



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 07:30 AM UTC

PDB ID : 4V6B / pdb_00004v6b
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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

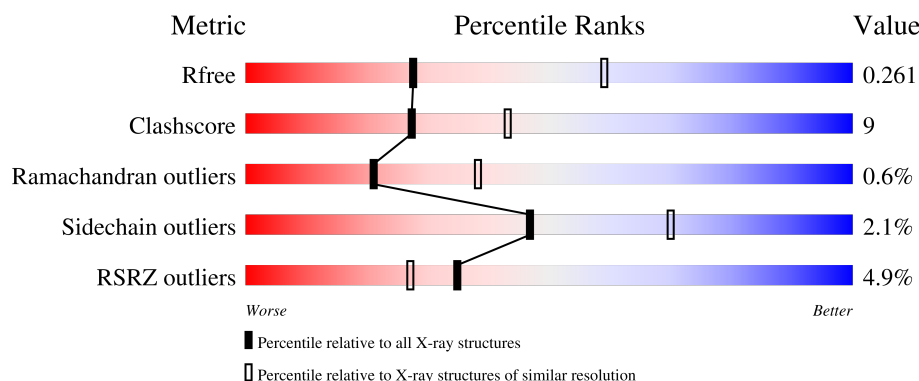
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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

Mol	Chain	Length	Quality of chain
1	AA	192	% 61% 21% 18%
1	AB	192	3% 67% 17% 14%
1	AC	192	2% 68% 15% 16%
1	AD	192	% 65% 17% 17%
1	AE	192	4% 63% 19% 14%

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Mol	Chain	Length	Quality of chain
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	Aa	192	
1	Ab	192	
1	Ac	192	
1	Ad	192	
1	Ae	192	
1	Af	192	

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Mol	Chain	Length	Quality of chain
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	

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Mol	Chain	Length	Quality of chain
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	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	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	

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Mol	Chain	Length	Quality of chain
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	

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Mol	Chain	Length	Quality of chain
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	

2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ferritin.

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

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

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

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

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

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

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

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

There are 144 discrepancies between the modelled and reference sequences:

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

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

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

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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AA	1	Total Ca 1 1	0	0
2	Aa	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
2	Ac	1	Total Ca 1 1	0	0
2	Ad	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Ae	1	Total 1	Ca 1	0	0
2	AF	1	Total 1	Ca 1	0	0
2	Ag	1	Total 1	Ca 1	0	0
2	AH	1	Total 1	Ca 1	0	0
2	Ah	1	Total 1	Ca 1	0	0
2	Aj	1	Total 1	Ca 1	0	0
2	AL	1	Total 1	Ca 1	0	0
2	AM	1	Total 1	Ca 1	0	0
2	An	1	Total 1	Ca 1	0	0
2	AO	1	Total 1	Ca 1	0	0
2	BA	1	Total 1	Ca 1	0	0
2	Ba	1	Total 1	Ca 1	0	0
2	BB	1	Total 1	Ca 1	0	0
2	Bb	1	Total 1	Ca 1	0	0
2	BC	1	Total 1	Ca 1	0	0
2	Bc	1	Total 1	Ca 1	0	0
2	BD	1	Total 1	Ca 1	0	0
2	Bd	1	Total 1	Ca 1	0	0
2	Be	1	Total 1	Ca 1	0	0
2	Bf	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	Bg	1	Total 1	Ca 1	0	0
2	BH	1	Total 1	Ca 1	0	0
2	BN	1	Total 1	Ca 1	0	0
2	BR	1	Total 1	Ca 1	0	0
2	Bu	1	Total 1	Ca 1	0	0
2	CA	1	Total 1	Ca 1	0	0
2	Ca	1	Total 1	Ca 1	0	0
2	CB	1	Total 1	Ca 1	0	0
2	Cb	1	Total 1	Ca 1	0	0
2	CC	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	Ce	1	Total 1	Ca 1	0	0
2	CF	1	Total 1	Ca 1	0	0
2	Cg	1	Total 1	Ca 1	0	0
2	CH	1	Total 1	Ca 1	0	0
2	Ck	1	Total 1	Ca 1	0	0
2	Cl	1	Total 1	Ca 1	0	0
2	Cn	1	Total 1	Ca 1	0	0
2	CO	1	Total 1	Ca 1	0	0
2	Cp	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Bh	19	Total 19	O 19	0	0
3	BI	20	Total 20	O 20	0	0
3	Bi	7	Total 7	O 7	0	0
3	BJ	8	Total 8	O 8	0	0
3	Bj	6	Total 6	O 6	0	0
3	BK	6	Total 6	O 6	0	0
3	Bk	6	Total 6	O 6	0	0
3	BL	10	Total 10	O 10	0	0
3	Bl	23	Total 23	O 23	0	0
3	BM	25	Total 25	O 25	0	0
3	Bm	25	Total 25	O 25	0	0
3	BN	18	Total 18	O 18	0	0
3	Bn	11	Total 11	O 11	0	0
3	BO	13	Total 13	O 13	0	0
3	Bo	9	Total 9	O 9	0	0
3	BP	10	Total 10	O 10	0	0
3	Bp	31	Total 31	O 31	0	0
3	BQ	30	Total 30	O 30	0	0
3	Bq	18	Total 18	O 18	0	0
3	BR	21	Total 21	O 21	0	0
3	Br	35	Total 35	O 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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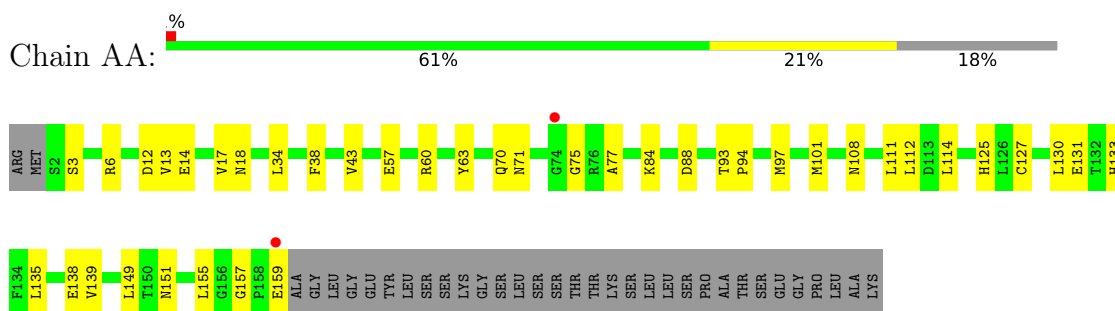
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	CP	14	Total 14	O 14	0	0
3	Cp	10	Total 10	O 10	0	0
3	CQ	41	Total 41	O 41	0	0
3	Cq	2	Total 2	O 2	0	0
3	CR	20	Total 20	O 20	0	0
3	Cr	4	Total 4	O 4	0	0
3	CS	28	Total 28	O 28	0	0
3	CT	15	Total 15	O 15	0	0
3	Ct	17	Total 17	O 17	0	0
3	CU	3	Total 3	O 3	0	0
3	Cu	12	Total 12	O 12	0	0
3	CV	8	Total 8	O 8	0	0
3	Cv	4	Total 4	O 4	0	0
3	CW	15	Total 15	O 15	0	0
3	Cw	10	Total 10	O 10	0	0
3	CX	21	Total 21	O 21	0	0
3	Cx	12	Total 12	O 12	0	0

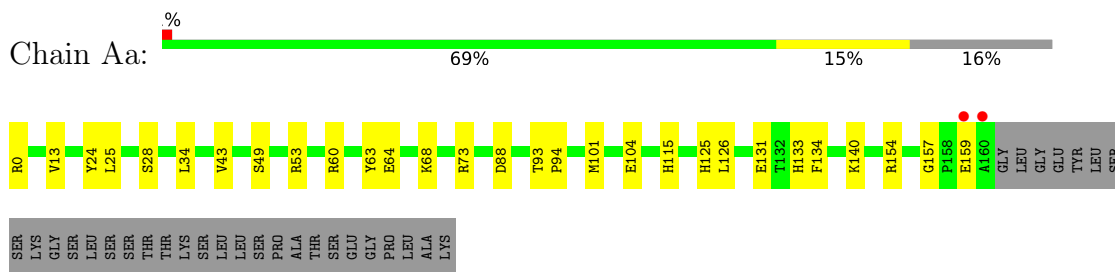
3 Residue-property plots [i](#)

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

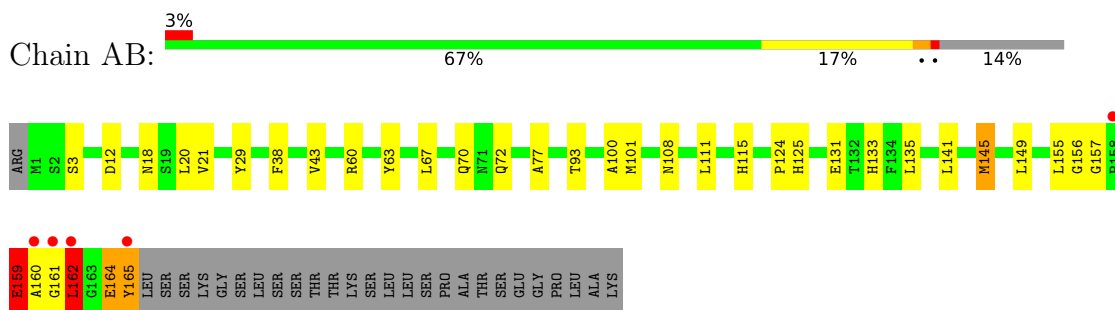
- Molecule 1: Ferritin



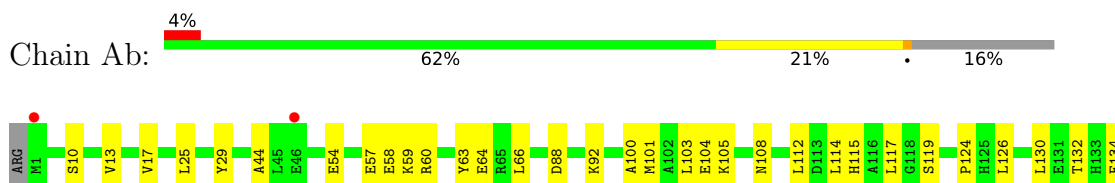
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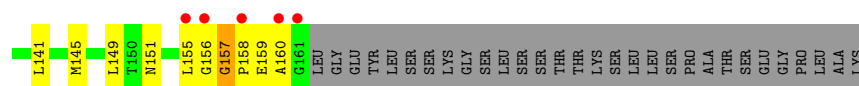


- Molecule 1: Ferritin

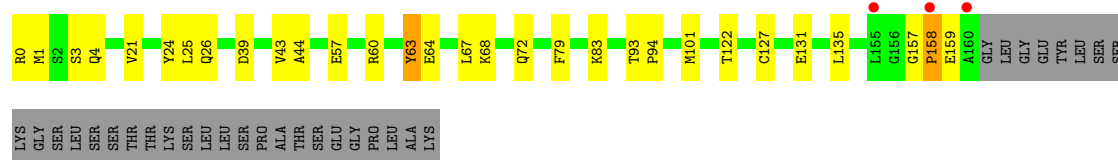


- Molecule 1: Ferritin

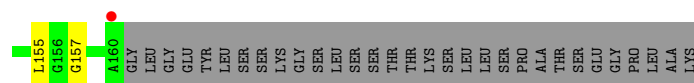




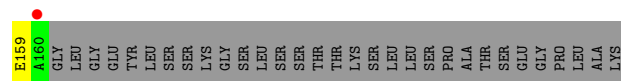
• Molecule 1: Ferritin



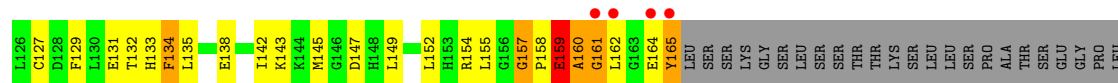
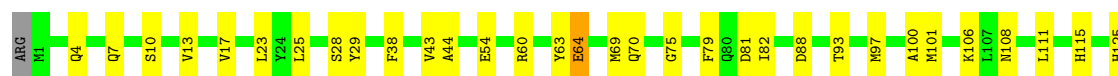
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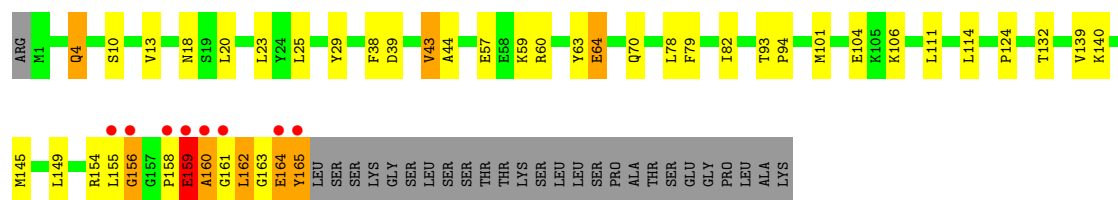
• Molecule 1: Ferritin



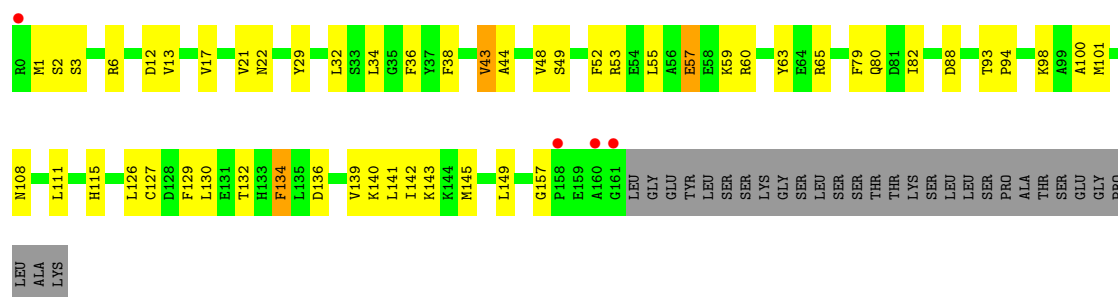
• Molecule 1: Ferritin



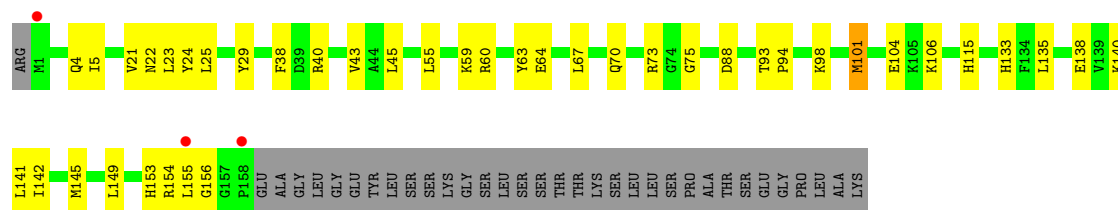
• Molecule 1: Ferritin



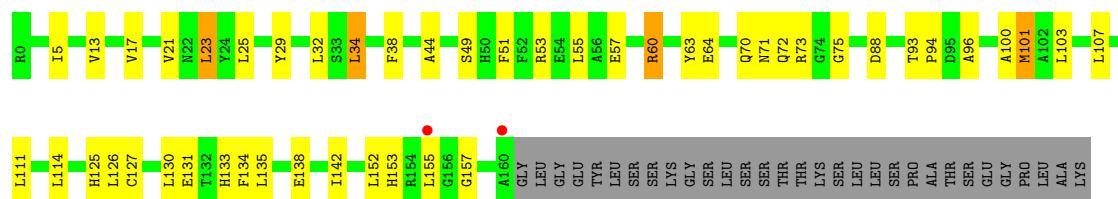
• Molecule 1: Ferritin



• Molecule 1: Ferritin

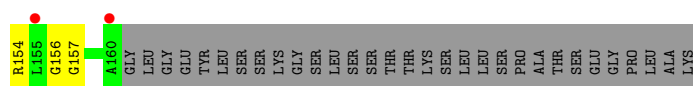


• Molecule 1: Ferritin

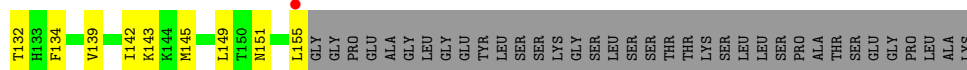


• Molecule 1: Ferritin

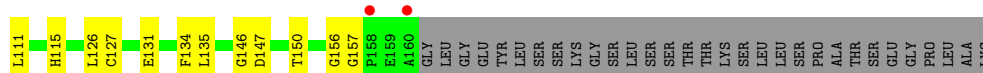




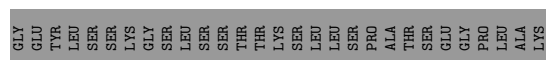
- Molecule 1: Ferritin



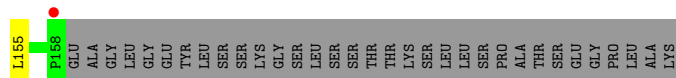
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



