



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:01 PM GMT

PDB ID : 4V98
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

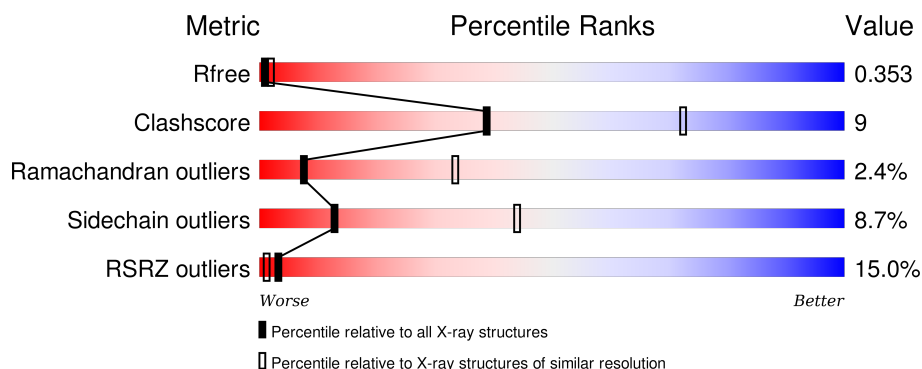
1 Overall quality at a glance

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>56%</div> <div>11% .. 31%</div> </div>
1	AI	119	<div> <div>57%</div> <div>10% .. 31%</div> </div>
1	AQ	119	<div> <div>56%</div> <div>11% .. 31%</div> </div>
1	AY	119	<div> <div>%</div> <div>58% 8% .. 31%</div> </div>
1	Ag	119	<div> <div>62%</div> <div>6% • 31%</div> </div>

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Mol	Chain	Length	Quality of chain
1	Ao	119	% 64% 31%
1	Aw	119	% 63% 5% 31%
1	BA	119	5% 57% 9% 31%
1	BI	119	12% 57% 9% 31%
1	BQ	119	% 57% 9% 31%
1	BY	119	61% 5% 31%
1	Bg	119	63% 5% 31%
1	Bo	119	62% 6% 31%
1	Bw	119	62% 6% 31%
1	CA	119	58% 9% 31%
1	CI	119	5% 57% 9% 31%
1	CQ	119	57% 9% 31%
1	CY	119	59% 8% 31%
1	Cg	119	62% 6% 31%
1	Co	119	8% 64% 31%
2	AB	118	% 69% 14% 15%
2	AJ	118	67% 17% 15%
2	AR	118	7% 66% 18% 15%
2	AZ	118	8% 69% 15% 15%
2	Ah	118	6% 78% 7% 15%
2	Ap	118	8% 82% 15%
2	Ax	118	3% 81% 15%
2	BB	118	24% 65% 18% 15%
2	BJ	118	32% 65% 17% 15%
2	BR	118	14% 66% 15% 15%

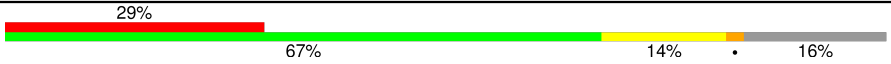
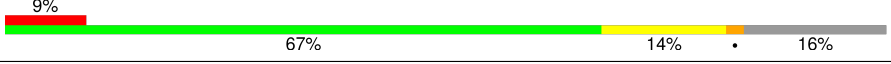
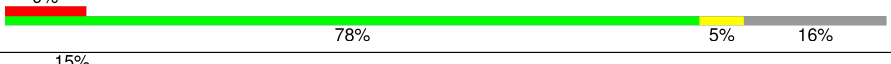


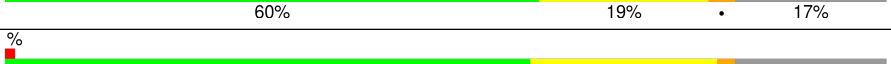
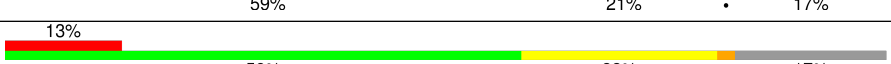
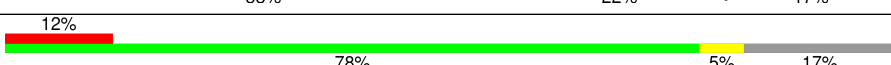
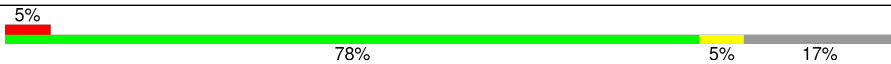


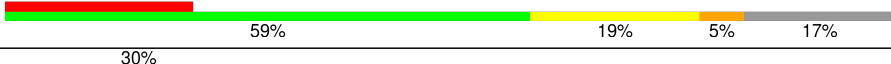
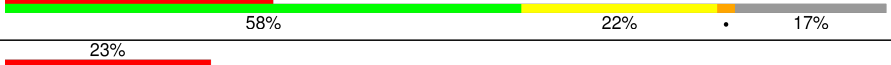

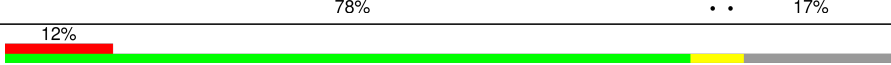










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Mol	Chain	Length	Quality of chain
2	BZ	118	
2	Bh	118	
2	Bp	118	
2	Bx	118	
2	CB	118	
2	CJ	118	
2	CR	118	
2	CZ	118	
2	Ch	118	
2	Cp	118	
3	AC	92	
3	AK	92	
3	AS	92	
3	Aa	92	
3	Ai	92	
3	Aq	92	
3	Ay	92	
3	BC	92	
3	BK	92	
3	BS	92	
3	Ba	92	
3	Bi	92	
3	Bq	92	
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	<div><div></div><div>29%</div><div></div><div>79%</div><div></div><div>12%</div><div></div><div>8%</div></div>
8	CX	76	<div><div></div><div>12%</div><div></div><div>79%</div><div></div><div>12%</div><div></div><div>8%</div></div>
8	Cf	76	<div><div></div><div>8%</div><div></div><div>88%</div><div></div><div></div><div></div><div>8%</div></div>
8	Cn	76	<div><div></div><div>30%</div><div></div><div>88%</div><div></div><div></div><div></div><div>8%</div></div>
8	Cv	76	<div><div></div><div>70%</div><div></div><div>88%</div><div></div><div></div><div></div><div>8%</div></div>

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	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Bm	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Bu	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	B3	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	CG	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	CO	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	CW	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Ce	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Cm	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Cu	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			

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.

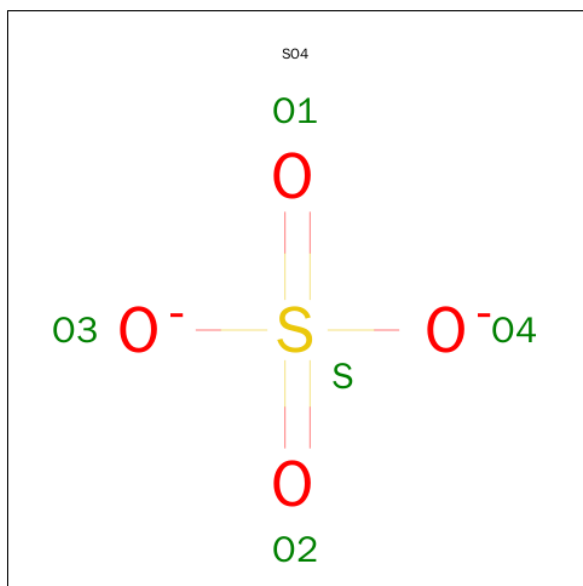
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AP	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	AH	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	AX	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Af	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	An	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
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 (three-letter code: 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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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		

- | MET | LI000 | LI001 | LI002 | LI009 | LI018 | LI047 | LI048 | LI049 | LI050 | LI053 | LI056 | LI061 | LI064 | LI069 | LI070 | LI071 | LI072 | LI081 | LI082 | LI083 | LI084 | LI085 | LI086 | LI087 | LI088 | LI089 | LI090 | LI091 | LI092 | LI093 | LI094 | LI095 | LI096 | LI097 | LI098 | LI099 | LI100 | LI101 | LI102 | LI103 | LI104 | LI105 | LI106 | LI107 | LI108 | LI109 | LI110 | LI111 | LI112 | LI113 | LI114 | LI115 | LI116 | LI117 | LI118 | LI119 | LI120 | LI121 | LI122 | LI123 | LI124 | LI125 | LI126 | LI127 | LI128 | LI129 | LI130 | LI131 | LI132 | LI133 | LI134 | LI135 | LI136 | LI137 | LI138 | LI139 | LI140 | LI141 | LI142 | LI143 | LI144 | LI145 | LI146 | LI147 | LI148 | LI149 | LI150 | LI151 | LI152 | LI153 | LI154 | LI155 | LI156 | LI157 | LI158 | LI159 | LI160 | LI161 | LI162 | LI163 | LI164 | LI165 | LI166 | LI167 | LI168 | LI169 | LI170 | LI171 | LI172 | LI173 | LI174 | LI175 | LI176 | LI177 | LI178 | LI179 | LI180 | LI181 | LI182 | LI183 | LI184 | LI185 | LI186 | LI187 | LI188 | LI189 | LI190 | LI191 | LI192 | LI193 | LI194 | LI195 | LI196 | LI197 | LI198 | LI199 | LI200 | LI201 | LI202 | LI203 | LI204 | LI205 | LI206 | LI207 | LI208 | LI209 | LI210 | LI211 | LI212 | LI213 | LI214 | LI215 | LI216 | LI217 | LI218 | LI219 | LI220 | LI221 | LI222 | LI223 | LI224 | LI225 | LI226 | LI227 | LI228 | LI229 | LI230 | LI231 | LI232 | LI233 | LI234 | LI235 | LI236 | LI237 | LI238 | LI239 | LI240 | LI241 | LI242 | LI243 | LI244 | LI245 | LI246 | LI247 | LI248 | LI249 | LI250 | LI251 | LI252 | LI253 | LI254 | LI255 | LI256 | LI257 | LI258 | LI259 | LI260 | LI261 | LI262 | LI263 | LI264 | LI265 | LI266 | LI267 | LI268 | LI269 | LI270 | LI271 | LI272 | LI273 | LI274 | LI275 | LI276 | LI277 | LI278 | LI279 | LI280 | LI281 | LI282 | LI283 | LI284 | LI285 | LI286 | LI287 | LI288 | LI289 | LI290 | LI291 | LI292 | LI293 | LI294 | LI295 | LI296 | LI297 | LI298 | LI299 | LI300 | LI301 | LI302 | LI303 | LI304 | LI305 | LI306 | LI307 | LI308 | LI309 | LI310 | LI311 | LI312 | LI313 | LI314 | LI315 | LI316 | LI317 | LI318 | LI319 | LI320 | LI321 | LI322 | LI323 | LI324 | LI325 | LI326 | LI327 | LI328 | LI329 | LI330 | LI331 | LI332 | LI333 | LI334 | LI335 | LI336 | LI337 | LI338 | LI339 | LI340 | LI341 | LI342 | LI343 | LI344 | LI345 | LI346 | LI347 | LI348 | LI349 | LI350 | LI351 | LI352 | LI353 | LI354 | LI355 | LI356 | LI357 | LI358 | LI359 | LI360 | LI361 | LI362 | LI363 | LI364 | LI365 | LI366 | LI367 | LI368 | LI369 | LI370 | LI371 | LI372 | LI373 | LI374 | LI375 | LI376 | LI377 | LI378 | LI379 | LI380 | LI381 | LI382 | LI383 | LI384 | LI385 | LI386 | LI387 | LI388 | LI389 | LI390 | LI391 | LI392 | LI393 | LI394 | LI395 | LI396 | LI397 | LI398 | LI399 | LI400 | LI401 | LI402 | LI403 | LI404 | LI405 | LI406 | LI407 | LI408 | LI409 | LI410 | LI411 | LI412 | LI413 | LI414 | LI415 | LI416 | LI417 | LI418 | LI419 | LI420 | LI421 | LI422 | LI423 | LI424 | LI425 | LI426 | LI427 | LI428 | LI429 | LI430 | LI431 | LI432 | LI433 | LI434 | LI435 | LI436 | LI437 | LI438 | LI439 | LI440 | LI441 | LI442 | LI443 | LI444 | LI445 | LI446 | LI447 | LI448 | LI449 | LI450 | LI451 | LI452 | LI453 | LI454 | LI455 | LI456 | LI457 | LI458 | LI459 | LI460 | LI461 | LI462 | LI463 | LI464 | LI465 | LI466 | LI467 | LI468 | LI469 | LI470 | LI471</ |
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|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|---------|

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| MET | K1000 | L1001 | V1002 | S1009 | K1018 | K1042 | N1047 | R1048 | R1064 | P1069 | D1070 | S1071 | L1072 | V1081 | GLU | PRO | LYS | VAL | LYS | SER | LYS | LYS | ARG | GLU | ALA | VAL | ALA | GLY | ARG | GLY | ARG | GLY | GLY | GLY | ARG | GLY | GLY | GLY | PRO | ARG |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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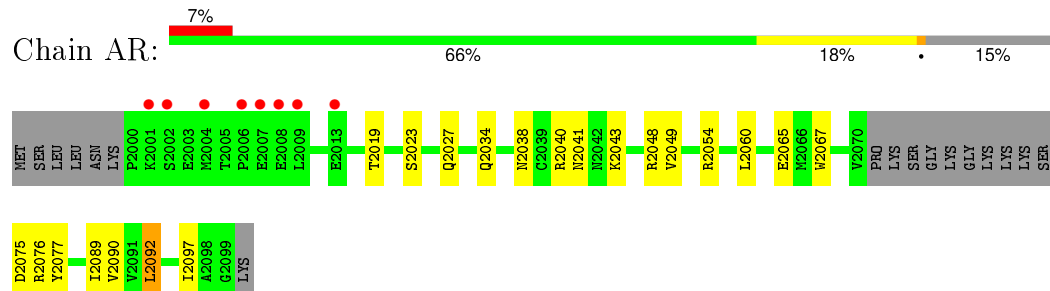
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| MET | SER | LEU | LEU | ASN | LYS | P2000 | E2016 | S2023 | Q2027 | Q2034 | N2038 | G2039 | R2040 | N2041 | N2042 | K2043 | R2048 | V2049 | R2054 | L2060 | E2065 | M2066 | W2067 | V2070 | PRO | LYS | LYS | GLY | GLY | LYS | LYS | LYS | LYS | SER | LYS | P2071 | D2075 | R2076 | Y2077 | I2089 | V2090 | Z2091 | L2092 | I2097 | A2098 |
|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

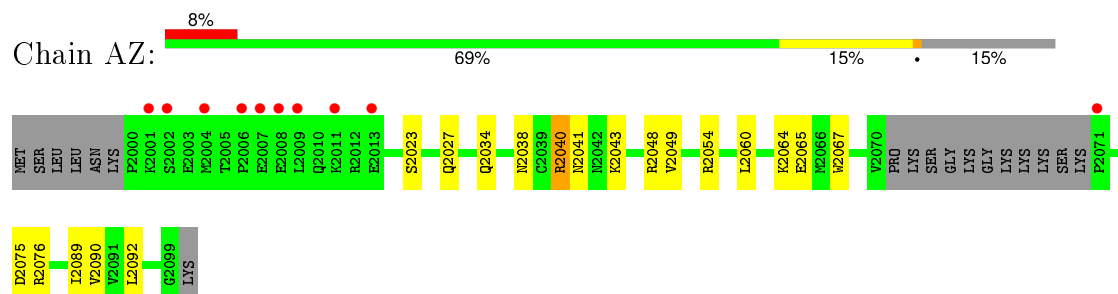
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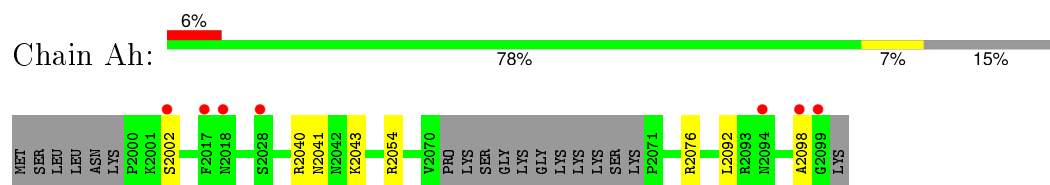
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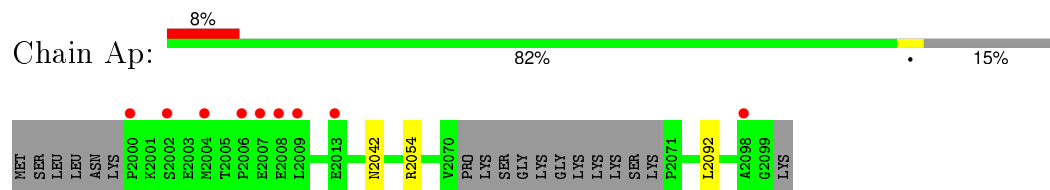
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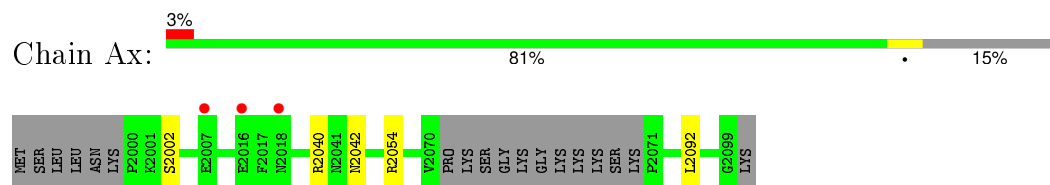
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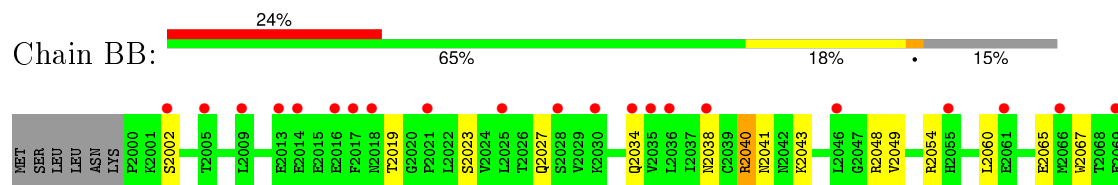
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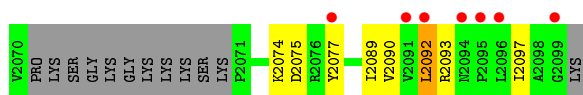


