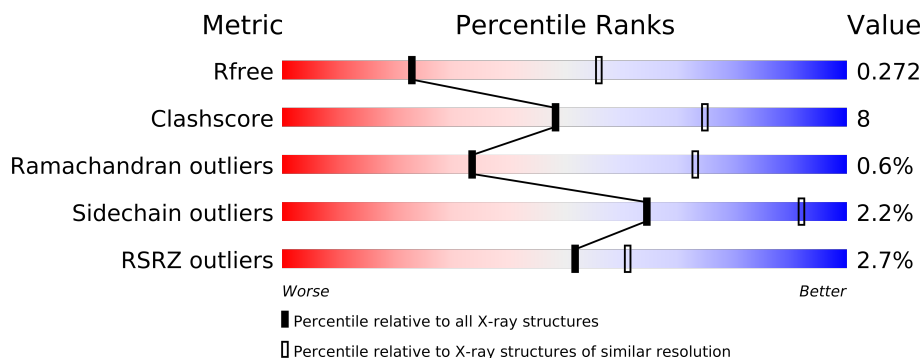
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	192	
1	AB	192	
1	AC	192	
1	AD	192	
1	AE	192	
1	AF	192	
1	AG	192	
1	AH	192	
1	AI	192	
1	AJ	192	
1	AK	192	
1	AL	192	
1	AM	192	
1	AN	192	

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
1	BI	192	
1	BJ	192	
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	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	
1	Bj	192	
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	





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

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Mol	Chain	Length	Quality of chain
1	Cu	192	
1	Cv	192	
1	Cw	192	
1	Cx	192	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	AA	201	-	X
2	CA	AB	201	-	X
2	CA	AC	201	-	X
2	CA	AF	201	-	X
2	CA	AH	201	-	X
2	CA	AL	201	-	X
2	CA	AM	201	-	X
2	CA	AO	201	-	X
2	CA	Aa	201	-	X
2	CA	Ac	201	-	X
2	CA	Ad	201	-	X
2	CA	Ae	201	-	X
2	CA	Ag	201	-	X
2	CA	Ah	201	-	X
2	CA	Aj	201	-	X
2	CA	An	201	-	X
2	CA	BA	201	-	X
2	CA	BC	201	-	X
2	CA	BG	201	-	X
2	CA	BH	201	-	X
2	CA	BN	201	-	X
2	CA	BR	201	-	X
2	CA	Ba	201	-	X
2	CA	Bb	201	-	X
2	CA	Bc	201	-	X
2	CA	Bd	201	-	X
2	CA	Be	201	-	X
2	CA	Bf	201	-	X
2	CA	Bg	201	-	X
2	CA	Bu	201	-	X
2	CA	CA	201	-	X
2	CA	CB	201	-	X
2	CA	CC	201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	CA	CE	201	-	X
2	CA	CF	201	-	X
2	CA	CO	201	-	X
2	CA	Ca	201	-	X
2	CA	Cb	201	-	X
2	CA	Ce	201	-	X
2	CA	Cg	201	-	X
2	CA	Ck	201	-	X
2	CA	Cl	201	-	X
2	CA	Cp	201	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 187090 atoms, of which 0 are hydrogen and 0 are deuterium.

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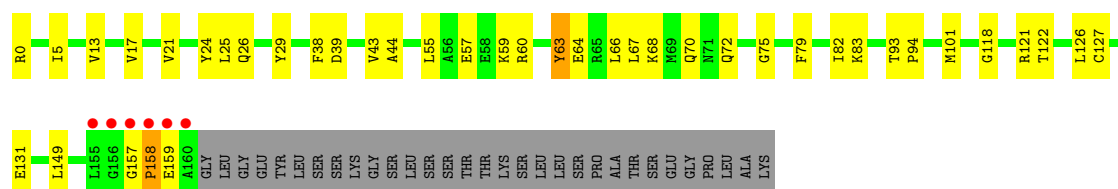
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Ce	6	Total 6	O 6	0	0
3	CF	25	Total 25	O 25	0	0
3	Cf	8	Total 8	O 8	0	0
3	CG	19	Total 19	O 19	0	0
3	Cg	16	Total 16	O 16	0	0
3	CH	10	Total 10	O 10	0	0
3	Ch	18	Total 18	O 18	0	0
3	CI	30	Total 30	O 30	0	0
3	Ci	9	Total 9	O 9	0	0
3	CJ	18	Total 18	O 18	0	0
3	Cj	9	Total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

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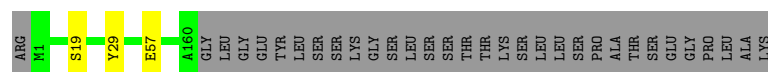
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	CP	14	Total 14	O 14	0	0
3	Cp	10	Total 10	O 10	0	0
3	CQ	41	Total 41	O 41	0	0
3	Cq	2	Total 2	O 2	0	0
3	CR	20	Total 20	O 20	0	0
3	Cr	4	Total 4	O 4	0	0
3	CS	28	Total 28	O 28	0	0
3	CT	15	Total 15	O 15	0	0
3	Ct	17	Total 17	O 17	0	0
3	CU	3	Total 3	O 3	0	0
3	Cu	12	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





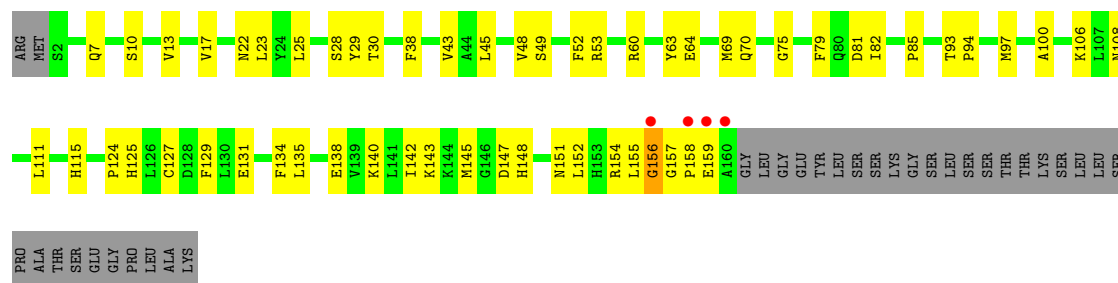
- Molecule 1: Ferritin

Chain Ac:



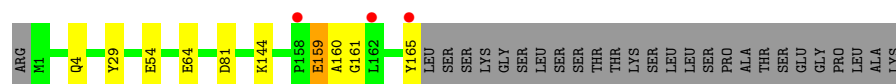
- Molecule 1: Ferritin

Chain AD:



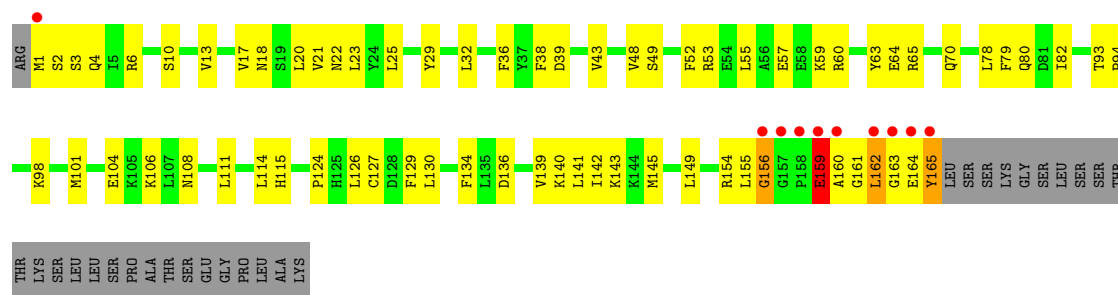
- Molecule 1: Ferritin

Chain Ad:



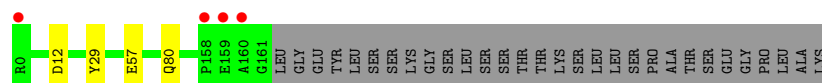
- Molecule 1: Ferritin

Chain AE:



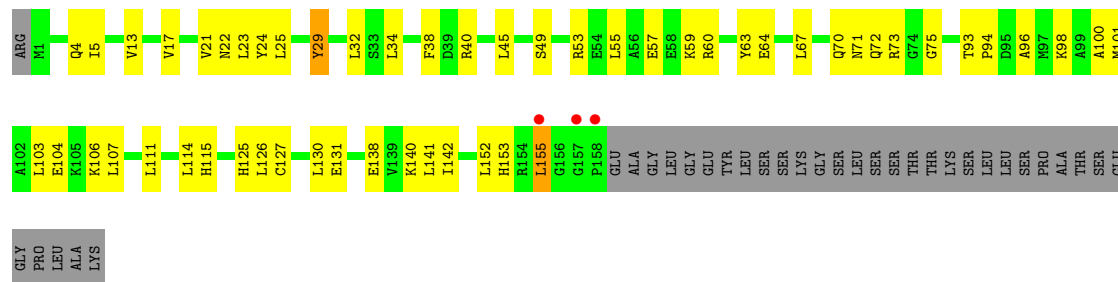
- Molecule 1: Ferritin

Chain Ae:



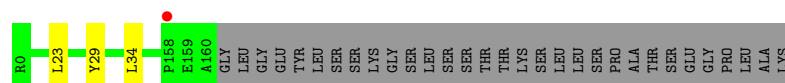
- Molecule 1: Ferritin

Chain AF:



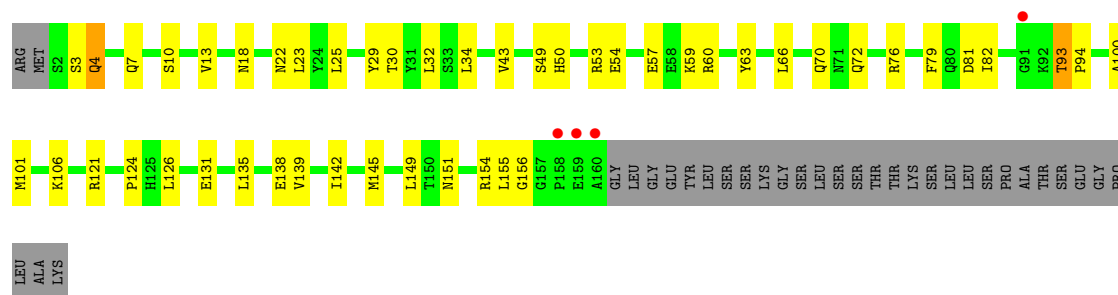
- Molecule 1: Ferritin

Chain Af:



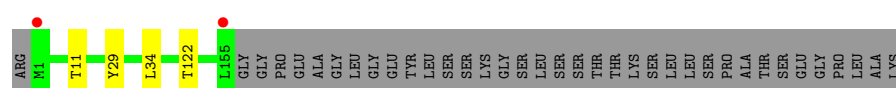
- Molecule 1: Ferritin

Chain AG:



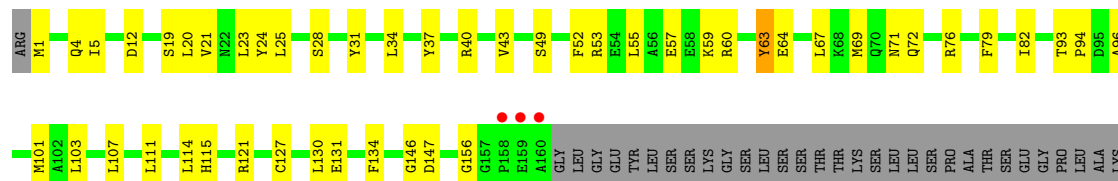
- Molecule 1: Ferritin

Chain Ag:



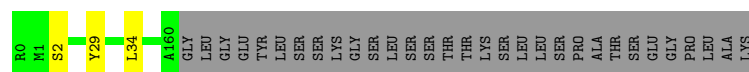
- Molecule 1: Ferritin

Chain AH:



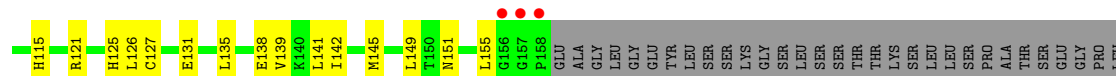
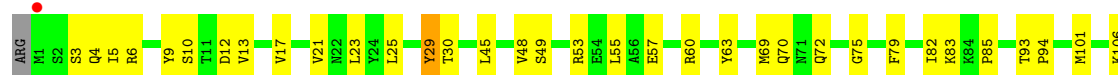
- Molecule 1: Ferritin

Chain Ah:



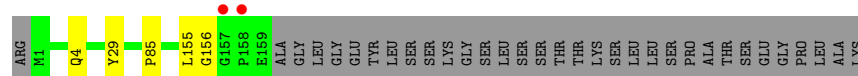
- Molecule 1: Ferritin

Chain AI:



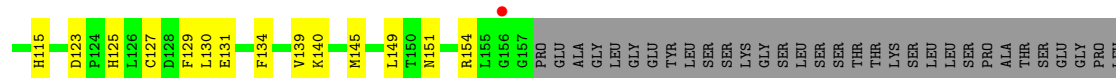
- Molecule 1: Ferritin

Chain Ai:



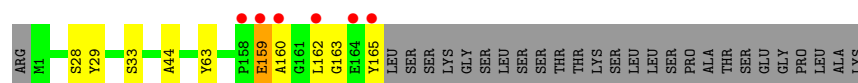
- Molecule 1: Ferritin

Chain AJ:



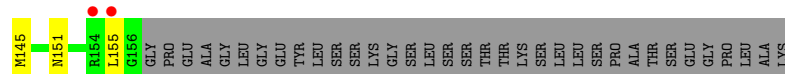
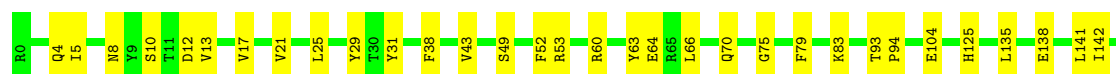
- Molecule 1: Ferritin

Chain Aj:



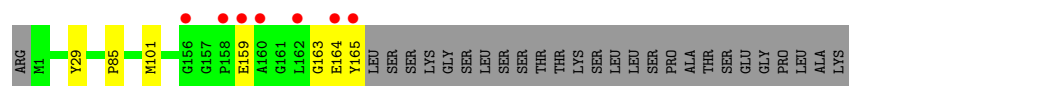
- Molecule 1: Ferritin

Chain AK:



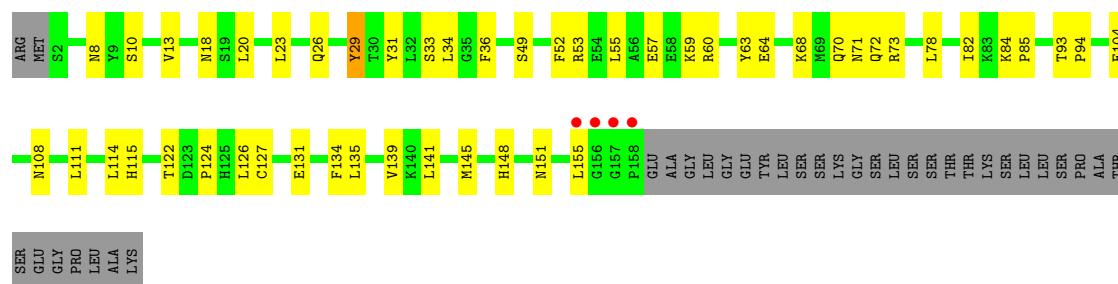
- Molecule 1: Ferritin

Chain Ak:



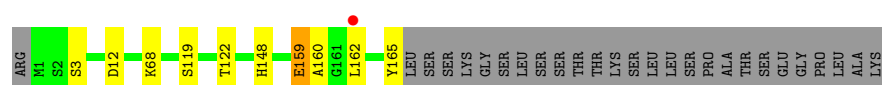
- Molecule 1: Ferritin

Chain AL:



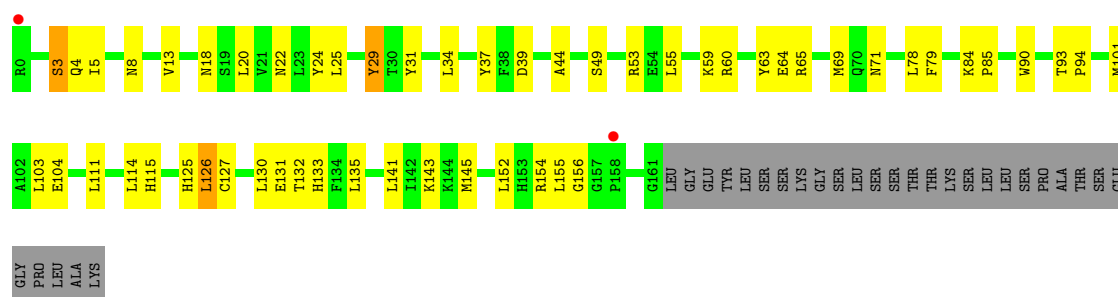
- Molecule 1: Ferritin

Chain Al:



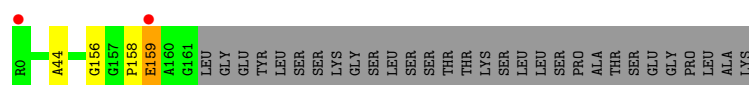
- Molecule 1: Ferritin

Chain AM:



- Molecule 1: Ferritin

Chain Am:



- Molecule 1: Ferritin

Chain AN:

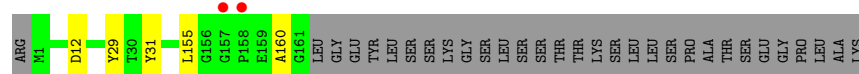






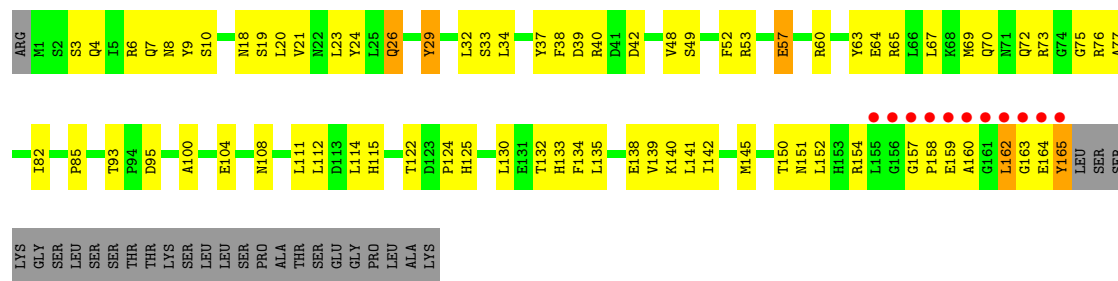
- Molecule 1: Ferritin

Chain An:



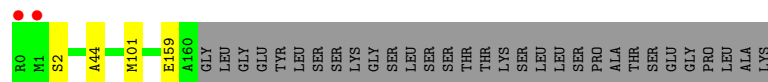
- Molecule 1: Ferritin

Chain AO:



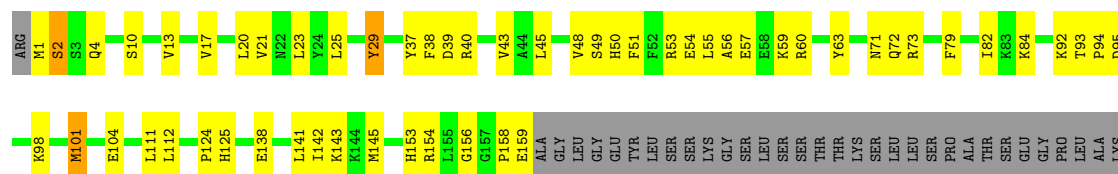
- Molecule 1: Ferritin

Chain Ao:



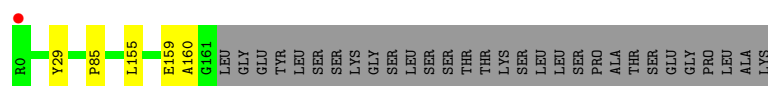
- Molecule 1: Ferritin

Chain AP:



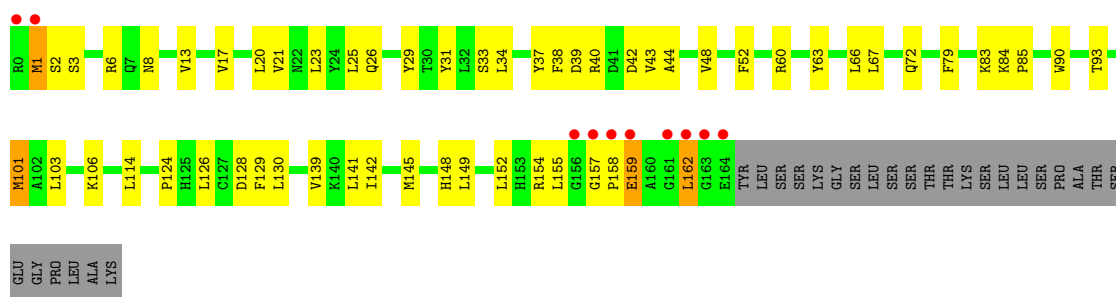
- Molecule 1: Ferritin

Chain Ap:



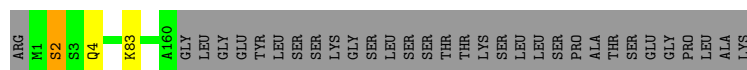
- Molecule 1: Ferritin

Chain AQ:



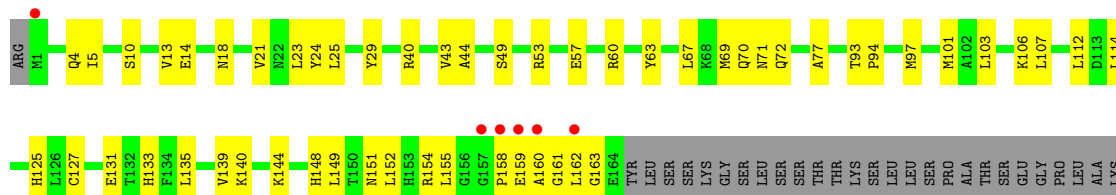
- Molecule 1: Ferritin

Chain Aq:



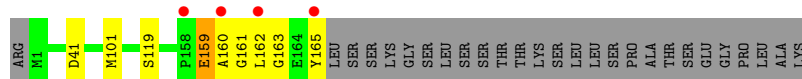
- Molecule 1: Ferritin

Chain AR:



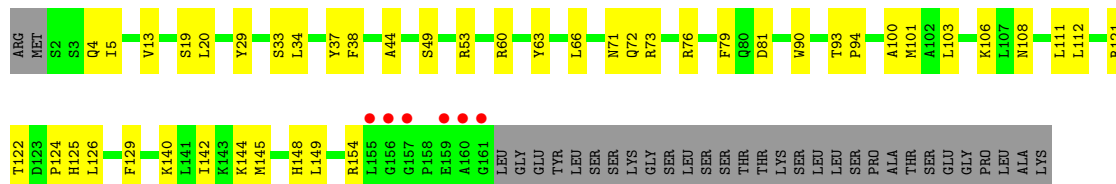
- Molecule 1: Ferritin

Chain Ar:



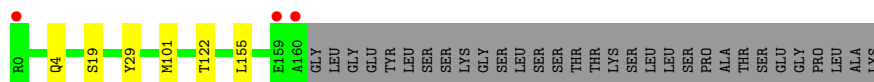
- Molecule 1: Ferritin

Chain AS:



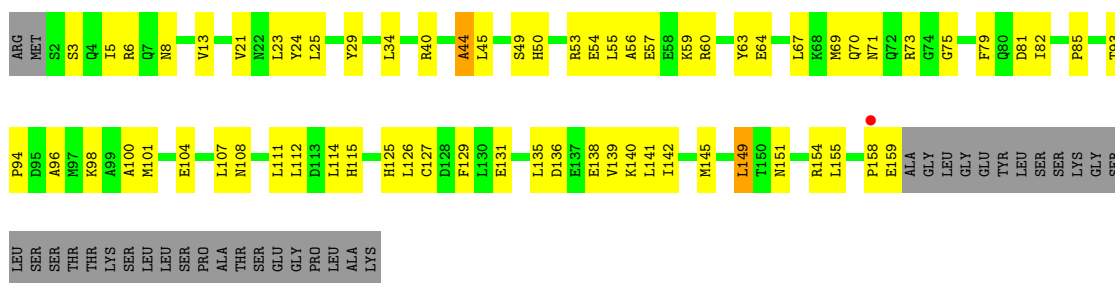
- Molecule 1: Ferritin

Chain As:



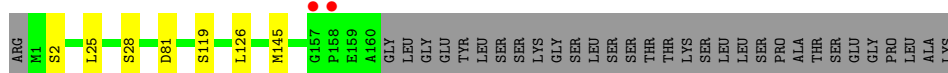
- Molecule 1: Ferritin

Chain AT:



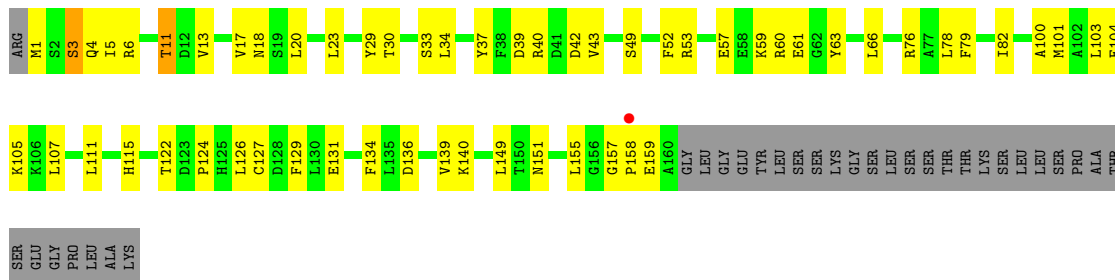
- Molecule 1: Ferritin

Chain At:



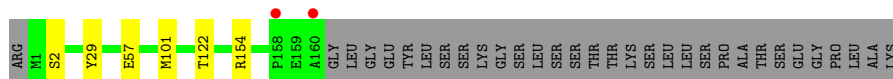
- Molecule 1: Ferritin

Chain AU:



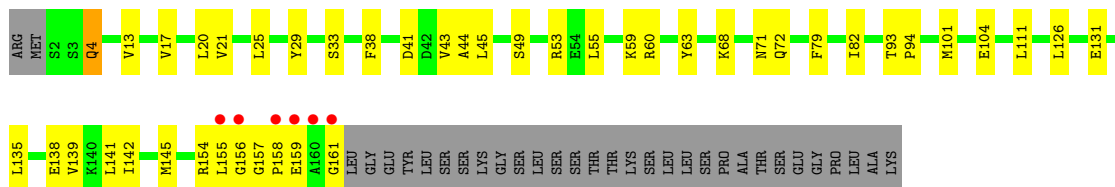
- Molecule 1: Ferritin

Chain Au:



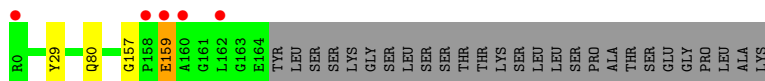
- Molecule 1: Ferritin

Chain AV:



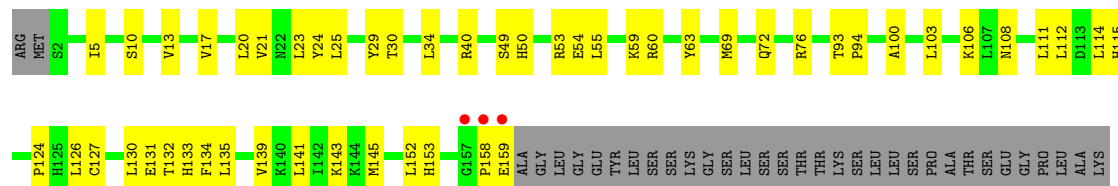
- Molecule 1: Ferritin

Chain Av:



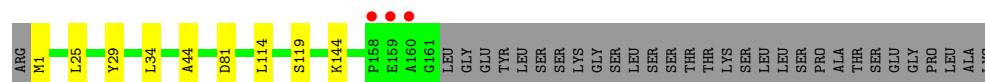
- Molecule 1: Ferritin

Chain AW:



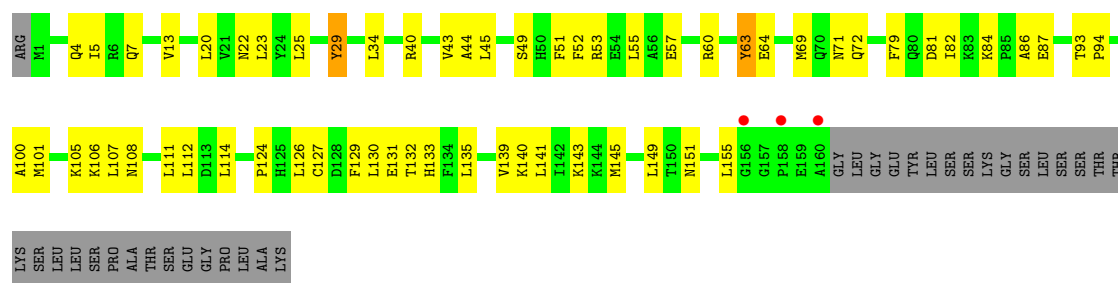
- Molecule 1: Ferritin

Chain Aw:



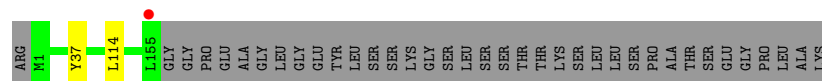
- Molecule 1: Ferritin

Chain AX:



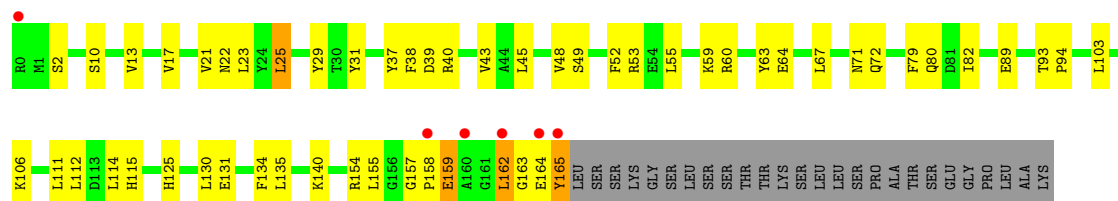
- Molecule 1: Ferritin

Chain Ax:



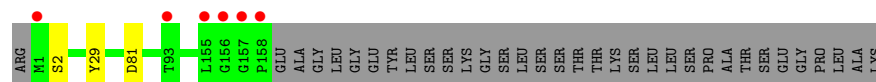
- Molecule 1: Ferritin

Chain BA:

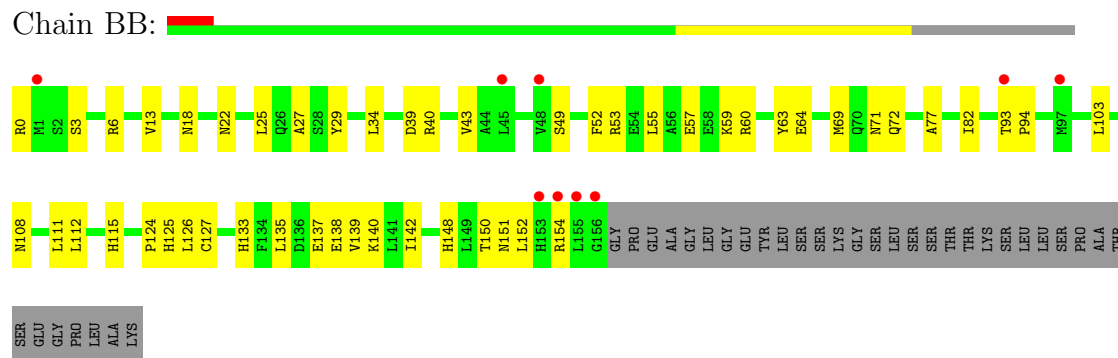


- Molecule 1: Ferritin

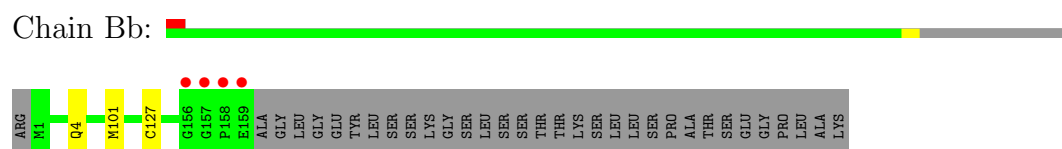
Chain Ba:



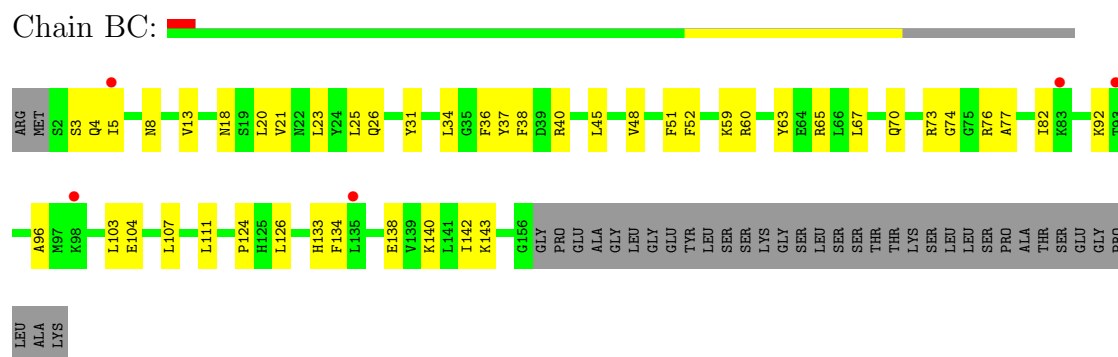
- Molecule 1: Ferritin



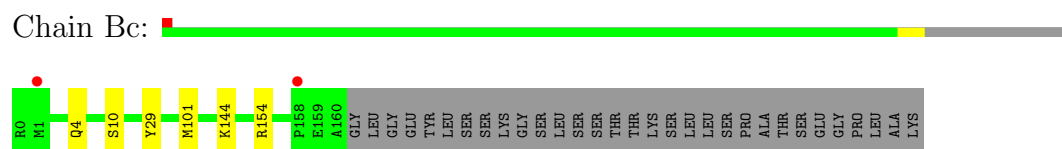
- Molecule 1: Ferritin



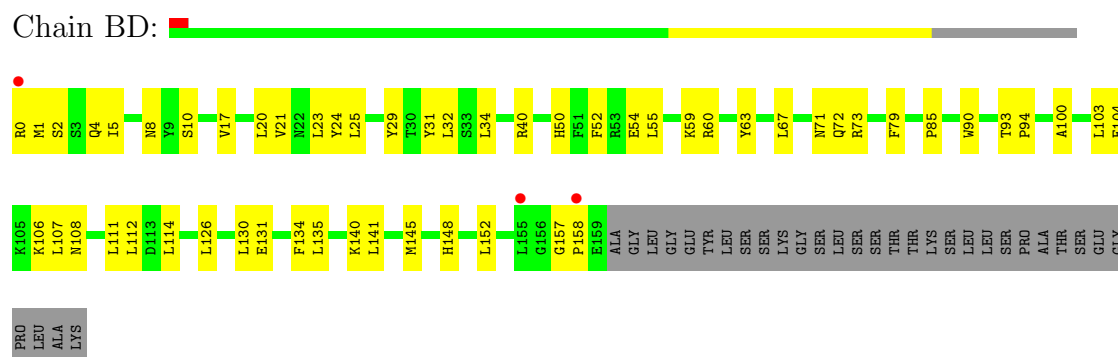
- Molecule 1: Ferritin



- Molecule 1: Ferritin

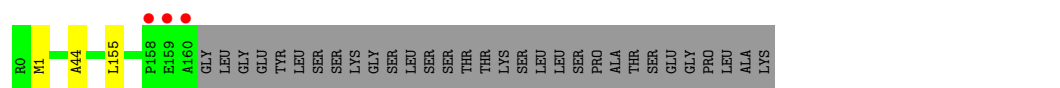


- Molecule 1: Ferritin



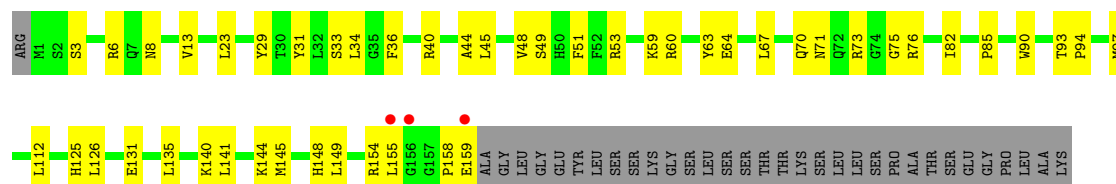
- Molecule 1: Ferritin

Chain Bd:



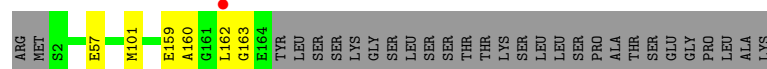
- Molecule 1: Ferritin

Chain BE:



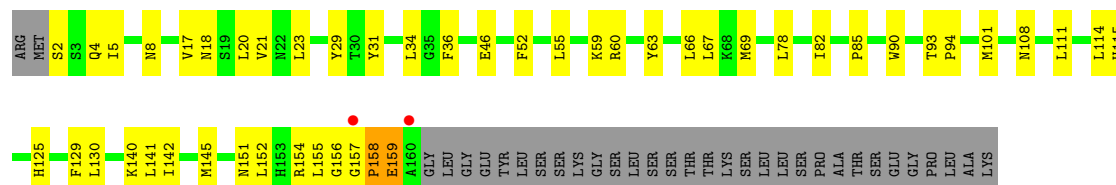
- Molecule 1: Ferritin

Chain Be:



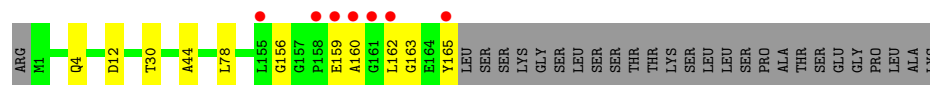
- Molecule 1: Ferritin

Chain BF:



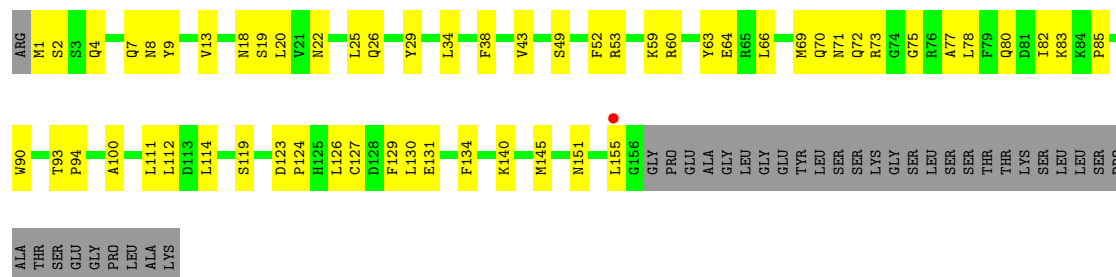
- Molecule 1: Ferritin

Chain Bf:



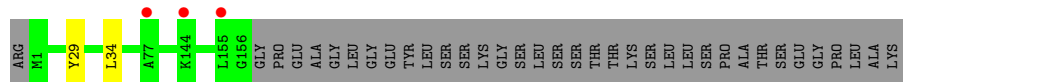
- Molecule 1: Ferritin

Chain BG:



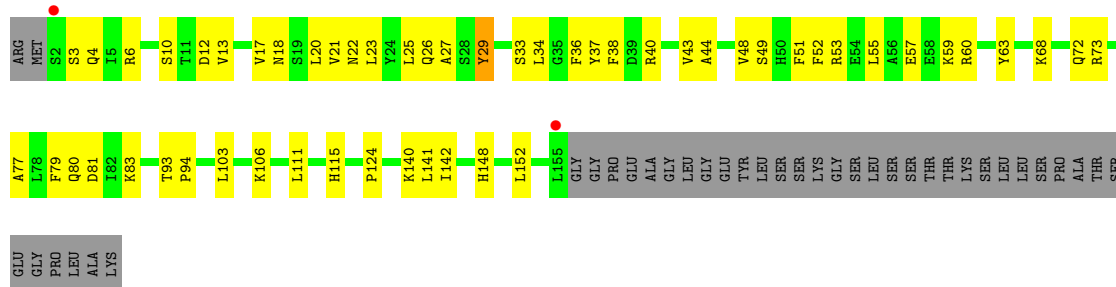
- Molecule 1: Ferritin

Chain Bg:



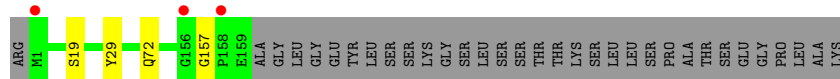
- Molecule 1: Ferritin

Chain BH:



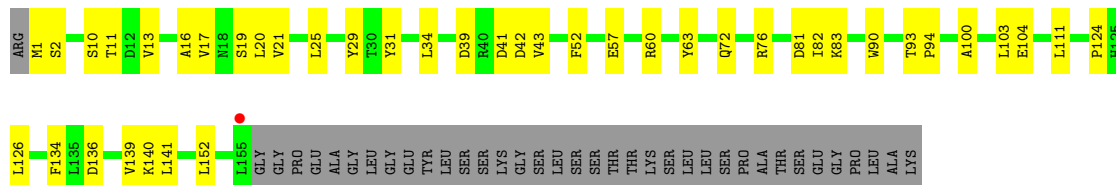
- Molecule 1: Ferritin

Chain Bh:



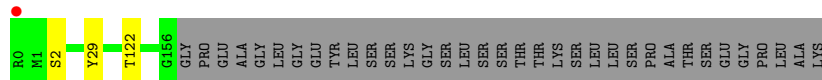
- Molecule 1: Ferritin

Chain BI:



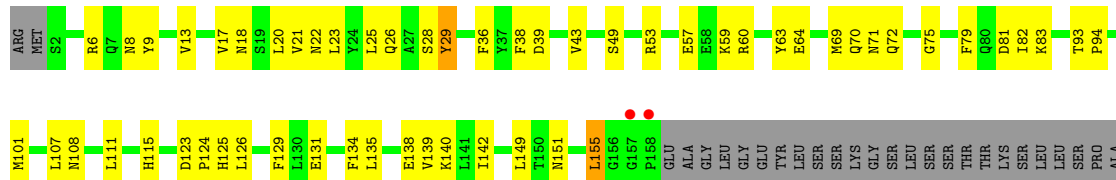
- Molecule 1: Ferritin

Chain Bi:



- Molecule 1: Ferritin

Chain BJ:



THR  
SER  
GLY  
PRO  
LEU  
ALA  
LYS

- Molecule 1: Ferritin

Chain Bj: 

ARG  
MET  
SER  
S3  
Q4  
D12  
Y29  
L78  
G156  
GLY  
PRO  
GLU  
ALA  
GLY  
LEU  
LEU  
GLY  
TYR  
LEU  
SER  
SER  
LYS  
GLY  
SER  
SER  
LEU  
SER  
PRO  
ALA  
THR  
SER  
GLY  
PRO  
LEU  
ALA  
LYS

- Molecule 1: Ferritin

Chain BK: 

ARG  
M1  
S2  
S3  
Q4  
I5  
R6  
S10  
T11  
D12  
V13  
E14  
N18  
S19  
L20  
V21  
N22  
L23  
Y24  
L26  
Q26  
A27  
S28  
Y29  
L34  
D39  
R40  
D41  
D42  
V43  
S49  
F52  
R53  
E54  
L55  
A56  
E57  
E58  
K59  
R60  
Y63  
L67  
Q70  
N71  
Q72  
R73  
A77  
Q80  
T93  
P94  
M97  
K98  
A99  
L103  
K106  
L107  
A110  
L111  
L112  
H115  
A116  
L117  
P124  
H125  
L126  
C127  
E131  
L135  
L141  
I142  
K143  
G146  
L149  
T150  
N151  
R154  
L155  
G156  
GLY  
PRO  
GLU  
ALA  
GLY  
LEU  
GLY  
TYR  
LEU  
SER  
SER  
LYS  
GLY  
SER  
LEU  
SER

THR  
THR  
LYS  
SER  
LEU  
LEU  
SER  
PRO  
ALA  
THR  
SER  
GLY  
GLY  
PRO  
LEU  
ALA  
LYS

- Molecule 1: Ferritin

Chain Bk: 

ARG  
M1  
Y29  
A44  
M101  
T122  
P158  
E159  
ALA  
GLY  
LEU  
GLY  
GLY  
TYR  
LEU  
SER  
SER  
SER  
SER  
THR  
THR  
LYS  
LYS  
SER  
LEU  
SER  
SER  
PRO  
ALA  
THR  
SER  
GLY  
PRO  
LEU  
ALA  
LYS

- Molecule 1: Ferritin

Chain BL: 

ARG  
M1  
I5  
R6  
Y9  
S10  
V13  
V17  
M18  
S19  
L20  
V21  
N22  
L23  
Y24  
L25  
L34  
F38  
D39  
R40  
R53  
E54  
L55  
K59  
R60  
Y63  
L67  
K68  
M69  
Q72  
R76  
A77  
I82  
T93  
P94  
M101  
K106  
L107  
L111  
L112  
D113  
L114  
P124  
F129  
L130  
F134  
I142  
K143  
D147  
H148  
L149  
L152  
L155  
GLY  
GLY  
PRO  
PRO  
GLY  
GLY  
ALA  
GLY  
GLY  
LEU  
GLY  
TYR  
LEU  
SER  
SER  
SER  
SER  
THR  
THR  
LYS  
LYS  
SER  
SER  
LEU  
SER  
SER  
PRO  
ALA  
THR  
SER  
GLY  
PRO  
LEU  
ALA  
LYS

- Molecule 1: Ferritin

Chain Bl: 

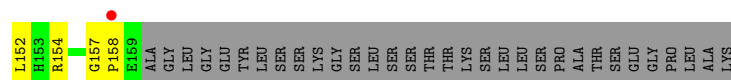
ARG  
M1  
Y29  
L34  
D81  
K98  
G156  
P158  
E159  
ALA  
GLY  
GLY  
GLY  
TYR  
LEU  
SER  
SER  
SER  
SER  
LYS  
GLY  
SER  
LEU  
SER  
SER  
THR  
THR  
LYS  
LYS  
SER  
SER  
LEU  
SER  
SER  
PRO  
ALA  
THR  
SER  
GLY  
PRO  
LEU  
ALA  
LYS

- Molecule 1: Ferritin

Chain BM: 

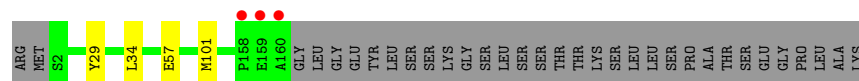
ARG  
MET  
S2  
V13  
S19  
N22  
L25  
Q26  
A27  
S28  
Y29  
Y31  
L32  
S49  
F52  
R53  
E54  
L55  
A56  
E57  
E58  
K59  
R60  
Y63  
L67  
R73  
L78  
I82  
T93  
P94  
K98  
D113  
A116  
H125  
L126  
E138  
V139  
I142  
H148





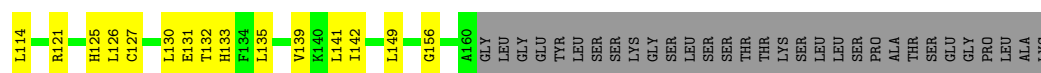
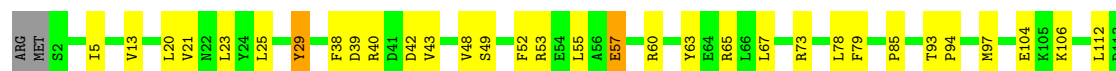
- Molecule 1: Ferritin

Chain Bm:



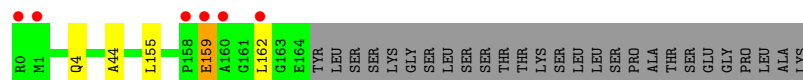
- Molecule 1: Ferritin

Chain BN:



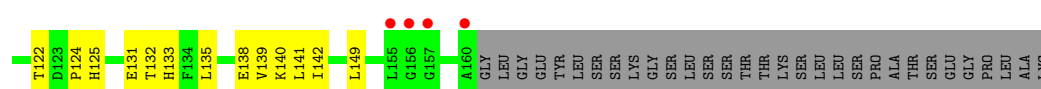
- Molecule 1: Ferritin

Chain Bn:



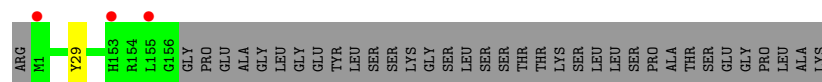
- Molecule 1: Ferritin

Chain BO:



- Molecule 1: Ferritin

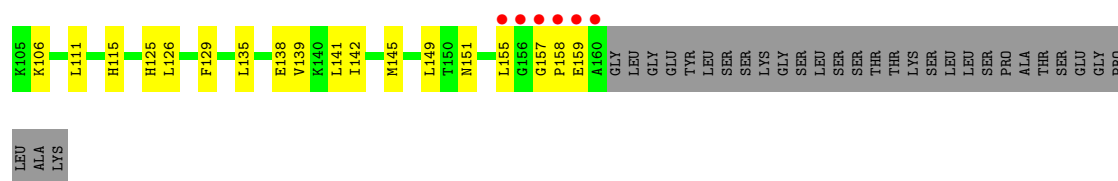
Chain Bo:



- Molecule 1: Ferritin

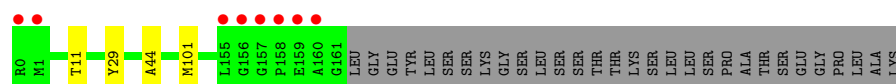
Chain BP:





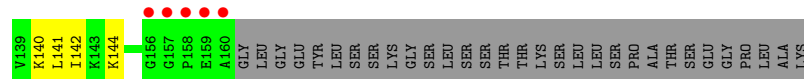
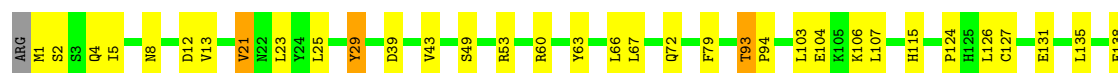
- Molecule 1: Ferritin

Chain Bp:



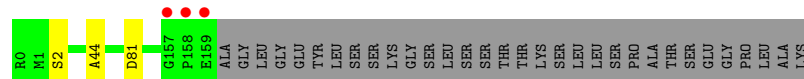
- Molecule 1: Ferritin

Chain BQ:



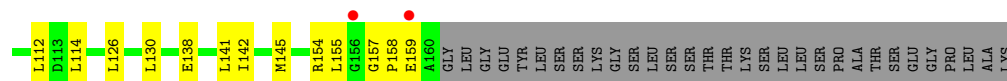
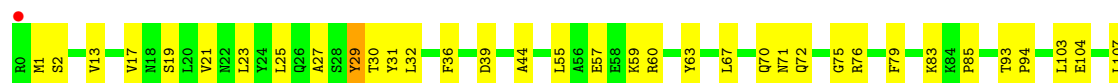
- Molecule 1: Ferritin

Chain Bq:



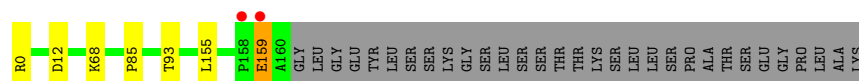
- Molecule 1: Ferritin

Chain BR:



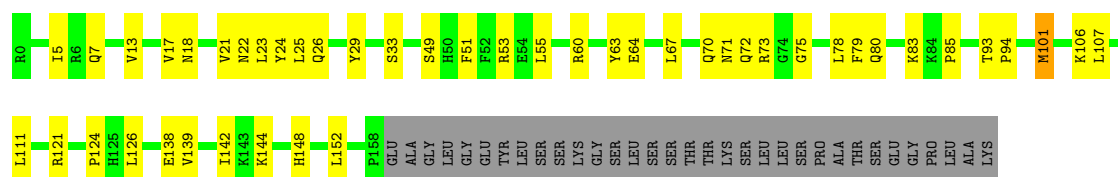
- Molecule 1: Ferritin

Chain Br:



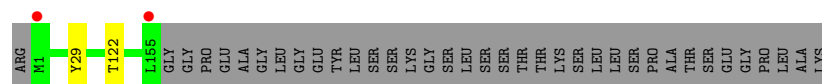
- Molecule 1: Ferritin

Chain BS:



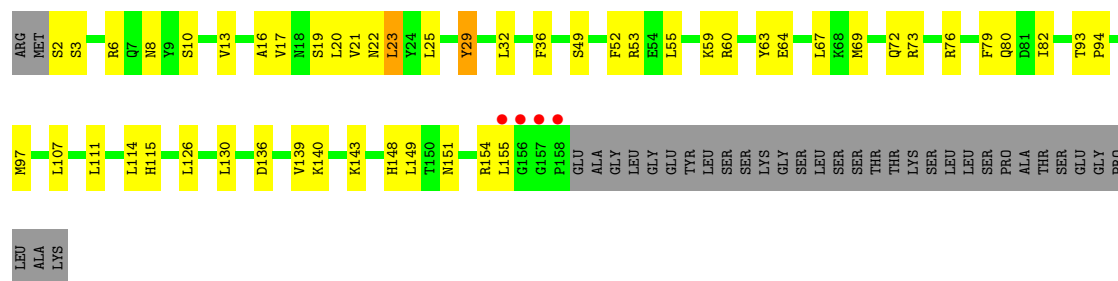
- Molecule 1: Ferritin

Chain Bs:



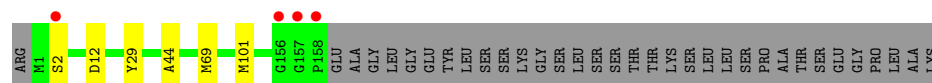
- Molecule 1: Ferritin

Chain BT:



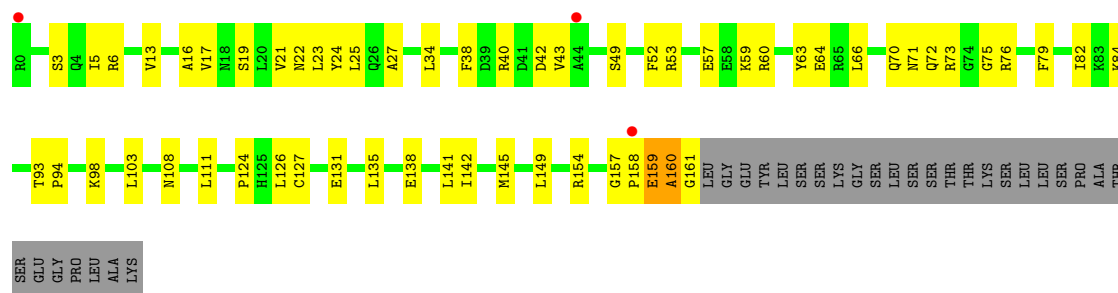
- Molecule 1: Ferritin

Chain Bt:



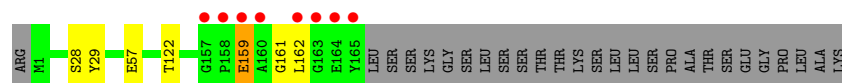
- Molecule 1: Ferritin

Chain BU:

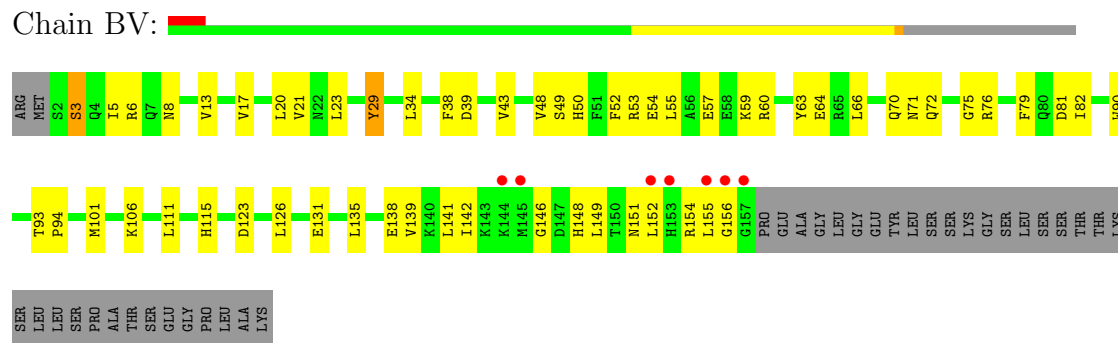


- Molecule 1: Ferritin

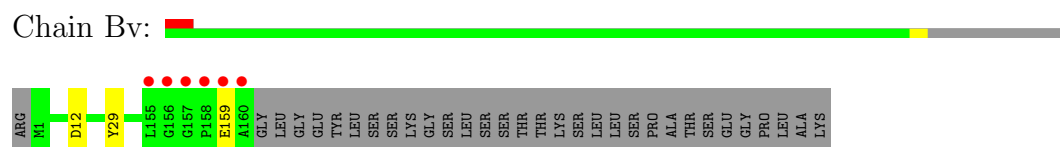
Chain Bu:



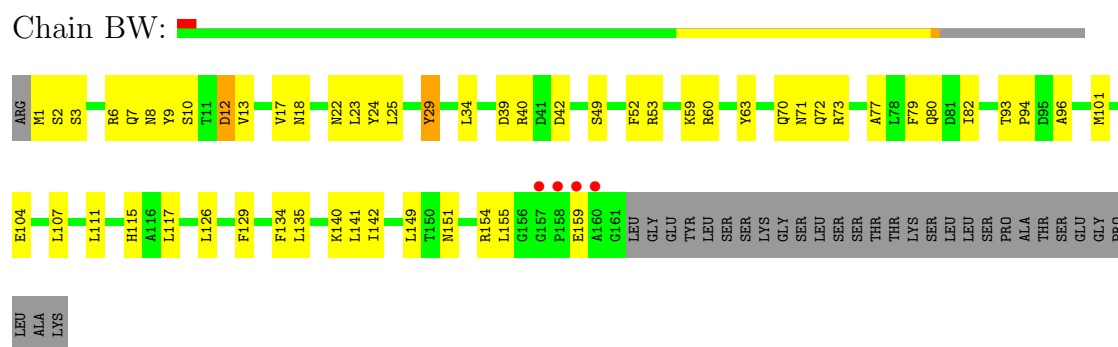
- Molecule 1: Ferritin



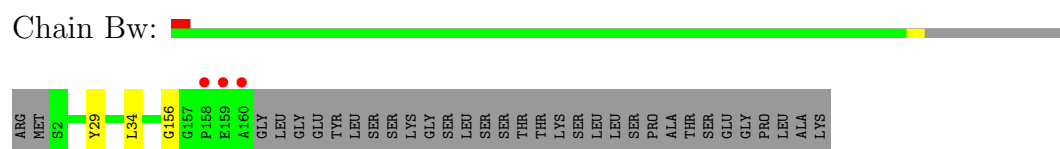
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin

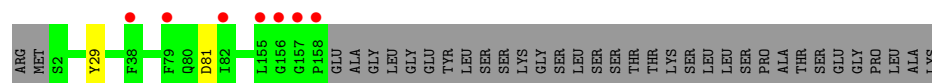


- Molecule 1: Ferritin



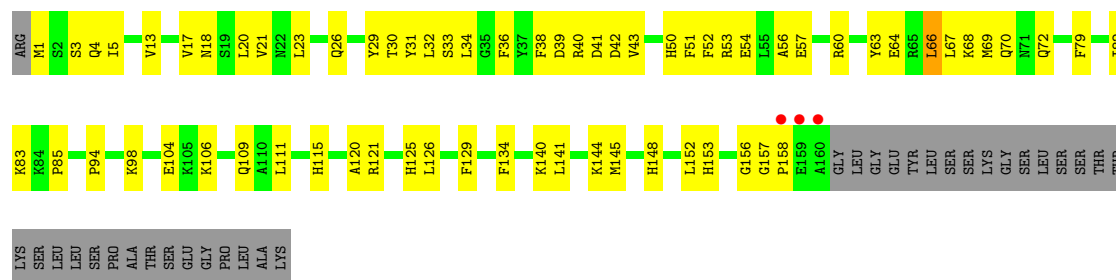
- Molecule 1: Ferritin

Chain Bx: 



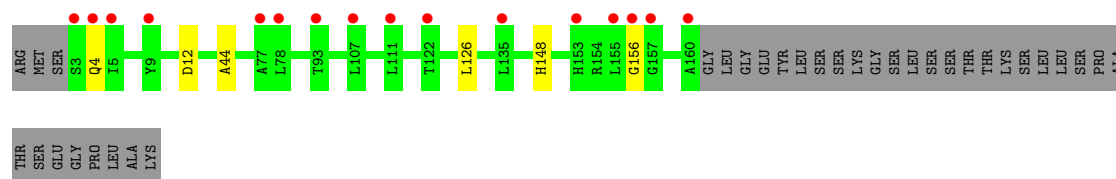
- Molecule 1: Ferritin

Chain CA: 



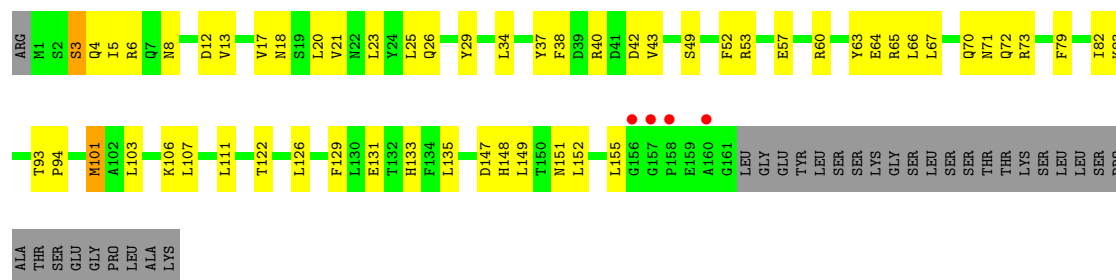
- Molecule 1: Ferritin

Chain Ca: 



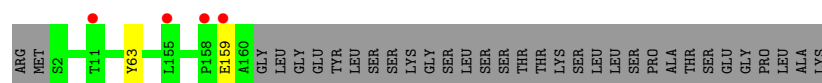
- Molecule 1: Ferritin

Chain CB: 



- Molecule 1: Ferritin

Chain Cb: 

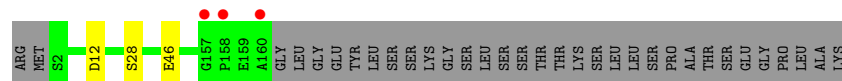


- Molecule 1: Ferritin

Chain CC: 

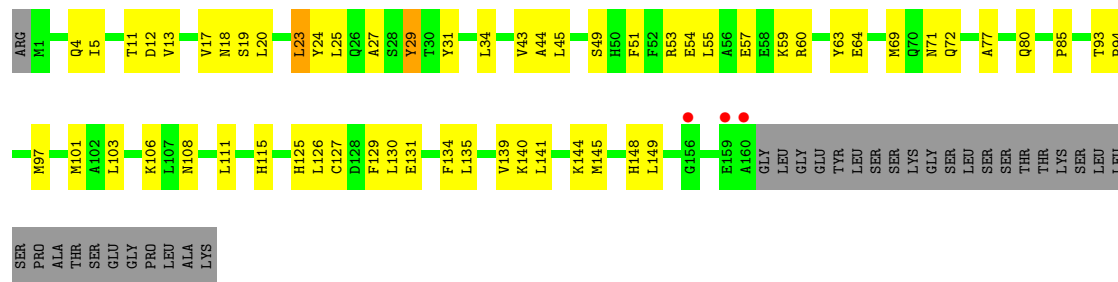






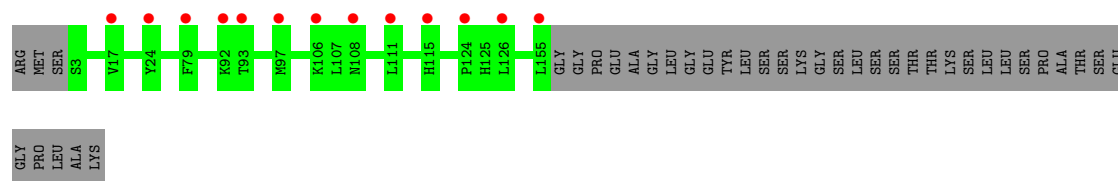
- Molecule 1: Ferritin

Chain CI:



- Molecule 1: Ferritin

Chain Ci:



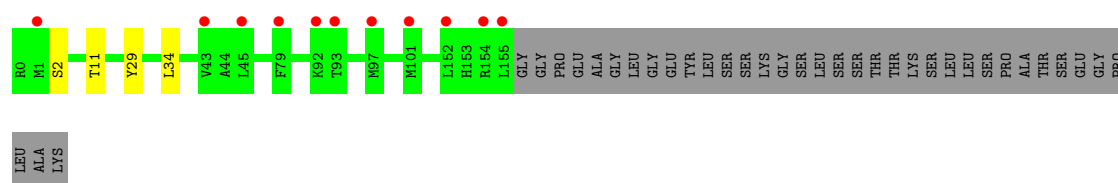
- Molecule 1: Ferritin

Chain CJ:



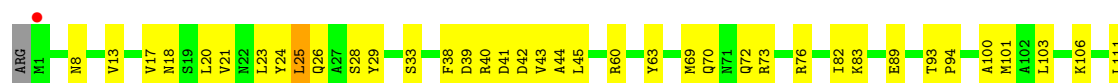
- Molecule 1: Ferritin

Chain Cj:

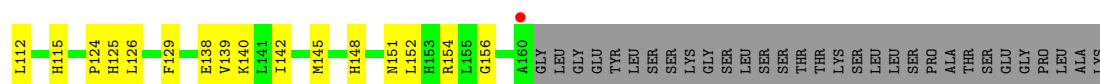


- Molecule 1: Ferritin

Chain CK:

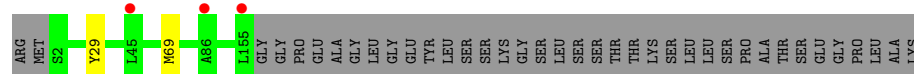






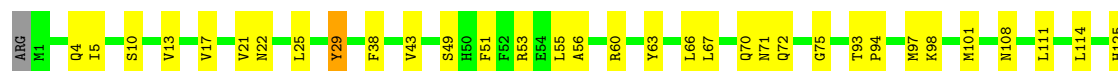
- Molecule 1: Ferritin

Chain Ck:



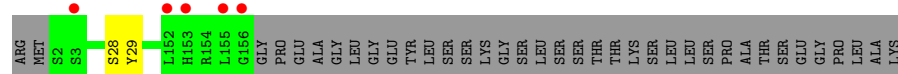
- Molecule 1: Ferritin

Chain CL:



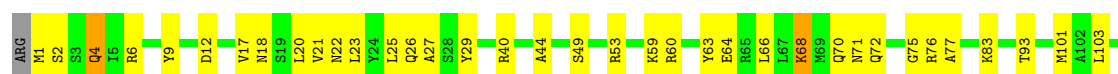
- Molecule 1: Ferritin

Chain Cl:



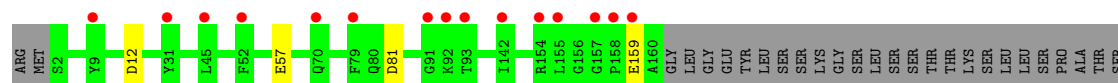
- Molecule 1: Ferritin

Chain CM:



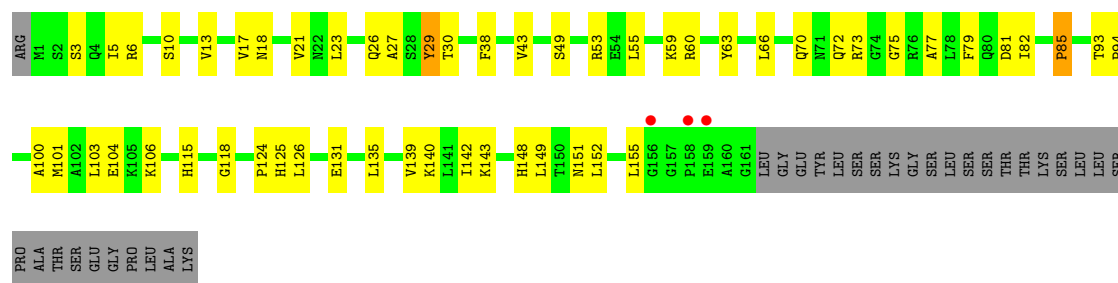
- Molecule 1: Ferritin

Chain Cm:



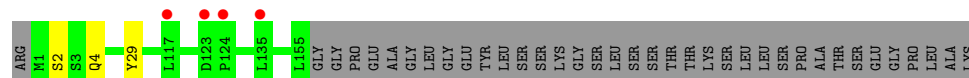
- Molecule 1: Ferritin

Chain CN:



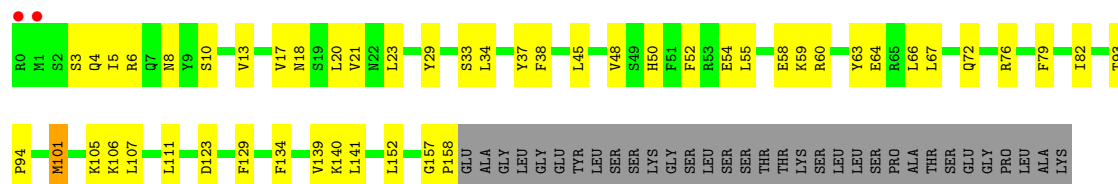
- Molecule 1: Ferritin

Chain Cn:



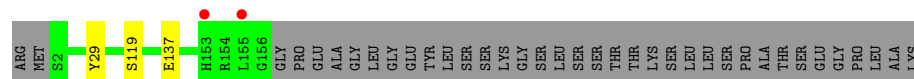
- Molecule 1: Ferritin

Chain CO:



- Molecule 1: Ferritin

Chain Co:



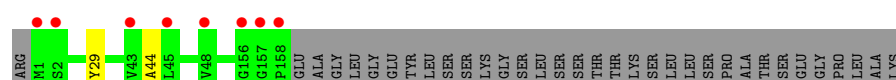
- Molecule 1: Ferritin

Chain CP:



- Molecule 1: Ferritin

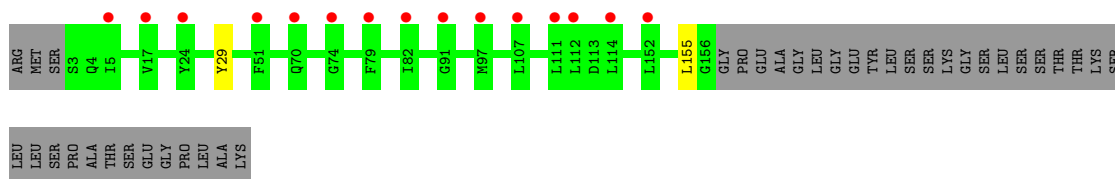
Chain Cp:



- Molecule 1: Ferritin

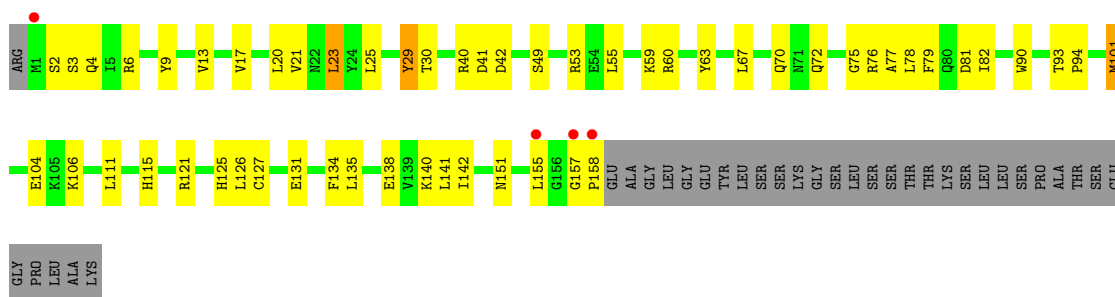
Chain CQ:





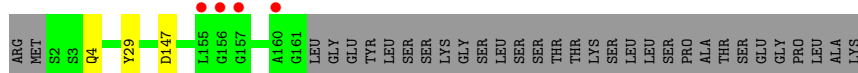
• Molecule 1: Ferritin

Chain CT:



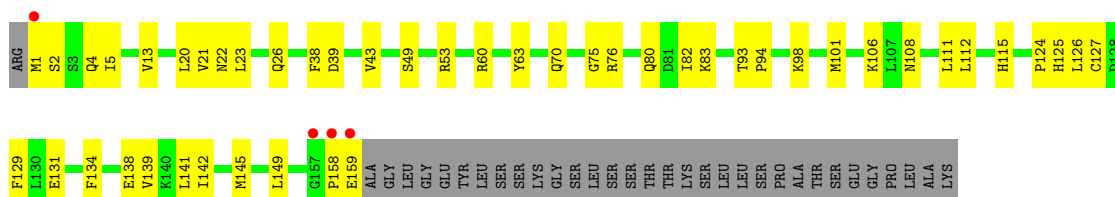
• Molecule 1: Ferritin

Chain Ct:



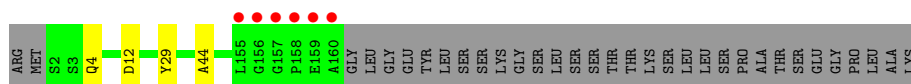
• Molecule 1: Ferritin

Chain CU:



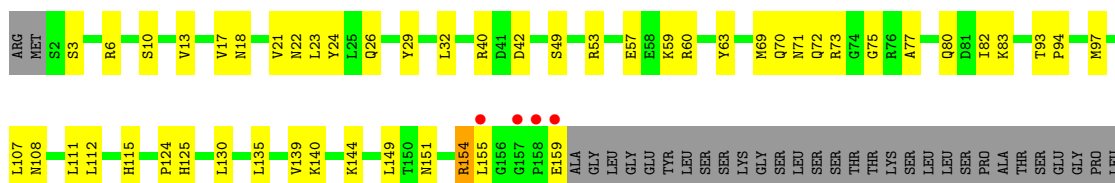
• Molecule 1: Ferritin

Chain Cu:



• Molecule 1: Ferritin

Chain CV:



ALA  
LYS

- Molecule 1: Ferritin

Chain Cv:

ARG	H1	Q4	Y29	Q80	P158	E159	A160	G161	LEU	GLY	GLY	TYR	LEU	SER	SER	LYS	GLY	SER	SER	LEU	SER	THR	LYS	SER	LEU	LEU	SER	PRO	ALA	THR	SER	GLU	GLY	PRO	LEU	ALA	LYS
-----	----	----	-----	-----	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: Ferritin

Chain CW:

ARG	H1	Q4	I5	S10	V13	V17	N18	N22	L25	Y29	F38	V43	K59	R60	Y63	E64	N71	Q72	R73	A77	L78	F79	I82	M97	K98	L103	L107	P124	H125	L126	C127	E131	L135	D136	E137	E138	V139	K140	L141
-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 1: Ferritin

Chain Cw:

ARG	ME1	S2	Y24	L107	L126	L155	G156	GLY	PRO	GLU	ALA	GLY	GLY	LEU	GLY	TYR	SER	SER	LYS	GLY	LEU	THR	THR	LYS	LEU	LEU	LEU	PRO	ALA	THR	SER	GLY	PRO	GLY	LEU	ALA	LYS
-----	-----	----	-----	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: Ferritin

Chain CX:

R0	M1	S2	N8	Y9	S10	T11	D12	V13	A16	V17	N18	V21	N22	L23	Y24	L25	Y29	L34	G35	F36	G37	F38	D39	R40	D41	D42	V43	A44	S49	F52	R53	R60	Y63	L67	K68	M69	Q70	N71	Q72	F79	I82	K83	K84	T93	P94
----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

K98	A99	M100	M101	K106	L107	M108	L111	L112	D113	L114	H115	A116	L126	C127	E131	T132	H133	E138	V139	K140	L141	T142	K143	K144	M145	G146	D147	H148	L149	T150	M151	R154	L155	G156	G157	P158	E159	A160	GLY	LEU	GLY	GLY	TYR	LEU	SER	SER	LYS	GLY	SER	LEU	SER	THR
-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: Ferritin

Chain Cx:

R0	H1	D12	Y29	E57	P85	L155	GLY	PRO	GLU	ALA	GLY	LEU	GLY	TYR	LEU	SER	SER	LYS	GLY	LEU	SER	THR	THR	LYS	SER	LEU	LEU	SER	PRO	ALA	THR	SER	GLY	PRO	GLY	LEU	ALA	LYS
----	----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 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 0.234 , 0.272	Depositor DCC
$R_{free}$ test set	42321 reflections (5.27%)	DCC
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> )	0.30 , 15.9	EDS
Estimated twinning fraction	0.000 for h,-h-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 845977 reflections	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.

