wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:00 PM GMT

PDB ID	:	4XQ2
Title	:	Ensemble refinement of cystathione gamma lyase (CalE6) D7G from Micromonospora echinospora
Authors	:	Wang, F.; Yennamalli, R.M.; Singh, S.; Tan, K.; Thorson, J.S.; Phillips Jr., G.N.; Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on	:	2015-01-18
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

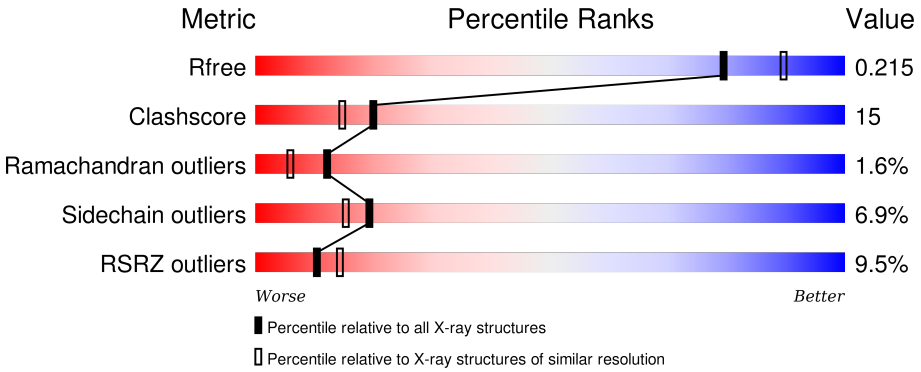
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk26765
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	1-A	384	10% 71% 23%
1	1-B	384	8% 70% 24%
1	1-C	384	9% 75% 20%
1	1-D	384	10% 69% 24% 5%
1	1-E	384	8% 71% 24%

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Mol	Chain	Length	Quality of chain
1	1-F	384	9% 68% 27%
1	1-G	384	10% 73% 22%
1	1-H	384	10% 69% 25%
1	10-A	384	10% 72% 21%
1	10-B	384	8% 68% 27%
1	10-C	384	9% 70% 26%
1	10-D	384	10% 67% 27%
1	10-E	384	8% 69% 25%
1	10-F	384	9% 67% 26%
1	10-G	384	10% 67% 26% 5%
1	10-H	384	10% 72% 23%
1	2-A	384	10% 76% 20%
1	2-B	384	8% 74% 20%
1	2-C	384	9% 72% 23%
1	2-D	384	10% 71% 22% 5%
1	2-E	384	8% 72% 24%
1	2-F	384	9% 75% 21%
1	2-G	384	10% 77% 18%
1	2-H	384	10% 70% 23% 5%
1	3-A	384	10% 73% 21%
1	3-B	384	8% 74% 21%
1	3-C	384	9% 70% 23% 5%
1	3-D	384	10% 69% 24% 5%
1	3-E	384	8% 71% 23%
1	3-F	384	9% 66% 29%

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Mol	Chain	Length	Quality of chain
1	3-G	384	10% 72% 23%
1	3-H	384	10% 67% 26%
1	4-A	384	10% 71% 23%
1	4-B	384	8% 72% 21% 5%
1	4-C	384	9% 72% 23%
1	4-D	384	10% 68% 26%
1	4-E	384	8% 66% 26% 5%
1	4-F	384	9% 67% 26% 5%
1	4-G	384	10% 71% 23%
1	4-H	384	10% 71% 24%
1	5-A	384	10% 71% 23%
1	5-B	384	8% 66% 28%
1	5-C	384	9% 70% 25%
1	5-D	384	10% 74% 20%
1	5-E	384	8% 66% 26% 6%
1	5-F	384	9% 73% 23%
1	5-G	384	10% 75% 19%
1	5-H	384	10% 72% 22%
1	6-A	384	10% 75% 20%
1	6-B	384	8% 69% 24%
1	6-C	384	9% 71% 24%
1	6-D	384	10% 68% 25%
1	6-E	384	8% 74% 19%
1	6-F	384	9% 70% 23% 5%
1	6-G	384	10% 72% 23%

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Mol	Chain	Length	Quality of chain
1	6-H	384	10% 74% 21%
1	7-A	384	10% 67% 24% 5%
1	7-B	384	8% 71% 23%
1	7-C	384	9% 70% 24%
1	7-D	384	10% 71% 22%
1	7-E	384	8% 73% 22%
1	7-F	384	9% 68% 28%
1	7-G	384	10% 75% 20%
1	7-H	384	10% 73% 23%
1	8-A	384	10% 77% 18%
1	8-B	384	8% 68% 28%
1	8-C	384	9% 71% 24%
1	8-D	384	10% 70% 24%
1	8-E	384	8% 70% 24%
1	8-F	384	9% 69% 25%
1	8-G	384	10% 73% 22%
1	8-H	384	10% 73% 23%
1	9-A	384	10% 70% 24%
1	9-B	384	8% 76% 20%
1	9-C	384	9% 70% 25%
1	9-D	384	10% 70% 24%
1	9-E	384	8% 69% 24%
1	9-F	384	9% 67% 27%
1	9-G	384	10% 75% 21%
1	9-H	384	10% 74% 22%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MES	10-B	401	-	-	X	-
2	MES	3-E	401	-	-	X	-
2	MES	4-C	401	-	-	X	-
2	MES	5-G	401	-	-	X	-
2	MES	6-F	401	-	-	X	-
2	MES	7-H	401	-	-	X	-
2	MES	8-C	401	-	-	X	-
2	MES	8-D	401	-	-	-	X
3	GOL	1-A	403	-	-	-	X
3	GOL	1-B	402	-	-	-	X
3	GOL	1-B	403	-	-	-	X
3	GOL	1-B	404	-	-	-	X
3	GOL	1-B	406	-	-	-	X
3	GOL	1-D	402	-	-	-	X
3	GOL	1-F	402	-	-	-	X
3	GOL	1-F	403	-	-	-	X
3	GOL	1-F	405	-	-	-	X
3	GOL	1-F	406	-	-	-	X
3	GOL	1-G	403	-	-	-	X
3	GOL	1-H	402	-	-	-	X
3	GOL	10-A	403	-	-	X	X
3	GOL	10-B	403	-	-	-	X
3	GOL	10-B	405	-	-	-	X
3	GOL	10-B	407	-	-	-	X
3	GOL	10-C	403	-	-	-	X
3	GOL	10-D	402	-	-	-	X
3	GOL	10-D	403	-	-	-	X
3	GOL	10-E	403	-	-	-	X
3	GOL	10-F	402	-	-	-	X
3	GOL	10-F	404	-	-	-	X
3	GOL	10-F	405	-	-	-	X
3	GOL	10-F	406	-	-	-	X
3	GOL	10-H	402	-	-	-	X
3	GOL	10-H	403	-	-	-	X
3	GOL	10-H	404	-	-	-	X
3	GOL	10-H	405	-	-	-	X
3	GOL	2-A	403	-	-	-	X
3	GOL	2-B	403	-	-	-	X
3	GOL	2-B	405	-	-	-	X
3	GOL	2-B	406	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	2-B	407	-	-	-	X
3	GOL	2-C	402	-	-	-	X
3	GOL	2-C	403	-	-	-	X
3	GOL	2-D	402	-	-	-	X
3	GOL	2-D	403	-	-	-	X
3	GOL	2-E	403	-	-	-	X
3	GOL	2-F	404	-	-	-	X
3	GOL	2-F	405	-	-	-	X
3	FMT	2-F	406	-	-	-	X
3	GOL	2-G	403	-	-	-	X
3	GOL	2-G	404	-	-	-	X
3	GOL	2-H	402	-	-	-	X
3	GOL	3-A	403	-	-	-	X
3	GOL	3-B	402	-	-	-	X
3	GOL	3-B	403	-	-	-	X
3	GOL	3-B	404	-	-	-	X
3	GOL	3-B	406	-	-	-	X
3	GOL	3-B	407	-	-	-	X
3	GOL	3-C	402	-	-	-	X
3	GOL	3-C	403	-	-	-	X
3	GOL	3-D	402	-	-	-	X
3	GOL	3-F	402	-	-	-	X
3	GOL	3-F	403	-	-	-	X
3	GOL	3-F	406	-	-	-	X
3	GOL	3-G	403	-	-	-	X
3	GOL	3-H	402	-	-	-	X
3	GOL	3-H	403	-	-	-	X
3	GOL	4-A	403	-	-	-	X
3	GOL	4-B	403	-	-	-	X
3	GOL	4-B	405	-	-	-	X
3	GOL	4-B	407	-	-	-	X
3	GOL	4-C	402	-	-	-	X
3	GOL	4-C	403	-	-	-	X
3	GOL	4-D	402	-	-	-	X
3	GOL	4-F	402	-	-	-	X
3	GOL	4-F	403	-	-	-	X
3	GOL	4-F	404	-	-	-	X
3	FMT	4-F	405	-	-	-	X
3	GOL	5-A	403	-	-	-	X
3	GOL	5-B	402	-	-	-	X
3	GOL	5-B	403	-	-	-	X
3	GOL	5-B	404	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	5-B	405	-	-	X	-
3	GOL	5-B	406	-	-	-	X
3	GOL	5-D	402	-	-	-	X
3	GOL	5-D	403	-	-	-	X
3	GOL	5-E	403	-	-	-	X
3	GOL	5-F	402	-	-	-	X
3	GOL	5-F	403	-	-	-	X
3	GOL	5-F	404	-	-	-	X
3	FMT	5-F	405	-	-	-	X
3	GOL	5-G	403	-	-	-	X
3	GOL	5-H	403	-	-	-	X
3	GOL	6-A	403	-	-	-	X
3	GOL	6-B	402	-	-	-	X
3	GOL	6-B	403	-	-	-	X
3	GOL	6-B	404	-	-	-	X
3	GOL	6-B	406	-	-	-	X
3	GOL	6-D	402	-	-	-	X
3	GOL	6-D	403	-	-	-	X
3	GOL	6-E	403	-	-	-	X
3	GOL	6-F	402	-	-	-	X
3	GOL	6-F	403	-	-	-	X
3	GOL	6-F	404	-	-	-	X
3	GOL	6-F	405	-	-	-	X
3	GOL	6-F	406	-	-	-	X
3	GOL	6-H	402	-	-	-	X
3	GOL	6-H	403	-	-	-	X
3	GOL	6-H	404	-	-	-	X
3	GOL	6-H	405	-	-	-	X
3	GOL	7-A	402	-	-	X	-
3	GOL	7-A	403	-	-	-	X
3	GOL	7-B	402	-	-	-	X
3	GOL	7-B	404	-	-	-	X
3	GOL	7-B	406	-	-	-	X
3	GOL	7-D	402	-	-	-	X
3	GOL	7-D	403	-	-	-	X
3	GOL	7-F	402	-	-	-	X
3	GOL	7-F	405	-	-	-	X
3	GOL	7-F	406	-	-	-	X
3	GOL	7-G	403	-	-	-	X
3	GOL	7-H	402	-	-	-	X
3	GOL	7-H	403	-	-	-	X
3	GOL	8-A	403	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	8-B	402	-	-	-	X
3	GOL	8-B	403	-	-	-	X
3	GOL	8-B	404	-	-	-	X
3	GOL	8-B	406	-	-	-	X
3	GOL	8-B	407	-	-	-	X
3	GOL	8-C	402	-	-	-	X
3	GOL	8-C	403	-	-	-	X
3	GOL	8-D	402	-	-	-	X
3	GOL	8-E	402	-	-	X	-
3	GOL	8-E	403	-	-	-	X
3	GOL	8-F	402	-	-	-	X
3	GOL	8-F	403	-	-	-	X
3	GOL	8-F	404	-	-	-	X
3	GOL	8-F	405	-	-	-	X
3	FMT	8-F	406	-	-	-	X
3	GOL	8-G	404	-	-	-	X
3	GOL	8-H	402	-	-	-	X
3	GOL	8-H	404	-	-	X	-
3	GOL	9-A	403	-	-	-	X
3	GOL	9-B	403	-	-	-	X
3	GOL	9-B	405	-	-	-	X
3	GOL	9-B	406	-	-	-	X
3	GOL	9-C	403	-	-	-	X
3	GOL	9-D	402	-	-	-	X
3	GOL	9-D	403	-	-	-	X
3	GOL	9-E	403	-	-	-	X
3	GOL	9-F	402	-	-	-	X
3	GOL	9-F	404	-	-	-	X
3	FMT	9-F	405	-	-	-	X
3	GOL	9-H	402	-	-	-	X
3	GOL	9-H	403	-	-	-	X
3	GOL	9-H	404	-	-	-	X
4	GOL	1-B	408	-	-	-	X
4	FMT	1-F	408	-	-	-	X
4	FMT	1-G	406	-	-	-	X
4	CL	10-E	404	-	-	X	-
4	CL	10-H	407	-	-	X	-
4	CL	2-H	406	-	-	X	-
4	GOL	3-A	405	-	-	-	X
4	GOL	3-E	404	-	-	-	X
4	CL	4-A	406	-	-	X	-
4	GOL	4-E	404	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMT	4-G	407	-	-	-	X
4	GOL	5-A	405	-	-	-	X
4	CL	5-D	405	-	-	X	-
4	GOL	5-E	404	-	-	-	X
4	GOL	6-A	405	-	-	-	X
4	CL	6-B	409	-	-	X	-
4	CL	6-D	405	-	-	X	-
4	CL	6-F	408	-	-	X	-
4	GOL	7-A	405	-	-	-	X
4	GOL	7-E	404	-	-	-	X
4	CL	7-F	408	-	-	X	-
4	GOL	8-B	408	-	-	-	X
4	GOL	8-E	404	-	-	-	X
4	GOL	9-A	405	-	-	-	X
4	GOL	9-E	404	-	-	-	X
5	FMT	10-F	407	-	-	-	X
5	GOL	2-C	404	-	-	-	X
5	FMT	3-C	404	-	-	-	X
5	FMT	3-F	407	-	-	X	X
5	GOL	3-G	405	-	-	-	X
5	GOL	4-C	404	-	-	-	X
5	GOL	4-G	405	-	-	-	X
5	GOL	5-G	405	-	-	-	X
5	FMT	6-F	407	-	-	-	X
5	FMT	7-F	407	-	-	X	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 243453 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 CalE6.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	1-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	2-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	3-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	4-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	5-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	6-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	7-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	8-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	9-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	10-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	1-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	2-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	3-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	4-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	5-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	6-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	7-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	8-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	9-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	10-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	1-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	2-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	3-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	4-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	5-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	6-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	7-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	8-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	9-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	10-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	1-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	2-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	3-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	4-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	5-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	6-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	7-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	8-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	9-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	10-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	1-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	2-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	3-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	4-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	5-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	6-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	7-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	8-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	9-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	10-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	1-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	2-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	3-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	4-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	5-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	6-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	7-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	8-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	9-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	10-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	1-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	2-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	3-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	4-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	5-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	6-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	7-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	8-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	9-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	10-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	1-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	2-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	3-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	4-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	5-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	6-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	7-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	8-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	9-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			

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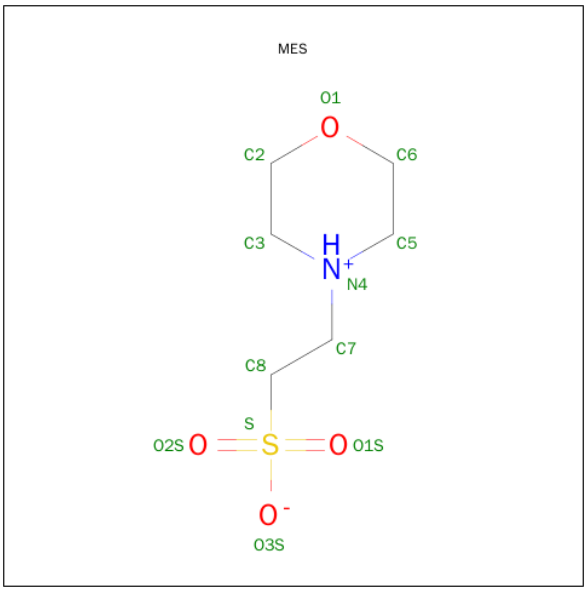
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	10-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8KNG3
A	-1	ASN	-	expression tag	UNP Q8KNG3
A	0	ALA	-	expression tag	UNP Q8KNG3
A	7	GLY	ASP	engineered mutation	UNP Q8KNG3
B	-2	SER	-	expression tag	UNP Q8KNG3
B	-1	ASN	-	expression tag	UNP Q8KNG3
B	0	ALA	-	expression tag	UNP Q8KNG3
B	7	GLY	ASP	engineered mutation	UNP Q8KNG3
C	-2	SER	-	expression tag	UNP Q8KNG3
C	-1	ASN	-	expression tag	UNP Q8KNG3
C	0	ALA	-	expression tag	UNP Q8KNG3
C	7	GLY	ASP	engineered mutation	UNP Q8KNG3
D	-2	SER	-	expression tag	UNP Q8KNG3
D	-1	ASN	-	expression tag	UNP Q8KNG3
D	0	ALA	-	expression tag	UNP Q8KNG3
D	7	GLY	ASP	engineered mutation	UNP Q8KNG3
E	-2	SER	-	expression tag	UNP Q8KNG3
E	-1	ASN	-	expression tag	UNP Q8KNG3
E	0	ALA	-	expression tag	UNP Q8KNG3
E	7	GLY	ASP	engineered mutation	UNP Q8KNG3
F	-2	SER	-	expression tag	UNP Q8KNG3
F	-1	ASN	-	expression tag	UNP Q8KNG3
F	0	ALA	-	expression tag	UNP Q8KNG3
F	7	GLY	ASP	engineered mutation	UNP Q8KNG3
G	-2	SER	-	expression tag	UNP Q8KNG3
G	-1	ASN	-	expression tag	UNP Q8KNG3
G	0	ALA	-	expression tag	UNP Q8KNG3
G	7	GLY	ASP	engineered mutation	UNP Q8KNG3
H	-2	SER	-	expression tag	UNP Q8KNG3
H	-1	ASN	-	expression tag	UNP Q8KNG3
H	0	ALA	-	expression tag	UNP Q8KNG3
H	7	GLY	ASP	engineered mutation	UNP Q8KNG3

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	2-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	4-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	5-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	6-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	7-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	8-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	9-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	10-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	2-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	4-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	6-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	8-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	10-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	5-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	6-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	7-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	8-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	2-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	4-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	5-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	8-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	10-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	2-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	4-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	5-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	6-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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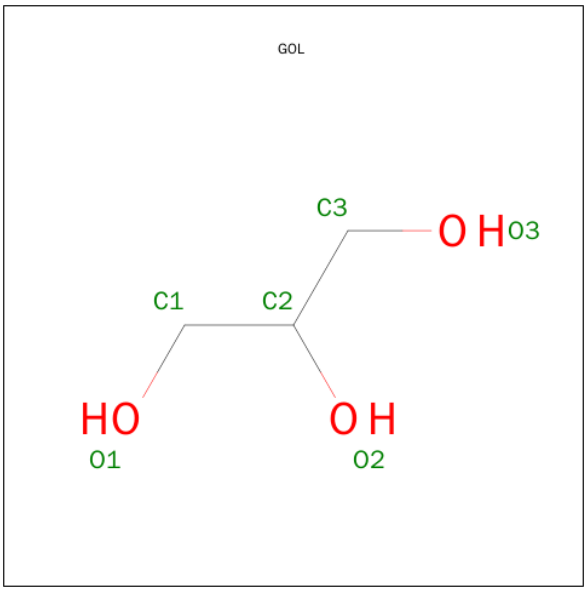
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	7-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	8-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	9-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	10-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	10-F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	2-G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	6-G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	7-G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	4-H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	7-H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL, FMT, CL) (formula: $C_3H_8O_3$, CH_2O_2, Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	1	Total C O 6 3 3	0	0
3	2-A	1	Total C O 6 3 3	0	0
3	3-A	1	Total C O 6 3 3	0	0
3	4-A	1	Total C O 6 3 3	0	0
3	5-A	1	Total C O 6 3 3	0	0
3	6-A	1	Total C O 6 3 3	0	0
3	7-A	1	Total C O 6 3 3	0	0
3	8-A	1	Total C O 6 3 3	0	0
3	9-A	1	Total C O 6 3 3	0	0
3	10-A	1	Total C O 6 3 3	0	0
3	1-A	1	Total C O 6 3 3	0	0
3	2-A	1	Total C O 6 3 3	0	0
3	3-A	1	Total C O 6 3 3	0	0
3	4-A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	5-A	1	Total	C	O	0	0
			6	3	3		
3	6-A	1	Total	C	O	0	0
			6	3	3		
3	7-A	1	Total	C	O	0	0
			6	3	3		
3	8-A	1	Total	C	O	0	0
			6	3	3		
3	9-A	1	Total	C	O	0	0
			6	3	3		
3	10-A	1	Total	C	O	0	0
			6	3	3		
3	1-A	1	Total	C	O	0	0
			6	3	3		
3	2-A	1	Total	C	O	0	0
			6	3	3		
3	3-A	1	Total	C	O	0	0
			6	3	3		
3	4-A	1	Total	C	O	0	0
			6	3	3		
3	5-A	1	Total	C	O	0	0
			6	3	3		
3	6-A	1	Total	C	O	0	0
			6	3	3		
3	7-A	1	Total	C	O	0	0
			6	3	3		
3	8-A	1	Total	C	O	0	0
			6	3	3		
3	9-A	1	Total	C	O	0	0
			6	3	3		
3	10-A	1	Total	C	O	0	0
			6	3	3		
3	1-B	1	Total	C	O	0	0
			6	3	3		
3	2-B	1	Total	C	O	0	0
			6	3	3		
3	4-B	1	Total	C	O	0	0
			6	3	3		
3	6-B	1	Total	C	O	0	0
			6	3	3		
3	8-B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	10-B	1	Total	C	O	0	0
			6	3	3		
3	1-B	1	Total	C	O	0	0
			6	3	3		
3	2-B	1	Total	C	O	0	0
			6	3	3		
3	3-B	1	Total	C	O	0	0
			6	3	3		
3	4-B	1	Total	C	O	0	0
			6	3	3		
3	5-B	1	Total	C	O	0	0
			6	3	3		
3	6-B	1	Total	C	O	0	0
			6	3	3		
3	7-B	1	Total	C	O	0	0
			6	3	3		
3	8-B	1	Total	C	O	0	0
			6	3	3		
3	9-B	1	Total	C	O	0	0
			6	3	3		
3	10-B	1	Total	C	O	0	0
			6	3	3		
3	1-B	1	Total	C	O	0	0
			6	3	3		
3	2-B	1	Total	C	O	0	0
			6	3	3		
3	3-B	1	Total	C	O	0	0
			6	3	3		
3	4-B	1	Total	C	O	0	0
			6	3	3		
3	5-B	1	Total	C	O	0	0
			6	3	3		
3	6-B	1	Total	C	O	0	0
			6	3	3		
3	7-B	1	Total	C	O	0	0
			6	3	3		
3	8-B	1	Total	C	O	0	0
			6	3	3		
3	9-B	1	Total	C	O	0	0
			6	3	3		
3	10-B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-B	1	Total C O 6 3 3	0	0
3	2-B	1	Total C O 6 3 3	0	0
3	3-B	1	Total C O 6 3 3	0	0
3	4-B	1	Total C O 6 3 3	0	0
3	5-B	1	Total C O 6 3 3	0	0
3	6-B	1	Total C O 6 3 3	0	0
3	7-B	1	Total C O 6 3 3	0	0
3	8-B	1	Total C O 6 3 3	0	0
3	9-B	1	Total C O 6 3 3	0	0
3	10-B	1	Total C O 6 3 3	0	0
3	1-B	1	Total C O 6 3 3	0	0
3	2-B	1	Total C O 6 3 3	0	0
3	3-B	1	Total C O 6 3 3	0	0
3	4-B	1	Total C O 6 3 3	0	0
3	5-B	1	Total C O 6 3 3	0	0
3	6-B	1	Total C O 6 3 3	0	0
3	7-B	1	Total C O 6 3 3	0	0
3	8-B	1	Total C O 6 3 3	0	0
3	9-B	1	Total C O 6 3 3	0	0
3	10-B	1	Total C O 6 3 3	0	0
3	1-B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	2-B	1	Total C O 6 3 3	0	0
3	3-B	1	Total C O 6 3 3	0	0
3	4-B	1	Total C O 6 3 3	0	0
3	5-B	1	Total C O 6 3 3	0	0
3	6-B	1	Total C O 6 3 3	0	0
3	7-B	1	Total C O 6 3 3	0	0
3	8-B	1	Total C O 6 3 3	0	0
3	9-B	1	Total C O 6 3 3	0	0
3	10-B	1	Total C O 6 3 3	0	0
3	1-B	1	Total C O 6 3 3	0	0
3	3-B	1	Total C O 6 3 3	0	0
3	5-B	1	Total C O 6 3 3	0	0
3	7-B	1	Total C O 6 3 3	0	0
3	8-B	1	Total C O 6 3 3	0	0
3	1-C	1	Total C O 6 3 3	0	0
3	2-C	1	Total C O 6 3 3	0	0
3	3-C	1	Total C O 6 3 3	0	0
3	4-C	1	Total C O 6 3 3	0	0
3	5-C	1	Total C O 6 3 3	0	0
3	6-C	1	Total C O 6 3 3	0	0
3	7-C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	8-C	1	Total C O 6 3 3	0	0
3	9-C	1	Total C O 6 3 3	0	0
3	10-C	1	Total C O 6 3 3	0	0
3	1-D	1	Total C O 6 3 3	0	0
3	2-D	1	Total C O 6 3 3	0	0
3	3-D	1	Total C O 6 3 3	0	0
3	4-D	1	Total C O 6 3 3	0	0
3	5-D	1	Total C O 6 3 3	0	0
3	6-D	1	Total C O 6 3 3	0	0
3	7-D	1	Total C O 6 3 3	0	0
3	8-D	1	Total C O 6 3 3	0	0
3	9-D	1	Total C O 6 3 3	0	0
3	10-D	1	Total C O 6 3 3	0	0
3	1-D	1	Total C O 6 3 3	0	0
3	2-D	1	Total C O 6 3 3	0	0
3	3-D	1	Total C O 6 3 3	0	0
3	4-D	1	Total C O 6 3 3	0	0
3	5-D	1	Total C O 6 3 3	0	0
3	6-D	1	Total C O 6 3 3	0	0
3	7-D	1	Total C O 6 3 3	0	0
3	8-D	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	9-D	1	Total	C	O	0	0
			6	3	3		
3	10-D	1	Total	C	O	0	0
			6	3	3		
3	1-D	1	Total	C	O	0	0
			6	3	3		
3	5-D	1	Total	C	O	0	0
			6	3	3		
3	10-D	1	Total	C	O	0	0
			6	3	3		
3	1-E	1	Total	C	O	0	0
			6	3	3		
3	2-E	1	Total	C	O	0	0
			6	3	3		
3	3-E	1	Total	C	O	0	0
			6	3	3		
3	4-E	1	Total	C	O	0	0
			6	3	3		
3	5-E	1	Total	C	O	0	0
			6	3	3		
3	6-E	1	Total	C	O	0	0
			6	3	3		
3	7-E	1	Total	C	O	0	0
			6	3	3		
3	8-E	1	Total	C	O	0	0
			6	3	3		
3	9-E	1	Total	C	O	0	0
			6	3	3		
3	10-E	1	Total	C	O	0	0
			6	3	3		
3	1-E	1	Total	C	O	0	0
			6	3	3		
3	2-E	1	Total	C	O	0	0
			6	3	3		
3	3-E	1	Total	C	O	0	0
			6	3	3		
3	4-E	1	Total	C	O	0	0
			6	3	3		
3	5-E	1	Total	C	O	0	0
			6	3	3		
3	6-E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	7-E	1	Total C O 6 3 3	0	0
3	8-E	1	Total C O 6 3 3	0	0
3	9-E	1	Total C O 6 3 3	0	0
3	10-E	1	Total C O 6 3 3	0	0
3	1-F	1	Total C O 6 3 3	0	0
3	10-F	1	Total C O 6 3 3	0	0
3	1-F	1	Total C O 6 3 3	0	0
3	3-F	1	Total C O 6 3 3	0	0
3	4-F	1	Total C O 6 3 3	0	0
3	6-F	1	Total C O 6 3 3	0	0
3	7-F	1	Total C O 6 3 3	0	0
3	8-F	1	Total C O 6 3 3	0	0
3	10-F	1	Total C O 6 3 3	0	0
3	1-F	1	Total C O 6 3 3	0	0
3	2-F	1	Total C O 6 3 3	0	0
3	3-F	1	Total C O 6 3 3	0	0
3	4-F	1	Total C O 6 3 3	0	0
3	5-F	1	Total C O 6 3 3	0	0
3	6-F	1	Total C O 6 3 3	0	0
3	7-F	1	Total C O 6 3 3	0	0
3	8-F	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	9-F	1	Total C O 6 3 3	0	0
3	10-F	1	Total C O 6 3 3	0	0
3	1-F	1	Total C O 6 3 3	0	0
3	2-F	1	Total C O 6 3 3	0	0
3	3-F	1	Total C O 6 3 3	0	0
3	4-F	1	Total C O 6 3 3	0	0
3	5-F	1	Total C O 6 3 3	0	0
3	6-F	1	Total C O 6 3 3	0	0
3	7-F	1	Total C O 6 3 3	0	0
3	8-F	1	Total C O 6 3 3	0	0
3	9-F	1	Total C O 6 3 3	0	0
3	10-F	1	Total C O 6 3 3	0	0
3	1-F	1	Total C O 6 3 3	0	0
3	2-F	1	Total C O 6 3 3	0	0
3	3-F	1	Total C O 6 3 3	0	0
3	5-F	1	Total C O 6 3 3	0	0
3	6-F	1	Total C O 6 3 3	0	0
3	7-F	1	Total C O 6 3 3	0	0
3	8-F	1	Total C O 6 3 3	0	0
3	9-F	1	Total C O 6 3 3	0	0
3	10-F	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-F	1	Total	C	O	0	0
			6	3	3		
3	2-F	1	Total	C	O	0	0
			6	3	3		
3	3-F	1	Total	C	O	0	0
			6	3	3		
3	6-F	1	Total	C	O	0	0
			6	3	3		
3	7-F	1	Total	C	O	0	0
			6	3	3		
3	1-G	1	Total	C	O	0	0
			6	3	3		
3	2-G	1	Total	C	O	0	0
			6	3	3		
3	3-G	1	Total	C	O	0	0
			6	3	3		
3	4-G	1	Total	C	O	0	0
			6	3	3		
3	5-G	1	Total	C	O	0	0
			6	3	3		
3	6-G	1	Total	C	O	0	0
			6	3	3		
3	7-G	1	Total	C	O	0	0
			6	3	3		
3	8-G	1	Total	C	O	0	0
			6	3	3		
3	9-G	1	Total	C	O	0	0
			6	3	3		
3	10-G	1	Total	C	O	0	0
			6	3	3		
3	1-G	1	Total	C	O	0	0
			6	3	3		
3	2-G	1	Total	C	O	0	0
			6	3	3		
3	3-G	1	Total	C	O	0	0
			6	3	3		
3	4-G	1	Total	C	O	0	0
			6	3	3		
3	5-G	1	Total	C	O	0	0
			6	3	3		
3	6-G	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	7-G	1	Total C O 6 3 3	0	0
3	8-G	1	Total C O 6 3 3	0	0
3	9-G	1	Total C O 6 3 3	0	0
3	10-G	1	Total C O 6 3 3	0	0
3	1-G	1	Total C O 6 3 3	0	0
3	2-G	1	Total C O 6 3 3	0	0
3	3-G	1	Total C O 6 3 3	0	0
3	4-G	1	Total C O 6 3 3	0	0
3	5-G	1	Total C O 6 3 3	0	0
3	7-G	1	Total C O 6 3 3	0	0
3	8-G	1	Total C O 6 3 3	0	0
3	1-G	1	Total C O 6 3 3	0	0
3	3-G	1	Total C O 6 3 3	0	0
3	1-H	1	Total C O 6 3 3	0	0
3	2-H	1	Total C O 6 3 3	0	0
3	3-H	1	Total C O 6 3 3	0	0
3	4-H	1	Total C O 6 3 3	0	0
3	5-H	1	Total C O 6 3 3	0	0
3	6-H	1	Total C O 6 3 3	0	0
3	7-H	1	Total C O 6 3 3	0	0
3	8-H	1	Total C O 6 3 3	0	0