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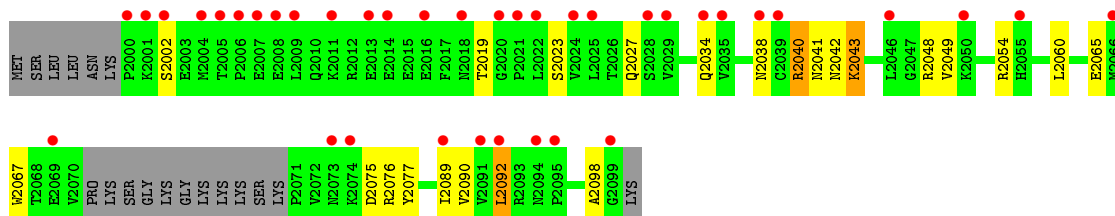


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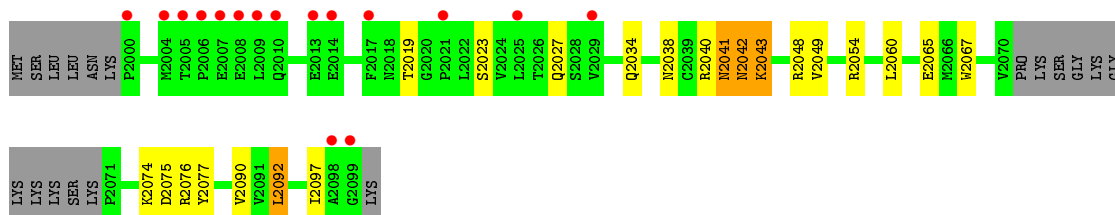




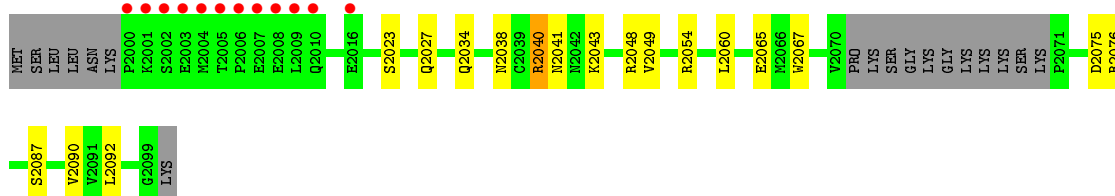
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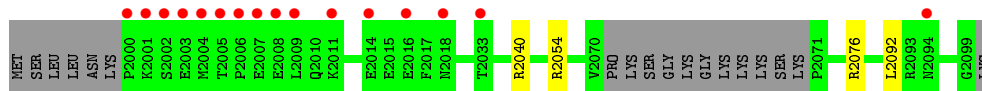
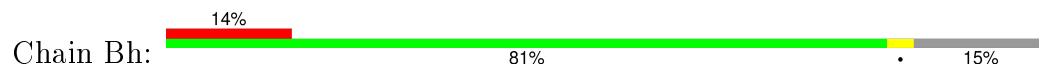
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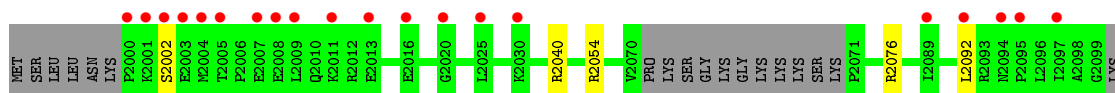
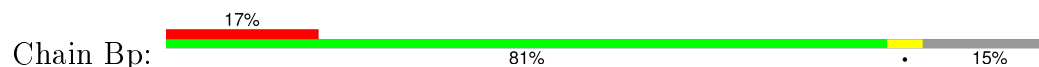
- Molecule 2: Small nuclear ribonucleoprotein Sm D2



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

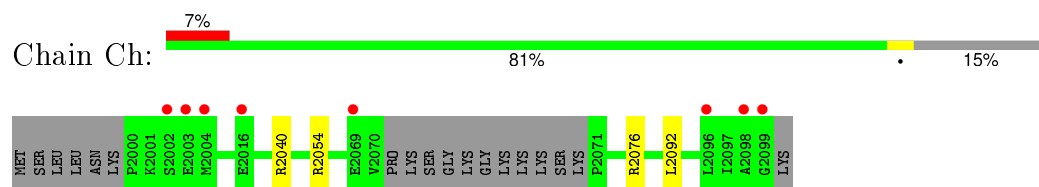


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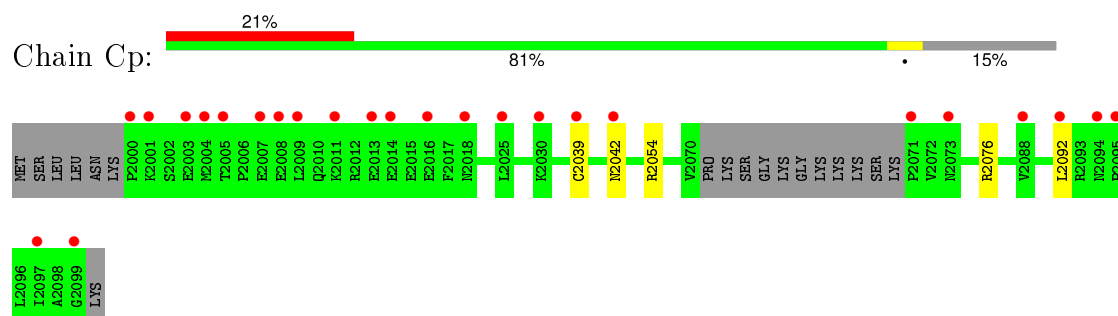


- Chain CZ:
-
- | Category | Percentage |
|----------|------------|
| Green | 69% |
| Yellow | 14% |
| Red | 7% |
| Grey | 15% |
- Legend: MET, SER, LEU, ASN, LYS, P2000, K2001, S2002, E2003, K2004, E2008, E2014, P2017, S2023, Q2027, Q2034, M2038, C2039, R2040, M2041, E2042, K2043, R2048, R2054, E2065, M2066, W2067, V2070, PRO, LYS, SER, GLY, LYS, LYS, LYS, LYS, SER, LYS, P2071, D2075, R2076, S2087, V2090, C2099, LYS.

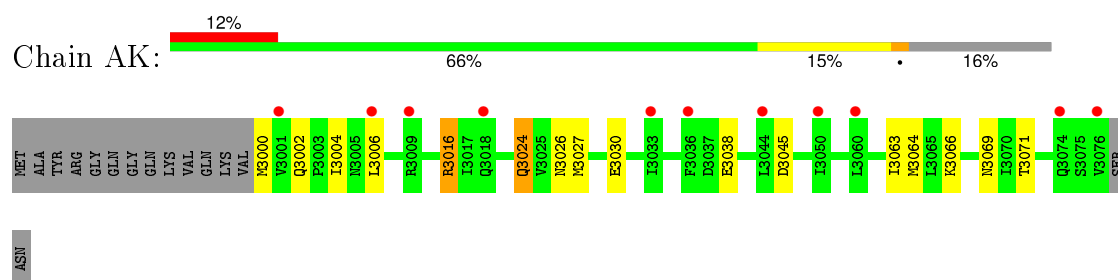
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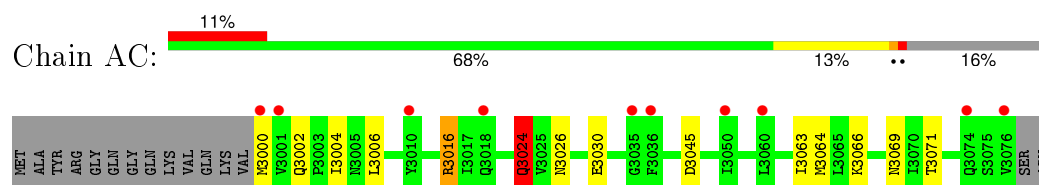
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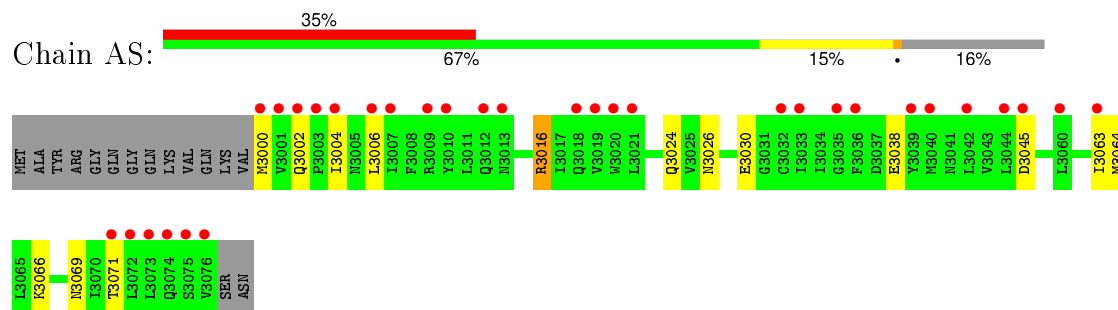
- Molecule 3: Small nuclear ribonucleoprotein E



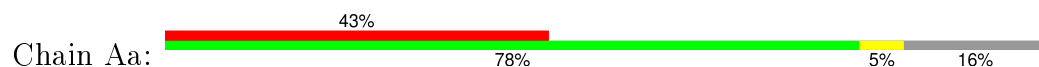
- Molecule 3: Small nuclear ribonucleoprotein E

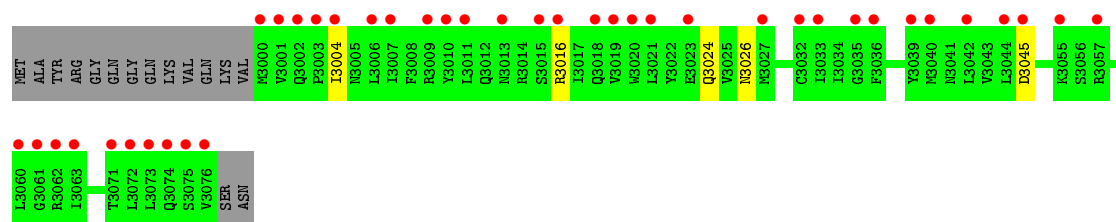


- Molecule 3: Small nuclear ribonucleoprotein E

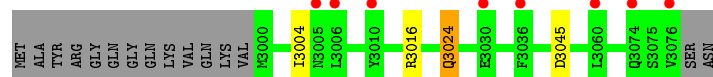
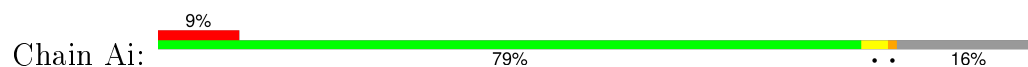


- Molecule 3: Small nuclear ribonucleoprotein E

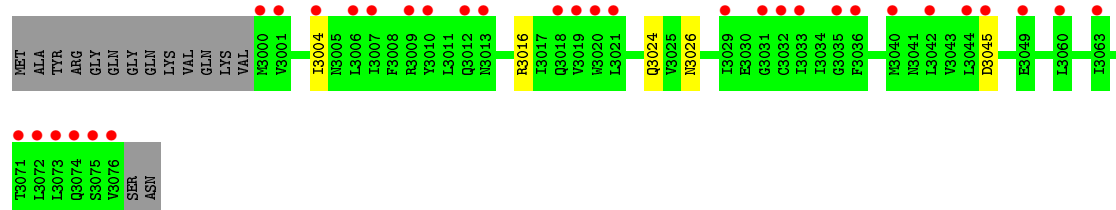
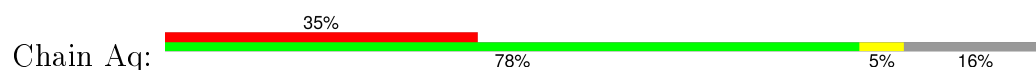




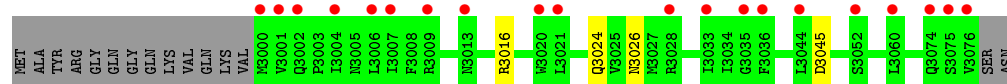
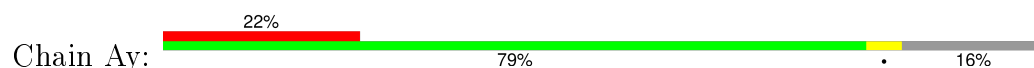
• Molecule 3: Small nuclear ribonucleoprotein E



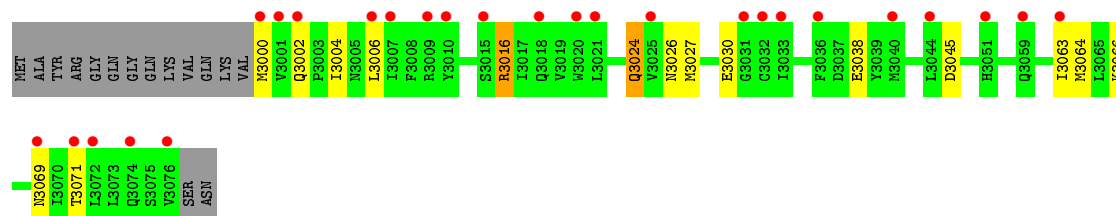
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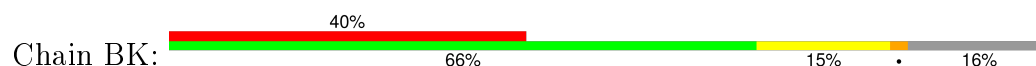
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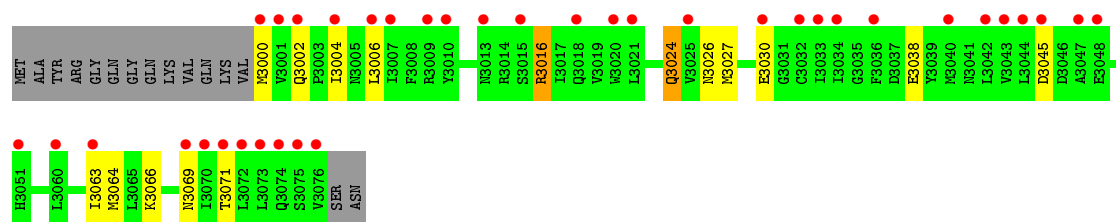


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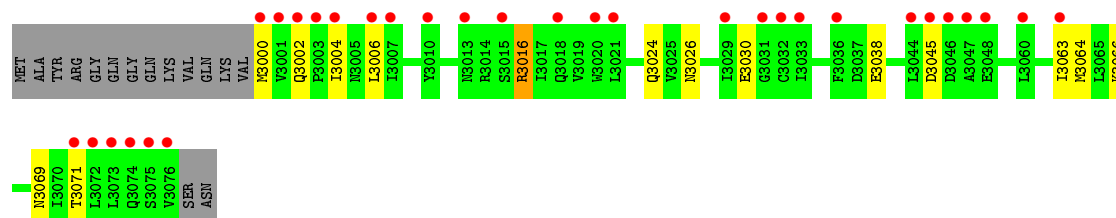


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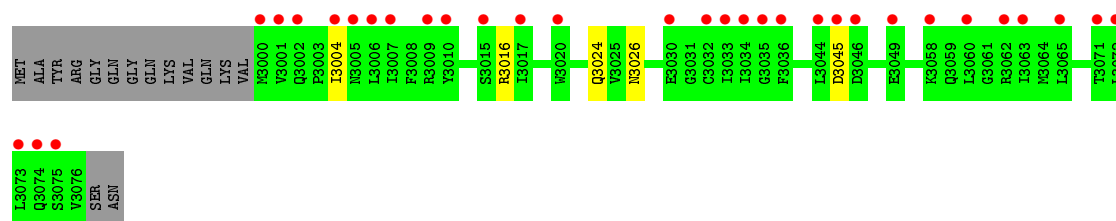
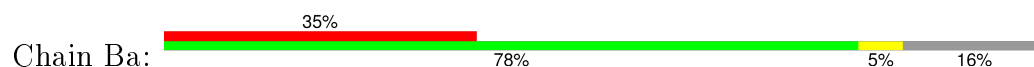