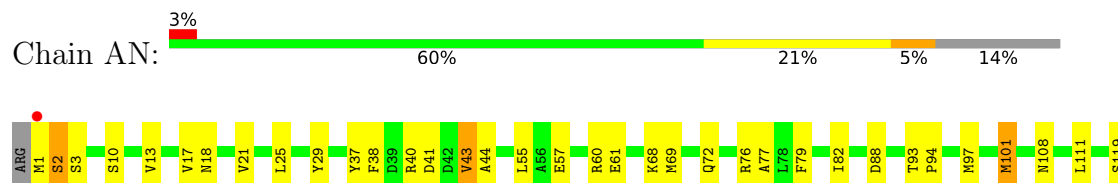


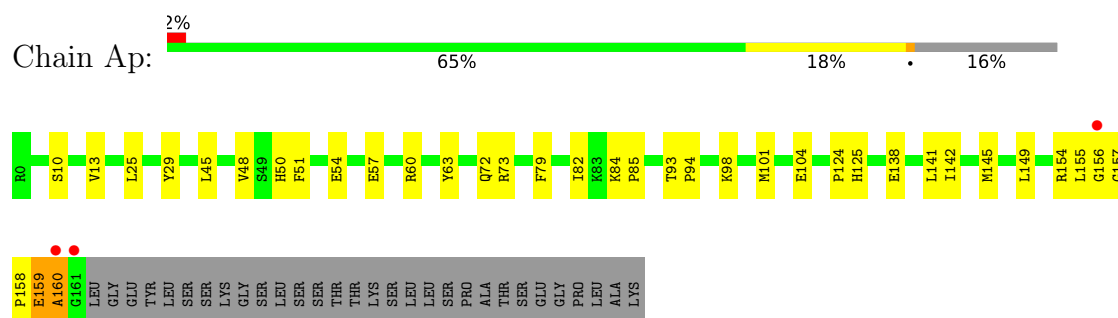
- Molecule 1: Ferritin

- Molecule 1: Ferritin

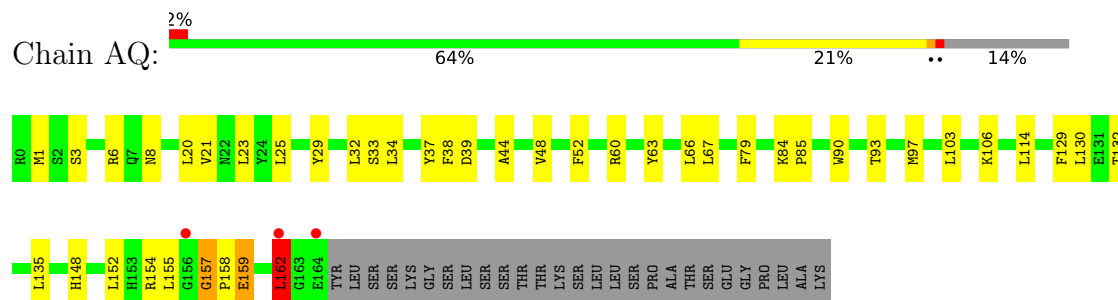
- Molecule 1: Ferritin

- Molecule 1: Ferritin

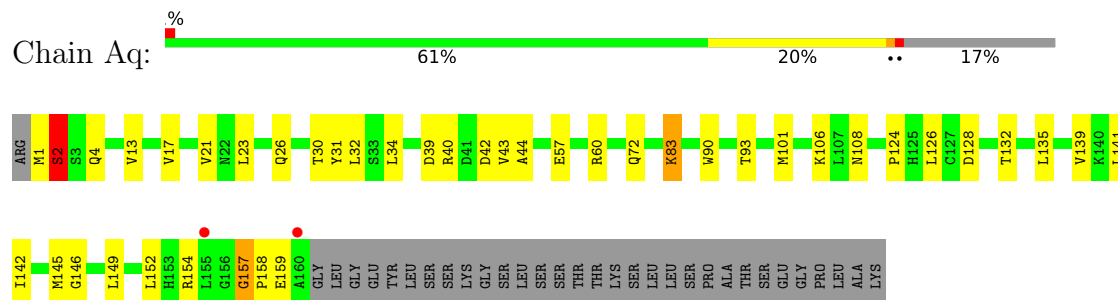




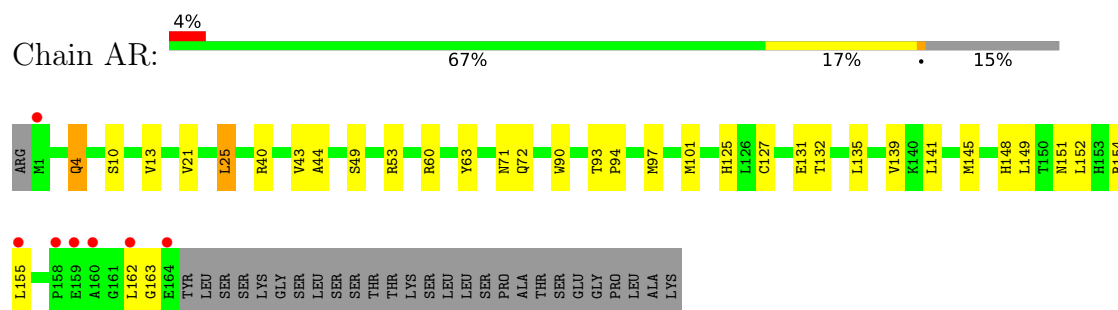
- Molecule 1: Ferritin



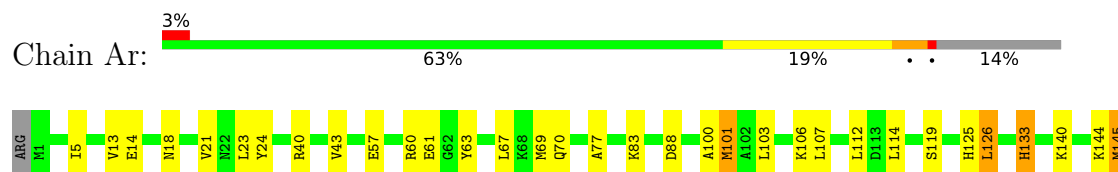
- Molecule 1: Ferritin

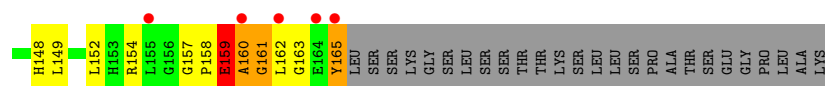


- Molecule 1: Ferritin

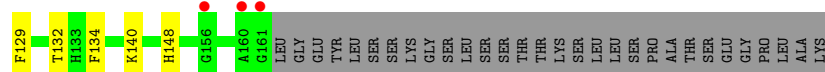


- Molecule 1: Ferritin

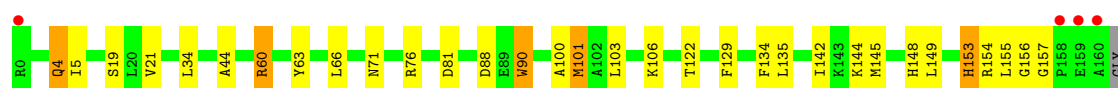




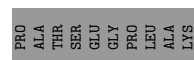
• Molecule 1: Ferritin



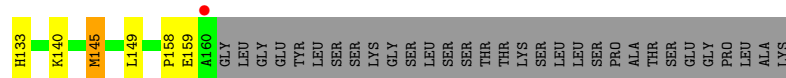
• Molecule 1: Ferritin



• Molecule 1: Ferritin

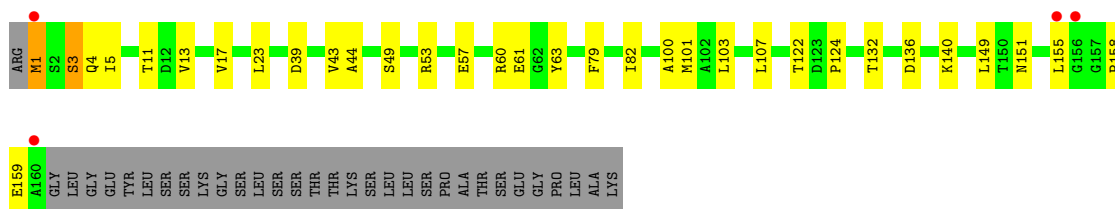


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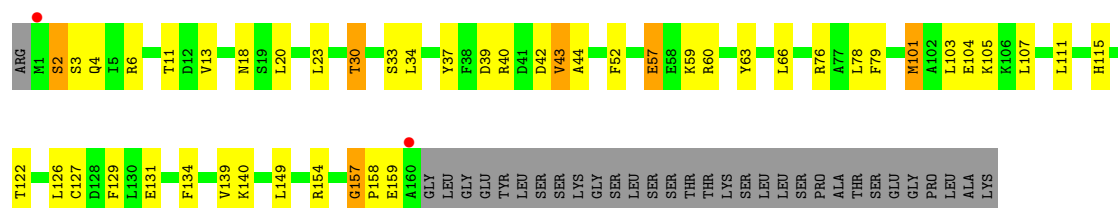


• Molecule 1: Ferritin

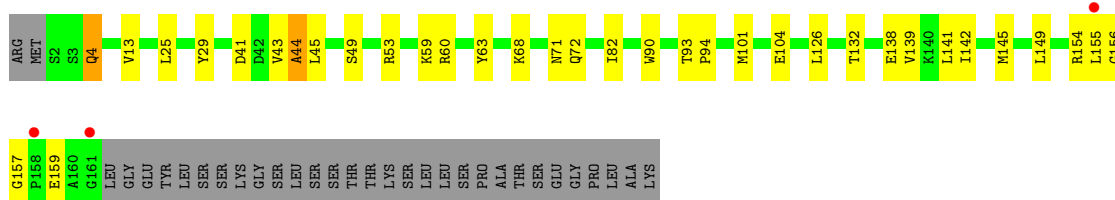




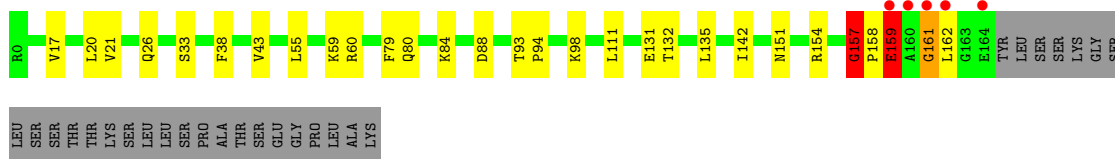
• Molecule 1: Ferritin



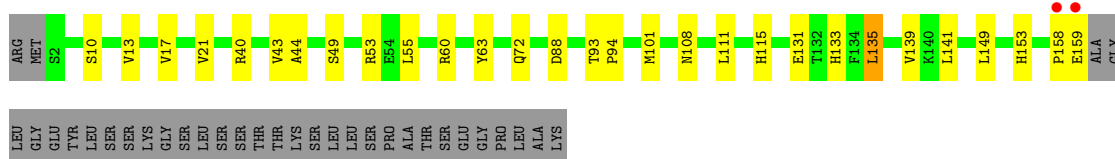
• Molecule 1: Ferritin



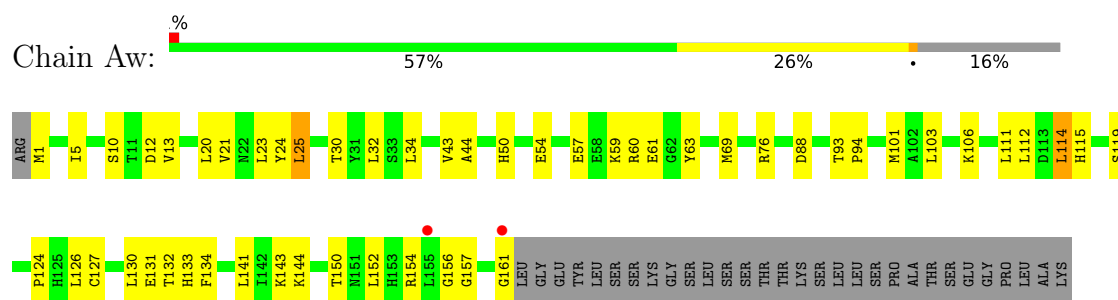
• Molecule 1: Ferritin



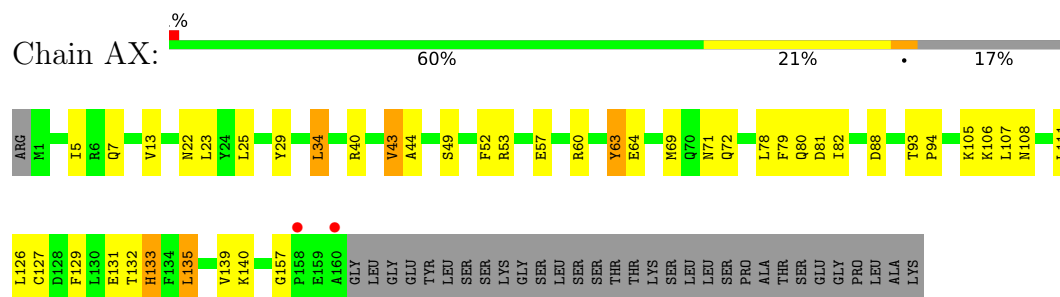
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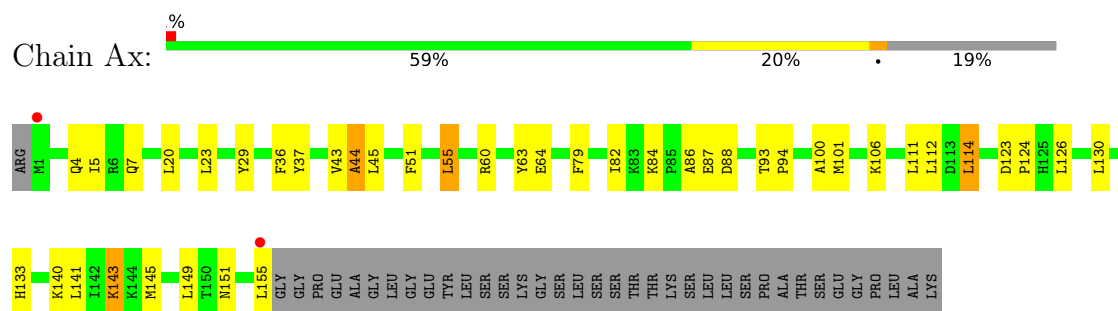
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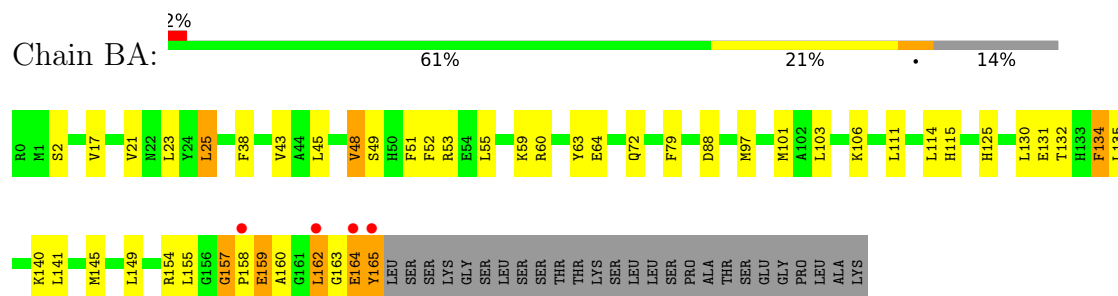
● Molecule 1: Ferritin



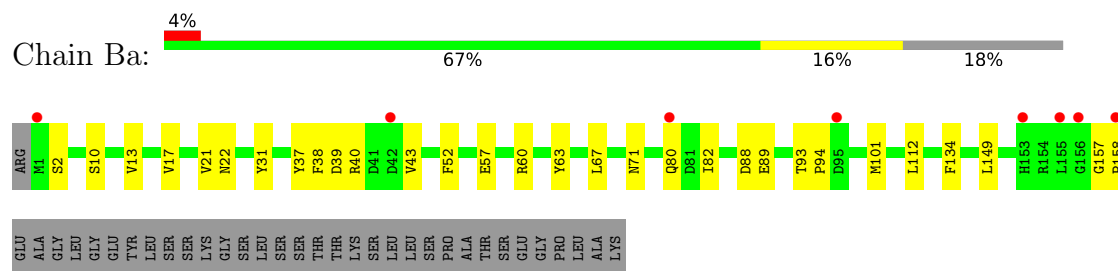
● Molecule 1: Ferritin



● Molecule 1: Ferritin



● Molecule 1: Ferritin



Chain BB:

23% 62% 19% 18%

Residue	Category
R0	Green
M1	Red
Y9	Green
S10	Green
T11	Red
D12	Red
V13	Red
V17	Green
N18	Yellow
N22	Yellow
L23	Green
Y24	Red
L25	Yellow
Q26	Red
A27	Red
L34	Green
G35	Green
F36	Green
Y37	Green
F38	Green
D39	Green
R40	Yellow
V43	Red
A44	Red
L45	Red
E46	Green
G47	Green
V48	Red
S49	Yellow
F52	Yellow
R53	Yellow
E54	Yellow
L55	Yellow
A56	Yellow
E57	Yellow
E58	Yellow
K59	Yellow
R60	Yellow
Y63	Red
M69	Yellow
Q70	Red
N71	Red
Q72	Red
R73	Red
G74	Red
G75	Red
R76	Yellow
A77	Yellow
L78	Yellow
F79	Red
L80	Yellow
A86	Red
E87	Red
D88	Red
F89	Red
Y90	Red
T93	Red
P94	Yellow
K97	Red
K98	Red
A99	Red
A100	Red
M101	Red
A102	Red
L103	Red
A110	Red
L111	Red
L112	Red
H115	Red
A120	Red
D123	Red
P124	Red
H125	Red
L126	Red
F129	Red
L130	Red
L135	Red
V139	Yellow
K140	Yellow
L141	Yellow
I142	Red
H148	Yellow
L149	Yellow
T150	Yellow
N151	Yellow
L152	Red
H153	Red
R154	Red
L155	Red
G156	Red
GLY	Grey
PRO	Grey
GLU	Grey
GLU	Grey
ALA	Grey
GLY	Grey
GLY	Grey
GLU	Grey
TYR	Grey
LEU	Grey

Chain Bb:

Segment Color	Percentage	Amino Acids
Red	3%	ARG
Green	62%	M1, S2, Q3, I5, R6, N8, Y9, V13, L25, D39, S49, R53, E57, F58, K59, R60, Y63, E64, M69, Q72, D88, T93, P94, M97, M101, M108, L111, H115, P124, L126, C127, T132, H133, F134, L135, L136, E137, F138
Yellow	19%	S4, I5, Q4, R7, V13, L25, D39, S49, R53, E57, F58, K59, R60, Y63, E64, M69, Q72, D88, T93, P94, M97, M101, M108, L111, H115, P124, L126, C127, T132, H133, F134, L135, L136, E137, F138
Orange	1%	M101
Grey	17%	ALA, GLY, LEU, TYR, SER, LYS, THR, LEU, SER, THR, LYS, LEU, SER, PRO, ALA, THR, SER, GLU, GLY, PRO, LEU, ALA, LYS

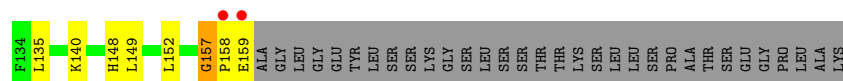
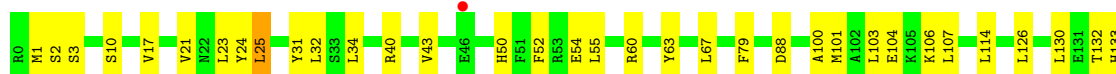
Chain BC:

Amino Acid	Frequency (%)
ARG	19%
MET	19%
S2	64%
S3	64%
Q4	64%
I5	64%
R6	64%
Q7	64%
V13	64%
M18	64%
S19	64%
L20	64%
L23	64%
Y24	64%
L25	64%
Q26	64%
A27	64%
S28	64%
Y29	64%
T30	64%
Y31	64%
L34	64%
G35	64%
F36	64%
Y37	64%
F38	64%
D39	64%
R40	64%
L45	64%
V48	64%
F51	64%
F52	64%
R60	64%
Y63	64%
E64	64%
R65	64%
L66	64%
L67	64%
K68	64%
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Q72	64%
R73	64%
A77	64%
L78	64%
F79	64%
I82	64%
K83	64%

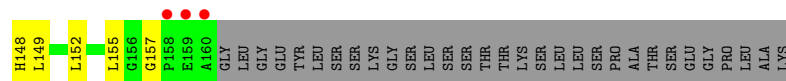
Chain Bc:

Amino Acid	Frequency (%)
R0	2%
M1	2%
Q4	17%
H8	66%
Y9	66%
S10	17%
V13	66%
M18	17%
V21	66%
N22	66%
L23	17%
L34	66%
Y37	17%
R40	17%
V43	66%
A44	66%
L45	17%
K59	66%
R60	66%
Y63	17%
L67	17%
Q70	17%
R73	66%
G74	17%
G75	66%
R76	66%
A77	17%
K92	17%
A96	17%
M101	2%
A102	66%
L103	66%
E104	17%
L107	17%
P124	17%
T132	17%
K143	66%
K144	66%
M145	66%