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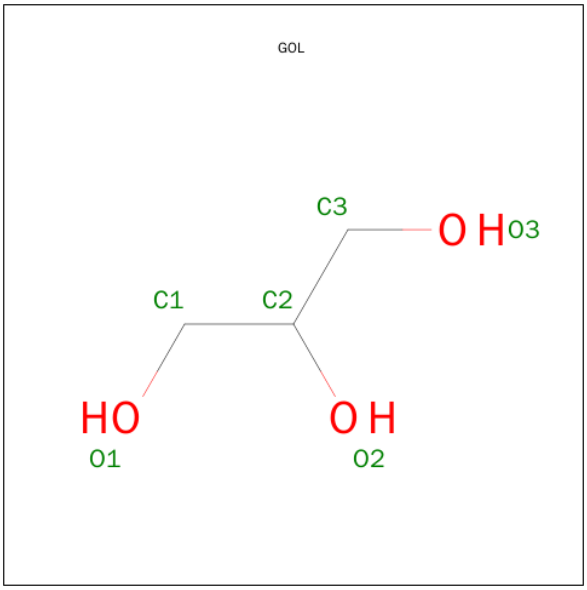
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	9-H	1	Total C O 6 3 3	0	0
3	10-H	1	Total C O 6 3 3	0	0
3	1-H	1	Total C O 6 3 3	0	0
3	2-H	1	Total C O 6 3 3	0	0
3	3-H	1	Total C O 6 3 3	0	0
3	4-H	1	Total C O 6 3 3	0	0
3	5-H	1	Total C O 6 3 3	0	0
3	6-H	1	Total C O 6 3 3	0	0
3	7-H	1	Total C O 6 3 3	0	0
3	8-H	1	Total C O 6 3 3	0	0
3	9-H	1	Total C O 6 3 3	0	0
3	10-H	1	Total C O 6 3 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: GOL, FMT, CL) (formula: $C_3H_8O_3$, CH_2O_2, Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	9-H	2	Total Cl 2 2	0	0
4	7-C	1	Total Cl 1 1	0	0
4	2-F	1	Total Cl 1 1	0	0
4	1-B	1	Total Cl 1 1	0	0
4	9-D	2	Total Cl 3 3	0	0
4	6-C	1	Total Cl 1 1	0	0
4	5-A	1	Total Cl 2 2	0	0
4	8-A	2	Total Cl 2 2	0	0
4	2-H	2	Total Cl 2 2	0	0
4	7-F	1	Total Cl 1 1	0	0
4	4-D	2	Total Cl 3 3	0	0
4	3-H	2	Total Cl 2 2	0	0
4	4-H	1	Total Cl 1 1	0	0
4	1-D	2	Total Cl 2 2	0	0
4	7-B	1	Total Cl 1 1	0	0
4	4-A	2	Total Cl 2 2	0	0
4	3-C	1	Total Cl 1 1	0	0
4	7-H	1	Total Cl 1 1	0	0
4	2-C	1	Total Cl 1 1	0	0
4	1-A	2	Total Cl 2 2	0	0
4	9-C	1	Total Cl 1 1	0	0
4	5-D	2	Total Cl 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	8-B	1	Total Cl 1 1	0	0
4	7-A	1	Total Cl 2 2	0	0
4	10-C	2	Total Cl 2 2	0	0
4	6-D	2	Total Cl 3 3	0	0
4	3-B	1	Total Cl 1 1	0	0
4	1-G	1	Total Cl 1 1	0	0
4	5-C	2	Total Cl 2 2	0	0
4	3-G	1	Total Cl 1 1	0	0
4	4-G	1	Total Cl 2 2	0	0
4	7-D	2	Total Cl 3 3	0	0
4	2-D	2	Total Cl 3 3	0	0
4	3-F	1	Total Cl 1 1	0	0
4	10-D	2	Total Cl 2 2	0	0
4	6-A	1	Total Cl 1 1	0	0
4	8-C	1	Total Cl 1 1	0	0
4	6-H	2	Total Cl 2 2	0	0
4	8-H	2	Total Cl 2 2	0	0
4	3-A	1	Total Cl 2 2	0	0
4	5-B	1	Total Cl 1 1	0	0
4	1-H	2	Total Cl 2 2	0	0
4	8-D	2	Total Cl 3 3	0	0

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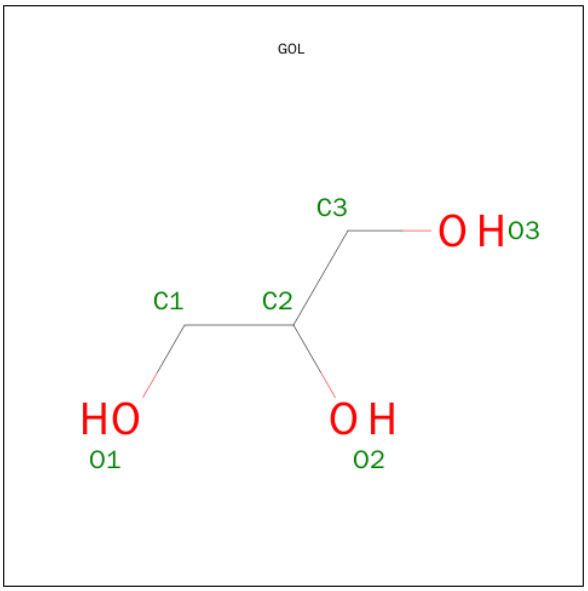
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-E	1	Total Cl 1 1	0	0
4	4-C	1	Total Cl 1 1	0	0
4	1-C	2	Total Cl 2 2	0	0
4	10-E	1	Total Cl 1 1	0	0
4	6-B	1	Total Cl 2 2	0	0
4	3-D	2	Total Cl 3 3	0	0
4	10-H	2	Total Cl 2 2	0	0
4	7-G	1	Total Cl 2 2	0	0
4	2-A	2	Total Cl 2 2	0	0
4	5-H	2	Total Cl 2 2	0	0
4	10-A	2	Total Cl 2 2	0	0
4	9-A	1	Total Cl 2 2	0	0
4	6-F	1	Total Cl 1 1	0	0
4	1-F	1	Total Cl 1 1	0	0

- Molecule 5 is FORMIC ACID (three-letter code: GOL, FMT, CL) (formula: $C_3H_8O_3$, CH_2O_2, Cl).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	1-C	1	Total	C	O		0	0
			3	1	2			
5	5-C	1	Total	C	O		0	0
			3	1	2			
5	6-C	1	Total	C	O		0	0
			3	1	2			
5	7-C	1	Total	C	O		0	0
			3	1	2			
5	9-C	1	Total	C	O		0	0
			3	1	2			
5	10-C	1	Total	C	O		0	0
			3	1	2			
5	1-F	1	Total	C	O		0	0
			3	1	2			
5	2-F	1	Total	C	O		0	0
			3	1	2			
5	3-F	1	Total	C	O		0	0
			3	1	2			
5	6-F	1	Total	C	O		0	0
			3	1	2			
5	7-F	1	Total	C	O		0	0
			3	1	2			
5	1-G	1	Total	C	O		0	0
			3	1	2			
5	3-G	1	Total	C	O		0	0
			3	1	2			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1-A	180	Total O 180 180	0	0
6	2-A	190	Total O 190 190	0	0
6	3-A	183	Total O 183 183	0	0
6	4-A	184	Total O 184 184	0	0
6	5-A	197	Total O 197 197	0	0
6	6-A	179	Total O 179 179	0	0
6	7-A	192	Total O 192 192	0	0
6	8-A	183	Total O 183 183	0	0
6	9-A	188	Total O 188 188	0	0
6	10-A	173	Total O 173 173	0	0
6	1-B	198	Total O 198 198	0	0
6	2-B	189	Total O 189 189	0	0
6	3-B	183	Total O 183 183	0	0
6	4-B	189	Total O 189 189	0	0
6	5-B	189	Total O 189 189	0	0
6	6-B	195	Total O 195 195	0	0
6	7-B	196	Total O 196 196	0	0
6	8-B	185	Total O 185 185	0	0
6	9-B	198	Total O 198 198	0	0
6	10-B	195	Total O 195 195	0	0
6	1-C	178	Total O 178 178	0	0
6	2-C	178	Total O 178 178	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	3-C	181	Total O 181 181	0	0
6	4-C	176	Total O 176 176	0	0
6	5-C	178	Total O 178 178	0	0
6	6-C	174	Total O 174 174	0	0
6	7-C	196	Total O 196 196	0	0
6	8-C	183	Total O 183 183	0	0
6	9-C	178	Total O 178 178	0	0
6	10-C	188	Total O 188 188	0	0
6	1-D	183	Total O 183 183	0	0
6	2-D	159	Total O 159 159	0	0
6	3-D	188	Total O 188 188	0	0
6	4-D	179	Total O 179 179	0	0
6	5-D	179	Total O 179 179	0	0
6	6-D	161	Total O 161 161	0	0
6	7-D	177	Total O 177 177	0	0
6	8-D	179	Total O 179 179	0	0
6	9-D	179	Total O 179 179	0	0
6	10-D	177	Total O 177 177	0	0
6	1-E	178	Total O 178 178	0	0
6	2-E	177	Total O 177 177	0	0
6	3-E	196	Total O 196 196	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	4-E	197	Total O 197 197	0	0
6	5-E	173	Total O 173 173	0	0
6	6-E	191	Total O 191 191	0	0
6	7-E	180	Total O 180 180	0	0
6	8-E	194	Total O 194 194	0	0
6	9-E	181	Total O 181 181	0	0
6	10-E	182	Total O 182 182	0	0
6	1-F	178	Total O 178 178	0	0
6	2-F	175	Total O 175 175	0	0
6	3-F	159	Total O 159 159	0	0
6	4-F	177	Total O 177 177	0	0
6	5-F	166	Total O 166 166	0	0
6	6-F	189	Total O 189 189	0	0
6	7-F	179	Total O 179 179	0	0
6	8-F	162	Total O 162 162	0	0
6	9-F	176	Total O 176 176	0	0
6	10-F	167	Total O 167 167	0	0
6	1-G	186	Total O 186 186	0	0
6	2-G	175	Total O 175 175	0	0
6	3-G	183	Total O 183 183	0	0
6	4-G	185	Total O 185 185	0	0

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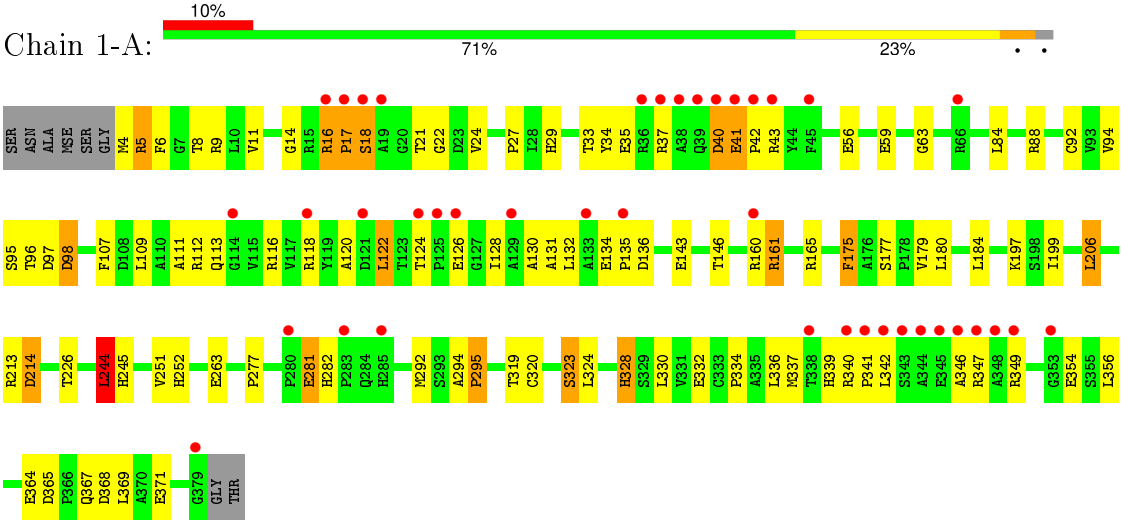
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	5-G	172	Total O 172 172	0	0
6	6-G	176	Total O 176 176	0	0
6	7-G	187	Total O 187 187	0	0
6	8-G	179	Total O 179 179	0	0
6	9-G	197	Total O 197 197	0	0
6	10-G	182	Total O 182 182	0	0
6	1-H	172	Total O 172 172	0	0
6	2-H	185	Total O 185 185	0	0
6	3-H	163	Total O 163 163	0	0
6	4-H	184	Total O 184 184	0	0
6	5-H	183	Total O 183 183	0	0
6	6-H	184	Total O 184 184	0	0
6	7-H	183	Total O 183 183	0	0
6	8-H	191	Total O 191 191	0	0
6	9-H	168	Total O 168 168	0	0
6	10-H	194	Total O 194 194	0	0

3 Residue-property plots (i)

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

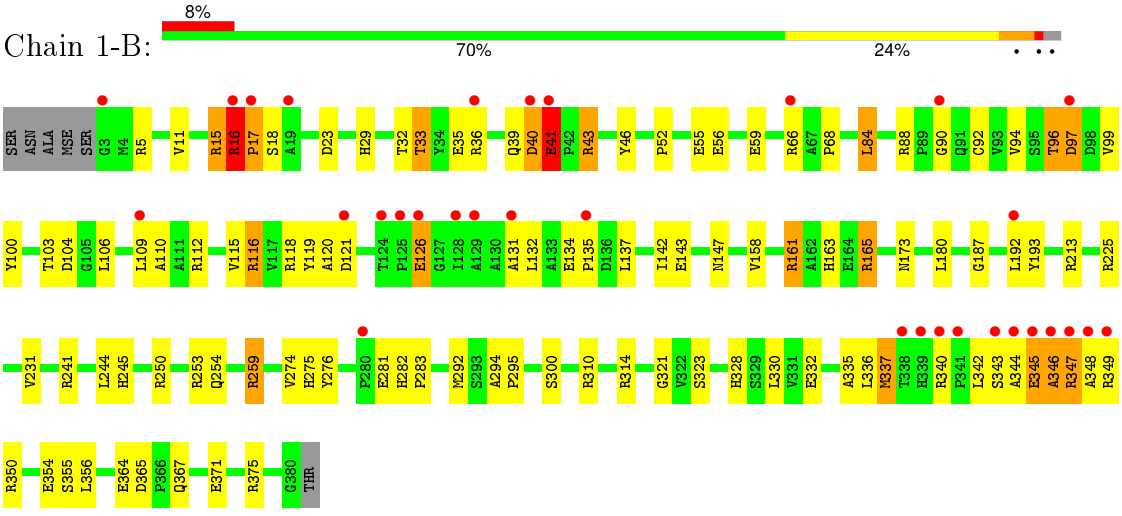
- Molecule 1: CalE6

Chain 1-A:



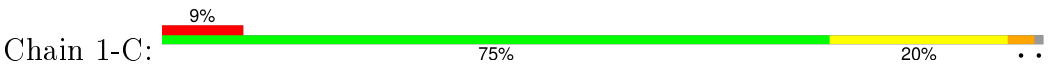
- Molecule 1: CalE6

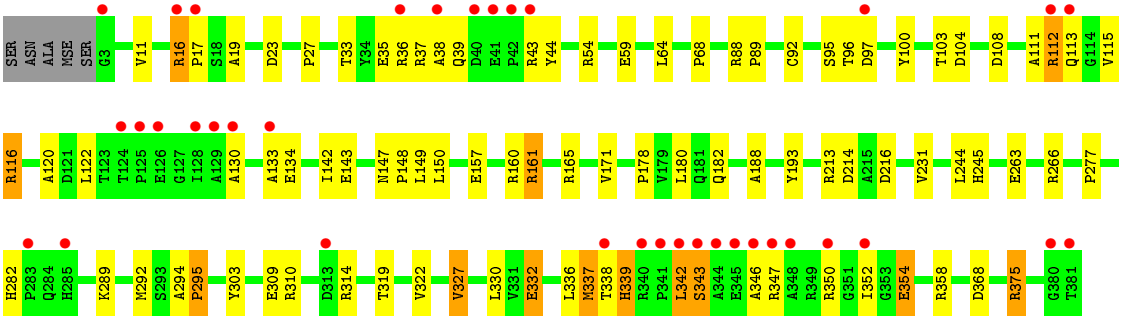
Chain 1-B:



- Molecule 1: CalE6

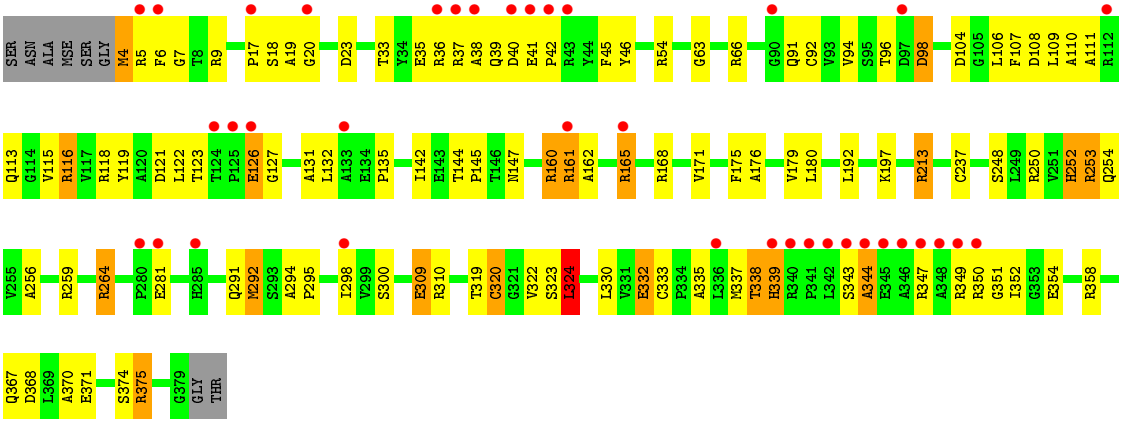
Chain 1-C:





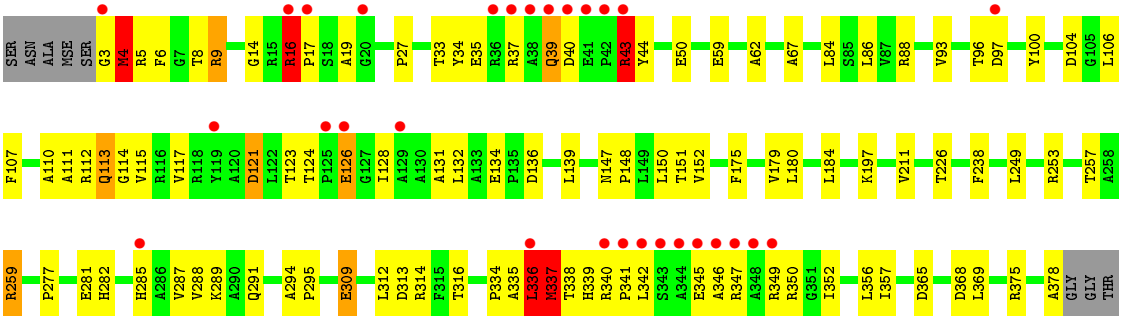
• Molecule 1: CalE6

Chain 1-D:



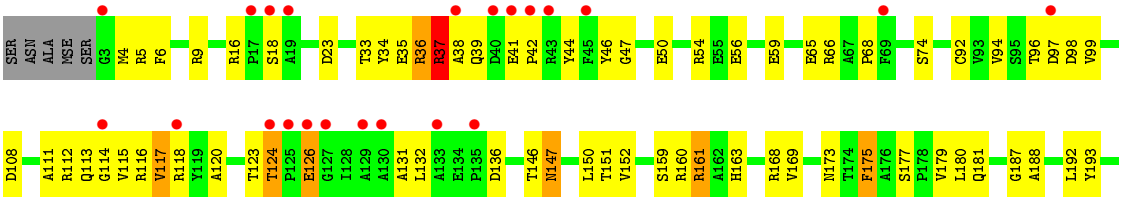
• Molecule 1: CalE6

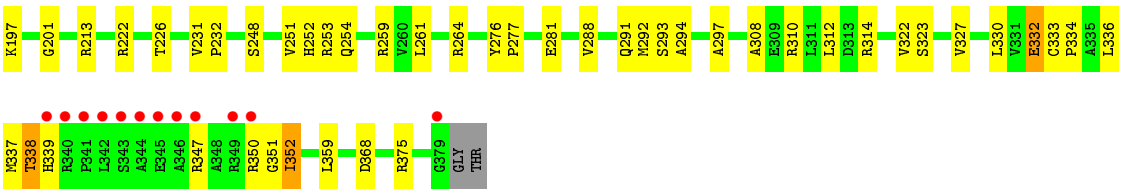
Chain 1-E:



• Molecule 1: CalE6

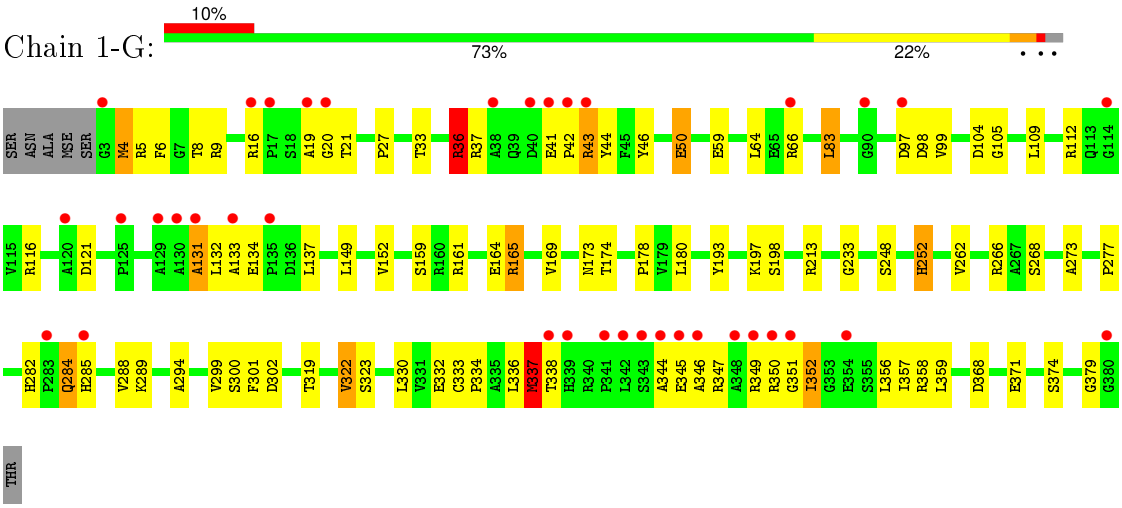
Chain 1-F:





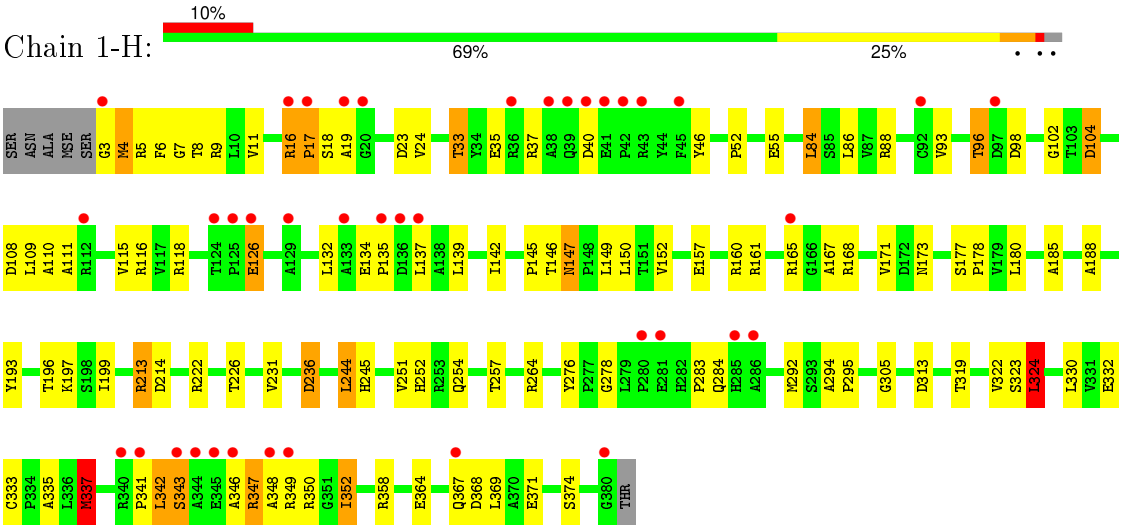
• Molecule 1: CalE6

Chain 1-G:



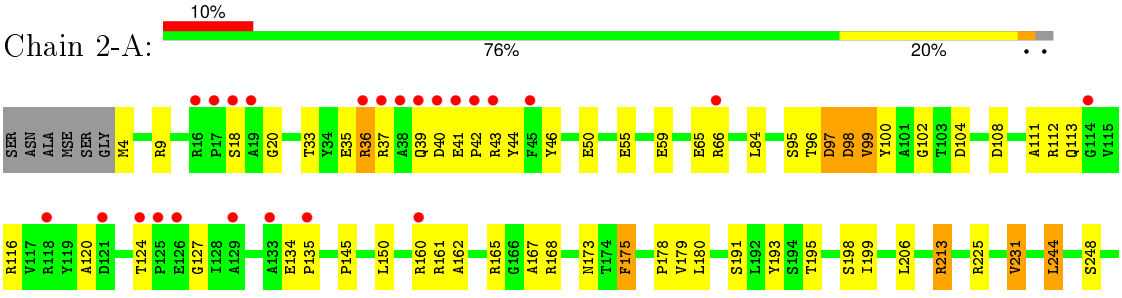
• Molecule 1: CalE6

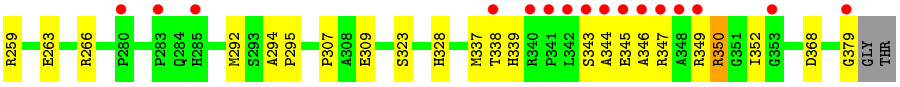
Chain 1-H:



• Molecule 1: CalE6

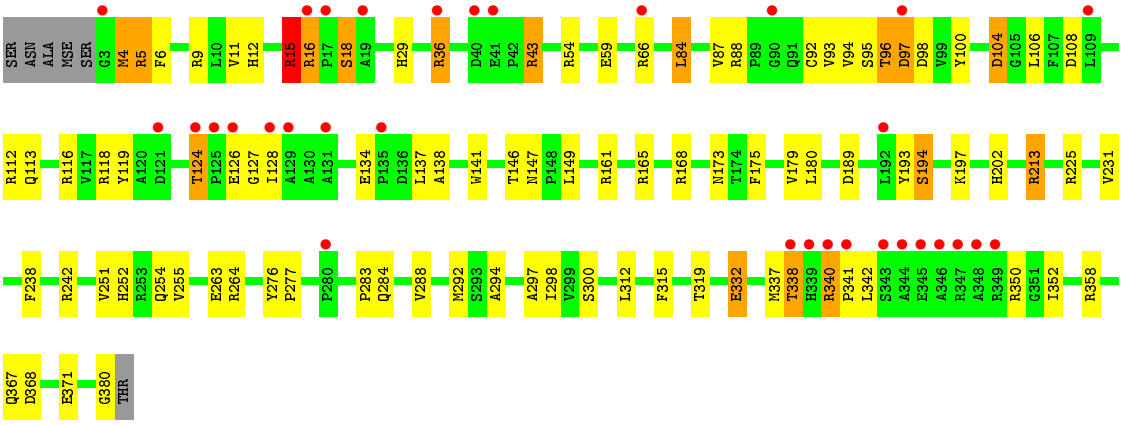
Chain 2-A:





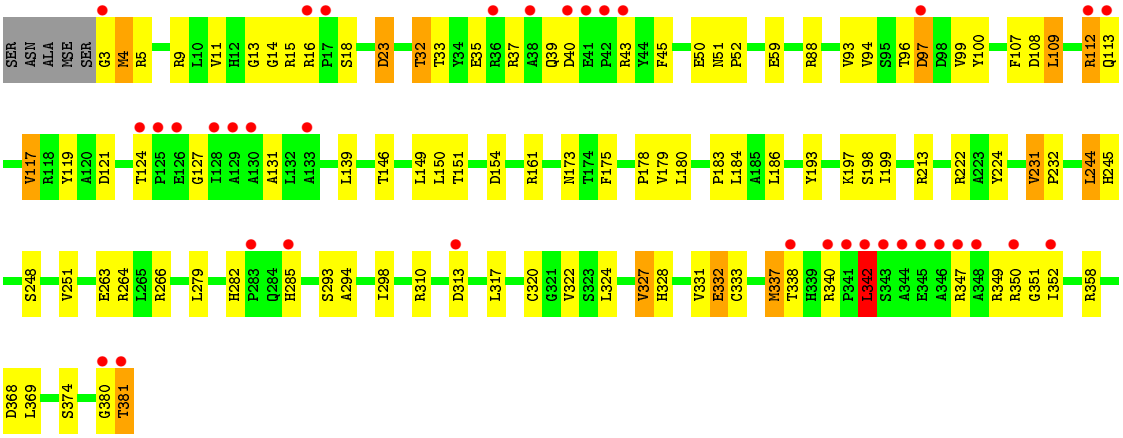
- Molecule 1: CalE6

Chain 2-B:



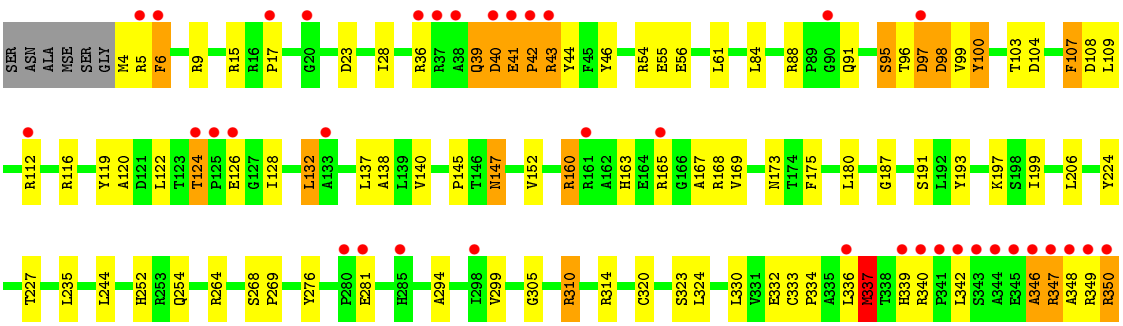
- Molecule 1: CalE6

Chain 2-C:



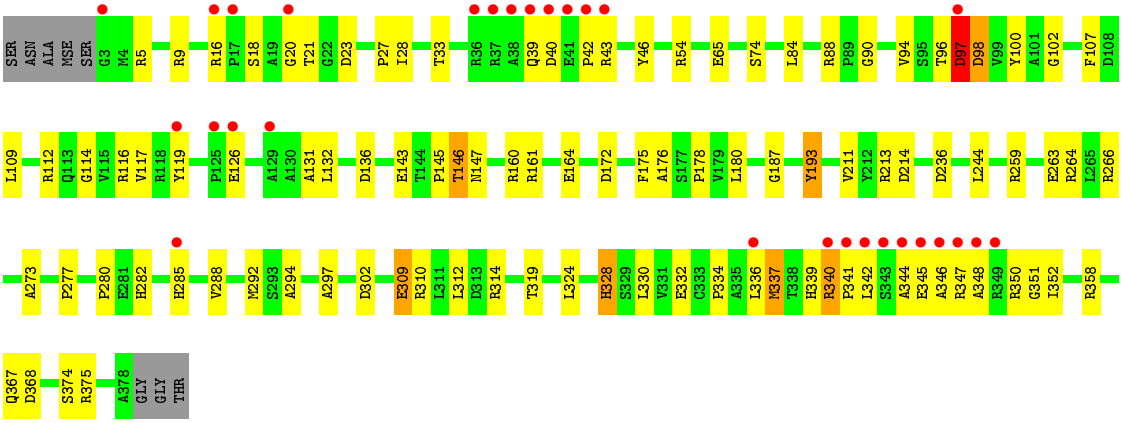
- Molecule 1: CalE6

Chain 2-D:



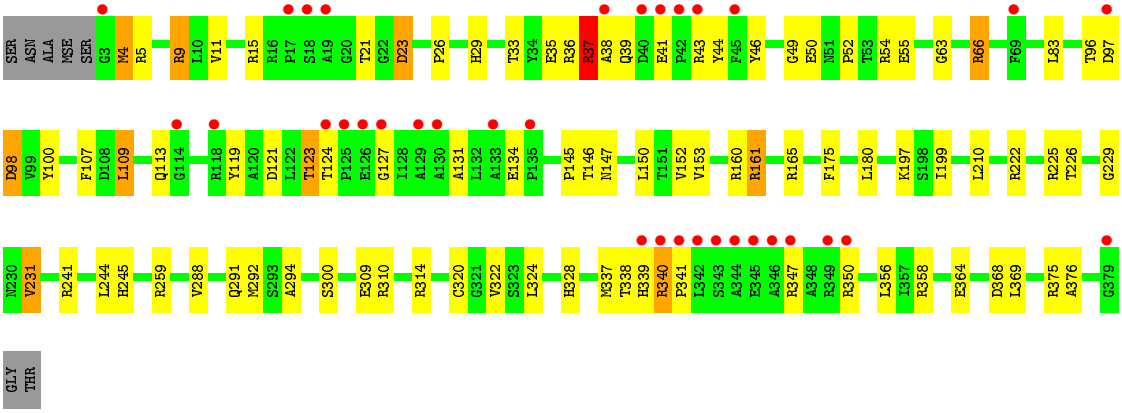
• Molecule 1: CalE6

Chain 2-E:



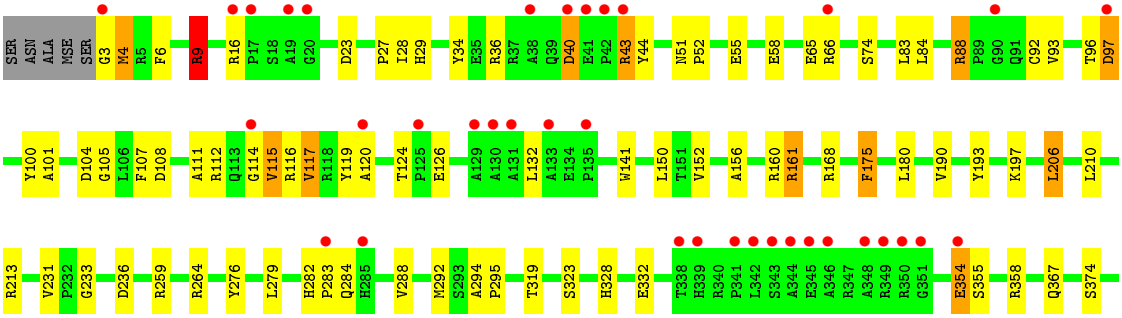
• Molecule 1: CalE6

Chain 2-F:



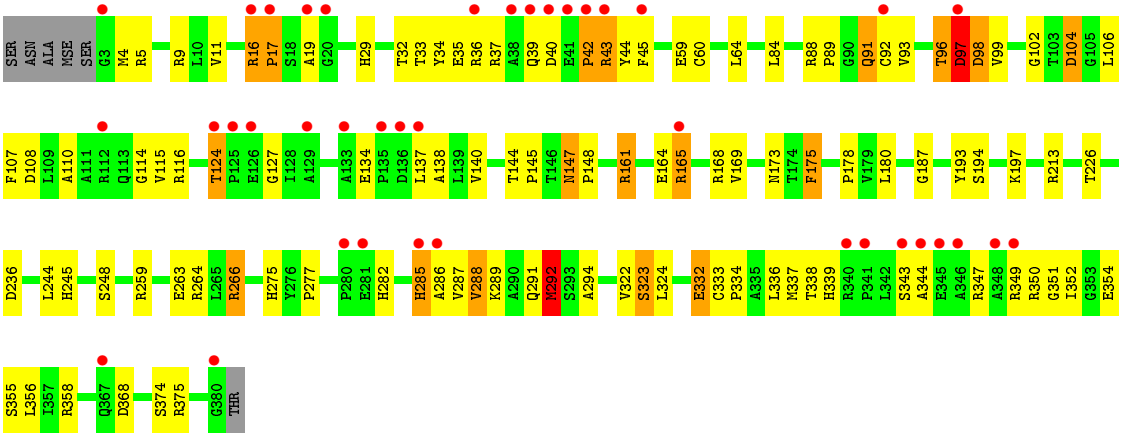
• Molecule 1: CalE6

Chain 2-G:



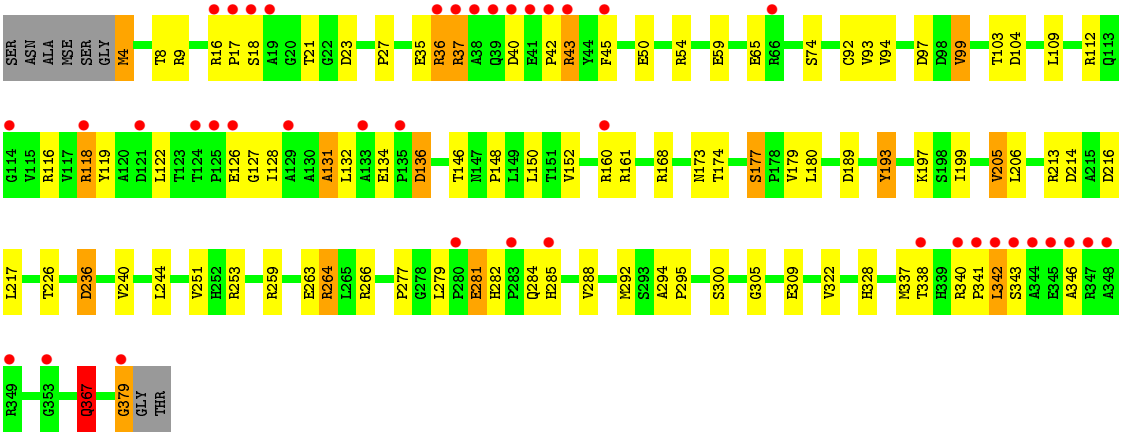
• Molecule 1: CalE6

Chain 2-H:



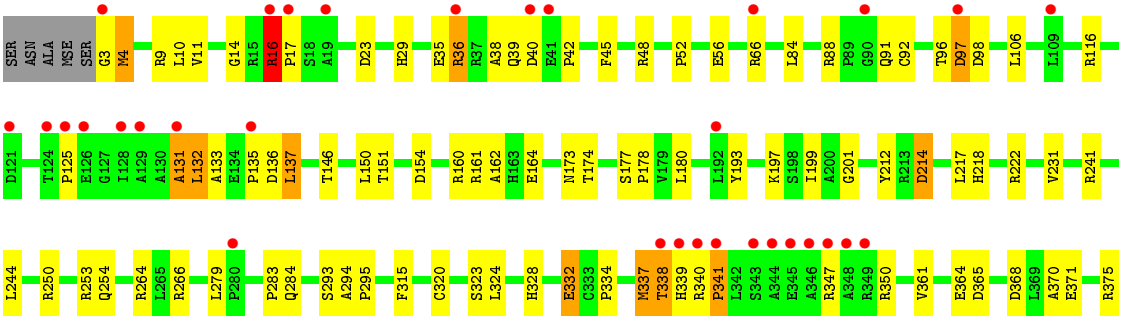
• Molecule 1: CalE6

Chain 3-A:



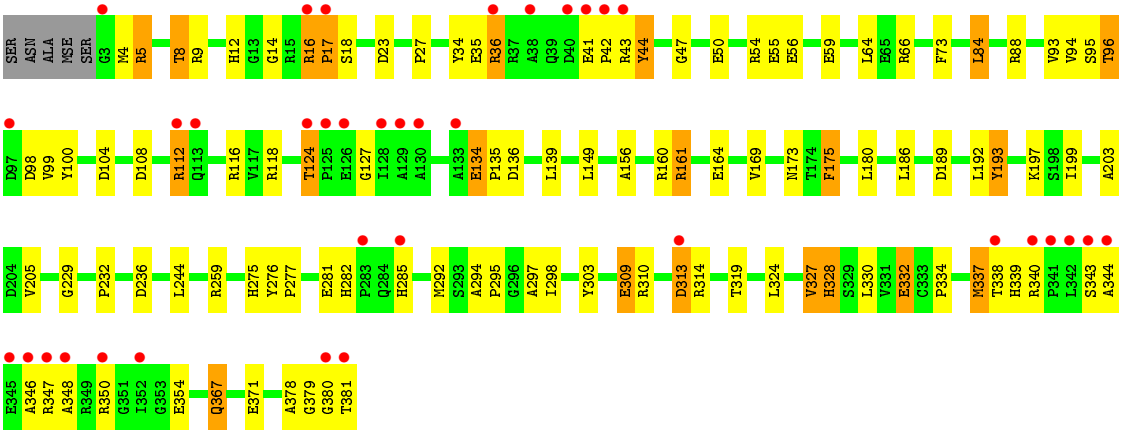
• Molecule 1: CalE6

Chain 3-B:



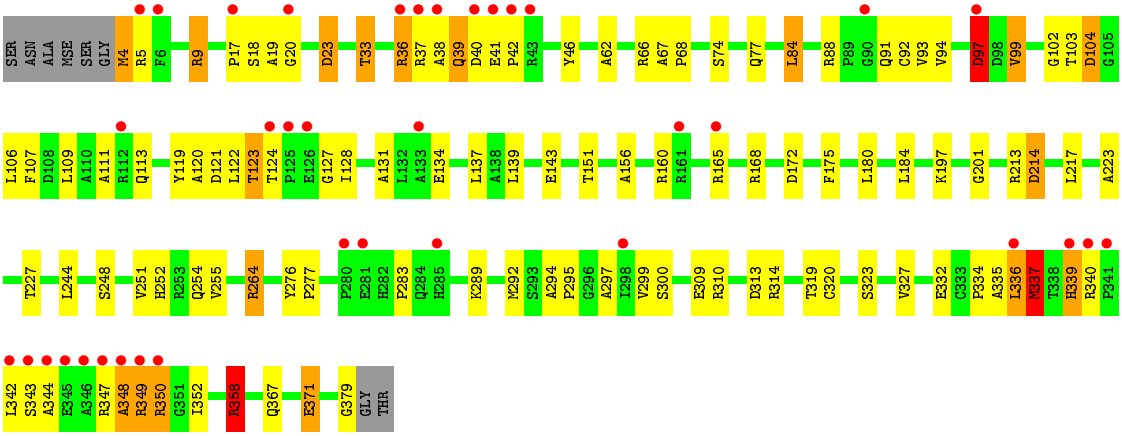
- Molecule 1: CalE6

Chain 3-C:



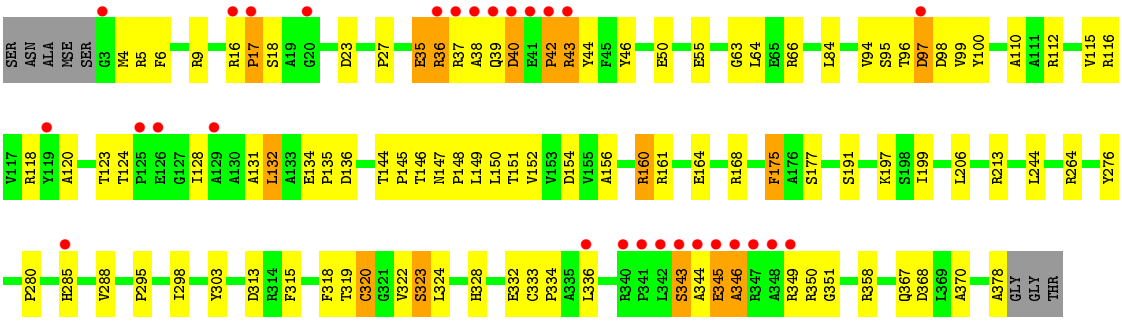
- Molecule 1: CalE6

Chain 3-D:



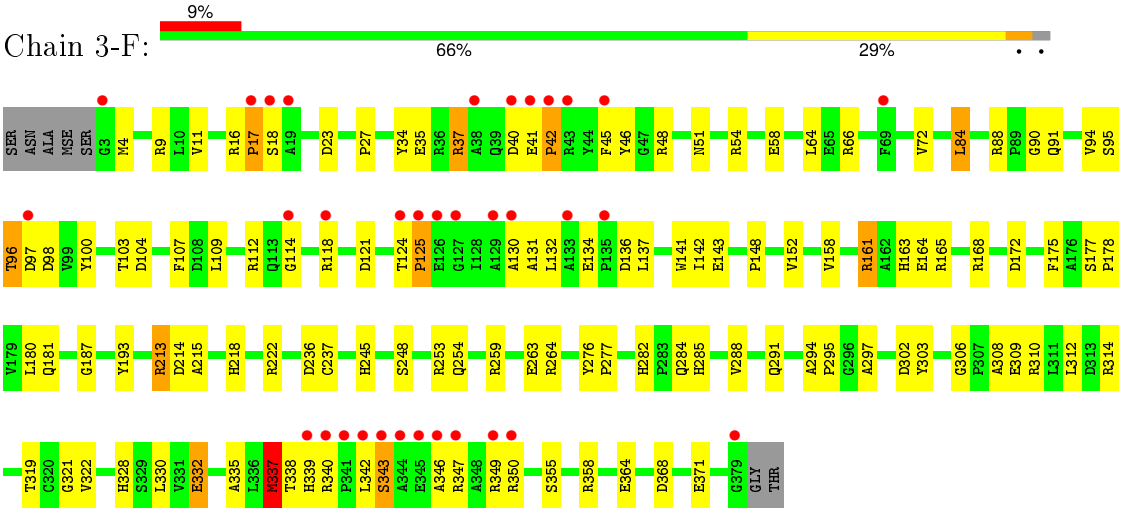
- Molecule 1: CalE6

Chain 3-E:



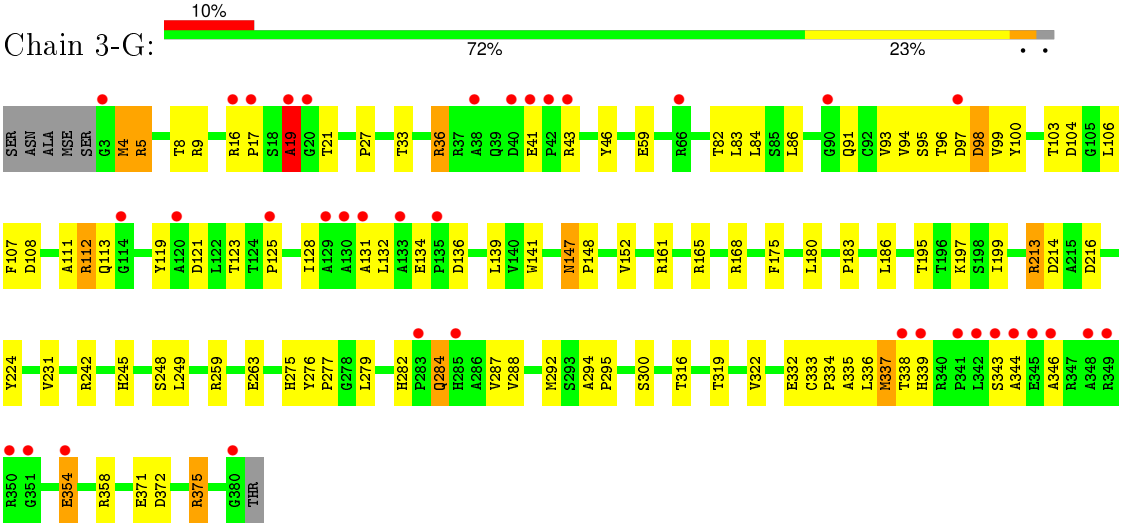
• Molecule 1: CalE6

Chain 3-F:



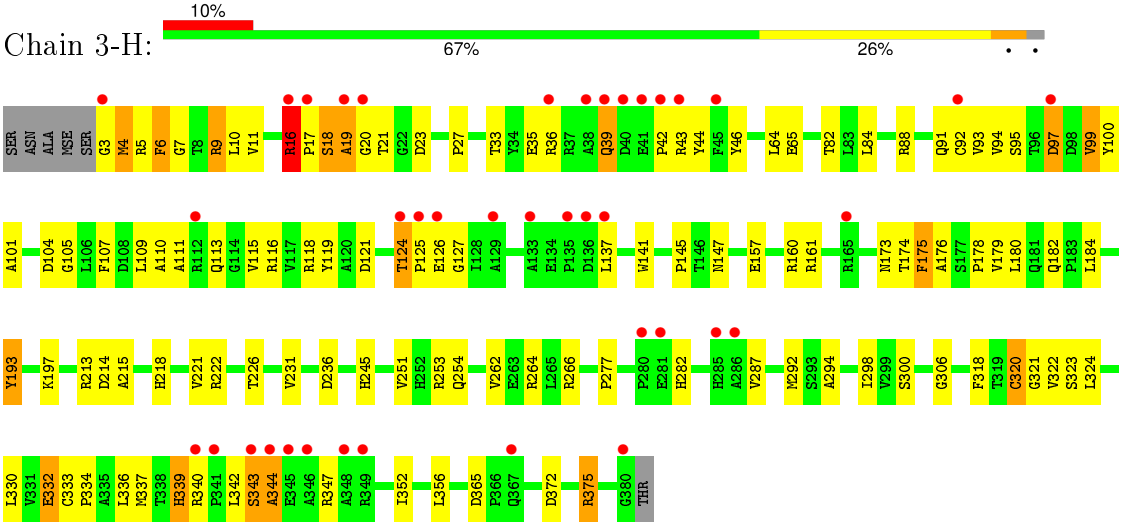
• Molecule 1: CalE6

Chain 3-G:



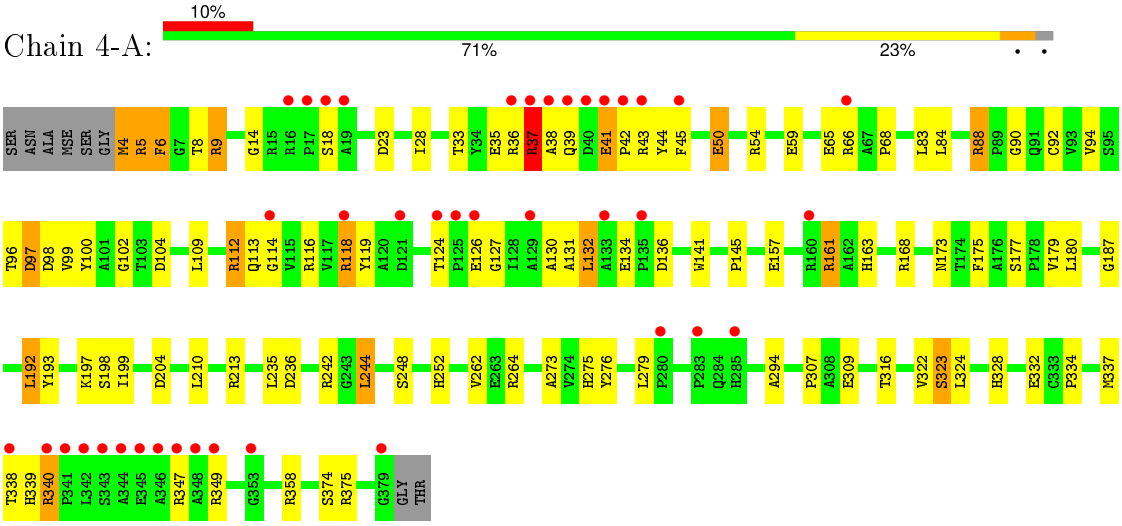
• Molecule 1: CalE6

Chain 3-H:



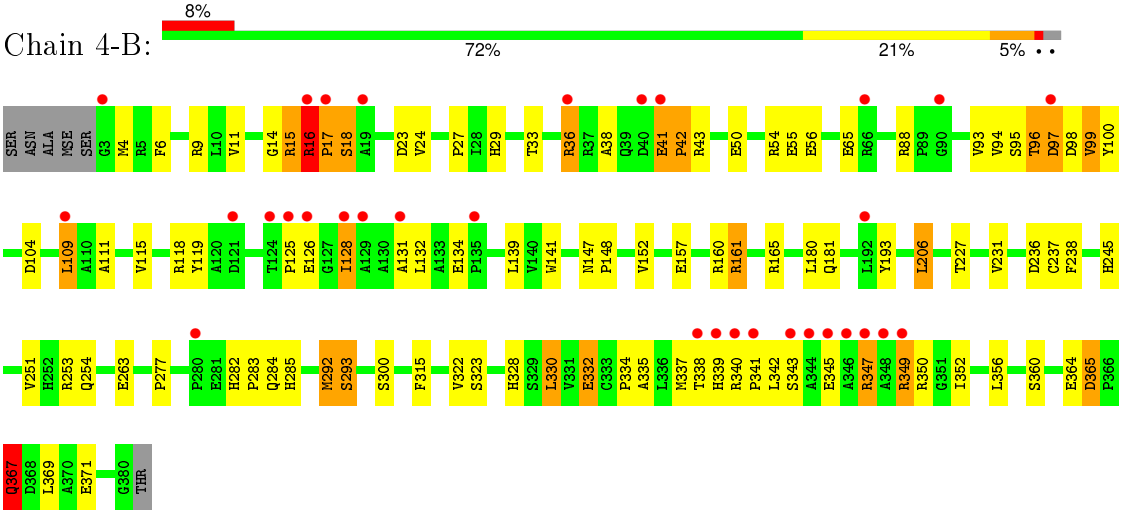
- Molecule 1: CalE6

Chain 4-A:



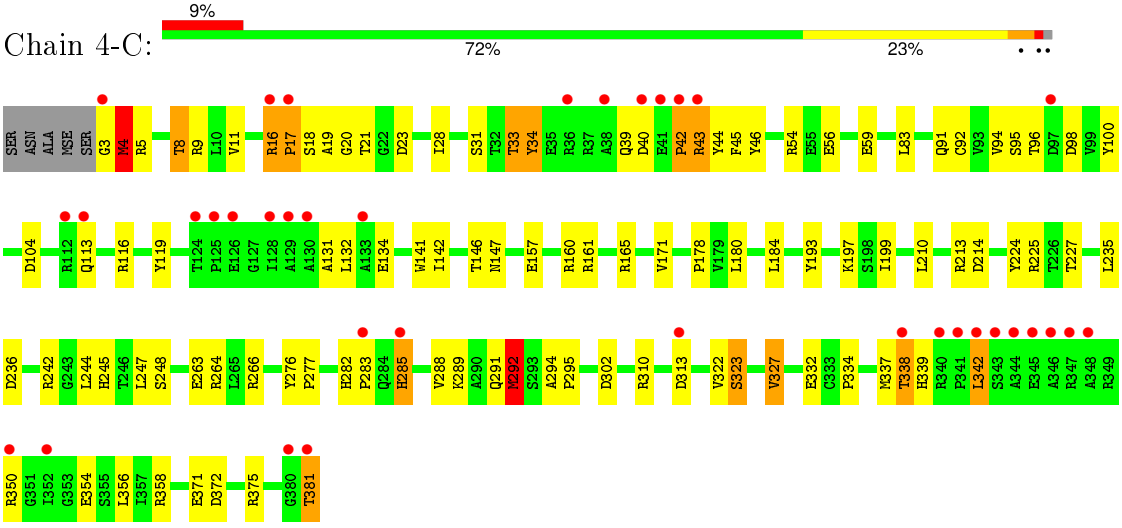
- Molecule 1: CalE6

Chain 4-B:



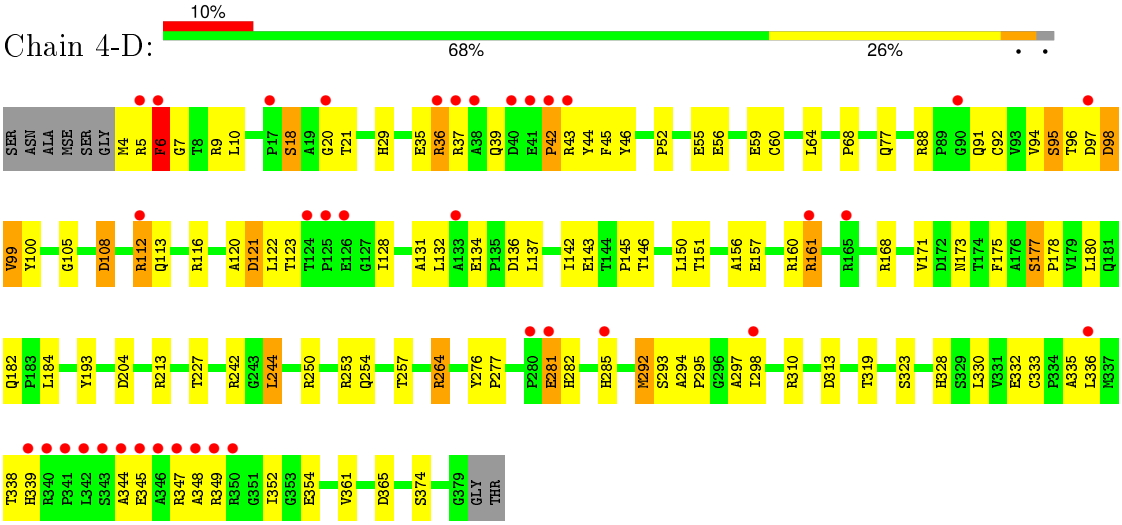
- Molecule 1: CalE6

Chain 4-C:



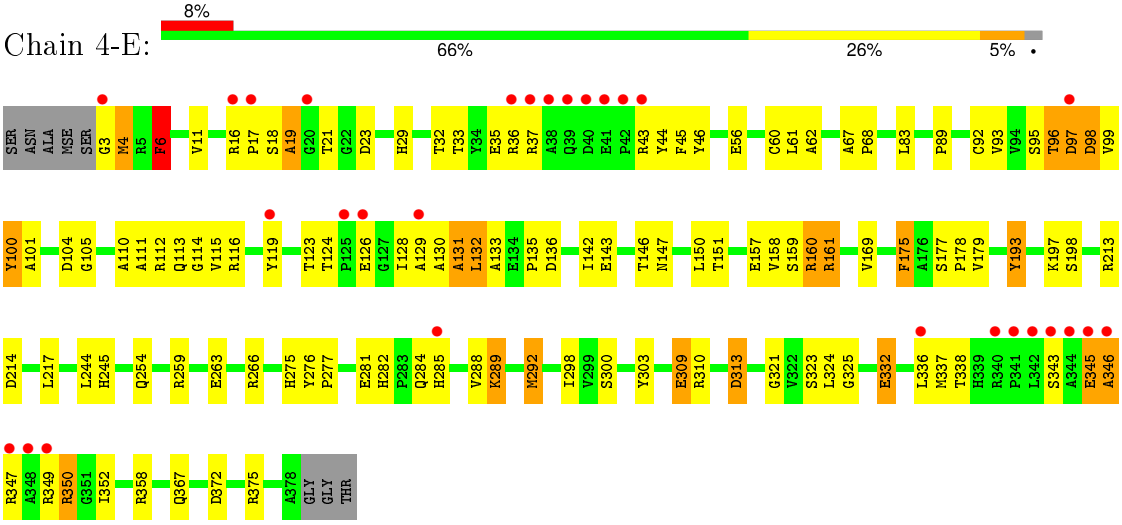
- Molecule 1: CalE6

Chain 4-D:



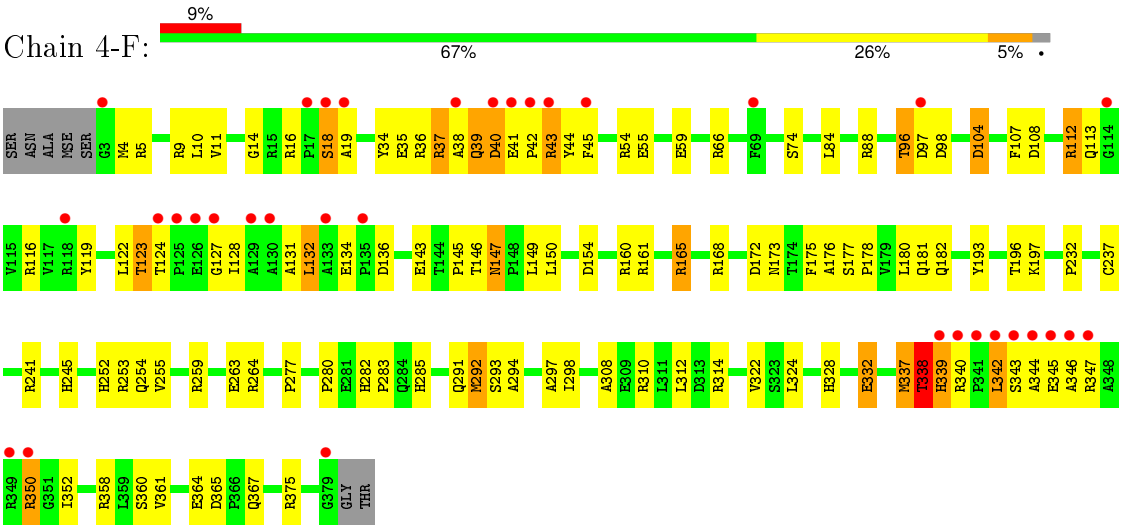
- Molecule 1: CalE6

Chain 4-E:



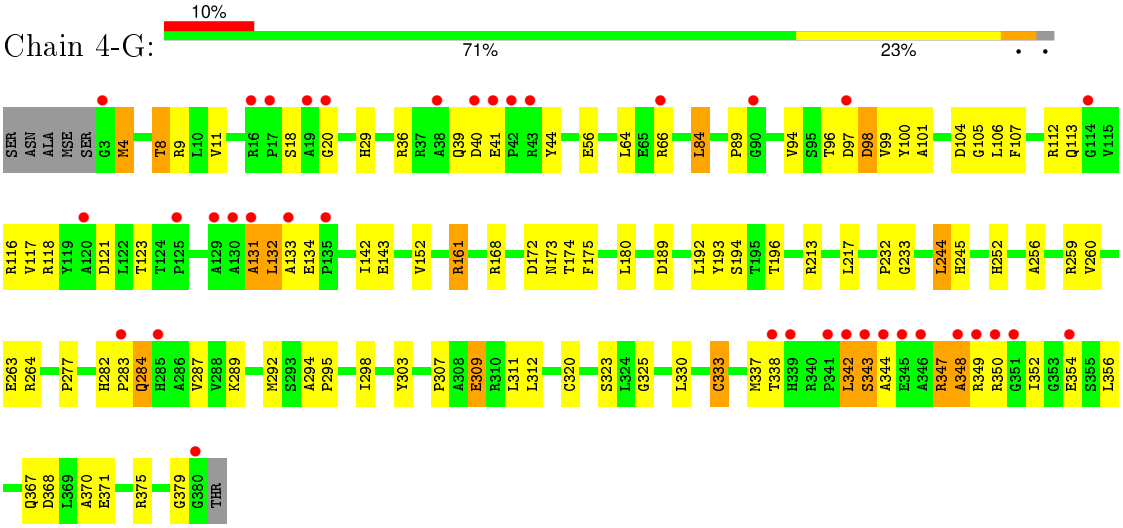
- Molecule 1: CalE6

Chain 4-F:



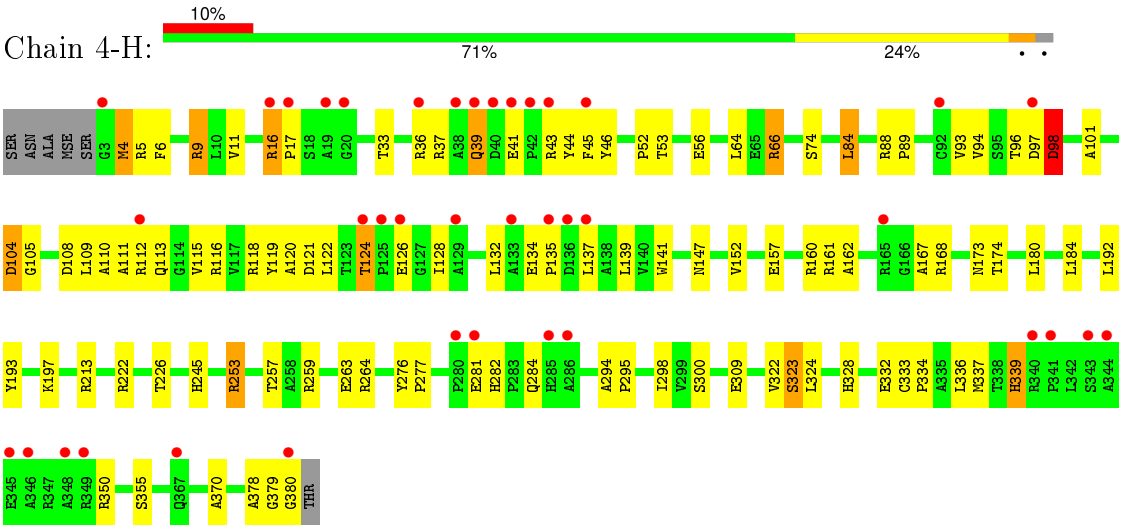
- Molecule 1: CalE6

Chain 4-G:



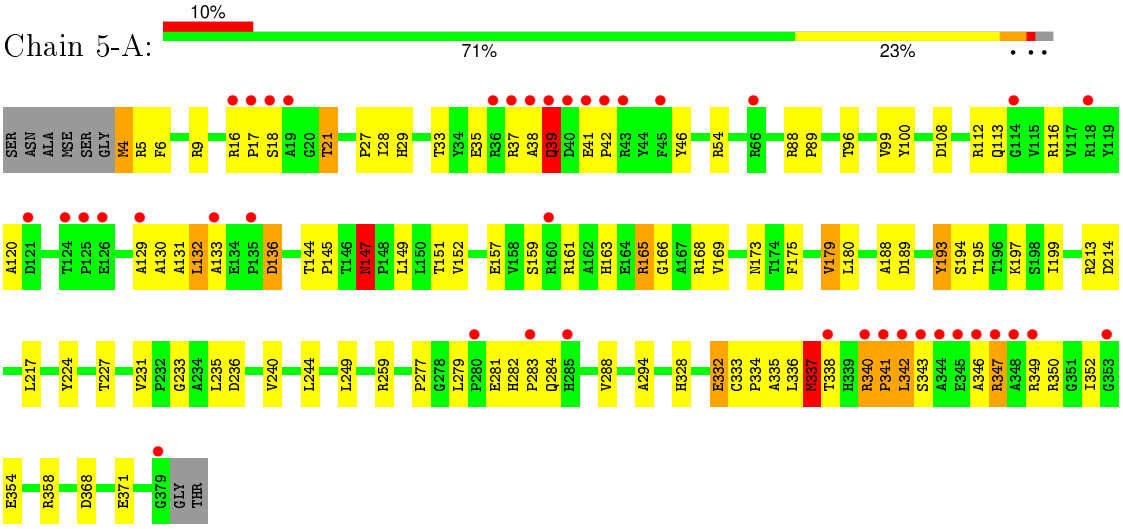
- Molecule 1: CalE6

Chain 4-H:



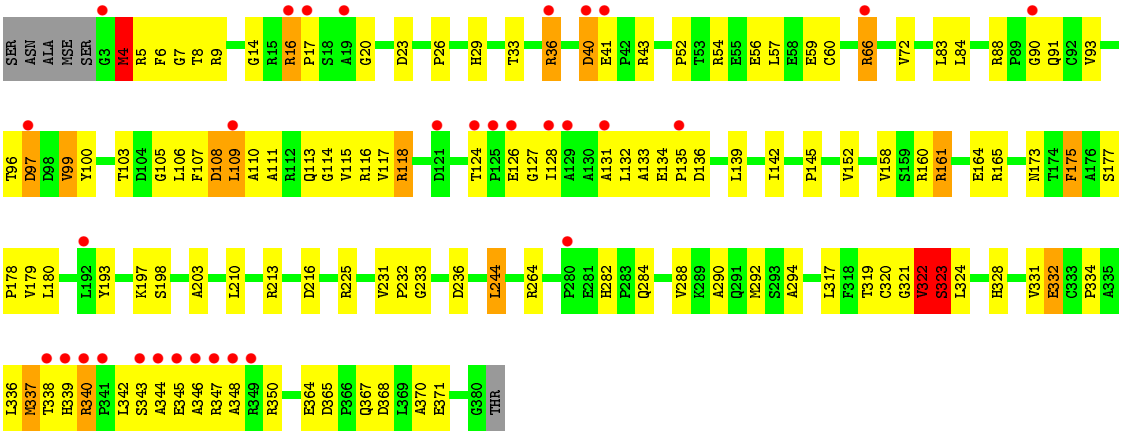
- Molecule 1: CalE6

Chain 5-A:



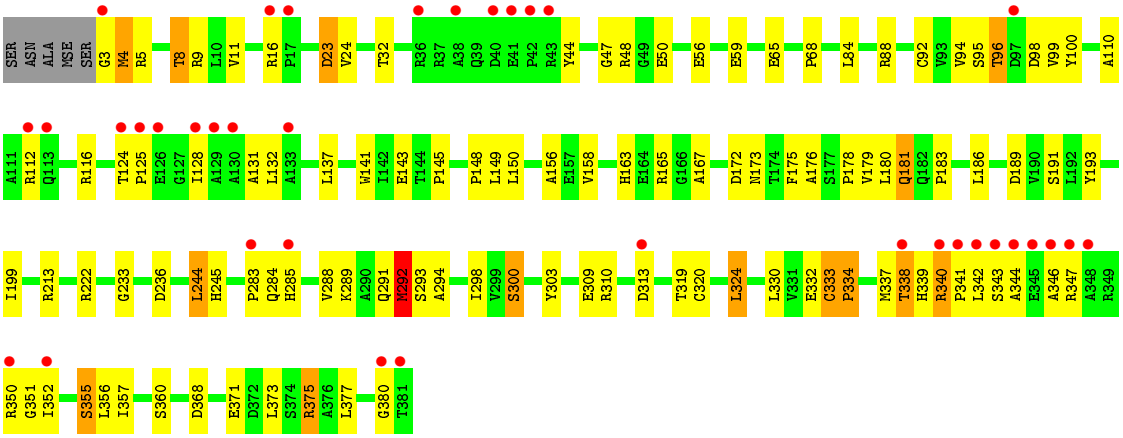
• Molecule 1: CalE6

Chain 5-B:



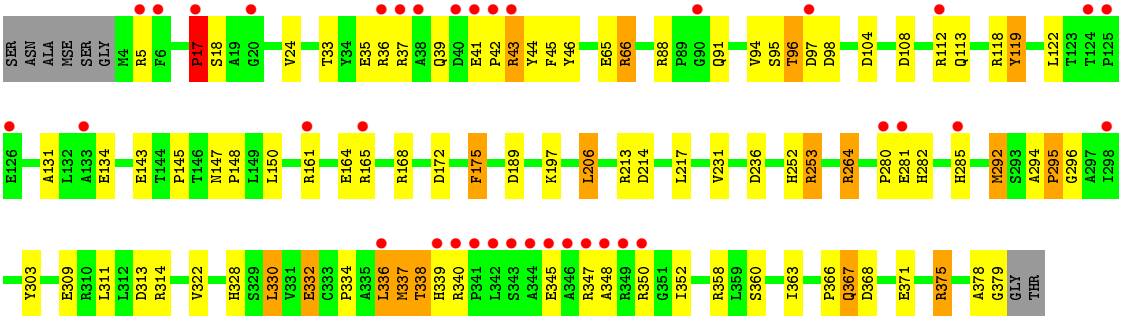
• Molecule 1: CalE6

Chain 5-C:



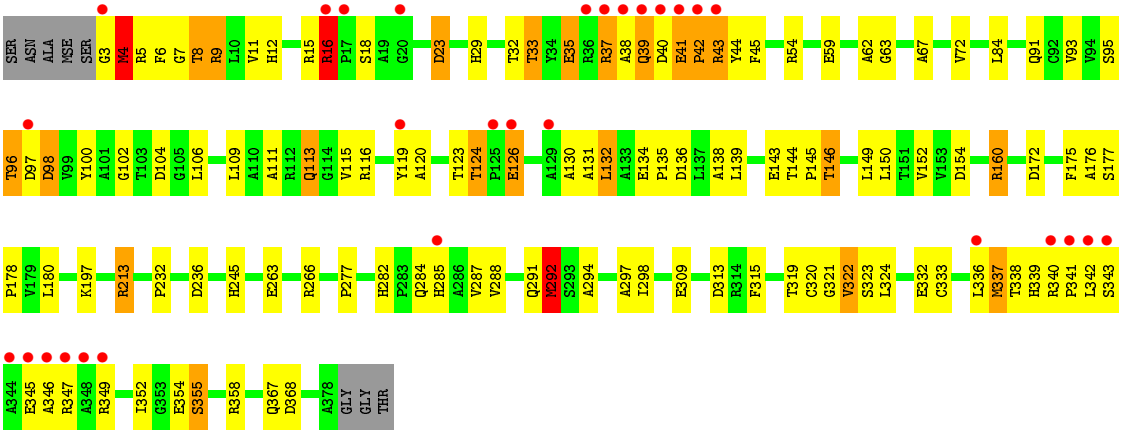
• Molecule 1: CalE6

Chain 5-D:



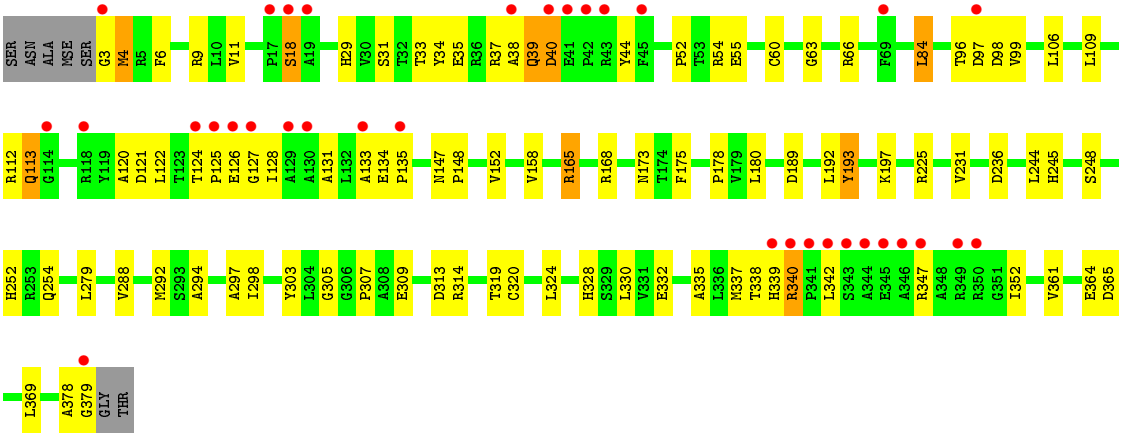
• Molecule 1: CalE6

Chain 5-E:



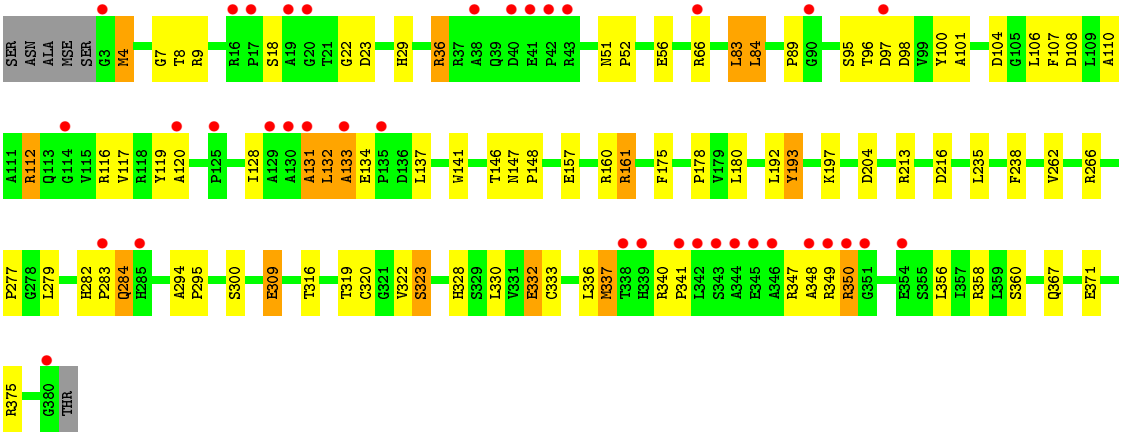
• Molecule 1: CalE6

Chain 5-F:



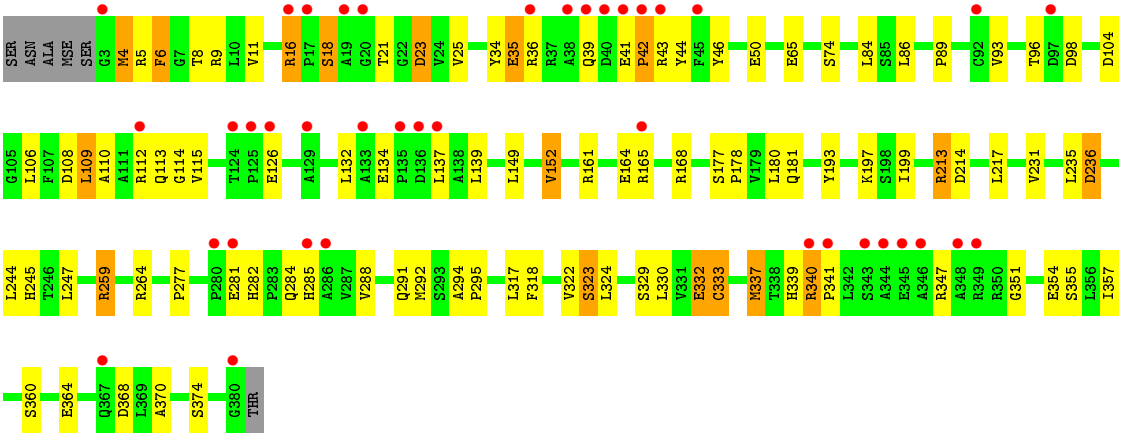
• Molecule 1: CalE6

Chain 5-G:



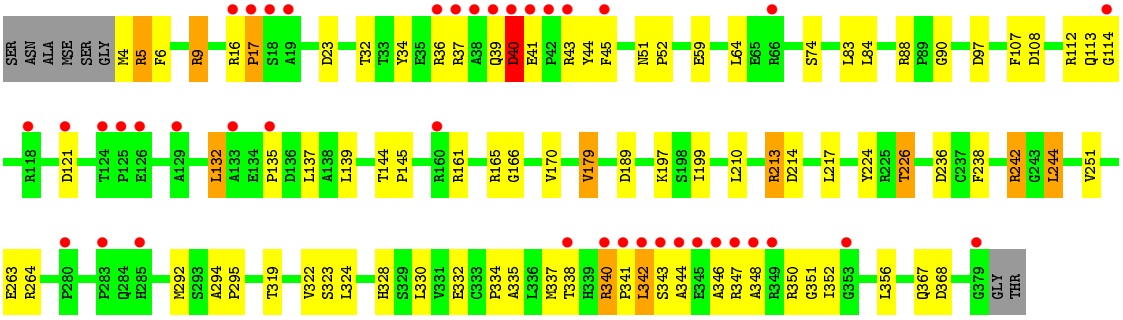
• Molecule 1: CalE6

Chain 5-H:



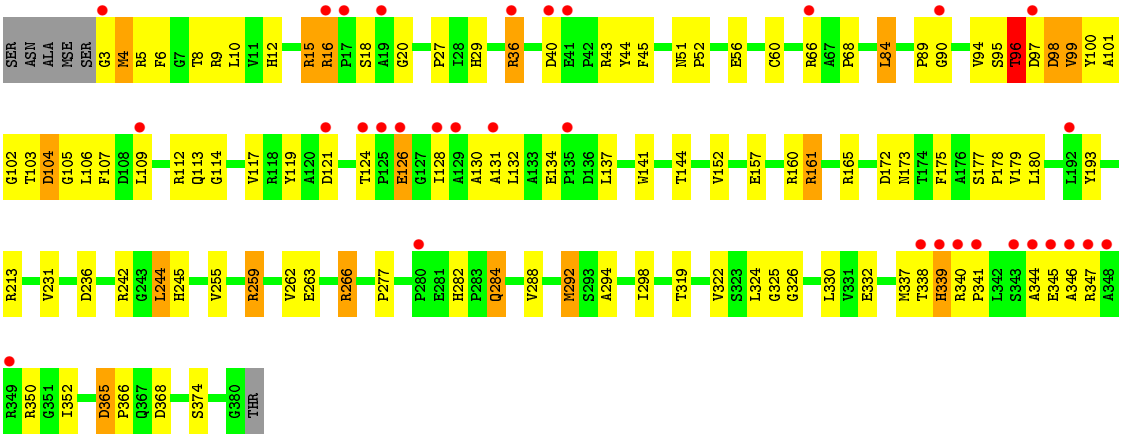
• Molecule 1: CalE6

Chain 6-A:



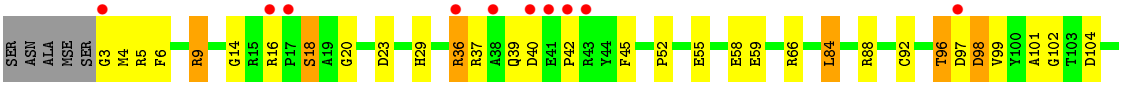
• Molecule 1: CalE6

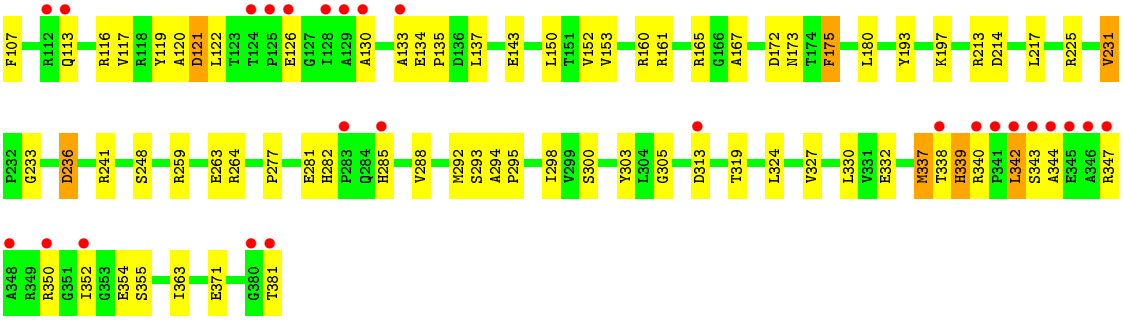
Chain 6-B:



• Molecule 1: CalE6

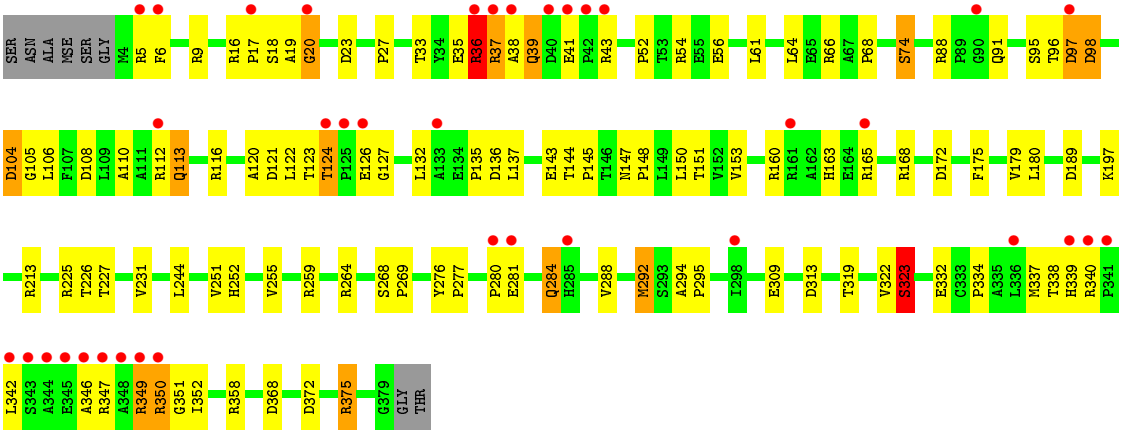
Chain 6-C:





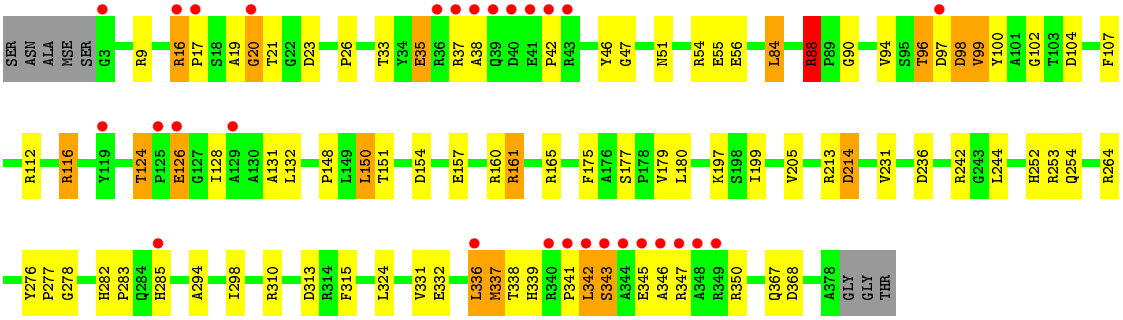
• Molecule 1: CalE6

Chain 6-D:



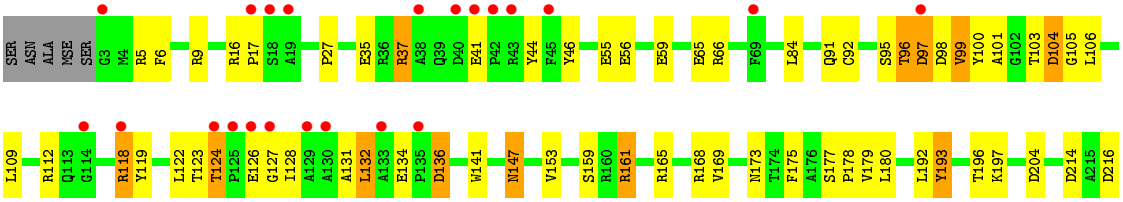
• Molecule 1: CalE6

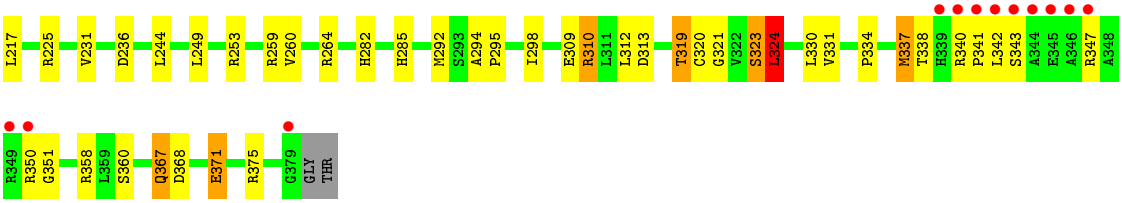
Chain 6-E:



• Molecule 1: CalE6

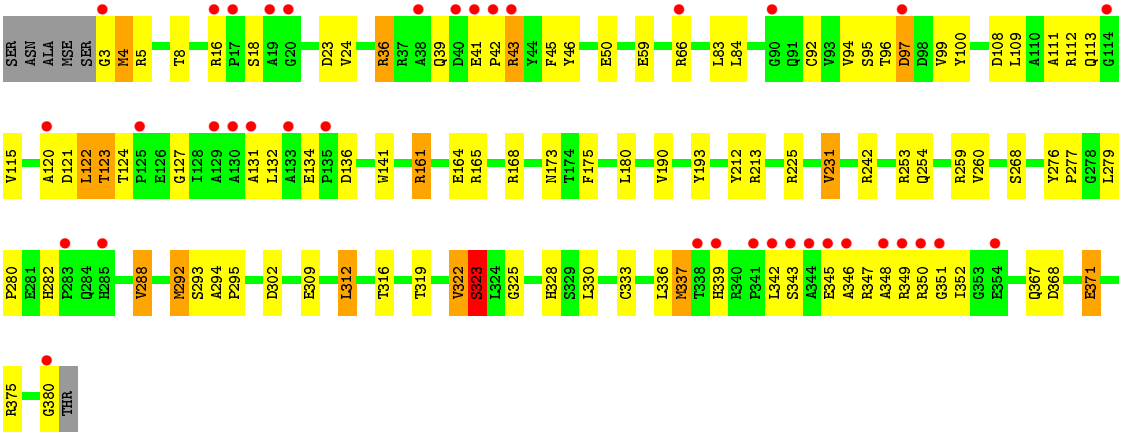
Chain 6-F:





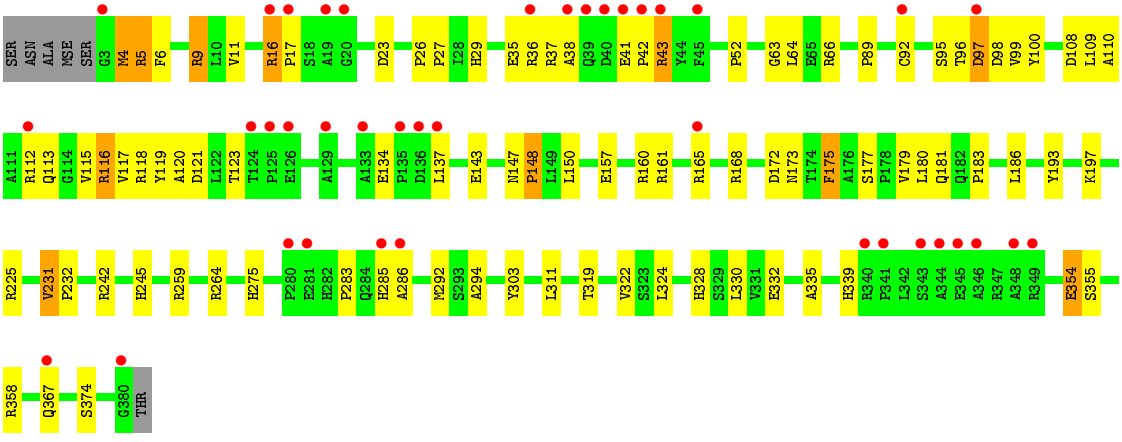
• Molecule 1: CalE6

Chain 6-G:



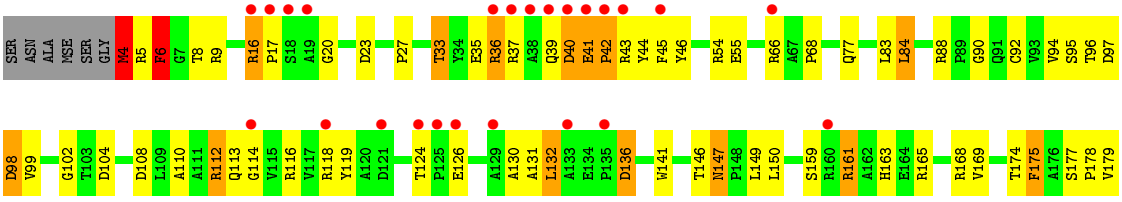
• Molecule 1: CalE6

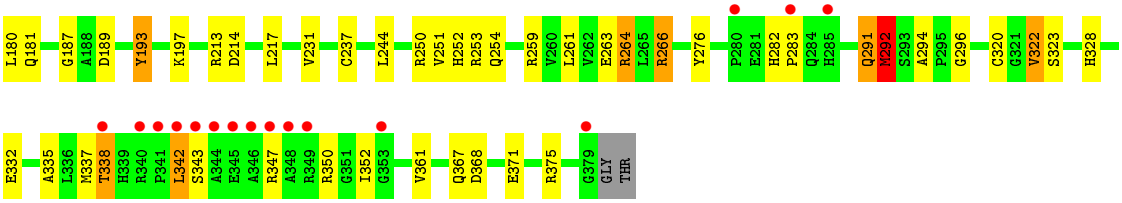
Chain 6-H:



• Molecule 1: CalE6

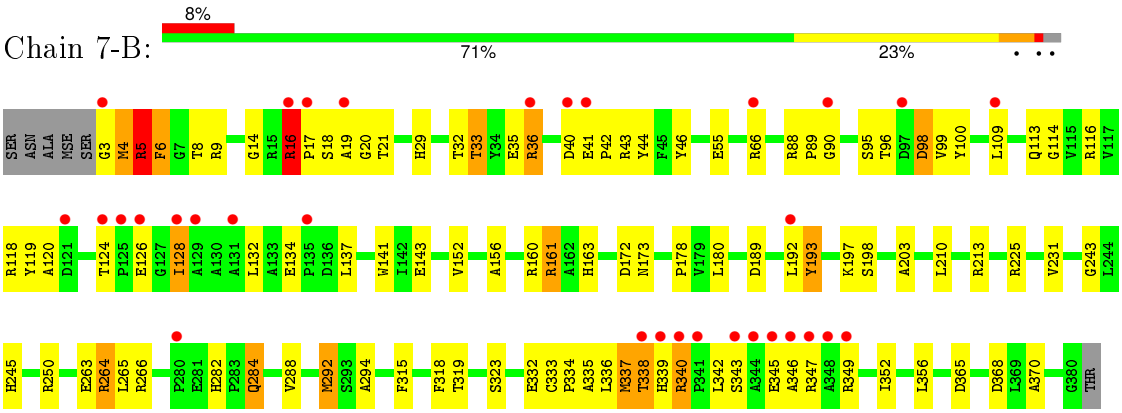
Chain 7-A:





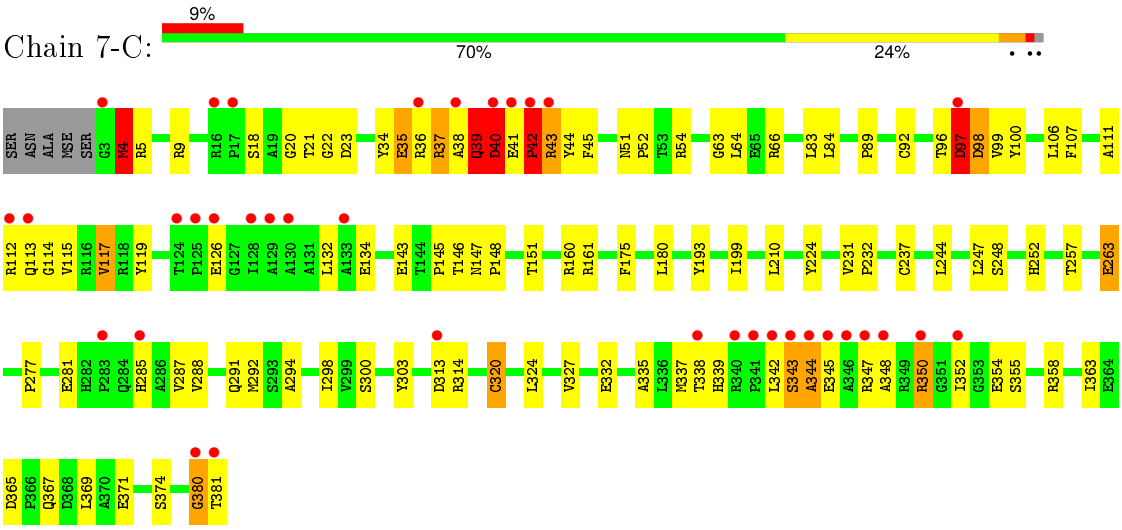
• Molecule 1: CalE6

Chain 7-B:



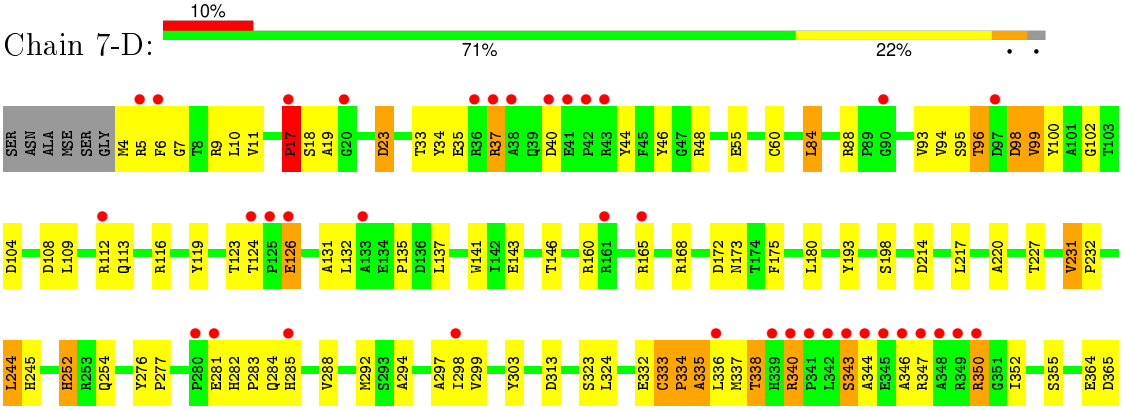
• Molecule 1: CalE6

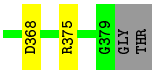
Chain 7-C:



• Molecule 1: CalE6

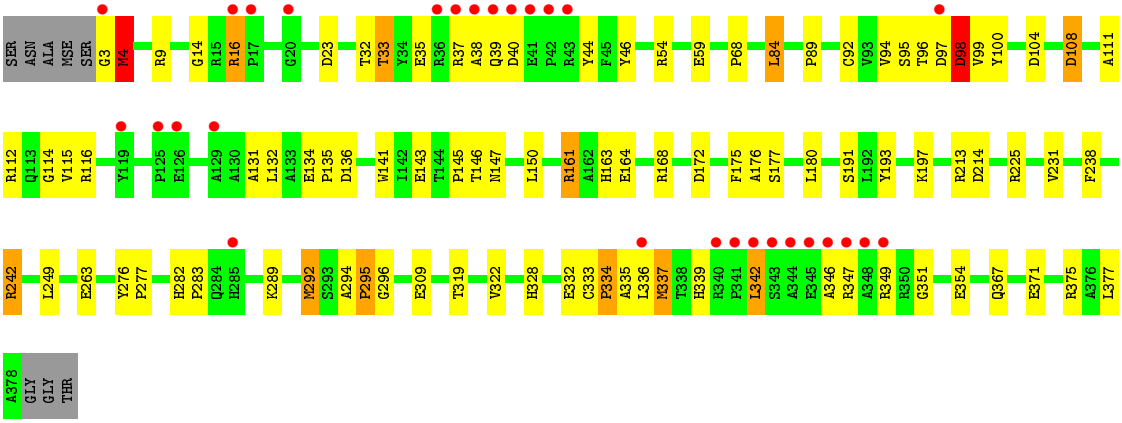
Chain 7-D:





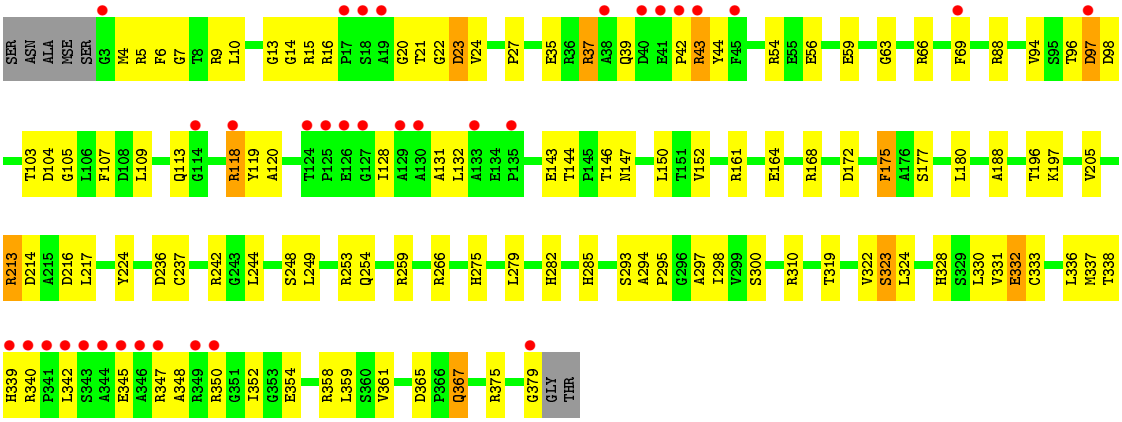
• Molecule 1: CalE6

Chain 7-E:



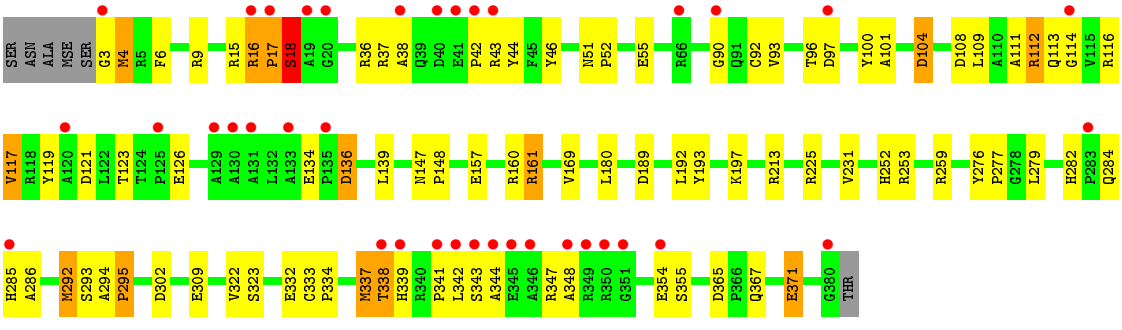
• Molecule 1: CalE6

Chain 7-F:



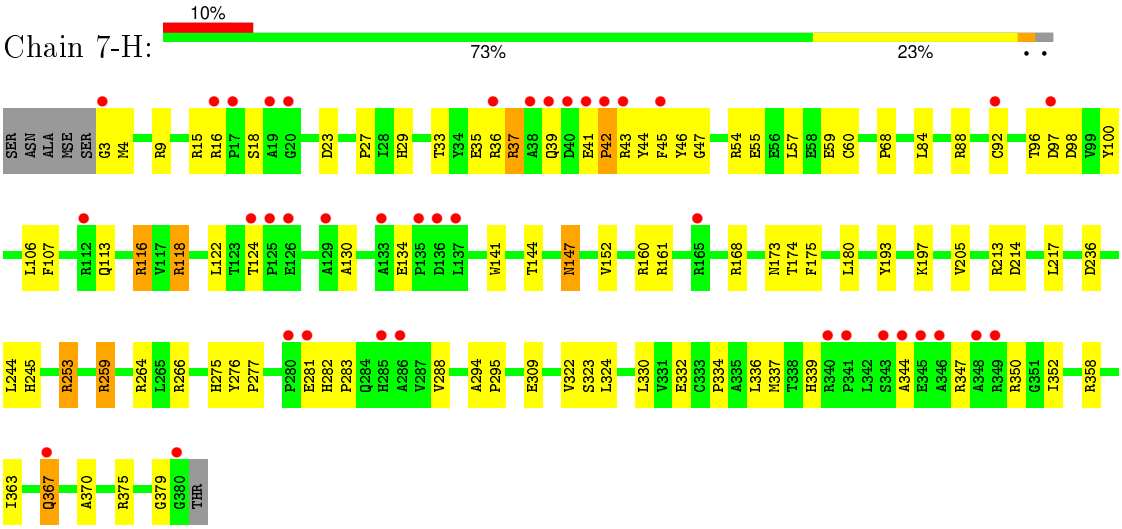
• Molecule 1: CalE6

Chain 7-G:



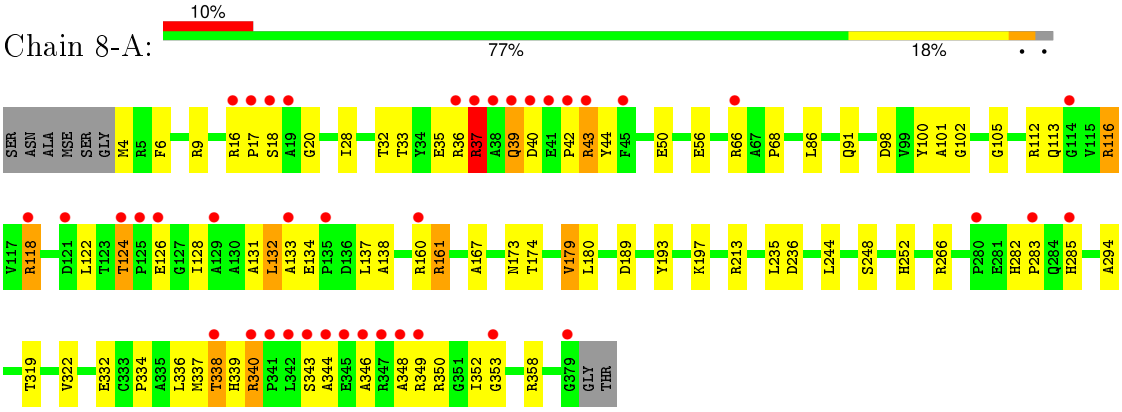
• Molecule 1: CalE6

Chain 7-H:



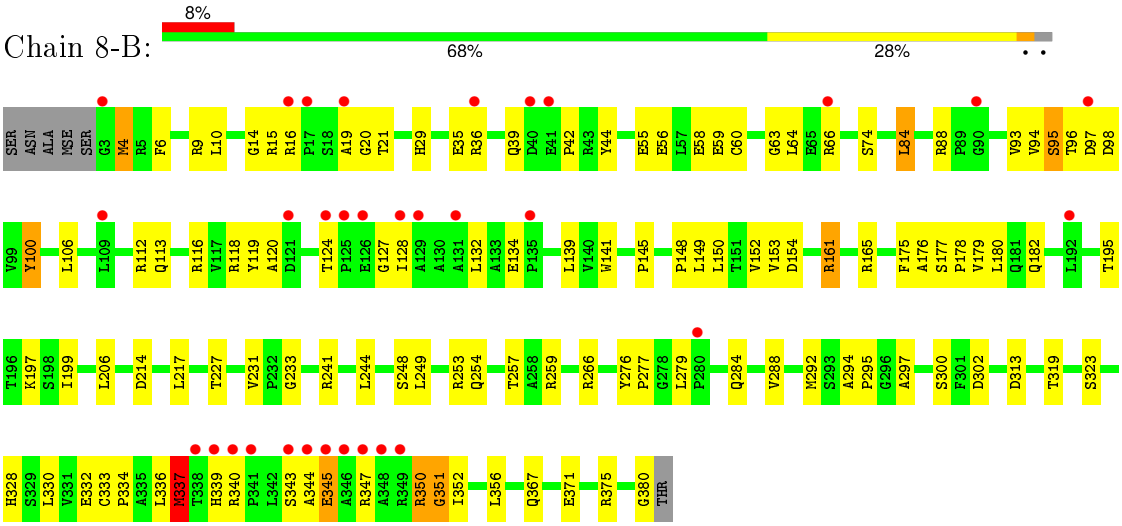
• Molecule 1: CalE6

Chain 8-A:



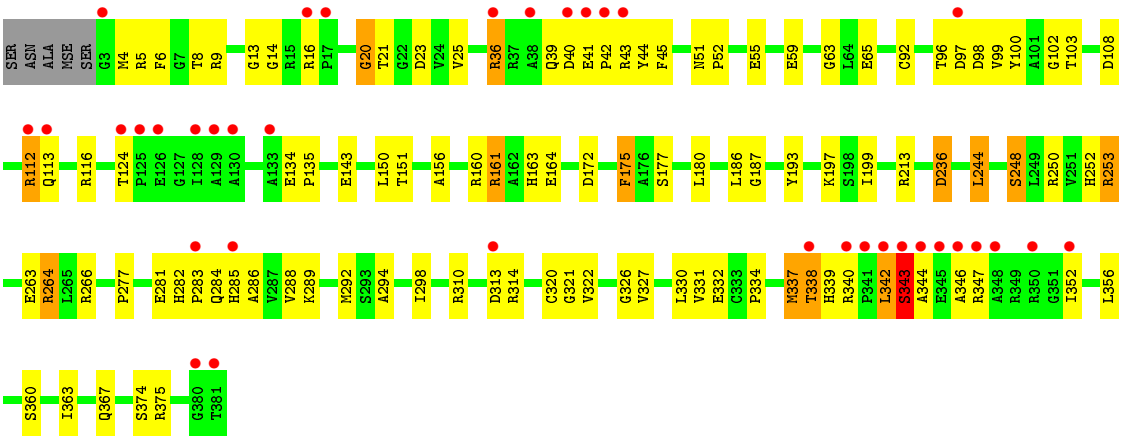
• Molecule 1: CalE6

Chain 8-B:



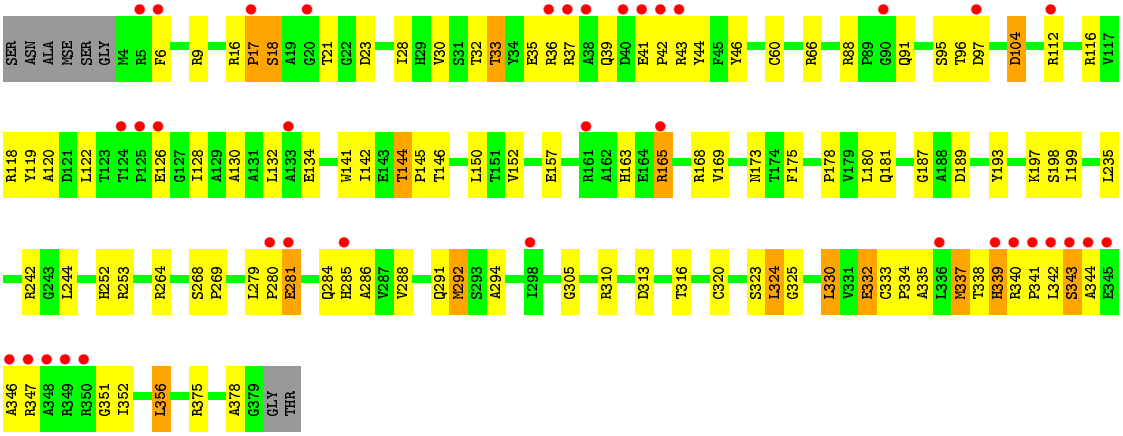
• Molecule 1: CalE6

Chain 8-C:



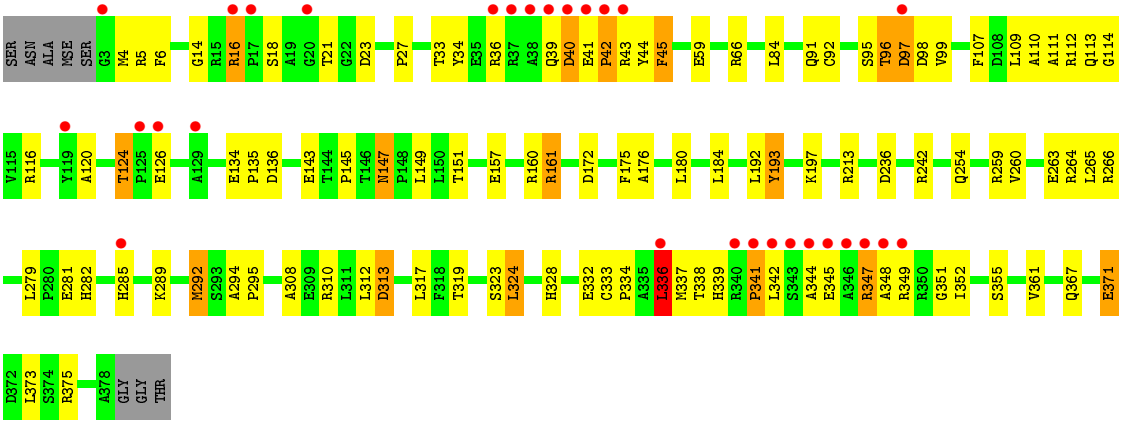
• Molecule 1: CalE6

Chain 8-D:



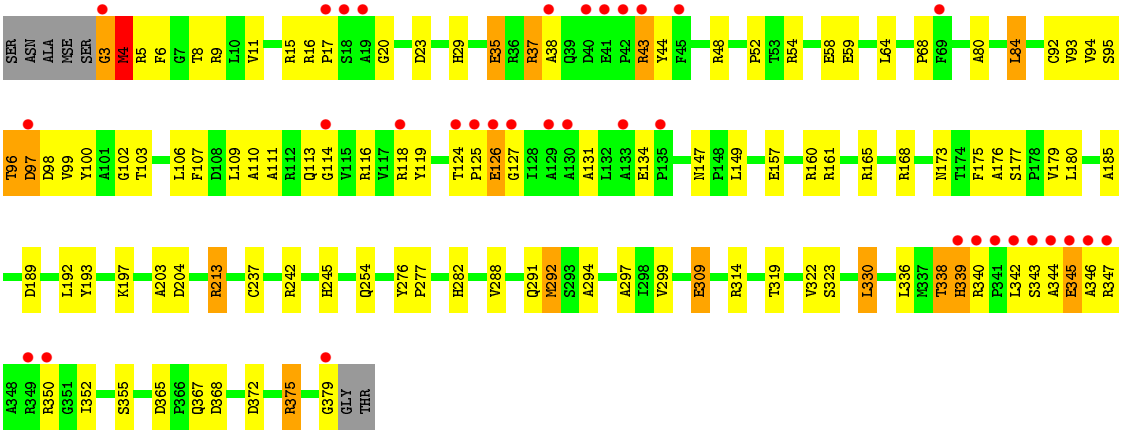
• Molecule 1: CalE6

Chain 8-E:



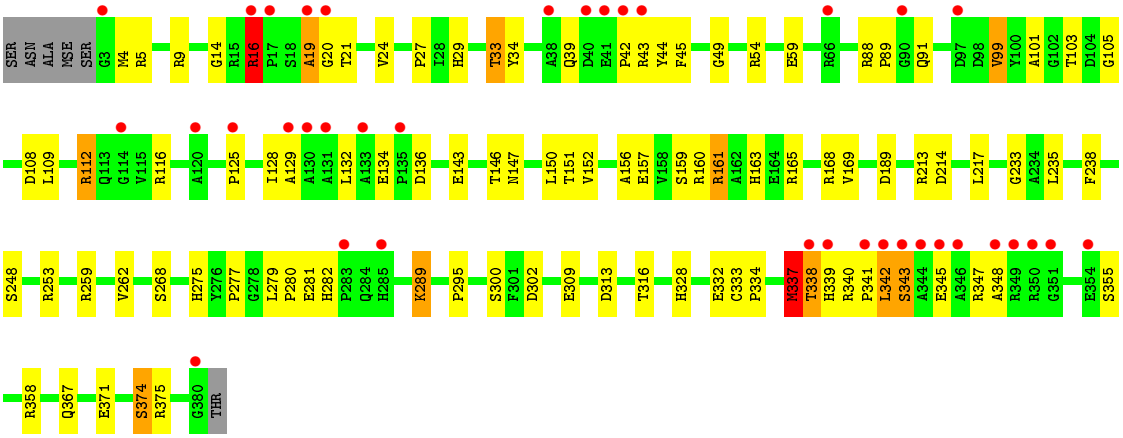
• Molecule 1: CalE6

Chain 8-F:



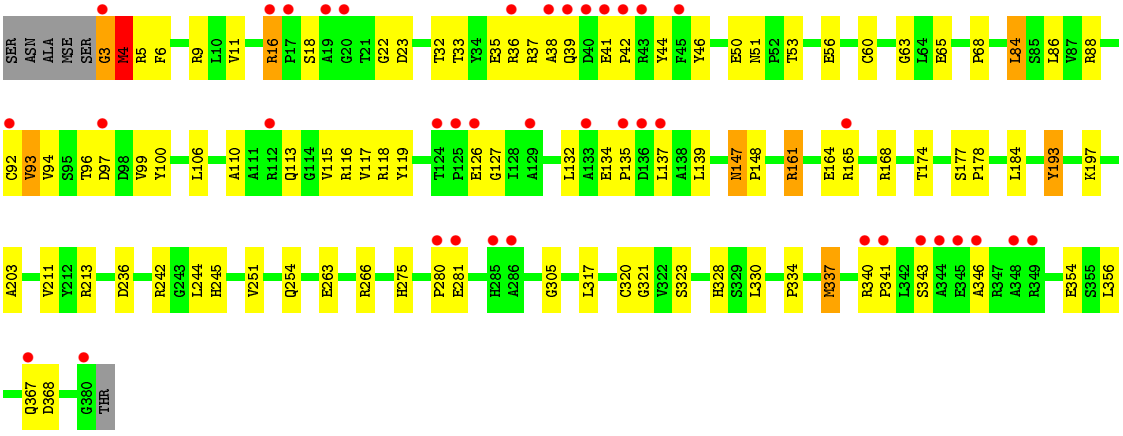
• Molecule 1: CalE6

Chain 8-G:



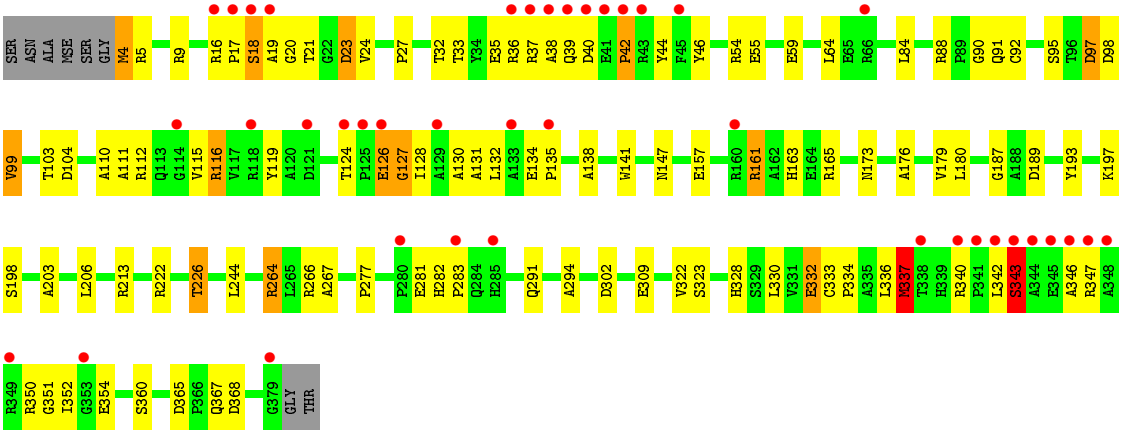
• Molecule 1: CalE6

Chain 8-H:



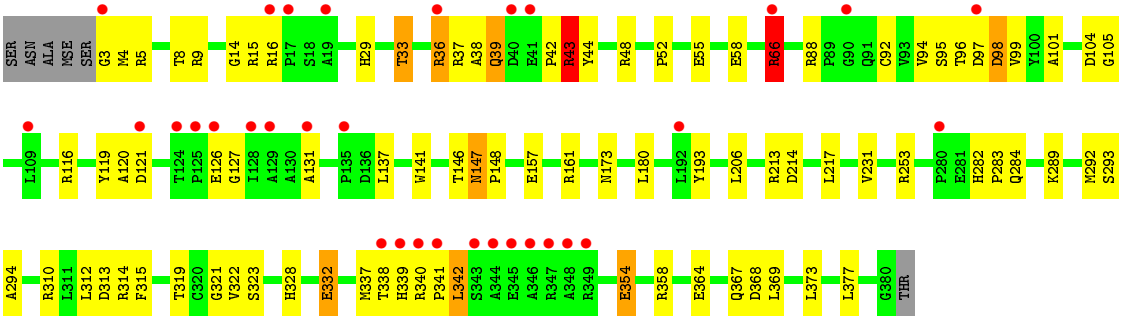
• Molecule 1: CalE6

Chain 9-A:



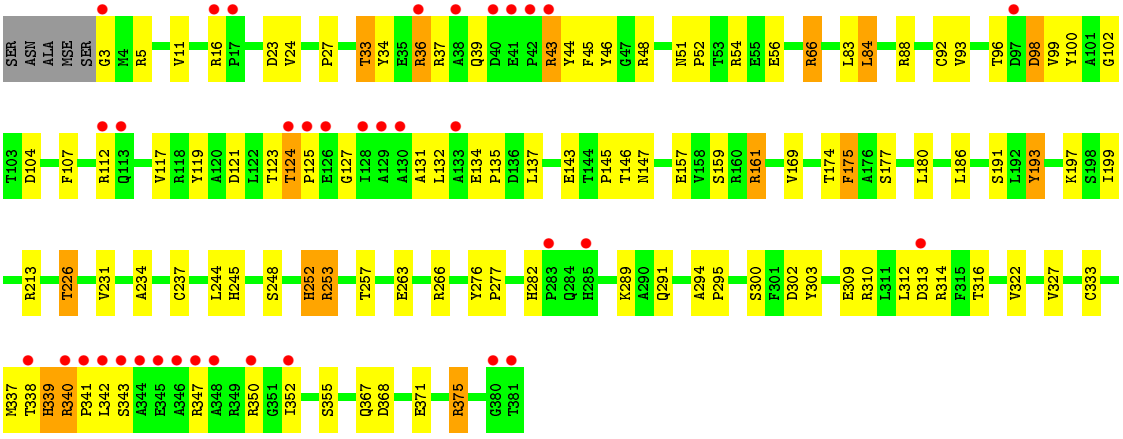
• Molecule 1: CalE6

Chain 9-B:



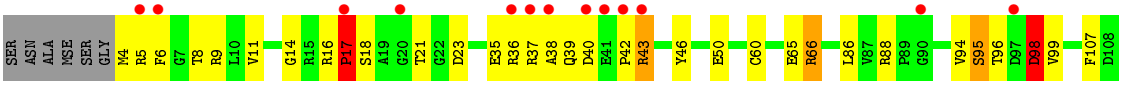
• Molecule 1: CalE6

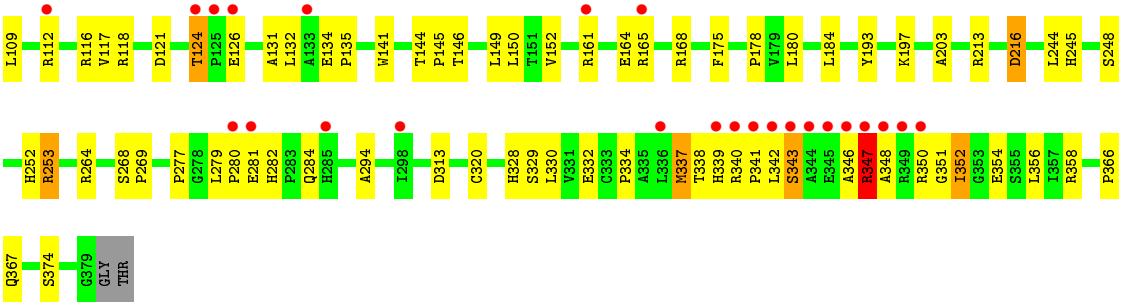
Chain 9-C:



• Molecule 1: CalE6

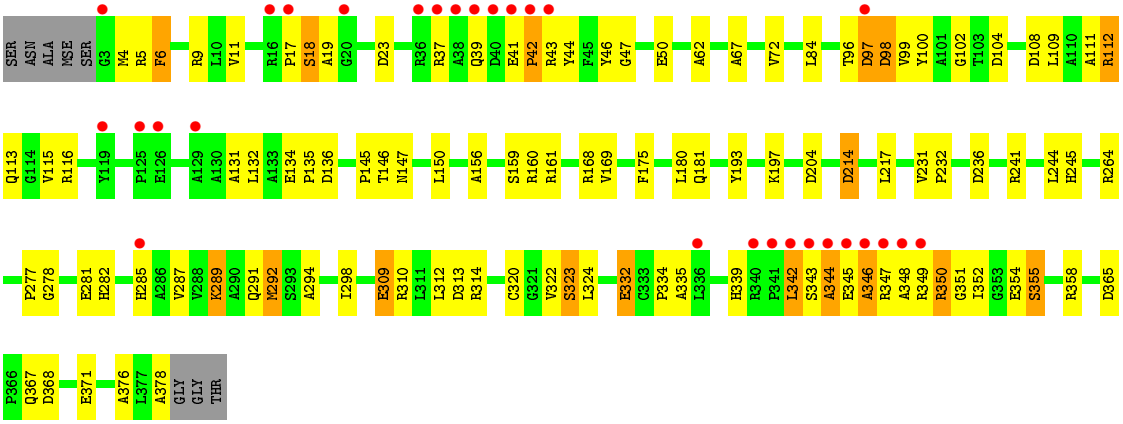
Chain 9-D:





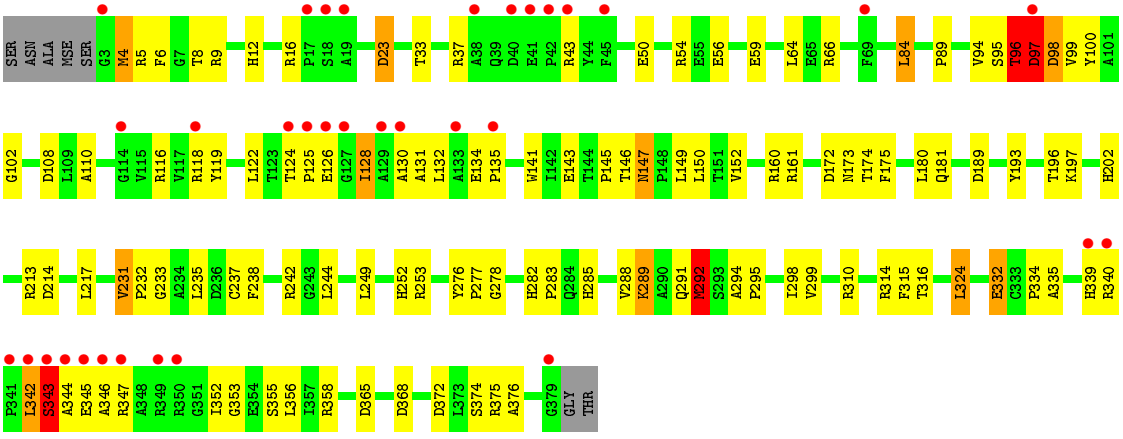
- Molecule 1: CalE6

Chain 9-E:



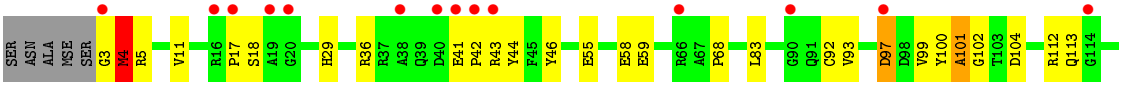
- Molecule 1: CalE6

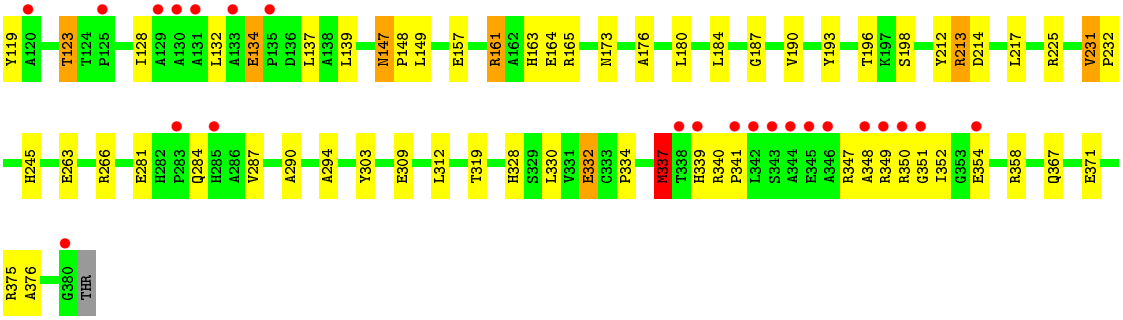
Chain 9-F:



- Molecule 1: CalE6

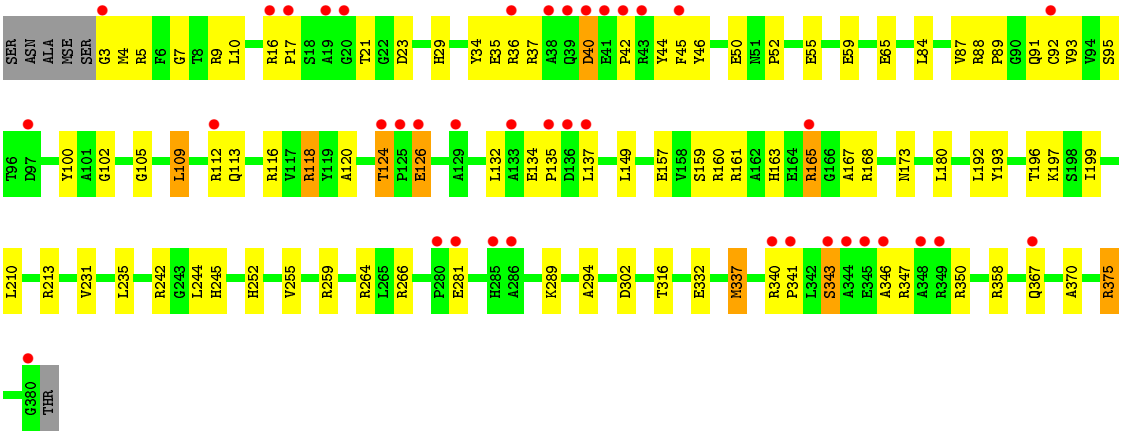
Chain 9-G:





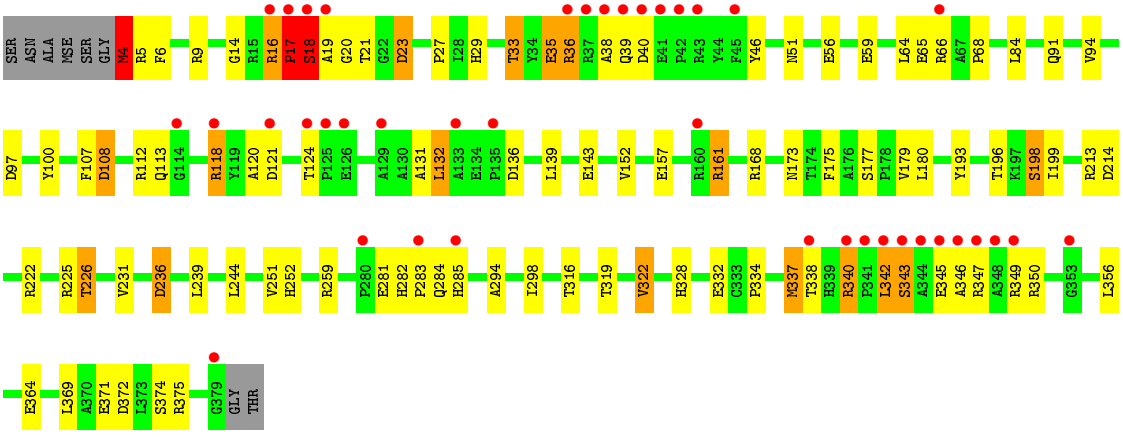
- Molecule 1: CalE6

Chain 9-H:



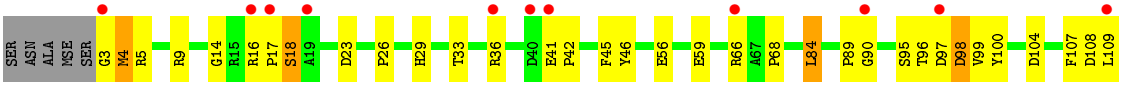
- Molecule 1: CalE6

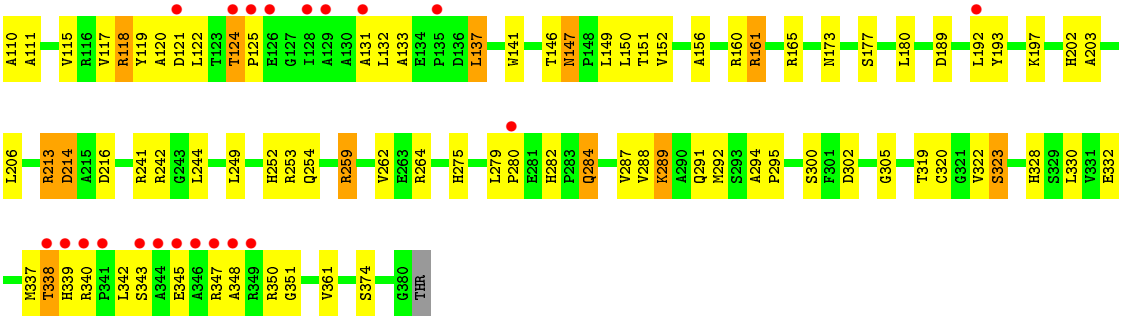
Chain 10-A:



- Molecule 1: CalE6

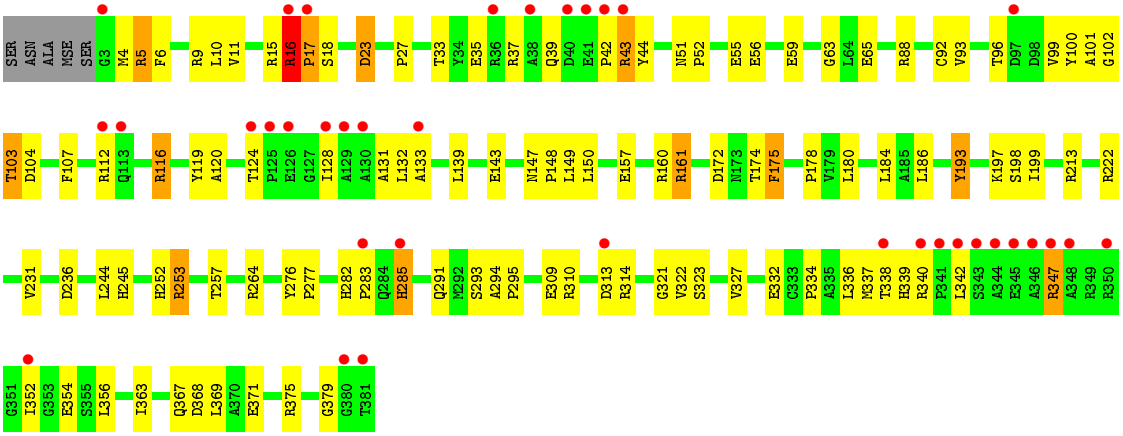
Chain 10-B:





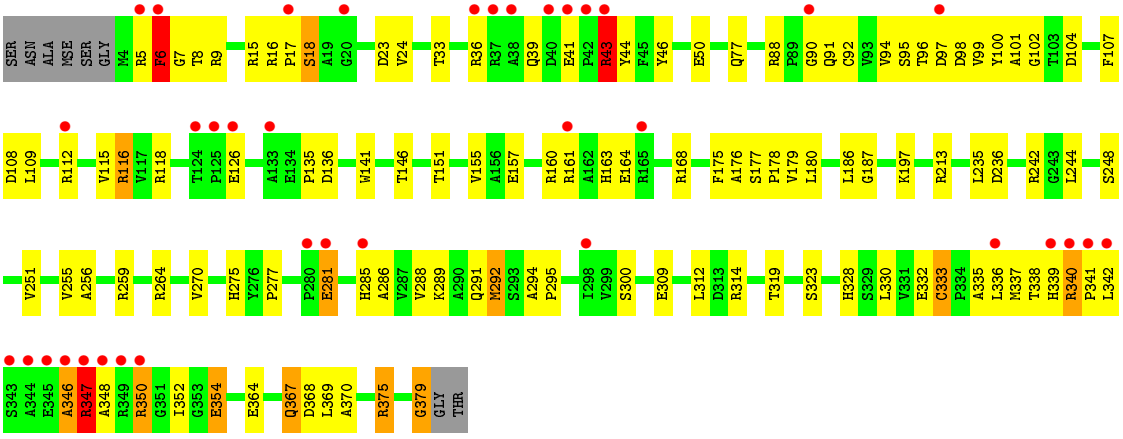
• Molecule 1: CalE6

Chain 10-C:



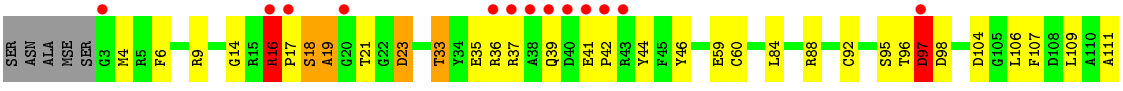
• Molecule 1: CalE6

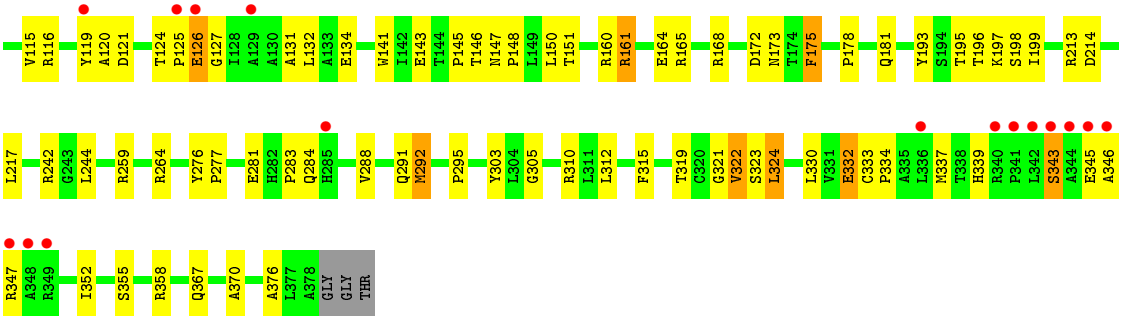
Chain 10-D:



• Molecule 1: CalE6

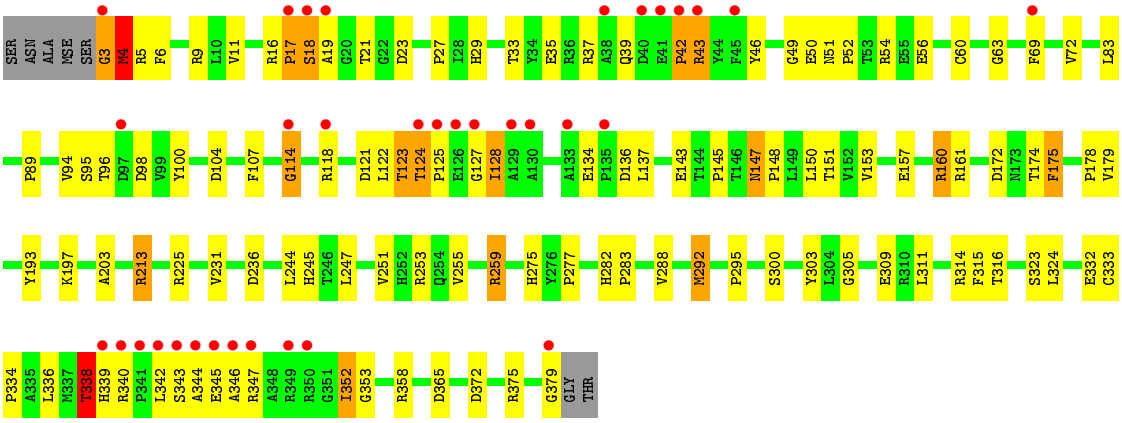
Chain 10-E:





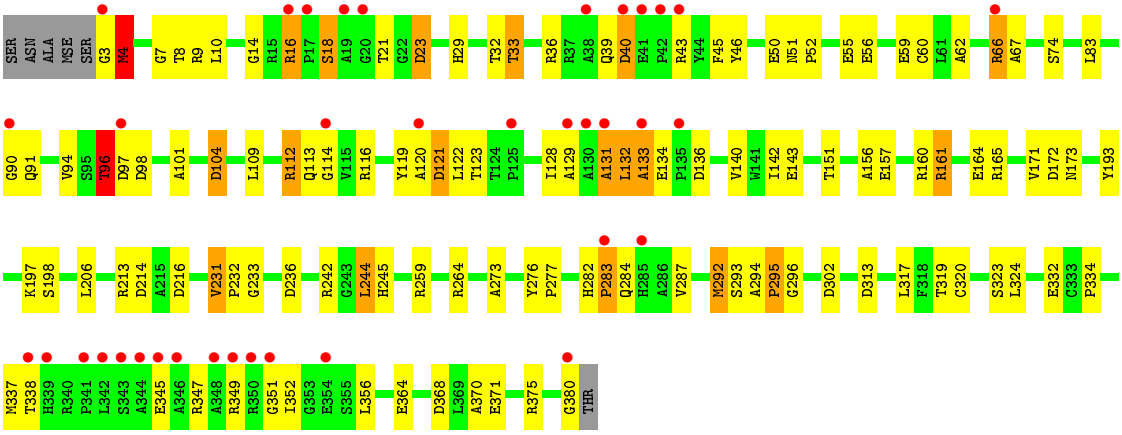
- Molecule 1: CalE6

Chain 10-F:



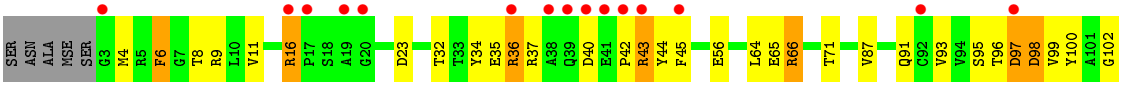
- Molecule 1: CalE6

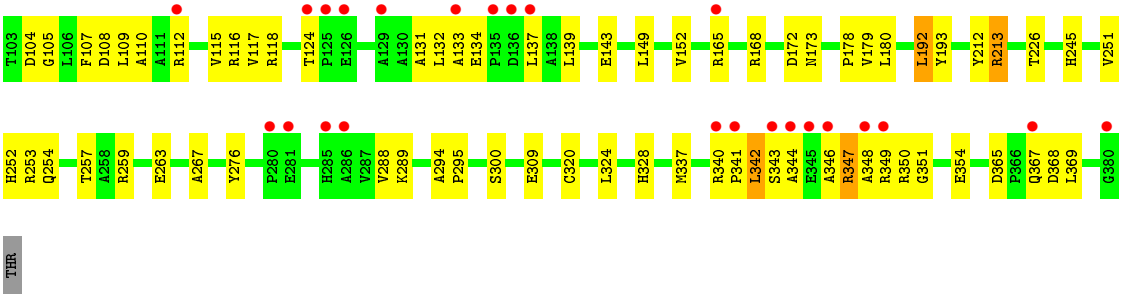
Chain 10-G:



- Molecule 1: CalE6

Chain 10-H:




T103 D104 G105 L106 F107 D108 L109 A110 A111 R112 V115 R116 Y117 R118 T124 P125 E126 A129 A130 A131 L132 A133 E134 P135 D136 L137 A138 L139 E143 L149 V152 R165 R168 D172 N173 P178 V179 L180 L192 Y193 Y212 R213 T226 H245 V251
H252 R253 Q254 T257 A258 R259 E263 A267 Y276 P280 E281 H285 A286 V287 V288 K289 A294 P295 S300 E309 C320 L324 H328 M337 R340 P341 L342 S343 A344 E345 A346 R347 A348 R349 R350 G351 E354 D365 P366 Q367 D368 L369 G380
THR

4 Data and refinement statistics (i)

Property	Value	So
Space group	I 2 2 2	Dep
Cell constants a, b, c, α, β, γ	146.85Å 146.98Å 349.90Å 90.00° 90.00° 90.00°	Dep
Resolution (Å)	33.97 – 2.10 33.97 – 2.10	Dep E
% Data completeness (in resolution range)	100.0 (33.97-2.10) 94.7 (33.97-2.10)	Dep E
R_{merge}	0.14	Dep
R_{sym}	(Not available)	Dep
$< I/\sigma(I) >$ [1]	3.37 (at 2.10Å)	Xt
Refinement program	PHENIX (PHENIX.ENSEMBLE_REFINEMENT: DEV_1839)	Dep
R, R_{free}	0.143 , 0.183 0.180 , 0.215	Dep D
R_{free} test set	11002 reflections (5.58%)	D
Wilson B-factor (Å^2)	23.6	Xt
Anisotropy	0.192	Xt
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 97.8	E
Estimated twinning fraction	0.055 for k,h,-l	Xt
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xt
Outliers	0 of 219087 reflections	Xt
F_o,F_c correlation	0.94	E
Total number of atoms	243453	wwP
Average B, all atoms (Å^2)	25.0	wwP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, LLP, MES, CL

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	1-A	0.50	3/2868 (0.1%)	0.63	1/3906 (0.0%)
1	1-B	0.45	0/2874	0.64	0/3912
1	1-C	0.43	0/2865	0.62	0/3903
1	1-D	0.51	1/2841 (0.0%)	0.65	2/3874 (0.1%)
1	1-E	0.47	0/2843	0.68	3/3874 (0.1%)
1	1-F	0.40	0/2840	0.59	0/3871
1	1-G	0.42	0/2842	0.62	2/3874 (0.1%)
1	1-H	0.44	0/2859	0.64	2/3893 (0.1%)
1	2-A	0.42	0/2868	0.63	0/3906
1	2-B	0.43	0/2874	0.64	3/3912 (0.1%)
1	2-C	0.45	0/2865	0.64	2/3903 (0.1%)
1	2-D	0.42	0/2841	0.66	3/3874 (0.1%)
1	2-E	0.44	0/2843	0.63	2/3874 (0.1%)
1	2-F	0.42	0/2840	0.59	0/3871
1	2-G	0.40	0/2842	0.63	3/3874 (0.1%)
1	2-H	0.44	0/2859	0.63	1/3893 (0.0%)
1	3-A	0.45	1/2868 (0.0%)	0.61	1/3906 (0.0%)
1	3-B	0.42	0/2874	0.63	1/3912 (0.0%)
1	3-C	0.45	0/2865	0.64	1/3903 (0.0%)
1	3-D	0.44	0/2841	0.72	7/3874 (0.2%)
1	3-E	0.46	1/2843 (0.0%)	0.63	0/3874
1	3-F	0.44	1/2840 (0.0%)	0.61	1/3871 (0.0%)
1	3-G	0.41	0/2842	0.64	3/3874 (0.1%)
1	3-H	0.43	0/2859	0.63	0/3893
1	4-A	0.44	1/2868 (0.0%)	0.61	0/3906
1	4-B	0.47	1/2874 (0.0%)	0.65	3/3912 (0.1%)
1	4-C	0.47	2/2865 (0.1%)	0.64	1/3903 (0.0%)
1	4-D	0.48	2/2841 (0.1%)	0.60	0/3874
1	4-E	0.44	0/2843	0.64	0/3874
1	4-F	0.42	0/2840	0.61	0/3871
1	4-G	0.43	0/2842	0.62	1/3874 (0.0%)
1	4-H	0.43	0/2859	0.60	0/3893

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	5-A	0.46	0/2868	0.63	3/3906 (0.1%)
1	5-B	0.49	1/2874 (0.0%)	0.64	2/3912 (0.1%)
1	5-C	0.47	1/2865 (0.0%)	0.66	2/3903 (0.1%)
1	5-D	0.44	0/2841	0.64	0/3874
1	5-E	0.53	2/2843 (0.1%)	0.68	3/3874 (0.1%)
1	5-F	0.45	1/2840 (0.0%)	0.63	2/3871 (0.1%)
1	5-G	0.42	0/2842	0.62	1/3874 (0.0%)
1	5-H	0.43	0/2859	0.62	0/3893
1	6-A	0.45	2/2868 (0.1%)	0.60	0/3906
1	6-B	0.44	0/2874	0.62	1/3912 (0.0%)
1	6-C	0.46	1/2865 (0.0%)	0.61	1/3903 (0.0%)
1	6-D	0.43	0/2841	0.65	0/3874
1	6-E	0.43	0/2843	0.68	4/3874 (0.1%)
1	6-F	0.42	0/2840	0.61	1/3871 (0.0%)
1	6-G	0.41	0/2842	0.61	1/3874 (0.0%)
1	6-H	0.47	0/2859	0.63	1/3893 (0.0%)
1	7-A	0.45	0/2868	0.64	2/3906 (0.1%)
1	7-B	0.43	0/2874	0.63	2/3912 (0.1%)
1	7-C	0.50	1/2865 (0.0%)	0.70	4/3903 (0.1%)
1	7-D	0.46	1/2841 (0.0%)	0.70	4/3874 (0.1%)
1	7-E	0.46	1/2843 (0.0%)	0.62	2/3874 (0.1%)
1	7-F	0.44	0/2840	0.65	0/3871
1	7-G	0.43	0/2842	0.65	2/3874 (0.1%)
1	7-H	0.42	0/2859	0.61	0/3893
1	8-A	0.44	0/2868	0.61	0/3906
1	8-B	0.43	0/2874	0.65	1/3912 (0.0%)
1	8-C	0.44	0/2865	0.62	0/3903
1	8-D	0.44	0/2841	0.64	2/3874 (0.1%)
1	8-E	0.47	1/2843 (0.0%)	0.64	1/3874 (0.0%)
1	8-F	0.43	0/2840	0.62	2/3871 (0.1%)
1	8-G	0.41	0/2842	0.61	1/3874 (0.0%)
1	8-H	0.42	0/2859	0.63	1/3893 (0.0%)
1	9-A	0.44	0/2868	0.63	1/3906 (0.0%)
1	9-B	0.48	2/2874 (0.1%)	0.66	4/3912 (0.1%)
1	9-C	0.48	1/2865 (0.0%)	0.64	1/3903 (0.0%)
1	9-D	0.41	0/2841	0.63	0/3874
1	9-E	0.42	0/2843	0.64	0/3874
1	9-F	0.45	1/2840 (0.0%)	0.65	2/3871 (0.1%)
1	9-G	0.41	0/2842	0.62	2/3874 (0.1%)
1	9-H	0.43	0/2859	0.60	0/3893
1	10-A	0.45	0/2868	0.63	0/3906
1	10-B	0.44	0/2874	0.62	2/3912 (0.1%)
1	10-C	0.45	1/2865 (0.0%)	0.65	0/3903

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	10-D	0.43	0/2841	0.67	1/3874 (0.0%)
1	10-E	0.46	0/2843	0.63	2/3874 (0.1%)
1	10-F	0.42	0/2840	0.63	0/3871
1	10-G	0.44	0/2842	0.64	0/3874
1	10-H	0.41	0/2859	0.61	1/3893 (0.0%)
All	All	0.44	30/228320 (0.0%)	0.63	105/311070 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-C	0	1
1	2-D	0	2
1	2-E	0	1
1	2-G	0	1
1	3-A	0	1
1	3-B	0	1
1	3-C	0	1
1	3-H	0	1
1	4-B	0	1
1	4-C	0	2
1	4-E	0	1
1	5-A	0	3
1	5-D	0	1
1	5-F	0	1
1	5-G	0	1
1	6-E	0	1
1	6-F	0	1
1	6-G	0	1
1	7-A	0	1
1	7-B	0	1
1	7-C	0	1
1	7-D	0	2
1	7-E	0	1
1	7-H	0	1
1	8-B	0	1
1	8-C	0	2
1	8-E	0	2
1	8-F	0	2
1	8-H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	9-C	0	1
1	9-E	0	1
1	9-F	0	1
1	10-A	0	1
1	10-C	0	1
1	10-D	0	1
1	10-E	0	1
1	10-F	0	1
All	All	0	45

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-B	322	VAL	CB-CG2	-11.16	1.29	1.52
1	1-D	344	ALA	CA-CB	-11.10	1.29	1.52
1	1-A	281	GLU	CB-CG	-9.85	1.33	1.52
1	9-C	66	ARG	CG-CD	-8.89	1.29	1.51
1	5-E	146	THR	CB-CG2	-8.80	1.23	1.52

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	7-A	4	MSE	CB-CG-SE	-10.95	79.84	112.70
1	3-D	97	ASP	CB-CG-OD1	-10.80	108.58	118.30
1	7-D	37	ARG	CG-CD-NE	10.78	134.44	111.80
1	9-A	337	MSE	CB-CG-SE	-10.36	81.63	112.70
1	7-C	97	ASP	CB-CG-OD1	-9.41	109.83	118.30

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2-C	32	THR	Peptide
1	2-D	336	LEU	Peptide
1	2-D	41	GLU	Peptide
1	2-E	193	TYR	Peptide
1	2-G	193	TYR	Peptide

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	1-A	2839	0	2836	79	0
1	1-B	2846	0	2840	83	0
1	1-C	2837	0	2821	68	0
1	1-D	2812	0	2793	100	0
1	1-E	2815	0	2796	91	0
1	1-F	2812	0	2789	93	0
1	1-G	2814	0	2788	87	0
1	1-H	2831	0	2820	92	0
1	2-A	2839	0	2836	67	0
1	2-B	2846	0	2839	89	0
1	2-C	2837	0	2820	88	0
1	2-D	2812	0	2793	88	0
1	2-E	2815	0	2796	84	0
1	2-F	2812	0	2788	76	0
1	2-G	2814	0	2788	59	0
1	2-H	2831	0	2819	95	0
1	3-A	2839	0	2835	85	0
1	3-B	2846	0	2840	81	0
1	3-C	2837	0	2820	100	0
1	3-D	2812	0	2793	91	0
1	3-E	2815	0	2795	84	0
1	3-F	2812	0	2788	88	0
1	3-G	2814	0	2788	86	0
1	3-H	2831	0	2819	97	0
1	4-A	2839	0	2835	99	0
1	4-B	2846	0	2839	95	0
1	4-C	2837	0	2821	87	0
1	4-D	2812	0	2793	84	0
1	4-E	2815	0	2796	105	0
1	4-F	2812	0	2788	96	0
1	4-G	2814	0	2788	87	0
1	4-H	2831	0	2820	89	0
1	5-A	2839	0	2835	103	0
1	5-B	2846	0	2840	115	0
1	5-C	2837	0	2820	102	0
1	5-D	2812	0	2792	79	0
1	5-E	2815	0	2796	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5-F	2812	0	2789	84	0
1	5-G	2814	0	2788	80	0
1	5-H	2831	0	2819	101	0
1	6-A	2839	0	2836	68	0
1	6-B	2846	0	2839	90	0
1	6-C	2837	0	2820	91	0
1	6-D	2812	0	2792	92	0
1	6-E	2815	0	2796	80	0
1	6-F	2812	0	2788	88	0
1	6-G	2814	0	2787	81	0
1	6-H	2831	0	2819	70	0
1	7-A	2839	0	2835	110	0
1	7-B	2846	0	2839	98	0
1	7-C	2837	0	2820	90	0
1	7-D	2812	0	2792	85	0
1	7-E	2815	0	2795	88	0
1	7-F	2812	0	2788	94	0
1	7-G	2814	0	2788	87	0
1	7-H	2831	0	2819	76	0
1	8-A	2839	0	2836	76	0
1	8-B	2846	0	2840	95	0
1	8-C	2837	0	2820	86	0
1	8-D	2812	0	2793	92	0
1	8-E	2815	0	2795	100	0
1	8-F	2812	0	2789	101	0
1	8-G	2814	0	2788	79	0
1	8-H	2831	0	2819	79	0
1	9-A	2839	0	2836	84	0
1	9-B	2846	0	2839	77	0
1	9-C	2837	0	2820	99	0
1	9-D	2812	0	2792	93	0
1	9-E	2815	0	2796	96	0
1	9-F	2812	0	2788	104	0
1	9-G	2814	0	2787	79	0
1	9-H	2831	0	2819	76	0
1	10-A	2839	0	2835	86	0
1	10-B	2846	0	2839	114	0
1	10-C	2837	0	2820	90	0
1	10-D	2812	0	2792	93	0
1	10-E	2815	0	2796	97	0
1	10-F	2812	0	2789	87	0
1	10-G	2814	0	2788	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10-H	2831	0	2820	83	0
2	1-A	12	0	12	1	0
2	1-B	12	0	12	0	0
2	1-C	12	0	12	1	0
2	1-D	12	0	12	3	0
2	1-E	12	0	12	2	0
2	1-F	12	0	12	2	0
2	1-G	12	0	12	3	0
2	1-H	12	0	12	2	0
2	2-A	12	0	13	0	0
2	2-B	12	0	12	3	0
2	2-C	12	0	12	5	0
2	2-D	12	0	12	2	0
2	2-E	12	0	12	4	0
2	2-F	12	0	12	3	0
2	2-G	12	0	12	2	0
2	2-H	12	0	12	2	0
2	3-A	12	0	12	0	0
2	3-B	12	0	12	1	0
2	3-C	12	0	12	2	0
2	3-D	12	0	12	1	0
2	3-E	12	0	12	6	0
2	3-F	12	0	12	2	0
2	3-G	12	0	12	3	0
2	3-H	12	0	12	5	0
2	4-A	12	0	12	4	0
2	4-B	12	0	12	5	0
2	4-C	12	0	12	8	0
2	4-D	12	0	12	2	0
2	4-E	12	0	12	4	0
2	4-F	12	0	12	2	0
2	4-G	12	0	12	1	0
2	4-H	12	0	12	2	0
2	5-A	12	0	12	0	0
2	5-B	12	0	12	3	0
2	5-C	12	0	12	3	0
2	5-D	12	0	12	2	0
2	5-E	12	0	12	5	0
2	5-F	12	0	12	2	0
2	5-G	12	0	12	7	0
2	5-H	12	0	12	1	0
2	6-A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-B	12	0	12	3	0
2	6-C	12	0	12	1	0
2	6-D	12	0	12	3	0
2	6-E	12	0	12	3	0
2	6-F	12	0	12	8	0
2	6-G	12	0	12	1	0
2	6-H	12	0	12	4	0
2	7-A	12	0	12	0	0
2	7-B	12	0	12	5	0
2	7-C	12	0	12	2	0
2	7-D	12	0	12	2	0
2	7-E	12	0	12	2	0
2	7-F	12	0	12	1	0
2	7-G	12	0	12	3	0
2	7-H	12	0	12	6	0
2	8-A	12	0	12	2	0
2	8-B	12	0	12	2	0
2	8-C	12	0	12	8	0
2	8-D	12	0	12	3	0
2	8-E	12	0	12	0	0
2	8-F	12	0	12	1	0
2	8-G	12	0	12	1	0
2	8-H	12	0	12	2	0
2	9-A	12	0	12	1	0
2	9-B	12	0	12	1	0
2	9-C	12	0	12	2	0
2	9-D	12	0	12	3	0
2	9-E	12	0	12	2	0
2	9-F	12	0	12	0	0
2	9-G	12	0	12	0	0
2	9-H	12	0	12	3	0
2	10-A	12	0	12	2	0
2	10-B	12	0	12	6	0
2	10-C	12	0	12	2	0
2	10-D	12	0	12	0	0
2	10-E	12	0	12	2	0
2	10-F	12	0	12	5	0
2	10-G	12	0	12	0	0
2	10-H	12	0	12	5	0
3	1-A	18	0	24	2	0
3	1-B	42	0	48	5	0
3	1-C	6	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1-D	18	0	23	0	0
3	1-E	12	0	16	2	0
3	1-F	36	0	39	3	0
3	1-G	24	0	24	4	0
3	1-H	12	0	16	4	0
3	2-A	18	0	24	2	0
3	2-B	36	0	47	2	0
3	2-C	18	0	16	2	0
3	2-D	12	0	16	1	0
3	2-E	24	0	24	3	0
3	2-F	24	0	33	0	0
3	2-G	18	0	24	2	0
3	2-H	18	0	24	4	0
3	3-A	24	0	24	2	0
3	3-B	36	0	48	5	0
3	3-C	12	0	16	0	0
3	3-D	12	0	16	1	0
3	3-E	18	0	16	6	0
3	3-F	30	0	40	4	0
3	3-G	24	0	24	4	0
3	3-H	12	0	16	1	0
3	4-A	18	0	24	3	0
3	4-B	36	0	48	4	0
3	4-C	18	0	16	2	0
3	4-D	12	0	16	3	0
3	4-E	18	0	16	1	0
3	4-F	18	0	25	1	0
3	4-G	30	0	24	3	0
3	4-H	18	0	24	4	0
3	5-A	24	0	24	5	0
3	5-B	36	0	48	7	0
3	5-C	6	0	9	0	0
3	5-D	18	0	24	3	0
3	5-E	24	0	24	3	0
3	5-F	18	0	25	3	0
3	5-G	24	0	24	2	0
3	5-H	18	0	24	4	0
3	6-A	24	0	24	2	0
3	6-B	36	0	48	2	0
3	6-C	6	0	9	1	0
3	6-D	18	0	24	4	0
3	6-E	18	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	6-F	30	0	40	7	0
3	6-G	12	0	17	3	0
3	6-H	24	0	32	0	0
3	7-A	24	0	24	6	0
3	7-B	36	0	48	1	0
3	7-C	6	0	9	0	0
3	7-D	18	0	24	2	0
3	7-E	18	0	16	4	0
3	7-F	30	0	40	5	0
3	7-G	18	0	24	2	0
3	7-H	18	0	24	1	0
3	8-A	18	0	24	2	0
3	8-B	42	0	48	4	0
3	8-C	12	0	16	1	0
3	8-D	12	0	16	1	0
3	8-E	18	0	16	6	0
3	8-F	24	0	33	5	0
3	8-G	24	0	24	2	0
3	8-H	18	0	24	4	0
3	9-A	24	0	24	0	0
3	9-B	30	0	40	0	0
3	9-C	12	0	16	2	0
3	9-D	18	0	24	5	0
3	9-E	24	0	24	1	0
3	9-F	18	0	25	2	0
3	9-G	18	0	24	3	0
3	9-H	24	0	32	4	0
3	10-A	18	0	24	5	0
3	10-B	36	0	48	3	0
3	10-C	12	0	16	1	0
3	10-D	18	0	24	3	0
3	10-E	12	0	16	1	0
3	10-F	30	0	40	2	0
3	10-G	18	0	24	4	0
3	10-H	24	0	32	4	0
4	1-A	2	0	0	0	0
4	1-B	1	0	8	0	0
4	1-C	2	0	0	0	0
4	1-D	2	0	0	0	0
4	1-E	1	0	0	0	0
4	1-F	1	0	1	0	0
4	1-G	1	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1-H	2	0	0	0	0
4	2-A	2	0	0	1	0
4	2-B	1	0	0	0	0
4	2-C	1	0	1	0	0
4	2-D	3	0	0	1	0
4	2-E	1	0	8	0	0
4	2-F	1	0	0	0	0
4	2-G	1	0	0	1	0
4	2-H	2	0	0	2	0
4	3-A	2	0	8	2	0
4	3-B	1	0	0	0	0
4	3-C	1	0	0	0	0
4	3-D	3	0	0	0	0
4	3-E	1	0	8	0	0
4	3-F	1	0	0	0	0
4	3-G	1	0	1	2	0
4	3-H	2	0	0	0	0
4	4-A	2	0	0	2	0
4	4-B	1	0	0	0	0
4	4-C	1	0	1	1	0
4	4-D	3	0	0	1	0
4	4-E	1	0	8	1	0
4	4-F	1	0	0	0	0
4	4-G	2	0	9	4	0
4	4-H	1	0	0	0	0
4	5-A	2	0	8	4	0
4	5-B	1	0	0	0	0
4	5-C	2	0	0	1	0
4	5-D	2	0	0	2	0
4	5-E	1	0	8	0	0
4	5-F	1	0	0	0	0
4	5-G	1	0	1	0	0
4	5-H	2	0	0	1	0
4	6-A	1	0	8	1	0
4	6-B	2	0	0	2	0
4	6-C	1	0	0	0	0
4	6-D	3	0	0	3	0
4	6-E	1	0	8	0	0
4	6-F	1	0	0	3	0
4	6-G	1	0	0	0	0
4	6-H	2	0	0	1	0
4	7-A	2	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	7-B	1	0	0	0	0
4	7-C	1	0	0	0	0
4	7-D	3	0	0	0	0
4	7-E	1	0	8	0	0
4	7-F	1	0	0	2	0
4	7-G	2	0	0	1	0
4	7-H	1	0	0	0	0
4	8-A	2	0	0	1	0
4	8-B	1	0	8	0	0
4	8-C	1	0	0	0	0
4	8-D	3	0	0	0	0
4	8-E	1	0	8	2	0
4	8-F	1	0	0	0	0
4	8-G	1	0	1	1	0
4	8-H	2	0	0	0	0
4	9-A	2	0	8	0	0
4	9-B	1	0	0	0	0
4	9-C	1	0	0	0	0
4	9-D	3	0	0	0	0
4	9-E	1	0	8	1	0
4	9-F	1	0	0	0	0
4	9-G	1	0	0	0	0
4	9-H	2	0	0	1	0
4	10-A	2	0	0	1	0
4	10-B	1	0	0	0	0
4	10-C	2	0	0	1	0
4	10-D	2	0	0	0	0
4	10-E	1	0	0	2	0
4	10-F	1	0	0	1	0
4	10-G	1	0	0	0	0
4	10-H	2	0	0	3	0
5	1-C	3	0	0	0	0
5	1-F	3	0	8	0	0
5	1-G	3	0	8	0	0
5	2-C	3	0	8	1	0
5	2-F	3	0	0	0	0
5	2-G	3	0	1	0	0
5	3-C	3	0	1	0	0
5	3-F	3	0	1	2	0
5	3-G	3	0	8	0	0
5	4-C	3	0	8	1	0
5	4-F	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4-G	3	0	8	0	0
5	5-C	3	0	0	0	0
5	5-F	3	0	0	0	0
5	5-G	3	0	8	1	0
5	6-C	3	0	0	1	0
5	6-F	3	0	1	0	0
5	6-G	3	0	0	0	0
5	7-C	3	0	0	0	0
5	7-F	3	0	1	2	0
5	7-G	3	0	1	0	0
5	8-C	3	0	1	0	0
5	8-F	3	0	0	1	0
5	8-G	3	0	8	0	0
5	9-C	3	0	1	0	0
5	9-F	3	0	0	0	0
5	9-G	3	0	1	0	0
5	10-C	3	0	1	0	0
5	10-F	3	0	1	1	0
5	10-G	3	0	1	0	0
6	1-A	180	0	0	15	0
6	1-B	198	0	0	14	0
6	1-C	178	0	0	14	0
6	1-D	183	0	0	26	0
6	1-E	178	0	0	11	0
6	1-F	178	0	0	14	0
6	1-G	186	0	0	15	0
6	1-H	172	0	0	14	0
6	2-A	190	0	0	11	0
6	2-B	189	0	0	18	0
6	2-C	178	0	0	22	0
6	2-D	159	0	0	12	0
6	2-E	177	0	0	19	0
6	2-F	175	0	0	14	0
6	2-G	175	0	0	14	0
6	2-H	185	0	0	15	0
6	3-A	183	0	0	23	0
6	3-B	183	0	0	13	0
6	3-C	181	0	0	26	0
6	3-D	188	0	0	17	0
6	3-E	196	0	0	15	0
6	3-F	159	0	0	10	0
6	3-G	183	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	3-H	163	0	0	15	0
6	4-A	184	0	0	15	0
6	4-B	189	0	0	20	0
6	4-C	176	0	0	14	0
6	4-D	179	0	0	9	0
6	4-E	197	0	0	19	0
6	4-F	177	0	0	32	0
6	4-G	185	0	0	21	0
6	4-H	184	0	0	17	0
6	5-A	197	0	0	25	0
6	5-B	189	0	0	11	0
6	5-C	178	0	0	26	0
6	5-D	179	0	0	12	0
6	5-E	173	0	0	27	0
6	5-F	166	0	0	15	0
6	5-G	172	0	0	11	0
6	5-H	183	0	0	21	0
6	6-A	179	0	0	12	0
6	6-B	195	0	0	16	0
6	6-C	174	0	0	22	0
6	6-D	161	0	0	8	0
6	6-E	191	0	0	21	0
6	6-F	189	0	0	14	0
6	6-G	176	0	0	11	0
6	6-H	184	0	0	12	0
6	7-A	192	0	0	18	0
6	7-B	196	0	0	10	0
6	7-C	196	0	0	22	0
6	7-D	177	0	0	14	0
6	7-E	180	0	0	20	0
6	7-F	179	0	0	19	0
6	7-G	187	0	0	20	0
6	7-H	183	0	0	13	0
6	8-A	183	0	0	13	0
6	8-B	185	0	0	21	0
6	8-C	183	0	0	24	0
6	8-D	179	0	0	18	0
6	8-E	194	0	0	25	0
6	8-F	162	0	0	18	0
6	8-G	179	0	0	14	0
6	8-H	191	0	0	14	0
6	9-A	188	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	9-B	198	0	0	18	0
6	9-C	178	0	0	21	0
6	9-D	179	0	0	14	0
6	9-E	181	0	0	19	0
6	9-F	176	0	0	18	0
6	9-G	197	0	0	18	0
6	9-H	168	0	0	20	0
6	10-A	173	0	0	9	0
6	10-B	195	0	0	26	0
6	10-C	188	0	0	27	0
6	10-D	177	0	0	15	0
6	10-E	182	0	0	21	0
6	10-F	167	0	0	11	0
6	10-G	182	0	0	10	0
6	10-H	194	0	0	22	0
All	All	243453	0	228016	6762	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 15.