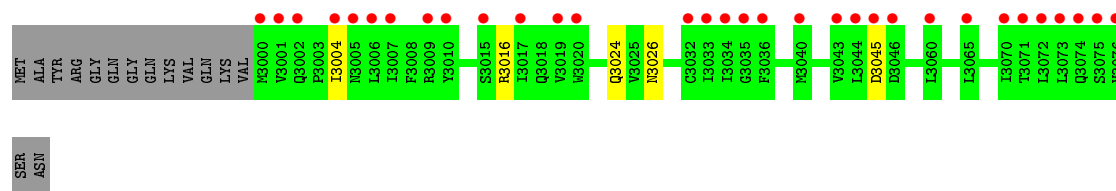
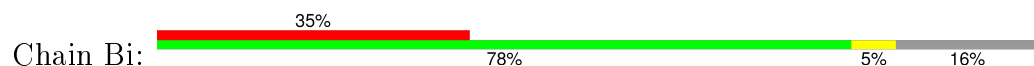
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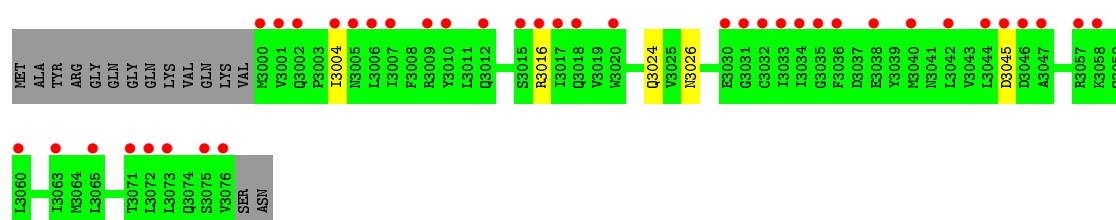
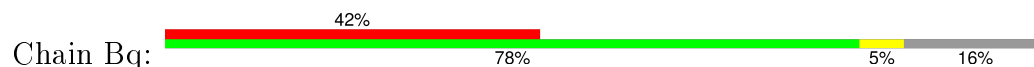
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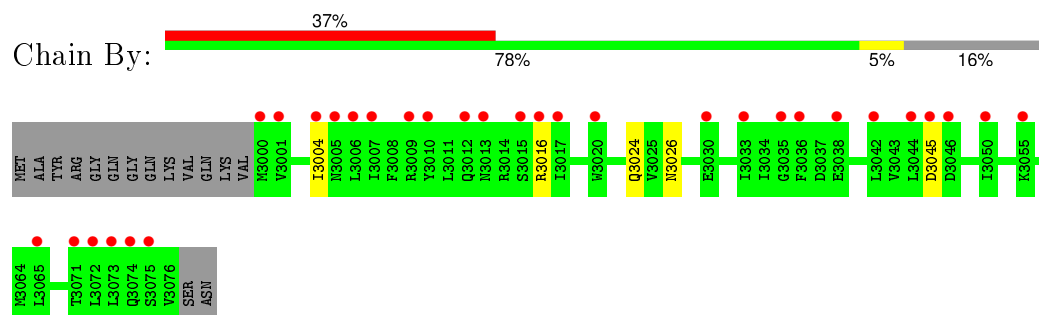
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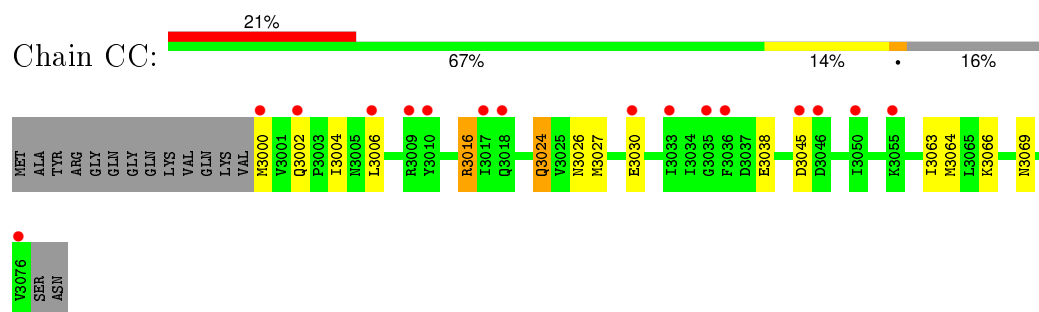
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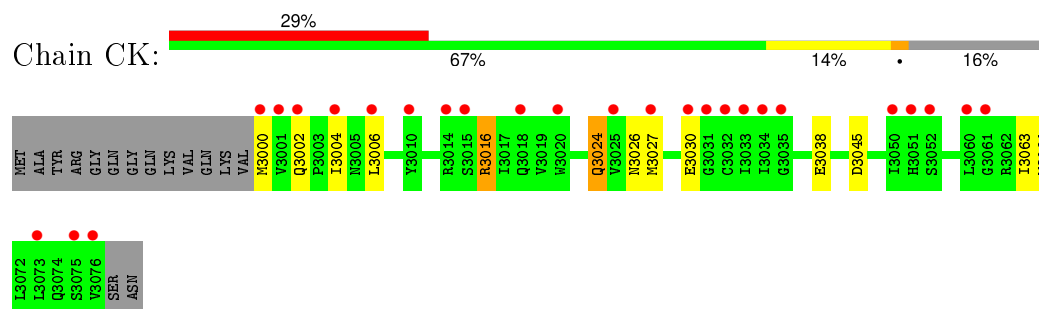
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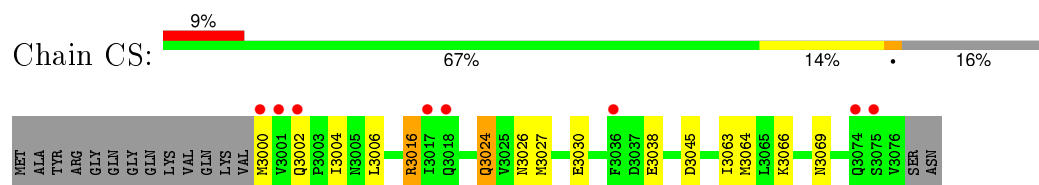
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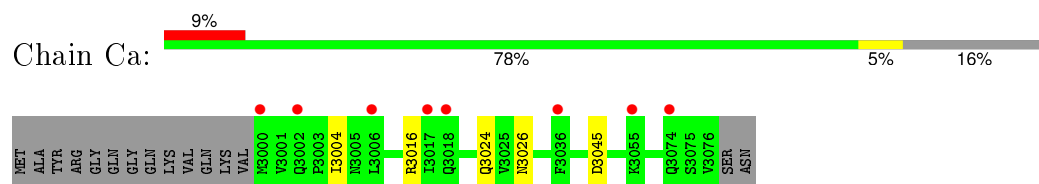
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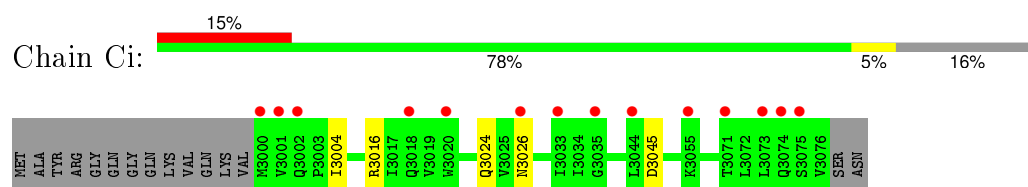
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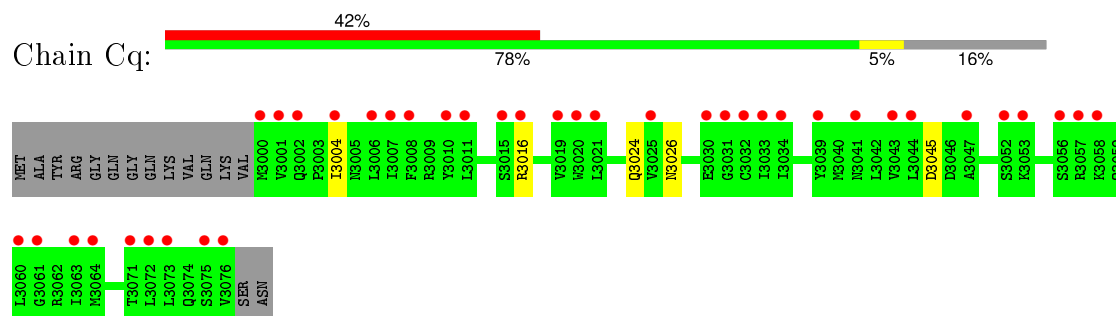
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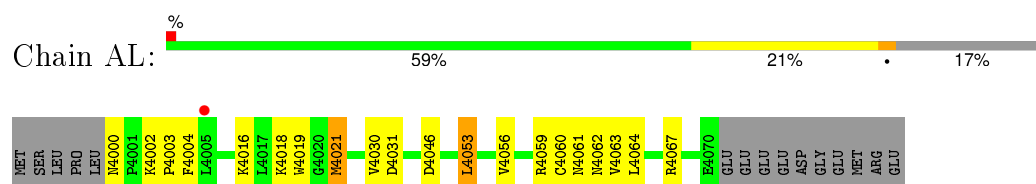
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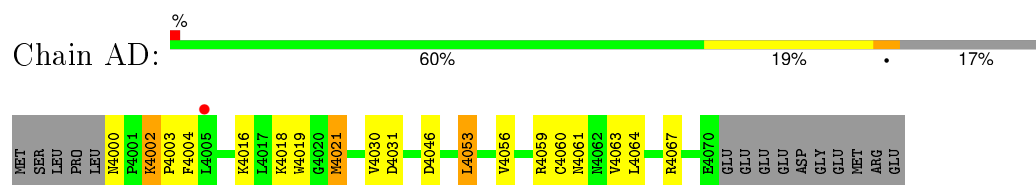
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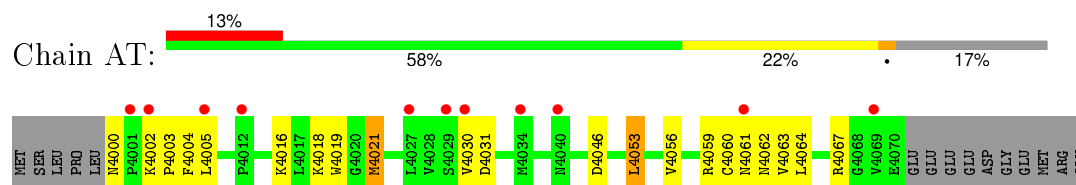
• Molecule 4: Small nuclear ribonucleoprotein F



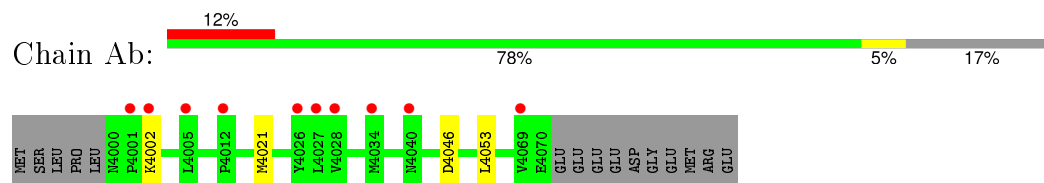
• Molecule 4: Small nuclear ribonucleoprotein F



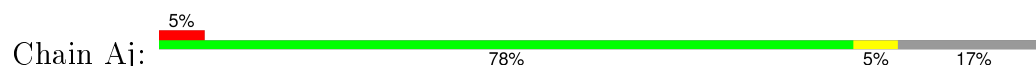
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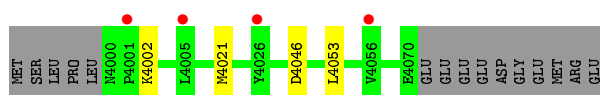


• Molecule 4: Small nuclear ribonucleoprotein F

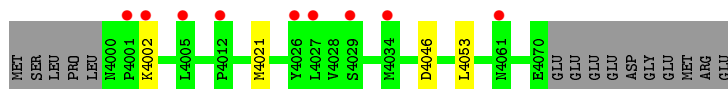
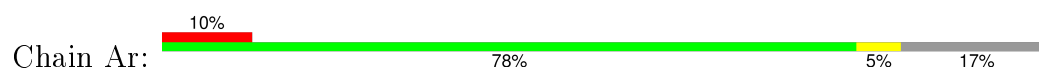


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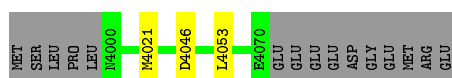
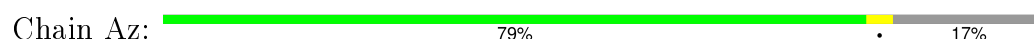




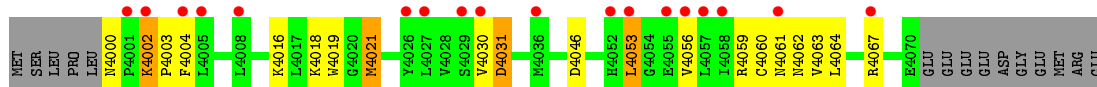
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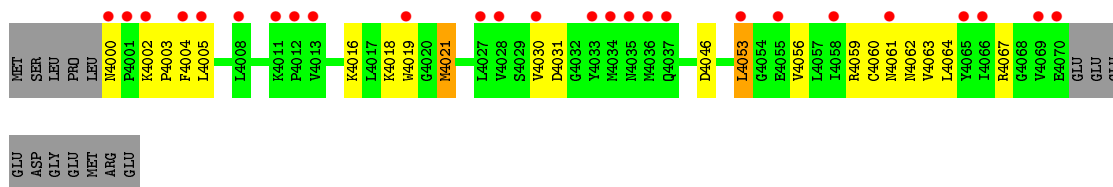
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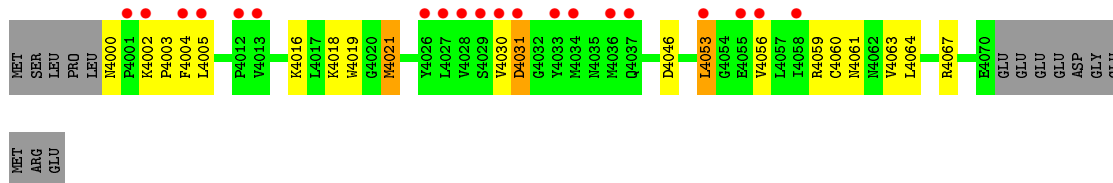
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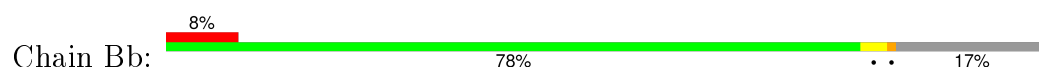
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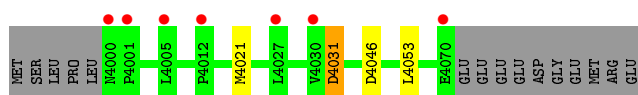


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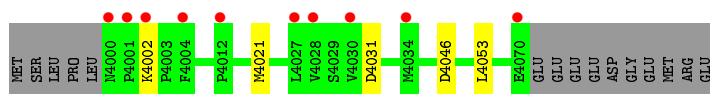
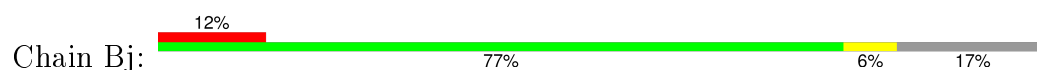


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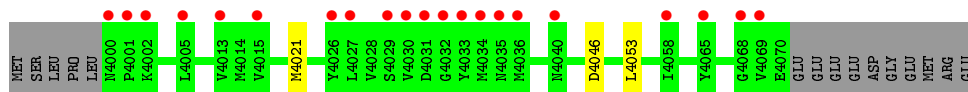
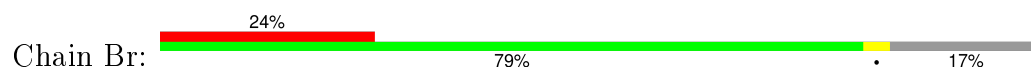




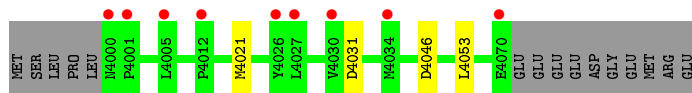
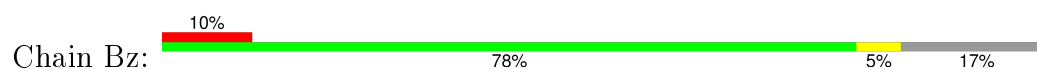
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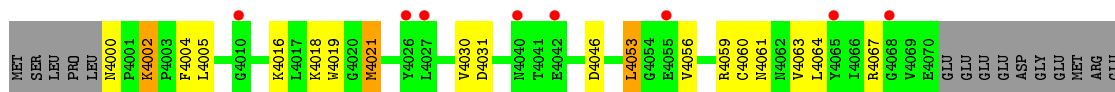
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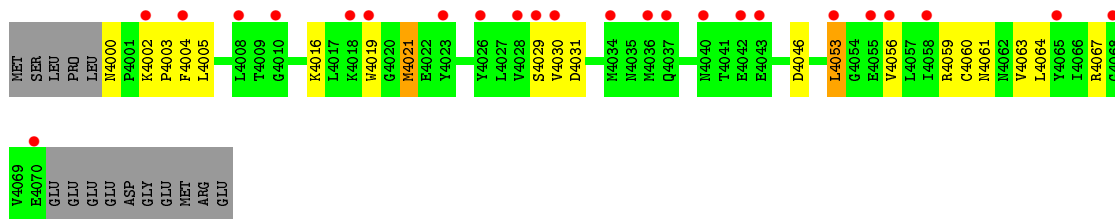
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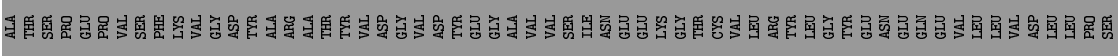
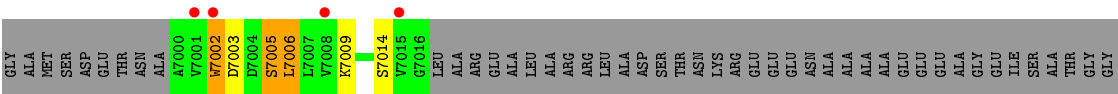


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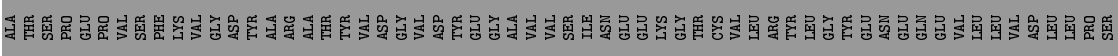
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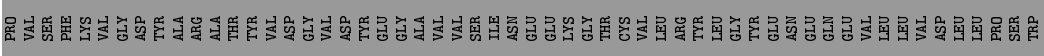
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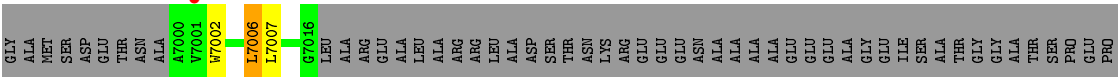


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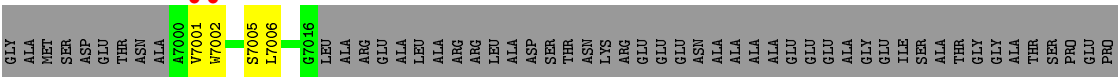
• Molecule 5: LD23602p



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• Molecule 5: LD23602p



GLY ALA SER ASP THR ASN ALA A7000 A7001 W7002 S7005 L7006 I7010 G7016 LEU

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• Molecule 5: LD23602p



GLY ALA MET SER ASP GLU THR ASN ALA A7000 A7001 W7002 W7003 L7006 L7007 G7016 LEU

PRO VAL SER PHE LYS VAL GLY ASP TYR ALA ARG ALA THR TYR VAL ASP GLY VAL ASP TYR TYR ASN LYS VAL LEU ARG TYR LEU ASN GLY TYR ALA ALA ASN GLU GLN GLU VAL LEU VAL LEU VAL ASP LEU PRO SER TRP

