



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 08:40 PM EDT

PDB ID : 4V98 / pdb_00004v98
Title : The 8S snRNP Assembly Intermediate
Authors : Grimm, C.; Pelz, J.P.; Schindelin, H.; Diederichs, K.; Kuper, J.; Kisker, C.
Deposited on : 2012-05-15
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

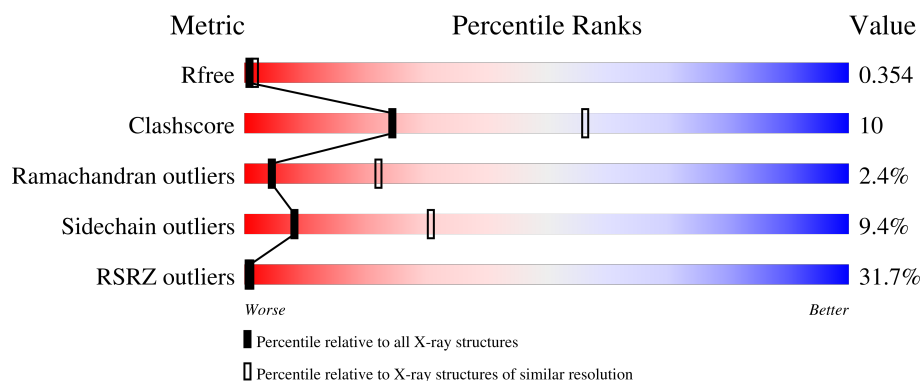
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	119	 3% 54% 13% 31%
1	AI	119	 3% 55% 13% 31%
1	AQ	119	 4% 54% 13% 31%
1	AY	119	 26% 53% 13% 31%
1	Ag	119	 5% 55% 12% 31%

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Mol	Chain	Length	Quality of chain
1	Ao	119	
1	Aw	119	
1	BA	119	
1	BI	119	
1	BQ	119	
1	BY	119	
1	Bg	119	
1	Bo	119	
1	Bw	119	
1	CA	119	
1	CI	119	
1	CQ	119	
1	CY	119	
1	Cg	119	
1	Co	119	
2	AB	118	
2	AJ	118	
2	AR	118	
2	AZ	118	
2	Ah	118	
2	Ap	118	
2	Ax	118	
2	BB	118	
2	BJ	118	
2	BR	118	

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Mol	Chain	Length	Quality of chain
2	BZ	118	
2	Bh	118	
2	Bp	118	
2	Bx	118	
2	CB	118	
2	CJ	118	
2	CR	118	
2	CZ	118	
2	Ch	118	
2	Cp	118	
3	AC	92	
3	AK	92	
3	AS	92	
3	Aa	92	
3	Ai	92	
3	Aq	92	
3	Ay	92	
3	BC	92	
3	BK	92	
3	BS	92	
3	Ba	92	
3	Bi	92	
3	Bq	92	
3	By	92	
3	CC	92	

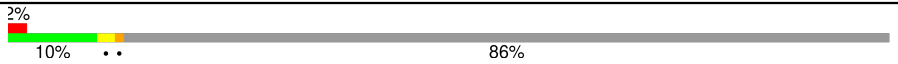
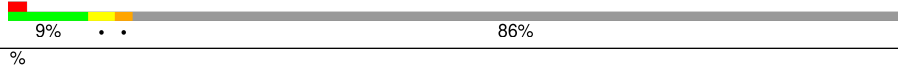
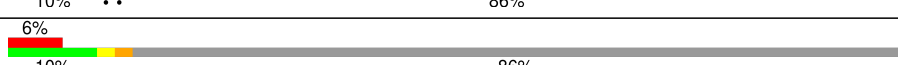
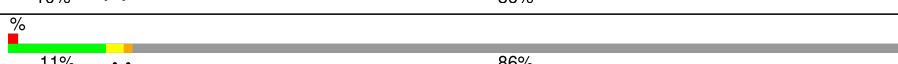
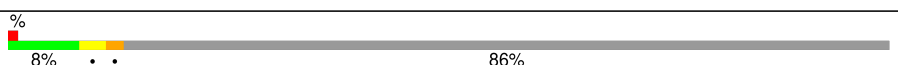
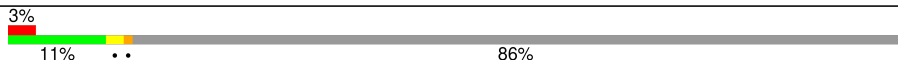
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Mol	Chain	Length	Quality of chain
3	CK	92	
3	CS	92	
3	Ca	92	
3	Ci	92	
3	Cq	92	
4	AD	86	
4	AL	86	
4	AT	86	
4	Ab	86	
4	Aj	86	
4	Ar	86	
4	Az	86	
4	BD	86	
4	BL	86	
4	BT	86	
4	Bb	86	
4	Bj	86	
4	Br	86	
4	Bz	86	
4	CD	86	
4	CL	86	
4	CT	86	
4	Cb	86	
4	Cj	86	
4	Cr	86	

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Mol	Chain	Length	Quality of chain
5	A1	124	
5	AE	124	
5	AM	124	
5	AU	124	
5	Ac	124	
5	Ak	124	
5	As	124	
5	B1	124	
5	BE	124	
5	BM	124	
5	BU	124	
5	Bc	124	
5	Bk	124	
5	Bs	124	
5	CE	124	
5	CM	124	
5	CU	124	
5	Cc	124	
5	Ck	124	
5	Cs	124	
6	A2	247	
6	AF	247	
6	AN	247	
6	AV	247	
6	Ad	247	

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Mol	Chain	Length	Quality of chain
6	Al	247	
6	At	247	
6	B2	247	
6	BF	247	
6	BN	247	
6	BV	247	
6	Bd	247	
6	Bl	247	
6	Bt	247	
6	CF	247	
6	CN	247	
6	CV	247	
6	Cd	247	
6	Cl	247	
6	Ct	247	
7	A3	186	
7	AG	186	
7	AO	186	
7	AW	186	
7	Ae	186	
7	Am	186	
7	Au	186	
7	B3	186	
7	BG	186	
7	BO	186	

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Mol	Chain	Length	Quality of chain
7	BW	186	
7	Be	186	
7	Bm	186	
7	Bu	186	
7	CG	186	
7	CO	186	
7	CW	186	
7	Ce	186	
7	Cm	186	
7	Cu	186	
8	A4	76	
8	AH	76	
8	AP	76	
8	AX	76	
8	Af	76	
8	An	76	
8	Av	76	
8	B4	76	
8	BH	76	
8	BP	76	
8	BX	76	
8	Bf	76	
8	Bn	76	
8	Bv	76	
8	CH	76	

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Mol	Chain	Length	Quality of chain
8	CP	76	41% 74% 17% 8%
8	CX	76	37% 74% 17% 8%
8	Cf	76	24% 75% 16% 8%
8	Cn	76	63% 72% 18% 8%
8	Cv	76	57% 74% 17% 8%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 121990 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 Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AI	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	AA	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	AQ	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	AY	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Ag	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Ao	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Aw	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	BA	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	BI	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	BQ	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	BY	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Bg	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Bo	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Bw	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	CA	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	CI	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CQ	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	CY	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Cg	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Co	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			

- Molecule 2 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AJ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	AB	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	AR	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	AZ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Ah	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Ap	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Ax	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	BB	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	BJ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	BR	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	BZ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Bh	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Bp	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Bx	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	CB	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CJ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	CR	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	CZ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Ch	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Cp	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			

- Molecule 3 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AK	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	AC	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	AS	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Aa	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Ai	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Aq	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Ay	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	BC	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	BK	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	BS	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Ba	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Bi	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Bq	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	By	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CC	77	Total 638	C 405	N 113	O 115	S 5	0	0	0
3	CK	77	Total 638	C 405	N 113	O 115	S 5	0	0	0
3	CS	77	Total 638	C 405	N 113	O 115	S 5	0	0	0
3	Ca	77	Total 638	C 405	N 113	O 115	S 5	0	0	0
3	Ci	77	Total 638	C 405	N 113	O 115	S 5	0	0	0
3	Cq	77	Total 638	C 405	N 113	O 115	S 5	0	0	0

- Molecule 4 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AL	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	AD	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	AT	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Ab	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Aj	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Ar	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Az	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	BD	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	BL	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	BT	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Bb	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Bj	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Br	71	Total 556	C 358	N 92	O 101	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Bz	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	CD	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	CL	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	CT	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Cb	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Cj	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Cr	71	Total 556	C 358	N 92	O 101	S 5	0	0	0

- Molecule 5 is a protein called LD23602p.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AM	17	Total 133	C 85	N 19	O 29	0	0	0
5	AE	17	Total 133	C 85	N 19	O 29	0	0	0
5	AU	17	Total 133	C 85	N 19	O 29	0	0	0
5	Ac	17	Total 133	C 85	N 19	O 29	0	0	0
5	Ak	17	Total 133	C 85	N 19	O 29	0	0	0
5	As	17	Total 133	C 85	N 19	O 29	0	0	0
5	A1	17	Total 133	C 85	N 19	O 29	0	0	0
5	BE	17	Total 133	C 85	N 19	O 29	0	0	0
5	BM	17	Total 133	C 85	N 19	O 29	0	0	0
5	BU	17	Total 133	C 85	N 19	O 29	0	0	0
5	Bc	17	Total 133	C 85	N 19	O 29	0	0	0
5	Bk	17	Total 133	C 85	N 19	O 29	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Bs	17	Total 133	C 85	N 19	O 29	0	0	0
5	B1	17	Total 133	C 85	N 19	O 29	0	0	0
5	CE	17	Total 133	C 85	N 19	O 29	0	0	0
5	CM	17	Total 133	C 85	N 19	O 29	0	0	0
5	CU	17	Total 133	C 85	N 19	O 29	0	0	0
5	Cc	17	Total 133	C 85	N 19	O 29	0	0	0
5	Ck	17	Total 133	C 85	N 19	O 29	0	0	0
5	Cs	17	Total 133	C 85	N 19	O 29	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	6991	GLY	-	expression tag	UNP Q9VV74
AM	6992	ALA	-	expression tag	UNP Q9VV74
AE	6991	GLY	-	expression tag	UNP Q9VV74
AE	6992	ALA	-	expression tag	UNP Q9VV74
AU	6991	GLY	-	expression tag	UNP Q9VV74
AU	6992	ALA	-	expression tag	UNP Q9VV74
Ac	6991	GLY	-	expression tag	UNP Q9VV74
Ac	6992	ALA	-	expression tag	UNP Q9VV74
Ak	6991	GLY	-	expression tag	UNP Q9VV74
Ak	6992	ALA	-	expression tag	UNP Q9VV74
As	6991	GLY	-	expression tag	UNP Q9VV74
As	6992	ALA	-	expression tag	UNP Q9VV74
A1	6991	GLY	-	expression tag	UNP Q9VV74
A1	6992	ALA	-	expression tag	UNP Q9VV74
BE	6991	GLY	-	expression tag	UNP Q9VV74
BE	6992	ALA	-	expression tag	UNP Q9VV74
BM	6991	GLY	-	expression tag	UNP Q9VV74
BM	6992	ALA	-	expression tag	UNP Q9VV74
BU	6991	GLY	-	expression tag	UNP Q9VV74
BU	6992	ALA	-	expression tag	UNP Q9VV74
Bc	6991	GLY	-	expression tag	UNP Q9VV74
Bc	6992	ALA	-	expression tag	UNP Q9VV74
Bk	6991	GLY	-	expression tag	UNP Q9VV74

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Chain	Residue	Modelled	Actual	Comment	Reference
Bk	6992	ALA	-	expression tag	UNP Q9VV74
Bs	6991	GLY	-	expression tag	UNP Q9VV74
Bs	6992	ALA	-	expression tag	UNP Q9VV74
B1	6991	GLY	-	expression tag	UNP Q9VV74
B1	6992	ALA	-	expression tag	UNP Q9VV74
CE	6991	GLY	-	expression tag	UNP Q9VV74
CE	6992	ALA	-	expression tag	UNP Q9VV74
CM	6991	GLY	-	expression tag	UNP Q9VV74
CM	6992	ALA	-	expression tag	UNP Q9VV74
CU	6991	GLY	-	expression tag	UNP Q9VV74
CU	6992	ALA	-	expression tag	UNP Q9VV74
Cc	6991	GLY	-	expression tag	UNP Q9VV74
Cc	6992	ALA	-	expression tag	UNP Q9VV74
Ck	6991	GLY	-	expression tag	UNP Q9VV74
Ck	6992	ALA	-	expression tag	UNP Q9VV74
Cs	6991	GLY	-	expression tag	UNP Q9VV74
Cs	6992	ALA	-	expression tag	UNP Q9VV74

- Molecule 6 is a protein called CG10419.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AN	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	AF	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	AV	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Ad	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Al	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	At	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	A2	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	BF	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	BN	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	BV	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Bd	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B1	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Bt	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	B2	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	CF	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	CN	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	CV	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Cd	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Cl	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Ct	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	7969	GLY	-	expression tag	UNP Q9V VX0
AN	7970	ALA	-	expression tag	UNP Q9V VX0
AF	7969	GLY	-	expression tag	UNP Q9V VX0
AF	7970	ALA	-	expression tag	UNP Q9V VX0
AV	7969	GLY	-	expression tag	UNP Q9V VX0
AV	7970	ALA	-	expression tag	UNP Q9V VX0
Ad	7969	GLY	-	expression tag	UNP Q9V VX0
Ad	7970	ALA	-	expression tag	UNP Q9V VX0
Al	7969	GLY	-	expression tag	UNP Q9V VX0
Al	7970	ALA	-	expression tag	UNP Q9V VX0
At	7969	GLY	-	expression tag	UNP Q9V VX0
At	7970	ALA	-	expression tag	UNP Q9V VX0
A2	7969	GLY	-	expression tag	UNP Q9V VX0
A2	7970	ALA	-	expression tag	UNP Q9V VX0
BF	7969	GLY	-	expression tag	UNP Q9V VX0
BF	7970	ALA	-	expression tag	UNP Q9V VX0
BN	7969	GLY	-	expression tag	UNP Q9V VX0
BN	7970	ALA	-	expression tag	UNP Q9V VX0
BV	7969	GLY	-	expression tag	UNP Q9V VX0
BV	7970	ALA	-	expression tag	UNP Q9V VX0
Bd	7969	GLY	-	expression tag	UNP Q9V VX0

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Chain	Residue	Modelled	Actual	Comment	Reference
Bd	7970	ALA	-	expression tag	UNP Q9V VX0
Bl	7969	GLY	-	expression tag	UNP Q9V VX0
Bl	7970	ALA	-	expression tag	UNP Q9V VX0
Bt	7969	GLY	-	expression tag	UNP Q9V VX0
Bt	7970	ALA	-	expression tag	UNP Q9V VX0
B2	7969	GLY	-	expression tag	UNP Q9V VX0
B2	7970	ALA	-	expression tag	UNP Q9V VX0
CF	7969	GLY	-	expression tag	UNP Q9V VX0
CF	7970	ALA	-	expression tag	UNP Q9V VX0
CN	7969	GLY	-	expression tag	UNP Q9V VX0
CN	7970	ALA	-	expression tag	UNP Q9V VX0
CV	7969	GLY	-	expression tag	UNP Q9V VX0
CV	7970	ALA	-	expression tag	UNP Q9V VX0
Cd	7969	GLY	-	expression tag	UNP Q9V VX0
Cd	7970	ALA	-	expression tag	UNP Q9V VX0
Cl	7969	GLY	-	expression tag	UNP Q9V VX0
Cl	7970	ALA	-	expression tag	UNP Q9V VX0
Ct	7969	GLY	-	expression tag	UNP Q9V VX0
Ct	7970	ALA	-	expression tag	UNP Q9V VX0

- Molecule 7 is a protein called Icln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AO	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	AG	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	AW	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Ae	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Am	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Au	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	A3	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	BG	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	BO	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	BW	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Be	127	Total 984	C 626	N 161	O 188	S 9	0	0	0
7	Bm	127	Total 984	C 626	N 161	O 188	S 9	0	0	0
7	Bu	127	Total 984	C 626	N 161	O 188	S 9	0	0	0
7	B3	127	Total 984	C 626	N 161	O 188	S 9	0	0	0
7	CG	127	Total 984	C 626	N 161	O 188	S 9	0	0	0
7	CO	127	Total 984	C 626	N 161	O 188	S 9	0	0	0
7	CW	127	Total 984	C 626	N 161	O 188	S 9	0	0	0
7	Ce	127	Total 984	C 626	N 161	O 188	S 9	0	0	0
7	Cm	127	Total 984	C 626	N 161	O 188	S 9	0	0	0
7	Cu	127	Total 984	C 626	N 161	O 188	S 9	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	6180	HIS	-	expression tag	UNP Q9U3W1
AO	6181	HIS	-	expression tag	UNP Q9U3W1
AO	6182	HIS	-	expression tag	UNP Q9U3W1
AO	6183	HIS	-	expression tag	UNP Q9U3W1
AO	6184	HIS	-	expression tag	UNP Q9U3W1
AO	6185	HIS	-	expression tag	UNP Q9U3W1
AG	6180	HIS	-	expression tag	UNP Q9U3W1
AG	6181	HIS	-	expression tag	UNP Q9U3W1
AG	6182	HIS	-	expression tag	UNP Q9U3W1
AG	6183	HIS	-	expression tag	UNP Q9U3W1
AG	6184	HIS	-	expression tag	UNP Q9U3W1
AG	6185	HIS	-	expression tag	UNP Q9U3W1
AW	6180	HIS	-	expression tag	UNP Q9U3W1
AW	6181	HIS	-	expression tag	UNP Q9U3W1
AW	6182	HIS	-	expression tag	UNP Q9U3W1
AW	6183	HIS	-	expression tag	UNP Q9U3W1
AW	6184	HIS	-	expression tag	UNP Q9U3W1
AW	6185	HIS	-	expression tag	UNP Q9U3W1
Ae	6180	HIS	-	expression tag	UNP Q9U3W1

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Chain	Residue	Modelled	Actual	Comment	Reference
Ae	6181	HIS	-	expression tag	UNP Q9U3W1
Ae	6182	HIS	-	expression tag	UNP Q9U3W1
Ae	6183	HIS	-	expression tag	UNP Q9U3W1
Ae	6184	HIS	-	expression tag	UNP Q9U3W1
Ae	6185	HIS	-	expression tag	UNP Q9U3W1
Am	6180	HIS	-	expression tag	UNP Q9U3W1
Am	6181	HIS	-	expression tag	UNP Q9U3W1
Am	6182	HIS	-	expression tag	UNP Q9U3W1
Am	6183	HIS	-	expression tag	UNP Q9U3W1
Am	6184	HIS	-	expression tag	UNP Q9U3W1
Am	6185	HIS	-	expression tag	UNP Q9U3W1
Au	6180	HIS	-	expression tag	UNP Q9U3W1
Au	6181	HIS	-	expression tag	UNP Q9U3W1
Au	6182	HIS	-	expression tag	UNP Q9U3W1
Au	6183	HIS	-	expression tag	UNP Q9U3W1
Au	6184	HIS	-	expression tag	UNP Q9U3W1
Au	6185	HIS	-	expression tag	UNP Q9U3W1
A3	6180	HIS	-	expression tag	UNP Q9U3W1
A3	6181	HIS	-	expression tag	UNP Q9U3W1
A3	6182	HIS	-	expression tag	UNP Q9U3W1
A3	6183	HIS	-	expression tag	UNP Q9U3W1
A3	6184	HIS	-	expression tag	UNP Q9U3W1
A3	6185	HIS	-	expression tag	UNP Q9U3W1
BG	6180	HIS	-	expression tag	UNP Q9U3W1
BG	6181	HIS	-	expression tag	UNP Q9U3W1
BG	6182	HIS	-	expression tag	UNP Q9U3W1
BG	6183	HIS	-	expression tag	UNP Q9U3W1
BG	6184	HIS	-	expression tag	UNP Q9U3W1
BG	6185	HIS	-	expression tag	UNP Q9U3W1
BO	6180	HIS	-	expression tag	UNP Q9U3W1
BO	6181	HIS	-	expression tag	UNP Q9U3W1
BO	6182	HIS	-	expression tag	UNP Q9U3W1
BO	6183	HIS	-	expression tag	UNP Q9U3W1
BO	6184	HIS	-	expression tag	UNP Q9U3W1
BO	6185	HIS	-	expression tag	UNP Q9U3W1
BW	6180	HIS	-	expression tag	UNP Q9U3W1
BW	6181	HIS	-	expression tag	UNP Q9U3W1
BW	6182	HIS	-	expression tag	UNP Q9U3W1
BW	6183	HIS	-	expression tag	UNP Q9U3W1
BW	6184	HIS	-	expression tag	UNP Q9U3W1
BW	6185	HIS	-	expression tag	UNP Q9U3W1
Be	6180	HIS	-	expression tag	UNP Q9U3W1

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Chain	Residue	Modelled	Actual	Comment	Reference
Be	6181	HIS	-	expression tag	UNP Q9U3W1
Be	6182	HIS	-	expression tag	UNP Q9U3W1
Be	6183	HIS	-	expression tag	UNP Q9U3W1
Be	6184	HIS	-	expression tag	UNP Q9U3W1
Be	6185	HIS	-	expression tag	UNP Q9U3W1
Bm	6180	HIS	-	expression tag	UNP Q9U3W1
Bm	6181	HIS	-	expression tag	UNP Q9U3W1
Bm	6182	HIS	-	expression tag	UNP Q9U3W1
Bm	6183	HIS	-	expression tag	UNP Q9U3W1
Bm	6184	HIS	-	expression tag	UNP Q9U3W1
Bm	6185	HIS	-	expression tag	UNP Q9U3W1
Bu	6180	HIS	-	expression tag	UNP Q9U3W1
Bu	6181	HIS	-	expression tag	UNP Q9U3W1
Bu	6182	HIS	-	expression tag	UNP Q9U3W1
Bu	6183	HIS	-	expression tag	UNP Q9U3W1
Bu	6184	HIS	-	expression tag	UNP Q9U3W1
Bu	6185	HIS	-	expression tag	UNP Q9U3W1
B3	6180	HIS	-	expression tag	UNP Q9U3W1
B3	6181	HIS	-	expression tag	UNP Q9U3W1
B3	6182	HIS	-	expression tag	UNP Q9U3W1
B3	6183	HIS	-	expression tag	UNP Q9U3W1
B3	6184	HIS	-	expression tag	UNP Q9U3W1
B3	6185	HIS	-	expression tag	UNP Q9U3W1
CG	6180	HIS	-	expression tag	UNP Q9U3W1
CG	6181	HIS	-	expression tag	UNP Q9U3W1
CG	6182	HIS	-	expression tag	UNP Q9U3W1
CG	6183	HIS	-	expression tag	UNP Q9U3W1
CG	6184	HIS	-	expression tag	UNP Q9U3W1
CG	6185	HIS	-	expression tag	UNP Q9U3W1
CO	6180	HIS	-	expression tag	UNP Q9U3W1
CO	6181	HIS	-	expression tag	UNP Q9U3W1
CO	6182	HIS	-	expression tag	UNP Q9U3W1
CO	6183	HIS	-	expression tag	UNP Q9U3W1
CO	6184	HIS	-	expression tag	UNP Q9U3W1
CO	6185	HIS	-	expression tag	UNP Q9U3W1
CW	6180	HIS	-	expression tag	UNP Q9U3W1
CW	6181	HIS	-	expression tag	UNP Q9U3W1
CW	6182	HIS	-	expression tag	UNP Q9U3W1
CW	6183	HIS	-	expression tag	UNP Q9U3W1
CW	6184	HIS	-	expression tag	UNP Q9U3W1
CW	6185	HIS	-	expression tag	UNP Q9U3W1
Ce	6180	HIS	-	expression tag	UNP Q9U3W1

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Chain	Residue	Modelled	Actual	Comment	Reference
Ce	6181	HIS	-	expression tag	UNP Q9U3W1
Ce	6182	HIS	-	expression tag	UNP Q9U3W1
Ce	6183	HIS	-	expression tag	UNP Q9U3W1
Ce	6184	HIS	-	expression tag	UNP Q9U3W1
Ce	6185	HIS	-	expression tag	UNP Q9U3W1
Cm	6180	HIS	-	expression tag	UNP Q9U3W1
Cm	6181	HIS	-	expression tag	UNP Q9U3W1
Cm	6182	HIS	-	expression tag	UNP Q9U3W1
Cm	6183	HIS	-	expression tag	UNP Q9U3W1
Cm	6184	HIS	-	expression tag	UNP Q9U3W1
Cm	6185	HIS	-	expression tag	UNP Q9U3W1
Cu	6180	HIS	-	expression tag	UNP Q9U3W1
Cu	6181	HIS	-	expression tag	UNP Q9U3W1
Cu	6182	HIS	-	expression tag	UNP Q9U3W1
Cu	6183	HIS	-	expression tag	UNP Q9U3W1
Cu	6184	HIS	-	expression tag	UNP Q9U3W1
Cu	6185	HIS	-	expression tag	UNP Q9U3W1

- Molecule 8 is a protein called Small nuclear ribonucleoprotein G.