## 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1270	0	1243	31	0
1	AB	1320	0	1292	48	0
1	AC	1294	0	1273	34	0
1	AD	1275	0	1248	50	0
1	AE	1320	0	1292	70	0
1	AF	1269	0	1249	56	0
1	AG	1275	0	1248	46	0
1	AH	1283	0	1260	48	0
1	AI	1269	0	1249	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AJ	1262	0	1242	41	0
1	AK	1269	0	1252	27	0
1	AL	1261	0	1237	44	0
1	AM	1298	0	1276	57	0
1	AN	1320	0	1292	54	0
1	AO	1320	0	1292	69	0
1	AP	1278	0	1255	48	0
1	AQ	1319	0	1296	52	0
1	AR	1308	0	1283	48	0
1	AS	1279	0	1251	34	0
1	AT	1270	0	1243	65	0
1	AU	1283	0	1260	44	0
1	AV	1279	0	1251	36	0
1	AW	1270	0	1243	49	0
1	AX	1283	0	1260	56	0
1	Aa	1294	0	1273	0	0
1	Ab	1287	0	1263	0	0
1	Ac	1283	0	1260	0	0
1	Ad	1320	0	1292	0	0
1	Ae	1298	0	1276	0	0
1	Af	1294	0	1273	0	0
1	Ag	1254	0	1236	0	0
1	Ah	1294	0	1273	0	0
1	Ai	1278	0	1255	0	0
1	Aj	1320	0	1292	0	0
1	Ak	1320	0	1292	0	0
1	Al	1320	0	1292	0	0
1	Am	1298	0	1276	0	0
1	An	1287	0	1263	0	0
1	Ao	1294	0	1273	0	0
1	Ap	1298	0	1276	0	0
1	Aq	1283	0	1260	0	0
1	Ar	1320	0	1292	0	0
1	As	1294	0	1273	0	0
1	At	1283	0	1260	0	0
1	Au	1283	0	1260	0	0
1	Av	1319	0	1296	0	0
1	Aw	1287	0	1263	0	0
1	Ax	1254	0	1236	0	0
1	BA	1331	0	1305	49	0
1	BB	1269	0	1252	40	0
1	BC	1250	0	1227	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BD	1289	0	1268	53	0
1	BE	1278	0	1255	43	0
1	BF	1275	0	1248	39	0
1	BG	1258	0	1239	49	0
1	BH	1246	0	1224	47	0
1	BI	1254	0	1236	45	0
1	BJ	1261	0	1237	48	0
1	BK	1258	0	1239	47	0
1	BL	1254	0	1236	39	0
1	BM	1270	0	1243	29	0
1	BN	1275	0	1248	43	0
1	BO	1283	0	1260	46	0
1	BP	1275	0	1248	46	0
1	BQ	1283	0	1260	30	0
1	BR	1294	0	1273	41	0
1	BS	1280	0	1262	40	0
1	BT	1261	0	1237	49	0
1	BU	1298	0	1276	45	0
1	BV	1254	0	1230	49	0
1	BW	1287	0	1263	50	0
1	BX	1300	0	1271	65	0
1	Ba	1269	0	1249	0	0
1	Bb	1278	0	1255	0	0
1	Bc	1294	0	1273	0	0
1	Bd	1294	0	1273	0	0
1	Be	1300	0	1271	0	0
1	Bf	1320	0	1292	0	0
1	Bg	1258	0	1239	0	0
1	Bh	1278	0	1255	0	0
1	Bi	1269	0	1252	0	0
1	Bj	1244	0	1222	0	0
1	Bk	1278	0	1255	0	0
1	Bl	1278	0	1255	0	0
1	Bm	1275	0	1248	0	0
1	Bn	1319	0	1296	0	0
1	Bo	1258	0	1239	0	0
1	Bp	1298	0	1276	0	0
1	Bq	1289	0	1268	0	0
1	Br	1294	0	1273	0	0
1	Bs	1254	0	1236	0	0
1	Bt	1269	0	1249	0	0
1	Bu	1320	0	1292	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Bv	1283	0	1260	0	0
1	Bw	1275	0	1248	0	0
1	Bx	1261	0	1237	0	0
1	CA	1283	0	1260	57	0
1	CB	1287	0	1263	51	0
1	CC	1261	0	1237	30	0
1	CD	1294	0	1273	34	0
1	CE	1289	0	1268	36	0
1	CF	1279	0	1251	54	0
1	CG	1289	0	1268	37	0
1	CH	1278	0	1255	48	0
1	CI	1283	0	1260	46	0
1	CJ	1319	0	1296	77	0
1	CK	1283	0	1260	40	0
1	CL	1278	0	1255	41	0
1	CM	1278	0	1255	41	0
1	CN	1287	0	1263	45	0
1	CO	1280	0	1262	40	0
1	CP	1269	0	1249	32	0
1	CQ	1298	0	1276	50	0
1	CR	1331	0	1305	46	0
1	CS	1294	0	1273	65	0
1	CT	1269	0	1249	45	0
1	CU	1278	0	1255	31	0
1	CV	1270	0	1243	37	0
1	CW	1254	0	1236	34	0
1	CX	1294	0	1273	53	0
1	Ca	1269	0	1243	0	0
1	Cb	1275	0	1248	0	0
1	Cc	1264	0	1238	0	0
1	Cd	1240	0	1219	0	0
1	Ce	1246	0	1224	0	0
1	Cf	1238	0	1213	0	0
1	Cg	1279	0	1251	0	0
1	Ch	1275	0	1248	0	0
1	Ci	1240	0	1219	0	0
1	Cj	1265	0	1249	0	0
1	Ck	1246	0	1224	0	0
1	Cl	1250	0	1227	0	0
1	Cm	1275	0	1248	0	0
1	Cn	1254	0	1236	0	0
1	Co	1250	0	1227	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Cp	1269	0	1249	0	0
1	Cq	1250	0	1227	0	0
1	Cr	1246	0	1224	0	0
1	Cs	1244	0	1222	0	0
1	Ct	1279	0	1251	0	0
1	Cu	1275	0	1248	0	0
1	Cv	1287	0	1263	0	0
1	Cw	1250	0	1227	0	0
1	Cx	1265	0	1249	0	0
2	AA	1	0	0	0	0
2	AB	1	0	0	0	0
2	AC	1	0	0	0	0
2	AF	1	0	0	0	0
2	AH	1	0	0	0	0
2	AL	1	0	0	0	0
2	AM	1	0	0	0	0
2	AO	1	0	0	0	0
2	Aa	1	0	0	0	0
2	Ac	1	0	0	0	0
2	Ad	1	0	0	0	0
2	Ae	1	0	0	0	0
2	Ag	1	0	0	0	0
2	Ah	1	0	0	0	0
2	Aj	1	0	0	0	0
2	An	1	0	0	0	0
2	BA	1	0	0	0	0
2	BB	1	0	0	0	0
2	BC	1	0	0	0	0
2	BD	1	0	0	0	0
2	BG	1	0	0	0	0
2	BH	1	0	0	0	0
2	BN	1	0	0	0	0
2	BR	1	0	0	0	0
2	Ba	1	0	0	0	0
2	Bb	1	0	0	0	0
2	Bc	1	0	0	0	0
2	Bd	1	0	0	0	0
2	Be	1	0	0	0	0
2	Bf	1	0	0	0	0
2	Bg	1	0	0	0	0
2	Bu	1	0	0	0	0
2	CA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CB	1	0	0	0	0
2	CC	1	0	0	0	0
2	CD	1	0	0	0	0
2	CE	1	0	0	0	0
2	CF	1	0	0	0	0
2	CH	1	0	0	0	0
2	CO	1	0	0	0	0
2	Ca	1	0	0	0	0
2	Cb	1	0	0	0	0
2	Ce	1	0	0	0	0
2	Cg	1	0	0	0	0
2	Ck	1	0	0	0	0
2	Cl	1	0	0	0	0
2	Cn	1	0	0	0	0
2	Cp	1	0	0	0	0
3	AA	10	0	0	0	0
3	AB	14	0	0	0	0
3	AC	15	0	0	1	0
3	AD	8	0	0	1	0
3	AE	27	0	0	0	0
3	AF	16	0	0	0	0
3	AG	27	0	0	0	0
3	AH	28	0	0	1	0
3	AI	6	0	0	0	0
3	AJ	9	0	0	0	0
3	AK	15	0	0	0	0
3	AL	11	0	0	0	0
3	AM	26	0	0	2	0
3	AN	17	0	0	1	0
3	AO	20	0	0	2	0
3	AP	25	0	0	1	0
3	AQ	21	0	0	0	0
3	AR	18	0	0	0	0
3	AS	20	0	0	1	0
3	AT	22	0	0	2	0
3	AU	20	0	0	1	0
3	AV	17	0	0	0	0
3	AW	19	0	0	2	0
3	AX	33	0	0	1	0
3	Aa	47	0	0	0	0
3	Ab	30	0	0	0	0
3	Ac	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Ad	37	0	0	0	0
3	Ae	26	0	0	0	0
3	Af	48	0	0	0	0
3	Ag	37	0	0	0	0
3	Ah	28	0	0	0	0
3	Ai	40	0	0	0	0
3	Aj	28	0	0	0	0
3	Ak	37	0	0	0	0
3	Al	25	0	0	0	0
3	Am	45	0	0	0	0
3	An	41	0	0	0	0
3	Ao	39	0	0	0	0
3	Ap	32	0	0	0	0
3	Aq	33	0	0	0	0
3	Ar	40	0	0	0	0
3	As	44	0	0	0	0
3	At	31	0	0	0	0
3	Au	31	0	0	0	0
3	Av	19	0	0	0	0
3	Aw	34	0	0	0	0
3	Ax	31	0	0	0	0
3	BA	15	0	0	0	0
3	BB	5	0	0	0	0
3	BC	2	0	0	0	0
3	BD	10	0	0	2	0
3	BE	15	0	0	0	0
3	BF	32	0	0	0	0
3	BG	7	0	0	0	0
3	BH	11	0	0	0	0
3	BI	20	0	0	0	0
3	BJ	8	0	0	2	0
3	BK	6	0	0	0	0
3	BL	10	0	0	1	0
3	BM	25	0	0	1	0
3	BN	18	0	0	0	0
3	BO	13	0	0	0	0
3	BP	10	0	0	0	0
3	BQ	30	0	0	0	0
3	BR	21	0	0	0	0
3	BS	37	0	0	0	0
3	BT	12	0	0	2	0
3	BU	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BV	5	0	0	0	0
3	BW	25	0	0	1	0
3	BX	3	0	0	0	0
3	Ba	10	0	0	0	0
3	Bb	4	0	0	0	0
3	Bc	32	0	0	0	0
3	Bd	27	0	0	0	0
3	Be	26	0	0	0	0
3	Bf	26	0	0	0	0
3	Bg	7	0	0	0	0
3	Bh	19	0	0	0	0
3	Bi	7	0	0	0	0
3	Bj	6	0	0	0	0
3	Bk	6	0	0	0	0
3	Bl	23	0	0	0	0
3	Bm	25	0	0	0	0
3	Bn	11	0	0	0	0
3	Bo	9	0	0	0	0
3	Bp	31	0	0	0	0
3	Bq	18	0	0	0	0
3	Br	35	0	0	0	0
3	Bs	15	0	0	0	0
3	Bt	11	0	0	0	0
3	Bu	28	0	0	0	0
3	Bv	25	0	0	0	0
3	Bw	39	0	0	0	0
3	Bx	7	0	0	0	0
3	CA	29	0	0	0	0
3	CB	16	0	0	0	0
3	CC	7	0	0	0	0
3	CD	28	0	0	1	0
3	CE	15	0	0	0	0
3	CF	25	0	0	1	0
3	CG	19	0	0	0	0
3	CH	10	0	0	0	0
3	CI	30	0	0	1	0
3	CJ	18	0	0	2	0
3	CK	12	0	0	0	0
3	CL	7	0	0	0	0
3	CM	23	0	0	1	0
3	CN	25	0	0	0	0
3	CO	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CP	14	0	0	1	0
3	CQ	41	0	0	0	0
3	CR	20	0	0	0	0
3	CS	28	0	0	0	0
3	CT	15	0	0	0	0
3	CU	3	0	0	0	0
3	CV	8	0	0	0	0
3	CW	15	0	0	0	0
3	CX	21	0	0	1	0
3	Ca	11	0	0	0	0
3	Cb	6	0	0	0	0
3	Cc	7	0	0	0	0
3	Cd	6	0	0	0	0
3	Ce	6	0	0	0	0
3	Cf	8	0	0	0	0
3	Cg	16	0	0	0	0
3	Ch	18	0	0	0	0
3	Ci	9	0	0	0	0
3	Cj	9	0	0	0	0
3	Ck	11	0	0	0	0
3	Cl	2	0	0	0	0
3	Cm	2	0	0	0	0
3	Cn	4	0	0	0	0
3	Co	12	0	0	0	0
3	Cp	10	0	0	0	0
3	Cq	2	0	0	0	0
3	Cr	4	0	0	0	0
3	Ct	17	0	0	0	0
3	Cu	12	0	0	0	0
3	Cv	4	0	0	0	0
3	Cw	10	0	0	0	0
3	Cx	12	0	0	0	0
All	All	187090	0	181001	2777	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 2777 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AJ:1:MET:HG3	1:AJ:2:SER:H	1.19	1.02
1:AM:8:ASN:HD22	1:AR:112:LEU:HD13	2.24	1.01
1:CB:8:ASN:HD22	1:CJ:112:LEU:HD13	2.31	1.00

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AE:23:LEU:HD11	1:AE:106:LYS:HE2	1.50	0.94
1:BI:1:MET:HG3	1:BI:2:SER:H	1.32	0.93

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	156/192 (81%)	151 (97%)	5 (3%)	0	100	100
1	AB	163/192 (85%)	149 (91%)	10 (6%)	4 (2%)	9	30
1	AC	159/192 (83%)	146 (92%)	10 (6%)	3 (2%)	12	39
1	AD	157/192 (82%)	151 (96%)	5 (3%)	1 (1%)	33	73
1	AE	163/192 (85%)	147 (90%)	11 (7%)	5 (3%)	7	23
1	AF	156/192 (81%)	151 (97%)	4 (3%)	1 (1%)	33	73
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%)	33	73
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%)	18	51
1	AN	163/192 (85%)	154 (94%)	7 (4%)	2 (1%)	19	54
1	AO	163/192 (85%)	148 (91%)	11 (7%)	4 (2%)	9	30
1	AP	157/192 (82%)	152 (97%)	5 (3%)	0	100	100
1	AQ	163/192 (85%)	150 (92%)	10 (6%)	3 (2%)	13	41
1	AR	162/192 (84%)	152 (94%)	8 (5%)	2 (1%)	19	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AS	158/192 (82%)	149 (94%)	8 (5%)	1 (1%)	33	73
1	AT	156/192 (81%)	144 (92%)	10 (6%)	2 (1%)	18	51
1	AU	158/192 (82%)	152 (96%)	5 (3%)	1 (1%)	33	73
1	AV	158/192 (82%)	148 (94%)	8 (5%)	2 (1%)	18	51
1	AW	156/192 (81%)	150 (96%)	6 (4%)	0	100	100
1	AX	158/192 (82%)	149 (94%)	8 (5%)	1 (1%)	33	73
1	Aa	159/192 (83%)	153 (96%)	6 (4%)	0	100	100
1	Ab	159/192 (83%)	151 (95%)	6 (4%)	2 (1%)	18	51
1	Ac	158/192 (82%)	155 (98%)	3 (2%)	0	100	100
1	Ad	163/192 (85%)	152 (93%)	8 (5%)	3 (2%)	13	41
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
1	Ai	157/192 (82%)	150 (96%)	5 (3%)	2 (1%)	18	51
1	Aj	163/192 (85%)	147 (90%)	11 (7%)	5 (3%)	7	23
1	Ak	163/192 (85%)	153 (94%)	8 (5%)	2 (1%)	19	54
1	Al	163/192 (85%)	149 (91%)	10 (6%)	4 (2%)	9	30
1	Am	160/192 (83%)	149 (93%)	7 (4%)	4 (2%)	9	30
1	An	159/192 (83%)	149 (94%)	8 (5%)	2 (1%)	18	51
1	Ao	159/192 (83%)	150 (94%)	7 (4%)	2 (1%)	18	51
1	Ap	160/192 (83%)	150 (94%)	7 (4%)	3 (2%)	12	39
1	Aq	158/192 (82%)	146 (92%)	11 (7%)	1 (1%)	33	73
1	Ar	163/192 (85%)	152 (93%)	8 (5%)	3 (2%)	13	41
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%)	33	73
1	Av	163/192 (85%)	148 (91%)	13 (8%)	2 (1%)	19	54
1	Aw	159/192 (83%)	149 (94%)	9 (6%)	1 (1%)	33	73
1	Ax	153/192 (80%)	150 (98%)	3 (2%)	0	100	100
1	BA	164/192 (85%)	150 (92%)	12 (7%)	2 (1%)	19	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	12	39
1	BG	154/192 (80%)	145 (94%)	9 (6%)	0	100	100
1	BH	152/192 (79%)	146 (96%)	5 (3%)	1 (1%)	30	70
1	BI	153/192 (80%)	150 (98%)	3 (2%)	0	100	100
1	BJ	155/192 (81%)	147 (95%)	7 (4%)	1 (1%)	33	73
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%)	33	73
1	BO	158/192 (82%)	146 (92%)	11 (7%)	1 (1%)	33	73
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%)	33	73
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%)	33	73
1	BV	154/192 (80%)	149 (97%)	3 (2%)	2 (1%)	18	51
1	BW	159/192 (83%)	154 (97%)	5 (3%)	0	100	100
1	BX	161/192 (84%)	150 (93%)	7 (4%)	4 (2%)	9	30
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%)	12	39
1	Be	161/192 (84%)	146 (91%)	12 (8%)	3 (2%)	12	39
1	Bf	163/192 (85%)	147 (90%)	11 (7%)	5 (3%)	7	23
1	Bg	154/192 (80%)	150 (97%)	4 (3%)	0	100	100
1	Bh	157/192 (82%)	151 (96%)	5 (3%)	1 (1%)	33	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bi	155/192 (81%)	148 (96%)	6 (4%)	1 (1%)	33	73
1	Bj	152/192 (79%)	147 (97%)	5 (3%)	0	100	100
1	Bk	157/192 (82%)	148 (94%)	8 (5%)	1 (1%)	33	73
1	Bl	157/192 (82%)	150 (96%)	6 (4%)	1 (1%)	33	73
1	Bm	157/192 (82%)	151 (96%)	6 (4%)	0	100	100
1	Bn	163/192 (85%)	153 (94%)	7 (4%)	3 (2%)	13	41
1	Bo	154/192 (80%)	149 (97%)	5 (3%)	0	100	100
1	Bp	160/192 (83%)	148 (92%)	11 (7%)	1 (1%)	33	73
1	Bq	158/192 (82%)	150 (95%)	6 (4%)	2 (1%)	18	51
1	Br	159/192 (83%)	148 (93%)	9 (6%)	2 (1%)	18	51
1	Bs	153/192 (80%)	148 (97%)	5 (3%)	0	100	100
1	Bt	156/192 (81%)	147 (94%)	7 (4%)	2 (1%)	18	51
1	Bu	163/192 (85%)	152 (93%)	9 (6%)	2 (1%)	19	54
1	Bv	158/192 (82%)	149 (94%)	8 (5%)	1 (1%)	33	73
1	Bw	157/192 (82%)	150 (96%)	6 (4%)	1 (1%)	33	73
1	Bx	155/192 (81%)	147 (95%)	8 (5%)	0	100	100
1	CA	158/192 (82%)	153 (97%)	4 (2%)	1 (1%)	33	73
1	CB	159/192 (83%)	154 (97%)	5 (3%)	0	100	100
1	CC	155/192 (81%)	149 (96%)	5 (3%)	1 (1%)	33	73
1	CD	159/192 (83%)	152 (96%)	6 (4%)	1 (1%)	33	73
1	CE	158/192 (82%)	149 (94%)	7 (4%)	2 (1%)	18	51
1	CF	158/192 (82%)	150 (95%)	8 (5%)	0	100	100
1	CG	158/192 (82%)	153 (97%)	4 (2%)	1 (1%)	33	73
1	CH	157/192 (82%)	146 (93%)	10 (6%)	1 (1%)	33	73
1	CI	158/192 (82%)	147 (93%)	10 (6%)	1 (1%)	33	73
1	CJ	163/192 (85%)	153 (94%)	8 (5%)	2 (1%)	19	54
1	CK	158/192 (82%)	152 (96%)	5 (3%)	1 (1%)	33	73
1	CL	157/192 (82%)	150 (96%)	7 (4%)	0	100	100
1	CM	157/192 (82%)	148 (94%)	7 (4%)	2 (1%)	18	51
1	CN	159/192 (83%)	152 (96%)	7 (4%)	0	100	100
1	CO	157/192 (82%)	146 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	13	41
1	CS	159/192 (83%)	150 (94%)	9 (6%)	0	100	100
1	CT	156/192 (81%)	147 (94%)	8 (5%)	1 (1%)	33	73
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%)	18	51
1	Ca	156/192 (81%)	148 (95%)	5 (3%)	3 (2%)	12	39
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
1	Cf	151/192 (79%)	146 (97%)	5 (3%)	0	100	100
1	Cg	158/192 (82%)	150 (95%)	7 (4%)	1 (1%)	33	73
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%)	33	73
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%)	33	73
1	Cq	153/192 (80%)	146 (95%)	7 (5%)	0	100	100
1	Cr	152/192 (79%)	147 (97%)	4 (3%)	1 (1%)	30	70
1	Cs	152/192 (79%)	147 (97%)	4 (3%)	1 (1%)	30	70
1	Ct	158/192 (82%)	154 (98%)	4 (2%)	0	100	100
1	Cu	157/192 (82%)	149 (95%)	7 (4%)	1 (1%)	33	73
1	Cv	159/192 (83%)	151 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	33	73