WORLDWIDE
 PDB
PROTEIN DATA BANK



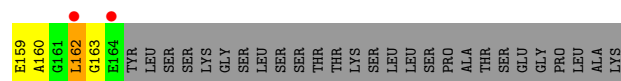
- Molecule 1: Ferritin



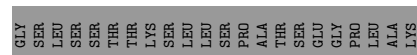
- Molecule 1: Ferritin



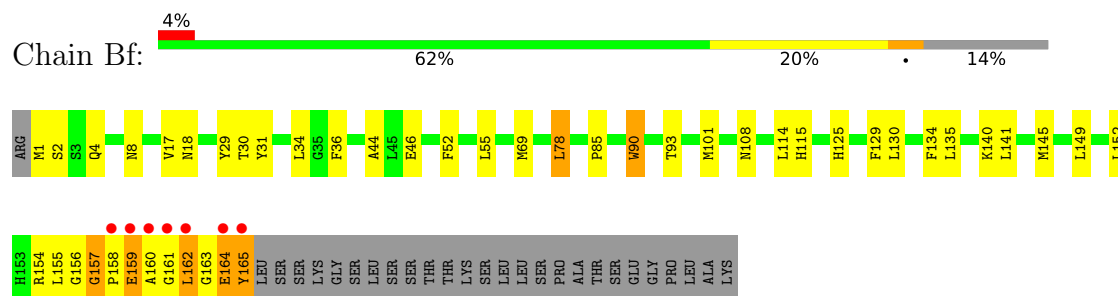
- Molecule 1: Ferritin



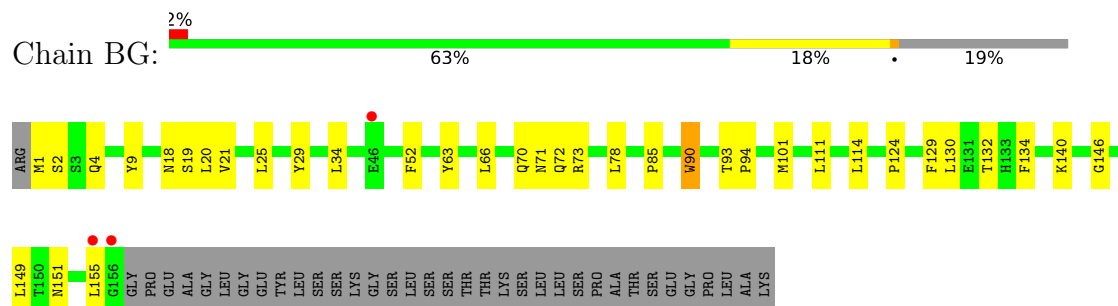
- Molecule 1: Ferritin



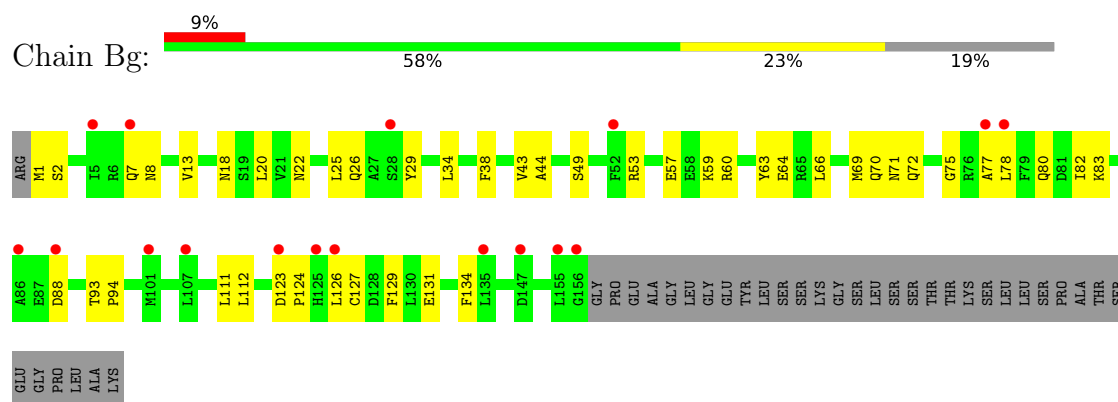
- Molecule 1: Ferritin



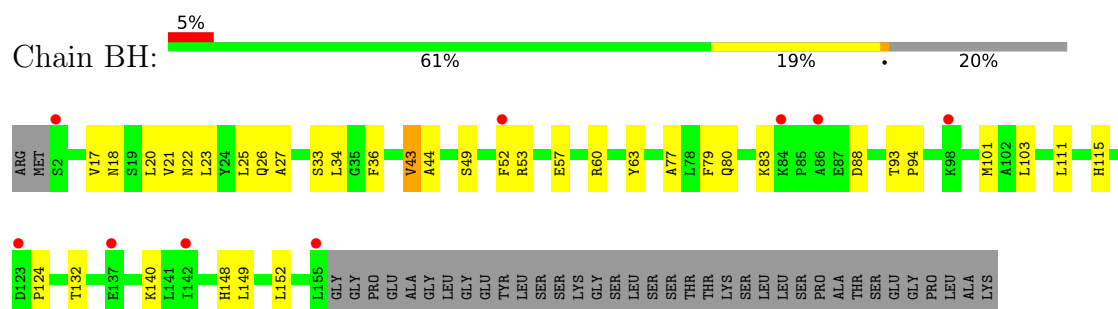
- Molecule 1: Ferritin



- Molecule 1: Ferritin

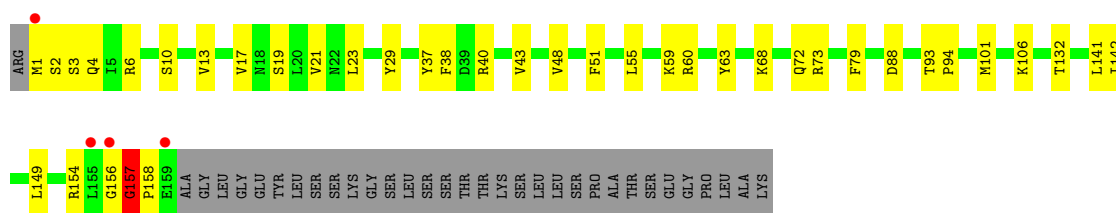


- Molecule 1: Ferritin

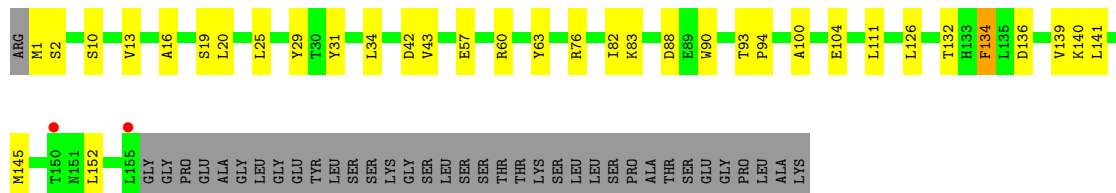


- Molecule 1: Ferritin

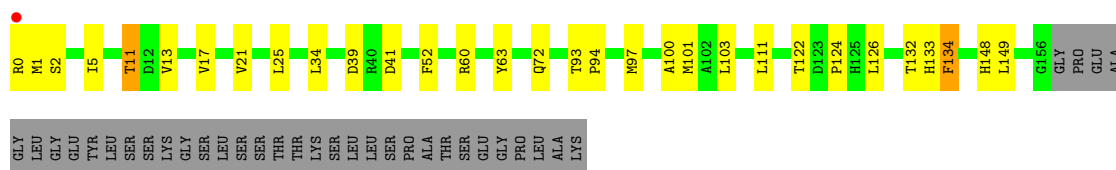




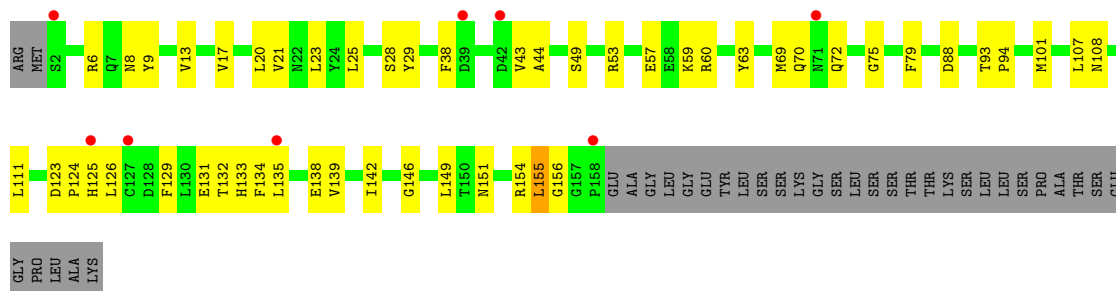
● Molecule 1: Ferritin



● Molecule 1: Ferritin

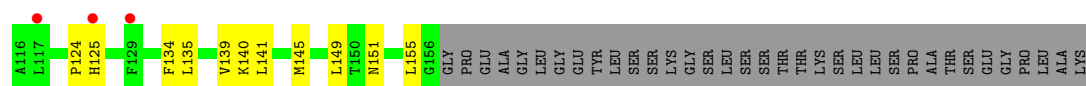


● Molecule 1: Ferritin

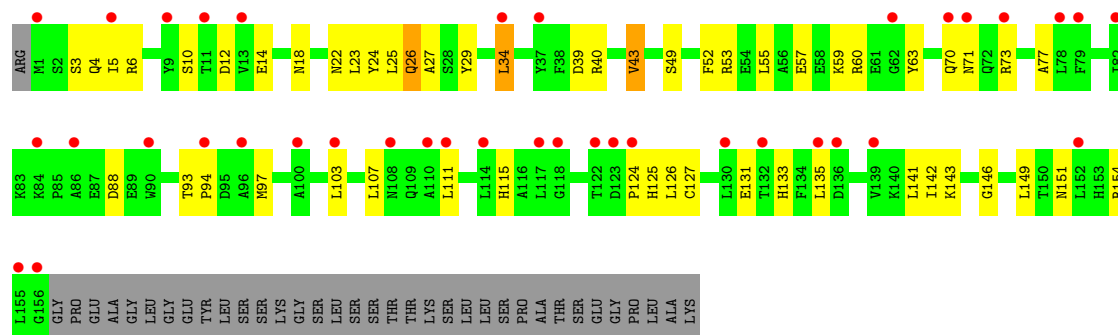


● Molecule 1: Ferritin

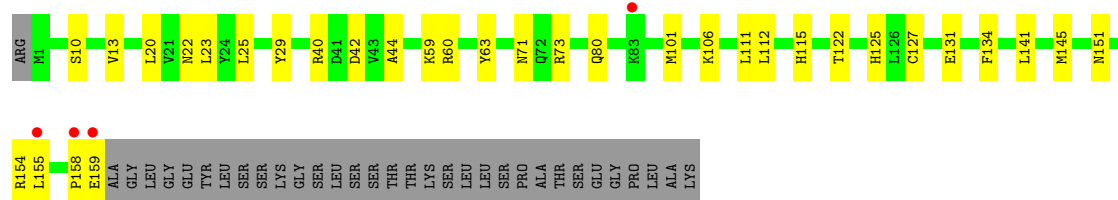




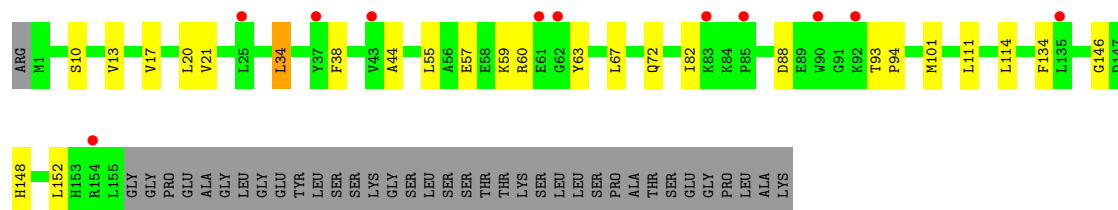
• Molecule 1: Ferritin



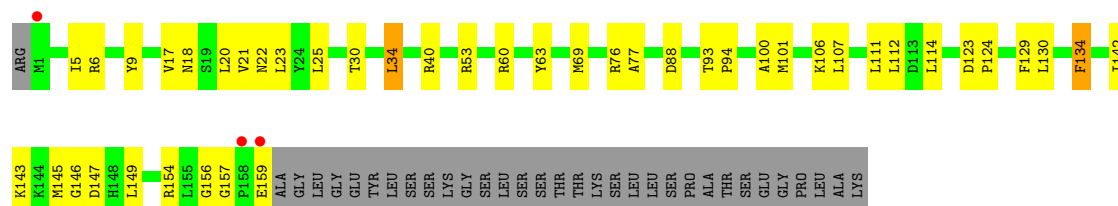
• Molecule 1: Ferritin



• Molecule 1: Ferritin

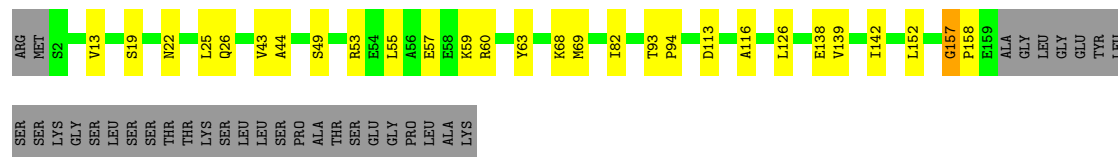


• Molecule 1: Ferritin



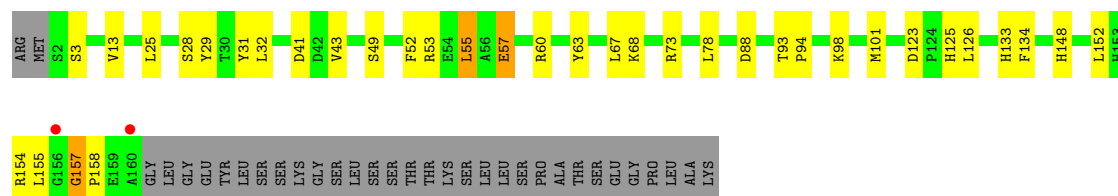
- Molecule 1: Ferritin

Chain BM: 



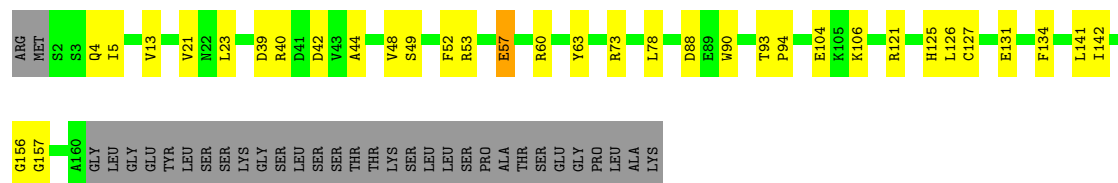
- Molecule 1: Ferritin

Chain Bm: 



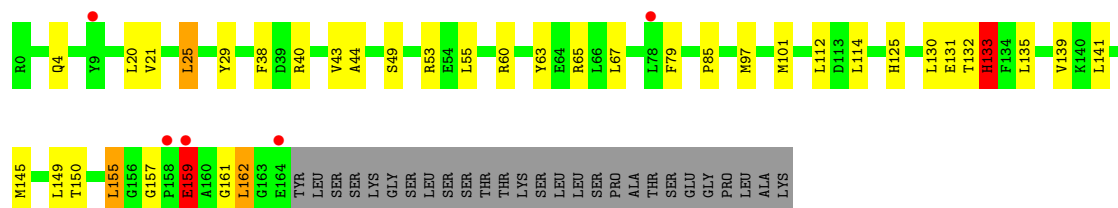
- Molecule 1: Ferritin

Chain BN: 



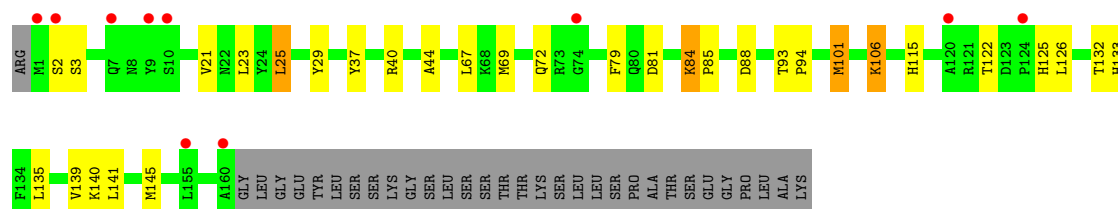
- Molecule 1: Ferritin

Chain Bn: 

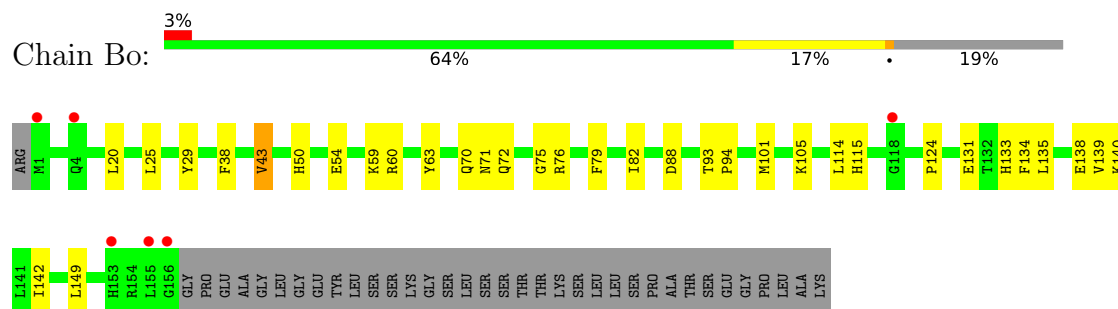


- Molecule 1: Ferritin

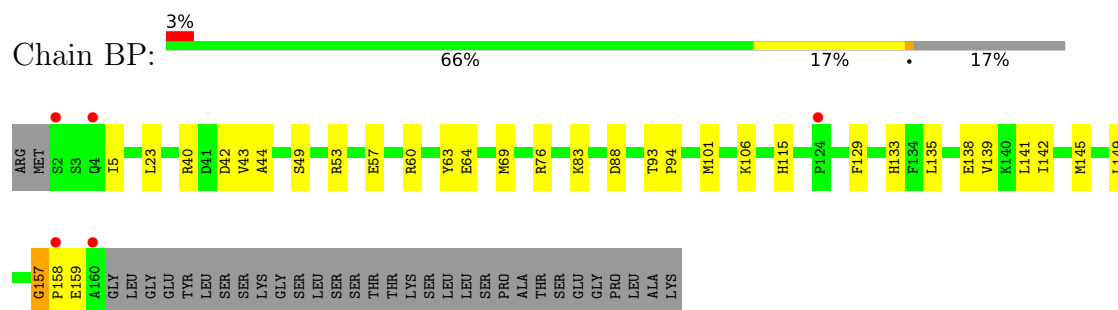
Chain BO: 



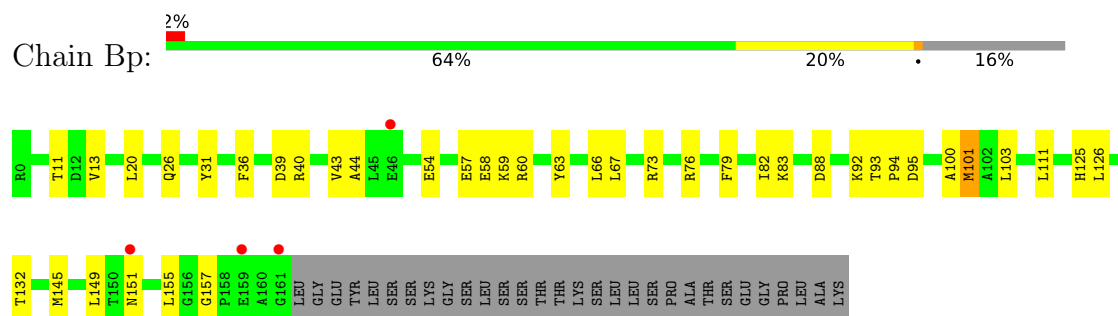
- Molecule 1: Ferritin



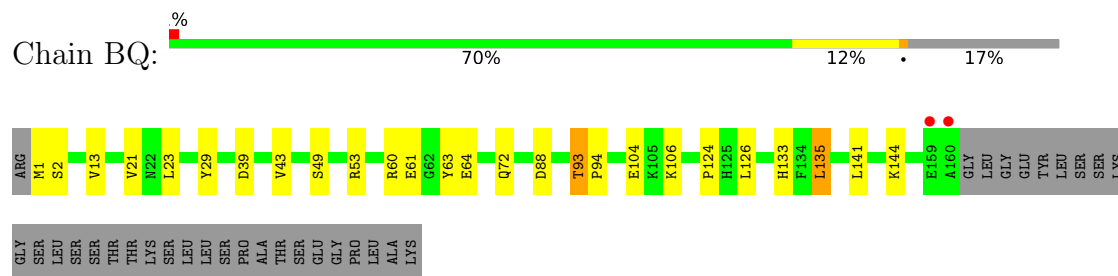
- Molecule 1: Ferritin



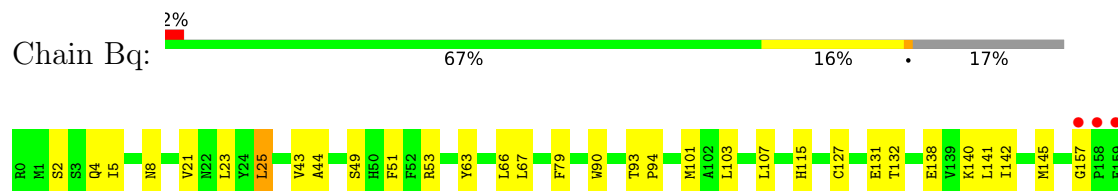
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



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

• Molecule 1: Ferritin

Chain BR:  %

R0 S19 V21 V22 L23 L24 Q26 A27 L34 D39 V43 A44 E57 E58 K59 R60 Y63 N71 Q72 R76 K83 W90 T93 P94 L103 E104 L107 L114 L130 H133 F134 E138 L141 I142 M145 R154 G157

P158 E159 A160 GLY LEU GLY TYR LEU SER SER LYS GLY SER LEU THR THR LYS SER LEU LEU SER PRO ALA THR SER GLY PRO LEU ALA LYS

• Molecule 1: Ferritin

Chain Br:  %

R0 M1 S2 S3 Q4 D12 V13 V17 V21 L25 Y29 T30 Y31 L32 F36 D39 L55 A56 E57 R60 Y63 L67 K68 M69 Q70 G75 F79 P85 D88 E89 W90 T93 M101 E104 L112 L126 T132 H133 F134

L135 E138 L141 M145 L149 L155 G156 G157 P158 E159 A160 GLY LEU GLY TYR LEU LEU SER SER LYS GLY SER SER SER THR THR LYS SER LEU SER PRO ALA THR SER GLY PRO LEU ALA LYS

• Molecule 1: Ferritin

Chain BS:  %

R0 T5 V21 Y24 L25 Y29 F51 L55 R60 Y63 E64 L67 Q70 N71 Q72 R73 G74 G75 F79 P85 D88 E89 W90 M101 L107 L111 R121 L136 E138 L141 I142 K143 M144 M145 P158 GLY ALA GLY LEU