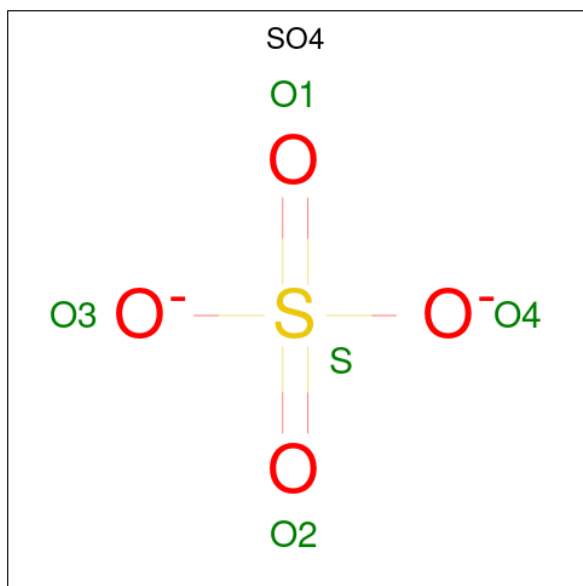
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AP	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	AH	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	AX	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Af	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	An	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Av	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	A4	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	BH	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	BP	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	BX	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Bf	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Bn	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Bv	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	B4	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	CH	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	CP	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	CX	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Cf	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Cn	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Cv	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

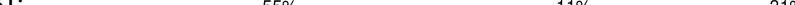


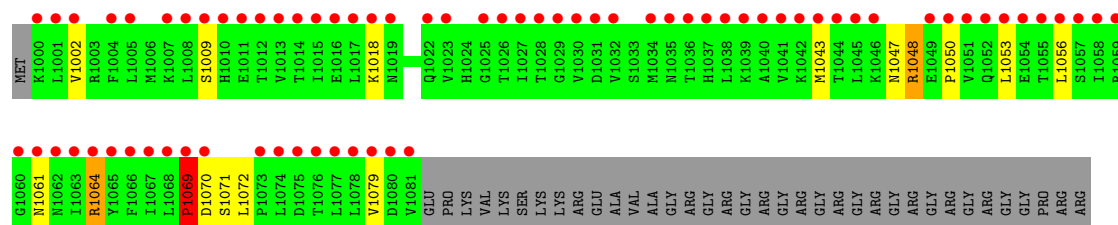
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	Ad	1	Total	O	S	0	0
			5	4	1		
9	At	1	Total	O	S	0	0
			5	4	1		

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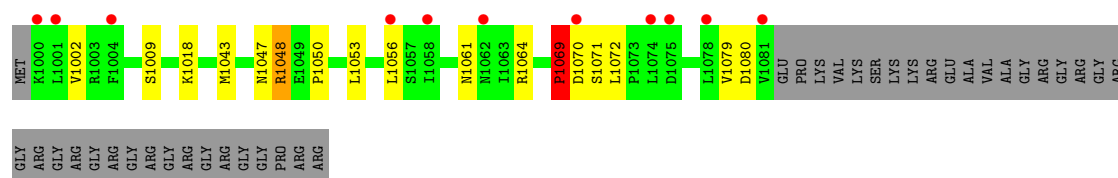
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A2	1	Total	O	S	0	0
			5	4	1		
9	BF	1	Total	O	S	0	0
			5	4	1		
9	BV	1	Total	O	S	0	0
			5	4	1		
9	Bd	1	Total	O	S	0	0
			5	4	1		
9	Bt	1	Total	O	S	0	0
			5	4	1		
9	B2	1	Total	O	S	0	0
			5	4	1		
9	CF	1	Total	O	S	0	0
			5	4	1		
9	Cl	1	Total	O	S	0	0
			5	4	1		

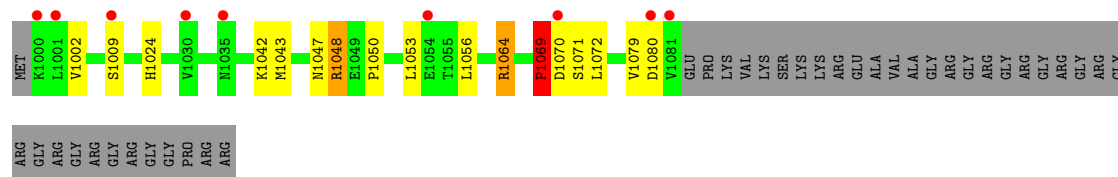
Chain BI: 



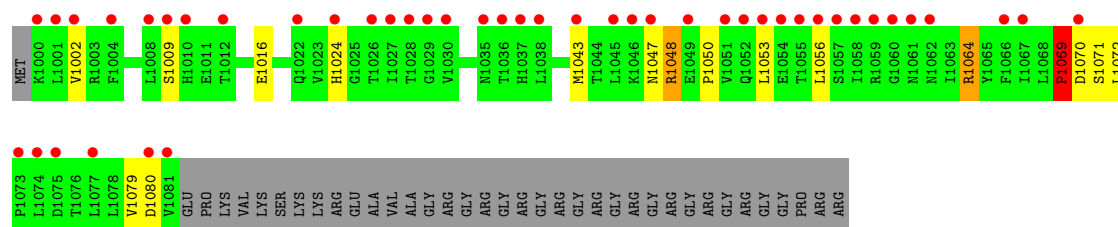
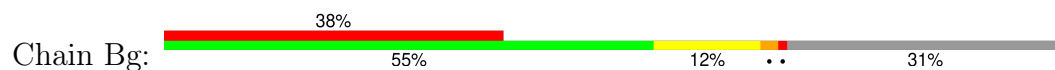
• Molecule 1: Small nuclear ribonucleoprotein Sm D1



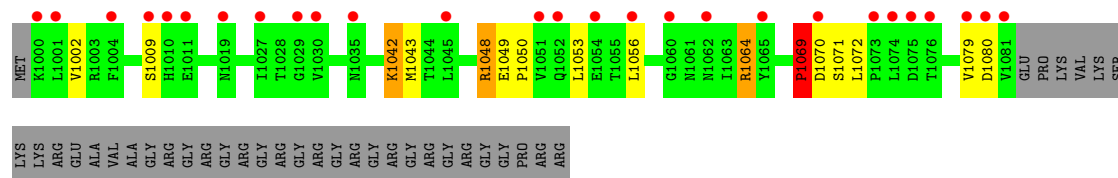
• Molecule 1: Small nuclear ribonucleoprotein Sm D1



• Molecule 1: Small nuclear ribonucleoprotein Sm D1



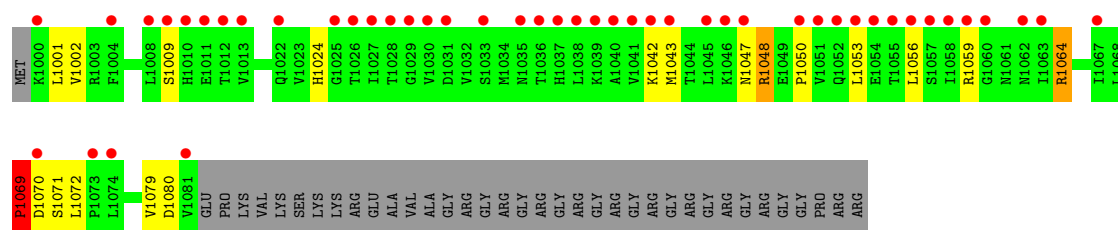
• Molecule 1: Small nuclear ribonucleoprotein Sm D1



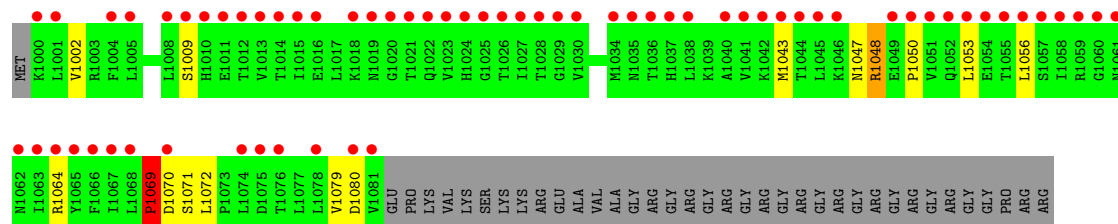
• Molecule 1: Small nuclear ribonucleoprotein Sm D1



Chain Cg:



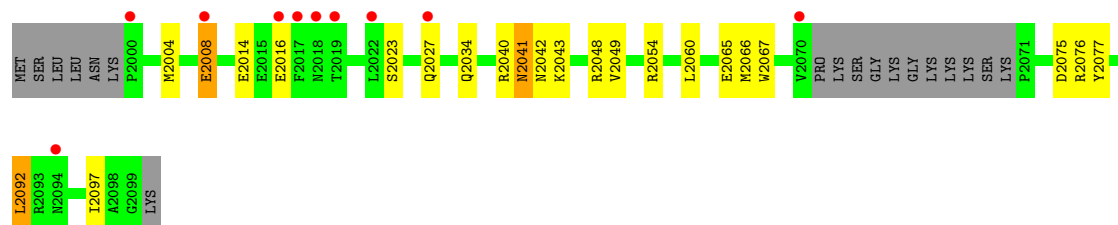
Chain Co:



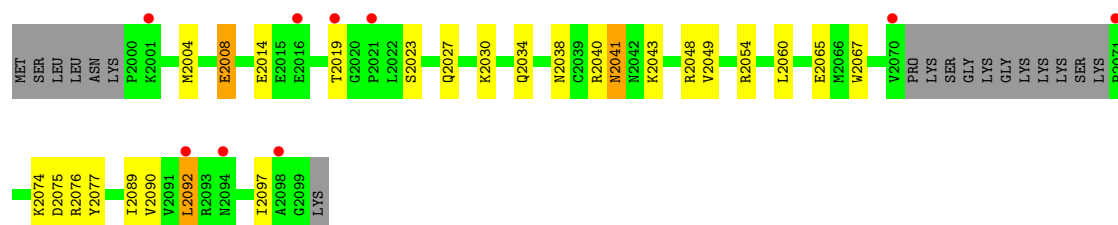
Chain A.J:



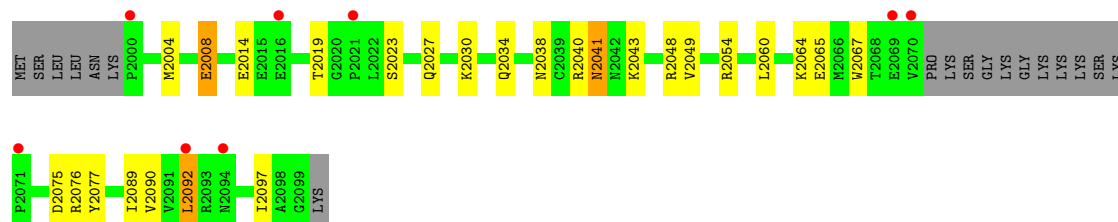
Chain AB:



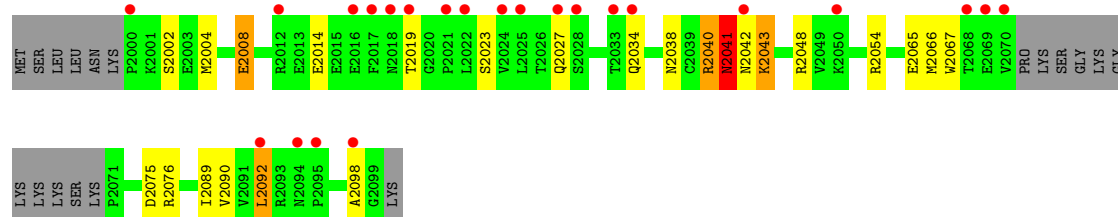
Chain AR:



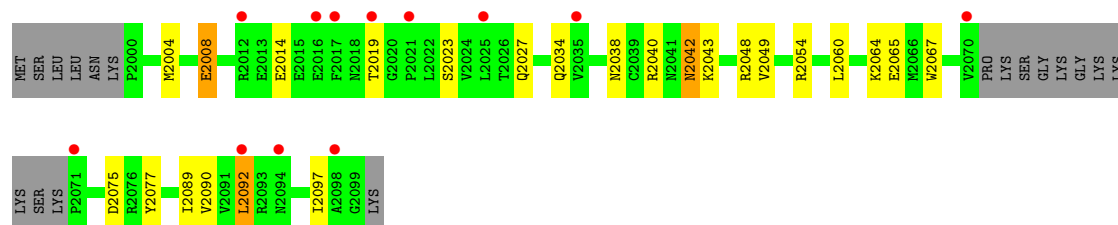
• Molecule 2: Small nuclear ribonucleoprotein Sm D2



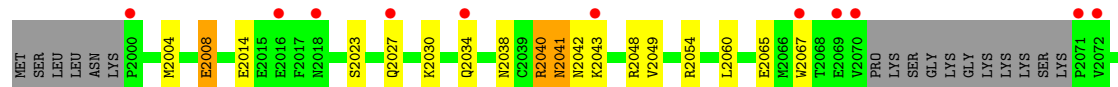
• Molecule 2: Small nuclear ribonucleoprotein Sm D2

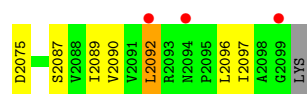


• Molecule 2: Small nuclear ribonucleoprotein Sm D2

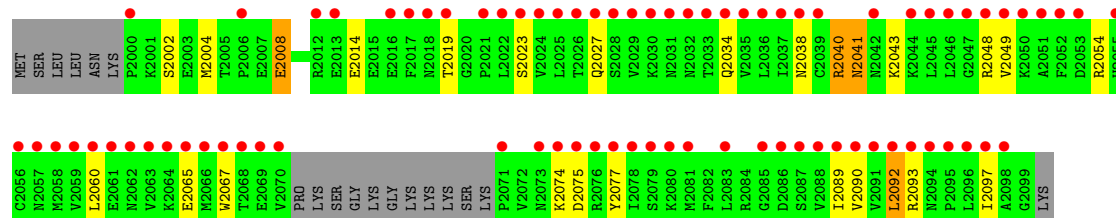


• Molecule 2: Small nuclear ribonucleoprotein Sm D2

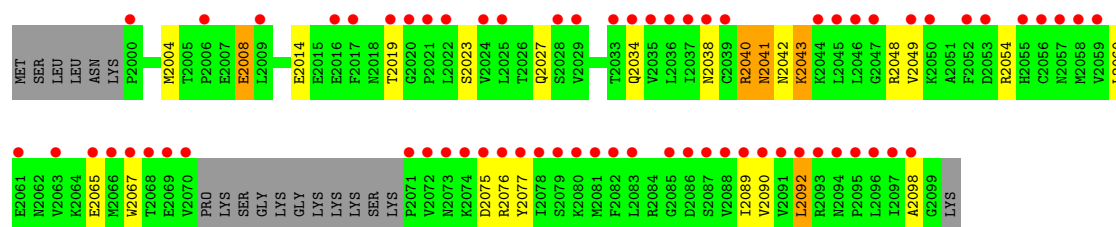




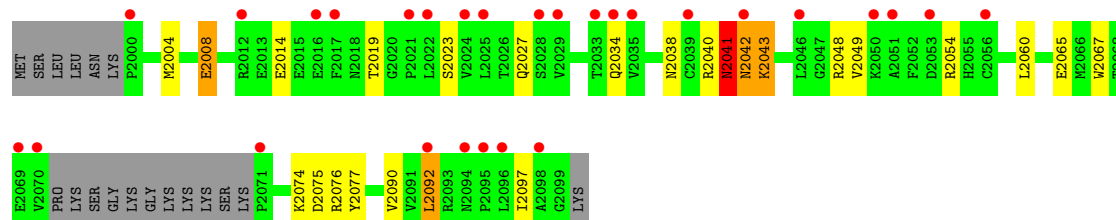
• Molecule 2: Small nuclear ribonucleoprotein Sm D2



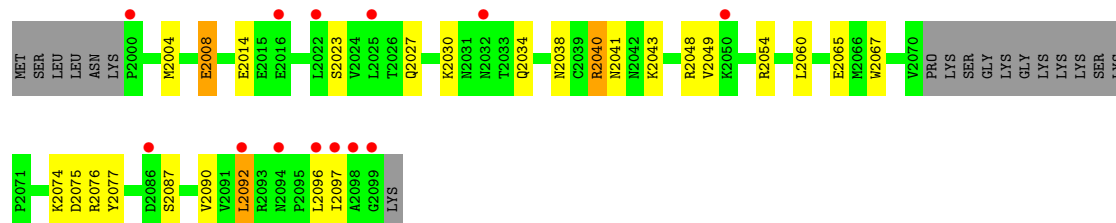
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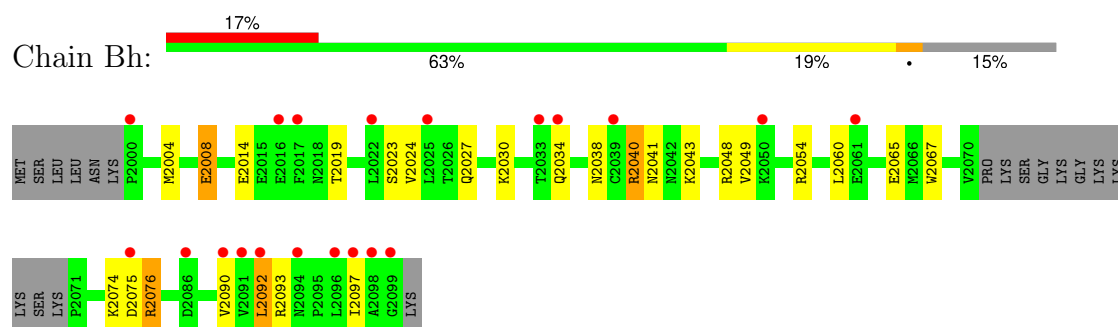
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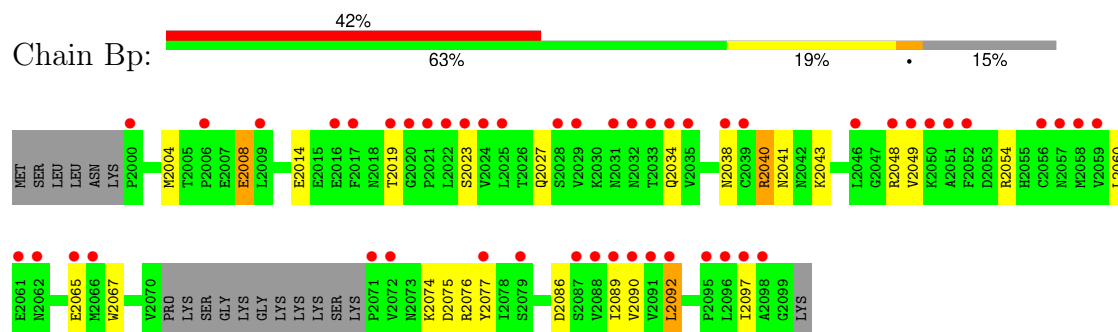
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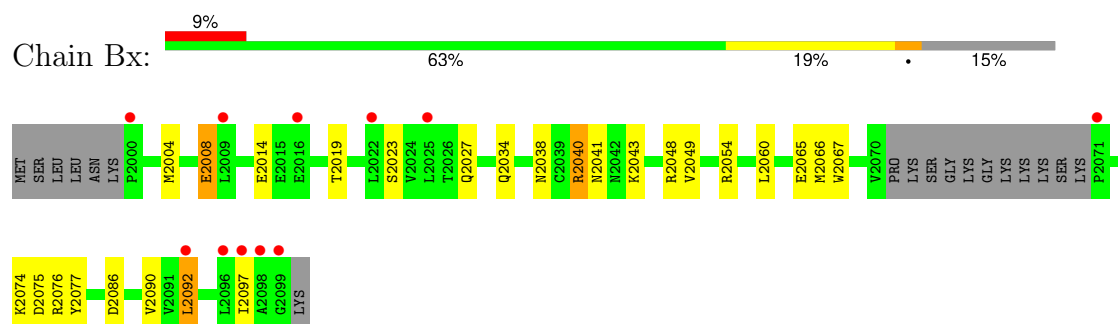
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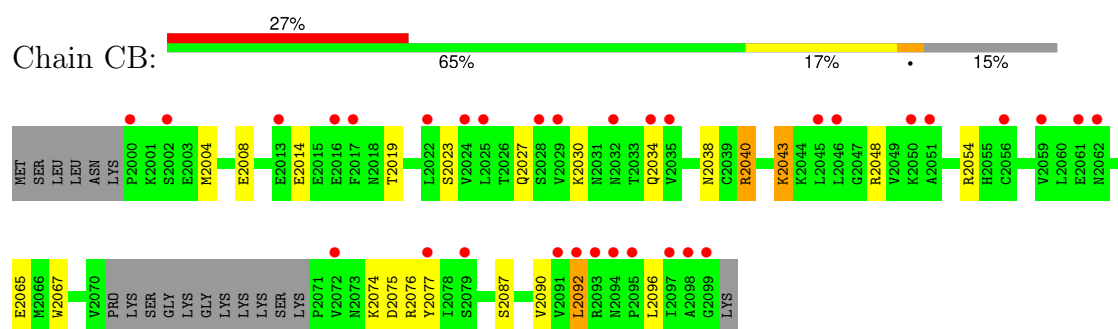
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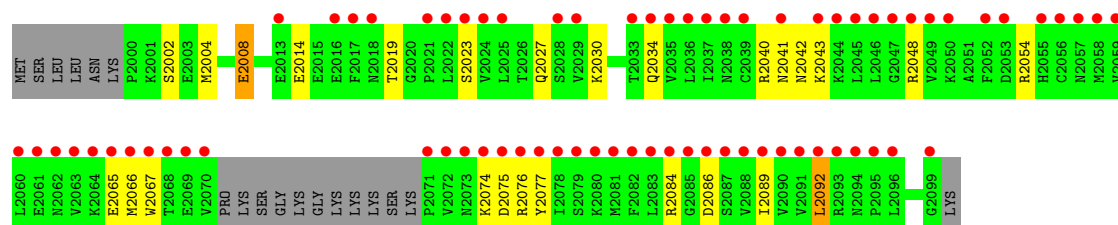


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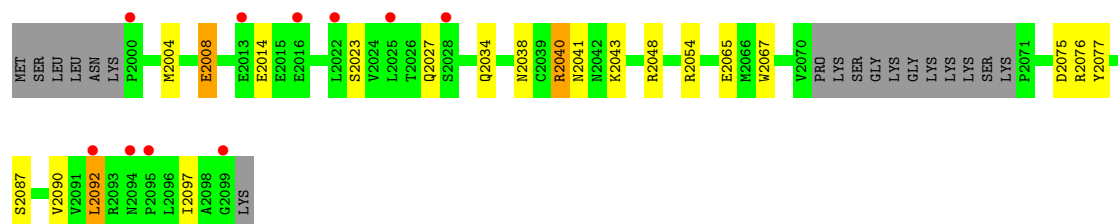


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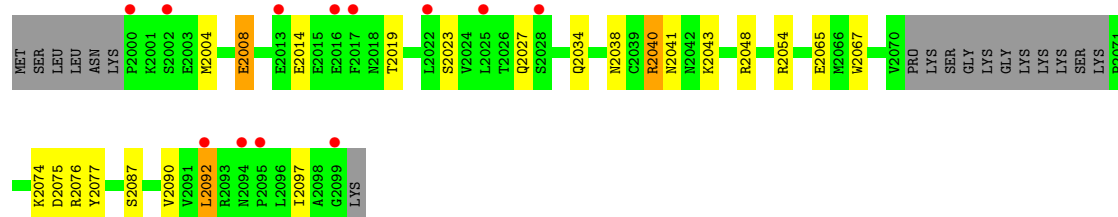