• Molecule 5: LD23602p



GLY ALA MET SER ASP GLU THR ASN ALA A7000 A7001 W7002 W7003 L7006 L7007 G7016 LEU

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• Molecule 5: LD23602p



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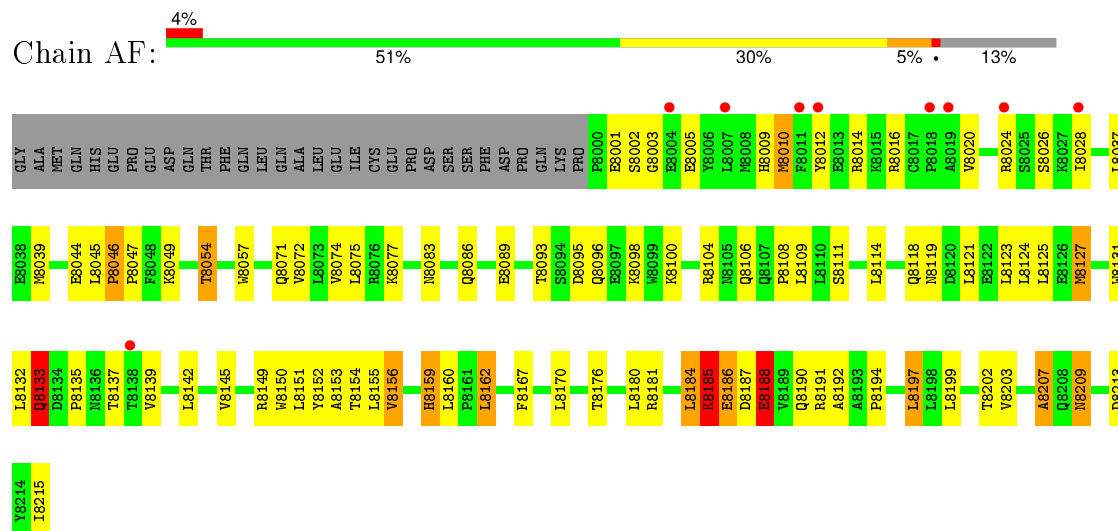
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TRP

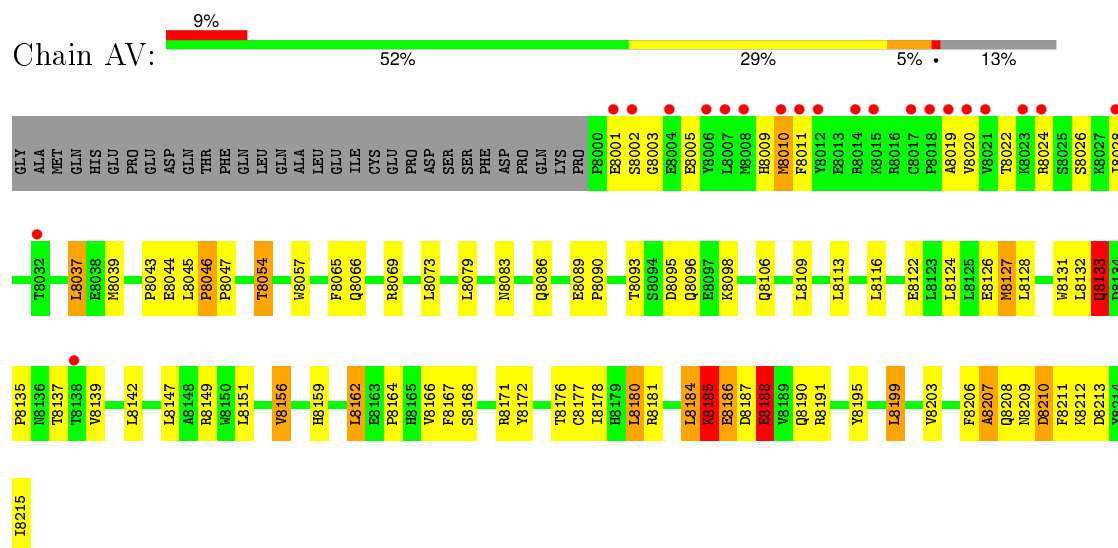
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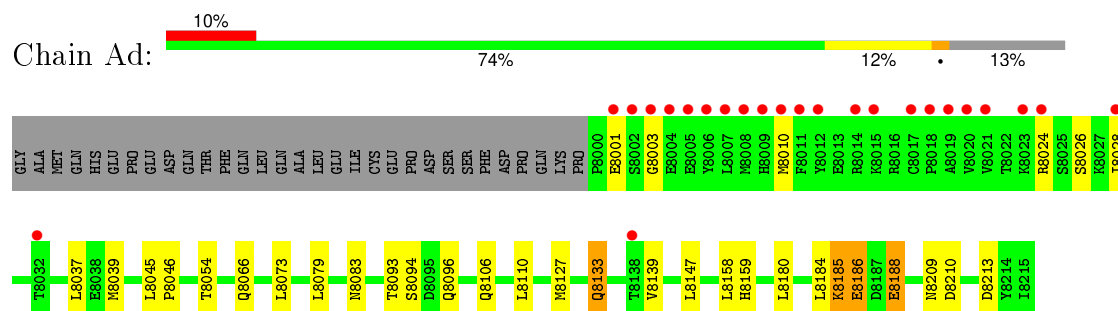
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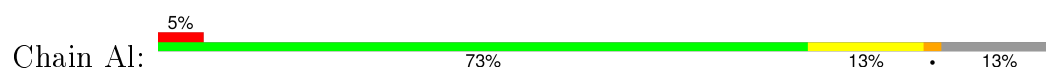
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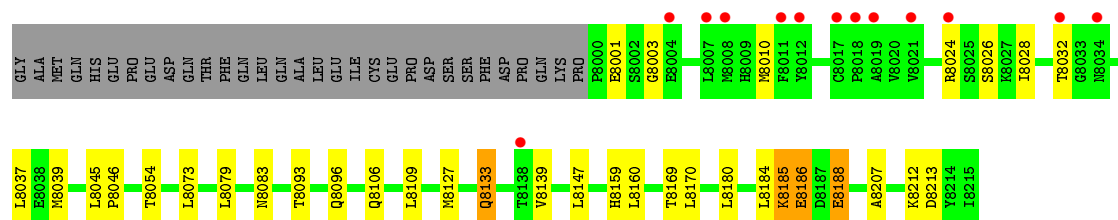


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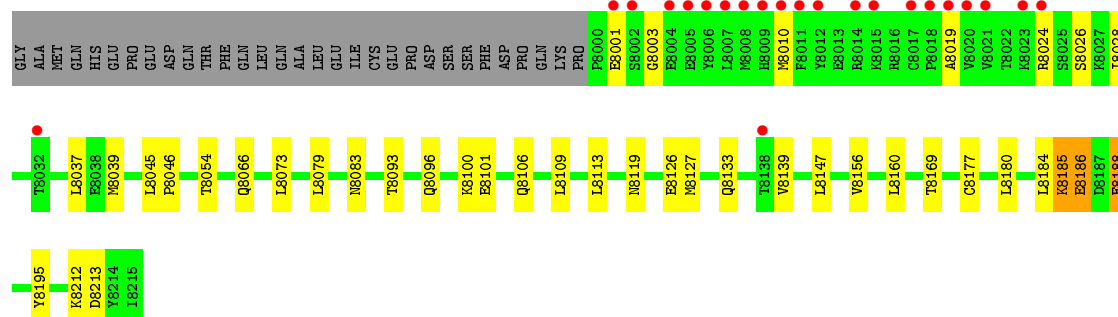


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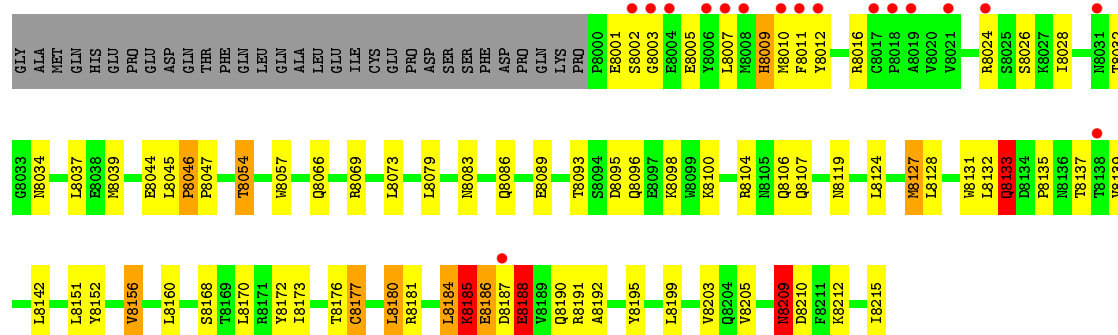




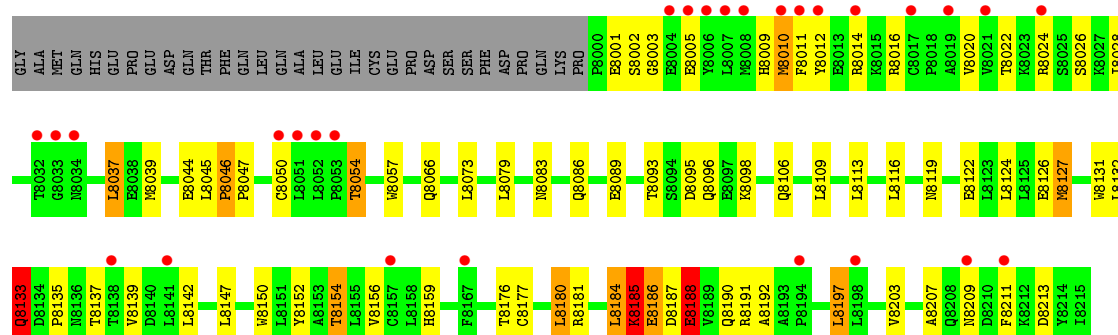
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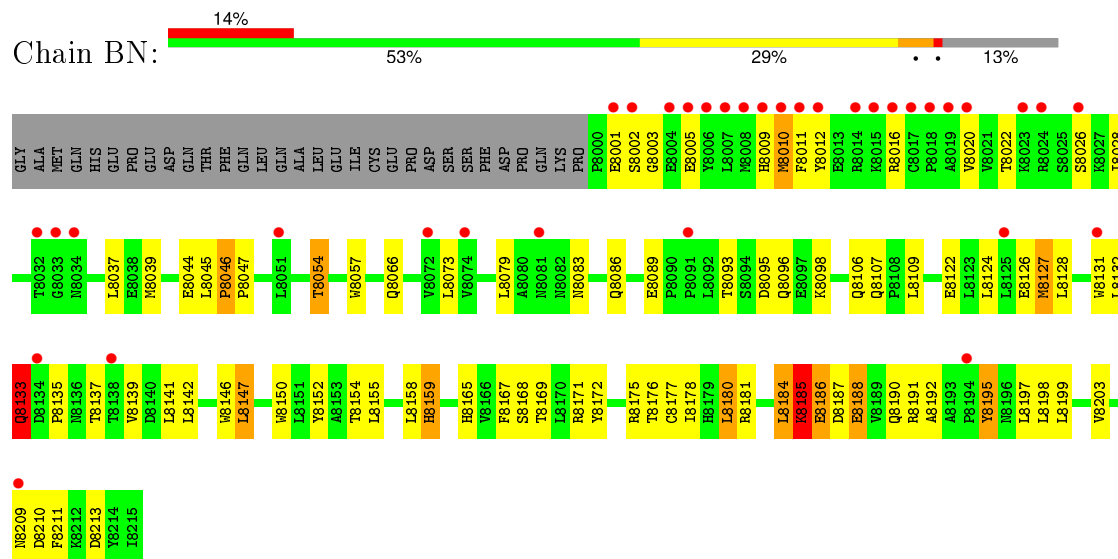
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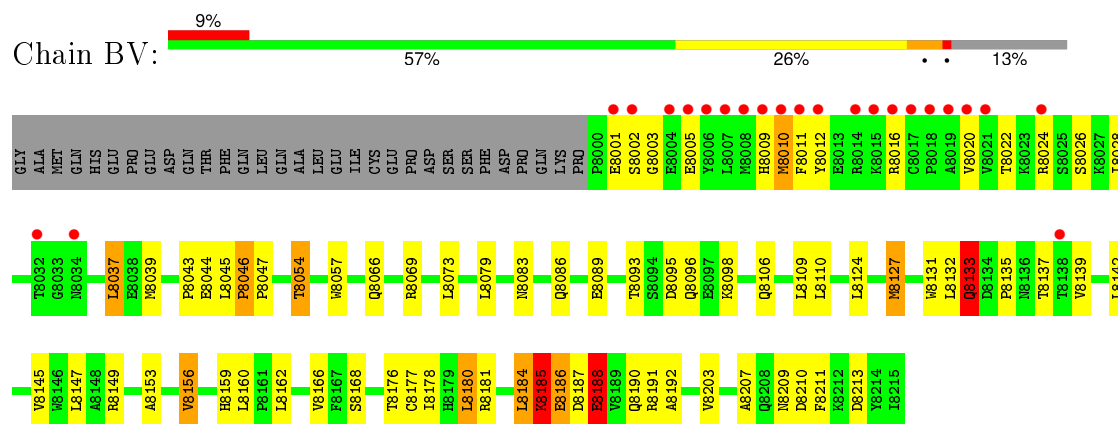
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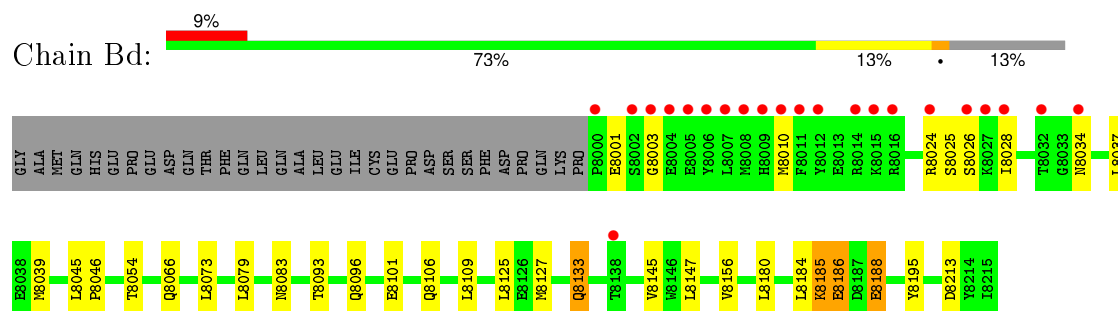
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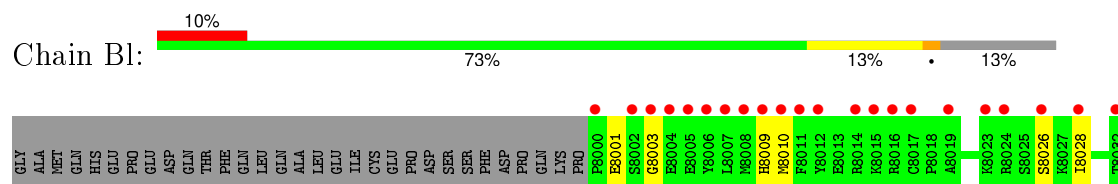
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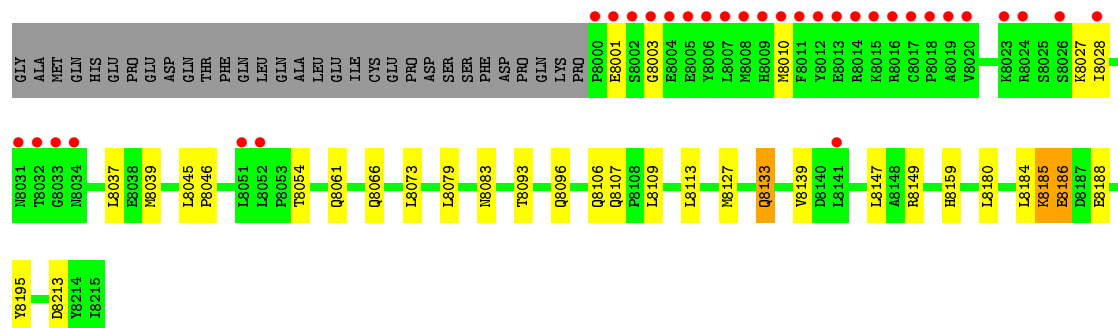


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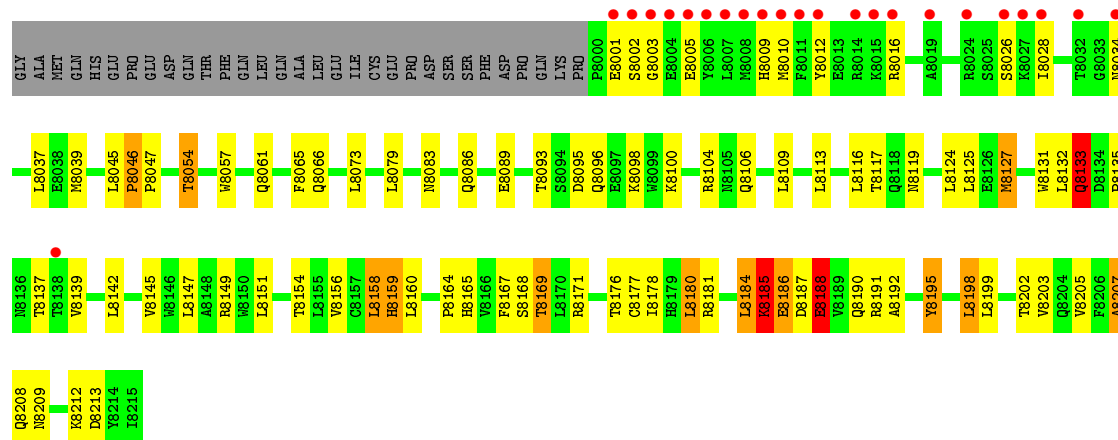