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

• Molecule 1: Ferritin

Chain Bs:  %

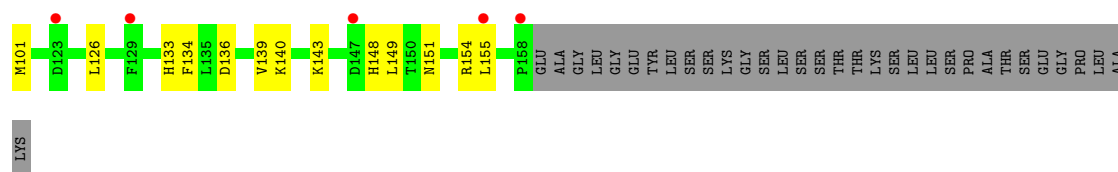
ARG H1 Q7 V13 V17 M18 N22 L23 Q26 S33 V43 S49 R53 R60 Y63 M69 Q72 L78 F79 Q80 K83 A86 T93 P94 K106 L107 T122 D123 P124 H125 L126 T132 H133 F134 L135 V139 H148

L152 L155 GLY PRO GLU ALA GLY LEU GLY GLU TYR LEU SER SER SER LYS GLY SER SER SER THR THR LYS SER LEU LEU SER PRO ALA THR SER GLY PRO LEU ALA LYS

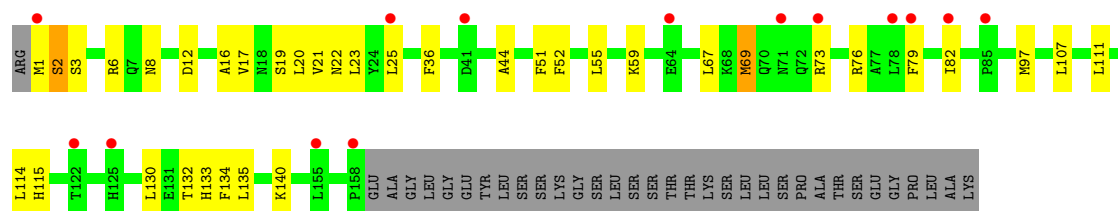
• Molecule 1: Ferritin

Chain BT:  %

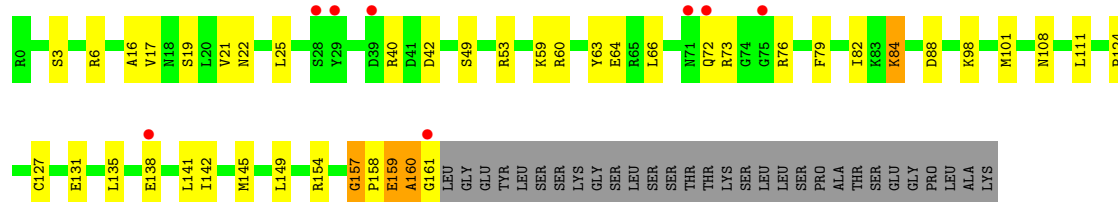
ARG MET S2 S3 R6 S10 V13 V17 V21 N22 L23 Y24 L25 Y29 L32 Y37 F38 D39 V43 A44 S49 R53 E54 L55 A56 K59 R60 Y63 E64 Q72 L78 F79 Q80 D81 I82 D88 E89 W90 T93 P94 M97



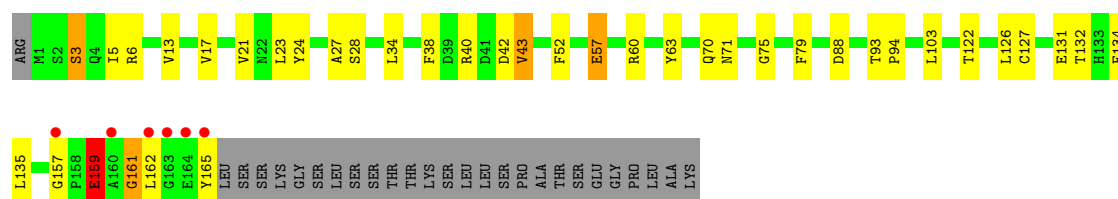
• Molecule 1: Ferritin



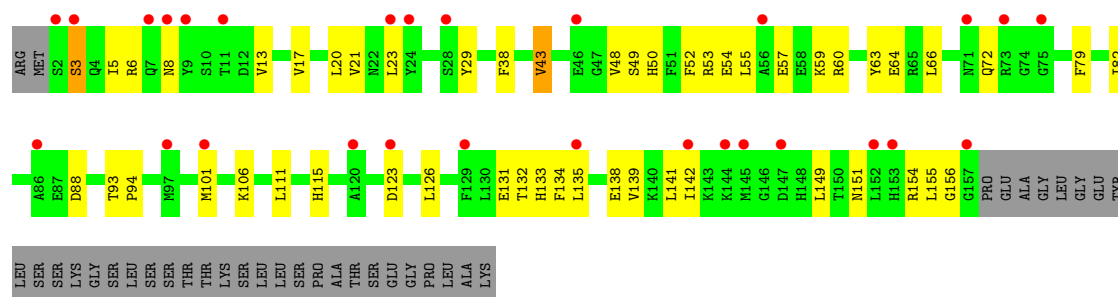
• Molecule 1: Ferritin



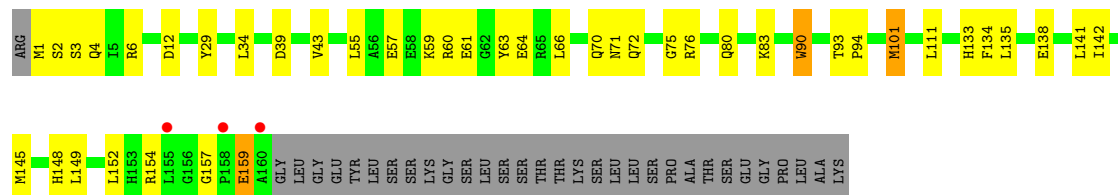
• Molecule 1: Ferritin



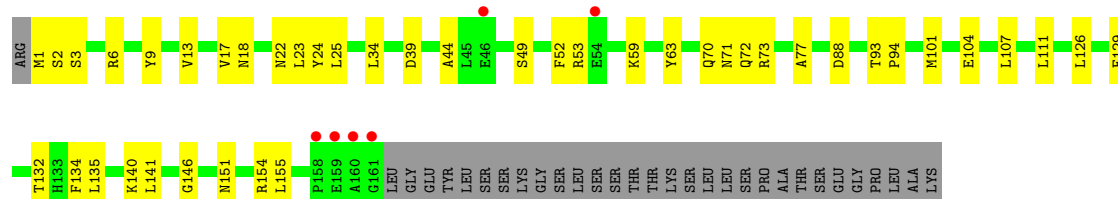
• Molecule 1: Ferritin



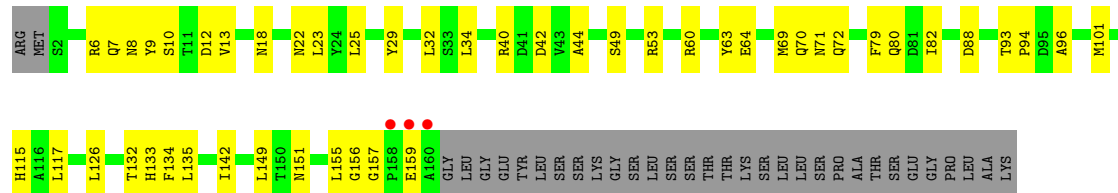
● Molecule 1: Ferritin



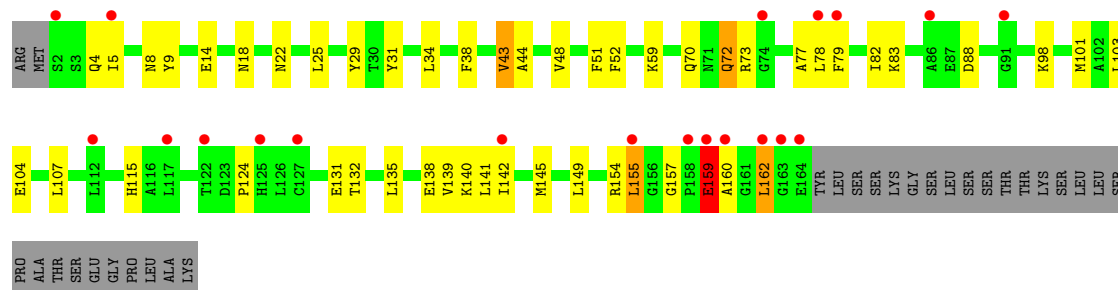
● Molecule 1: Ferritin



● Molecule 1: Ferritin

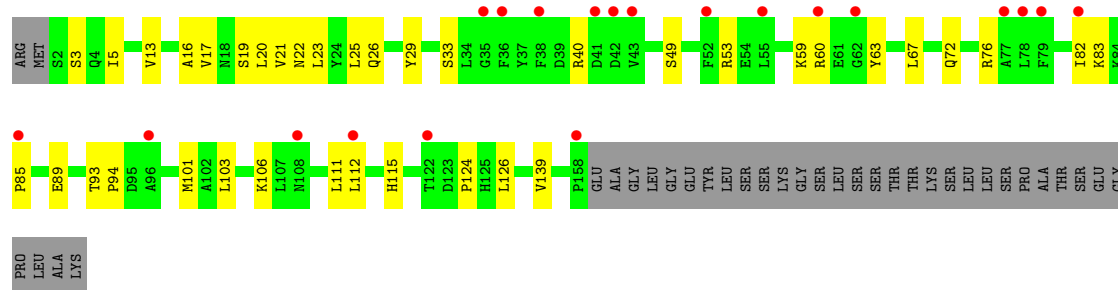


● Molecule 1: Ferritin

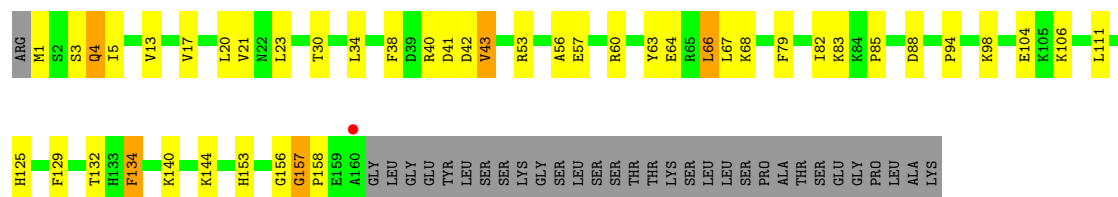


● Molecule 1: Ferritin

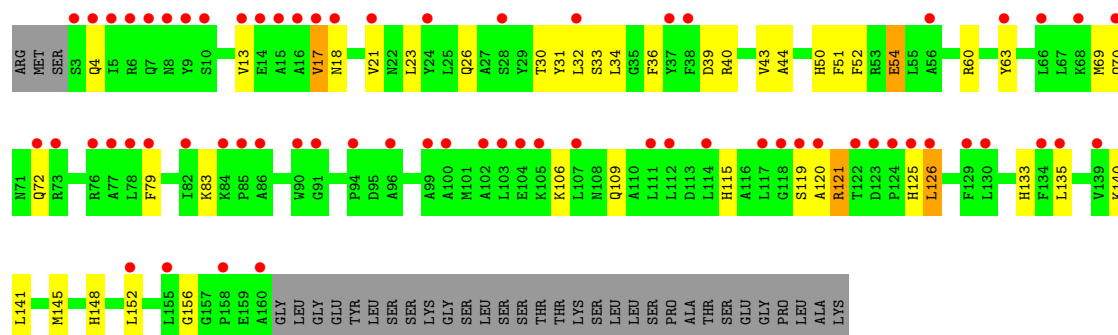




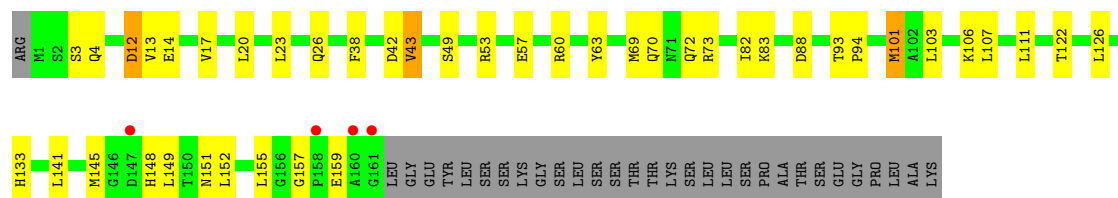
- Molecule 1: Ferritin



- Molecule 1: Ferritin

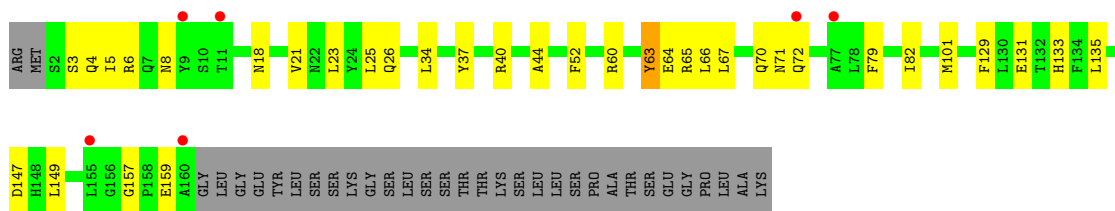


- Molecule 1: Ferritin

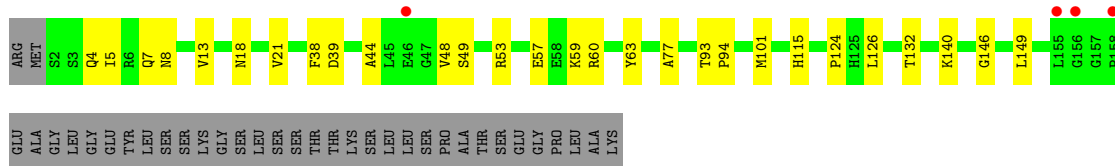


- Molecule 1: Ferritin

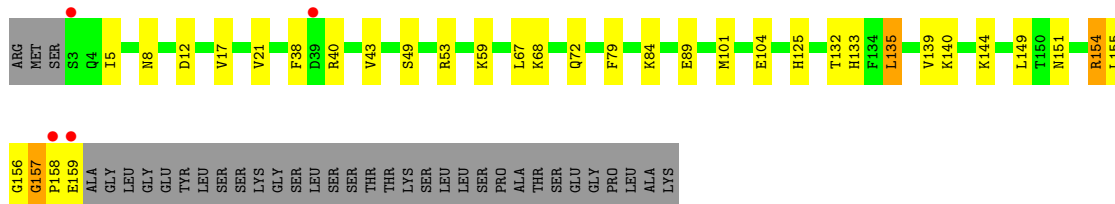




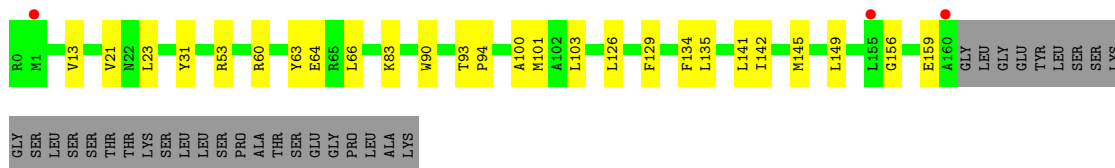
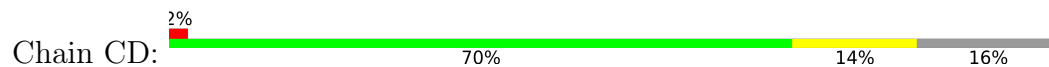
• Molecule 1: Ferritin



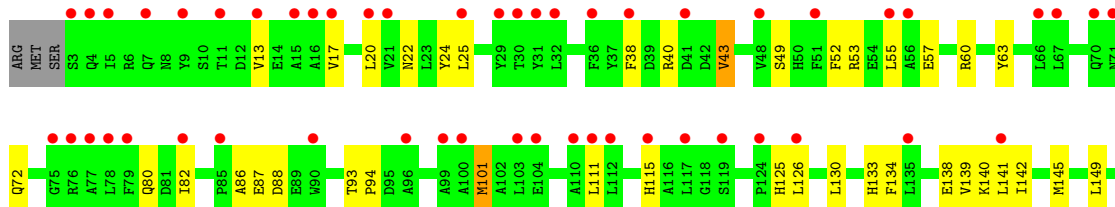
• Molecule 1: Ferritin

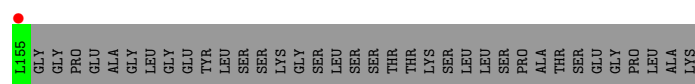


• Molecule 1: Ferritin

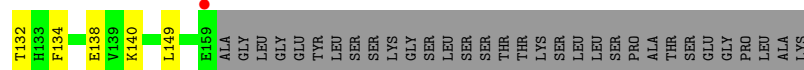


• Molecule 1: Ferritin

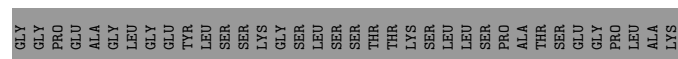
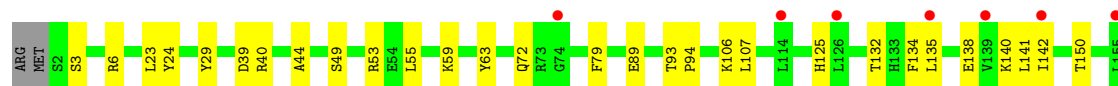




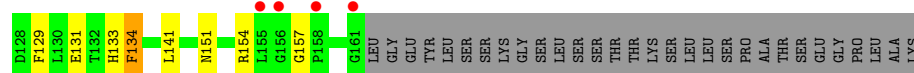
• Molecule 1: Ferritin



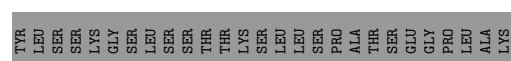
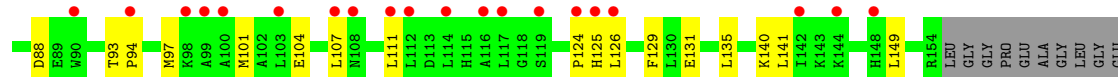
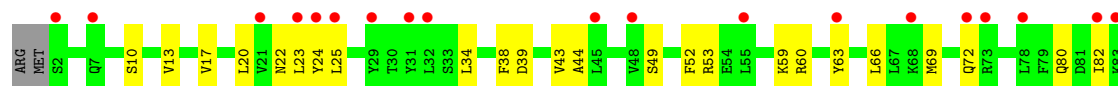
• Molecule 1: Ferritin