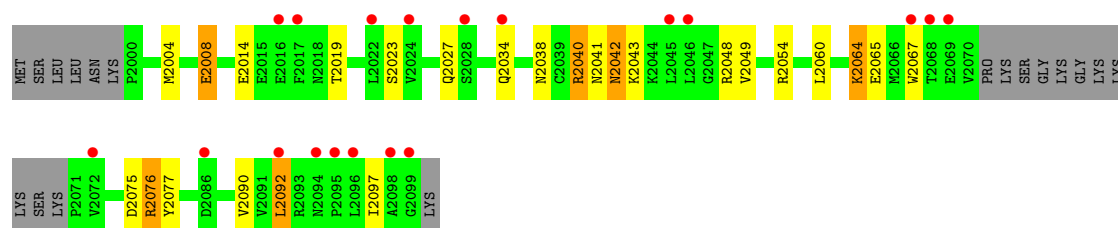
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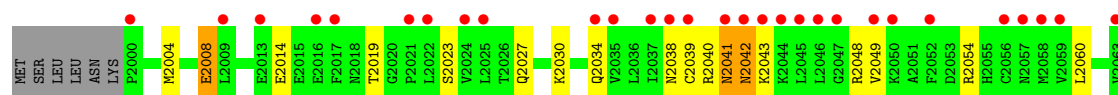
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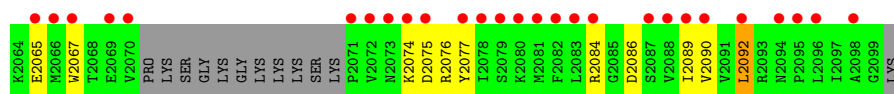


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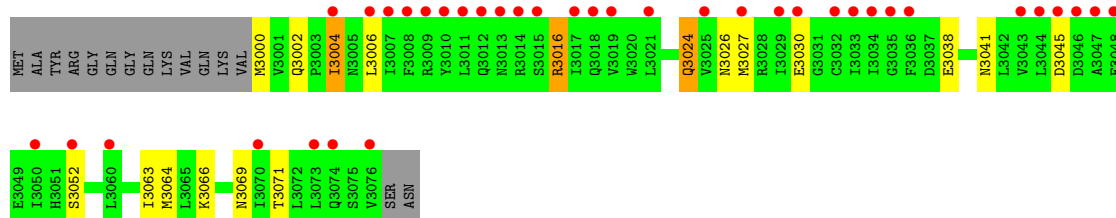
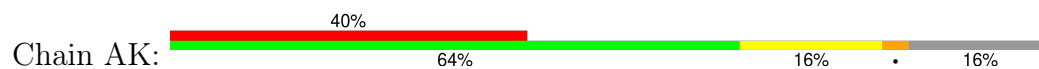


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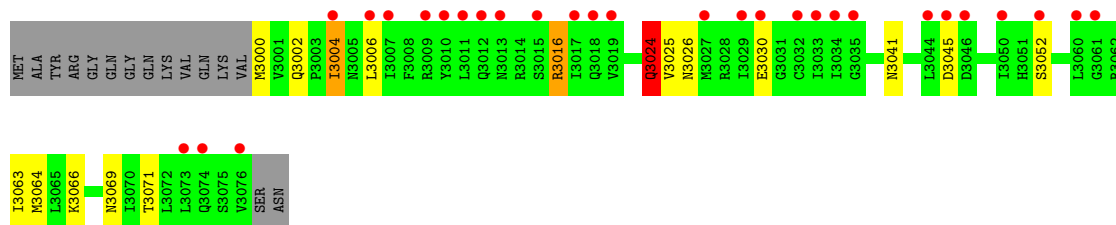




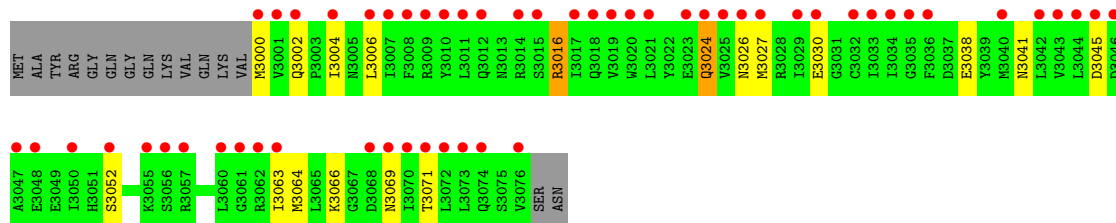
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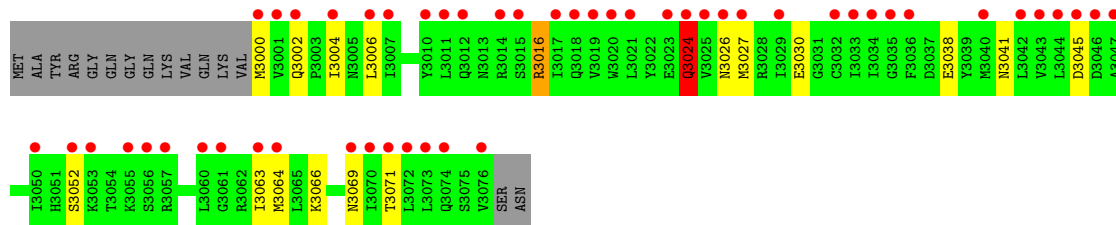
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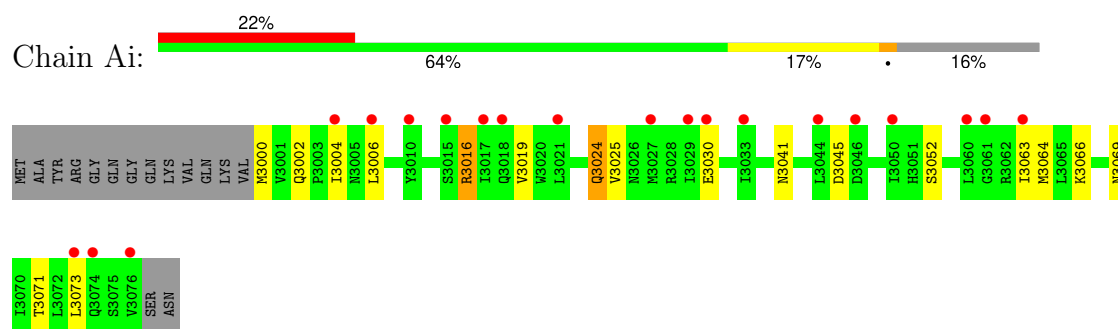
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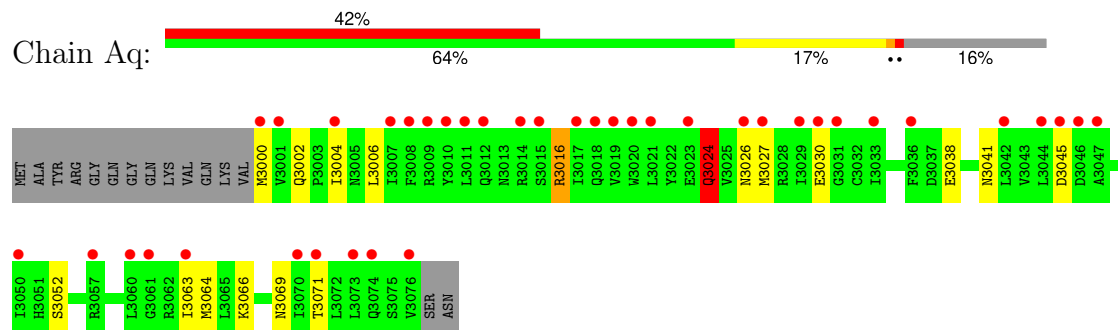
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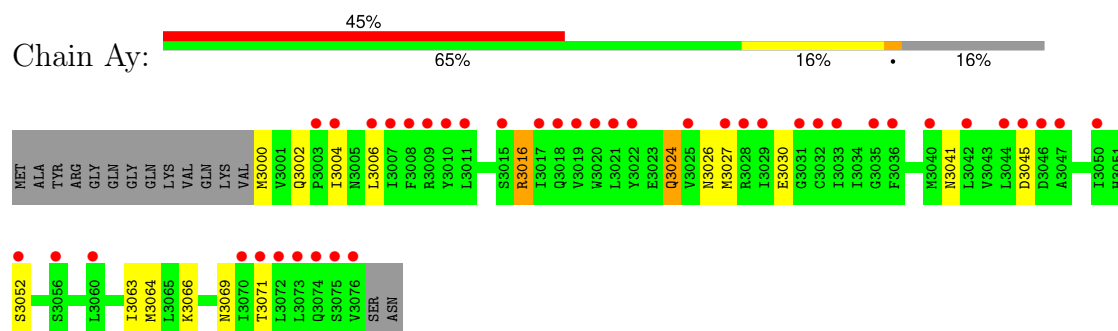
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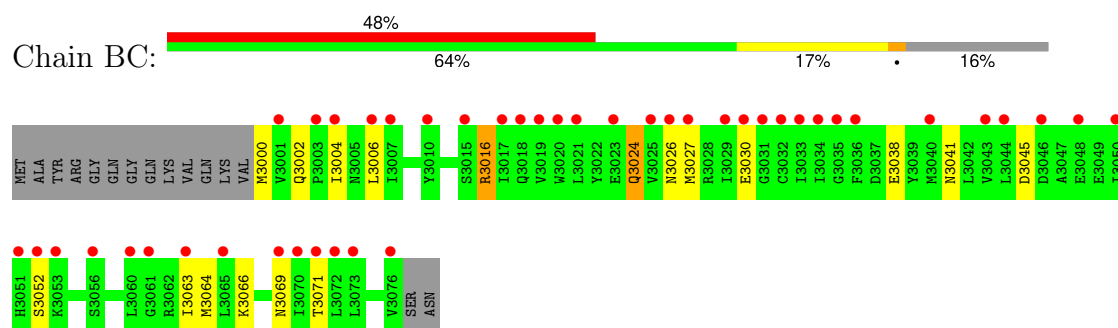
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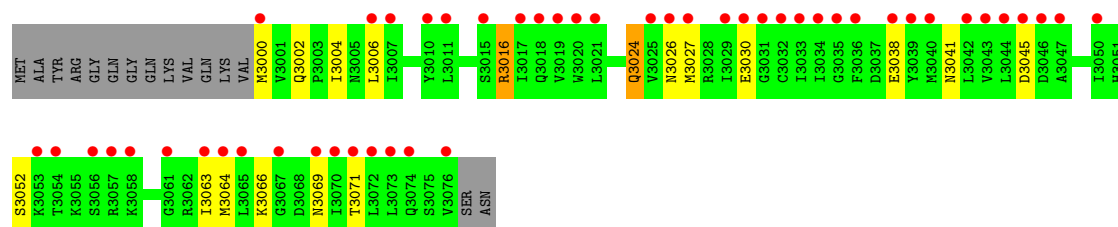


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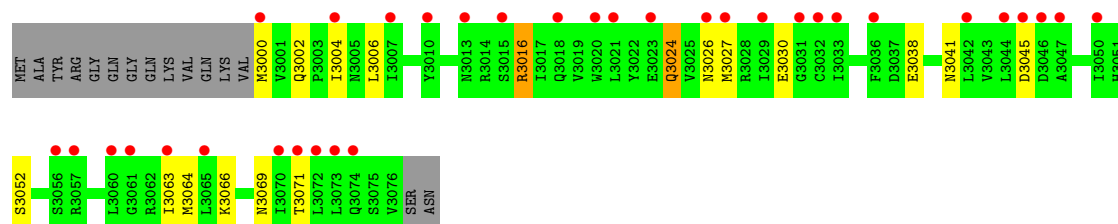
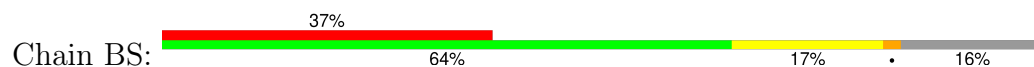


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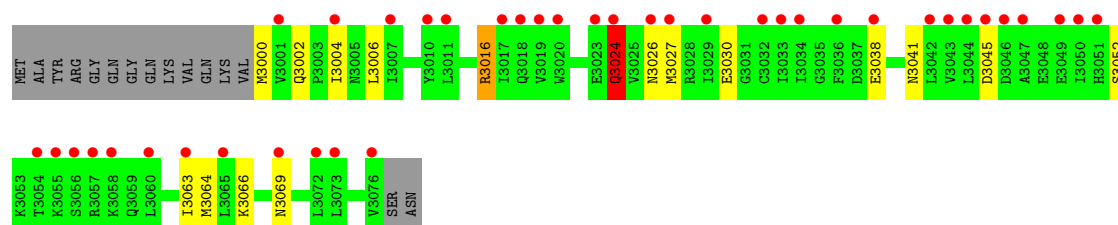




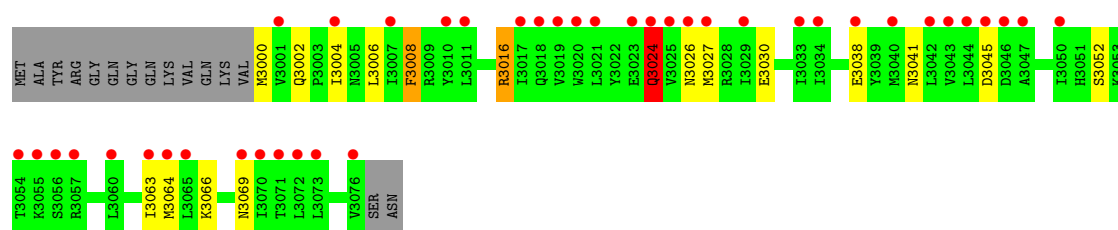
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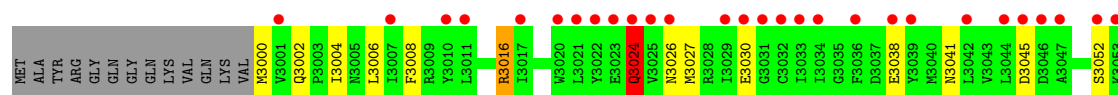
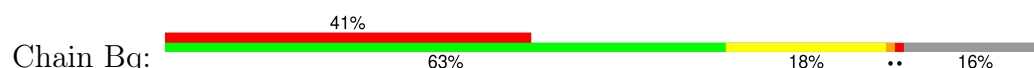
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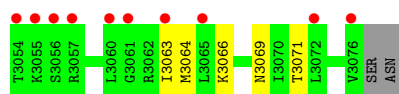


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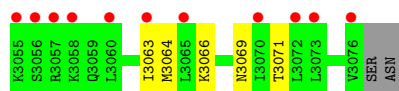
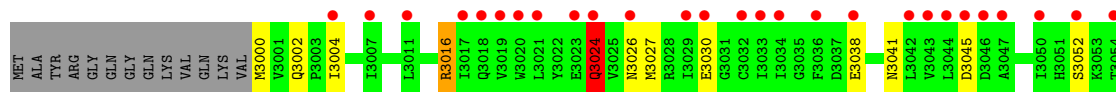
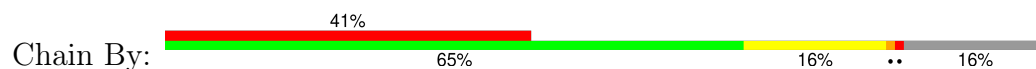


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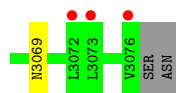
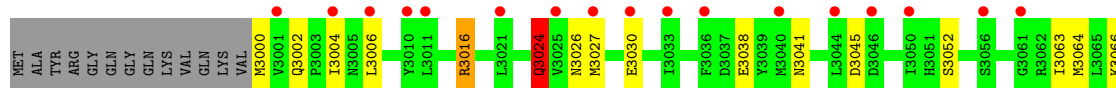




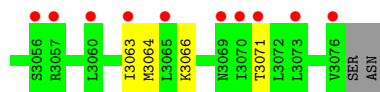
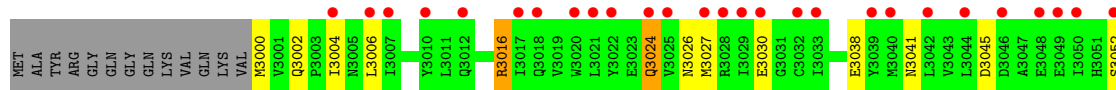
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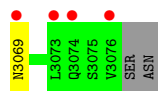
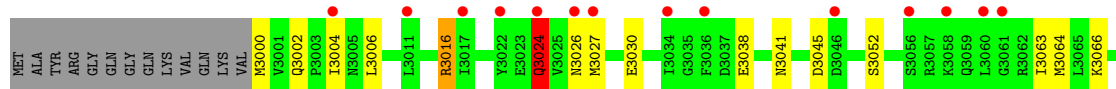
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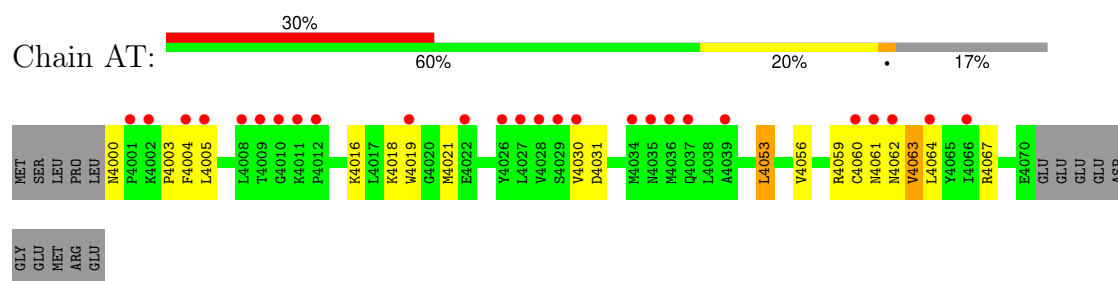
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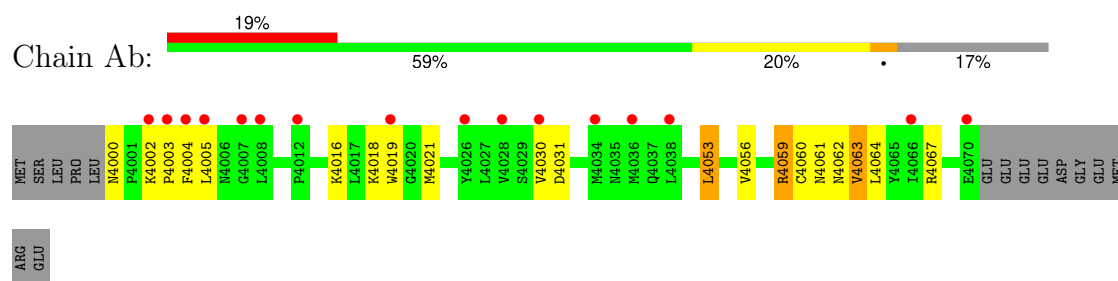
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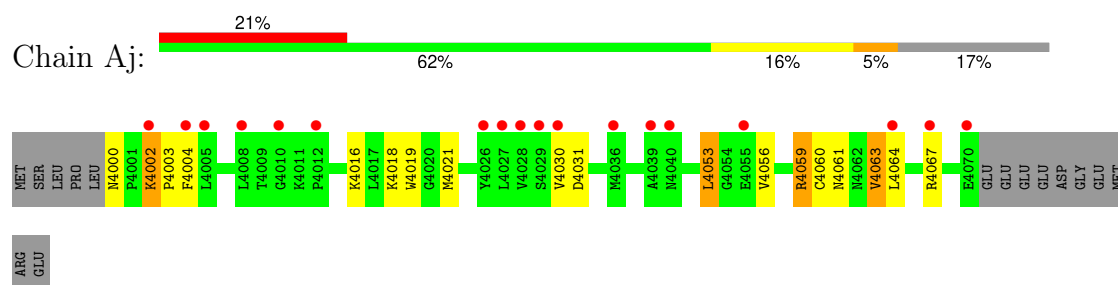
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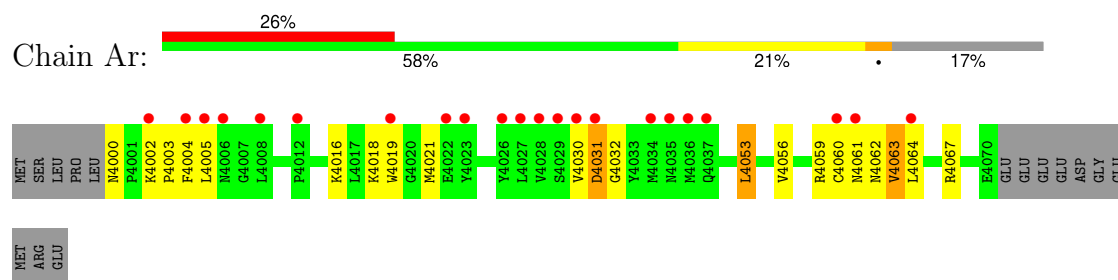
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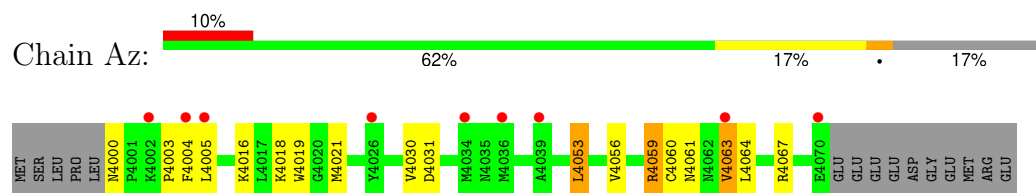
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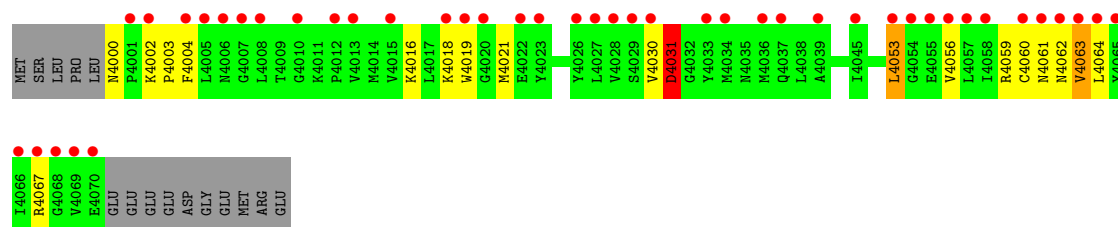


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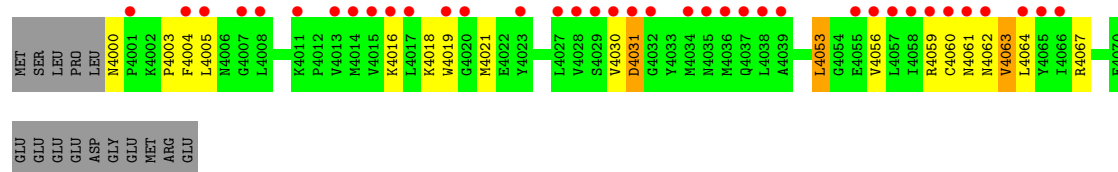
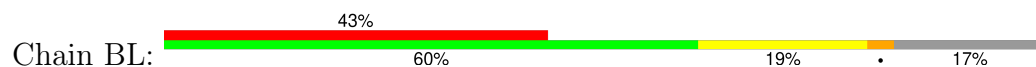