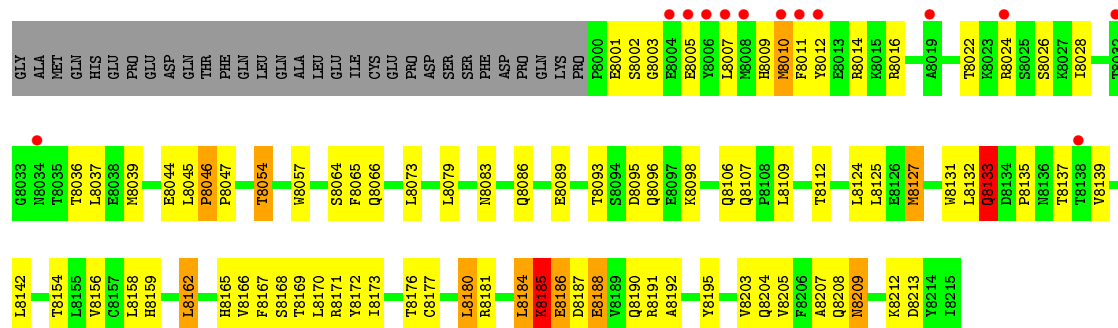
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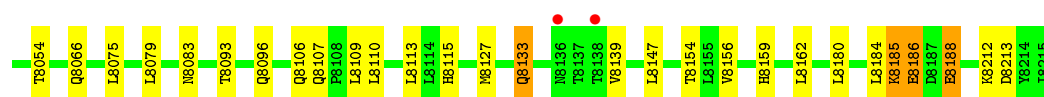
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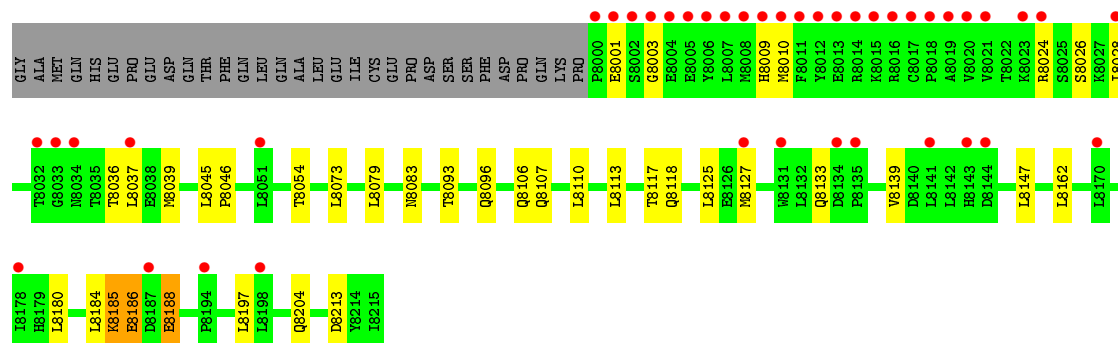
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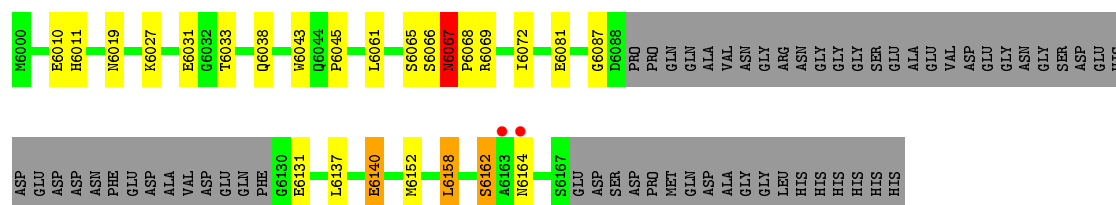
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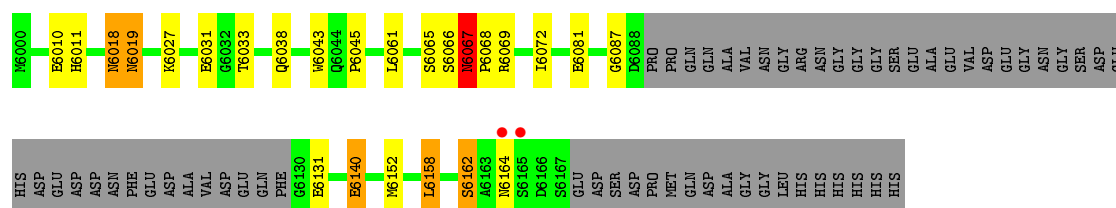
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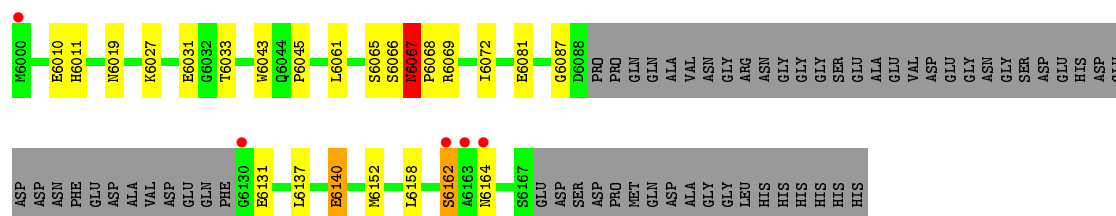
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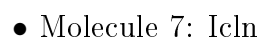
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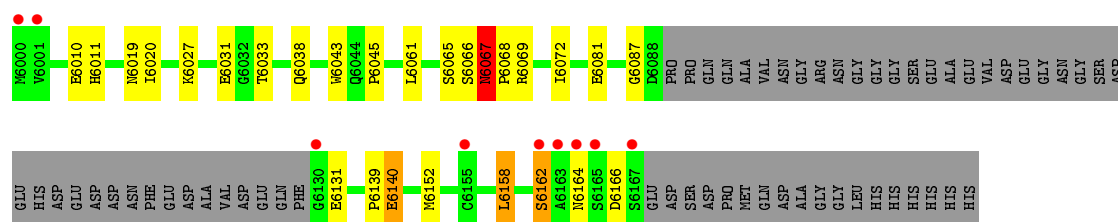


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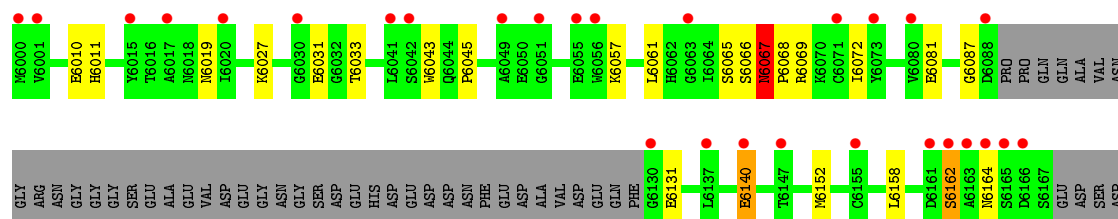


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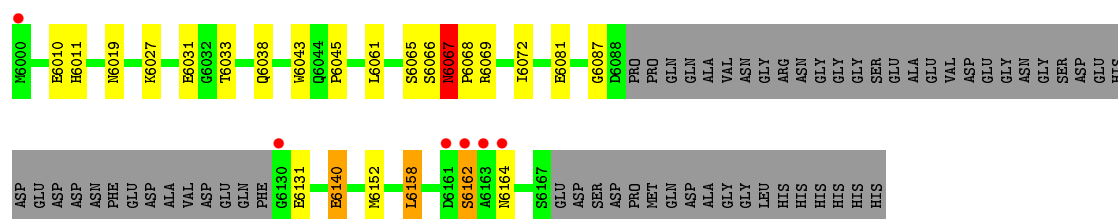




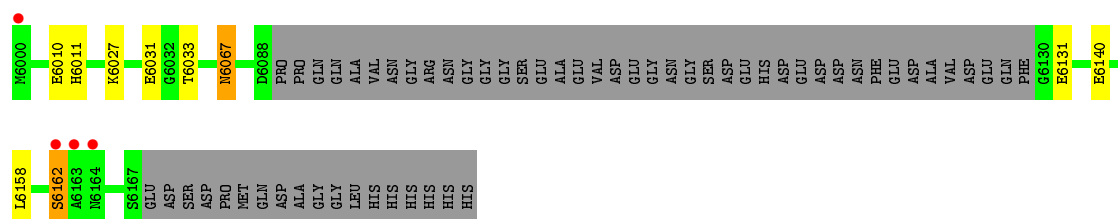
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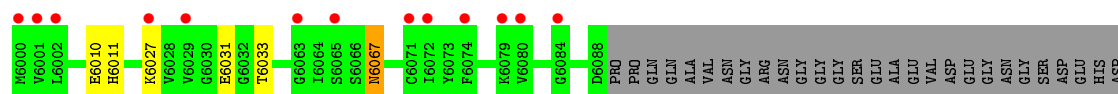
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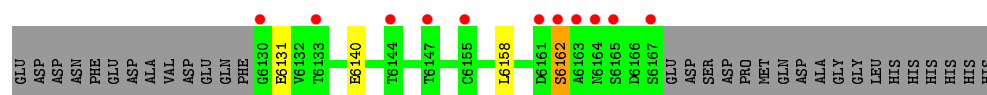


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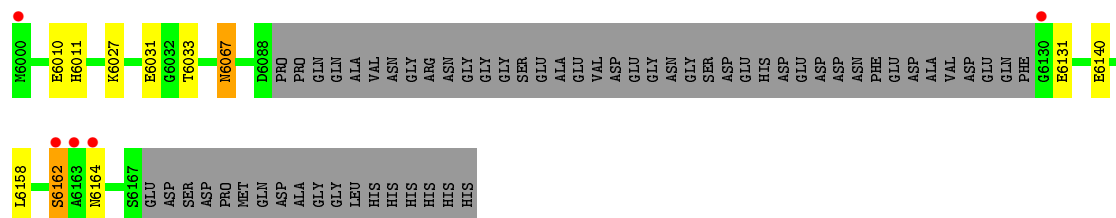


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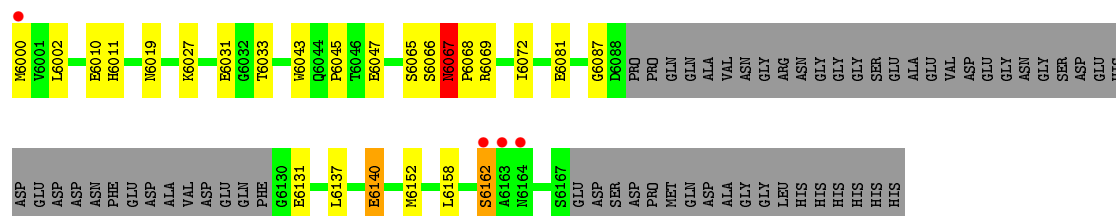




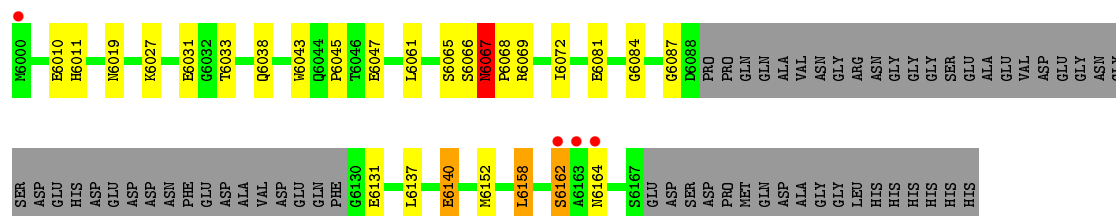
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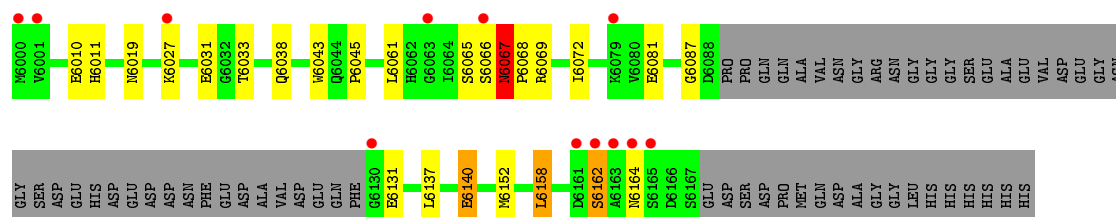
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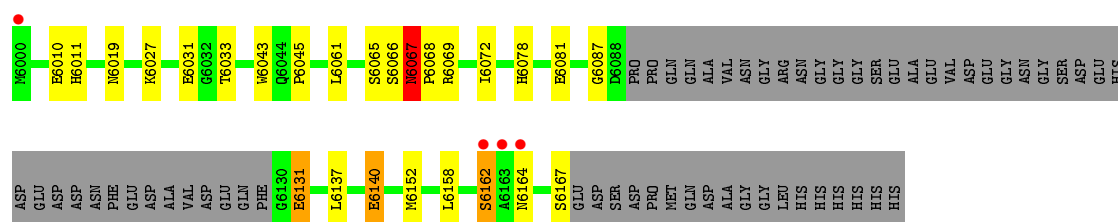


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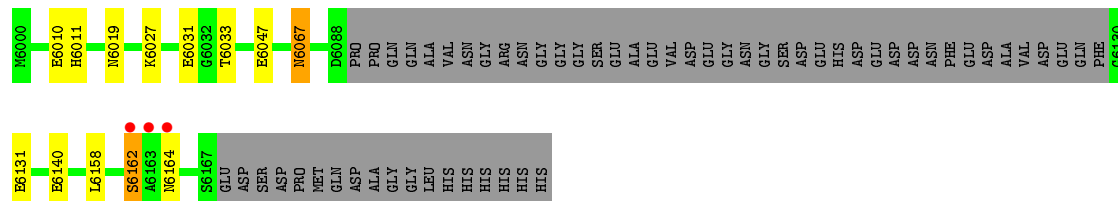


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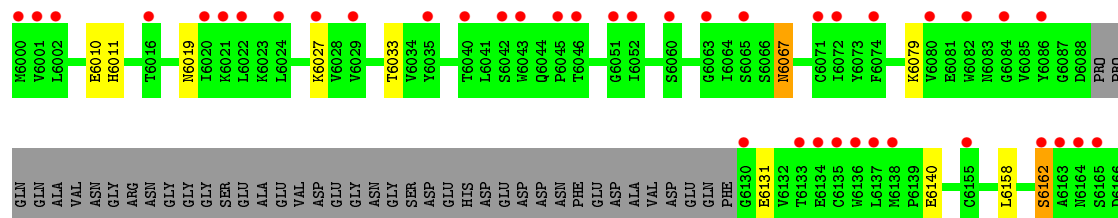




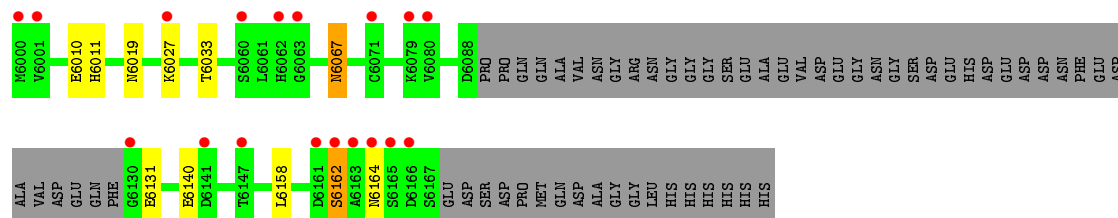
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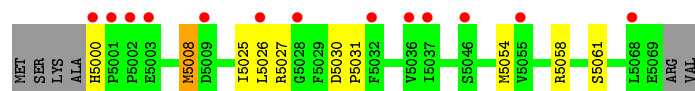
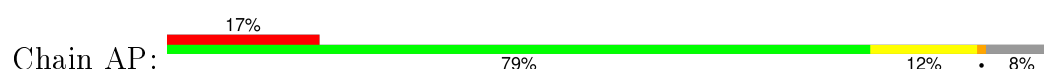
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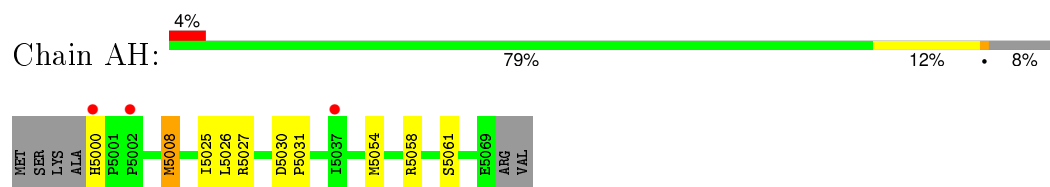
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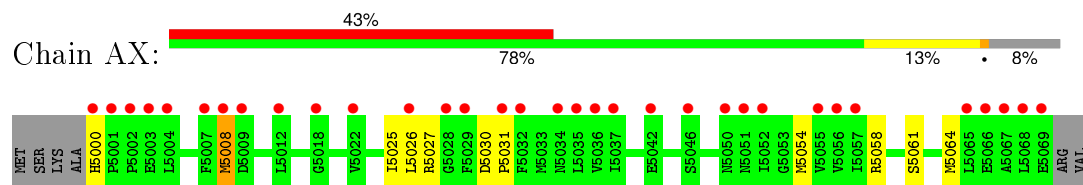
• Molecule 8: Small nuclear ribonucleoprotein G