5 of 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

### 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%)	38	76
1	AB	138/161 (86%)	133 (96%)	5 (4%)	47	84
1	AC	136/161 (84%)	132 (97%)	4 (3%)	55	88
1	AD	134/161 (83%)	133 (99%)	1 (1%)	91	98
1	AE	138/161 (86%)	136 (99%)	2 (1%)	78	95
1	AF	134/161 (83%)	131 (98%)	3 (2%)	64	92
1	AG	134/161 (83%)	131 (98%)	3 (2%)	64	92
1	AH	135/161 (84%)	131 (97%)	4 (3%)	53	88
1	AI	134/161 (83%)	131 (98%)	3 (2%)	64	92
1	AJ	133/161 (83%)	132 (99%)	1 (1%)	89	98
1	AK	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	AL	133/161 (83%)	130 (98%)	3 (2%)	63	91
1	AM	136/161 (84%)	133 (98%)	3 (2%)	64	92
1	AN	138/161 (86%)	135 (98%)	3 (2%)	64	92
1	AO	138/161 (86%)	127 (92%)	11 (8%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AP	135/161 (84%)	128 (95%)	7 (5%)	32	69
1	AQ	138/161 (86%)	136 (99%)	2 (1%)	78	95
1	AR	137/161 (85%)	135 (98%)	2 (2%)	76	95
1	AS	134/161 (83%)	130 (97%)	4 (3%)	53	88
1	AT	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	AU	135/161 (84%)	131 (97%)	4 (3%)	53	88
1	AV	134/161 (83%)	133 (99%)	1 (1%)	91	98
1	AW	134/161 (83%)	133 (99%)	1 (1%)	91	98
1	AX	135/161 (84%)	134 (99%)	1 (1%)	91	98
1	Aa	136/161 (84%)	133 (98%)	3 (2%)	64	92
1	Ab	135/161 (84%)	130 (96%)	5 (4%)	45	83
1	Ac	135/161 (84%)	132 (98%)	3 (2%)	64	92
1	Ad	138/161 (86%)	131 (95%)	7 (5%)	33	70
1	Ae	136/161 (84%)	132 (97%)	4 (3%)	55	88
1	Af	136/161 (84%)	133 (98%)	3 (2%)	64	92
1	Ag	133/161 (83%)	129 (97%)	4 (3%)	53	88
1	Ah	136/161 (84%)	133 (98%)	3 (2%)	64	92
1	Ai	135/161 (84%)	132 (98%)	3 (2%)	64	92
1	Aj	138/161 (86%)	132 (96%)	6 (4%)	40	77
1	Ak	138/161 (86%)	133 (96%)	5 (4%)	47	84
1	Al	138/161 (86%)	131 (95%)	7 (5%)	33	70
1	Am	136/161 (84%)	135 (99%)	1 (1%)	91	98
1	An	135/161 (84%)	133 (98%)	2 (2%)	76	95
1	Ao	136/161 (84%)	134 (98%)	2 (2%)	76	95
1	Ap	136/161 (84%)	134 (98%)	2 (2%)	76	95
1	Aq	135/161 (84%)	132 (98%)	3 (2%)	64	92
1	Ar	138/161 (86%)	133 (96%)	5 (4%)	47	84
1	As	136/161 (84%)	130 (96%)	6 (4%)	39	76
1	At	135/161 (84%)	128 (95%)	7 (5%)	32	69
1	Au	135/161 (84%)	130 (96%)	5 (4%)	45	83
1	Av	138/161 (86%)	135 (98%)	3 (2%)	64	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aw	135/161 (84%)	128 (95%)	7 (5%)	32	69
1	Ax	133/161 (83%)	132 (99%)	1 (1%)	89	98
1	BA	139/161 (86%)	134 (96%)	5 (4%)	47	84
1	BB	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	BC	132/161 (82%)	130 (98%)	2 (2%)	76	95
1	BD	136/161 (84%)	135 (99%)	1 (1%)	91	98
1	BE	135/161 (84%)	135 (100%)	0	100	100
1	BF	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	BG	133/161 (83%)	131 (98%)	2 (2%)	76	95
1	BH	132/161 (82%)	129 (98%)	3 (2%)	63	91
1	BI	133/161 (83%)	132 (99%)	1 (1%)	89	98
1	BJ	133/161 (83%)	130 (98%)	3 (2%)	63	91
1	BK	133/161 (83%)	128 (96%)	5 (4%)	44	82
1	BL	133/161 (83%)	132 (99%)	1 (1%)	89	98
1	BM	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	BN	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	BO	135/161 (84%)	132 (98%)	3 (2%)	64	92
1	BP	134/161 (83%)	131 (98%)	3 (2%)	64	92
1	BQ	135/161 (84%)	130 (96%)	5 (4%)	45	83
1	BR	136/161 (84%)	134 (98%)	2 (2%)	76	95
1	BS	135/161 (84%)	134 (99%)	1 (1%)	91	98
1	BT	133/161 (83%)	131 (98%)	2 (2%)	76	95
1	BU	136/161 (84%)	135 (99%)	1 (1%)	91	98
1	BV	132/161 (82%)	130 (98%)	2 (2%)	76	95
1	BW	135/161 (84%)	133 (98%)	2 (2%)	76	95
1	BX	136/161 (84%)	133 (98%)	3 (2%)	64	92
1	Ba	134/161 (83%)	131 (98%)	3 (2%)	64	92
1	Bb	135/161 (84%)	132 (98%)	3 (2%)	64	92
1	Bc	136/161 (84%)	130 (96%)	6 (4%)	39	76
1	Bd	136/161 (84%)	136 (100%)	0	100	100
1	Be	136/161 (84%)	133 (98%)	3 (2%)	64	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bf	138/161 (86%)	132 (96%)	6 (4%)	40	77
1	Bg	133/161 (83%)	131 (98%)	2 (2%)	76	95
1	Bh	135/161 (84%)	132 (98%)	3 (2%)	64	92
1	Bi	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	Bj	131/161 (81%)	128 (98%)	3 (2%)	63	91
1	Bk	135/161 (84%)	132 (98%)	3 (2%)	64	92
1	Bl	135/161 (84%)	131 (97%)	4 (3%)	53	88
1	Bm	134/161 (83%)	130 (97%)	4 (3%)	53	88
1	Bn	138/161 (86%)	135 (98%)	3 (2%)	64	92
1	Bo	133/161 (83%)	132 (99%)	1 (1%)	89	98
1	Bp	136/161 (84%)	133 (98%)	3 (2%)	64	92
1	Bq	136/161 (84%)	135 (99%)	1 (1%)	91	98
1	Br	136/161 (84%)	130 (96%)	6 (4%)	39	76
1	Bs	133/161 (83%)	131 (98%)	2 (2%)	76	95
1	Bt	134/161 (83%)	130 (97%)	4 (3%)	53	88
1	Bu	138/161 (86%)	133 (96%)	5 (4%)	47	84
1	Bv	135/161 (84%)	133 (98%)	2 (2%)	76	95
1	Bw	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	Bx	133/161 (83%)	131 (98%)	2 (2%)	76	95
1	CA	135/161 (84%)	131 (97%)	4 (3%)	53	88
1	CB	135/161 (84%)	130 (96%)	5 (4%)	45	83
1	CC	133/161 (83%)	131 (98%)	2 (2%)	76	95
1	CD	136/161 (84%)	136 (100%)	0	100	100
1	CE	136/161 (84%)	134 (98%)	2 (2%)	76	95
1	CF	134/161 (83%)	130 (97%)	4 (3%)	53	88
1	CG	136/161 (84%)	131 (96%)	5 (4%)	45	83
1	CH	135/161 (84%)	132 (98%)	3 (2%)	64	92
1	CI	135/161 (84%)	130 (96%)	5 (4%)	45	83
1	CJ	138/161 (86%)	133 (96%)	5 (4%)	47	84
1	CK	135/161 (84%)	131 (97%)	4 (3%)	53	88
1	CL	135/161 (84%)	133 (98%)	2 (2%)	76	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CM	135/161 (84%)	130 (96%)	5 (4%)	45	83
1	CN	135/161 (84%)	133 (98%)	2 (2%)	76	95
1	CO	135/161 (84%)	133 (98%)	2 (2%)	76	95
1	CP	134/161 (83%)	131 (98%)	3 (2%)	64	92
1	CQ	136/161 (84%)	129 (95%)	7 (5%)	33	70
1	CR	139/161 (86%)	136 (98%)	3 (2%)	64	92
1	CS	136/161 (84%)	131 (96%)	5 (4%)	45	83
1	CT	134/161 (83%)	130 (97%)	4 (3%)	53	88
1	CU	135/161 (84%)	135 (100%)	0	100	100
1	CV	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	CW	133/161 (83%)	132 (99%)	1 (1%)	89	98
1	CX	136/161 (84%)	134 (98%)	2 (2%)	76	95
1	Ca	133/161 (83%)	130 (98%)	3 (2%)	63	91
1	Cb	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	Cc	133/161 (83%)	131 (98%)	2 (2%)	76	95
1	Cd	131/161 (81%)	129 (98%)	2 (2%)	76	95
1	Ce	132/161 (82%)	129 (98%)	3 (2%)	63	91
1	Cf	131/161 (81%)	131 (100%)	0	100	100
1	Cg	134/161 (83%)	132 (98%)	2 (2%)	76	95
1	Ch	134/161 (83%)	131 (98%)	3 (2%)	64	92
1	Ci	131/161 (81%)	131 (100%)	0	100	100
1	Cj	134/161 (83%)	131 (98%)	3 (2%)	64	92
1	Ck	132/161 (82%)	130 (98%)	2 (2%)	76	95
1	Cl	132/161 (82%)	130 (98%)	2 (2%)	76	95
1	Cm	134/161 (83%)	130 (97%)	4 (3%)	53	88
1	Cn	133/161 (83%)	130 (98%)	3 (2%)	63	91
1	Co	132/161 (82%)	129 (98%)	3 (2%)	63	91
1	Cp	134/161 (83%)	133 (99%)	1 (1%)	91	98
1	Cq	132/161 (82%)	131 (99%)	1 (1%)	89	98
1	Cr	132/161 (82%)	130 (98%)	2 (2%)	76	95
1	Cs	131/161 (81%)	130 (99%)	1 (1%)	89	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ct	134/161 (83%)	131 (98%)	3 (2%)	64	92
1	Cu	134/161 (83%)	131 (98%)	3 (2%)	64	92
1	Cv	135/161 (84%)	132 (98%)	3 (2%)	64	92
1	Cw	132/161 (82%)	132 (100%)	0	100	100
1	Cx	134/161 (83%)	130 (97%)	4 (3%)	53	88
All	All	19400/23184 (84%)	18968 (98%)	432 (2%)	64	92

5 of 432 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Bc	154	ARG
1	BM	26	GLN
1	CR	63	TYR
1	BF	101	MET
1	Bi	29	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 253 such sidechains are listed below:

Mol	Chain	Res	Type
1	BM	8	ASN
1	Bv	72	GLN
1	Cs	72	GLN
1	Bo	50	HIS
1	Bs	26	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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.