• Molecule 4: Small nuclear ribonucleoprotein F

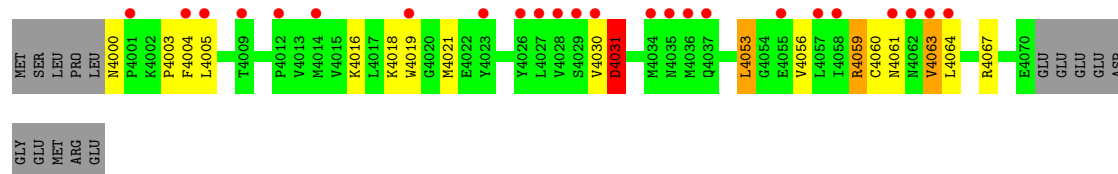




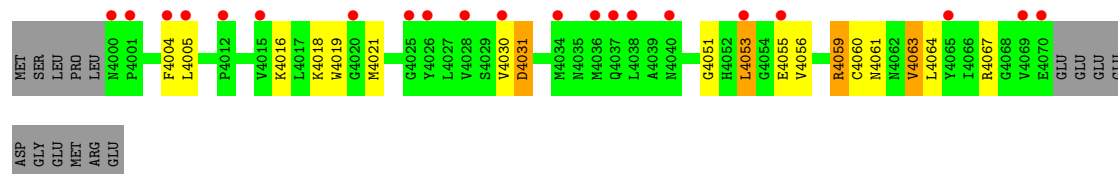
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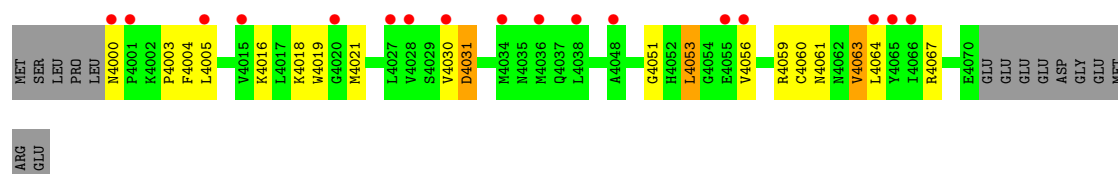
• Molecule 4: Small nuclear ribonucleoprotein F



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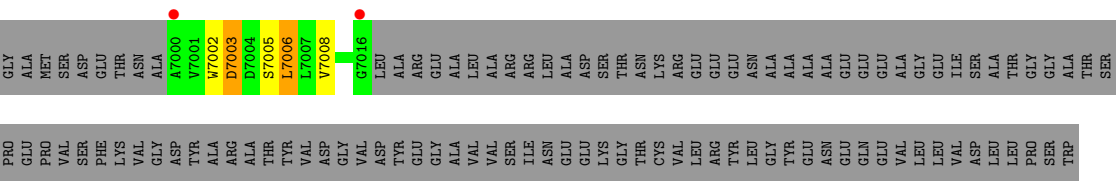
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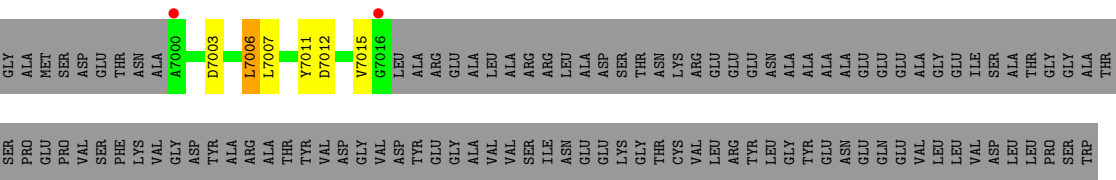
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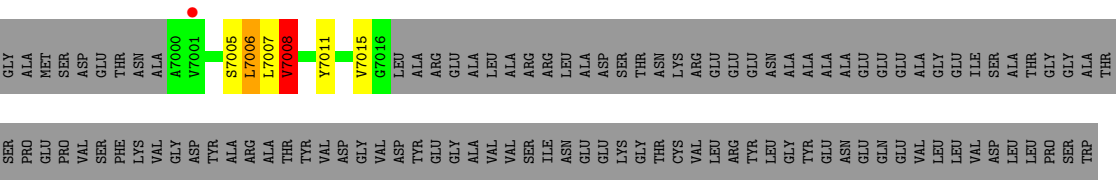
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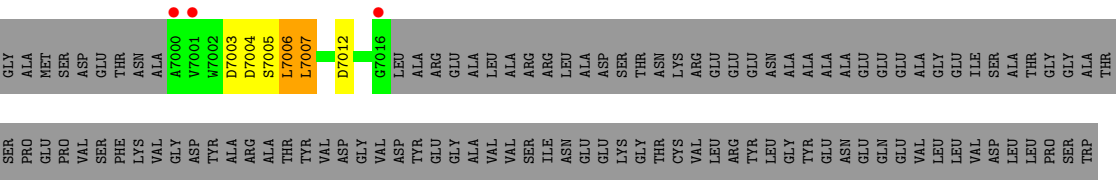
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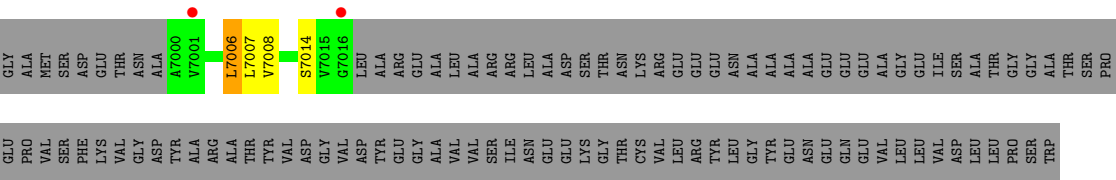
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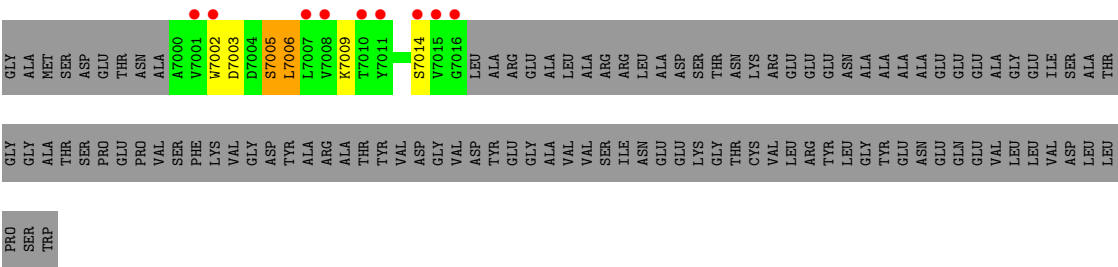


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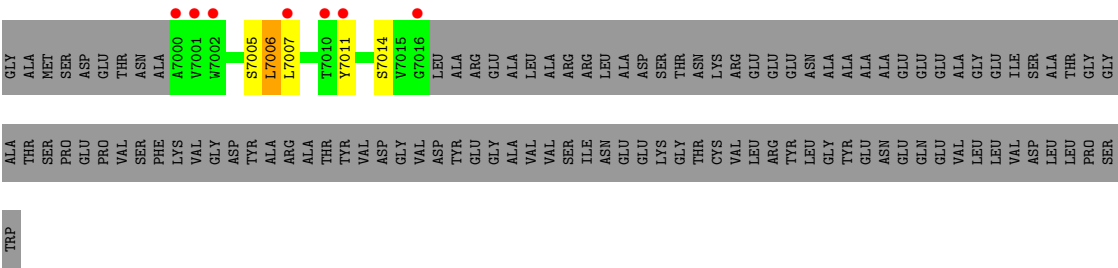


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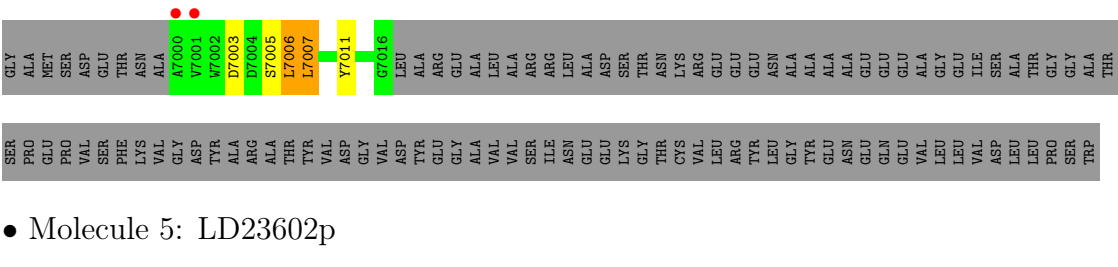




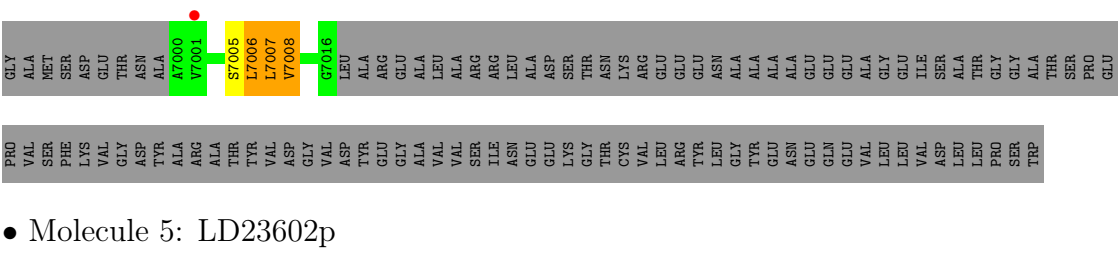
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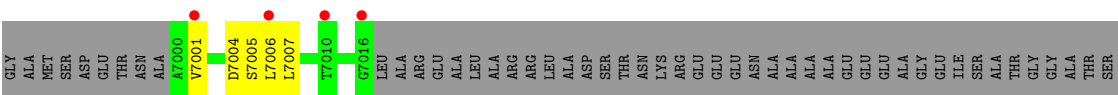
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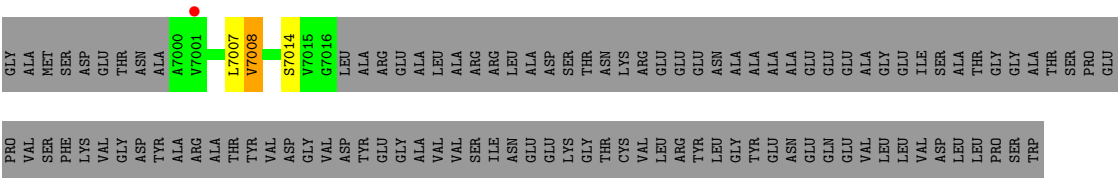


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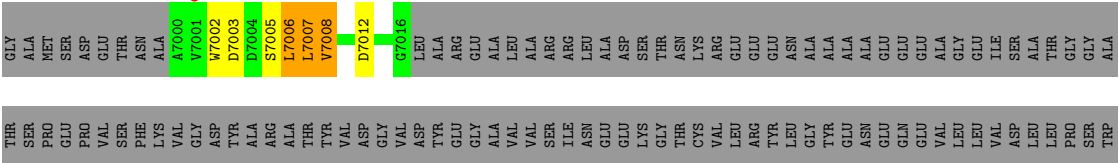


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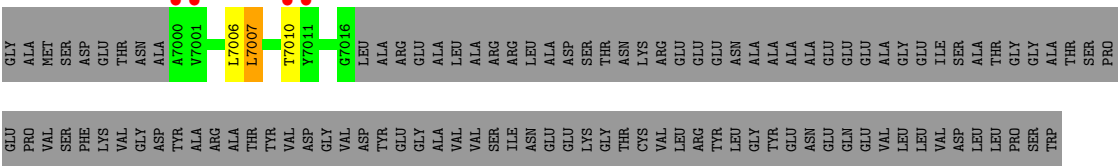




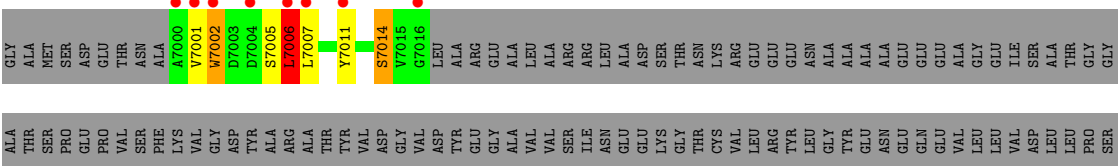
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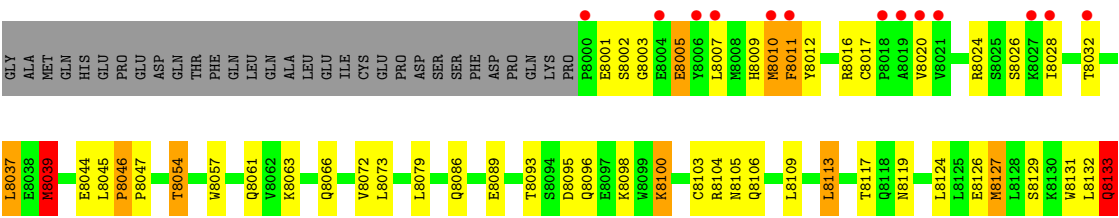


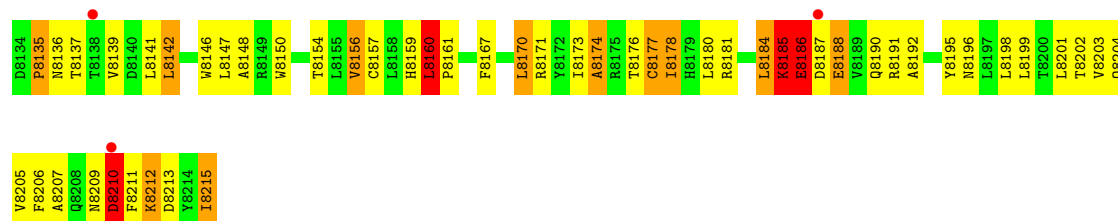
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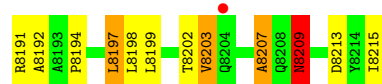
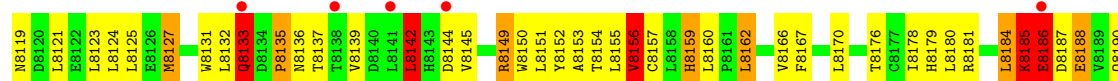
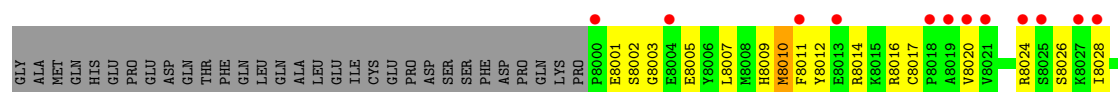
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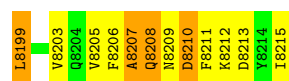
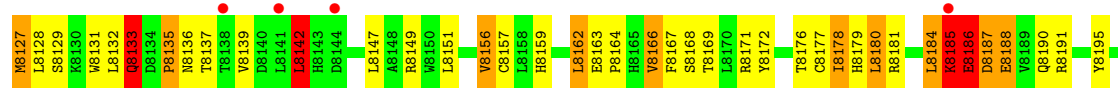
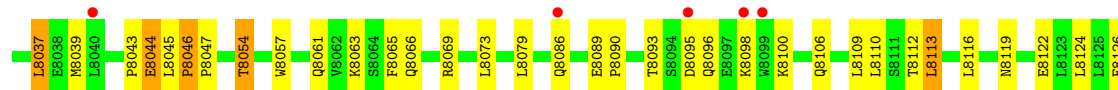
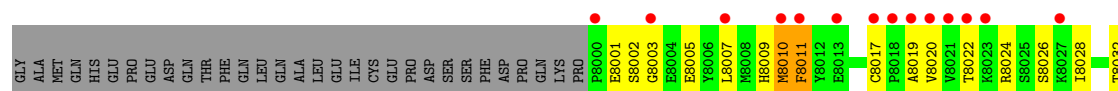




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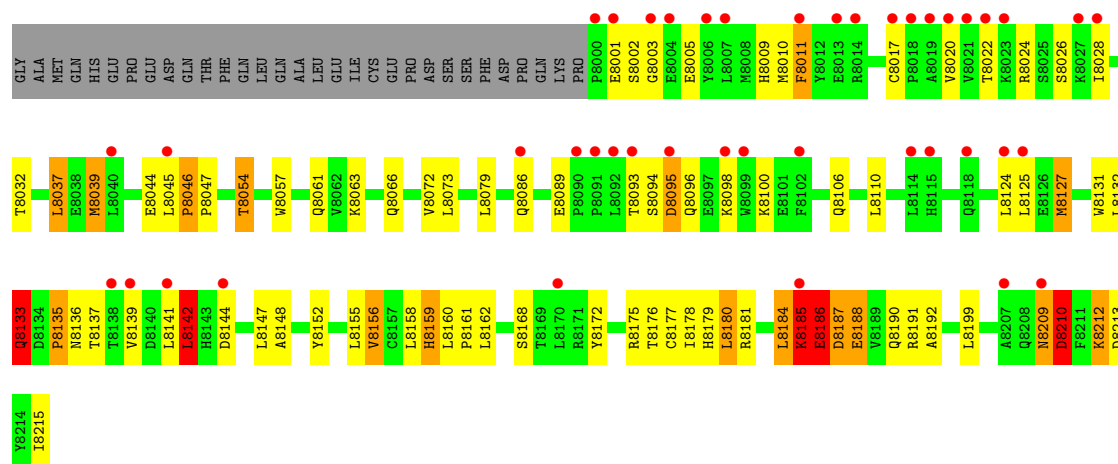


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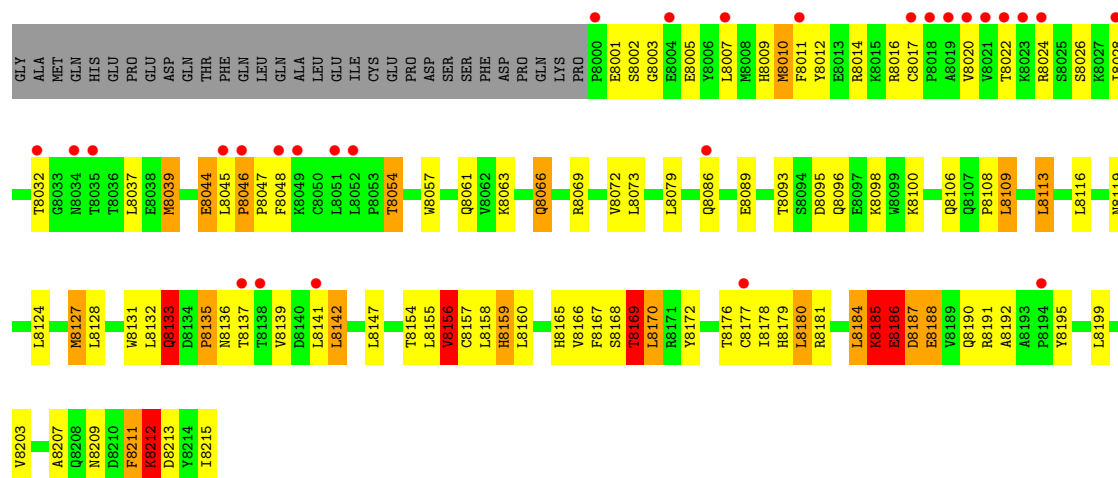


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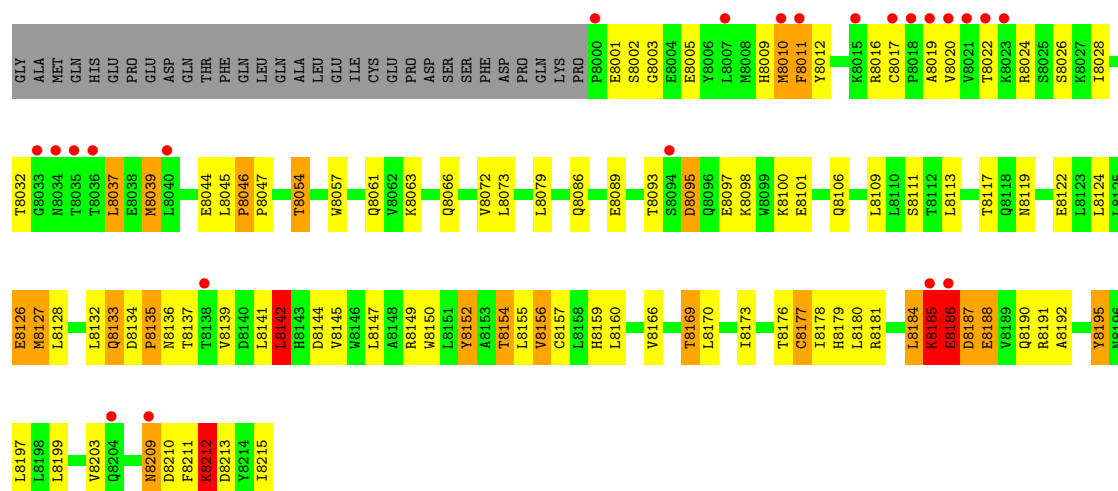




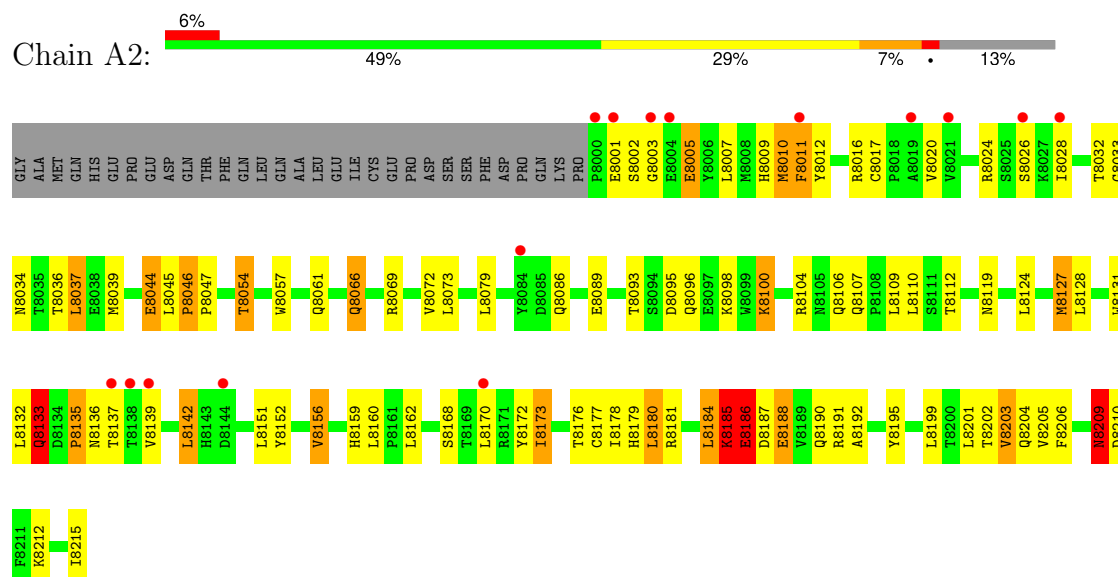
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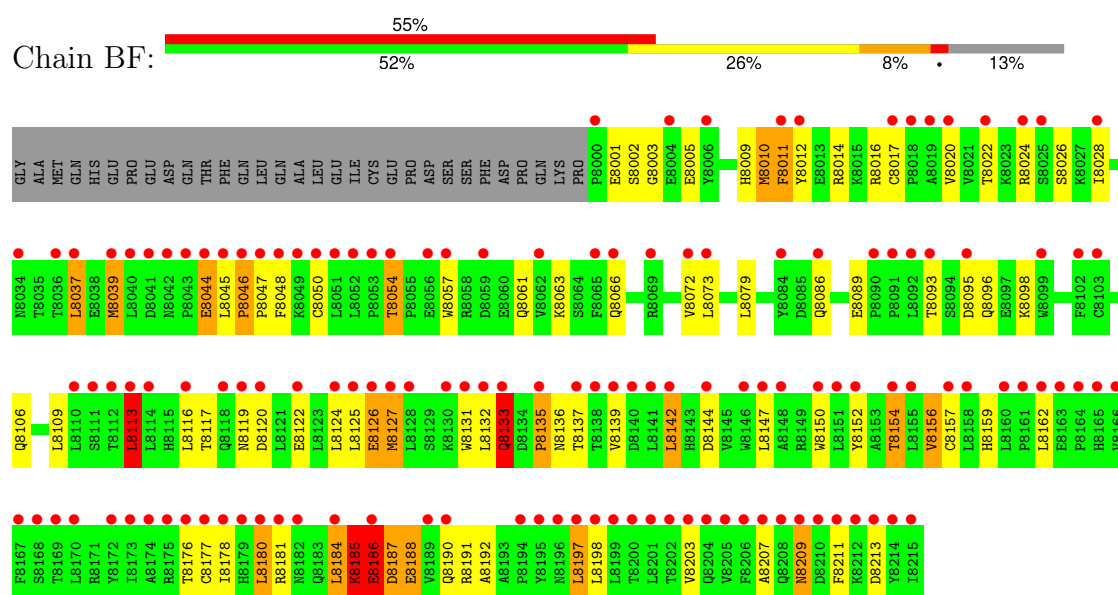
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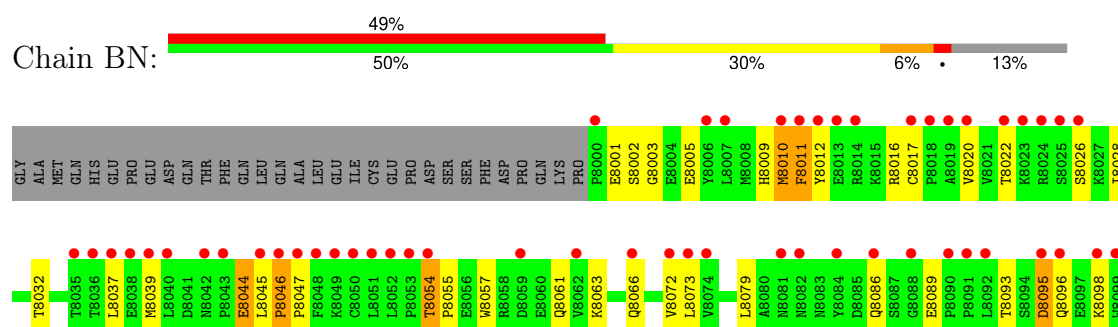
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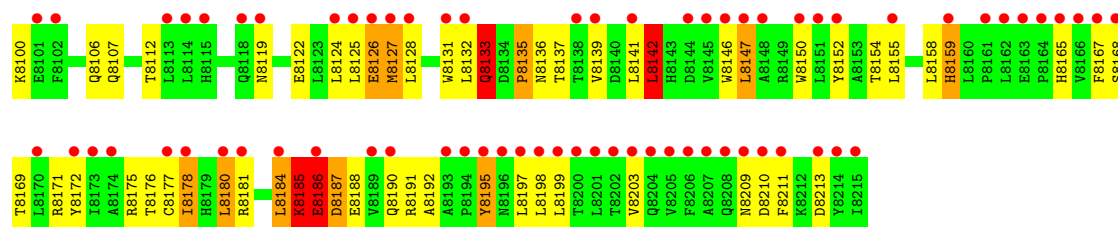