• Molecule 1: Ferritin

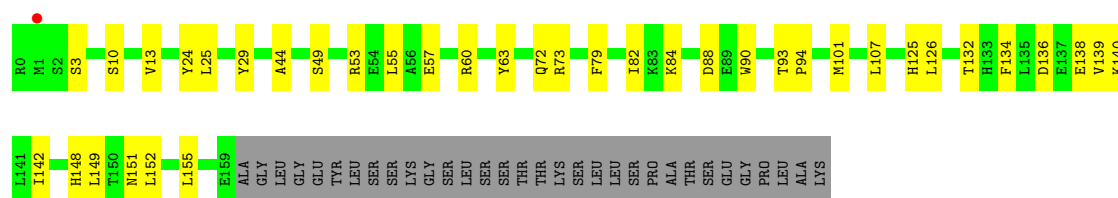


• Molecule 1: Ferritin

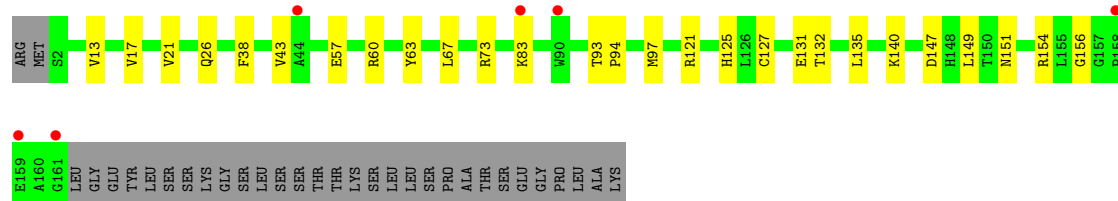


• Molecule 1: Ferritin

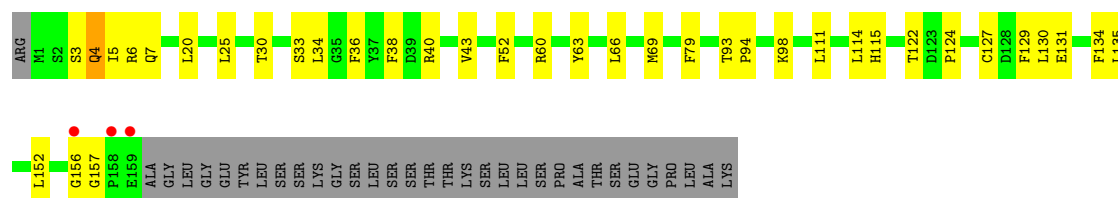




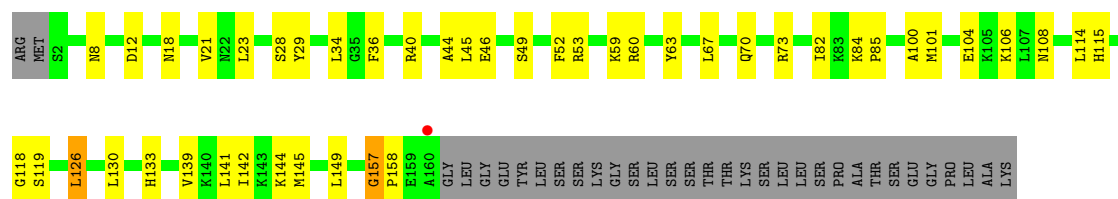
- Molecule 1: Ferritin



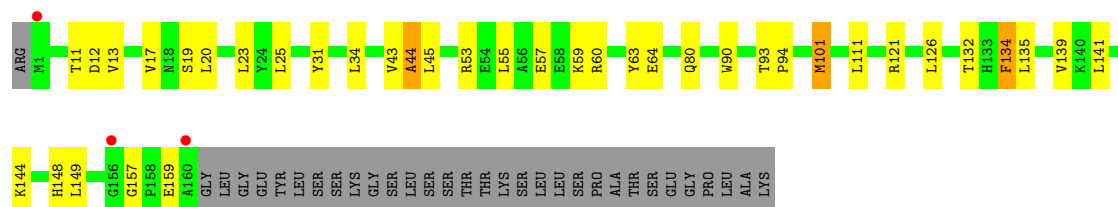
- Molecule 1: Ferritin



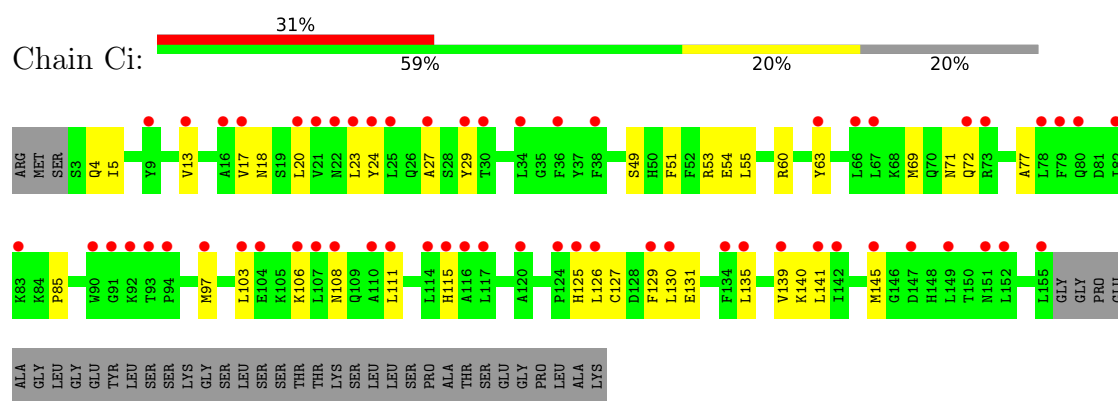
- Molecule 1: Ferritin



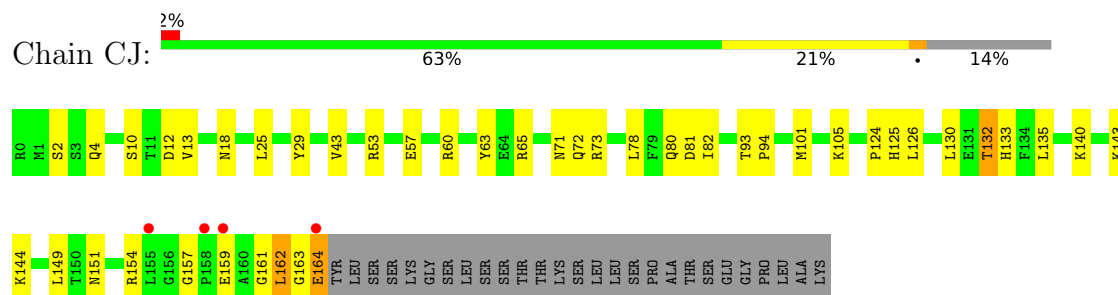
- Molecule 1: Ferritin



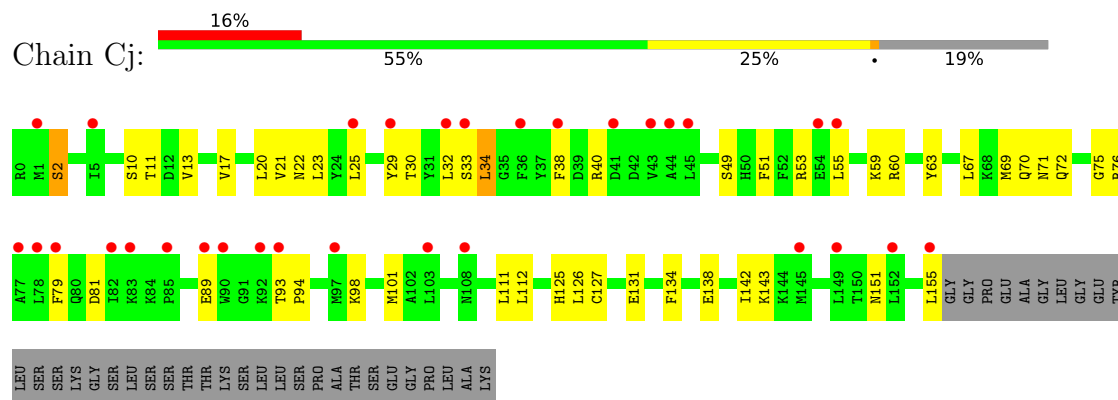
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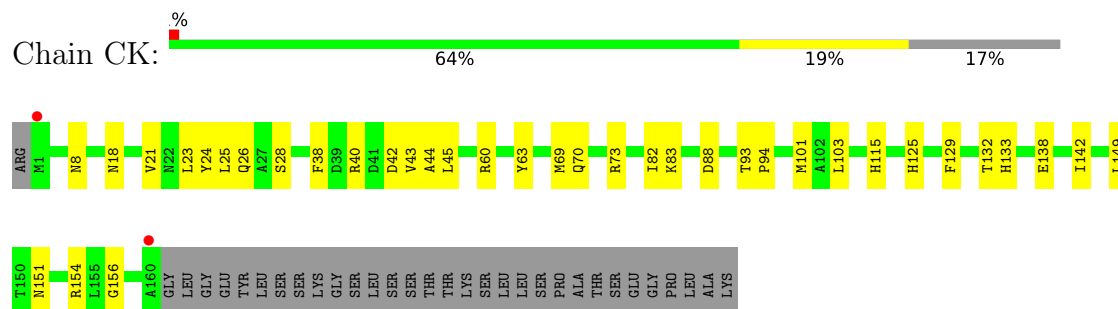
- Molecule 1: Ferritin



- Molecule 1: Ferritin

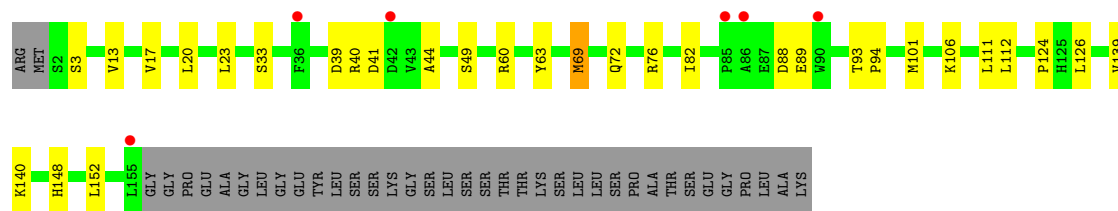


- Molecule 1: Ferritin

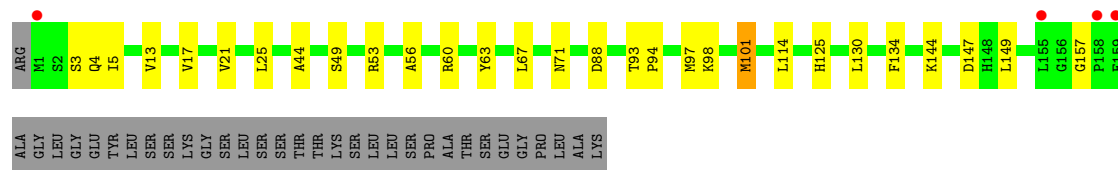


- Molecule 1: Ferritin

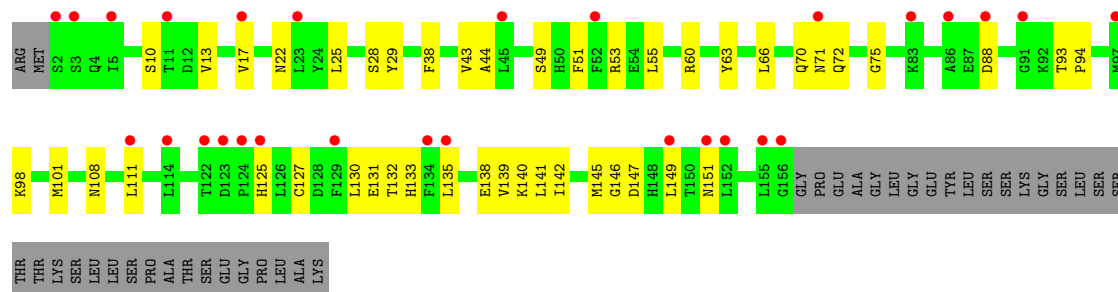




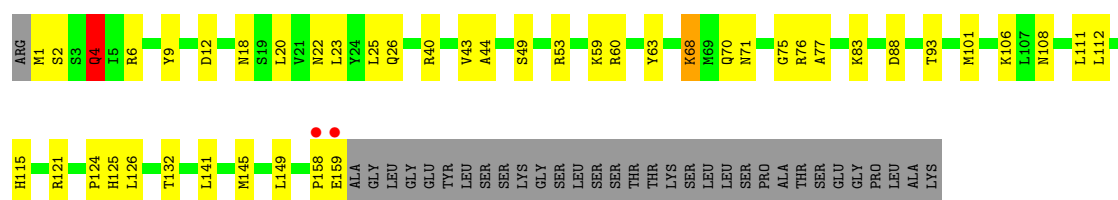
• Molecule 1: Ferritin



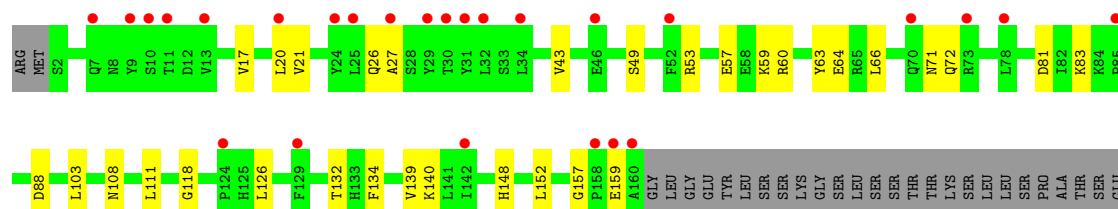
• Molecule 1: Ferritin

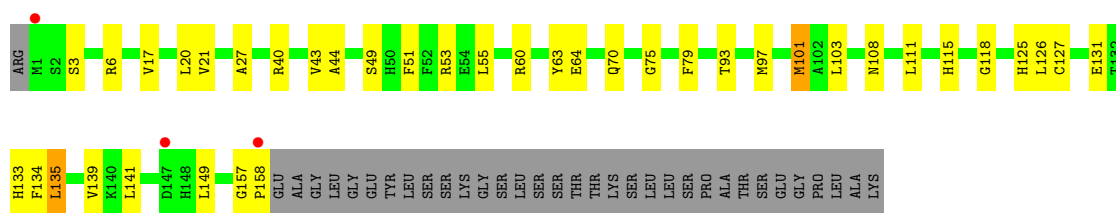


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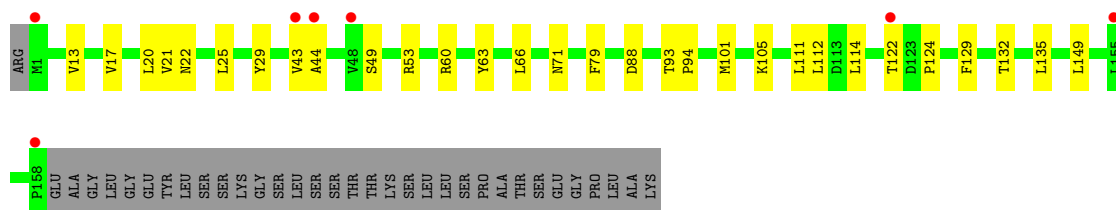


• Molecule 1: Ferritin

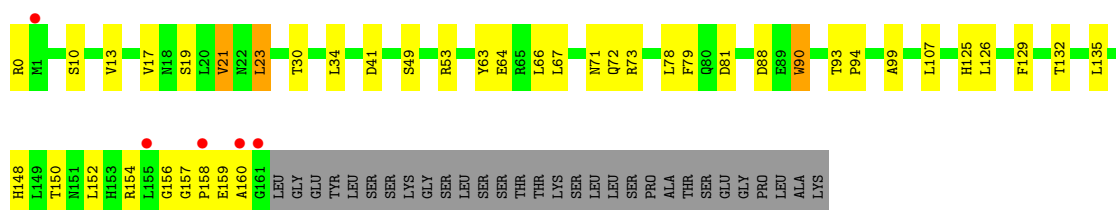




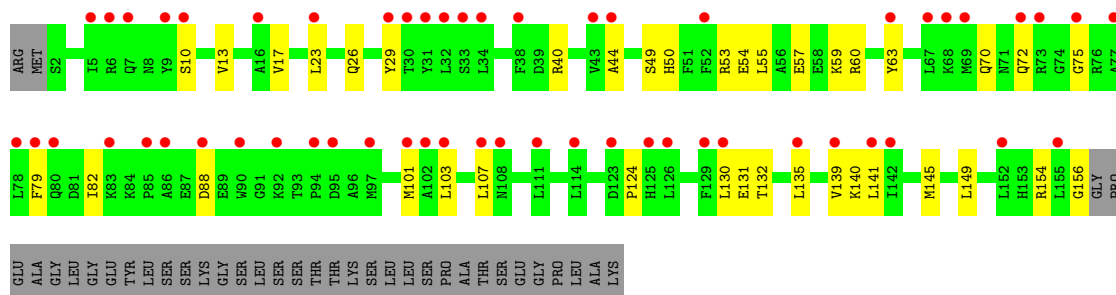
● Molecule 1: Ferritin



● Molecule 1: Ferritin

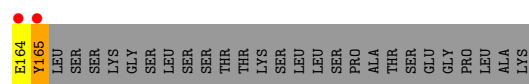


● Molecule 1: Ferritin

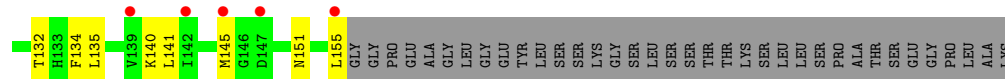
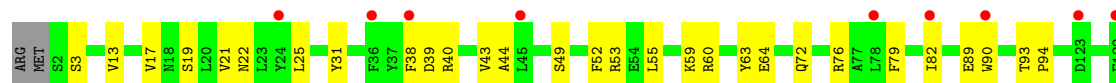


● Molecule 1: Ferritin

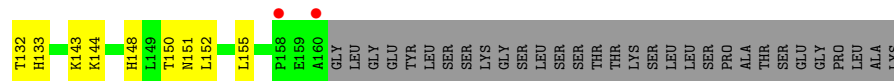




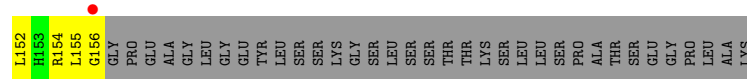
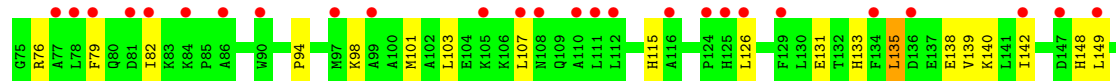
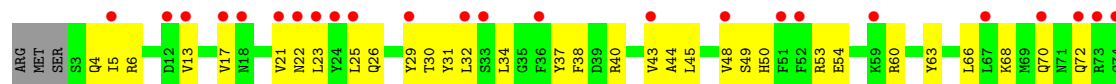
● Molecule 1: Ferritin



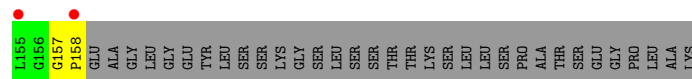
● Molecule 1: Ferritin



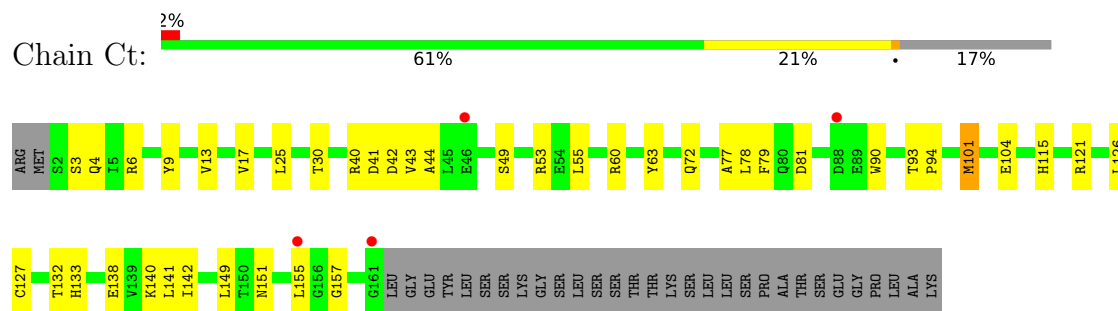
● Molecule 1: Ferritin



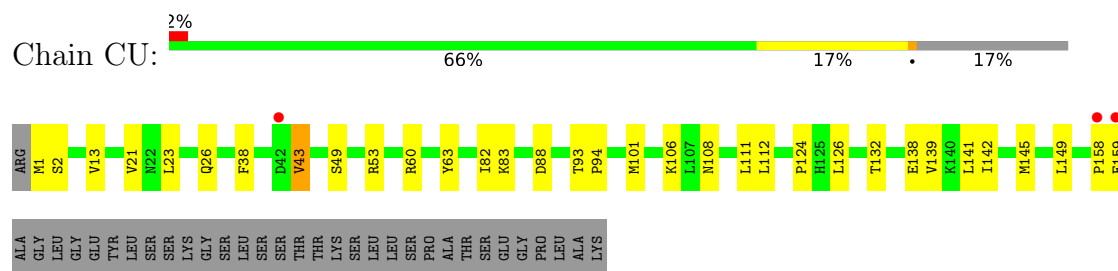
● Molecule 1: Ferritin



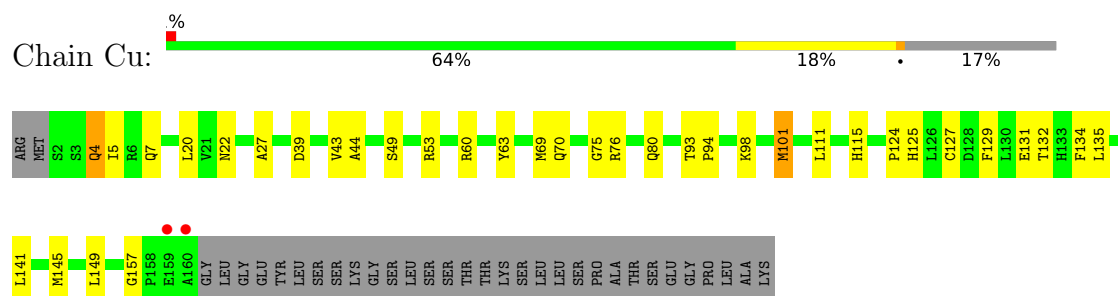
- Molecule 1: Ferritin



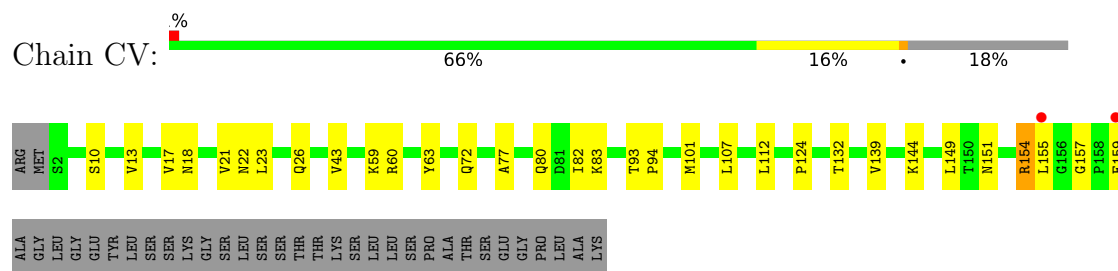
- Molecule 1: Ferritin



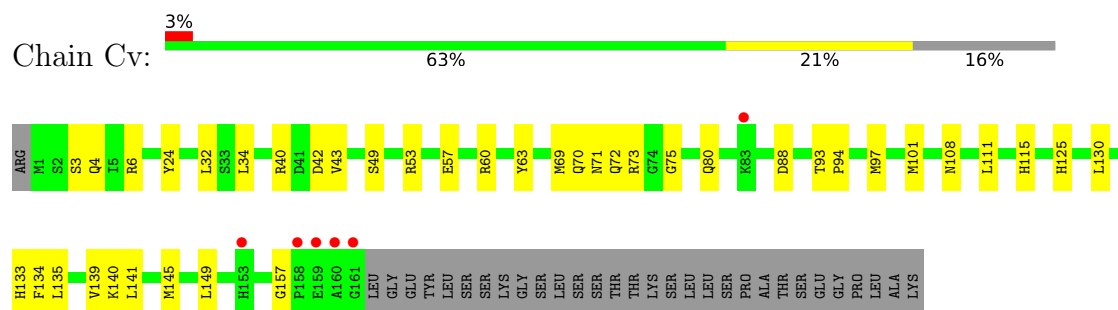
- Molecule 1: Ferritin



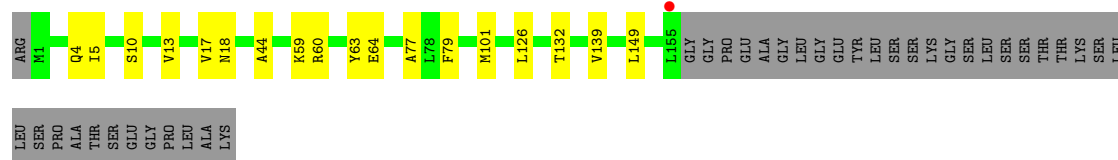
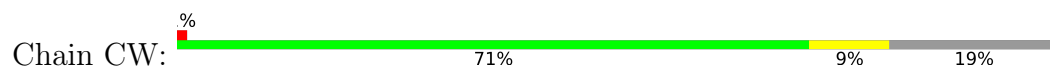
- Molecule 1: Ferritin