## 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%)	-0.36	5 (3%) 45 54	31, 61, 82, 117	0
1	AB	165/192 (85%)	-0.23	8 (4%) 29 35	26, 54, 95, 109	0
1	AC	161/192 (83%)	-0.34	6 (3%) 39 47	38, 58, 77, 111	0
1	AD	159/192 (82%)	-0.24	4 (2%) 54 64	51, 68, 82, 118	0
1	AE	165/192 (85%)	-0.44	10 (6%) 21 23	12, 34, 96, 112	0
1	AF	158/192 (82%)	-0.51	3 (1%) 64 72	19, 47, 66, 104	0
1	AG	159/192 (82%)	-0.48	4 (2%) 54 64	31, 47, 63, 123	0
1	AH	160/192 (83%)	-0.26	3 (1%) 64 72	21, 42, 69, 112	0
1	AI	158/192 (82%)	-0.27	4 (2%) 54 64	54, 70, 84, 114	0
1	AJ	157/192 (81%)	-0.33	1 (0%) 86 91	25, 60, 79, 99	0
1	AK	157/192 (81%)	-0.37	2 (1%) 74 82	33, 59, 75, 101	0
1	AL	157/192 (81%)	-0.18	4 (2%) 54 64	52, 68, 82, 120	0
1	AM	162/192 (84%)	-0.50	2 (1%) 75 83	17, 39, 69, 112	0
1	AN	165/192 (85%)	-0.35	5 (3%) 48 57	31, 48, 89, 107	0
1	AO	165/192 (85%)	-0.25	11 (6%) 17 20	17, 46, 87, 110	0
1	AP	159/192 (82%)	-0.56	0 100 100	7, 30, 51, 102	0
1	AQ	165/192 (85%)	-0.17	10 (6%) 21 23	33, 62, 90, 110	0
1	AR	164/192 (85%)	-0.34	6 (3%) 39 47	20, 46, 89, 111	0
1	AS	160/192 (83%)	-0.22	6 (3%) 38 45	32, 56, 87, 117	0
1	AT	158/192 (82%)	-0.53	1 (0%) 86 91	15, 43, 62, 110	0
1	AU	160/192 (83%)	-0.52	1 (0%) 86 91	24, 42, 68, 107	0
1	AV	160/192 (83%)	-0.19	6 (3%) 38 45	30, 49, 82, 115	0
1	AW	158/192 (82%)	-0.36	3 (1%) 64 72	26, 56, 76, 113	0
1	AX	160/192 (83%)	-0.35	3 (1%) 64 72	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%)	-0.54	3 (1%) 64 72	12, 30, 54, 109	0
1	Ab	161/192 (83%)	-0.62	0 100 100	13, 35, 65, 110	0
1	Ac	160/192 (83%)	-0.58	0 100 100	15, 35, 66, 103	0
1	Ad	165/192 (85%)	-0.60	3 (1%) 65 74	7, 26, 87, 107	0
1	Ae	162/192 (84%)	-0.34	4 (2%) 54 64	8, 29, 65, 113	0
1	Af	161/192 (83%)	-0.45	1 (0%) 86 91	10, 28, 56, 106	0
1	Ag	155/192 (80%)	-0.68	2 (1%) 74 82	8, 28, 45, 70	0
1	Ah	161/192 (83%)	-0.44	0 100 100	12, 32, 55, 109	0
1	Ai	159/192 (82%)	-0.54	2 (1%) 74 82	8, 23, 46, 96	0
1	Aj	165/192 (85%)	-0.24	6 (3%) 41 48	12, 31, 85, 109	0
1	Ak	165/192 (85%)	-0.32	7 (4%) 35 41	18, 37, 86, 107	0
1	Al	165/192 (85%)	-0.39	1 (0%) 86 91	8, 33, 81, 108	0
1	Am	162/192 (84%)	-0.50	2 (1%) 75 83	11, 31, 57, 102	0
1	An	161/192 (83%)	-0.61	2 (1%) 75 83	13, 28, 56, 96	0
1	Ao	161/192 (83%)	-0.53	2 (1%) 75 83	11, 32, 54, 105	0
1	Ap	162/192 (84%)	-0.60	1 (0%) 86 91	11, 30, 63, 101	0
1	Aq	160/192 (83%)	-0.53	0 100 100	9, 30, 58, 110	0
1	Ar	165/192 (85%)	-0.49	4 (2%) 56 65	9, 28, 81, 105	0
1	As	161/192 (83%)	-0.51	3 (1%) 64 72	9, 32, 60, 109	0
1	At	160/192 (83%)	-0.61	2 (1%) 74 82	9, 31, 67, 107	0
1	Au	160/192 (83%)	-0.30	2 (1%) 74 82	19, 40, 66, 104	0
1	Av	165/192 (85%)	-0.31	5 (3%) 48 57	16, 39, 85, 110	0
1	Aw	161/192 (83%)	-0.51	3 (1%) 64 72	8, 31, 58, 109	0
1	Ax	155/192 (80%)	-0.76	1 (0%) 86 91	11, 31, 45, 76	0
1	BA	166/192 (86%)	-0.20	6 (3%) 41 48	30, 51, 87, 108	0
1	BB	157/192 (81%)	0.46	9 (5%) 23 27	68, 86, 98, 109	0
1	BC	155/192 (80%)	0.29	5 (3%) 45 54	64, 84, 94, 103	0
1	BD	160/192 (83%)	-0.31	3 (1%) 64 72	22, 52, 76, 105	0
1	BE	159/192 (82%)	-0.37	3 (1%) 64 72	26, 46, 72, 111	0
1	BF	159/192 (82%)	-0.62	2 (1%) 74 82	13, 32, 53, 102	0
1	BG	156/192 (81%)	-0.27	1 (0%) 86 91	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%)	0.04	2 (1%) 74 82	40, 70, 86, 99	0
1	BI	155/192 (80%)	-0.40	1 (0%) 86 91	19, 52, 73, 97	0
1	BJ	157/192 (81%)	-0.10	2 (1%) 74 82	50, 69, 91, 111	0
1	BK	156/192 (81%)	0.42	10 (6%) 19 22	71, 87, 98, 105	0
1	BL	155/192 (80%)	-0.00	0 100 100	57, 74, 89, 92	0
1	BM	158/192 (82%)	-0.36	1 (0%) 86 91	9, 33, 54, 102	0
1	BN	159/192 (82%)	-0.35	0 100 100	20, 41, 63, 114	0
1	BO	160/192 (83%)	-0.08	6 (3%) 38 45	37, 62, 86, 114	0
1	BP	159/192 (82%)	-0.23	6 (3%) 38 45	29, 55, 83, 114	0
1	BQ	160/192 (83%)	-0.47	5 (3%) 47 56	17, 37, 63, 114	0
1	BR	161/192 (83%)	-0.48	3 (1%) 64 72	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%)	0.17	4 (2%) 54 64	58, 74, 92, 118	0
1	BU	162/192 (84%)	0.12	3 (1%) 64 72	55, 78, 91, 115	0
1	BV	156/192 (81%)	0.27	7 (4%) 32 38	69, 87, 96, 111	0
1	BW	161/192 (83%)	-0.15	4 (2%) 54 64	38, 60, 81, 117	0
1	BX	163/192 (84%)	0.31	9 (5%) 24 29	61, 78, 91, 110	0
1	Ba	158/192 (82%)	-0.04	6 (3%) 38 45	52, 71, 88, 111	0
1	Bb	159/192 (82%)	-0.03	4 (2%) 54 64	49, 72, 90, 118	0
1	Bc	161/192 (83%)	-0.43	2 (1%) 75 83	15, 38, 69, 109	0
1	Bd	161/192 (83%)	-0.48	3 (1%) 64 72	21, 40, 64, 114	0
1	Be	163/192 (84%)	-0.49	1 (0%) 86 91	13, 36, 77, 107	0
1	Bf	165/192 (85%)	-0.29	7 (4%) 35 41	14, 44, 85, 110	0
1	Bg	156/192 (81%)	0.05	3 (1%) 64 72	54, 76, 89, 108	0
1	Bh	159/192 (82%)	-0.43	3 (1%) 64 72	30, 48, 72, 108	0
1	Bi	157/192 (81%)	-0.19	1 (0%) 86 91	32, 58, 70, 94	0
1	Bj	154/192 (80%)	0.13	1 (0%) 86 91	55, 76, 85, 96	0
1	Bk	159/192 (82%)	-0.20	2 (1%) 74 82	37, 57, 80, 114	0
1	Bl	159/192 (82%)	-0.56	2 (1%) 74 82	12, 38, 61, 109	0
1	Bm	159/192 (82%)	-0.53	3 (1%) 64 72	18, 36, 59, 113	0
1	Bn	165/192 (85%)	-0.07	6 (3%) 41 48	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%)	-0.24	3 (1%)	64 72	44, 65, 84, 96	0
1	Bp	162/192 (84%)	-0.39	8 (4%)	28 34	17, 41, 79, 116	0
1	Bq	160/192 (83%)	-0.07	3 (1%)	64 72	26, 55, 76, 111	0
1	Br	161/192 (83%)	-0.61	2 (1%)	75 83	8, 28, 57, 105	0
1	Bs	155/192 (80%)	-0.27	2 (1%)	74 82	37, 57, 80, 97	0
1	Bt	158/192 (82%)	0.11	4 (2%)	54 64	61, 79, 93, 110	0
1	Bu	165/192 (85%)	-0.38	8 (4%)	29 35	14, 36, 83, 106	0
1	Bv	160/192 (83%)	-0.42	6 (3%)	38 45	23, 45, 72, 120	0
1	Bw	159/192 (82%)	-0.41	3 (1%)	64 72	11, 29, 55, 112	0
1	Bx	157/192 (81%)	0.21	7 (4%)	32 38	62, 83, 95, 113	0
1	CA	160/192 (83%)	-0.50	3 (1%)	64 72	12, 36, 61, 111	0
1	CB	161/192 (83%)	-0.23	4 (2%)	54 64	19, 52, 79, 108	0
1	CC	157/192 (81%)	-0.22	3 (1%)	64 72	45, 65, 78, 109	0
1	CD	161/192 (83%)	-0.50	2 (1%)	75 83	13, 39, 68, 107	0
1	CE	160/192 (83%)	-0.28	2 (1%)	74 82	29, 52, 80, 112	0
1	CF	160/192 (83%)	-0.54	3 (1%)	64 72	11, 35, 53, 101	0
1	CG	160/192 (83%)	-0.42	3 (1%)	64 72	21, 45, 72, 112	0
1	CH	159/192 (82%)	-0.12	3 (1%)	64 72	33, 62, 79, 119	0
1	CI	160/192 (83%)	-0.24	3 (1%)	64 72	15, 35, 74, 107	0
1	CJ	165/192 (85%)	-0.37	5 (3%)	48 57	24, 44, 85, 105	0
1	CK	160/192 (83%)	-0.29	2 (1%)	74 82	22, 60, 77, 115	0
1	CL	159/192 (82%)	-0.33	3 (1%)	64 72	38, 57, 73, 121	0
1	CM	159/192 (82%)	-0.46	3 (1%)	64 72	16, 42, 63, 112	0
1	CN	161/192 (83%)	-0.51	3 (1%)	64 72	16, 40, 77, 110	0
1	CO	159/192 (82%)	-0.37	2 (1%)	74 82	38, 58, 74, 99	0
1	CP	158/192 (82%)	-0.40	3 (1%)	64 72	25, 57, 76, 110	0
1	CQ	162/192 (84%)	-0.48	4 (2%)	54 64	9, 31, 61, 104	0
1	CR	166/192 (86%)	-0.39	6 (3%)	41 48	24, 42, 82, 107	0
1	CS	161/192 (83%)	-0.34	5 (3%)	47 56	10, 35, 65, 114	0
1	CT	158/192 (82%)	-0.42	4 (2%)	54 64	26, 50, 66, 106	0
1	CU	159/192 (82%)	-0.21	4 (2%)	54 64	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%)	-0.18	4 (2%) 54 64	55, 68, 84, 120	0
1	CW	155/192 (80%)	-0.49	1 (0%) 86 91	27, 47, 69, 87	0
1	CX	161/192 (83%)	-0.46	4 (2%) 54 64	20, 48, 70, 107	0
1	Ca	158/192 (82%)	0.61	16 (10%) 7 9	58, 89, 103, 121	0
1	Cb	159/192 (82%)	-0.05	4 (2%) 54 64	37, 69, 87, 109	0
1	Cc	157/192 (81%)	-0.05	6 (3%) 38 45	40, 69, 86, 118	0
1	Cd	153/192 (79%)	0.57	14 (9%) 9 11	76, 91, 104, 109	0
1	Ce	154/192 (80%)	0.12	6 (3%) 37 44	59, 81, 92, 95	0
1	Cf	153/192 (79%)	0.73	18 (11%) 5 6	83, 97, 107, 110	0
1	Cg	160/192 (83%)	0.02	5 (3%) 47 56	48, 68, 93, 126	0
1	Ch	159/192 (82%)	-0.47	3 (1%) 64 72	23, 49, 66, 114	0
1	Ci	153/192 (79%)	0.66	13 (8%) 11 13	69, 89, 104, 111	0
1	Cj	156/192 (81%)	0.31	11 (7%) 16 18	61, 81, 100, 112	0
1	Ck	154/192 (80%)	-0.05	3 (1%) 64 72	45, 74, 92, 104	0
1	Cl	155/192 (80%)	0.19	5 (3%) 45 54	56, 85, 97, 113	0
1	Cm	159/192 (82%)	0.41	15 (9%) 9 11	71, 88, 100, 113	0
1	Cn	155/192 (80%)	0.19	4 (2%) 53 63	65, 86, 101, 104	0
1	Co	155/192 (80%)	-0.35	2 (1%) 74 82	26, 52, 71, 100	0
1	Cp	158/192 (82%)	-0.05	8 (5%) 27 32	46, 67, 89, 109	0
1	Cq	155/192 (80%)	0.65	17 (10%) 6 7	83, 96, 106, 112	0
1	Cr	154/192 (80%)	0.26	8 (5%) 26 32	78, 91, 103, 111	0
1	Cs	154/192 (80%)	0.55	15 (9%) 8 10	83, 98, 106, 107	0
1	Ct	160/192 (83%)	-0.44	4 (2%) 54 64	34, 51, 79, 115	0
1	Cu	159/192 (82%)	-0.26	6 (3%) 38 45	44, 62, 81, 119	0
1	Cv	161/192 (83%)	-0.11	3 (1%) 64 72	39, 59, 81, 119	0
1	Cw	155/192 (80%)	0.24	5 (3%) 45 54	71, 89, 98, 107	0
1	Cx	156/192 (81%)	-0.22	2 (1%) 74 82	39, 59, 78, 99	0
All	All	22946/27648 (82%)	-0.24	618 (2%) 52 61	7, 52, 95, 126	0

The worst 5 of 618 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ci	155	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
1	Ar	162	LEU	6.5
1	Av	162	LEU	6.3
1	Cv	159	GLU	6.3
1	AC	158	PRO	6.0

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	Bd	201	1/1	0.28	16.51	61,61,61,61	0
2	CA	Bu	201	1/1	0.30	12.53	61,61,61,61	0
2	CA	CF	201	1/1	0.33	12.11	63,63,63,63	0
2	CA	BN	201	1/1	0.36	10.74	73,73,73,73	0
2	CA	Ac	201	1/1	0.30	9.49	70,70,70,70	0
2	CA	BH	201	1/1	0.32	9.38	96,96,96,96	0
2	CA	An	201	1/1	0.31	9.07	61,61,61,61	0
2	CA	CA	201	1/1	0.33	8.66	67,67,67,67	0
2	CA	Cb	201	1/1	0.26	8.65	80,80,80,80	0
2	CA	Ce	201	1/1	0.33	8.20	106,106,106,106	0
2	CA	Cl	201	1/1	0.48	8.08	85,85,85,85	1
2	CA	Be	201	1/1	0.33	7.63	66,66,66,66	0
2	CA	Bf	201	1/1	0.26	7.37	68,68,68,68	0
2	CA	Ae	201	1/1	0.26	7.10	70,70,70,70	0
2	CA	BA	201	1/1	0.25	7.01	78,78,78,78	0
2	CA	AC	201	1/1	0.33	6.90	86,86,86,86	0
2	CA	BG	201	1/1	0.33	6.49	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	Bb	201	1/1	0.29	6.16	98,98,98,98	0
2	CA	BC	201	1/1	0.46	5.96	73,73,73,73	1
2	CA	Ca	201	1/1	0.42	5.85	87,87,87,87	1
2	CA	AM	201	1/1	0.28	5.61	68,68,68,68	0
2	CA	AH	201	1/1	0.29	5.61	62,62,62,62	0
2	CA	CE	201	1/1	0.32	5.56	83,83,83,83	0
2	CA	Cp	201	1/1	0.27	5.41	69,69,69,69	0
2	CA	Ah	201	1/1	0.29	5.32	56,56,56,56	0
2	CA	BR	201	1/1	0.31	5.28	72,72,72,72	0
2	CA	Bg	201	1/1	0.27	4.87	88,88,88,88	0
2	CA	Aj	201	1/1	0.29	4.77	56,56,56,56	0
2	CA	Bc	201	1/1	0.31	4.67	73,73,73,73	0
2	CA	AO	201	1/1	0.23	4.58	67,67,67,67	0
2	CA	Ad	201	1/1	0.23	4.42	54,54,54,54	0
2	CA	Aa	201	1/1	0.25	4.36	58,58,58,58	0
2	CA	AF	201	1/1	0.25	4.27	68,68,68,68	0
2	CA	CC	201	1/1	0.28	4.19	96,96,96,96	0
2	CA	Ag	201	1/1	0.27	3.94	55,55,55,55	0
2	CA	CB	201	1/1	0.27	3.48	60,60,60,60	0
2	CA	CO	201	1/1	0.23	3.31	68,68,68,68	0
2	CA	Cg	201	1/1	0.21	3.25	85,85,85,85	0
2	CA	AA	201	1/1	0.24	3.18	106,106,106,106	0
2	CA	AB	201	1/1	0.22	2.74	75,75,75,75	0
2	CA	AL	201	1/1	0.22	2.63	84,84,84,84	0
2	CA	Ba	201	1/1	0.21	2.16	80,80,80,80	0
2	CA	Ck	201	1/1	0.21	2.04	78,78,78,78	0
2	CA	BD	201	1/1	0.22	1.63	81,81,81,81	0
2	CA	CD	201	1/1	0.18	1.61	68,68,68,68	0
2	CA	Cn	201	1/1	0.20	1.39	108,108,108,108	0
2	CA	CH	201	1/1	0.16	0.20	69,69,69,69	0
2	CA	BB	201	1/1	0.14	-1.50	86,86,86,86	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.