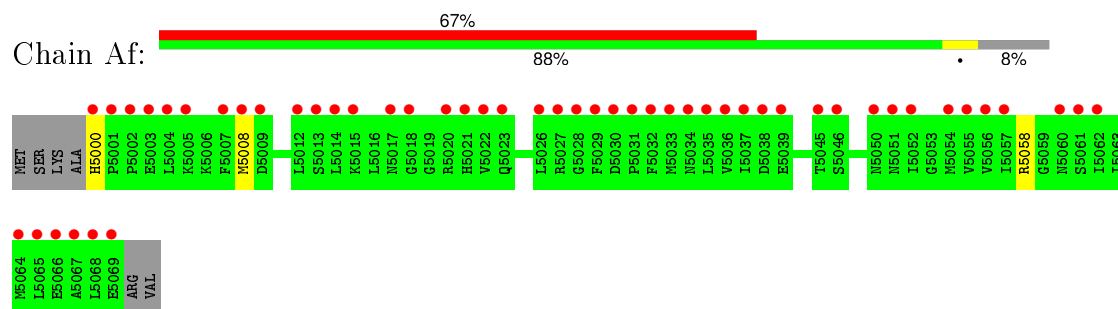
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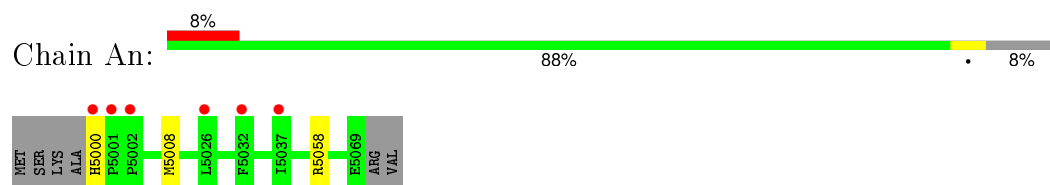
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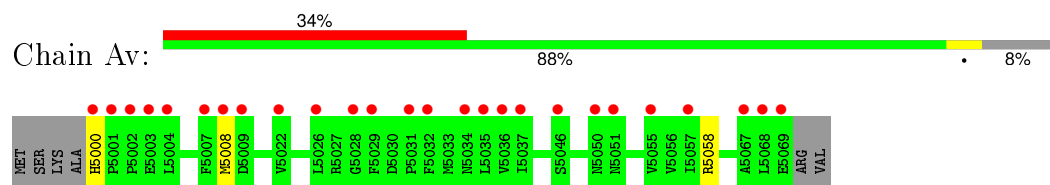
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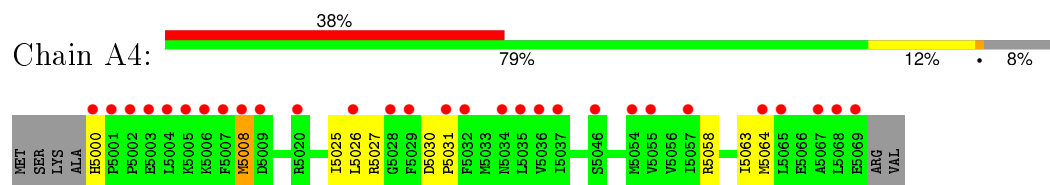
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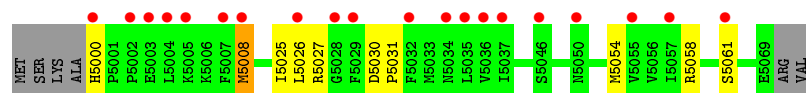
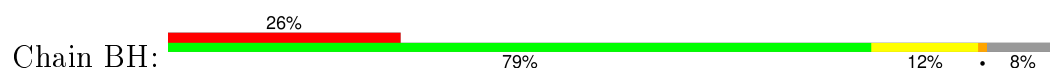
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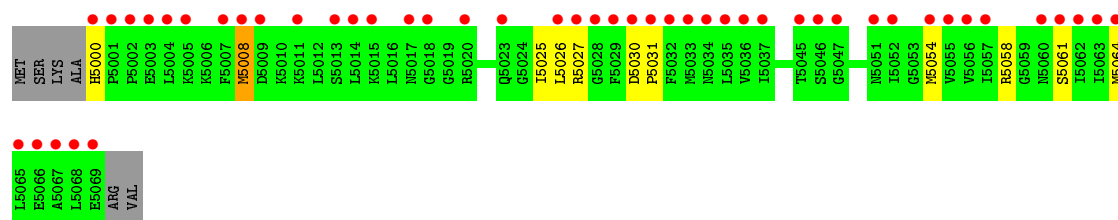
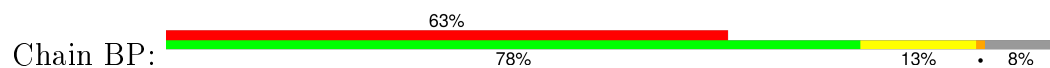
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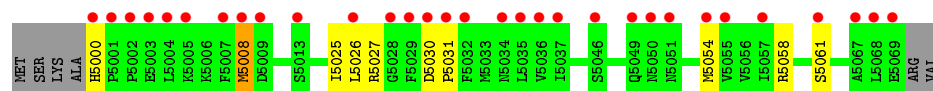
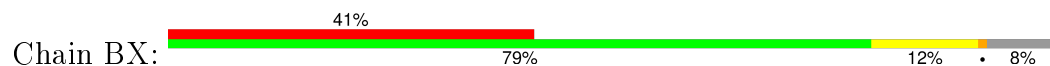
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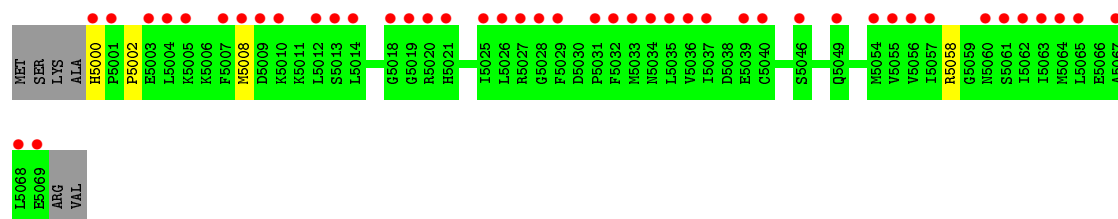
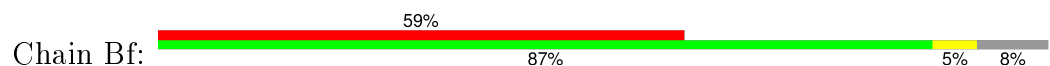
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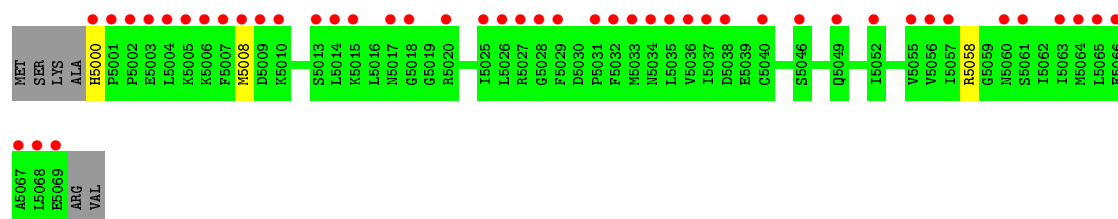
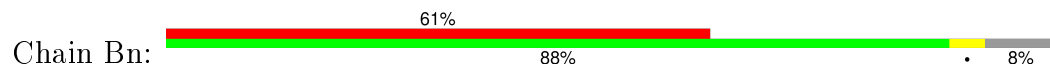
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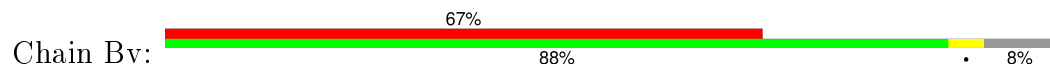
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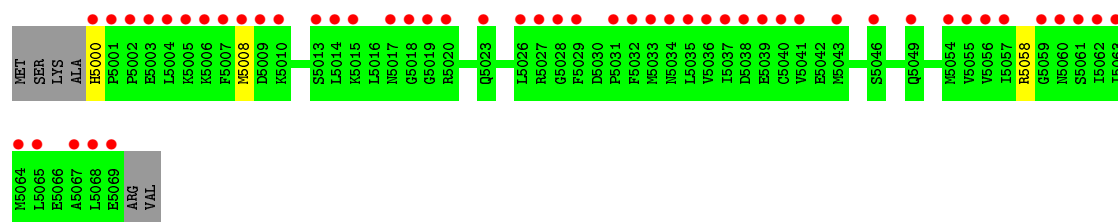


- Molecule 8: Small nuclear ribonucleoprotein G

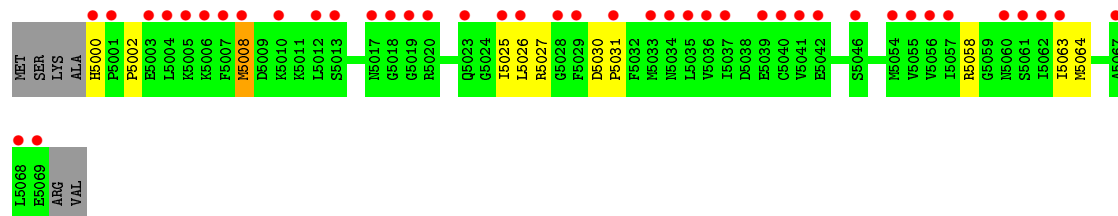
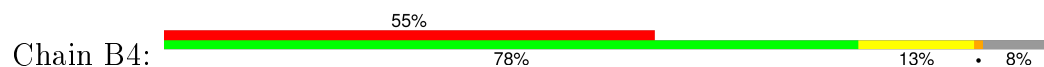


- Molecule 8: Small nuclear ribonucleoprotein G

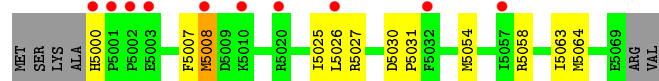
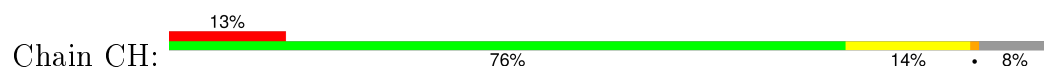




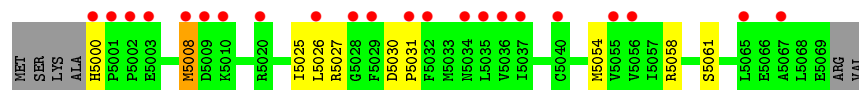
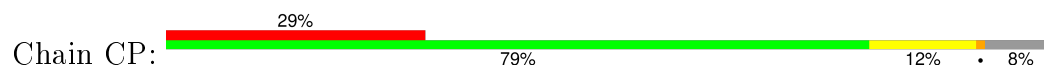
• Molecule 8: Small nuclear ribonucleoprotein G



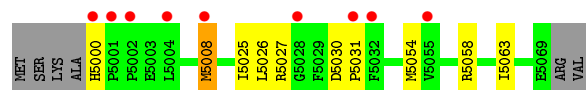
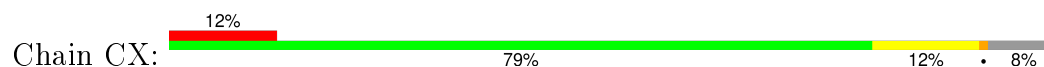
• Molecule 8: Small nuclear ribonucleoprotein G



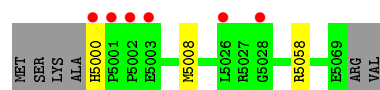
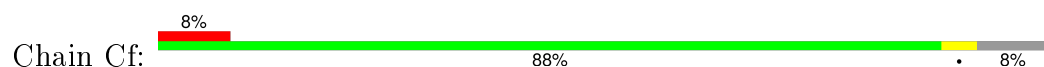
• Molecule 8: Small nuclear ribonucleoprotein G



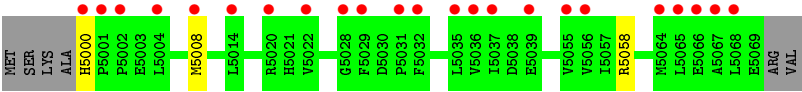
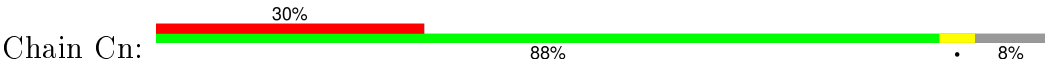
• Molecule 8: Small nuclear ribonucleoprotein G



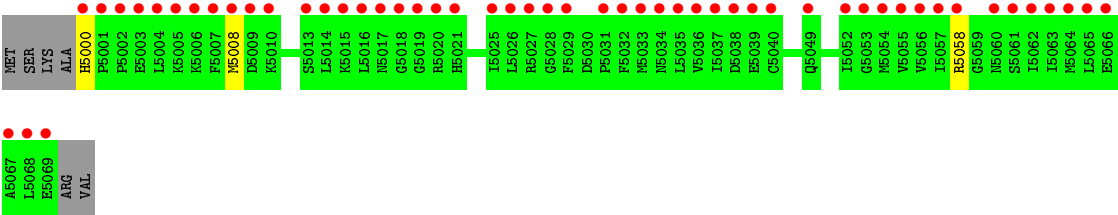
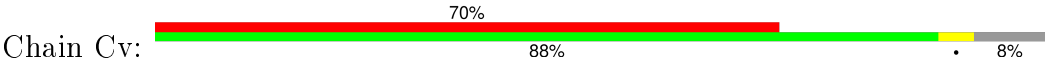
• Molecule 8: Small nuclear ribonucleoprotein G



• Molecule 8: Small nuclear ribonucleoprotein G



● Molecule 8: Small nuclear ribonucleoprotein G



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 , 0.353	Depositor DCC
R_{free} test set	2901 reflections (1.04%)	DCC
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 76.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	39 of 281573 reflections (0.014%)	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.51	0/656	0.75	1/888 (0.1%)
1	AI	0.51	0/656	0.74	1/888 (0.1%)
1	AQ	0.49	0/656	0.76	1/888 (0.1%)
1	AY	0.49	0/656	0.75	1/888 (0.1%)
1	Ag	0.49	0/656	0.74	1/888 (0.1%)
1	Ao	0.51	0/656	0.75	1/888 (0.1%)
1	Aw	0.46	0/656	0.74	1/888 (0.1%)
1	BA	0.45	0/656	0.73	1/888 (0.1%)
1	BI	0.46	0/656	0.72	1/888 (0.1%)
1	BQ	0.46	0/656	0.73	1/888 (0.1%)
1	BY	0.50	0/656	0.74	1/888 (0.1%)
1	Bg	0.46	0/656	0.74	1/888 (0.1%)
1	Bo	0.48	0/656	0.73	1/888 (0.1%)
1	Bw	0.52	0/656	0.75	1/888 (0.1%)
1	CA	0.47	0/656	0.74	1/888 (0.1%)
1	CI	0.46	0/656	0.70	1/888 (0.1%)
1	CQ	0.49	0/656	0.75	1/888 (0.1%)
1	CY	0.53	0/656	0.76	1/888 (0.1%)
1	Cg	0.45	0/656	0.73	1/888 (0.1%)
1	Co	0.45	0/656	0.71	1/888 (0.1%)
2	AB	0.52	0/817	0.70	0/1096
2	AJ	0.50	0/817	0.70	0/1096
2	AR	0.48	0/817	0.69	0/1096
2	AZ	0.47	0/817	0.68	0/1096
2	Ah	0.47	0/817	0.68	0/1096
2	Ap	0.47	0/817	0.67	0/1096
2	Ax	0.48	0/817	0.69	0/1096
2	BB	0.42	0/817	0.64	0/1096
2	BJ	0.44	0/817	0.68	0/1096
2	BR	0.45	0/817	0.68	0/1096
2	BZ	0.50	0/817	0.70	0/1096
2	Bh	0.46	0/817	0.68	0/1096

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Bp	0.46	0/817	0.68	0/1096
2	Bx	0.49	0/817	0.70	0/1096
2	CB	0.45	0/817	0.68	0/1096
2	CJ	0.44	0/817	0.68	0/1096
2	CR	0.46	0/817	0.68	0/1096
2	CZ	0.47	0/817	0.68	0/1096
2	Ch	0.45	0/817	0.67	0/1096
2	Cp	0.46	0/817	0.69	0/1096
3	AC	0.43	0/646	0.75	1/867 (0.1%)
3	AK	0.46	0/646	0.76	1/867 (0.1%)
3	AS	0.44	0/646	0.75	1/867 (0.1%)
3	Aa	0.40	0/646	0.74	1/867 (0.1%)
3	Ai	0.41	0/646	0.74	1/867 (0.1%)
3	Aq	0.43	0/646	0.74	1/867 (0.1%)
3	Ay	0.42	0/646	0.74	1/867 (0.1%)
3	BC	0.41	0/646	0.74	1/867 (0.1%)
3	BK	0.39	0/646	0.73	1/867 (0.1%)
3	BS	0.40	0/646	0.74	1/867 (0.1%)
3	Ba	0.41	0/646	0.74	1/867 (0.1%)
3	Bi	0.38	0/646	0.73	1/867 (0.1%)
3	Bq	0.37	0/646	0.73	1/867 (0.1%)
3	By	0.46	0/646	0.75	1/867 (0.1%)
3	CC	0.40	0/646	0.74	1/867 (0.1%)
3	CK	0.38	0/646	0.74	1/867 (0.1%)
3	CS	0.41	0/646	0.74	1/867 (0.1%)
3	Ca	0.41	0/646	0.74	1/867 (0.1%)
3	Ci	0.39	0/646	0.73	1/867 (0.1%)
3	Cq	0.37	0/646	0.73	1/867 (0.1%)
4	AD	0.39	0/567	0.65	0/765
4	AL	0.39	0/567	0.65	0/765
4	AT	0.40	0/567	0.64	0/765
4	Ab	0.40	0/567	0.64	0/765
4	Aj	0.39	0/567	0.64	0/765
4	Ar	0.39	0/567	0.67	0/765
4	Az	0.38	0/567	0.64	0/765
4	BD	0.38	0/567	0.65	0/765
4	BL	0.37	0/567	0.64	0/765
4	BT	0.37	0/567	0.64	0/765
4	Bb	0.40	0/567	0.68	1/765 (0.1%)
4	Bj	0.39	0/567	0.67	1/765 (0.1%)
4	Br	0.37	0/567	0.64	0/765
4	Bz	0.40	0/567	0.66	0/765
4	CD	0.38	0/567	0.68	0/765

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	CL	0.37	0/567	0.66	0/765
4	CT	0.38	0/567	0.64	0/765
4	Cb	0.40	0/567	0.69	1/765 (0.1%)
4	Cj	0.38	0/567	0.64	0/765
4	Cr	0.37	0/567	0.63	0/765
5	A1	0.65	0/135	0.90	0/184
5	AE	0.57	0/135	0.88	0/184
5	AM	0.63	0/135	0.89	0/184
5	AU	0.56	0/135	0.83	0/184
5	Ac	0.64	0/135	0.94	0/184
5	Ak	0.64	0/135	0.91	0/184
5	As	0.55	0/135	0.87	0/184
5	B1	0.60	0/135	0.88	0/184
5	BE	0.59	0/135	0.81	0/184
5	BM	0.59	0/135	0.86	0/184
5	BU	0.54	0/135	0.83	0/184
5	Bc	0.60	0/135	0.88	0/184
5	Bk	0.63	0/135	0.86	0/184
5	Bs	0.57	0/135	0.89	0/184
5	CE	0.66	0/135	0.92	0/184
5	CM	0.61	0/135	0.89	0/184
5	CU	0.67	0/135	0.90	0/184
5	Cc	0.69	0/135	0.94	0/184
5	Ck	0.64	0/135	0.89	0/184
5	Cs	0.58	0/135	0.86	0/184
6	A2	0.56	0/1830	0.88	2/2489 (0.1%)
6	AF	0.58	0/1830	0.89	2/2489 (0.1%)
6	AN	0.60	0/1830	0.91	2/2489 (0.1%)
6	AV	0.56	0/1830	0.87	2/2489 (0.1%)
6	Ad	0.53	0/1830	0.86	2/2489 (0.1%)
6	Al	0.58	0/1830	0.89	2/2489 (0.1%)
6	At	0.60	0/1830	0.89	2/2489 (0.1%)
6	B2	0.58	0/1830	0.89	2/2489 (0.1%)
6	BF	0.50	0/1830	0.84	2/2489 (0.1%)
6	BN	0.52	0/1830	0.83	2/2489 (0.1%)
6	BV	0.52	0/1830	0.85	2/2489 (0.1%)
6	Bd	0.56	0/1830	0.88	2/2489 (0.1%)
6	Bl	0.54	0/1830	0.86	2/2489 (0.1%)
6	Bt	0.55	0/1830	0.86	2/2489 (0.1%)
6	CF	0.54	0/1830	0.86	2/2489 (0.1%)
6	CN	0.52	0/1830	0.84	2/2489 (0.1%)
6	CV	0.54	0/1830	0.85	2/2489 (0.1%)
6	Cd	0.56	0/1830	0.90	3/2489 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	Cl	0.54	0/1830	0.86	2/2489 (0.1%)
6	Ct	0.53	0/1830	0.86	2/2489 (0.1%)
7	A3	0.46	0/1008	0.74	0/1373
7	AG	0.57	0/1008	0.76	0/1373
7	AO	0.55	0/1008	0.75	0/1373
7	AW	0.53	0/1008	0.75	0/1373
7	Ae	0.47	0/1008	0.72	0/1373
7	Am	0.57	0/1008	0.75	0/1373
7	Au	0.55	0/1008	0.75	0/1373
7	B3	0.53	0/1008	0.75	0/1373
7	BG	0.52	0/1008	0.74	0/1373
7	BO	0.50	0/1008	0.76	1/1373 (0.1%)
7	BW	0.54	0/1008	0.75	0/1373
7	Be	0.54	0/1008	0.75	0/1373
7	Bm	0.49	0/1008	0.72	0/1373
7	Bu	0.51	0/1008	0.75	0/1373
7	CG	0.53	0/1008	0.75	0/1373
7	CO	0.49	0/1008	0.73	0/1373
7	CW	0.55	0/1008	0.75	0/1373
7	Ce	0.57	0/1008	0.76	0/1373
7	Cm	0.49	0/1008	0.74	0/1373
7	Cu	0.48	0/1008	0.74	0/1373
8	A4	0.40	0/551	0.72	0/737
8	AH	0.42	0/551	0.73	0/737
8	AP	0.42	0/551	0.73	0/737
8	AX	0.42	0/551	0.73	0/737
8	Af	0.39	0/551	0.72	0/737
8	An	0.42	0/551	0.73	0/737
8	Av	0.41	0/551	0.73	0/737
8	B4	0.47	0/551	0.75	0/737
8	BH	0.40	0/551	0.72	0/737
8	BP	0.40	0/551	0.71	0/737
8	BX	0.40	0/551	0.69	0/737
8	Bf	0.44	0/551	0.74	0/737
8	Bn	0.40	0/551	0.74	0/737
8	Bv	0.42	0/551	0.73	0/737
8	CH	0.44	0/551	0.73	0/737
8	CP	0.41	0/551	0.73	0/737
8	CX	0.44	0/551	0.74	0/737
8	Cf	0.45	0/551	0.74	0/737
8	Cn	0.39	0/551	0.72	0/737
8	Cv	0.39	0/551	0.72	0/737
All	All	0.49	0/124200	0.77	85/167980 (0.1%)

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

There are no bond length outliers.