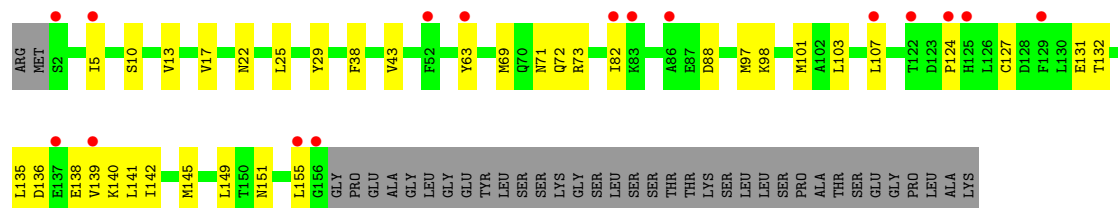
- Molecule 1: Ferritin



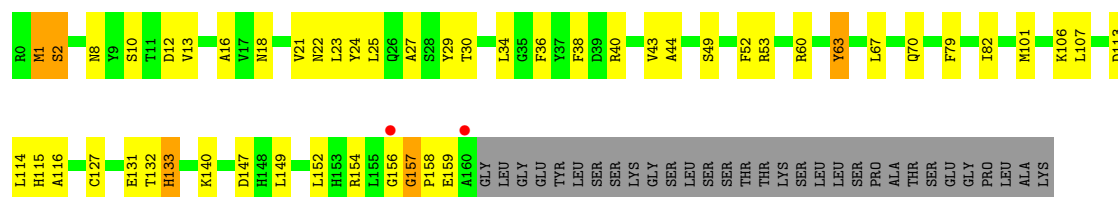
- Molecule 1: Ferritin



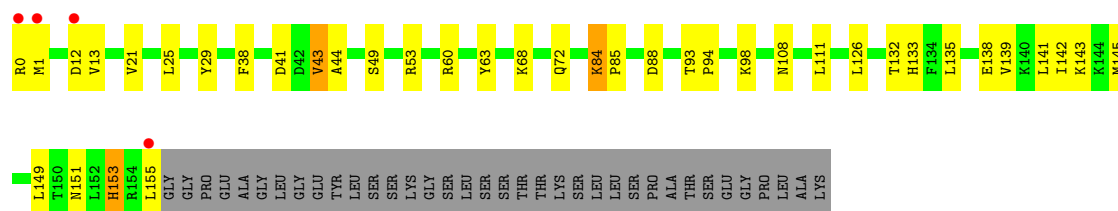
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	212.34Å 236.94Å 249.71Å 94.69° 115.06° 114.96°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.85) 95.3 (50.00-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.291 0.223 , 0.261	Depositor DCC
R_{free} test set	42321 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	187090	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.40	0/1294	0.95	4/1741 (0.2%)
1	AB	0.46	0/1345	1.04	6/1809 (0.3%)
1	AC	0.43	0/1318	0.95	3/1772 (0.2%)
1	AD	0.36	0/1299	0.99	6/1748 (0.3%)
1	AE	0.57	0/1345	1.00	4/1809 (0.2%)
1	AF	0.47	0/1293	0.95	4/1739 (0.2%)
1	AG	0.45	0/1299	1.02	8/1748 (0.5%)
1	AH	0.57	0/1307	1.01	9/1758 (0.5%)
1	AI	0.37	0/1293	0.94	3/1739 (0.2%)
1	AJ	0.42	0/1285	0.96	4/1727 (0.2%)
1	AK	0.41	0/1292	0.97	6/1736 (0.3%)
1	AL	0.38	0/1285	0.95	4/1729 (0.2%)
1	AM	0.52	0/1322	1.00	6/1777 (0.3%)
1	AN	0.47	0/1345	1.04	9/1809 (0.5%)
1	AO	0.56	0/1345	1.03	6/1809 (0.3%)
1	AP	0.59	0/1302	1.01	4/1751 (0.2%)
1	AQ	0.43	0/1343	0.96	7/1805 (0.4%)
1	AR	0.48	0/1332	0.93	2/1791 (0.1%)
1	AS	0.44	0/1303	0.91	5/1753 (0.3%)
1	AT	0.53	0/1294	1.04	4/1741 (0.2%)
1	AU	0.50	0/1307	0.94	3/1758 (0.2%)
1	AV	0.47	0/1303	0.96	5/1753 (0.3%)
1	AW	0.41	0/1294	0.94	5/1741 (0.3%)
1	AX	0.51	0/1307	1.07	7/1758 (0.4%)
1	Aa	0.60	0/1318	1.04	8/1772 (0.5%)
1	Ab	0.57	0/1311	0.96	6/1763 (0.3%)
1	Ac	0.53	0/1307	1.02	7/1758 (0.4%)
1	Ad	0.66	0/1345	1.05	8/1809 (0.4%)
1	Ae	0.58	0/1322	1.06	7/1777 (0.4%)
1	Af	0.61	0/1318	1.03	8/1772 (0.5%)
1	Ag	0.63	0/1277	0.97	4/1717 (0.2%)
1	Ah	0.59	0/1318	0.96	6/1772 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ai	0.67	0/1302	1.06	6/1751 (0.3%)
1	Aj	0.61	0/1345	1.06	10/1809 (0.6%)
1	Ak	0.53	0/1345	0.98	7/1809 (0.4%)
1	Al	0.58	0/1345	1.06	8/1809 (0.4%)
1	Am	0.63	0/1322	1.00	6/1777 (0.3%)
1	An	0.60	0/1311	1.00	7/1763 (0.4%)
1	Ao	0.59	0/1318	1.02	8/1772 (0.5%)
1	Ap	0.58	0/1322	1.02	4/1777 (0.2%)
1	Aq	0.61	0/1307	1.03	6/1758 (0.3%)
1	Ar	0.71	0/1345	1.10	5/1809 (0.3%)
1	As	0.58	1/1318 (0.1%)	1.03	8/1772 (0.5%)
1	At	0.57	0/1307	0.98	4/1758 (0.2%)
1	Au	0.57	0/1307	1.05	6/1758 (0.3%)
1	Av	0.57	0/1343	1.01	8/1805 (0.4%)
1	Aw	0.78	2/1311 (0.2%)	1.06	7/1763 (0.4%)
1	Ax	0.59	0/1277	1.03	7/1717 (0.4%)
1	BA	0.45	0/1356	1.01	6/1823 (0.3%)
1	BB	0.42	0/1292	0.97	4/1736 (0.2%)
1	BC	0.38	0/1273	0.90	1/1712 (0.1%)
1	BD	0.43	0/1313	1.01	8/1765 (0.5%)
1	BE	0.45	0/1302	0.96	4/1751 (0.2%)
1	BF	0.55	0/1299	0.98	4/1748 (0.2%)
1	BG	0.47	0/1281	0.93	3/1722 (0.2%)
1	BH	0.41	0/1269	0.95	3/1707 (0.2%)
1	BI	0.45	0/1277	0.95	3/1717 (0.2%)
1	BJ	0.38	0/1285	0.96	4/1729 (0.2%)
1	BK	0.40	0/1281	0.93	3/1722 (0.2%)
1	BL	0.38	0/1277	0.94	3/1717 (0.2%)
1	BM	0.54	0/1294	1.01	4/1741 (0.2%)
1	BN	0.53	0/1299	1.00	7/1748 (0.4%)
1	BO	0.43	0/1307	0.91	4/1758 (0.2%)
1	BP	0.42	0/1299	1.00	6/1748 (0.3%)
1	BQ	0.53	0/1307	0.94	5/1758 (0.3%)
1	BR	0.49	0/1318	0.93	6/1772 (0.3%)
1	BS	0.56	0/1304	0.91	3/1753 (0.2%)
1	BT	0.36	0/1285	0.99	5/1729 (0.3%)
1	BU	0.37	0/1322	0.95	5/1777 (0.3%)
1	BV	0.36	0/1277	0.97	5/1717 (0.3%)
1	BW	0.42	0/1311	0.91	4/1763 (0.2%)
1	BX	0.40	0/1324	0.99	6/1781 (0.3%)
1	Ba	0.36	0/1293	0.91	2/1739 (0.1%)
1	Bb	0.41	0/1302	0.92	5/1751 (0.3%)
1	Bc	0.52	0/1318	0.99	5/1772 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Bd	0.54	0/1318	0.98	7/1772 (0.4%)
1	Be	0.56	0/1324	1.02	4/1781 (0.2%)
1	Bf	0.53	0/1345	1.02	6/1809 (0.3%)
1	Bg	0.38	0/1281	0.93	3/1722 (0.2%)
1	Bh	0.43	0/1302	0.95	4/1751 (0.2%)
1	Bi	0.45	0/1292	0.92	3/1736 (0.2%)
1	Bj	0.36	0/1267	0.92	2/1704 (0.1%)
1	Bk	0.42	0/1302	0.89	1/1751 (0.1%)
1	Bl	0.50	0/1302	0.97	6/1751 (0.3%)
1	Bm	0.53	0/1299	1.05	10/1748 (0.6%)
1	Bn	0.44	0/1343	0.97	3/1805 (0.2%)
1	Bo	0.39	0/1281	0.95	4/1722 (0.2%)
1	Bp	0.54	0/1322	1.00	4/1777 (0.2%)
1	Bq	0.44	0/1313	0.91	4/1765 (0.2%)
1	Br	0.63	0/1318	1.04	8/1772 (0.5%)
1	Bs	0.42	0/1277	0.96	4/1717 (0.2%)
1	Bt	0.38	0/1293	0.92	4/1739 (0.2%)
1	Bu	0.56	0/1345	1.03	10/1809 (0.6%)
1	Bv	0.49	0/1307	0.96	8/1758 (0.5%)
1	Bw	0.60	0/1299	1.02	8/1748 (0.5%)
1	Bx	0.36	0/1285	0.92	0/1729
1	CA	0.54	0/1307	0.98	7/1758 (0.4%)
1	CB	0.47	0/1311	1.02	6/1763 (0.3%)
1	CC	0.40	0/1285	0.89	1/1729 (0.1%)
1	CD	0.54	0/1318	0.95	3/1772 (0.2%)
1	CE	0.45	0/1313	0.90	3/1765 (0.2%)
1	CF	0.57	0/1303	0.99	6/1753 (0.3%)
1	CG	0.48	0/1313	0.94	5/1765 (0.3%)
1	CH	0.42	0/1302	0.90	5/1751 (0.3%)
1	CI	0.57	0/1307	1.00	7/1758 (0.4%)
1	CJ	0.58	1/1343 (0.1%)	1.03	6/1805 (0.3%)
1	CK	0.41	0/1307	0.93	3/1758 (0.2%)
1	CL	0.41	0/1302	0.91	6/1751 (0.3%)
1	CM	0.54	0/1302	0.99	3/1751 (0.2%)
1	CN	0.51	0/1311	0.99	6/1763 (0.3%)
1	CO	0.45	0/1304	0.90	2/1753 (0.1%)
1	CP	0.41	0/1293	0.93	5/1739 (0.3%)
1	CQ	0.63	0/1322	1.03	10/1777 (0.6%)
1	CR	0.56	0/1356	1.04	5/1823 (0.3%)
1	CS	0.63	0/1318	0.96	2/1772 (0.1%)
1	CT	0.46	0/1293	0.91	4/1739 (0.2%)
1	CU	0.37	0/1302	0.89	3/1751 (0.2%)
1	CV	0.37	0/1294	0.99	4/1741 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CW	0.42	0/1277	0.92	2/1717 (0.1%)
1	CX	0.49	0/1318	1.04	5/1772 (0.3%)
1	Ca	0.41	0/1293	1.04	5/1740 (0.3%)
1	Cb	0.42	0/1299	0.93	3/1748 (0.2%)
1	Cc	0.39	0/1288	0.98	7/1733 (0.4%)
1	Cd	0.39	0/1263	0.97	4/1699 (0.2%)
1	Ce	0.38	0/1269	0.95	4/1707 (0.2%)
1	Cf	0.38	0/1261	0.93	2/1696 (0.1%)
1	Cg	0.40	0/1303	0.92	2/1753 (0.1%)
1	Ch	0.45	0/1299	0.97	2/1748 (0.1%)
1	Ci	0.42	0/1263	0.95	0/1699
1	Cj	0.39	0/1288	0.99	2/1731 (0.1%)
1	Ck	0.39	0/1269	0.92	4/1707 (0.2%)
1	Cl	0.36	0/1273	0.97	4/1712 (0.2%)
1	Cm	0.39	0/1299	1.00	6/1748 (0.3%)
1	Cn	0.37	0/1277	0.94	5/1717 (0.3%)
1	Co	0.45	0/1273	1.01	3/1712 (0.2%)
1	Cp	0.41	0/1293	0.92	4/1739 (0.2%)
1	Cq	0.37	0/1273	0.94	3/1712 (0.2%)
1	Cr	0.37	0/1269	0.95	5/1707 (0.3%)
1	Cs	0.35	0/1267	0.95	2/1704 (0.1%)
1	Ct	0.45	0/1303	0.99	6/1753 (0.3%)
1	Cu	0.41	0/1299	0.97	6/1748 (0.3%)
1	Cv	0.41	0/1311	0.93	6/1763 (0.3%)
1	Cw	0.38	0/1273	0.94	2/1712 (0.1%)
1	Cx	0.42	0/1288	0.99	8/1731 (0.5%)
All	All	0.49	4/187767 (0.0%)	0.98	710/252515 (0.3%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aw	1	MET	SD-CE	-12.49	1.48	1.79
1	Aw	1	MET	CG-SD	-8.39	1.59	1.80
1	As	21	VAL	CA-CB	5.11	1.60	1.54
1	CJ	162	LEU	N-CA	5.05	1.52	1.46

The worst 5 of 710 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bc	43	VAL	N-CA-C	-11.53	102.51	111.62
1	AB	164	GLU	N-CA-C	11.51	123.51	110.97
1	Ar	43	VAL	N-CA-C	-10.92	103.00	111.62
1	CX	43	VAL	N-CA-C	-10.63	103.22	111.62
1	BA	164	GLU	N-CA-C	10.18	123.44	111.02