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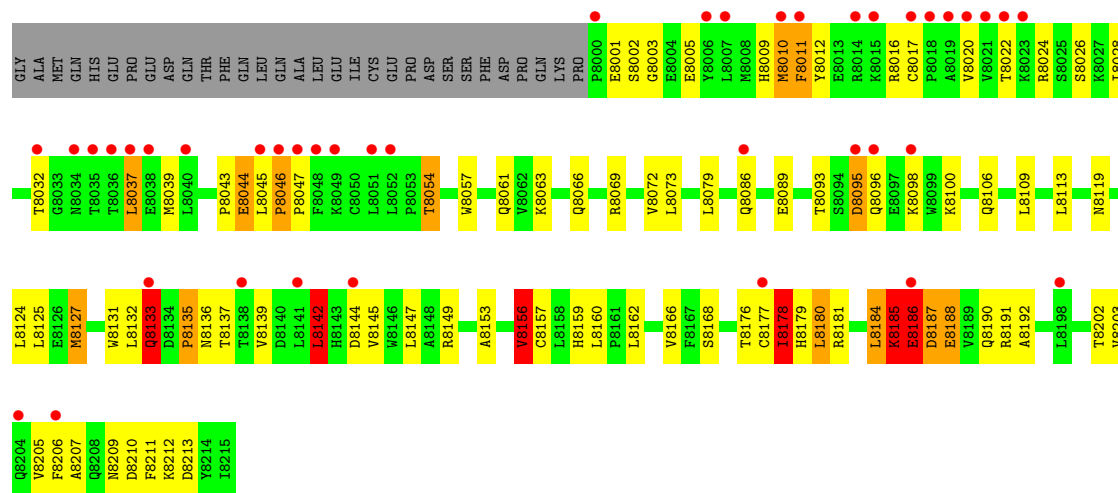


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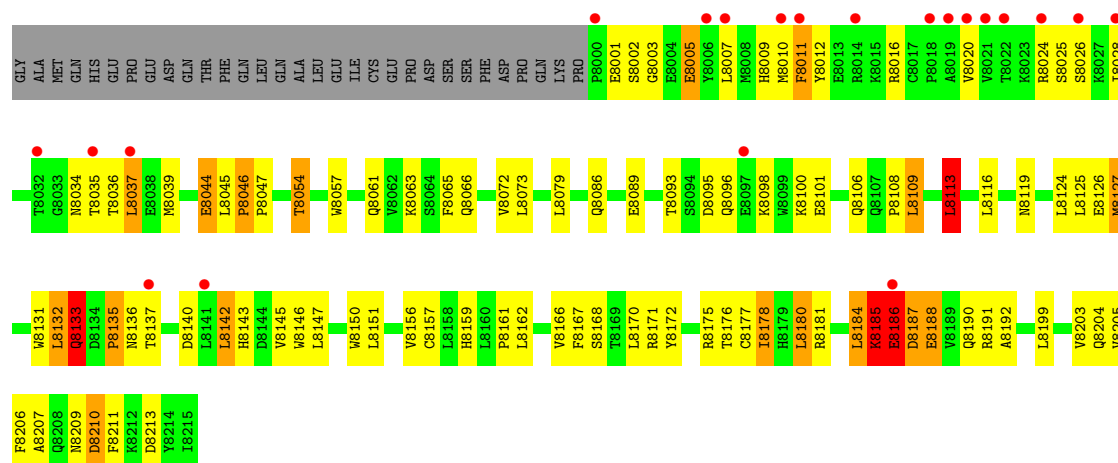




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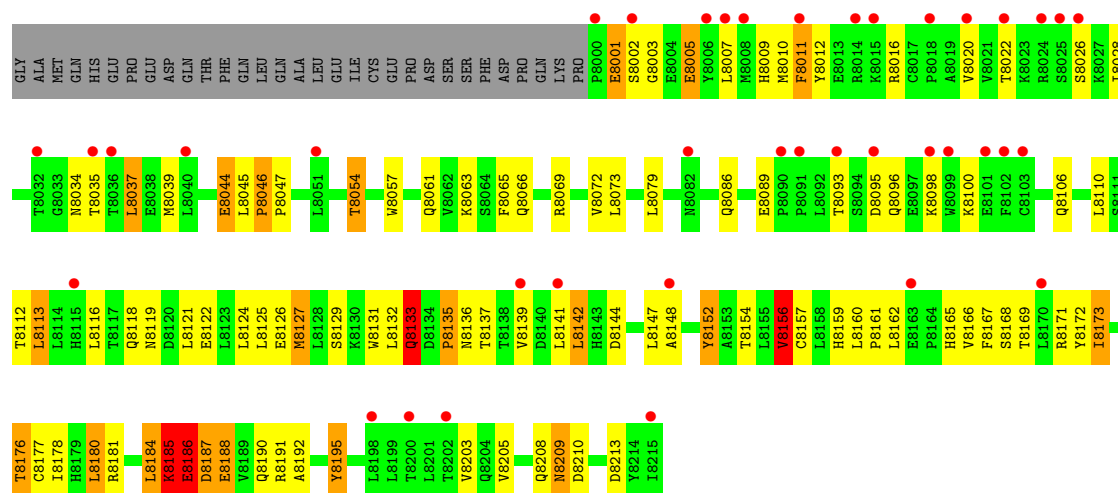


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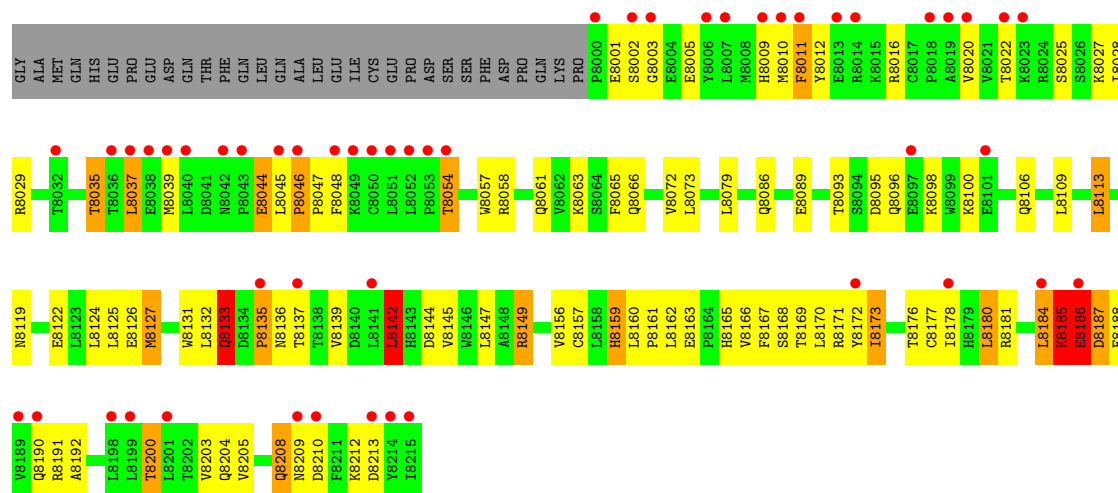


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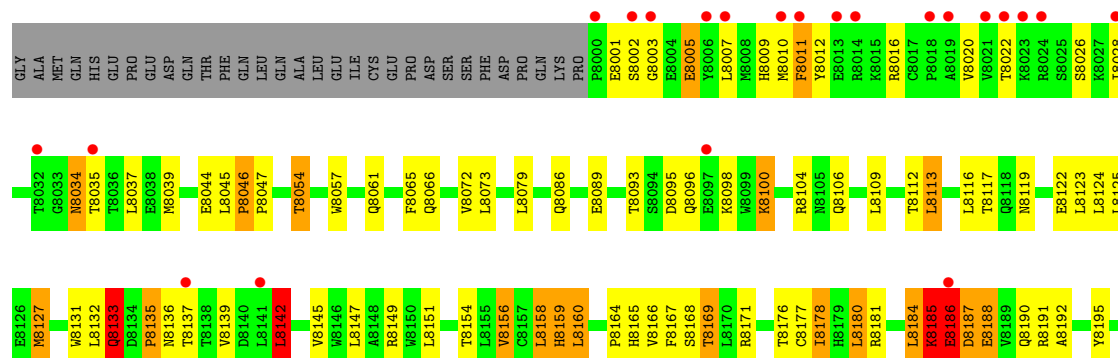




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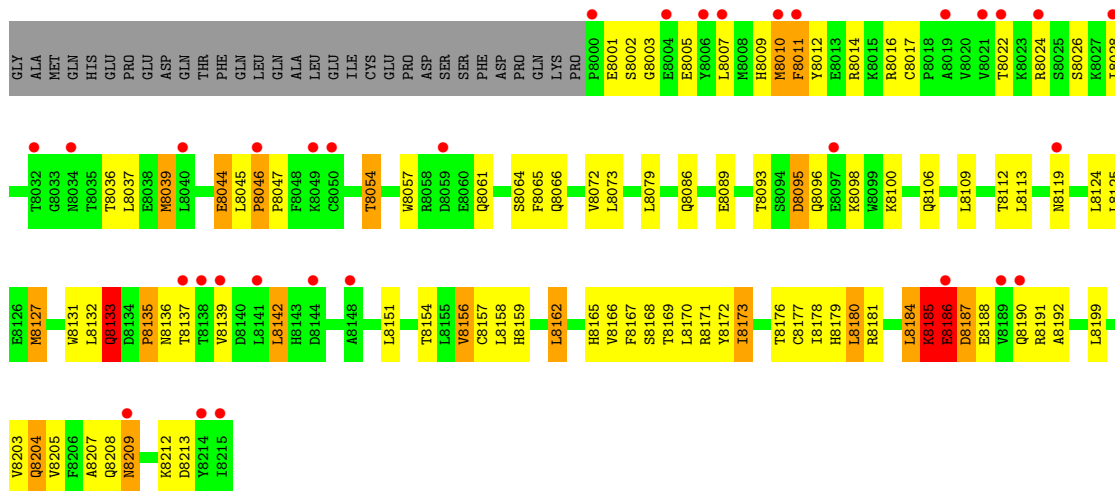


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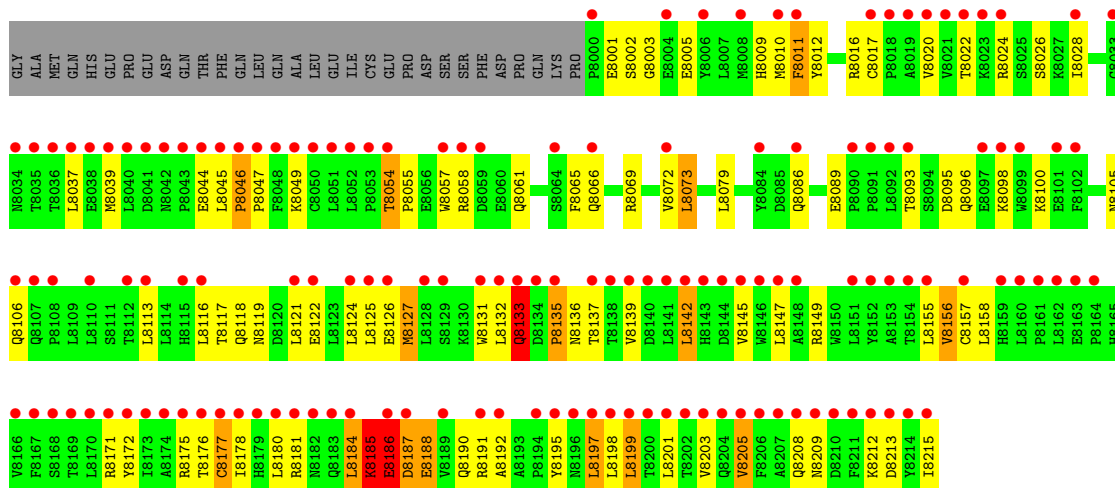




• Molecule 6: CG10419

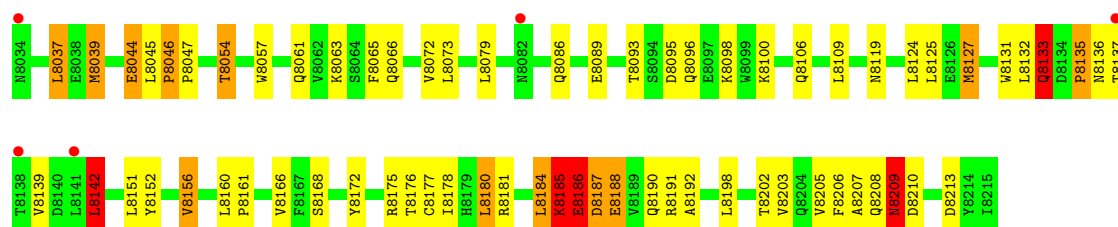


• Molecule 6: CG10419

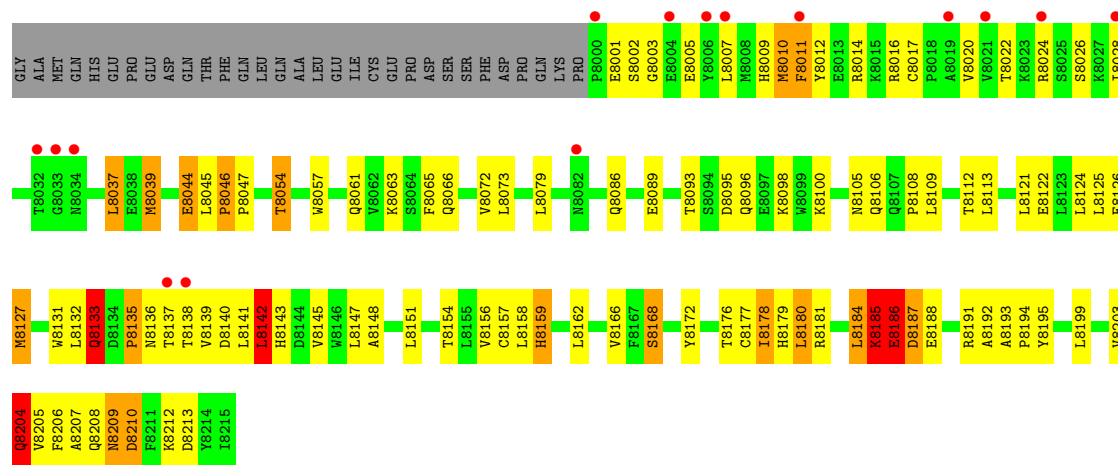


• Molecule 6: CG10419

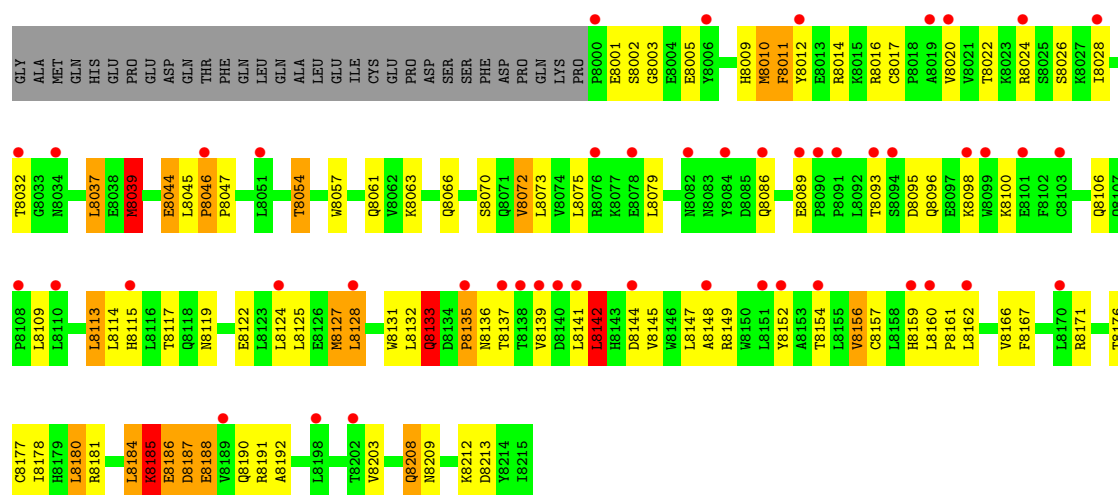




• Molecule 6: CG10419

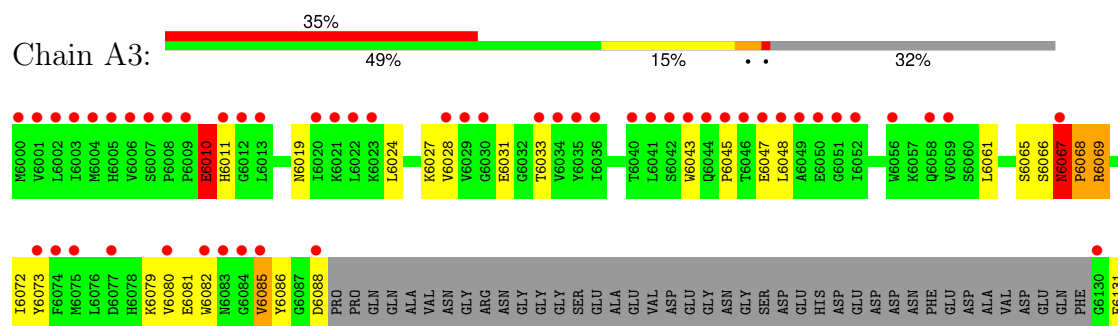


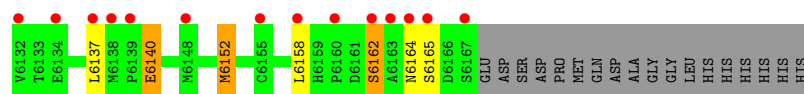
• Molecule 6: CG10419



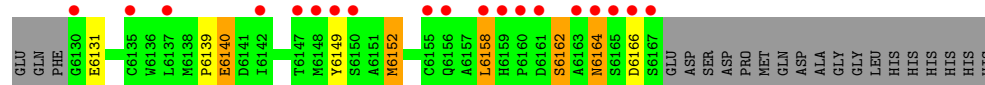
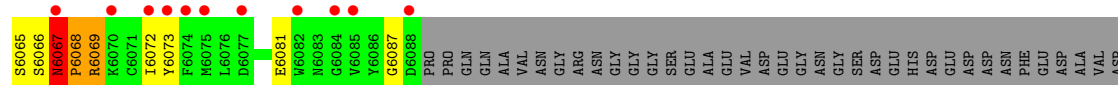
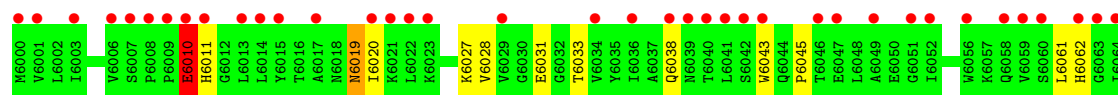
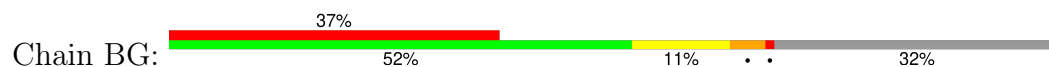
• Molecule 6: CG10419



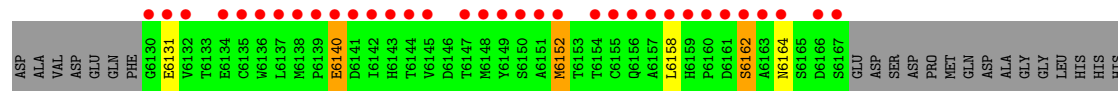
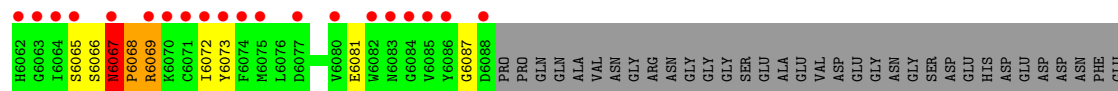
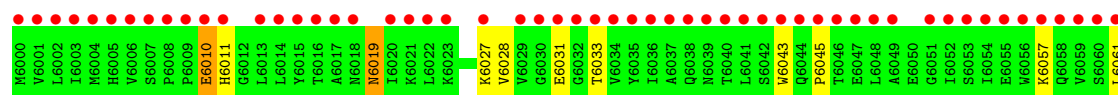




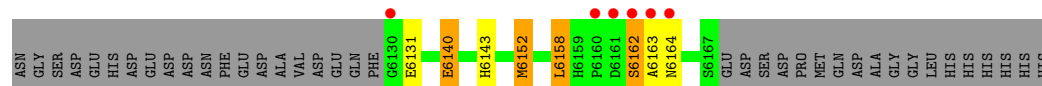
• Molecule 7: Icln



• Molecule 7: Icln

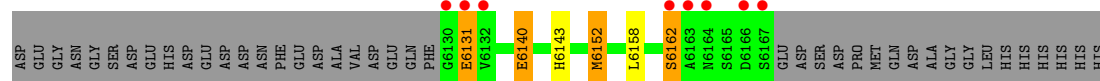


• Molecule 7: Icln

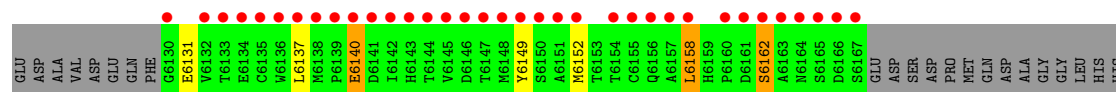
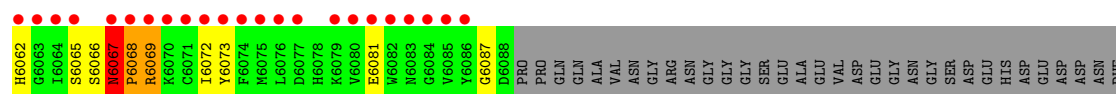
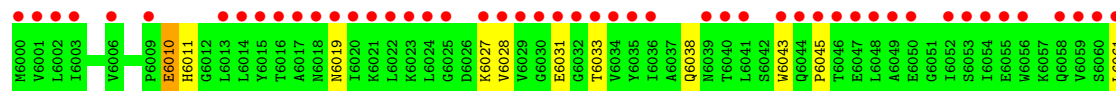