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AN	8185	LYS	C-N-CA	7.12	139.50	121.70
6	AF	8185	LYS	C-N-CA	7.10	139.44	121.70
6	A2	8185	LYS	C-N-CA	7.08	139.40	121.70
6	Bd	8185	LYS	C-N-CA	7.07	139.36	121.70
6	Cd	8185	LYS	C-N-CA	7.06	139.34	121.70

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AG	6067	ASN	Mainchain

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Mol	Chain	Res	Type	Group
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	648	0	690	6	0
1	AI	648	0	690	10	0
1	AQ	648	0	690	10	0
1	AY	648	0	690	7	0
1	Ag	648	0	690	0	0
1	Ao	648	0	690	0	0
1	Aw	648	0	690	0	0
1	BA	648	0	690	10	0
1	BI	648	0	690	9	0
1	BQ	648	0	690	11	0
1	BY	648	0	690	6	0
1	Bg	648	0	690	0	0
1	Bo	648	0	690	0	0
1	Bw	648	0	690	0	0
1	CA	648	0	690	8	0
1	CI	648	0	690	10	0
1	CQ	648	0	690	10	0
1	CY	648	0	690	8	0
1	Cg	648	0	690	0	0
1	Co	648	0	690	0	0
2	AB	807	0	833	13	0
2	AJ	807	0	833	18	0
2	AR	807	0	833	19	0
2	AZ	807	0	833	9	0
2	Ah	807	0	833	0	0
2	Ap	807	0	833	0	0
2	Ax	807	0	833	0	0
2	BB	807	0	833	19	0
2	BJ	807	0	833	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BR	807	0	833	16	0
2	BZ	807	0	833	9	0
2	Bh	807	0	833	0	0
2	Bp	807	0	833	0	0
2	Bx	807	0	833	0	0
2	CB	807	0	833	16	0
2	CJ	807	0	833	18	0
2	CR	807	0	833	15	0
2	CZ	807	0	833	8	0
2	Ch	807	0	833	0	0
2	Cp	807	0	833	0	0
3	AC	638	0	657	13	0
3	AK	638	0	657	15	0
3	AS	638	0	657	13	0
3	Aa	638	0	657	0	0
3	Ai	638	0	657	0	0
3	Aq	638	0	657	0	0
3	Ay	638	0	657	0	0
3	BC	638	0	657	13	0
3	BK	638	0	657	15	0
3	BS	638	0	657	13	0
3	Ba	638	0	657	0	0
3	Bi	638	0	657	0	0
3	Bq	638	0	657	0	0
3	By	638	0	657	0	0
3	CC	638	0	657	12	0
3	CK	638	0	657	12	0
3	CS	638	0	657	13	0
3	Ca	638	0	657	0	0
3	Ci	638	0	657	0	0
3	Cq	638	0	657	0	0
4	AD	556	0	561	16	0
4	AL	556	0	561	17	0
4	AT	556	0	561	17	0
4	Ab	556	0	561	0	0
4	Aj	556	0	561	0	0
4	Ar	556	0	561	0	0
4	Az	556	0	561	0	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Bj	556	0	561	0	0
4	Br	556	0	561	0	0
4	Bz	556	0	561	0	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	0	0
4	Cj	556	0	561	0	0
4	Cr	556	0	561	0	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	0	0
5	Ak	133	0	123	0	0
5	As	133	0	123	0	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	0	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	0	0
5	Ck	133	0	123	0	0
5	Cs	133	0	123	0	0
6	A2	1787	0	1779	37	0
6	AF	1787	0	1779	51	0
6	AN	1787	0	1779	57	0
6	AV	1787	0	1779	55	0
6	Ad	1787	0	1779	0	0
6	Al	1787	0	1779	0	0
6	At	1787	0	1779	0	0
6	B2	1787	0	1779	40	0
6	BF	1787	0	1779	45	0
6	BN	1787	0	1779	50	0
6	BV	1787	0	1779	45	0
6	Bd	1787	0	1779	0	0
6	Bl	1787	0	1779	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Bt	1787	0	1779	0	0
6	CF	1787	0	1779	46	0
6	CN	1787	0	1779	48	0
6	CV	1787	0	1779	39	0
6	Cd	1787	0	1779	0	0
6	Cl	1787	0	1779	0	0
6	Ct	1787	0	1779	0	0
7	A3	984	0	943	19	0
7	AG	984	0	943	21	0
7	AO	984	0	943	19	0
7	AW	984	0	943	19	0
7	Ae	984	0	943	0	0
7	Am	984	0	943	0	0
7	Au	984	0	943	0	0
7	B3	984	0	943	18	0
7	BG	984	0	943	20	0
7	BO	984	0	943	19	0
7	BW	984	0	943	17	0
7	Be	984	0	943	0	0
7	Bm	984	0	943	0	0
7	Bu	984	0	943	0	0
7	CG	984	0	943	22	0
7	CO	984	0	943	19	0
7	CW	984	0	943	22	0
7	Ce	984	0	943	0	0
7	Cm	984	0	943	0	0
7	Cu	984	0	943	0	0
8	A4	544	0	563	6	0
8	AH	544	0	563	7	0
8	AP	544	0	563	7	0
8	AX	544	0	563	8	0
8	Af	544	0	563	0	0
8	An	544	0	563	0	0
8	Av	544	0	563	0	0
8	B4	544	0	563	4	0
8	BH	544	0	563	7	0
8	BP	544	0	563	9	0
8	BX	544	0	563	7	0
8	Bf	544	0	563	0	0
8	Bn	544	0	563	0	0
8	Bv	544	0	563	0	0
8	CH	544	0	563	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	CP	544	0	563	7	0
8	CX	544	0	563	7	0
8	Cf	544	0	563	0	0
8	Cn	544	0	563	0	0
8	Cv	544	0	563	0	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	1154	0

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

The worst 5 of 1154 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:AR:2043:LYS:HG2	2:AR:2067:TRP:HB3	1.49	0.94
7:AO:6067:ASN:HB2	7:AO:6068:PRO:HD3	1.49	0.92
2:AR:2092:LEU:HD23	4:AT:4056:VAL:HG22	1.51	0.91
7:CG:6067:ASN:HB2	7:CG:6068:PRO:HD3	1.50	0.91
2:AB:2092:LEU:HD23	4:AD:4056:VAL:HG22	1.51	0.91

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	AI	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	AQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	AY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Ag	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Ao	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	7	32
1	Aw	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	7	32
1	BA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	BI	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	7	32
1	BQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	BY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Bg	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Bo	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Bw	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	CA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	CI	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	CQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	CY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Cg	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Co	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
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%)	5	27
2	Ap	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Ax	96/118 (81%)	92 (96%)	3 (3%)	1 (1%)	19	58
2	BB	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	BJ	96/118 (81%)	90 (94%)	4 (4%)	2 (2%)	9	37
2	BR	96/118 (81%)	90 (94%)	4 (4%)	2 (2%)	9	37
2	BZ	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Bh	96/118 (81%)	90 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	19	58
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	9
5	AE	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	AM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	AU	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	Ac	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	1	9
5	Ak	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	9
5	As	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
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	9
5	BM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	BU	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	Bc	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	9
5	Bk	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	Bs	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CE	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	9
5	CM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	CU	15/124 (12%)	10 (67%)	5 (33%)	0	100	100
5	Cc	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	1	9
5	Ck	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	Cs	15/124 (12%)	10 (67%)	2 (13%)	3 (20%)	0	0
6	A2	214/247 (87%)	187 (87%)	17 (8%)	10 (5%)	3	17
6	AF	214/247 (87%)	182 (85%)	22 (10%)	10 (5%)	3	17
6	AN	214/247 (87%)	174 (81%)	31 (14%)	9 (4%)	3	19
6	AV	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	2	15
6	Ad	214/247 (87%)	183 (86%)	20 (9%)	11 (5%)	2	15
6	Al	214/247 (87%)	183 (86%)	21 (10%)	10 (5%)	3	17
6	At	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	2	15
6	B2	214/247 (87%)	179 (84%)	23 (11%)	12 (6%)	2	13
6	BF	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	4	23
6	BN	214/247 (87%)	185 (86%)	22 (10%)	7 (3%)	5	26
6	BV	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	4	23
6	Bd	214/247 (87%)	185 (86%)	19 (9%)	10 (5%)	3	17
6	Bl	214/247 (87%)	186 (87%)	18 (8%)	10 (5%)	3	17
6	Bt	214/247 (87%)	181 (85%)	27 (13%)	6 (3%)	6	30
6	CF	214/247 (87%)	187 (87%)	19 (9%)	8 (4%)	4	23
6	CN	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	4	23
6	CV	214/247 (87%)	182 (85%)	24 (11%)	8 (4%)	4	23
6	Cd	214/247 (87%)	185 (86%)	19 (9%)	10 (5%)	3	17
6	Cl	214/247 (87%)	186 (87%)	19 (9%)	9 (4%)	3	19
6	Ct	214/247 (87%)	178 (83%)	26 (12%)	10 (5%)	3	17
7	A3	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	AG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	AO	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	AW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Ae	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Am	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Au	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	B3	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	7	33
7	BG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	BO	123/186 (66%)	115 (94%)	4 (3%)	4 (3%)	5	26
7	BW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Be	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	7	33
7	Bm	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	7	33
7	Bu	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	CG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	CO	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	CW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Ce	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Cm	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	7	33
7	Cu	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
8	A4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	AH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	AP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	AX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Af	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	An	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Av	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	B4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	BH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	BP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	BX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Bf	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Bn	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Bv	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	CH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	CP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Cf	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Cn	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Cv	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
All	All	14800/20960 (71%)	13553 (92%)	894 (6%)	353 (2%)	7	33

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%)	12	40
1	AI	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	AQ	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	AY	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	Ag	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	Ao	77/101 (76%)	73 (95%)	4 (5%)	29	65
1	Aw	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	BA	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	BI	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	BQ	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	BY	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	Bg	77/101 (76%)	72 (94%)	5 (6%)	21	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bo	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	Bw	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	CA	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	CI	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	CQ	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	CY	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	Cg	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	Co	77/101 (76%)	73 (95%)	4 (5%)	29	65
2	AB	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	AJ	94/110 (86%)	92 (98%)	2 (2%)	61	86
2	AR	94/110 (86%)	91 (97%)	3 (3%)	46	79
2	AZ	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	Ah	94/110 (86%)	89 (95%)	5 (5%)	28	64
2	Ap	94/110 (86%)	91 (97%)	3 (3%)	46	79
2	Ax	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	BB	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	BJ	94/110 (86%)	88 (94%)	6 (6%)	22	57
2	BR	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	BZ	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	Bh	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	Bp	94/110 (86%)	89 (95%)	5 (5%)	28	64
2	Bx	94/110 (86%)	88 (94%)	6 (6%)	22	57
2	CB	94/110 (86%)	89 (95%)	5 (5%)	28	64
2	CJ	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	CR	94/110 (86%)	91 (97%)	3 (3%)	46	79
2	CZ	94/110 (86%)	88 (94%)	6 (6%)	22	57
2	Ch	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	Cp	94/110 (86%)	89 (95%)	5 (5%)	28	64
3	AC	72/84 (86%)	67 (93%)	5 (7%)	19	55
3	AK	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	AS	72/84 (86%)	68 (94%)	4 (6%)	26	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Aa	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Ai	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Aq	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Ay	72/84 (86%)	69 (96%)	3 (4%)	36	73
3	BC	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	BK	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	BS	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Ba	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Bi	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Bq	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	By	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	CC	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	CK	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	CS	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Ca	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Ci	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Cq	72/84 (86%)	68 (94%)	4 (6%)	26	62
4	AD	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	AL	60/74 (81%)	57 (95%)	3 (5%)	30	67
4	AT	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Ab	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Aj	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Ar	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Az	60/74 (81%)	57 (95%)	3 (5%)	30	67
4	BD	60/74 (81%)	55 (92%)	5 (8%)	14	46
4	BL	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	BT	60/74 (81%)	55 (92%)	5 (8%)	14	46
4	Bb	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Bj	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Br	60/74 (81%)	57 (95%)	3 (5%)	30	67
4	Bz	60/74 (81%)	56 (93%)	4 (7%)	20	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	60/74 (81%)	55 (92%)	5 (8%)	14	46
4	CL	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	CT	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Cb	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Cj	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Cr	60/74 (81%)	56 (93%)	4 (7%)	20	56
5	A1	15/97 (16%)	11 (73%)	4 (27%)	0	1
5	AE	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	AM	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	AU	15/97 (16%)	13 (87%)	2 (13%)	5	20
5	Ac	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	Ak	15/97 (16%)	13 (87%)	2 (13%)	5	20
5	As	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	B1	15/97 (16%)	13 (87%)	2 (13%)	5	20
5	BE	15/97 (16%)	11 (73%)	4 (27%)	0	1
5	BM	15/97 (16%)	11 (73%)	4 (27%)	0	1
5	BU	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	Bc	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	Bk	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	Bs	15/97 (16%)	13 (87%)	2 (13%)	5	20
5	CE	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	CM	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	CU	15/97 (16%)	11 (73%)	4 (27%)	0	1
5	Cc	15/97 (16%)	13 (87%)	2 (13%)	5	20
5	Ck	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	Cs	15/97 (16%)	10 (67%)	5 (33%)	0	0
6	A2	203/231 (88%)	176 (87%)	27 (13%)	5	20
6	AF	203/231 (88%)	170 (84%)	33 (16%)	3	12
6	AN	203/231 (88%)	171 (84%)	32 (16%)	3	13
6	AV	203/231 (88%)	177 (87%)	26 (13%)	5	21
6	Ad	203/231 (88%)	178 (88%)	25 (12%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Al	203/231 (88%)	176 (87%)	27 (13%)	5	20
6	At	203/231 (88%)	172 (85%)	31 (15%)	3	14
6	B2	203/231 (88%)	169 (83%)	34 (17%)	3	11
6	BF	203/231 (88%)	176 (87%)	27 (13%)	5	20
6	BN	203/231 (88%)	177 (87%)	26 (13%)	5	21
6	BV	203/231 (88%)	178 (88%)	25 (12%)	6	23
6	Bd	203/231 (88%)	176 (87%)	27 (13%)	5	20
6	Bl	203/231 (88%)	175 (86%)	28 (14%)	4	19
6	Bt	203/231 (88%)	174 (86%)	29 (14%)	4	17
6	CF	203/231 (88%)	172 (85%)	31 (15%)	3	14
6	CN	203/231 (88%)	178 (88%)	25 (12%)	6	23
6	CV	203/231 (88%)	175 (86%)	28 (14%)	4	19
6	Cd	203/231 (88%)	174 (86%)	29 (14%)	4	17
6	Cl	203/231 (88%)	172 (85%)	31 (15%)	3	14
6	Ct	203/231 (88%)	174 (86%)	29 (14%)	4	17
7	A3	108/159 (68%)	98 (91%)	10 (9%)	11	39
7	AG	108/159 (68%)	98 (91%)	10 (9%)	11	39
7	AO	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	AW	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Ae	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Am	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Au	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	B3	108/159 (68%)	98 (91%)	10 (9%)	11	39
7	BG	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	BO	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	BW	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Be	108/159 (68%)	100 (93%)	8 (7%)	17	51
7	Bm	108/159 (68%)	100 (93%)	8 (7%)	17	51
7	Bu	108/159 (68%)	100 (93%)	8 (7%)	17	51
7	CG	108/159 (68%)	98 (91%)	10 (9%)	11	39
7	CO	108/159 (68%)	99 (92%)	9 (8%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	CW	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Ce	108/159 (68%)	98 (91%)	10 (9%)	11	39
7	Cm	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Cu	108/159 (68%)	100 (93%)	8 (7%)	17	51
8	A4	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	AH	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	AP	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	AX	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Af	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	An	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Av	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	B4	61/66 (92%)	58 (95%)	3 (5%)	31	68
8	BH	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	BP	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	BX	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Bf	61/66 (92%)	58 (95%)	3 (5%)	31	68
8	Bn	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Bv	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	CH	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	CP	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	CX	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Cf	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Cn	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Cv	61/66 (92%)	59 (97%)	2 (3%)	45	79
All	All	13800/18440 (75%)	12594 (91%)	1206 (9%)	13	44