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 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1270	0	1243	21	0
1	AB	1320	0	1292	25	0
1	AC	1294	0	1273	16	0
1	AD	1275	0	1248	20	0
1	AE	1320	0	1292	38	0
1	AF	1269	0	1249	34	0
1	AG	1275	0	1248	30	0
1	AH	1283	0	1260	31	0
1	AI	1269	0	1249	19	0
1	AJ	1262	0	1242	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AK	1269	0	1252	19	0
1	AL	1261	0	1237	20	0
1	AM	1298	0	1276	35	0
1	AN	1320	0	1292	42	0
1	AO	1320	0	1292	49	0
1	AP	1278	0	1255	33	0
1	AQ	1319	0	1296	30	0
1	AR	1308	0	1283	22	0
1	AS	1279	0	1251	22	0
1	AT	1270	0	1243	46	0
1	AU	1283	0	1260	19	0
1	AV	1279	0	1251	29	0
1	AW	1270	0	1243	15	0
1	AX	1283	0	1260	34	0
1	Aa	1294	0	1273	12	0
1	Ab	1287	0	1263	27	0
1	Ac	1283	0	1260	25	0
1	Ad	1320	0	1292	41	0
1	Ae	1298	0	1276	42	0
1	Af	1294	0	1273	34	0
1	Ag	1254	0	1236	29	0
1	Ah	1294	0	1273	22	0
1	Ai	1278	0	1255	29	0
1	Aj	1320	0	1292	25	0
1	Ak	1320	0	1292	23	0
1	Al	1320	0	1292	45	0
1	Am	1298	0	1276	29	0
1	An	1287	0	1263	23	0
1	Ao	1294	0	1273	33	0
1	Ap	1298	0	1276	27	0
1	Aq	1283	0	1260	29	0
1	Ar	1320	0	1292	38	0
1	As	1294	0	1273	22	0
1	At	1283	0	1260	33	0
1	Au	1283	0	1260	32	0
1	Av	1319	0	1296	16	0
1	Aw	1287	0	1263	42	0
1	Ax	1254	0	1236	27	0
1	BA	1331	0	1305	40	0
1	BB	1269	0	1252	26	0
1	BC	1250	0	1227	30	0
1	BD	1289	0	1268	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BE	1278	0	1255	27	0
1	BF	1275	0	1248	16	0
1	BG	1258	0	1239	24	0
1	BH	1246	0	1224	28	0
1	BI	1254	0	1236	32	0
1	BJ	1261	0	1237	32	0
1	BK	1258	0	1239	35	0
1	BL	1254	0	1236	17	0
1	BM	1270	0	1243	18	0
1	BN	1275	0	1248	20	0
1	BO	1283	0	1260	25	0
1	BP	1275	0	1248	21	0
1	BQ	1283	0	1260	14	0
1	BR	1294	0	1273	20	0
1	BS	1280	0	1262	22	0
1	BT	1261	0	1237	32	0
1	BU	1298	0	1276	28	0
1	BV	1254	0	1230	37	0
1	BW	1287	0	1263	28	0
1	BX	1300	0	1271	47	0
1	Ba	1269	0	1249	20	0
1	Bb	1278	0	1255	27	0
1	Bc	1294	0	1273	24	0
1	Bd	1294	0	1273	28	0
1	Be	1300	0	1271	27	0
1	Bf	1320	0	1292	36	0
1	Bg	1258	0	1239	31	0
1	Bh	1278	0	1255	30	0
1	Bi	1269	0	1252	23	0
1	Bj	1244	0	1222	27	0
1	Bk	1278	0	1255	17	0
1	Bl	1278	0	1255	30	0
1	Bm	1275	0	1248	21	0
1	Bn	1319	0	1296	37	0
1	Bo	1258	0	1239	28	0
1	Bp	1298	0	1276	29	0
1	Bq	1289	0	1268	22	0
1	Br	1294	0	1273	32	0
1	Bs	1254	0	1236	20	0
1	Bt	1269	0	1249	26	0
1	Bu	1320	0	1292	24	0
1	Bv	1283	0	1260	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Bw	1275	0	1248	30	0
1	Bx	1261	0	1237	29	0
1	CA	1283	0	1260	32	0
1	CB	1287	0	1263	27	0
1	CC	1261	0	1237	17	0
1	CD	1294	0	1273	16	0
1	CE	1289	0	1268	26	0
1	CF	1279	0	1251	30	0
1	CG	1289	0	1268	26	0
1	CH	1278	0	1255	24	0
1	CI	1283	0	1260	23	0
1	CJ	1319	0	1296	39	0
1	CK	1283	0	1260	23	0
1	CL	1278	0	1255	16	0
1	CM	1278	0	1255	32	0
1	CN	1287	0	1263	25	0
1	CO	1280	0	1262	17	0
1	CP	1269	0	1249	24	0
1	CQ	1298	0	1276	19	0
1	CR	1331	0	1305	28	0
1	CS	1294	0	1273	29	0
1	CT	1269	0	1249	21	0
1	CU	1278	0	1255	18	0
1	CV	1270	0	1243	22	0
1	CW	1254	0	1236	13	0
1	CX	1294	0	1273	35	0
1	Ca	1269	0	1243	30	0
1	Cb	1275	0	1248	31	0
1	Cc	1264	0	1238	23	0
1	Cd	1240	0	1219	26	0
1	Ce	1246	0	1224	16	0
1	Cf	1238	0	1213	31	0
1	Cg	1279	0	1251	14	0
1	Ch	1275	0	1248	33	0
1	Ci	1240	0	1219	29	0
1	Cj	1265	0	1249	45	0
1	Ck	1246	0	1224	23	0
1	Cl	1250	0	1227	34	0
1	Cm	1275	0	1248	16	0
1	Cn	1254	0	1236	28	0
1	Co	1250	0	1227	25	0
1	Cp	1269	0	1249	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Cq	1250	0	1227	38	0
1	Cr	1246	0	1224	23	0
1	Cs	1244	0	1222	44	0
1	Ct	1279	0	1251	25	0
1	Cu	1275	0	1248	21	0
1	Cv	1287	0	1263	21	0
1	Cw	1250	0	1227	28	0
1	Cx	1265	0	1249	22	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
2	CB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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	1	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	1	0
3	Ad	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Ae	26	0	0	0	0
3	Af	48	0	0	2	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	1	0
3	Am	45	0	0	0	0
3	An	41	0	0	0	0
3	Ao	39	0	0	3	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	1	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	1	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	1	0
3	BK	6	0	0	0	0
3	BL	10	0	0	0	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
3	BV	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	1	0
3	Bi	7	0	0	0	0
3	Bj	6	0	0	1	0
3	Bk	6	0	0	0	0
3	Bl	23	0	0	1	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	1	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	1	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
3	CP	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
3	Ch	18	0	0	0	0
3	Ci	9	0	0	0	0
3	Cj	9	0	0	1	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	3312	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 3312 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:1:MET:HG3	1:AJ:2:SER:H	1.19	1.02
1:Am:8:ASN:HD22	1:Ar:112:LEU:HD13	1.19	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cb:8:ASN:HD22	1:Cj:112:LEU:HD13	1.26	1.00
1:AE:23:LEU:HD11	1:AE:106:LYS:HE2	1.50	0.94
1:Ad:155:LEU:HD11	1:Ad:162:LEU:HD11	1.45	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%)	4	10
1	AC	159/192 (83%)	146 (92%)	10 (6%)	3 (2%)	6	14
1	AD	157/192 (82%)	151 (96%)	5 (3%)	1 (1%)	21	38
1	AE	163/192 (85%)	147 (90%)	11 (7%)	5 (3%)	3	7
1	AF	156/192 (81%)	151 (97%)	4 (3%)	1 (1%)	21	38
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%)	21	38
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%)	9	21
1	AN	163/192 (85%)	154 (94%)	7 (4%)	2 (1%)	10	22
1	AO	163/192 (85%)	148 (91%)	11 (7%)	4 (2%)	4	10
1	AP	157/192 (82%)	152 (97%)	5 (3%)	0	100	100
1	AQ	163/192 (85%)	150 (92%)	10 (6%)	3 (2%)	6	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AR	162/192 (84%)	152 (94%)	8 (5%)	2 (1%)	10	22
1	AS	158/192 (82%)	149 (94%)	8 (5%)	1 (1%)	21	38
1	AT	156/192 (81%)	144 (92%)	10 (6%)	2 (1%)	9	21
1	AU	158/192 (82%)	152 (96%)	5 (3%)	1 (1%)	21	38
1	AV	158/192 (82%)	148 (94%)	8 (5%)	2 (1%)	9	21
1	AW	156/192 (81%)	150 (96%)	6 (4%)	0	100	100
1	AX	158/192 (82%)	149 (94%)	8 (5%)	1 (1%)	21	38
1	Aa	159/192 (83%)	153 (96%)	6 (4%)	0	100	100
1	Ab	159/192 (83%)	151 (95%)	6 (4%)	2 (1%)	9	21
1	Ac	158/192 (82%)	155 (98%)	3 (2%)	0	100	100
1	Ad	163/192 (85%)	152 (93%)	8 (5%)	3 (2%)	6	15
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%)	9	21
1	Aj	163/192 (85%)	147 (90%)	11 (7%)	5 (3%)	3	7
1	Ak	163/192 (85%)	153 (94%)	8 (5%)	2 (1%)	10	22
1	Al	163/192 (85%)	149 (91%)	10 (6%)	4 (2%)	4	10
1	Am	160/192 (83%)	149 (93%)	7 (4%)	4 (2%)	4	10
1	An	159/192 (83%)	149 (94%)	8 (5%)	2 (1%)	9	21
1	Ao	159/192 (83%)	150 (94%)	7 (4%)	2 (1%)	9	21
1	Ap	160/192 (83%)	150 (94%)	7 (4%)	3 (2%)	6	14
1	Aq	158/192 (82%)	146 (92%)	11 (7%)	1 (1%)	21	38
1	Ar	163/192 (85%)	152 (93%)	8 (5%)	3 (2%)	6	15
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%)	21	38
1	Av	163/192 (85%)	148 (91%)	13 (8%)	2 (1%)	10	22
1	Aw	159/192 (83%)	149 (94%)	9 (6%)	1 (1%)	21	38
1	Ax	153/192 (80%)	150 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	164/192 (85%)	150 (92%)	12 (7%)	2 (1%)	10	22
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%)	6	14
1	BG	154/192 (80%)	145 (94%)	9 (6%)	0	100	100
1	BH	152/192 (79%)	146 (96%)	5 (3%)	1 (1%)	18	35
1	BI	153/192 (80%)	150 (98%)	3 (2%)	0	100	100
1	BJ	155/192 (81%)	147 (95%)	7 (4%)	1 (1%)	21	38
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%)	21	38
1	BO	158/192 (82%)	146 (92%)	11 (7%)	1 (1%)	21	38
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%)	21	38
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%)	21	38
1	BV	154/192 (80%)	149 (97%)	3 (2%)	2 (1%)	9	21
1	BW	159/192 (83%)	154 (97%)	5 (3%)	0	100	100
1	BX	161/192 (84%)	150 (93%)	7 (4%)	4 (2%)	4	10
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%)	6	14
1	Be	161/192 (84%)	146 (91%)	12 (8%)	3 (2%)	6	14
1	Bf	163/192 (85%)	147 (90%)	11 (7%)	5 (3%)	3	7
1	Bg	154/192 (80%)	150 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bh	157/192 (82%)	151 (96%)	5 (3%)	1 (1%)	21	38
1	Bi	155/192 (81%)	148 (96%)	6 (4%)	1 (1%)	21	38
1	Bj	152/192 (79%)	147 (97%)	5 (3%)	0	100	100
1	Bk	157/192 (82%)	148 (94%)	8 (5%)	1 (1%)	21	38
1	Bl	157/192 (82%)	150 (96%)	6 (4%)	1 (1%)	21	38
1	Bm	157/192 (82%)	151 (96%)	6 (4%)	0	100	100
1	Bn	163/192 (85%)	153 (94%)	7 (4%)	3 (2%)	6	15
1	Bo	154/192 (80%)	149 (97%)	5 (3%)	0	100	100
1	Bp	160/192 (83%)	148 (92%)	11 (7%)	1 (1%)	21	38
1	Bq	158/192 (82%)	150 (95%)	6 (4%)	2 (1%)	9	21
1	Br	159/192 (83%)	148 (93%)	9 (6%)	2 (1%)	9	21
1	Bs	153/192 (80%)	148 (97%)	5 (3%)	0	100	100
1	Bt	156/192 (81%)	147 (94%)	7 (4%)	2 (1%)	9	21
1	Bu	163/192 (85%)	152 (93%)	9 (6%)	2 (1%)	10	22
1	Bv	158/192 (82%)	149 (94%)	8 (5%)	1 (1%)	21	38
1	Bw	157/192 (82%)	150 (96%)	6 (4%)	1 (1%)	21	38
1	Bx	155/192 (81%)	147 (95%)	8 (5%)	0	100	100
1	CA	158/192 (82%)	153 (97%)	4 (2%)	1 (1%)	21	38
1	CB	159/192 (83%)	154 (97%)	5 (3%)	0	100	100
1	CC	155/192 (81%)	149 (96%)	5 (3%)	1 (1%)	21	38
1	CD	159/192 (83%)	152 (96%)	6 (4%)	1 (1%)	21	38
1	CE	158/192 (82%)	149 (94%)	7 (4%)	2 (1%)	9	21
1	CF	158/192 (82%)	150 (95%)	8 (5%)	0	100	100
1	CG	158/192 (82%)	153 (97%)	4 (2%)	1 (1%)	21	38
1	CH	157/192 (82%)	146 (93%)	10 (6%)	1 (1%)	21	38
1	CI	158/192 (82%)	147 (93%)	10 (6%)	1 (1%)	21	38
1	CJ	163/192 (85%)	153 (94%)	8 (5%)	2 (1%)	10	22
1	CK	158/192 (82%)	152 (96%)	5 (3%)	1 (1%)	21	38
1	CL	157/192 (82%)	150 (96%)	7 (4%)	0	100	100
1	CM	157/192 (82%)	148 (94%)	7 (4%)	2 (1%)	9	21
1	CN	159/192 (83%)	152 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CO	157/192 (82%)	146 (93%)	11 (7%)	0	100	100
1	CP	156/192 (81%)	152 (97%)	4 (3%)	0	100	100
1	CQ	160/192 (83%)	150 (94%)	10 (6%)	0	100	100
1	CR	164/192 (85%)	150 (92%)	11 (7%)	3 (2%)	6	15
1	CS	159/192 (83%)	150 (94%)	9 (6%)	0	100	100
1	CT	156/192 (81%)	147 (94%)	8 (5%)	1 (1%)	21	38
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%)	9	21
1	Ca	156/192 (81%)	148 (95%)	5 (3%)	3 (2%)	6	14
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%)	21	38
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%)	21	38
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%)	21	38
1	Cq	153/192 (80%)	146 (95%)	7 (5%)	0	100	100
1	Cr	152/192 (79%)	147 (97%)	4 (3%)	1 (1%)	18	35
1	Cs	152/192 (79%)	147 (97%)	4 (3%)	1 (1%)	18	35
1	Ct	158/192 (82%)	154 (98%)	4 (2%)	0	100	100
1	Cu	157/192 (82%)	149 (95%)	7 (4%)	1 (1%)	21	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Cv	159/192 (83%)	151 (95%)	8 (5%)	0	100	100
1	Cw	153/192 (80%)	149 (97%)	4 (3%)	0	100	100
1	Cx	154/192 (80%)	151 (98%)	3 (2%)	0	100	100
All	All	22658/27648 (82%)	21530 (95%)	982 (4%)	146 (1%)	21	38

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%)	130 (97%)	4 (3%)	36	61
1	AB	138/161 (86%)	133 (96%)	5 (4%)	31	56
1	AC	136/161 (84%)	132 (97%)	4 (3%)	37	61
1	AD	134/161 (83%)	133 (99%)	1 (1%)	76	87
1	AE	138/161 (86%)	134 (97%)	4 (3%)	37	61
1	AF	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	AG	134/161 (83%)	131 (98%)	3 (2%)	45	69
1	AH	135/161 (84%)	129 (96%)	6 (4%)	25	49
1	AI	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	AJ	133/161 (83%)	132 (99%)	1 (1%)	73	86
1	AK	134/161 (83%)	133 (99%)	1 (1%)	76	87
1	AL	133/161 (83%)	132 (99%)	1 (1%)	73	86
1	AM	136/161 (84%)	131 (96%)	5 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AN	138/161 (86%)	133 (96%)	5 (4%)	31	56
1	AO	138/161 (86%)	126 (91%)	12 (9%)	9	21
1	AP	135/161 (84%)	129 (96%)	6 (4%)	25	49
1	AQ	138/161 (86%)	137 (99%)	1 (1%)	76	87
1	AR	137/161 (85%)	135 (98%)	2 (2%)	57	77
1	AS	134/161 (83%)	130 (97%)	4 (3%)	36	61
1	AT	134/161 (83%)	130 (97%)	4 (3%)	36	61
1	AU	135/161 (84%)	132 (98%)	3 (2%)	45	69
1	AV	134/161 (83%)	133 (99%)	1 (1%)	76	87
1	AW	134/161 (83%)	134 (100%)	0	100	100
1	AX	135/161 (84%)	132 (98%)	3 (2%)	45	69
1	Aa	136/161 (84%)	133 (98%)	3 (2%)	45	69
1	Ab	135/161 (84%)	133 (98%)	2 (2%)	57	77
1	Ac	135/161 (84%)	131 (97%)	4 (3%)	36	61
1	Ad	138/161 (86%)	132 (96%)	6 (4%)	26	50
1	Ae	136/161 (84%)	133 (98%)	3 (2%)	45	69
1	Af	136/161 (84%)	133 (98%)	3 (2%)	45	69
1	Ag	133/161 (83%)	129 (97%)	4 (3%)	36	61
1	Ah	136/161 (84%)	133 (98%)	3 (2%)	45	69
1	Ai	135/161 (84%)	131 (97%)	4 (3%)	36	61
1	Aj	138/161 (86%)	134 (97%)	4 (3%)	37	61
1	Ak	138/161 (86%)	134 (97%)	4 (3%)	37	61
1	Al	138/161 (86%)	133 (96%)	5 (4%)	31	56
1	Am	136/161 (84%)	129 (95%)	7 (5%)	21	43
1	An	135/161 (84%)	135 (100%)	0	100	100
1	Ao	136/161 (84%)	134 (98%)	2 (2%)	57	77
1	Ap	136/161 (84%)	134 (98%)	2 (2%)	57	77
1	Aq	135/161 (84%)	131 (97%)	4 (3%)	36	61
1	Ar	138/161 (86%)	129 (94%)	9 (6%)	15	32
1	As	136/161 (84%)	130 (96%)	6 (4%)	25	49
1	At	135/161 (84%)	130 (96%)	5 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Au	135/161 (84%)	129 (96%)	6 (4%)	25	49
1	Av	138/161 (86%)	134 (97%)	4 (3%)	37	61
1	Aw	135/161 (84%)	129 (96%)	6 (4%)	25	49
1	Ax	133/161 (83%)	129 (97%)	4 (3%)	36	61
1	BA	139/161 (86%)	134 (96%)	5 (4%)	31	56
1	BB	134/161 (83%)	133 (99%)	1 (1%)	76	87
1	BC	132/161 (82%)	130 (98%)	2 (2%)	57	77
1	BD	136/161 (84%)	134 (98%)	2 (2%)	57	77
1	BE	135/161 (84%)	135 (100%)	0	100	100
1	BF	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	BG	133/161 (83%)	130 (98%)	3 (2%)	44	68
1	BH	132/161 (82%)	132 (100%)	0	100	100
1	BI	133/161 (83%)	133 (100%)	0	100	100
1	BJ	133/161 (83%)	132 (99%)	1 (1%)	73	86
1	BK	133/161 (83%)	128 (96%)	5 (4%)	29	54
1	BL	133/161 (83%)	132 (99%)	1 (1%)	73	86
1	BM	134/161 (83%)	131 (98%)	3 (2%)	45	69
1	BN	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	BO	135/161 (84%)	132 (98%)	3 (2%)	45	69
1	BP	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	BQ	135/161 (84%)	131 (97%)	4 (3%)	36	61
1	BR	136/161 (84%)	133 (98%)	3 (2%)	45	69
1	BS	135/161 (84%)	133 (98%)	2 (2%)	57	77
1	BT	133/161 (83%)	132 (99%)	1 (1%)	73	86
1	BU	136/161 (84%)	135 (99%)	1 (1%)	76	87
1	BV	132/161 (82%)	132 (100%)	0	100	100
1	BW	135/161 (84%)	135 (100%)	0	100	100
1	BX	136/161 (84%)	134 (98%)	2 (2%)	57	77
1	Ba	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	Bb	135/161 (84%)	132 (98%)	3 (2%)	45	69
1	Bc	136/161 (84%)	131 (96%)	5 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bd	136/161 (84%)	135 (99%)	1 (1%)	76	87
1	Be	136/161 (84%)	133 (98%)	3 (2%)	45	69
1	Bf	138/161 (86%)	132 (96%)	6 (4%)	26	50
1	Bg	133/161 (83%)	132 (99%)	1 (1%)	73	86
1	Bh	135/161 (84%)	134 (99%)	1 (1%)	76	87
1	Bi	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	Bj	131/161 (81%)	129 (98%)	2 (2%)	57	77
1	Bk	135/161 (84%)	131 (97%)	4 (3%)	36	61
1	Bl	135/161 (84%)	134 (99%)	1 (1%)	76	87
1	Bm	134/161 (83%)	131 (98%)	3 (2%)	45	69
1	Bn	138/161 (86%)	133 (96%)	5 (4%)	31	56
1	Bo	133/161 (83%)	133 (100%)	0	100	100
1	Bp	136/161 (84%)	133 (98%)	3 (2%)	45	69
1	Bq	136/161 (84%)	135 (99%)	1 (1%)	76	87
1	Br	136/161 (84%)	130 (96%)	6 (4%)	25	49
1	Bs	133/161 (83%)	132 (99%)	1 (1%)	73	86
1	Bt	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	Bu	138/161 (86%)	133 (96%)	5 (4%)	31	56
1	Bv	135/161 (84%)	131 (97%)	4 (3%)	36	61
1	Bw	134/161 (83%)	130 (97%)	4 (3%)	36	61
1	Bx	133/161 (83%)	133 (100%)	0	100	100
1	CA	135/161 (84%)	131 (97%)	4 (3%)	36	61
1	CB	135/161 (84%)	130 (96%)	5 (4%)	30	55
1	CC	133/161 (83%)	131 (98%)	2 (2%)	57	77
1	CD	136/161 (84%)	134 (98%)	2 (2%)	57	77
1	CE	136/161 (84%)	135 (99%)	1 (1%)	76	87
1	CF	134/161 (83%)	130 (97%)	4 (3%)	36	61
1	CG	136/161 (84%)	136 (100%)	0	100	100
1	CH	135/161 (84%)	132 (98%)	3 (2%)	45	69
1	CI	135/161 (84%)	128 (95%)	7 (5%)	21	43
1	CJ	138/161 (86%)	134 (97%)	4 (3%)	37	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CK	135/161 (84%)	134 (99%)	1 (1%)	76	87
1	CL	135/161 (84%)	134 (99%)	1 (1%)	76	87
1	CM	135/161 (84%)	131 (97%)	4 (3%)	36	61
1	CN	135/161 (84%)	134 (99%)	1 (1%)	76	87
1	CO	135/161 (84%)	133 (98%)	2 (2%)	57	77
1	CP	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	CQ	136/161 (84%)	130 (96%)	6 (4%)	25	49
1	CR	139/161 (86%)	137 (99%)	2 (1%)	59	78
1	CS	136/161 (84%)	130 (96%)	6 (4%)	25	49
1	CT	134/161 (83%)	130 (97%)	4 (3%)	36	61
1	CU	135/161 (84%)	135 (100%)	0	100	100
1	CV	134/161 (83%)	133 (99%)	1 (1%)	76	87
1	CW	133/161 (83%)	133 (100%)	0	100	100
1	CX	136/161 (84%)	132 (97%)	4 (3%)	37	61
1	Ca	133/161 (83%)	128 (96%)	5 (4%)	29	54
1	Cb	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	Cc	133/161 (83%)	130 (98%)	3 (2%)	44	68
1	Cd	131/161 (81%)	130 (99%)	1 (1%)	73	86
1	Ce	132/161 (82%)	131 (99%)	1 (1%)	73	86
1	Cf	131/161 (81%)	131 (100%)	0	100	100
1	Cg	134/161 (83%)	133 (99%)	1 (1%)	76	87
1	Ch	134/161 (83%)	129 (96%)	5 (4%)	30	55
1	Ci	131/161 (81%)	131 (100%)	0	100	100
1	Cj	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	Ck	132/161 (82%)	131 (99%)	1 (1%)	73	86
1	Cl	132/161 (82%)	131 (99%)	1 (1%)	73	86
1	Cm	134/161 (83%)	131 (98%)	3 (2%)	45	69
1	Cn	133/161 (83%)	132 (99%)	1 (1%)	73	86
1	Co	132/161 (82%)	129 (98%)	3 (2%)	44	68
1	Cp	134/161 (83%)	133 (99%)	1 (1%)	76	87
1	Cq	132/161 (82%)	131 (99%)	1 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Cr	132/161 (82%)	131 (99%)	1 (1%)	73	86
1	Cs	131/161 (81%)	129 (98%)	2 (2%)	57	77
1	Ct	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	Cu	134/161 (83%)	132 (98%)	2 (2%)	57	77
1	Cv	135/161 (84%)	132 (98%)	3 (2%)	45	69
1	Cw	132/161 (82%)	132 (100%)	0	100	100
1	Cx	134/161 (83%)	131 (98%)	3 (2%)	45	69
All	All	19400/23184 (84%)	19000 (98%)	400 (2%)	47	70