• Molecule 7: Icln

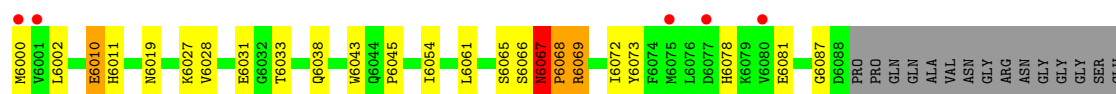




• Molecule 7: Icln



• Molecule 7: Icln



• Molecule 7: Icln



Chain CG:

Category	Percentage
ASP	5%
GLU	52%
SER	12%
PHE	5%
HIS	32%

Chain CO:

39% 53% 11% 1% 32%

Chain CO	Percentage
39%	39%
53%	53%
11%	11%
1%	1%
32%	32%

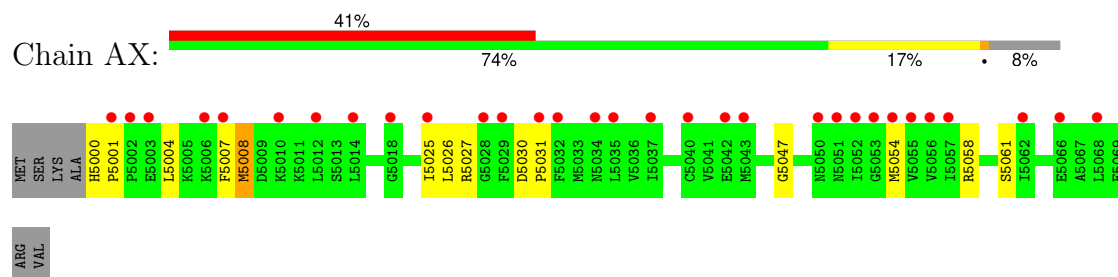
Chain CW:

7% 52% 12% 32%

[illegible]

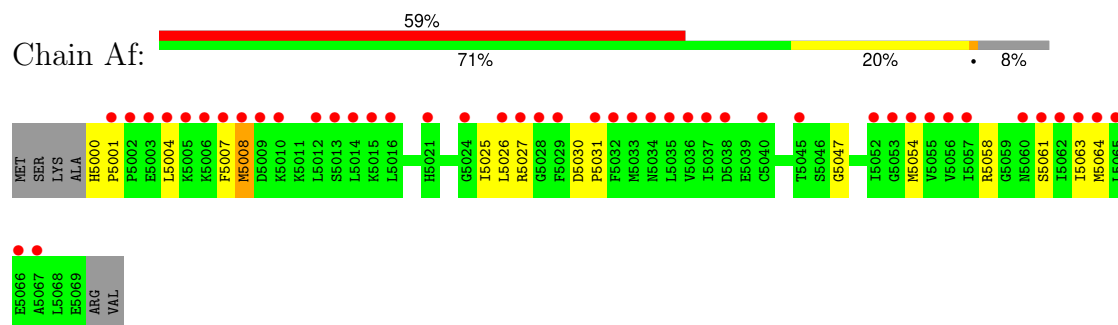
• Molecule 8: Small nuclear ribonucleoprotein G

Chain AX:



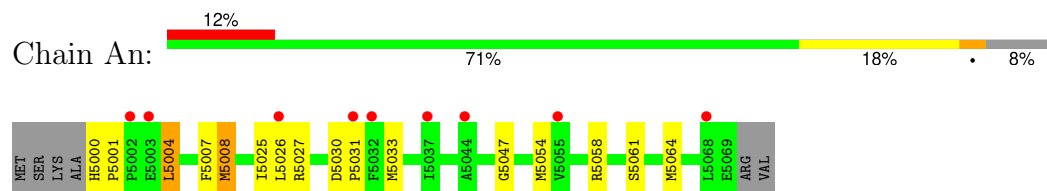
• Molecule 8: Small nuclear ribonucleoprotein G

Chain Af:



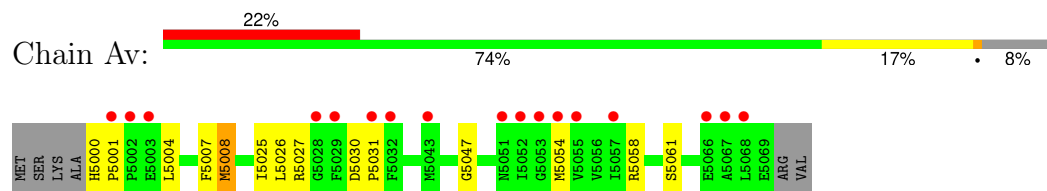
• Molecule 8: Small nuclear ribonucleoprotein G

Chain An:



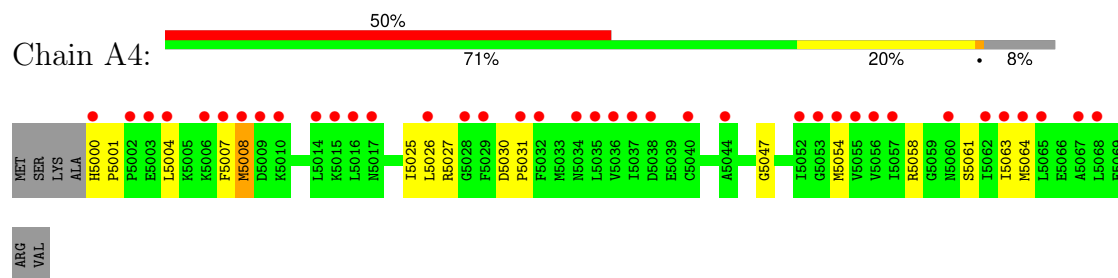
• Molecule 8: Small nuclear ribonucleoprotein G

Chain Av:



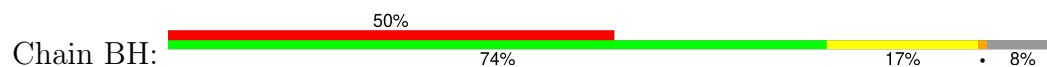
• Molecule 8: Small nuclear ribonucleoprotein G

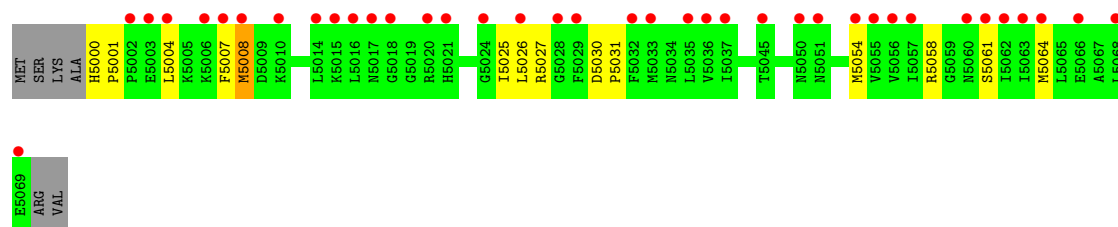
Chain A4:



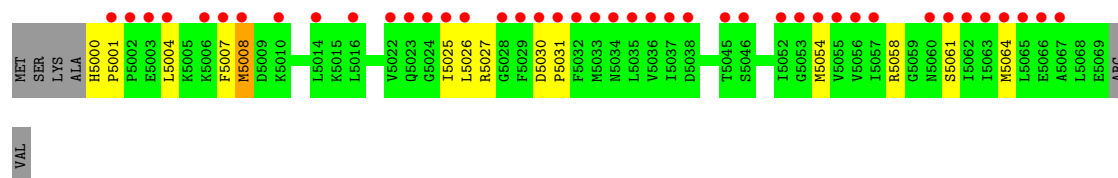
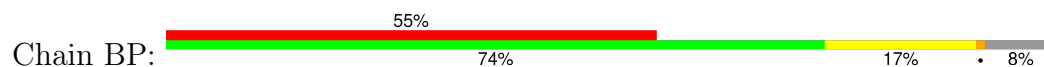
• Molecule 8: Small nuclear ribonucleoprotein G

Chain BH:

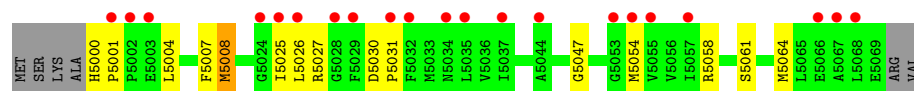
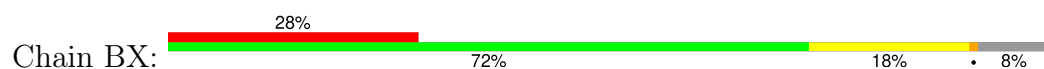




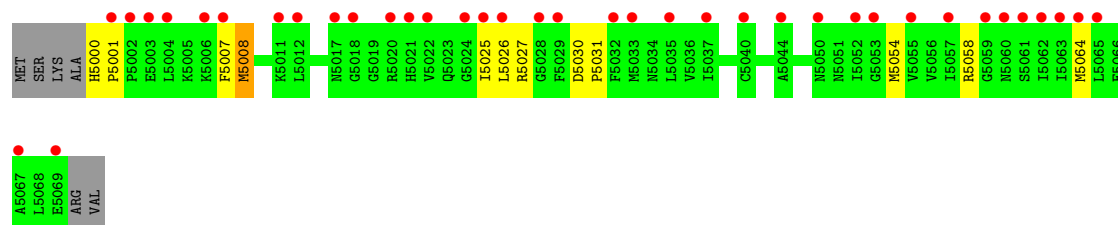
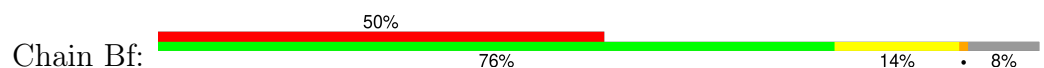
• Molecule 8: Small nuclear ribonucleoprotein G



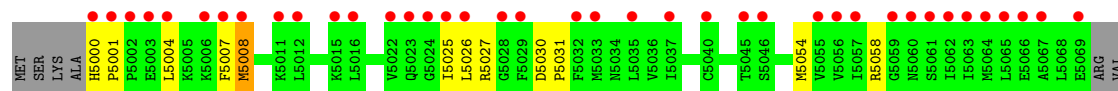
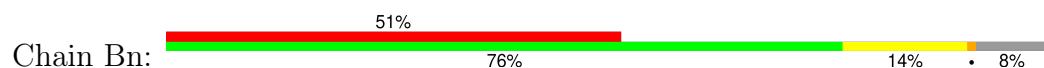
• Molecule 8: Small nuclear ribonucleoprotein G



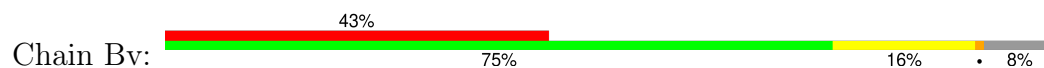
• Molecule 8: Small nuclear ribonucleoprotein G

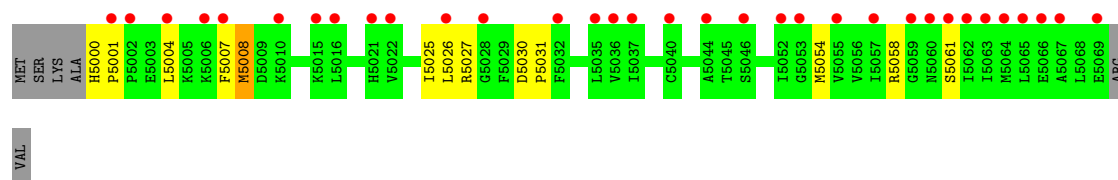


• Molecule 8: Small nuclear ribonucleoprotein G

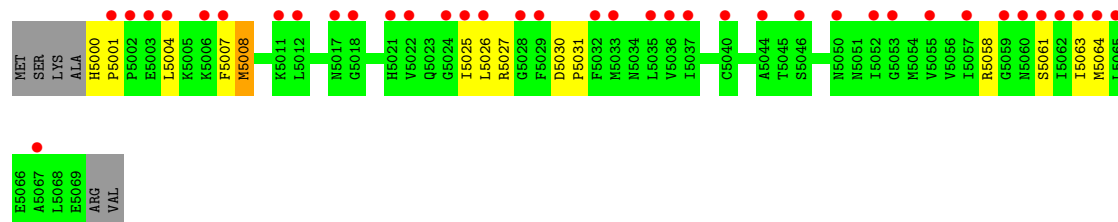
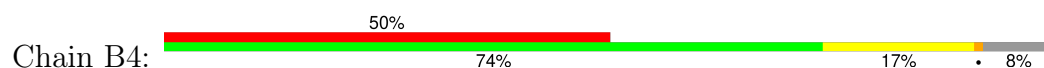


• Molecule 8: Small nuclear ribonucleoprotein G

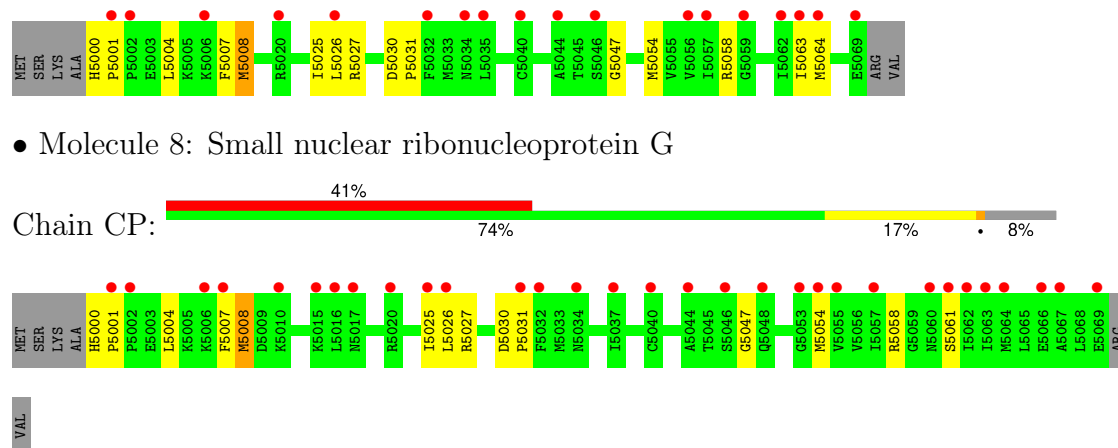
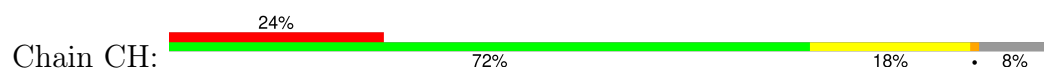




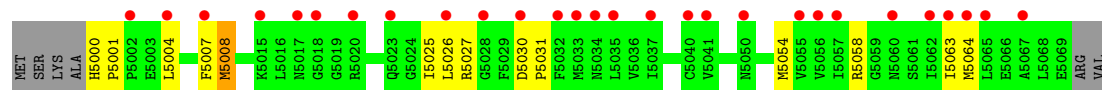
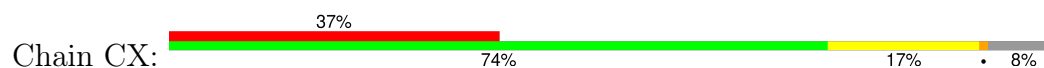
• Molecule 8: Small nuclear ribonucleoprotein G



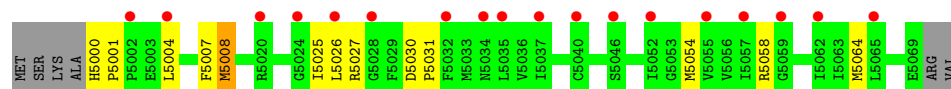
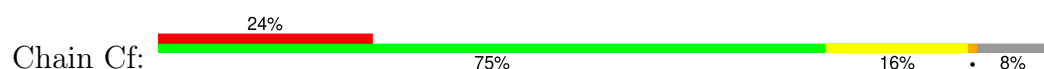
• Molecule 8: Small nuclear ribonucleoprotein G



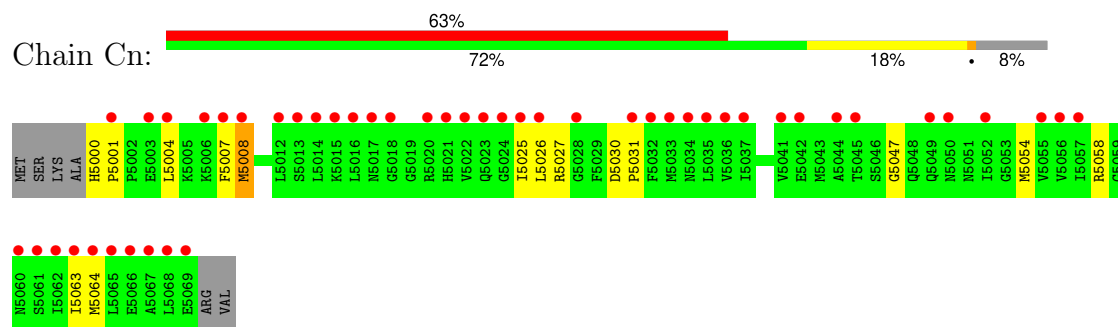
• Molecule 8: Small nuclear ribonucleoprotein G



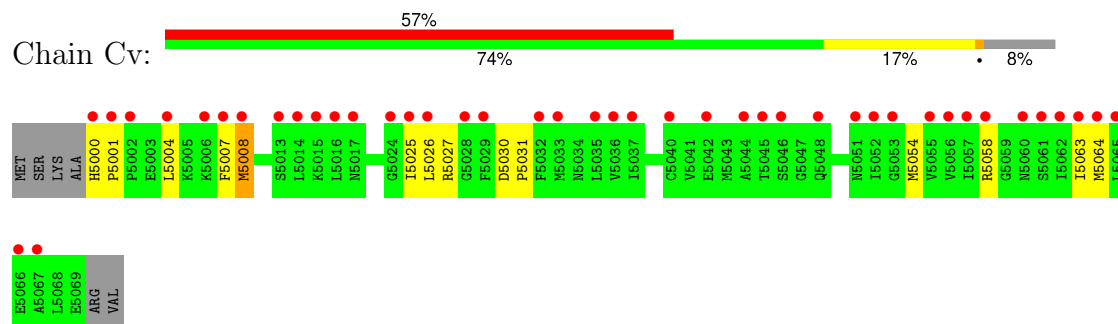
• Molecule 8: Small nuclear ribonucleoprotein G



Chain Cn:



Chain Cv:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	150.93Å 356.81Å 230.75Å 90.00° 97.31° 90.00°	Depositor
Resolution (Å)	59.47 – 3.10 59.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	64.6 (59.47-3.10) 64.6 (59.47-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.232 , 0.256 0.348 , 0.354	Depositor DCC
R_{free} test set	2901 reflections (1.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 109.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	121990	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7504e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.80	0/656	1.17	4/888 (0.5%)
1	AI	0.80	0/656	1.16	3/888 (0.3%)
1	AQ	0.77	0/656	1.16	3/888 (0.3%)
1	AY	0.77	0/656	1.16	3/888 (0.3%)
1	Ag	0.77	0/656	1.15	2/888 (0.2%)
1	Ao	0.80	0/656	1.16	2/888 (0.2%)
1	Aw	0.75	0/656	1.16	4/888 (0.5%)
1	BA	0.70	0/656	1.13	1/888 (0.1%)
1	BI	0.73	0/656	1.12	1/888 (0.1%)
1	BQ	0.73	0/656	1.13	2/888 (0.2%)
1	BY	0.78	0/656	1.15	3/888 (0.3%)
1	Bg	0.75	0/656	1.15	4/888 (0.5%)
1	Bo	0.76	0/656	1.14	3/888 (0.3%)
1	Bw	0.80	0/656	1.16	4/888 (0.5%)
1	CA	0.75	0/656	1.14	3/888 (0.3%)
1	CI	0.74	0/656	1.12	3/888 (0.3%)
1	CQ	0.77	0/656	1.14	3/888 (0.3%)
1	CY	0.83	0/656	1.15	3/888 (0.3%)
1	Cg	0.72	0/656	1.13	3/888 (0.3%)
1	Co	0.72	0/656	1.12	3/888 (0.3%)
2	AB	0.82	1/817 (0.1%)	1.17	3/1096 (0.3%)
2	AJ	0.81	0/817	1.17	1/1096 (0.1%)
2	AR	0.77	0/817	1.17	3/1096 (0.3%)
2	AZ	0.76	0/817	1.20	3/1096 (0.3%)
2	Ah	0.76	1/817 (0.1%)	1.17	3/1096 (0.3%)
2	Ap	0.76	0/817	1.16	2/1096 (0.2%)
2	Ax	0.77	0/817	1.21	3/1096 (0.3%)
2	BB	0.73	0/817	1.14	3/1096 (0.3%)
2	BJ	0.74	0/817	1.19	3/1096 (0.3%)
2	BR	0.74	0/817	1.18	3/1096 (0.3%)
2	BZ	0.81	0/817	1.22	2/1096 (0.2%)
2	Bh	0.77	0/817	1.21	2/1096 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Bp	0.75	0/817	1.19	3/1096 (0.3%)
2	Bx	0.79	0/817	1.21	3/1096 (0.3%)
2	CB	0.75	0/817	1.18	0/1096
2	CJ	0.74	1/817 (0.1%)	1.15	2/1096 (0.2%)
2	CR	0.75	0/817	1.18	2/1096 (0.2%)
2	CZ	0.77	0/817	1.18	2/1096 (0.2%)
2	Ch	0.75	0/817	1.18	4/1096 (0.4%)
2	Cp	0.75	0/817	1.20	4/1096 (0.4%)
3	AC	0.65	0/646	1.18	7/867 (0.8%)
3	AK	0.68	0/646	1.22	4/867 (0.5%)
3	AS	0.66	0/646	1.21	3/867 (0.3%)
3	Aa	0.61	0/646	1.20	3/867 (0.3%)
3	Ai	0.63	0/646	1.19	6/867 (0.7%)
3	Aq	0.64	0/646	1.20	3/867 (0.3%)
3	Ay	0.63	0/646	1.20	3/867 (0.3%)
3	BC	0.63	0/646	1.20	3/867 (0.3%)
3	BK	0.60	0/646	1.18	3/867 (0.3%)
3	BS	0.61	0/646	1.19	3/867 (0.3%)
3	Ba	0.62	0/646	1.20	3/867 (0.3%)
3	Bi	0.60	0/646	1.20	4/867 (0.5%)
3	Bq	0.58	0/646	1.19	4/867 (0.5%)
3	By	0.68	0/646	1.21	3/867 (0.3%)
3	CC	0.62	0/646	1.19	3/867 (0.3%)
3	CK	0.60	0/646	1.19	3/867 (0.3%)
3	CS	0.62	0/646	1.20	3/867 (0.3%)
3	Ca	0.63	0/646	1.19	3/867 (0.3%)
3	Ci	0.61	0/646	1.19	3/867 (0.3%)
3	Cq	0.58	0/646	1.20	4/867 (0.5%)
4	AD	0.58	0/567	0.99	2/765 (0.3%)
4	AL	0.58	0/567	0.98	2/765 (0.3%)
4	AT	0.60	0/567	0.98	0/765
4	Ab	0.61	0/567	1.00	2/765 (0.3%)
4	Aj	0.58	0/567	0.98	2/765 (0.3%)
4	Ar	0.59	0/567	1.03	1/765 (0.1%)
4	Az	0.57	0/567	0.98	2/765 (0.3%)
4	BD	0.58	0/567	0.99	1/765 (0.1%)
4	BL	0.56	0/567	1.01	1/765 (0.1%)
4	BT	0.57	0/567	1.00	3/765 (0.4%)
4	Bb	0.60	0/567	1.05	4/765 (0.5%)
4	Bj	0.60	0/567	1.04	2/765 (0.3%)
4	Br	0.57	0/567	1.00	1/765 (0.1%)
4	Bz	0.60	0/567	1.01	1/765 (0.1%)
4	CD	0.59	0/567	1.06	1/765 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	CL	0.56	0/567	1.00	3/765 (0.4%)
4	CT	0.58	0/567	0.99	0/765
4	Cb	0.60	0/567	1.04	2/765 (0.3%)
4	Cj	0.58	0/567	1.00	1/765 (0.1%)
4	Cr	0.57	0/567	1.00	3/765 (0.4%)
5	A1	1.11	0/135	1.75	0/184
5	AE	0.95	0/135	1.72	3/184 (1.6%)
5	AM	1.08	0/135	1.77	0/184
5	AU	0.96	0/135	1.72	2/184 (1.1%)
5	Ac	1.11	0/135	1.93	3/184 (1.6%)
5	Ak	1.06	0/135	1.72	1/184 (0.5%)
5	As	0.93	0/135	1.75	3/184 (1.6%)
5	B1	1.01	0/135	1.88	5/184 (2.7%)
5	BE	0.99	0/135	1.57	0/184
5	BM	1.03	0/135	1.71	0/184
5	BU	0.94	0/135	1.74	4/184 (2.2%)
5	Bc	1.02	0/135	1.76	1/184 (0.5%)
5	Bk	1.08	0/135	1.67	1/184 (0.5%)
5	Bs	0.99	0/135	1.84	8/184 (4.3%)
5	CE	1.11	0/135	1.87	2/184 (1.1%)
5	CM	1.06	0/135	1.77	2/184 (1.1%)
5	CU	1.10	0/135	1.76	1/184 (0.5%)
5	Cc	1.13	0/135	1.85	2/184 (1.1%)
5	Ck	1.08	0/135	1.73	0/184
5	Cs	1.03	0/135	1.76	0/184
6	A2	0.92	0/1830	1.70	25/2489 (1.0%)
6	AF	0.95	0/1830	1.69	27/2489 (1.1%)
6	AN	0.98	0/1830	1.68	30/2489 (1.2%)
6	AV	0.92	0/1830	1.66	29/2489 (1.2%)
6	Ad	0.88	0/1830	1.65	25/2489 (1.0%)
6	Al	0.96	0/1830	1.71	30/2489 (1.2%)
6	At	0.96	0/1830	1.66	29/2489 (1.2%)
6	B2	0.93	1/1830 (0.1%)	1.66	23/2489 (0.9%)
6	BF	0.86	0/1830	1.66	24/2489 (1.0%)
6	BN	0.88	0/1830	1.63	20/2489 (0.8%)
6	BV	0.87	0/1830	1.66	29/2489 (1.2%)
6	Bd	0.91	0/1830	1.68	24/2489 (1.0%)
6	Bl	0.89	0/1830	1.65	31/2489 (1.2%)
6	Bt	0.91	0/1830	1.66	23/2489 (0.9%)
6	CF	0.89	0/1830	1.66	25/2489 (1.0%)
6	CN	0.86	0/1830	1.64	25/2489 (1.0%)
6	CV	0.89	0/1830	1.64	20/2489 (0.8%)
6	Cd	0.91	0/1830	1.70	32/2489 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	Cl	0.89	0/1830	1.67	25/2489 (1.0%)
6	Ct	0.89	0/1830	1.68	21/2489 (0.8%)
7	A3	0.76	1/1008 (0.1%)	1.18	6/1373 (0.4%)
7	AG	0.89	1/1008 (0.1%)	1.19	7/1373 (0.5%)
7	AO	0.87	1/1008 (0.1%)	1.17	9/1373 (0.7%)
7	AW	0.85	1/1008 (0.1%)	1.17	7/1373 (0.5%)
7	Ae	0.76	1/1008 (0.1%)	1.15	9/1373 (0.7%)
7	Am	0.91	1/1008 (0.1%)	1.19	7/1373 (0.5%)
7	Au	0.87	1/1008 (0.1%)	1.17	7/1373 (0.5%)
7	B3	0.85	0/1008	1.19	7/1373 (0.5%)
7	BG	0.83	1/1008 (0.1%)	1.17	7/1373 (0.5%)
7	BO	0.82	1/1008 (0.1%)	1.20	7/1373 (0.5%)
7	BW	0.86	1/1008 (0.1%)	1.17	8/1373 (0.6%)
7	Be	0.90	2/1008 (0.2%)	1.18	6/1373 (0.4%)
7	Bm	0.81	0/1008	1.16	6/1373 (0.4%)
7	Bu	0.83	1/1008 (0.1%)	1.19	10/1373 (0.7%)
7	CG	0.86	0/1008	1.18	7/1373 (0.5%)
7	CO	0.79	0/1008	1.17	7/1373 (0.5%)
7	CW	0.88	1/1008 (0.1%)	1.19	6/1373 (0.4%)
7	Ce	0.92	1/1008 (0.1%)	1.20	6/1373 (0.4%)
7	Cm	0.80	0/1008	1.17	6/1373 (0.4%)
7	Cu	0.79	0/1008	1.17	9/1373 (0.7%)
8	A4	0.64	0/551	1.11	3/737 (0.4%)
8	AH	0.68	0/551	1.14	2/737 (0.3%)
8	AP	0.69	0/551	1.14	3/737 (0.4%)
8	AX	0.68	0/551	1.12	3/737 (0.4%)
8	Af	0.63	0/551	1.11	3/737 (0.4%)
8	An	0.69	0/551	1.14	3/737 (0.4%)
8	Av	0.67	0/551	1.12	3/737 (0.4%)
8	B4	0.71	0/551	1.13	2/737 (0.3%)
8	BH	0.64	0/551	1.13	2/737 (0.3%)
8	BP	0.67	0/551	1.11	2/737 (0.3%)
8	BX	0.65	0/551	1.10	3/737 (0.4%)
8	Bf	0.68	0/551	1.13	1/737 (0.1%)
8	Bn	0.65	0/551	1.13	2/737 (0.3%)
8	Bv	0.66	0/551	1.12	2/737 (0.3%)
8	CH	0.71	0/551	1.13	3/737 (0.4%)
8	CP	0.66	0/551	1.11	3/737 (0.4%)
8	CX	0.71	0/551	1.13	2/737 (0.3%)
8	Cf	0.70	0/551	1.13	2/737 (0.3%)
8	Cn	0.64	0/551	1.12	3/737 (0.4%)
8	Cv	0.63	0/551	1.12	2/737 (0.3%)
All	All	0.80	19/124200 (0.0%)	1.34	961/167980 (0.6%)