5 of 1206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BR	2092	LEU
6	Bl	8037	LEU
6	Cl	8096	GLN
6	BV	8037	LEU
5	Bc	7006	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
6	BN	8209	ASN
2	Bh	2031	ASN
7	Cm	6018	ASN
2	BR	2031	ASN
2	BZ	2031	ASN

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 carbohydrates 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	A2	8301	-	4,4,4	0.26	0	6,6,6	0.41	0
9	SO4	Ad	8301	-	4,4,4	0.38	0	6,6,6	0.25	0
9	SO4	At	8301	-	4,4,4	0.56	0	6,6,6	0.38	0
9	SO4	B2	8301	-	4,4,4	0.33	0	6,6,6	0.30	0
9	SO4	BF	8301	-	4,4,4	0.22	0	6,6,6	0.27	0
9	SO4	BV	8301	-	4,4,4	0.40	0	6,6,6	0.34	0
9	SO4	Bd	8301	-	4,4,4	0.27	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	Bt	8301	-	4,4,4	0.42	0	6,6,6	0.27	0
9	SO4	CF	8301	-	4,4,4	0.38	0	6,6,6	0.28	0
9	SO4	Cl	8301	-	4,4,4	0.41	0	6,6,6	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SO4	A2	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	Ad	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	At	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	B2	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	BF	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	BV	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	Bd	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	Bt	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	CF	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	Cl	8301	-	-	0/0/0/0	0/0/0/0

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%)	-0.24	0 100 100	16, 44, 80, 155	0
1	AI	82/119 (68%)	-0.40	0 100 100	17, 41, 83, 141	0
1	AQ	82/119 (68%)	-0.28	0 100 100	26, 48, 92, 145	0
1	AY	82/119 (68%)	0.39	1 (1%) 81 64	48, 76, 117, 154	0
1	Ag	82/119 (68%)	-0.29	0 100 100	14, 47, 94, 167	0
1	Ao	82/119 (68%)	-0.32	1 (1%) 81 64	18, 43, 87, 158	0
1	Aw	82/119 (68%)	0.35	1 (1%) 81 64	48, 76, 115, 154	0
1	BA	82/119 (68%)	1.08	6 (7%) 18 6	69, 92, 131, 175	0
1	BI	82/119 (68%)	1.27	14 (17%) 2 1	66, 92, 127, 175	0
1	BQ	82/119 (68%)	0.01	1 (1%) 81 64	34, 60, 107, 179	0
1	BY	82/119 (68%)	-0.17	0 100 100	25, 54, 88, 130	0
1	Bg	82/119 (68%)	0.53	0 100 100	58, 81, 117, 151	0
1	Bo	82/119 (68%)	0.20	0 100 100	41, 68, 117, 164	0
1	Bw	82/119 (68%)	-0.15	0 100 100	24, 53, 90, 142	0
1	CA	82/119 (68%)	0.11	0 100 100	36, 64, 105, 132	0
1	CI	82/119 (68%)	1.11	6 (7%) 18 6	61, 86, 127, 164	0
1	CQ	82/119 (68%)	-0.23	0 100 100	29, 54, 88, 136	0
1	CY	82/119 (68%)	-0.24	0 100 100	17, 47, 88, 130	0
1	Cg	82/119 (68%)	0.55	0 100 100	52, 82, 119, 162	0
1	Co	82/119 (68%)	1.10	10 (12%) 5 2	64, 88, 130, 168	0
2	AB	100/118 (84%)	-0.02	1 (1%) 84 69	19, 63, 168, 181	0
2	AJ	100/118 (84%)	-0.06	0 100 100	20, 63, 167, 179	0
2	AR	100/118 (84%)	0.25	8 (8%) 15 5	29, 69, 190, 201	0
2	AZ	100/118 (84%)	0.43	10 (10%) 9 3	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%)	0.33	7 (7%) 19 7	44, 82, 207, 217	0
2	Ap	100/118 (84%)	0.30	9 (9%) 12 4	34, 72, 215, 219	0
2	Ax	100/118 (84%)	0.11	3 (3%) 54 29	31, 73, 210, 225	0
2	BB	100/118 (84%)	1.48	28 (28%) 1 0	87, 124, 220, 226	0
2	BJ	100/118 (84%)	1.70	38 (38%) 0 0	77, 113, 245, 255	0
2	BR	100/118 (84%)	0.79	16 (16%) 3 1	45, 94, 235, 237	0
2	BZ	100/118 (84%)	0.45	12 (12%) 6 2	37, 76, 216, 232	0
2	Bh	100/118 (84%)	0.76	16 (16%) 3 1	51, 90, 235, 253	0
2	Bp	100/118 (84%)	1.20	20 (20%) 1 0	56, 111, 242, 250	0
2	Bx	100/118 (84%)	0.47	10 (10%) 9 3	32, 75, 230, 243	0
2	CB	100/118 (84%)	0.71	15 (15%) 3 1	48, 92, 223, 238	0
2	CJ	100/118 (84%)	1.47	26 (26%) 1 0	79, 118, 224, 231	0
2	CR	100/118 (84%)	0.24	7 (7%) 19 7	35, 76, 183, 203	0
2	CZ	100/118 (84%)	0.15	8 (8%) 15 5	28, 72, 184, 205	0
2	Ch	100/118 (84%)	0.64	8 (8%) 15 5	55, 90, 212, 223	0
2	Cp	100/118 (84%)	1.48	25 (25%) 1 0	67, 112, 233, 247	0
3	AC	77/92 (83%)	0.62	10 (12%) 5 2	70, 120, 150, 162	0
3	AK	77/92 (83%)	0.90	11 (14%) 4 2	79, 125, 164, 170	0
3	AS	77/92 (83%)	2.16	32 (41%) 0 0	128, 181, 261, 265	0
3	Aa	77/92 (83%)	2.44	40 (51%) 0 0	134, 199, 268, 274	0
3	Ai	77/92 (83%)	0.80	8 (10%) 8 3	86, 135, 164, 173	0
3	Aq	77/92 (83%)	1.82	32 (41%) 0 0	126, 179, 246, 254	0
3	Ay	77/92 (83%)	1.34	20 (25%) 1 0	87, 140, 220, 227	0
3	BC	77/92 (83%)	1.66	26 (33%) 0 0	128, 157, 177, 185	0
3	BK	77/92 (83%)	2.70	37 (48%) 0 0	177, 242, 280, 286	0
3	BS	77/92 (83%)	2.04	31 (40%) 0 0	148, 203, 244, 256	0
3	Ba	77/92 (83%)	1.95	32 (41%) 0 0	133, 188, 260, 264	0
3	Bi	77/92 (83%)	2.17	32 (41%) 0 0	144, 203, 278, 279	0
3	Bq	77/92 (83%)	2.22	39 (50%) 0 0	200, 257, 282, 293	0
3	By	77/92 (83%)	1.88	34 (44%) 0 0	143, 207, 268, 274	0
3	CC	77/92 (83%)	1.08	19 (24%) 1 0	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%)	1.67	27 (35%) 0 0	131, 181, 212, 222	0
3	CS	77/92 (83%)	0.72	8 (10%) 8 3	81, 121, 161, 172	0
3	Ca	77/92 (83%)	0.67	8 (10%) 8 3	82, 122, 165, 177	0
3	Ci	77/92 (83%)	1.10	14 (18%) 2 1	107, 148, 200, 206	0
3	Cq	77/92 (83%)	2.56	39 (50%) 0 0	172, 241, 284, 286	0
4	AD	71/86 (82%)	0.03	1 (1%) 78 60	46, 93, 120, 142	0
4	AL	71/86 (82%)	0.03	1 (1%) 78 60	50, 89, 113, 143	0
4	AT	71/86 (82%)	0.67	11 (15%) 3 1	64, 115, 159, 182	0
4	Ab	71/86 (82%)	0.81	10 (14%) 4 2	73, 116, 166, 193	0
4	Aj	71/86 (82%)	0.48	4 (5%) 28 11	71, 125, 153, 185	0
4	Ar	71/86 (82%)	0.70	9 (12%) 5 2	66, 122, 172, 191	0
4	Az	71/86 (82%)	0.17	0 100 100	60, 105, 133, 163	0
4	BD	71/86 (82%)	1.41	18 (25%) 1 0	104, 169, 199, 208	0
4	BL	71/86 (82%)	1.68	26 (36%) 0 0	118, 165, 251, 260	0
4	BT	71/86 (82%)	1.12	20 (28%) 1 0	98, 144, 212, 220	0
4	Bb	71/86 (82%)	0.70	7 (9%) 9 3	64, 121, 161, 193	0
4	Bj	71/86 (82%)	0.95	10 (14%) 4 2	80, 130, 174, 203	0
4	Br	71/86 (82%)	1.55	21 (29%) 1 0	118, 183, 264, 271	0
4	Bz	71/86 (82%)	0.76	9 (12%) 5 2	71, 128, 179, 219	0
4	CD	71/86 (82%)	0.65	8 (11%) 7 2	77, 126, 152, 195	0
4	CL	71/86 (82%)	1.67	24 (33%) 0 0	111, 166, 197, 201	0
4	CT	71/86 (82%)	0.04	1 (1%) 78 60	64, 101, 128, 156	0
4	Cb	71/86 (82%)	0.06	2 (2%) 56 32	60, 102, 128, 157	0
4	Cj	71/86 (82%)	0.37	3 (4%) 40 19	79, 117, 152, 178	0
4	Cr	71/86 (82%)	1.63	23 (32%) 1 0	111, 166, 244, 257	0
5	A1	17/124 (13%)	0.70	3 (17%) 2 1	73, 98, 162, 164	0
5	AE	17/124 (13%)	0.28	0 100 100	67, 81, 121, 128	0
5	AM	17/124 (13%)	0.18	1 (5%) 26 11	64, 80, 131, 133	0
5	AU	17/124 (13%)	0.26	1 (5%) 26 11	58, 85, 120, 125	0
5	Ac	17/124 (13%)	0.57	3 (17%) 2 1	52, 86, 141, 144	0
5	Ak	17/124 (13%)	0.44	1 (5%) 26 11	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%)	0.15	1 (5%) 26 11	59, 76, 128, 128	0
5	B1	17/124 (13%)	0.19	1 (5%) 26 11	56, 69, 129, 130	0
5	BE	17/124 (13%)	1.30	4 (23%) 1 0	115, 129, 153, 167	0
5	BM	17/124 (13%)	1.32	3 (17%) 2 1	96, 109, 152, 152	0
5	BU	17/124 (13%)	0.51	1 (5%) 26 11	83, 94, 129, 132	0
5	Bc	17/124 (13%)	0.34	1 (5%) 26 11	60, 81, 133, 136	0
5	Bk	17/124 (13%)	1.06	2 (11%) 6 2	85, 98, 150, 153	0
5	Bs	17/124 (13%)	0.66	3 (17%) 2 1	81, 95, 149, 151	0
5	CE	17/124 (13%)	0.58	2 (11%) 6 2	77, 93, 139, 142	0
5	CM	17/124 (13%)	1.97	5 (29%) 1 0	111, 124, 163, 163	0
5	CU	17/124 (13%)	0.43	3 (17%) 2 1	54, 78, 134, 134	0
5	Cc	17/124 (13%)	0.28	2 (11%) 6 2	53, 72, 132, 134	0
5	Ck	17/124 (13%)	1.34	3 (17%) 2 1	79, 92, 156, 160	0
5	Cs	17/124 (13%)	1.18	3 (17%) 2 1	101, 114, 151, 152	0
6	A2	216/247 (87%)	0.08	17 (7%) 15 5	24, 73, 196, 212	0
6	AF	216/247 (87%)	-0.00	9 (4%) 40 19	14, 56, 168, 208	0
6	AN	216/247 (87%)	-0.02	10 (4%) 36 17	11, 54, 167, 187	0
6	AV	216/247 (87%)	0.18	21 (9%) 10 3	17, 59, 201, 226	0
6	Ad	216/247 (87%)	0.52	24 (11%) 7 2	27, 75, 214, 236	0
6	Al	216/247 (87%)	0.09	13 (6%) 25 10	16, 62, 189, 235	0
6	At	216/247 (87%)	0.12	22 (10%) 9 3	14, 55, 202, 219	0
6	B2	216/247 (87%)	0.25	23 (10%) 8 3	20, 58, 225, 240	0
6	BF	216/247 (87%)	1.04	28 (12%) 5 2	71, 108, 202, 230	0
6	BN	216/247 (87%)	1.27	35 (16%) 3 1	57, 99, 235, 247	0
6	BV	216/247 (87%)	0.46	23 (10%) 8 3	31, 78, 219, 245	0
6	Bd	216/247 (87%)	0.24	22 (10%) 9 3	24, 61, 215, 236	0
6	Bl	216/247 (87%)	0.57	25 (11%) 6 2	38, 78, 226, 246	0
6	Bt	216/247 (87%)	0.71	32 (14%) 3 1	41, 78, 233, 250	0
6	CF	216/247 (87%)	0.24	13 (6%) 25 10	35, 73, 195, 229	0
6	CN	216/247 (87%)	1.14	35 (16%) 3 1	64, 107, 196, 224	0
6	CV	216/247 (87%)	-0.03	7 (3%) 51 27	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%)	-0.08	9 (4%) 40 19	14, 55, 181, 211	0
6	Cl	216/247 (87%)	0.37	11 (5%) 32 13	32, 76, 204, 225	0
6	Ct	216/247 (87%)	1.28	42 (19%) 1 1	63, 103, 224, 240	0
7	A3	127/186 (68%)	0.99	14 (11%) 7 2	74, 126, 154, 172	0
7	AG	127/186 (68%)	-0.04	2 (1%) 74 55	21, 47, 108, 144	0
7	AO	127/186 (68%)	-0.01	2 (1%) 74 55	19, 58, 119, 143	0
7	AW	127/186 (68%)	0.00	5 (3%) 43 21	29, 60, 122, 152	0
7	Ae	127/186 (68%)	1.61	33 (25%) 1 0	78, 122, 162, 170	0
7	Am	127/186 (68%)	-0.28	5 (3%) 43 21	13, 43, 110, 149	0
7	Au	127/186 (68%)	0.02	6 (4%) 35 16	20, 51, 122, 152	0
7	B3	127/186 (68%)	0.08	4 (3%) 52 28	31, 58, 113, 162	0
7	BG	127/186 (68%)	0.91	9 (7%) 19 7	51, 82, 135, 167	0
7	BO	127/186 (68%)	1.68	28 (22%) 1 0	73, 107, 149, 178	0
7	BW	127/186 (68%)	0.02	6 (4%) 35 16	28, 54, 115, 153	0
7	Be	127/186 (68%)	0.05	4 (3%) 52 28	33, 62, 120, 162	0
7	Bm	127/186 (68%)	1.44	24 (18%) 2 1	62, 110, 152, 178	0
7	Bu	127/186 (68%)	0.14	5 (3%) 43 21	34, 63, 122, 167	0
7	CG	127/186 (68%)	-0.07	4 (3%) 52 28	22, 57, 116, 158	0
7	CO	127/186 (68%)	0.88	12 (9%) 11 4	55, 85, 133, 174	0
7	CW	127/186 (68%)	-0.08	4 (3%) 52 28	23, 59, 126, 158	0
7	Ce	127/186 (68%)	-0.11	3 (2%) 62 39	20, 53, 115, 158	0
7	Cm	127/186 (68%)	1.80	41 (32%) 1 0	67, 125, 157, 179	0
7	Cu	127/186 (68%)	1.32	18 (14%) 4 2	73, 100, 146, 174	0
8	A4	70/76 (92%)	2.36	29 (41%) 0 0	158, 202, 224, 228	0
8	AH	70/76 (92%)	0.32	3 (4%) 39 18	69, 116, 151, 158	0
8	AP	70/76 (92%)	0.98	13 (18%) 2 1	81, 137, 167, 178	0
8	AX	70/76 (92%)	2.54	33 (47%) 0 0	121, 196, 220, 225	0
8	Af	70/76 (92%)	4.55	51 (72%) 0 0	200, 237, 255, 258	0
8	An	70/76 (92%)	0.41	6 (8%) 13 4	67, 110, 152, 158	0
8	Av	70/76 (92%)	1.78	26 (37%) 0 0	109, 176, 200, 214	0
8	B4	70/76 (92%)	3.05	42 (60%) 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%)	1.39	20 (28%)	1	0	102, 140, 170, 178	0
8	BP	70/76 (92%)	4.03	48 (68%)	0	0	180, 237, 261, 266	0
8	BX	70/76 (92%)	2.32	31 (44%)	0	0	114, 173, 192, 201	0
8	Bf	70/76 (92%)	3.09	45 (64%)	0	0	178, 226, 252, 255	0
8	Bn	70/76 (92%)	3.73	46 (65%)	0	0	221, 251, 273, 278	0
8	Bv	70/76 (92%)	3.51	51 (72%)	0	0	185, 237, 271, 277	0
8	CH	70/76 (92%)	0.91	10 (14%)	4	2	106, 144, 166, 172	0
8	CP	70/76 (92%)	1.72	22 (31%)	1	0	135, 167, 187, 206	0
8	CX	70/76 (92%)	0.91	9 (12%)	5	2	103, 135, 162, 171	0
8	Cf	70/76 (92%)	0.64	6 (8%)	13	4	97, 140, 160, 170	0
8	Cn	70/76 (92%)	1.87	23 (32%)	0	0	146, 178, 204, 210	0
8	Cv	70/76 (92%)	4.43	53 (75%)	0	0	231, 267, 287, 290	0
All	All	15200/20960 (72%)	0.77	2274 (14%)	3	1	11, 97, 231, 293	0

The worst 5 of 2274 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	Af	5055	VAL	22.6
8	BP	5055	VAL	21.6
7	BO	6164	ASN	21.3
8	Af	5028	GLY	20.6
7	BG	6164	ASN	19.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
9	SO4	Bt	8301	5/5	0.93	0.20	-0.19	111,113,114,115	0
9	SO4	Cl	8301	5/5	0.76	0.25	-0.27	129,131,132,132	0
9	SO4	Ad	8301	5/5	0.72	0.27	-0.28	137,139,139,140	0
9	SO4	BF	8301	5/5	0.86	0.21	-0.63	129,129,130,131	0
9	SO4	B2	8301	5/5	0.95	0.17	-1.04	97,99,99,103	0
9	SO4	A2	8301	5/5	0.85	0.16	-1.11	150,150,150,151	0
9	SO4	At	8301	5/5	0.89	0.17	-1.29	92,93,96,99	0
9	SO4	BV	8301	5/5	0.90	0.14	-1.42	111,113,114,116	0
9	SO4	CF	8301	5/5	0.94	0.14	-1.47	100,103,104,106	0
9	SO4	Bd	8301	5/5	0.94	0.12	-1.59	108,108,109,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.