5 of 400 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BL	34	LEU
1	Bw	64	GLU
1	Cx	153	HIS
1	Bm	101	MET
1	BR	21	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 392 such sidechains are listed below:

Mol	Chain	Res	Type
1	BV	115	HIS
1	Cg	26	GLN
1	BW	125	HIS
1	CC	4	GLN
1	Ci	72	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	158/192 (82%)	0.26	2 (1%) 75 68	31, 61, 82, 117	0
1	AB	165/192 (85%)	0.22	5 (3%) 52 44	26, 54, 95, 109	0
1	AC	161/192 (83%)	0.11	3 (1%) 66 59	38, 58, 77, 111	0
1	AD	159/192 (82%)	0.25	2 (1%) 75 68	51, 68, 82, 118	0
1	AE	165/192 (85%)	-0.27	8 (4%) 35 28	12, 34, 96, 112	0
1	AF	158/192 (82%)	-0.03	3 (1%) 66 59	19, 47, 66, 104	0
1	AG	159/192 (82%)	0.00	2 (1%) 75 68	31, 47, 63, 123	0
1	AH	160/192 (83%)	-0.07	2 (1%) 75 68	21, 42, 69, 112	0
1	AI	158/192 (82%)	0.35	2 (1%) 75 68	54, 70, 84, 114	0
1	AJ	157/192 (81%)	0.36	4 (2%) 58 49	25, 60, 79, 99	0
1	AK	157/192 (81%)	0.20	2 (1%) 75 68	33, 59, 75, 101	0
1	AL	157/192 (81%)	0.41	2 (1%) 75 68	52, 68, 82, 120	0
1	AM	162/192 (84%)	-0.21	3 (1%) 66 59	17, 39, 69, 112	0
1	AN	165/192 (85%)	0.15	5 (3%) 52 44	31, 48, 89, 107	0
1	AO	165/192 (85%)	0.16	10 (6%) 27 20	17, 46, 87, 110	0
1	AP	159/192 (82%)	-0.46	1 (0%) 85 82	7, 30, 51, 102	0
1	AQ	165/192 (85%)	0.29	3 (1%) 67 61	33, 62, 90, 110	0
1	AR	164/192 (85%)	-0.04	7 (4%) 40 31	20, 46, 89, 111	0
1	AS	160/192 (83%)	0.28	3 (1%) 66 59	32, 56, 87, 117	0
1	AT	158/192 (82%)	-0.16	0 100 100	15, 43, 62, 110	0
1	AU	160/192 (83%)	-0.18	4 (2%) 58 49	24, 42, 68, 107	0
1	AV	160/192 (83%)	0.01	3 (1%) 66 59	30, 49, 82, 115	0
1	AW	158/192 (82%)	0.09	2 (1%) 75 68	26, 56, 76, 113	0
1	AX	160/192 (83%)	0.01	2 (1%) 75 68	23, 45, 78, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	Aa	161/192 (83%)	-0.47	2 (1%)	76 71	12, 30, 54, 109	0
1	Ab	161/192 (83%)	-0.27	7 (4%)	40 31	13, 35, 65, 110	0
1	Ac	160/192 (83%)	-0.36	2 (1%)	75 68	15, 35, 66, 103	0
1	Ad	165/192 (85%)	-0.43	4 (2%)	59 51	7, 26, 87, 107	0
1	Ae	162/192 (84%)	-0.33	4 (2%)	58 49	8, 29, 65, 113	0
1	Af	161/192 (83%)	-0.44	2 (1%)	76 71	10, 28, 56, 106	0
1	Ag	155/192 (80%)	-0.55	1 (0%)	85 82	8, 28, 45, 70	0
1	Ah	161/192 (83%)	-0.40	3 (1%)	66 59	12, 32, 55, 109	0
1	Ai	159/192 (82%)	-0.63	2 (1%)	75 68	8, 23, 46, 96	0
1	Aj	165/192 (85%)	-0.27	6 (3%)	46 36	12, 31, 85, 109	0
1	Ak	165/192 (85%)	-0.36	4 (2%)	59 51	18, 37, 86, 107	0
1	Al	165/192 (85%)	-0.31	5 (3%)	52 44	8, 33, 81, 108	0
1	Am	162/192 (84%)	-0.31	3 (1%)	66 59	11, 31, 57, 102	0
1	An	161/192 (83%)	-0.45	3 (1%)	66 59	13, 28, 56, 96	0
1	Ao	161/192 (83%)	-0.29	3 (1%)	66 59	11, 32, 54, 105	0
1	Ap	162/192 (84%)	-0.47	3 (1%)	66 59	11, 30, 63, 101	0
1	Aq	160/192 (83%)	-0.41	2 (1%)	75 68	9, 30, 58, 110	0
1	Ar	165/192 (85%)	-0.30	5 (3%)	52 44	9, 28, 81, 105	0
1	As	161/192 (83%)	-0.47	4 (2%)	58 49	9, 32, 60, 109	0
1	At	160/192 (83%)	-0.34	1 (0%)	85 82	9, 31, 67, 107	0
1	Au	160/192 (83%)	-0.19	2 (1%)	75 68	19, 40, 66, 104	0
1	Av	165/192 (85%)	-0.14	5 (3%)	52 44	16, 39, 85, 110	0
1	Aw	161/192 (83%)	-0.42	2 (1%)	76 71	8, 31, 58, 109	0
1	Ax	155/192 (80%)	-0.43	2 (1%)	75 68	11, 31, 45, 76	0
1	BA	166/192 (86%)	0.12	4 (2%)	59 51	30, 51, 87, 108	0
1	BB	157/192 (81%)	1.52	44 (28%)	1 1	68, 86, 98, 109	0
1	BC	155/192 (80%)	1.49	36 (23%)	2 2	64, 84, 94, 103	0
1	BD	160/192 (83%)	0.26	3 (1%)	66 59	22, 52, 76, 105	0
1	BE	159/192 (82%)	-0.05	3 (1%)	66 59	26, 46, 72, 111	0
1	BF	159/192 (82%)	-0.51	1 (0%)	85 82	13, 32, 53, 102	0
1	BG	156/192 (81%)	0.34	3 (1%)	66 59	31, 58, 70, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	BH	154/192 (80%)	0.82	9 (5%) 29 21	40, 70, 86, 99	0
1	BI	155/192 (80%)	0.13	2 (1%) 75 68	19, 52, 73, 97	0
1	BJ	157/192 (81%)	0.75	8 (5%) 33 26	50, 69, 91, 111	0
1	BK	156/192 (81%)	1.52	38 (24%) 2 1	71, 87, 98, 105	0
1	BL	155/192 (80%)	1.12	11 (7%) 22 16	57, 74, 89, 92	0
1	BM	158/192 (82%)	-0.38	0 100 100	9, 33, 54, 102	0
1	BN	159/192 (82%)	-0.23	0 100 100	20, 41, 63, 114	0
1	BO	160/192 (83%)	0.66	10 (6%) 26 19	37, 62, 86, 114	0
1	BP	159/192 (82%)	0.22	5 (3%) 51 43	29, 55, 83, 114	0
1	BQ	160/192 (83%)	-0.32	2 (1%) 75 68	17, 37, 63, 114	0
1	BR	161/192 (83%)	-0.20	1 (0%) 85 82	18, 42, 68, 103	0
1	BS	159/192 (82%)	-0.48	1 (0%) 85 82	18, 34, 54, 98	0
1	BT	157/192 (81%)	1.05	14 (8%) 15 12	58, 74, 92, 118	0
1	BU	162/192 (84%)	0.94	8 (4%) 35 27	55, 78, 91, 115	0
1	BV	156/192 (81%)	1.43	28 (17%) 3 3	69, 87, 96, 111	0
1	BW	161/192 (83%)	0.41	6 (3%) 45 35	38, 60, 81, 117	0
1	BX	163/192 (84%)	1.16	20 (12%) 8 6	61, 78, 91, 110	0
1	Ba	158/192 (82%)	0.79	8 (5%) 33 26	52, 71, 88, 111	0
1	Bb	159/192 (82%)	0.80	5 (3%) 51 43	49, 72, 90, 118	0
1	Bc	161/192 (83%)	-0.23	4 (2%) 58 49	15, 38, 69, 109	0
1	Bd	161/192 (83%)	-0.27	3 (1%) 66 59	21, 40, 64, 114	0
1	Be	163/192 (84%)	-0.28	3 (1%) 67 61	13, 36, 77, 107	0
1	Bf	165/192 (85%)	-0.05	7 (4%) 40 32	14, 44, 85, 110	0
1	Bg	156/192 (81%)	1.22	17 (10%) 10 8	54, 76, 89, 108	0
1	Bh	159/192 (82%)	0.09	4 (2%) 58 49	30, 48, 72, 108	0
1	Bi	157/192 (81%)	0.21	1 (0%) 85 82	32, 58, 70, 94	0
1	Bj	154/192 (80%)	1.04	13 (8%) 17 12	55, 76, 85, 96	0
1	Bk	159/192 (82%)	0.29	4 (2%) 58 49	37, 57, 80, 114	0
1	Bl	159/192 (82%)	-0.30	3 (1%) 66 59	12, 38, 61, 109	0
1	Bm	159/192 (82%)	-0.30	2 (1%) 75 68	18, 36, 59, 113	0
1	Bn	165/192 (85%)	0.68	5 (3%) 52 44	33, 61, 89, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	Bo	156/192 (81%)	0.71	6 (3%)	44	35	44, 65, 84, 96	0
1	Bp	162/192 (84%)	-0.14	4 (2%)	58	49	17, 41, 79, 116	0
1	Bq	160/192 (83%)	0.23	3 (1%)	66	59	26, 55, 76, 111	0
1	Br	161/192 (83%)	-0.51	1 (0%)	85	82	8, 28, 57, 105	0
1	Bs	155/192 (80%)	0.35	3 (1%)	66	59	37, 57, 80, 97	0
1	Bt	158/192 (82%)	1.14	14 (8%)	15	12	61, 79, 93, 110	0
1	Bu	165/192 (85%)	-0.31	6 (3%)	46	36	14, 36, 83, 106	0
1	Bv	160/192 (83%)	-0.16	3 (1%)	66	59	23, 45, 72, 120	0
1	Bw	159/192 (82%)	-0.45	3 (1%)	66	59	11, 29, 55, 112	0
1	Bx	157/192 (81%)	1.37	20 (12%)	8	5	62, 83, 95, 113	0
1	CA	160/192 (83%)	-0.24	1 (0%)	85	82	12, 36, 61, 111	0
1	CB	161/192 (83%)	0.27	4 (2%)	58	49	19, 52, 79, 108	0
1	CC	157/192 (81%)	0.32	4 (2%)	58	49	45, 65, 78, 109	0
1	CD	161/192 (83%)	-0.26	3 (1%)	66	59	13, 39, 68, 107	0
1	CE	160/192 (83%)	0.05	1 (0%)	85	82	29, 52, 80, 112	0
1	CF	160/192 (83%)	-0.29	4 (2%)	58	49	11, 35, 53, 101	0
1	CG	160/192 (83%)	-0.06	1 (0%)	85	82	21, 45, 72, 112	0
1	CH	159/192 (82%)	0.38	3 (1%)	66	59	33, 62, 79, 119	0
1	CI	160/192 (83%)	-0.32	3 (1%)	66	59	15, 35, 74, 107	0
1	CJ	165/192 (85%)	0.01	4 (2%)	59	51	24, 44, 85, 105	0
1	CK	160/192 (83%)	0.31	2 (1%)	75	68	22, 60, 77, 115	0
1	CL	159/192 (82%)	0.06	4 (2%)	58	49	38, 57, 73, 121	0
1	CM	159/192 (82%)	-0.08	2 (1%)	75	68	16, 42, 63, 112	0
1	CN	161/192 (83%)	-0.22	1 (0%)	85	82	16, 40, 77, 110	0
1	CO	159/192 (82%)	0.23	2 (1%)	75	68	38, 58, 74, 99	0
1	CP	158/192 (82%)	0.16	3 (1%)	66	59	25, 57, 76, 110	0
1	CQ	162/192 (84%)	-0.31	5 (3%)	51	43	9, 31, 61, 104	0
1	CR	166/192 (86%)	-0.07	5 (3%)	52	44	24, 42, 82, 107	0
1	CS	161/192 (83%)	-0.31	3 (1%)	66	59	10, 35, 65, 114	0
1	CT	158/192 (82%)	0.13	3 (1%)	66	59	26, 50, 66, 106	0
1	CU	159/192 (82%)	0.33	3 (1%)	66	59	51, 67, 82, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	CV	158/192 (82%)	0.41	2 (1%) 75 68	55, 68, 84, 120	0
1	CW	155/192 (80%)	-0.16	1 (0%) 85 82	27, 47, 69, 87	0
1	CX	161/192 (83%)	0.05	2 (1%) 76 71	20, 48, 70, 107	0
1	Ca	158/192 (82%)	1.95	67 (42%) 0 0	58, 89, 103, 121	0
1	Cb	159/192 (82%)	0.70	6 (3%) 44 35	37, 69, 87, 109	0
1	Cc	157/192 (81%)	0.67	4 (2%) 58 49	40, 69, 86, 118	0
1	Cd	153/192 (79%)	1.71	52 (33%) 1 1	76, 91, 104, 109	0
1	Ce	154/192 (80%)	0.87	7 (4%) 38 29	59, 81, 92, 95	0
1	Cf	153/192 (79%)	1.50	39 (25%) 1 1	83, 97, 107, 110	0
1	Cg	160/192 (83%)	0.60	6 (3%) 44 35	48, 68, 93, 126	0
1	Ch	159/192 (82%)	-0.00	1 (0%) 85 82	23, 49, 66, 114	0
1	Ci	153/192 (79%)	1.92	60 (39%) 1 0	69, 89, 104, 111	0
1	Cj	156/192 (81%)	1.38	31 (19%) 3 3	61, 81, 100, 112	0
1	Ck	154/192 (80%)	0.74	6 (3%) 43 34	45, 74, 92, 104	0
1	Cl	155/192 (80%)	1.41	28 (18%) 3 3	56, 85, 97, 113	0
1	Cm	159/192 (82%)	1.23	26 (16%) 4 4	71, 88, 100, 113	0
1	Cn	155/192 (80%)	1.15	19 (12%) 8 6	65, 86, 101, 104	0
1	Co	155/192 (80%)	0.13	2 (1%) 75 68	26, 52, 71, 100	0
1	Cp	158/192 (82%)	0.61	7 (4%) 39 30	46, 67, 89, 109	0
1	Cq	155/192 (80%)	1.74	55 (35%) 1 1	83, 96, 106, 112	0
1	Cr	154/192 (80%)	1.07	14 (9%) 15 11	78, 91, 103, 111	0
1	Cs	154/192 (80%)	1.63	51 (33%) 1 1	83, 98, 106, 107	0
1	Ct	160/192 (83%)	0.07	4 (2%) 58 49	34, 51, 79, 115	0
1	Cu	159/192 (82%)	0.27	2 (1%) 75 68	44, 62, 81, 119	0
1	Cv	161/192 (83%)	0.24	6 (3%) 45 35	39, 59, 81, 119	0
1	Cw	155/192 (80%)	1.15	16 (10%) 12 10	71, 89, 98, 107	0
1	Cx	156/192 (81%)	0.31	4 (2%) 57 48	39, 59, 78, 99	0
All	All	22946/27648 (82%)	0.23	1135 (4%) 35 27	7, 52, 95, 126	0

The worst 5 of 1135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BX	164	GLU	6.1

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Mol	Chain	Res	Type	RSRZ
1	Bf	165	TYR	5.8
1	AO	165	TYR	5.7
1	CF	161	GLY	5.5
1	At	160	ALA	5.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	Cl	201	1/1	0.69	0.27	85,85,85,85	1
2	CA	BN	201	1/1	0.76	0.16	73,73,73,73	0
2	CA	Aa	201	1/1	0.76	0.13	58,58,58,58	0
2	CA	BC	201	1/1	0.79	0.24	73,73,73,73	1
2	CA	Cn	201	1/1	0.79	0.10	108,108,108,108	0
2	CA	BR	201	1/1	0.80	0.15	72,72,72,72	0
2	CA	Cg	201	1/1	0.80	0.13	85,85,85,85	0
2	CA	Bb	201	1/1	0.81	0.14	98,98,98,98	0
2	CA	AC	201	1/1	0.83	0.15	86,86,86,86	0
2	CA	BD	201	1/1	0.84	0.09	81,81,81,81	0
2	CA	AA	201	1/1	0.84	0.15	106,106,106,106	0
2	CA	Ck	201	1/1	0.85	0.09	78,78,78,78	0
2	CA	Bd	201	1/1	0.86	0.12	61,61,61,61	0
2	CA	An	201	1/1	0.86	0.14	61,61,61,61	0
2	CA	Ae	201	1/1	0.86	0.11	70,70,70,70	0
2	CA	CE	201	1/1	0.86	0.15	83,83,83,83	0
2	CA	CC	201	1/1	0.87	0.11	96,96,96,96	0
2	CA	BG	201	1/1	0.87	0.12	94,94,94,94	0
2	CA	Ca	201	1/1	0.87	0.22	87,87,87,87	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	AL	201	1/1	0.89	0.10	84,84,84,84	0
2	CA	BB	201	1/1	0.89	0.07	86,86,86,86	0
2	CA	AM	201	1/1	0.89	0.13	68,68,68,68	0
2	CA	CA	201	1/1	0.89	0.17	67,67,67,67	0
2	CA	Be	201	1/1	0.89	0.17	66,66,66,66	0
2	CA	Cb	201	1/1	0.89	0.11	80,80,80,80	0
2	CA	AB	201	1/1	0.90	0.12	75,75,75,75	0
2	CA	Ac	201	1/1	0.90	0.14	70,70,70,70	0
2	CA	Ba	201	1/1	0.90	0.08	80,80,80,80	0
2	CA	BH	201	1/1	0.91	0.11	96,96,96,96	0
2	CA	AH	201	1/1	0.91	0.12	62,62,62,62	0
2	CA	BA	201	1/1	0.91	0.13	78,78,78,78	0
2	CA	Bg	201	1/1	0.91	0.13	88,88,88,88	0
2	CA	Ag	201	1/1	0.92	0.12	55,55,55,55	0
2	CA	AO	201	1/1	0.92	0.07	67,67,67,67	0
2	CA	AF	201	1/1	0.92	0.10	68,68,68,68	0
2	CA	CF	201	1/1	0.93	0.18	63,63,63,63	0
2	CA	Bu	201	1/1	0.93	0.14	61,61,61,61	0
2	CA	Ah	201	1/1	0.93	0.13	56,56,56,56	0
2	CA	Bc	201	1/1	0.93	0.17	73,73,73,73	0
2	CA	Ce	201	1/1	0.93	0.12	106,106,106,106	0
2	CA	Aj	201	1/1	0.94	0.12	56,56,56,56	0
2	CA	CH	201	1/1	0.94	0.05	69,69,69,69	0
2	CA	Ad	201	1/1	0.94	0.10	54,54,54,54	0
2	CA	CB	201	1/1	0.94	0.11	60,60,60,60	0
2	CA	Bf	201	1/1	0.94	0.10	68,68,68,68	0
2	CA	CD	201	1/1	0.95	0.09	68,68,68,68	0
2	CA	CO	201	1/1	0.96	0.09	68,68,68,68	0
2	CA	Cp	201	1/1	0.97	0.13	69,69,69,69	0

6.5 Other polymers

There are no such residues in this entry.