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
7	A3	0	1
7	AG	0	1
7	AO	0	1
7	AW	0	1
7	Ae	0	1
7	Am	0	1
7	Au	0	1
7	B3	0	1
7	BG	0	1
7	BO	0	1
7	BW	0	1
7	Be	0	1
7	Bm	0	1
7	Bu	0	1
7	CG	0	1
7	CO	0	1
7	CW	0	1
7	Ce	0	1
7	Cm	0	1
7	Cu	0	1
All	All	0	20

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	BO	6152	MET	SD-CE	-7.26	1.61	1.79
7	Ce	6152	MET	SD-CE	-6.75	1.62	1.79
7	Au	6152	MET	SD-CE	-6.63	1.62	1.79
7	BW	6152	MET	SD-CE	-6.51	1.63	1.79
7	AG	6152	MET	SD-CE	-6.41	1.63	1.79

The worst 5 of 961 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Ct	8178	ILE	N-CA-C	-12.68	99.20	110.74
3	Bq	3024	GLN	N-CA-C	11.34	127.24	112.72
3	Ay	3024	GLN	N-CA-C	10.95	126.79	112.12
3	AK	3024	GLN	N-CA-C	10.92	126.76	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CK	3024	GLN	N-CA-C	10.91	126.75	112.12

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AG	6067	ASN	Mainchain
7	AO	6067	ASN	Mainchain
7	AW	6067	ASN	Mainchain
7	Ae	6067	ASN	Mainchain
7	Am	6067	ASN	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	648	0	690	7	0
1	AI	648	0	690	11	0
1	AQ	648	0	690	11	0
1	AY	648	0	690	12	0
1	Ag	648	0	690	10	0
1	Ao	648	0	690	12	0
1	Aw	648	0	690	10	0
1	BA	648	0	690	11	0
1	BI	648	0	690	10	0
1	BQ	648	0	690	12	0
1	BY	648	0	690	11	0
1	Bg	648	0	690	11	0
1	Bo	648	0	690	10	0
1	Bw	648	0	690	9	0
1	CA	648	0	690	9	0
1	CI	648	0	690	11	0
1	CQ	648	0	690	11	0
1	CY	648	0	690	12	0
1	Cg	648	0	690	12	0
1	Co	648	0	690	10	0
2	AB	807	0	833	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AJ	807	0	833	21	0
2	AR	807	0	833	20	0
2	AZ	807	0	833	19	0
2	Ah	807	0	833	17	0
2	Ap	807	0	833	16	0
2	Ax	807	0	833	17	0
2	BB	807	0	833	20	0
2	BJ	807	0	833	17	0
2	BR	807	0	833	17	0
2	BZ	807	0	833	18	0
2	Bh	807	0	833	18	0
2	Bp	807	0	833	21	0
2	Bx	807	0	833	17	0
2	CB	807	0	833	17	0
2	CJ	807	0	833	19	0
2	CR	807	0	833	16	0
2	CZ	807	0	833	18	0
2	Ch	807	0	833	22	0
2	Cp	807	0	833	20	0
3	AC	638	0	657	14	0
3	AK	638	0	657	16	0
3	AS	638	0	657	16	0
3	Aa	638	0	657	15	0
3	Ai	638	0	657	13	0
3	Aq	638	0	657	17	0
3	Ay	638	0	657	16	0
3	BC	638	0	657	15	0
3	BK	638	0	657	17	0
3	BS	638	0	657	16	0
3	Ba	638	0	657	16	0
3	Bi	638	0	657	17	0
3	Bq	638	0	657	17	0
3	By	638	0	657	15	0
3	CC	638	0	657	14	0
3	CK	638	0	657	14	0
3	CS	638	0	657	14	0
3	Ca	638	0	657	15	0
3	Ci	638	0	657	14	0
3	Cq	638	0	657	16	0
4	AD	556	0	561	16	0
4	AL	556	0	561	17	0
4	AT	556	0	561	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Ab	556	0	561	17	0
4	Aj	556	0	561	19	0
4	Ar	556	0	561	17	0
4	Az	556	0	561	16	0
4	BD	556	0	561	18	0
4	BL	556	0	561	17	0
4	BT	556	0	561	15	0
4	Bb	556	0	561	17	0
4	Bj	556	0	561	17	0
4	Br	556	0	561	18	0
4	Bz	556	0	561	16	0
4	CD	556	0	561	14	0
4	CL	556	0	561	15	0
4	CT	556	0	561	16	0
4	Cb	556	0	561	16	0
4	Cj	556	0	561	17	0
4	Cr	556	0	561	14	0
5	A1	133	0	123	0	0
5	AE	133	0	123	2	0
5	AM	133	0	123	2	0
5	AU	133	0	123	2	0
5	Ac	133	0	123	1	0
5	Ak	133	0	123	4	0
5	As	133	0	123	2	0
5	B1	133	0	123	1	0
5	BE	133	0	123	2	0
5	BM	133	0	123	2	0
5	BU	133	0	123	1	0
5	Bc	133	0	123	2	0
5	Bk	133	0	123	0	0
5	Bs	133	0	123	0	0
5	CE	133	0	123	1	0
5	CM	133	0	123	2	0
5	CU	133	0	123	0	0
5	Cc	133	0	123	3	0
5	Ck	133	0	123	1	0
5	Cs	133	0	123	3	0
6	A2	1787	0	1779	46	0
6	AF	1787	0	1779	53	0
6	AN	1787	0	1779	61	0
6	AV	1787	0	1779	58	0
6	Ad	1787	0	1779	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Al	1787	0	1779	48	0
6	At	1787	0	1779	52	0
6	B2	1787	0	1779	52	0
6	BF	1787	0	1779	47	0
6	BN	1787	0	1779	52	0
6	BV	1787	0	1779	47	0
6	Bd	1787	0	1779	51	0
6	Bl	1787	0	1779	51	0
6	Bt	1787	0	1779	53	0
6	CF	1787	0	1779	48	0
6	CN	1787	0	1779	52	0
6	CV	1787	0	1779	41	0
6	Cd	1787	0	1779	53	0
6	Cl	1787	0	1779	49	0
6	Ct	1787	0	1779	48	0
7	A3	984	0	943	27	0
7	AG	984	0	943	26	0
7	AO	984	0	943	24	0
7	AW	984	0	943	21	0
7	Ae	984	0	943	24	0
7	Am	984	0	943	25	0
7	Au	984	0	943	21	0
7	B3	984	0	943	25	0
7	BG	984	0	943	27	0
7	BO	984	0	943	24	0
7	BW	984	0	943	21	0
7	Be	984	0	943	24	0
7	Bm	984	0	943	23	0
7	Bu	984	0	943	25	0
7	CG	984	0	943	25	0
7	CO	984	0	943	23	0
7	CW	984	0	943	26	0
7	Ce	984	0	943	24	0
7	Cm	984	0	943	26	0
7	Cu	984	0	943	28	0
8	A4	544	0	563	9	0
8	AH	544	0	563	8	0
8	AP	544	0	563	9	0
8	AX	544	0	563	8	0
8	Af	544	0	563	9	0
8	An	544	0	563	10	0
8	Av	544	0	563	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B4	544	0	563	7	0
8	BH	544	0	563	9	0
8	BP	544	0	563	10	0
8	BX	544	0	563	8	0
8	Bf	544	0	563	8	0
8	Bn	544	0	563	7	0
8	Bv	544	0	563	8	0
8	CH	544	0	563	9	0
8	CP	544	0	563	8	0
8	CX	544	0	563	8	0
8	Cf	544	0	563	9	0
8	Cn	544	0	563	10	0
8	Cv	544	0	563	8	0
9	A2	5	0	0	0	0
9	Ad	5	0	0	0	0
9	At	5	0	0	0	0
9	B2	5	0	0	0	0
9	BF	5	0	0	0	0
9	BV	5	0	0	0	0
9	Bd	5	0	0	0	0
9	Bt	5	0	0	0	0
9	CF	5	0	0	0	0
9	Cl	5	0	0	0	0
All	All	121990	0	122980	2413	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 10.

The worst 5 of 2413 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)
2:BZ:2092:LEU:HD23	4:Bb:4056:VAL:HG22	1.48	0.94
2:AR:2043:LYS:HG2	2:AR:2067:TRP:HB3	1.49	0.94
3:Ci:3066:LYS:HG3	4:Cj:4063:VAL:HG13	1.46	0.94
2:Bx:2092:LEU:HD23	4:Bz:4056:VAL:HG22	1.49	0.93
3:Bq:3024:GLN:HE22	3:Bq:3027:MET:HE2	1.34	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	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	AI	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	AQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	AY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	Ag	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	Ao	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	4	21
1	Aw	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	4	21
1	BA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	BI	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	4	21
1	BQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	BY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	Bg	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	Bo	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	Bw	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	CA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	CI	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	CQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	CY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	Cg	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
1	Co	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	4	21
2	AB	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
2	AJ	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	AR	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	AZ	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
2	Ah	96/118 (81%)	90 (94%)	3 (3%)	3 (3%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ap	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Ax	96/118 (81%)	92 (96%)	3 (3%)	1 (1%)	12	41
2	BB	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	BJ	96/118 (81%)	90 (94%)	4 (4%)	2 (2%)	5	25
2	BR	96/118 (81%)	90 (94%)	4 (4%)	2 (2%)	5	25
2	BZ	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Bh	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	Bp	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Bx	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	CB	96/118 (81%)	90 (94%)	5 (5%)	1 (1%)	12	41
2	CJ	96/118 (81%)	89 (93%)	7 (7%)	0	100	100
2	CR	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	CZ	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	Ch	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Cp	96/118 (81%)	89 (93%)	7 (7%)	0	100	100
3	AC	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	AK	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	AS	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Aa	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Ai	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Aq	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Ay	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	BC	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	BK	75/92 (82%)	74 (99%)	1 (1%)	0	100	100
3	BS	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Ba	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Bi	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Bq	75/92 (82%)	74 (99%)	1 (1%)	0	100	100
3	By	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	CC	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	CK	75/92 (82%)	73 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CS	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Ca	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Ci	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Cq	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
4	AD	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	AL	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	AT	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
4	Ab	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Aj	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
4	Ar	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Az	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	BD	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
4	BL	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
4	BT	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Bb	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Bj	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Br	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Bz	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	CD	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	CL	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	CT	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Cb	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Cj	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Cr	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
5	A1	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6
5	AE	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6
5	AM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6
5	AU	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6
5	Ac	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	1	6
5	Ak	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	6
5	As	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B1	15/124 (12%)	10 (67%)	3 (20%)	2 (13%)	0	1
5	BE	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6
5	BM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6
5	BU	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6
5	Bc	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	6
5	Bk	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6
5	Bs	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	6
5	CE	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	6
5	CM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6
5	CU	15/124 (12%)	10 (67%)	5 (33%)	0	100	100
5	Cc	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	1	6
5	Ck	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	6
5	Cs	15/124 (12%)	10 (67%)	2 (13%)	3 (20%)	0	0
6	A2	214/247 (87%)	187 (87%)	17 (8%)	10 (5%)	2	11
6	AF	214/247 (87%)	182 (85%)	22 (10%)	10 (5%)	2	11
6	AN	214/247 (87%)	174 (81%)	31 (14%)	9 (4%)	2	13
6	AV	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	1	10
6	Ad	214/247 (87%)	183 (86%)	20 (9%)	11 (5%)	1	10
6	Al	214/247 (87%)	183 (86%)	21 (10%)	10 (5%)	2	11
6	At	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	1	10
6	B2	214/247 (87%)	179 (84%)	23 (11%)	12 (6%)	1	8
6	BF	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	2	15
6	BN	214/247 (87%)	185 (86%)	22 (10%)	7 (3%)	3	17
6	BV	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	2	15
6	Bd	214/247 (87%)	185 (86%)	19 (9%)	10 (5%)	2	11
6	Bl	214/247 (87%)	186 (87%)	18 (8%)	10 (5%)	2	11
6	Bt	214/247 (87%)	181 (85%)	27 (13%)	6 (3%)	4	20
6	CF	214/247 (87%)	187 (87%)	19 (9%)	8 (4%)	2	15
6	CN	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	2	15
6	CV	214/247 (87%)	182 (85%)	24 (11%)	8 (4%)	2	15
6	Cd	214/247 (87%)	185 (86%)	19 (9%)	10 (5%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Cl	214/247 (87%)	186 (87%)	19 (9%)	9 (4%)	2	13
6	Ct	214/247 (87%)	178 (83%)	26 (12%)	10 (5%)	2	11
7	A3	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	AG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	AO	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	AW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	Ae	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	Am	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	Au	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	B3	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	4	22
7	BG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	BO	123/186 (66%)	115 (94%)	4 (3%)	4 (3%)	3	17
7	BW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	Be	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	4	22
7	Bm	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	4	22
7	Bu	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	CG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	CO	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	CW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	Ce	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
7	Cm	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	4	22
7	Cu	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	3	17
8	A4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	AH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	AP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	AX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	Af	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	An	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	Av	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	B4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	BH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	BP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	BX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	Bf	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	Bn	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	Bv	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	CH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	CP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	CX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	Cf	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	Cn	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
8	Cv	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	8	32
All	All	14800/20960 (71%)	13553 (92%)	894 (6%)	353 (2%)	4	22

5 of 353 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AM	7006	LEU
6	AN	8028	ILE
6	AN	8185	LYS
6	AN	8186	GLU
6	AN	8212	LYS

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	77/101 (76%)	70 (91%)	7 (9%)	9	32
1	AI	77/101 (76%)	71 (92%)	6 (8%)	11	38
1	AQ	77/101 (76%)	71 (92%)	6 (8%)	11	38
1	AY	77/101 (76%)	71 (92%)	6 (8%)	11	38
1	Ag	77/101 (76%)	70 (91%)	7 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ao	77/101 (76%)	72 (94%)	5 (6%)	15	44
1	Aw	77/101 (76%)	72 (94%)	5 (6%)	15	44
1	BA	77/101 (76%)	71 (92%)	6 (8%)	11	38
1	BI	77/101 (76%)	71 (92%)	6 (8%)	11	38
1	BQ	77/101 (76%)	72 (94%)	5 (6%)	15	44
1	BY	77/101 (76%)	70 (91%)	7 (9%)	9	32
1	Bg	77/101 (76%)	71 (92%)	6 (8%)	11	38
1	Bo	77/101 (76%)	70 (91%)	7 (9%)	9	32
1	Bw	77/101 (76%)	70 (91%)	7 (9%)	9	32
1	CA	77/101 (76%)	70 (91%)	7 (9%)	9	32
1	CI	77/101 (76%)	70 (91%)	7 (9%)	9	32
1	CQ	77/101 (76%)	70 (91%)	7 (9%)	9	32
1	CY	77/101 (76%)	70 (91%)	7 (9%)	9	32
1	Cg	77/101 (76%)	70 (91%)	7 (9%)	9	32
1	Co	77/101 (76%)	72 (94%)	5 (6%)	15	44
2	AB	94/110 (86%)	89 (95%)	5 (5%)	20	51
2	AJ	94/110 (86%)	90 (96%)	4 (4%)	26	57
2	AR	94/110 (86%)	89 (95%)	5 (5%)	20	51
2	AZ	94/110 (86%)	89 (95%)	5 (5%)	20	51
2	Ah	94/110 (86%)	88 (94%)	6 (6%)	16	44
2	Ap	94/110 (86%)	90 (96%)	4 (4%)	26	57
2	Ax	94/110 (86%)	89 (95%)	5 (5%)	20	51
2	BB	94/110 (86%)	89 (95%)	5 (5%)	20	51
2	BJ	94/110 (86%)	88 (94%)	6 (6%)	16	44
2	BR	94/110 (86%)	89 (95%)	5 (5%)	20	51
2	BZ	94/110 (86%)	88 (94%)	6 (6%)	16	44
2	Bh	94/110 (86%)	88 (94%)	6 (6%)	16	44
2	Bp	94/110 (86%)	89 (95%)	5 (5%)	20	51
2	Bx	94/110 (86%)	87 (93%)	7 (7%)	13	40
2	CB	94/110 (86%)	88 (94%)	6 (6%)	16	44
2	CJ	94/110 (86%)	88 (94%)	6 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CR	94/110 (86%)	89 (95%)	5 (5%)	20	51
2	CZ	94/110 (86%)	89 (95%)	5 (5%)	20	51
2	Ch	94/110 (86%)	87 (93%)	7 (7%)	13	40
2	Cp	94/110 (86%)	87 (93%)	7 (7%)	13	40
3	AC	72/84 (86%)	67 (93%)	5 (7%)	14	41
3	AK	72/84 (86%)	68 (94%)	4 (6%)	19	49
3	AS	72/84 (86%)	68 (94%)	4 (6%)	19	49
3	Aa	72/84 (86%)	67 (93%)	5 (7%)	14	41
3	Ai	72/84 (86%)	68 (94%)	4 (6%)	19	49
3	Aq	72/84 (86%)	67 (93%)	5 (7%)	14	41
3	Ay	72/84 (86%)	69 (96%)	3 (4%)	26	58
3	BC	72/84 (86%)	68 (94%)	4 (6%)	19	49
3	BK	72/84 (86%)	68 (94%)	4 (6%)	19	49
3	BS	72/84 (86%)	68 (94%)	4 (6%)	19	49
3	Ba	72/84 (86%)	67 (93%)	5 (7%)	14	41
3	Bi	72/84 (86%)	67 (93%)	5 (7%)	14	41
3	Bq	72/84 (86%)	67 (93%)	5 (7%)	14	41
3	By	72/84 (86%)	67 (93%)	5 (7%)	14	41
3	CC	72/84 (86%)	67 (93%)	5 (7%)	14	41
3	CK	72/84 (86%)	68 (94%)	4 (6%)	19	49
3	CS	72/84 (86%)	67 (93%)	5 (7%)	14	41
3	Ca	72/84 (86%)	67 (93%)	5 (7%)	14	41
3	Ci	72/84 (86%)	68 (94%)	4 (6%)	19	49
3	Cq	72/84 (86%)	67 (93%)	5 (7%)	14	41
4	AD	60/74 (81%)	57 (95%)	3 (5%)	22	53
4	AL	60/74 (81%)	58 (97%)	2 (3%)	33	63
4	AT	60/74 (81%)	58 (97%)	2 (3%)	33	63
4	Ab	60/74 (81%)	57 (95%)	3 (5%)	22	53
4	Aj	60/74 (81%)	57 (95%)	3 (5%)	22	53
4	Ar	60/74 (81%)	57 (95%)	3 (5%)	22	53
4	Az	60/74 (81%)	58 (97%)	2 (3%)	33	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BD	60/74 (81%)	57 (95%)	3 (5%)	22	53
4	BL	60/74 (81%)	58 (97%)	2 (3%)	33	63
4	BT	60/74 (81%)	57 (95%)	3 (5%)	22	53
4	Bb	60/74 (81%)	57 (95%)	3 (5%)	22	53
4	Bj	60/74 (81%)	58 (97%)	2 (3%)	33	63
4	Br	60/74 (81%)	58 (97%)	2 (3%)	33	63
4	Bz	60/74 (81%)	58 (97%)	2 (3%)	33	63
4	CD	60/74 (81%)	57 (95%)	3 (5%)	22	53
4	CL	60/74 (81%)	59 (98%)	1 (2%)	53	74
4	CT	60/74 (81%)	56 (93%)	4 (7%)	15	43
4	Cb	60/74 (81%)	56 (93%)	4 (7%)	15	43
4	Cj	60/74 (81%)	58 (97%)	2 (3%)	33	63
4	Cr	60/74 (81%)	59 (98%)	1 (2%)	53	74
5	A1	15/97 (16%)	11 (73%)	4 (27%)	0	2
5	AE	15/97 (16%)	13 (87%)	2 (13%)	4	17
5	AM	15/97 (16%)	13 (87%)	2 (13%)	4	17
5	AU	15/97 (16%)	14 (93%)	1 (7%)	15	43
5	Ac	15/97 (16%)	13 (87%)	2 (13%)	4	17
5	Ak	15/97 (16%)	13 (87%)	2 (13%)	4	17
5	As	15/97 (16%)	13 (87%)	2 (13%)	4	17
5	B1	15/97 (16%)	14 (93%)	1 (7%)	15	43
5	BE	15/97 (16%)	12 (80%)	3 (20%)	1	6
5	BM	15/97 (16%)	12 (80%)	3 (20%)	1	6
5	BU	15/97 (16%)	13 (87%)	2 (13%)	4	17
5	Bc	15/97 (16%)	13 (87%)	2 (13%)	4	17
5	Bk	15/97 (16%)	12 (80%)	3 (20%)	1	6
5	Bs	15/97 (16%)	14 (93%)	1 (7%)	15	43
5	CE	15/97 (16%)	13 (87%)	2 (13%)	4	17
5	CM	15/97 (16%)	13 (87%)	2 (13%)	4	17
5	CU	15/97 (16%)	12 (80%)	3 (20%)	1	6
5	Cc	15/97 (16%)	13 (87%)	2 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Ck	15/97 (16%)	13 (87%)	2 (13%)	4	17
5	Cs	15/97 (16%)	10 (67%)	5 (33%)	0	0
6	A2	203/231 (88%)	174 (86%)	29 (14%)	3	14
6	AF	203/231 (88%)	164 (81%)	39 (19%)	1	7
6	AN	203/231 (88%)	166 (82%)	37 (18%)	2	8
6	AV	203/231 (88%)	171 (84%)	32 (16%)	2	12
6	Ad	203/231 (88%)	172 (85%)	31 (15%)	3	12
6	Al	203/231 (88%)	169 (83%)	34 (17%)	2	10
6	At	203/231 (88%)	167 (82%)	36 (18%)	2	9
6	B2	203/231 (88%)	165 (81%)	38 (19%)	1	7
6	BF	203/231 (88%)	170 (84%)	33 (16%)	2	11
6	BN	203/231 (88%)	172 (85%)	31 (15%)	3	12
6	BV	203/231 (88%)	172 (85%)	31 (15%)	3	12
6	Bd	203/231 (88%)	171 (84%)	32 (16%)	2	12
6	Bl	203/231 (88%)	172 (85%)	31 (15%)	3	12
6	Bt	203/231 (88%)	170 (84%)	33 (16%)	2	11
6	CF	203/231 (88%)	171 (84%)	32 (16%)	2	12
6	CN	203/231 (88%)	175 (86%)	28 (14%)	3	15
6	CV	203/231 (88%)	172 (85%)	31 (15%)	3	12
6	Cd	203/231 (88%)	172 (85%)	31 (15%)	3	12
6	Cl	203/231 (88%)	169 (83%)	34 (17%)	2	10
6	Ct	203/231 (88%)	168 (83%)	35 (17%)	2	10
7	A3	108/159 (68%)	97 (90%)	11 (10%)	7	28
7	AG	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	AO	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	AW	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	Ae	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	Am	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	Au	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	B3	108/159 (68%)	98 (91%)	10 (9%)	8	31
7	BG	108/159 (68%)	99 (92%)	9 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	BO	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	BW	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	Be	108/159 (68%)	100 (93%)	8 (7%)	13	40
7	Bm	108/159 (68%)	100 (93%)	8 (7%)	13	40
7	Bu	108/159 (68%)	100 (93%)	8 (7%)	13	40
7	CG	108/159 (68%)	98 (91%)	10 (9%)	8	31
7	CO	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	CW	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	Ce	108/159 (68%)	98 (91%)	10 (9%)	8	31
7	Cm	108/159 (68%)	99 (92%)	9 (8%)	10	35
7	Cu	108/159 (68%)	100 (93%)	8 (7%)	13	40
8	A4	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	AH	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	AP	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	AX	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	Af	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	An	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	Av	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	B4	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	BH	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	BP	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	BX	61/66 (92%)	58 (95%)	3 (5%)	22	53
8	Bf	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	Bn	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	Bv	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	CH	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	CP	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	CX	61/66 (92%)	58 (95%)	3 (5%)	22	53
8	Cf	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	Cn	61/66 (92%)	59 (97%)	2 (3%)	33	63
8	Cv	61/66 (92%)	59 (97%)	2 (3%)	33	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	13800/18440 (75%)	12497 (91%)	1303 (9%)	8 31

5 of 1303 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CC	3045	ASP
6	Cd	8142	LEU
6	CF	8139	VAL
3	CC	3026	ASN
1	CQ	1064	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 254 such sidechains are listed below:

Mol	Chain	Res	Type
2	BR	2094	ASN
6	Cd	8096	GLN
3	Bi	3002	GLN
3	Ca	3024	GLN
7	Cm	6058	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SO4	Bt	8301	-	4,4,4	0.19	0	6,6,6	0.34	0
9	SO4	BV	8301	-	4,4,4	0.27	0	6,6,6	0.41	0
9	SO4	B2	8301	-	4,4,4	0.36	0	6,6,6	0.33	0
9	SO4	Bd	8301	-	4,4,4	0.35	0	6,6,6	0.40	0
9	SO4	Ad	8301	-	4,4,4	0.38	0	6,6,6	0.28	0
9	SO4	BF	8301	-	4,4,4	0.19	0	6,6,6	0.28	0
9	SO4	A2	8301	-	4,4,4	0.22	0	6,6,6	0.40	0
9	SO4	At	8301	-	4,4,4	0.44	0	6,6,6	0.57	0
9	SO4	Cl	8301	-	4,4,4	0.42	0	6,6,6	0.25	0
9	SO4	CF	8301	-	4,4,4	0.38	0	6,6,6	0.37	0

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	82/119 (68%)	0.46	4 (4%) 35 18	16, 44, 80, 155	0
1	AI	82/119 (68%)	0.38	4 (4%) 35 18	17, 41, 83, 141	0
1	AQ	82/119 (68%)	0.49	5 (6%) 27 15	26, 48, 92, 145	0
1	AY	82/119 (68%)	1.93	31 (37%) 1 0	48, 76, 117, 154	0
1	Ag	82/119 (68%)	0.70	6 (7%) 21 11	14, 47, 94, 167	0
1	Ao	82/119 (68%)	0.44	4 (4%) 35 18	18, 43, 87, 158	0
1	Aw	82/119 (68%)	1.81	30 (36%) 1 0	48, 76, 115, 154	0
1	BA	82/119 (68%)	3.10	75 (91%) 0 0	69, 92, 131, 175	0
1	BI	82/119 (68%)	3.25	72 (87%) 0 0	66, 92, 127, 175	0
1	BQ	82/119 (68%)	1.03	11 (13%) 7 4	34, 60, 107, 179	0
1	BY	82/119 (68%)	0.80	9 (10%) 10 5	25, 54, 88, 130	0
1	Bg	82/119 (68%)	2.19	45 (54%) 0 0	58, 81, 117, 151	0
1	Bo	82/119 (68%)	1.59	27 (32%) 1 0	41, 68, 117, 164	0
1	Bw	82/119 (68%)	0.76	6 (7%) 21 11	24, 53, 90, 142	0
1	CA	82/119 (68%)	1.36	18 (21%) 2 1	36, 64, 105, 132	0
1	CI	82/119 (68%)	3.05	69 (84%) 0 0	61, 86, 127, 164	0
1	CQ	82/119 (68%)	0.60	5 (6%) 27 15	29, 54, 88, 136	0
1	CY	82/119 (68%)	0.69	7 (8%) 16 9	17, 47, 88, 130	0
1	Cg	82/119 (68%)	2.27	47 (57%) 0 0	52, 82, 119, 162	0
1	Co	82/119 (68%)	3.00	65 (79%) 0 0	64, 88, 130, 168	0
2	AB	100/118 (84%)	0.92	10 (10%) 12 6	19, 63, 168, 181	0
2	AJ	100/118 (84%)	0.86	12 (12%) 9 5	20, 63, 167, 179	0
2	AR	100/118 (84%)	0.92	9 (9%) 15 8	29, 69, 190, 201	0
2	AZ	100/118 (84%)	1.10	8 (8%) 18 10	39, 82, 226, 242	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
2	Ah	100/118 (84%)	1.49	23 (23%)	2	1	44, 82, 207, 217	0
2	Ap	100/118 (84%)	1.07	12 (12%)	9	5	34, 72, 215, 219	0
2	Ax	100/118 (84%)	1.12	14 (14%)	6	4	31, 73, 210, 225	0
2	BB	100/118 (84%)	3.11	79 (79%)	0	0	87, 124, 220, 226	0
2	BJ	100/118 (84%)	2.59	68 (68%)	0	0	77, 113, 245, 255	0
2	BR	100/118 (84%)	1.64	28 (28%)	1	1	45, 94, 235, 237	0
2	BZ	100/118 (84%)	1.09	13 (13%)	7	4	37, 76, 216, 232	0
2	Bh	100/118 (84%)	1.43	20 (20%)	3	1	50, 90, 235, 253	0
2	Bp	100/118 (84%)	1.98	49 (49%)	0	0	56, 111, 242, 250	0
2	Bx	100/118 (84%)	1.03	11 (11%)	10	5	32, 75, 230, 243	0
2	CB	100/118 (84%)	1.71	32 (32%)	1	0	48, 92, 223, 238	0
2	CJ	100/118 (84%)	2.92	72 (72%)	0	0	79, 118, 224, 231	0
2	CR	100/118 (84%)	0.90	10 (10%)	12	6	35, 76, 183, 203	0
2	CZ	100/118 (84%)	0.88	12 (12%)	9	5	28, 72, 184, 205	0
2	Ch	100/118 (84%)	1.44	19 (19%)	3	1	55, 90, 212, 223	0
2	Cp	100/118 (84%)	2.29	56 (56%)	0	0	67, 112, 233, 247	0
3	AC	77/92 (83%)	1.69	29 (37%)	1	0	70, 120, 150, 162	0
3	AK	77/92 (83%)	2.02	37 (48%)	0	0	79, 125, 164, 170	0
3	AS	77/92 (83%)	2.70	55 (71%)	0	0	128, 181, 261, 265	0
3	Aa	77/92 (83%)	2.46	51 (66%)	0	0	134, 199, 268, 274	0
3	Ai	77/92 (83%)	1.55	20 (25%)	1	1	86, 135, 164, 173	0
3	Aq	77/92 (83%)	2.23	39 (50%)	0	0	126, 179, 246, 254	0
3	Ay	77/92 (83%)	2.15	41 (53%)	0	0	87, 140, 220, 227	0
3	BC	77/92 (83%)	2.27	44 (57%)	0	0	128, 157, 177, 185	0
3	BK	77/92 (83%)	2.70	49 (63%)	0	0	177, 242, 280, 286	0
3	BS	77/92 (83%)	2.08	34 (44%)	0	0	148, 203, 244, 256	0
3	Ba	77/92 (83%)	2.38	40 (51%)	0	0	133, 188, 260, 264	0
3	Bi	77/92 (83%)	2.36	41 (53%)	0	0	144, 203, 278, 279	0
3	Bq	77/92 (83%)	2.22	38 (49%)	0	0	200, 257, 282, 293	0
3	By	77/92 (83%)	2.15	38 (49%)	0	0	143, 207, 268, 274	0
3	CC	77/92 (83%)	1.60	20 (25%)	1	1	107, 151, 185, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
3	CK	77/92 (83%)	2.18	37 (48%)	0	0	131, 181, 212, 222	0
3	CS	77/92 (83%)	1.50	18 (23%)	2	1	81, 121, 161, 172	0
3	Ca	77/92 (83%)	1.42	21 (27%)	1	1	82, 122, 165, 177	0
3	Ci	77/92 (83%)	2.02	31 (40%)	0	0	107, 148, 200, 206	0
3	Cq	77/92 (83%)	2.02	37 (48%)	0	0	172, 241, 284, 286	0
4	AD	71/86 (82%)	1.24	11 (15%)	5	2	46, 93, 120, 142	0
4	AL	71/86 (82%)	1.17	11 (15%)	5	2	50, 89, 113, 143	0
4	AT	71/86 (82%)	1.69	26 (36%)	1	0	64, 115, 159, 182	0
4	Ab	71/86 (82%)	1.40	16 (22%)	2	1	73, 116, 166, 193	0
4	Aj	71/86 (82%)	1.59	18 (25%)	1	1	71, 125, 153, 185	0
4	Ar	71/86 (82%)	1.67	22 (30%)	1	1	66, 122, 172, 191	0
4	Az	71/86 (82%)	1.14	9 (12%)	8	4	60, 105, 133, 163	0
4	BD	71/86 (82%)	2.41	44 (61%)	0	0	104, 169, 199, 208	0
4	BL	71/86 (82%)	2.26	37 (52%)	0	0	118, 165, 251, 260	0
4	BT	71/86 (82%)	1.75	24 (33%)	1	0	98, 144, 212, 220	0
4	Bb	71/86 (82%)	1.66	21 (29%)	1	1	64, 121, 161, 193	0
4	Bj	71/86 (82%)	1.61	17 (23%)	2	1	80, 130, 174, 203	0
4	Br	71/86 (82%)	2.31	45 (63%)	0	0	118, 183, 264, 271	0
4	Bz	71/86 (82%)	1.57	24 (33%)	1	0	71, 128, 179, 219	0
4	CD	71/86 (82%)	1.67	17 (23%)	2	1	77, 126, 152, 195	0
4	CL	71/86 (82%)	2.86	51 (71%)	0	0	111, 166, 197, 201	0
4	CT	71/86 (82%)	1.11	7 (9%)	13	7	64, 101, 128, 156	0
4	Cb	71/86 (82%)	1.19	9 (12%)	8	4	60, 102, 128, 157	0
4	Cj	71/86 (82%)	1.30	12 (16%)	4	2	79, 117, 152, 178	0
4	Cr	71/86 (82%)	2.19	34 (47%)	0	0	111, 166, 244, 257	0
5	A1	17/124 (13%)	0.80	2 (11%)	9	5	73, 98, 162, 164	0
5	AE	17/124 (13%)	0.77	0	100	100	67, 81, 121, 128	0
5	AM	17/124 (13%)	0.78	0	100	100	64, 80, 131, 133	0
5	AU	17/124 (13%)	0.89	2 (11%)	9	5	58, 85, 120, 125	0
5	Ac	17/124 (13%)	0.90	2 (11%)	9	5	52, 86, 141, 144	0
5	Ak	17/124 (13%)	0.82	1 (5%)	28	15	63, 78, 125, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	As	17/124 (13%)	0.75	3 (17%) 4 2	59, 76, 128, 128	0
5	B1	17/124 (13%)	0.81	1 (5%) 28 15	56, 69, 129, 130	0
5	BE	17/124 (13%)	2.00	9 (52%) 0 0	115, 129, 153, 167	0
5	BM	17/124 (13%)	1.66	7 (41%) 0 0	96, 109, 152, 152	0
5	BU	17/124 (13%)	0.82	2 (11%) 9 5	83, 94, 129, 132	0
5	Bc	17/124 (13%)	0.80	1 (5%) 28 15	60, 81, 133, 136	0
5	Bk	17/124 (13%)	1.51	4 (23%) 2 1	85, 98, 150, 153	0
5	Bs	17/124 (13%)	1.34	3 (17%) 4 2	81, 95, 149, 151	0
5	CE	17/124 (13%)	1.12	3 (17%) 4 2	77, 93, 139, 142	0
5	CM	17/124 (13%)	1.94	8 (47%) 0 0	111, 124, 163, 163	0
5	CU	17/124 (13%)	0.68	1 (5%) 28 15	54, 78, 134, 134	0
5	Cc	17/124 (13%)	0.89	1 (5%) 28 15	53, 72, 132, 134	0
5	Ck	17/124 (13%)	1.62	4 (23%) 2 1	79, 92, 156, 160	0
5	Cs	17/124 (13%)	1.71	8 (47%) 0 0	101, 114, 151, 152	0
6	A2	216/247 (87%)	0.64	15 (6%) 23 12	24, 73, 196, 212	0
6	AF	216/247 (87%)	0.74	21 (9%) 13 7	14, 56, 168, 208	0
6	AN	216/247 (87%)	0.65	16 (7%) 20 11	11, 54, 167, 187	0
6	AV	216/247 (87%)	0.75	23 (10%) 11 6	17, 59, 201, 226	0
6	Ad	216/247 (87%)	1.22	42 (19%) 3 1	27, 75, 214, 236	0
6	Al	216/247 (87%)	0.92	28 (12%) 7 4	16, 62, 189, 235	0
6	At	216/247 (87%)	0.78	23 (10%) 11 6	14, 55, 202, 219	0
6	B2	216/247 (87%)	0.88	22 (10%) 12 6	20, 58, 225, 240	0
6	BF	216/247 (87%)	2.51	136 (62%) 0 0	71, 108, 202, 230	0
6	BN	216/247 (87%)	2.29	122 (56%) 0 0	57, 99, 235, 247	0
6	BV	216/247 (87%)	1.19	41 (18%) 3 1	31, 78, 219, 245	0
6	Bd	216/247 (87%)	0.85	21 (9%) 13 7	24, 61, 215, 236	0
6	Bl	216/247 (87%)	1.31	39 (18%) 3 1	38, 78, 226, 246	0
6	Bt	216/247 (87%)	1.43	51 (23%) 2 1	41, 78, 233, 250	0
6	CF	216/247 (87%)	1.20	32 (14%) 5 3	35, 73, 195, 229	0
6	CN	216/247 (87%)	2.58	144 (66%) 0 0	64, 107, 196, 224	0
6	CV	216/247 (87%)	0.66	12 (5%) 30 16	23, 61, 175, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	Cd	216/247 (87%)	0.71	15 (6%) 23 12	14, 55, 181, 211	0
6	Cl	216/247 (87%)	1.36	48 (22%) 2 1	32, 76, 204, 225	0
6	Ct	216/247 (87%)	2.37	129 (59%) 0 0	63, 103, 224, 240	0
7	A3	127/186 (68%)	2.25	66 (51%) 0 0	74, 126, 154, 172	0
7	AG	127/186 (68%)	0.80	11 (8%) 16 9	21, 47, 108, 144	0
7	AO	127/186 (68%)	0.94	12 (9%) 14 8	19, 58, 119, 143	0
7	AW	127/186 (68%)	0.88	11 (8%) 16 9	29, 60, 122, 152	0
7	Ae	127/186 (68%)	3.74	114 (89%) 0 0	78, 122, 162, 170	0
7	Am	127/186 (68%)	0.50	8 (6%) 26 14	13, 43, 110, 149	0
7	Au	127/186 (68%)	0.91	13 (10%) 12 6	20, 51, 122, 152	0
7	B3	127/186 (68%)	1.06	14 (11%) 10 5	31, 58, 113, 162	0
7	BG	127/186 (68%)	2.25	68 (53%) 0 0	51, 82, 135, 167	0
7	BO	127/186 (68%)	3.37	109 (85%) 0 0	73, 107, 149, 178	0
7	BW	127/186 (68%)	0.67	10 (7%) 18 10	28, 54, 115, 153	0
7	Be	127/186 (68%)	1.00	15 (11%) 9 5	33, 62, 120, 162	0
7	Bm	127/186 (68%)	3.31	107 (84%) 0 0	62, 110, 152, 178	0
7	Bu	127/186 (68%)	1.00	10 (7%) 18 10	34, 63, 122, 167	0
7	CG	127/186 (68%)	0.74	9 (7%) 22 12	22, 57, 116, 158	0
7	CO	127/186 (68%)	2.21	73 (57%) 0 0	55, 85, 133, 174	0
7	CW	127/186 (68%)	0.88	13 (10%) 12 6	23, 59, 126, 158	0
7	Ce	127/186 (68%)	0.78	14 (11%) 10 5	20, 53, 115, 158	0
7	Cm	127/186 (68%)	4.12	117 (92%) 0 0	67, 125, 157, 179	0
7	Cu	127/186 (68%)	2.81	91 (71%) 0 0	73, 100, 146, 174	0
8	A4	70/76 (92%)	2.55	38 (54%) 0 0	158, 202, 224, 228	0
8	AH	70/76 (92%)	1.37	14 (20%) 3 1	69, 116, 150, 158	0
8	AP	70/76 (92%)	1.96	32 (45%) 0 0	81, 137, 167, 178	0
8	AX	70/76 (92%)	2.08	31 (44%) 0 0	121, 196, 220, 225	0
8	Af	70/76 (92%)	2.62	45 (64%) 0 0	200, 237, 255, 258	0
8	An	70/76 (92%)	1.27	9 (12%) 7 4	67, 110, 152, 158	0
8	Av	70/76 (92%)	1.59	17 (24%) 2 1	109, 176, 200, 214	0
8	B4	70/76 (92%)	2.37	38 (54%) 0 0	176, 224, 253, 261	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
8	BH	70/76 (92%)	2.28	38 (54%)	0	0	102, 140, 170, 178	0
8	BP	70/76 (92%)	2.59	42 (60%)	0	0	180, 237, 261, 266	0
8	BX	70/76 (92%)	1.72	21 (30%)	1	1	114, 173, 192, 201	0
8	Bf	70/76 (92%)	2.35	38 (54%)	0	0	178, 226, 252, 255	0
8	Bn	70/76 (92%)	2.43	39 (55%)	0	0	221, 251, 273, 278	0
8	Bv	70/76 (92%)	2.19	33 (47%)	0	0	185, 237, 271, 277	0
8	CH	70/76 (92%)	1.57	18 (25%)	1	1	106, 144, 166, 172	0
8	CP	70/76 (92%)	2.11	31 (44%)	0	0	135, 167, 187, 206	0
8	CX	70/76 (92%)	1.80	28 (40%)	1	0	103, 135, 162, 171	0
8	Cf	70/76 (92%)	1.70	18 (25%)	1	1	97, 140, 160, 170	0
8	Cn	70/76 (92%)	2.81	48 (68%)	0	0	146, 178, 204, 210	0
8	Cv	70/76 (92%)	2.50	43 (61%)	0	0	231, 267, 287, 290	0
All	All	15200/20960 (72%)	1.59	4820 (31%)	1	1	11, 97, 231, 293	0

The worst 5 of 4820 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	BG	6164	ASN	11.1
7	BO	6164	ASN	10.0
3	BK	3044	LEU	9.6
7	Ae	6164	ASN	9.4
8	A4	5055	VAL	8.8

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($\text{\AA}^2$)	Q<0.9
9	SO4	Cl	8301	5/5	0.54	0.17	129,131,132,132	0
9	SO4	Ad	8301	5/5	0.56	0.17	137,139,139,140	0
9	SO4	BF	8301	5/5	0.60	0.20	129,129,130,131	0
9	SO4	At	8301	5/5	0.67	0.18	92,93,96,99	0
9	SO4	Bt	8301	5/5	0.69	0.19	111,113,114,115	0
9	SO4	A2	8301	5/5	0.69	0.18	150,150,150,151	0
9	SO4	Bd	8301	5/5	0.74	0.17	108,108,109,112	0
9	SO4	BV	8301	5/5	0.77	0.18	111,113,114,116	0
9	SO4	CF	8301	5/5	0.79	0.15	100,103,104,106	0
9	SO4	B2	8301	5/5	0.82	0.16	97,99,99,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.