The worst 5 of 6762 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:MSE:CG	1:E:4:MSE:SE	2.14	1.44
1:C:292:MSE:CG	1:C:292:MSE:SE	2.21	1.37
1:A:4:MSE:HB3	1:A:8:THR:HB	1.26	1.15
1:B:5:ARG:NH1	1:C:368:ASP:OD1	1.83	1.12
1:H:333:CYS:H	1:H:337:MSE:SE	1.84	1.10

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	1-A	373/384 (97%)	347 (93%)	20 (5%)	6 (2%)	12 6
1	1-B	375/384 (98%)	350 (93%)	19 (5%)	6 (2%)	12 6
1	1-C	376/384 (98%)	346 (92%)	23 (6%)	7 (2%)	10 4
1	1-D	373/384 (97%)	338 (91%)	23 (6%)	12 (3%)	5 1
1	1-E	373/384 (97%)	347 (93%)	20 (5%)	6 (2%)	12 6
1	1-F	374/384 (97%)	352 (94%)	18 (5%)	4 (1%)	17 11
1	1-G	375/384 (98%)	341 (91%)	27 (7%)	7 (2%)	10 4
1	1-H	375/384 (98%)	341 (91%)	28 (8%)	6 (2%)	12 6
1	2-A	373/384 (97%)	348 (93%)	21 (6%)	4 (1%)	17 11
1	2-B	375/384 (98%)	345 (92%)	24 (6%)	6 (2%)	12 6
1	2-C	376/384 (98%)	348 (93%)	24 (6%)	4 (1%)	17 11
1	2-D	373/384 (97%)	350 (94%)	15 (4%)	8 (2%)	9 3
1	2-E	373/384 (97%)	350 (94%)	17 (5%)	6 (2%)	12 6
1	2-F	374/384 (97%)	345 (92%)	25 (7%)	4 (1%)	17 11
1	2-G	375/384 (98%)	344 (92%)	28 (8%)	3 (1%)	24 17
1	2-H	375/384 (98%)	345 (92%)	24 (6%)	6 (2%)	12 6
1	3-A	373/384 (97%)	341 (91%)	28 (8%)	4 (1%)	17 11
1	3-B	375/384 (98%)	347 (92%)	20 (5%)	8 (2%)	9 3
1	3-C	376/384 (98%)	341 (91%)	30 (8%)	5 (1%)	15 9
1	3-D	373/384 (97%)	342 (92%)	23 (6%)	8 (2%)	9 3
1	3-E	373/384 (97%)	345 (92%)	19 (5%)	9 (2%)	7 3
1	3-F	374/384 (97%)	346 (92%)	17 (4%)	11 (3%)	6 2
1	3-G	375/384 (98%)	339 (90%)	31 (8%)	5 (1%)	15 9
1	3-H	375/384 (98%)	346 (92%)	21 (6%)	8 (2%)	9 3
1	4-A	373/384 (97%)	348 (93%)	21 (6%)	4 (1%)	17 11
1	4-B	375/384 (98%)	350 (93%)	18 (5%)	7 (2%)	10 4
1	4-C	376/384 (98%)	353 (94%)	17 (4%)	6 (2%)	12 6
1	4-D	373/384 (97%)	342 (92%)	25 (7%)	6 (2%)	12 6
1	4-E	373/384 (97%)	347 (93%)	18 (5%)	8 (2%)	9 3
1	4-F	374/384 (97%)	340 (91%)	24 (6%)	10 (3%)	6 2
1	4-G	375/384 (98%)	344 (92%)	24 (6%)	7 (2%)	10 4
1	4-H	375/384 (98%)	348 (93%)	24 (6%)	3 (1%)	24 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	5-A	373/384 (97%)	333 (89%)	32 (9%)	8 (2%)	9 3
1	5-B	375/384 (98%)	352 (94%)	19 (5%)	4 (1%)	17 11
1	5-C	376/384 (98%)	347 (92%)	28 (7%)	1 (0%)	46 45
1	5-D	373/384 (97%)	345 (92%)	21 (6%)	7 (2%)	10 4
1	5-E	373/384 (97%)	343 (92%)	17 (5%)	13 (4%)	4 1
1	5-F	374/384 (97%)	349 (93%)	18 (5%)	7 (2%)	10 4
1	5-G	375/384 (98%)	339 (90%)	29 (8%)	7 (2%)	10 4
1	5-H	375/384 (98%)	345 (92%)	25 (7%)	5 (1%)	15 9
1	6-A	373/384 (97%)	342 (92%)	25 (7%)	6 (2%)	12 6
1	6-B	375/384 (98%)	343 (92%)	29 (8%)	3 (1%)	24 17
1	6-C	376/384 (98%)	345 (92%)	28 (7%)	3 (1%)	24 17
1	6-D	373/384 (97%)	340 (91%)	22 (6%)	11 (3%)	6 2
1	6-E	373/384 (97%)	351 (94%)	17 (5%)	5 (1%)	15 9
1	6-F	374/384 (97%)	347 (93%)	24 (6%)	3 (1%)	24 17
1	6-G	375/384 (98%)	351 (94%)	20 (5%)	4 (1%)	17 11
1	6-H	375/384 (98%)	347 (92%)	23 (6%)	5 (1%)	15 9
1	7-A	373/384 (97%)	345 (92%)	22 (6%)	6 (2%)	12 6
1	7-B	375/384 (98%)	349 (93%)	22 (6%)	4 (1%)	17 11
1	7-C	376/384 (98%)	340 (90%)	28 (7%)	8 (2%)	9 3
1	7-D	373/384 (97%)	343 (92%)	24 (6%)	6 (2%)	12 6
1	7-E	373/384 (97%)	344 (92%)	24 (6%)	5 (1%)	15 9
1	7-F	374/384 (97%)	344 (92%)	25 (7%)	5 (1%)	15 9
1	7-G	375/384 (98%)	339 (90%)	30 (8%)	6 (2%)	12 6
1	7-H	375/384 (98%)	349 (93%)	23 (6%)	3 (1%)	24 17
1	8-A	373/384 (97%)	344 (92%)	23 (6%)	6 (2%)	12 6
1	8-B	375/384 (98%)	347 (92%)	23 (6%)	5 (1%)	15 9
1	8-C	376/384 (98%)	347 (92%)	23 (6%)	6 (2%)	12 6
1	8-D	373/384 (97%)	345 (92%)	21 (6%)	7 (2%)	10 4
1	8-E	373/384 (97%)	353 (95%)	15 (4%)	5 (1%)	15 9
1	8-F	374/384 (97%)	341 (91%)	29 (8%)	4 (1%)	17 11
1	8-G	375/384 (98%)	347 (92%)	22 (6%)	6 (2%)	12 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	8-H	375/384 (98%)	346 (92%)	25 (7%)	4 (1%)	17 11
1	9-A	373/384 (97%)	344 (92%)	18 (5%)	11 (3%)	6 2
1	9-B	375/384 (98%)	345 (92%)	25 (7%)	5 (1%)	15 9
1	9-C	376/384 (98%)	349 (93%)	26 (7%)	1 (0%)	46 45
1	9-D	373/384 (97%)	335 (90%)	32 (9%)	6 (2%)	12 6
1	9-E	373/384 (97%)	342 (92%)	20 (5%)	11 (3%)	6 2
1	9-F	374/384 (97%)	351 (94%)	19 (5%)	4 (1%)	17 11
1	9-G	375/384 (98%)	347 (92%)	24 (6%)	4 (1%)	17 11
1	9-H	375/384 (98%)	350 (93%)	23 (6%)	2 (0%)	34 30
1	10-A	373/384 (97%)	343 (92%)	25 (7%)	5 (1%)	15 9
1	10-B	375/384 (98%)	342 (91%)	27 (7%)	6 (2%)	12 6
1	10-C	376/384 (98%)	340 (90%)	29 (8%)	7 (2%)	10 4
1	10-D	373/384 (97%)	345 (92%)	16 (4%)	12 (3%)	5 1
1	10-E	373/384 (97%)	346 (93%)	20 (5%)	7 (2%)	10 4
1	10-F	374/384 (97%)	347 (93%)	17 (4%)	10 (3%)	6 2
1	10-G	375/384 (98%)	341 (91%)	25 (7%)	9 (2%)	7 3
1	10-H	375/384 (98%)	349 (93%)	23 (6%)	3 (1%)	24 17
All	All	29940/30720 (98%)	27614 (92%)	1841 (6%)	485 (2%)	12 6

5 of 485 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	17	PRO
1	1-A	40	ASP
1	1-A	122	LEU
1	1-B	15	ARG
1	1-B	17	PRO

5.3.2 Protein sidechains (i)

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	1-A	291/293 (99%)	269 (92%)	22 (8%)	16 12
1	1-B	291/293 (99%)	263 (90%)	28 (10%)	10 6
1	1-C	289/293 (99%)	268 (93%)	21 (7%)	17 13
1	1-D	285/293 (97%)	261 (92%)	24 (8%)	14 9
1	1-E	286/293 (98%)	268 (94%)	18 (6%)	22 18
1	1-F	284/293 (97%)	261 (92%)	23 (8%)	15 10
1	1-G	285/293 (97%)	267 (94%)	18 (6%)	22 18
1	1-H	287/293 (98%)	263 (92%)	24 (8%)	14 9
1	2-A	291/293 (99%)	274 (94%)	17 (6%)	25 21
1	2-B	291/293 (99%)	270 (93%)	21 (7%)	18 14
1	2-C	289/293 (99%)	274 (95%)	15 (5%)	29 25
1	2-D	285/293 (97%)	263 (92%)	22 (8%)	16 12
1	2-E	286/293 (98%)	271 (95%)	15 (5%)	29 25
1	2-F	284/293 (97%)	266 (94%)	18 (6%)	22 18
1	2-G	285/293 (97%)	265 (93%)	20 (7%)	19 15
1	2-H	287/293 (98%)	263 (92%)	24 (8%)	14 9
1	3-A	291/293 (99%)	267 (92%)	24 (8%)	14 10
1	3-B	291/293 (99%)	281 (97%)	10 (3%)	44 45
1	3-C	289/293 (99%)	264 (91%)	25 (9%)	13 8
1	3-D	285/293 (97%)	260 (91%)	25 (9%)	12 8
1	3-E	286/293 (98%)	273 (96%)	13 (4%)	34 32
1	3-F	284/293 (97%)	264 (93%)	20 (7%)	19 15
1	3-G	285/293 (97%)	267 (94%)	18 (6%)	22 18
1	3-H	287/293 (98%)	267 (93%)	20 (7%)	19 15
1	4-A	291/293 (99%)	270 (93%)	21 (7%)	18 14
1	4-B	291/293 (99%)	268 (92%)	23 (8%)	15 11
1	4-C	289/293 (99%)	273 (94%)	16 (6%)	27 23
1	4-D	285/293 (97%)	263 (92%)	22 (8%)	16 12
1	4-E	286/293 (98%)	266 (93%)	20 (7%)	19 15
1	4-F	284/293 (97%)	261 (92%)	23 (8%)	15 10
1	4-G	285/293 (97%)	269 (94%)	16 (6%)	26 22
1	4-H	287/293 (98%)	265 (92%)	22 (8%)	16 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	5-A	291/293 (99%)	275 (94%)	16 (6%)	27 23
1	5-B	291/293 (99%)	269 (92%)	22 (8%)	16 12
1	5-C	289/293 (99%)	269 (93%)	20 (7%)	19 15
1	5-D	285/293 (97%)	260 (91%)	25 (9%)	12 8
1	5-E	286/293 (98%)	261 (91%)	25 (9%)	13 8
1	5-F	284/293 (97%)	273 (96%)	11 (4%)	39 39
1	5-G	285/293 (97%)	272 (95%)	13 (5%)	33 31
1	5-H	287/293 (98%)	266 (93%)	21 (7%)	17 13
1	6-A	291/293 (99%)	274 (94%)	17 (6%)	25 21
1	6-B	291/293 (99%)	270 (93%)	21 (7%)	18 14
1	6-C	289/293 (99%)	271 (94%)	18 (6%)	23 19
1	6-D	285/293 (97%)	260 (91%)	25 (9%)	12 8
1	6-E	286/293 (98%)	264 (92%)	22 (8%)	16 12
1	6-F	284/293 (97%)	259 (91%)	25 (9%)	12 8
1	6-G	285/293 (97%)	261 (92%)	24 (8%)	14 9
1	6-H	287/293 (98%)	269 (94%)	18 (6%)	22 18
1	7-A	291/293 (99%)	258 (89%)	33 (11%)	7 4
1	7-B	291/293 (99%)	267 (92%)	24 (8%)	14 10
1	7-C	289/293 (99%)	269 (93%)	20 (7%)	19 15
1	7-D	285/293 (97%)	261 (92%)	24 (8%)	14 9
1	7-E	286/293 (98%)	268 (94%)	18 (6%)	22 18
1	7-F	284/293 (97%)	265 (93%)	19 (7%)	20 16
1	7-G	285/293 (97%)	272 (95%)	13 (5%)	33 31
1	7-H	287/293 (98%)	269 (94%)	18 (6%)	22 18
1	8-A	291/293 (99%)	276 (95%)	15 (5%)	29 25
1	8-B	291/293 (99%)	277 (95%)	14 (5%)	31 29
1	8-C	289/293 (99%)	271 (94%)	18 (6%)	23 19
1	8-D	285/293 (97%)	267 (94%)	18 (6%)	22 18
1	8-E	286/293 (98%)	267 (93%)	19 (7%)	21 17
1	8-F	284/293 (97%)	265 (93%)	19 (7%)	20 16
1	8-G	285/293 (97%)	269 (94%)	16 (6%)	26 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	8-H	287/293 (98%)	271 (94%)	16 (6%)	26 22
1	9-A	291/293 (99%)	272 (94%)	19 (6%)	21 17
1	9-B	291/293 (99%)	272 (94%)	19 (6%)	21 17
1	9-C	289/293 (99%)	262 (91%)	27 (9%)	11 7
1	9-D	285/293 (97%)	269 (94%)	16 (6%)	26 22
1	9-E	286/293 (98%)	267 (93%)	19 (7%)	21 17
1	9-F	284/293 (97%)	263 (93%)	21 (7%)	17 13
1	9-G	285/293 (97%)	271 (95%)	14 (5%)	31 28
1	9-H	287/293 (98%)	271 (94%)	16 (6%)	26 22
1	10-A	291/293 (99%)	263 (90%)	28 (10%)	10 6
1	10-B	291/293 (99%)	270 (93%)	21 (7%)	18 14
1	10-C	289/293 (99%)	268 (93%)	21 (7%)	17 13
1	10-D	285/293 (97%)	263 (92%)	22 (8%)	16 12
1	10-E	286/293 (98%)	271 (95%)	15 (5%)	29 25
1	10-F	284/293 (97%)	266 (94%)	18 (6%)	22 18
1	10-G	285/293 (97%)	262 (92%)	23 (8%)	15 10
1	10-H	287/293 (98%)	270 (94%)	17 (6%)	24 20
All	All	22980/23440 (98%)	21389 (93%)	1591 (7%)	19 15

5 of 1591 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5-D	264	ARG
1	6-E	116	ARG
1	10-B	284	GLN
1	5-E	43	ARG
1	6-A	179	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 186 such sidechains are listed below:

Mol	Chain	Res	Type
1	5-D	147	ASN
1	6-D	113	GLN
1	10-B	284	GLN
1	5-E	113	GLN

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Mol	Chain	Res	Type
1	5-G	367	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

80 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	1-A	197	1	23,24,25	2.64	7 (30%)	28,32,34	1.38	6 (21%)
1	LLP	1-B	197	1	23,24,25	2.80	8 (34%)	28,32,34	1.23	1 (3%)
1	LLP	1-C	197	1	23,24,25	2.69	7 (30%)	28,32,34	1.38	5 (17%)
1	LLP	1-D	197	1	23,24,25	2.69	6 (26%)	28,32,34	1.12	4 (14%)
1	LLP	1-E	197	1	23,24,25	2.70	7 (30%)	28,32,34	1.15	5 (17%)
1	LLP	1-F	197	1	23,24,25	2.74	8 (34%)	28,32,34	1.30	5 (17%)
1	LLP	1-G	197	1	23,24,25	2.82	7 (30%)	28,32,34	1.19	4 (14%)
1	LLP	1-H	197	1	23,24,25	2.68	5 (21%)	28,32,34	1.22	4 (14%)
1	LLP	10-A	197	1	23,24,25	2.80	7 (30%)	28,32,34	1.23	3 (10%)
1	LLP	10-B	197	1	23,24,25	2.75	7 (30%)	28,32,34	1.37	6 (21%)
1	LLP	10-C	197	1	23,24,25	2.78	7 (30%)	28,32,34	1.26	3 (10%)
1	LLP	10-D	197	1	23,24,25	2.69	5 (21%)	28,32,34	1.06	3 (10%)
1	LLP	10-E	197	1	23,24,25	2.73	6 (26%)	28,32,34	1.11	3 (10%)
1	LLP	10-F	197	1	23,24,25	2.74	8 (34%)	28,32,34	1.26	5 (17%)
1	LLP	10-G	197	1	23,24,25	2.79	6 (26%)	28,32,34	1.41	3 (10%)
1	LLP	10-H	197	1	23,24,25	2.77	7 (30%)	28,32,34	1.29	3 (10%)
1	LLP	2-A	197	1	23,24,25	2.85	7 (30%)	28,32,34	1.40	2 (7%)
1	LLP	2-B	197	1	23,24,25	2.80	6 (26%)	28,32,34	1.16	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LLP	2-C	197	1	23,24,25	2.77	7 (30%)	28,32,34	1.33	4 (14%)
1	LLP	2-D	197	1	23,24,25	2.67	6 (26%)	28,32,34	1.13	4 (14%)
1	LLP	2-E	197	1	23,24,25	2.83	7 (30%)	28,32,34	1.31	3 (10%)
1	LLP	2-F	197	1	23,24,25	2.75	7 (30%)	28,32,34	1.34	6 (21%)
1	LLP	2-G	197	1	23,24,25	2.86	7 (30%)	28,32,34	1.21	2 (7%)
1	LLP	2-H	197	1	23,24,25	2.67	9 (39%)	28,32,34	1.62	8 (28%)
1	LLP	3-A	197	1	23,24,25	2.79	7 (30%)	28,32,34	1.36	5 (17%)
1	LLP	3-B	197	1	23,24,25	2.84	7 (30%)	28,32,34	1.45	5 (17%)
1	LLP	3-C	197	1	23,24,25	2.73	7 (30%)	28,32,34	1.38	5 (17%)
1	LLP	3-D	197	1	23,24,25	2.67	5 (21%)	28,32,34	1.15	4 (14%)
1	LLP	3-E	197	1	23,24,25	2.86	7 (30%)	28,32,34	1.18	2 (7%)
1	LLP	3-F	197	1	23,24,25	2.73	7 (30%)	28,32,34	1.27	4 (14%)
1	LLP	3-G	197	1	23,24,25	2.78	8 (34%)	28,32,34	1.27	4 (14%)
1	LLP	3-H	197	1	23,24,25	2.87	7 (30%)	28,32,34	1.28	3 (10%)
1	LLP	4-A	197	1	23,24,25	2.73	6 (26%)	28,32,34	1.37	4 (14%)
1	LLP	4-B	197	1	23,24,25	2.78	7 (30%)	28,32,34	1.25	3 (10%)
1	LLP	4-C	197	1	23,24,25	2.90	7 (30%)	28,32,34	1.46	5 (17%)
1	LLP	4-D	197	1	23,24,25	2.63	6 (26%)	28,32,34	1.23	2 (7%)
1	LLP	4-E	197	1	23,24,25	2.76	7 (30%)	28,32,34	1.25	4 (14%)
1	LLP	4-F	197	1	23,24,25	2.74	8 (34%)	28,32,34	1.28	6 (21%)
1	LLP	4-G	197	1	23,24,25	2.75	7 (30%)	28,32,34	1.30	3 (10%)
1	LLP	4-H	197	1	23,24,25	2.89	7 (30%)	28,32,34	1.31	3 (10%)
1	LLP	5-A	197	1	23,24,25	2.84	6 (26%)	28,32,34	1.25	4 (14%)
1	LLP	5-B	197	1	23,24,25	2.81	7 (30%)	28,32,34	1.16	3 (10%)
1	LLP	5-C	197	1	23,24,25	2.75	7 (30%)	28,32,34	1.45	6 (21%)
1	LLP	5-D	197	1	23,24,25	2.64	6 (26%)	28,32,34	1.29	4 (14%)
1	LLP	5-E	197	1	23,24,25	2.71	7 (30%)	28,32,34	1.19	5 (17%)
1	LLP	5-F	197	1	23,24,25	2.56	6 (26%)	28,32,34	1.35	5 (17%)
1	LLP	5-G	197	1	23,24,25	2.74	8 (34%)	28,32,34	1.36	3 (10%)
1	LLP	5-H	197	1	23,24,25	2.70	6 (26%)	28,32,34	1.35	4 (14%)
1	LLP	6-A	197	1	23,24,25	2.76	7 (30%)	28,32,34	1.29	4 (14%)
1	LLP	6-B	197	1	23,24,25	2.70	6 (26%)	28,32,34	1.31	4 (14%)
1	LLP	6-C	197	1	23,24,25	2.91	7 (30%)	28,32,34	1.44	6 (21%)
1	LLP	6-D	197	1	23,24,25	2.67	5 (21%)	28,32,34	1.20	4 (14%)
1	LLP	6-E	197	1	23,24,25	2.70	6 (26%)	28,32,34	1.21	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LLP	6-F	197	1	23,24,25	2.76	8 (34%)	28,32,34	1.25	5 (17%)
1	LLP	6-G	197	1	23,24,25	2.81	7 (30%)	28,32,34	1.34	4 (14%)
1	LLP	6-H	197	1	23,24,25	2.73	8 (34%)	28,32,34	1.32	4 (14%)
1	LLP	7-A	197	1	23,24,25	2.83	6 (26%)	28,32,34	1.35	5 (17%)
1	LLP	7-B	197	1	23,24,25	2.73	6 (26%)	28,32,34	1.35	4 (14%)
1	LLP	7-C	197	1	23,24,25	2.73	6 (26%)	28,32,34	1.31	4 (14%)
1	LLP	7-D	197	1	23,24,25	2.72	6 (26%)	28,32,34	1.56	6 (21%)
1	LLP	7-E	197	1	23,24,25	2.77	7 (30%)	28,32,34	1.13	2 (7%)
1	LLP	7-F	197	1	23,24,25	2.79	8 (34%)	28,32,34	1.34	5 (17%)
1	LLP	7-G	197	1	23,24,25	2.83	7 (30%)	28,32,34	1.23	3 (10%)
1	LLP	7-H	197	1	23,24,25	2.75	7 (30%)	28,32,34	1.58	7 (25%)
1	LLP	8-A	197	1	23,24,25	2.80	8 (34%)	28,32,34	1.30	4 (14%)
1	LLP	8-B	197	1	23,24,25	2.74	7 (30%)	28,32,34	1.23	4 (14%)
1	LLP	8-C	197	1	23,24,25	2.78	7 (30%)	28,32,34	1.27	4 (14%)
1	LLP	8-D	197	1	23,24,25	2.66	7 (30%)	28,32,34	1.38	6 (21%)
1	LLP	8-E	197	1	23,24,25	2.77	6 (26%)	28,32,34	1.19	4 (14%)
1	LLP	8-F	197	1	23,24,25	2.71	8 (34%)	28,32,34	1.35	5 (17%)
1	LLP	8-G	197	1	23,24,25	2.70	7 (30%)	28,32,34	1.37	5 (17%)
1	LLP	8-H	197	1	23,24,25	2.77	8 (34%)	28,32,34	1.29	4 (14%)
1	LLP	9-A	197	1	23,24,25	2.71	7 (30%)	28,32,34	1.25	5 (17%)
1	LLP	9-B	197	1	23,24,25	2.49	6 (26%)	28,32,34	1.59	7 (25%)
1	LLP	9-C	197	1	23,24,25	2.81	6 (26%)	28,32,34	1.14	3 (10%)
1	LLP	9-D	197	1	23,24,25	2.61	5 (21%)	28,32,34	1.18	4 (14%)
1	LLP	9-E	197	1	23,24,25	2.72	7 (30%)	28,32,34	1.24	5 (17%)
1	LLP	9-F	197	1	23,24,25	2.74	8 (34%)	28,32,34	1.29	5 (17%)
1	LLP	9-G	197	1	23,24,25	2.80	6 (26%)	28,32,34	1.18	3 (10%)
1	LLP	9-H	197	1	23,24,25	2.74	8 (34%)	28,32,34	1.26	4 (14%)

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
1	LLP	1-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-B	197	1	-	0/15/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	1-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-D	197	1	-	0/15/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	5-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-H	197	1	-	0/15/17/19	0/1/1/1

The worst 5 of 545 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-C	197	LLP	C4-C5	-3.90	1.36	1.42
1	4-C	197	LLP	C4-C5	-3.82	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	197	LLP	C4-C5	-3.82	1.36	1.42
1	5-A	197	LLP	C4-C5	-3.76	1.36	1.42
1	9-A	197	LLP	C4-C5	-3.66	1.37	1.42

The worst 5 of 333 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	197	LLP	CE-NZ-C4'	-4.05	107.28	118.97
1	7-H	197	LLP	CG-CB-CA	-3.96	97.52	114.16
1	4-G	197	LLP	CE-NZ-C4'	-3.83	107.91	118.97
1	9-B	197	LLP	CE-NZ-C4'	-3.78	108.05	118.97
1	10-G	197	LLP	CE-NZ-C4'	-3.77	108.09	118.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

62 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1-A	197	LLP	2	0
1	1-D	197	LLP	3	0
1	1-E	197	LLP	1	0
1	1-F	197	LLP	1	0
1	1-G	197	LLP	3	0
1	1-H	197	LLP	2	0
1	10-B	197	LLP	2	0
1	10-C	197	LLP	2	0
1	10-D	197	LLP	1	0
1	10-E	197	LLP	2	0
1	10-F	197	LLP	2	0
1	10-G	197	LLP	2	0
1	2-B	197	LLP	1	0
1	2-C	197	LLP	3	0
1	2-D	197	LLP	1	0
1	2-F	197	LLP	2	0
1	2-G	197	LLP	1	0
1	2-H	197	LLP	3	0
1	3-A	197	LLP	1	0
1	3-B	197	LLP	4	0
1	3-C	197	LLP	2	0
1	3-D	197	LLP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	3-E	197	LLP	1	0
1	3-G	197	LLP	1	0
1	3-H	197	LLP	1	0
1	4-A	197	LLP	1	0
1	4-C	197	LLP	1	0
1	4-E	197	LLP	1	0
1	4-F	197	LLP	3	0
1	4-H	197	LLP	3	0
1	5-A	197	LLP	1	0
1	5-B	197	LLP	1	0
1	5-D	197	LLP	1	0
1	5-E	197	LLP	1	0
1	5-F	197	LLP	1	0
1	5-G	197	LLP	1	0
1	5-H	197	LLP	2	0
1	6-A	197	LLP	2	0
1	6-C	197	LLP	1	0
1	6-D	197	LLP	1	0
1	6-E	197	LLP	1	0
1	6-F	197	LLP	2	0
1	6-H	197	LLP	2	0
1	7-A	197	LLP	1	0
1	7-B	197	LLP	1	0
1	7-E	197	LLP	1	0
1	7-F	197	LLP	2	0
1	7-G	197	LLP	2	0
1	7-H	197	LLP	3	0
1	8-A	197	LLP	3	0
1	8-B	197	LLP	3	0
1	8-C	197	LLP	1	0
1	8-D	197	LLP	2	0
1	8-E	197	LLP	1	0
1	8-F	197	LLP	2	0
1	8-H	197	LLP	1	0
1	9-A	197	LLP	2	0
1	9-C	197	LLP	2	0
1	9-D	197	LLP	1	0
1	9-E	197	LLP	1	0
1	9-F	197	LLP	3	0
1	9-H	197	LLP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 494 ligands modelled in this entry, 107 are monoatomic - leaving 387 for Mogul analysis.

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	$\#\|Z\| > 2$
2	MES	1-A	401	-	11,12,12	0.81	0	14,16,16	2.44	5 (35%)
3	GOL	1-A	402	-	5,5,5	0.33	0	5,5,5	0.20	0
3	GOL	1-A	403	-	5,5,5	0.36	0	5,5,5	0.43	0
3	GOL	1-A	404	-	5,5,5	0.40	0	5,5,5	0.38	0
2	MES	1-B	401	-	11,12,12	0.75	0	14,16,16	2.05	5 (35%)
3	GOL	1-B	402	-	5,5,5	0.37	0	5,5,5	0.37	0
3	GOL	1-B	403	-	5,5,5	0.37	0	5,5,5	0.23	0
3	GOL	1-B	404	-	5,5,5	0.30	0	5,5,5	0.74	0
3	GOL	1-B	405	-	5,5,5	0.37	0	5,5,5	0.50	0
3	GOL	1-B	406	-	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	1-B	407	-	5,5,5	0.38	0	5,5,5	0.37	0
4	GOL	1-B	408	-	5,5,5	0.35	0	5,5,5	0.25	0
2	MES	1-C	401	-	11,12,12	0.72	0	14,16,16	2.61	7 (50%)
3	GOL	1-C	402	-	5,5,5	0.30	0	5,5,5	0.36	0
3	FMT	1-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	1-D	401	-	11,12,12	0.76	0	14,16,16	2.53	7 (50%)
3	GOL	1-D	402	-	5,5,5	0.40	0	5,5,5	0.37	0
3	GOL	1-D	403	-	5,5,5	1.03	0	5,5,5	1.22	1 (20%)
3	GOL	1-D	404	-	5,5,5	0.42	0	5,5,5	0.13	0
2	MES	1-E	401	-	11,12,12	0.77	0	14,16,16	2.53	4 (28%)
3	GOL	1-E	402	-	5,5,5	0.26	0	5,5,5	0.65	0
3	GOL	1-E	403	-	5,5,5	0.39	0	5,5,5	0.18	0
2	MES	1-F	401	-	11,12,12	0.73	0	14,16,16	3.09	7 (50%)
3	GOL	1-F	402	-	5,5,5	0.39	0	5,5,5	0.21	0
3	GOL	1-F	403	-	5,5,5	0.34	0	5,5,5	0.43	0
3	GOL	1-F	404	-	5,5,5	0.37	0	5,5,5	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	1-F	405	-	5,5,5	0.35	0	5,5,5	0.28	0
3	GOL	1-F	406	-	5,5,5	1.39	1 (20%)	5,5,5	1.46	1 (20%)
5	GOL	1-F	407	-	5,5,5	0.38	0	5,5,5	0.25	0
4	FMT	1-F	408	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	1-G	401	-	11,12,12	0.69	0	14,16,16	2.25	6 (42%)
3	GOL	1-G	402	-	5,5,5	0.45	0	5,5,5	0.58	0
3	GOL	1-G	403	-	5,5,5	0.41	0	5,5,5	0.47	0
3	GOL	1-G	404	-	5,5,5	0.40	0	5,5,5	0.33	0
5	GOL	1-G	405	-	5,5,5	0.32	0	5,5,5	0.53	0
4	FMT	1-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	1-H	401	-	11,12,12	0.71	0	14,16,16	2.18	7 (50%)
3	GOL	1-H	402	-	5,5,5	0.40	0	5,5,5	0.42	0
3	GOL	1-H	403	-	5,5,5	0.35	0	5,5,5	0.24	0
2	MES	10-A	401	-	11,12,12	0.70	0	14,16,16	1.95	5 (35%)
3	GOL	10-A	402	-	5,5,5	0.33	0	5,5,5	0.19	0
3	GOL	10-A	403	-	5,5,5	0.39	0	5,5,5	0.34	0
3	GOL	10-A	404	-	5,5,5	0.34	0	5,5,5	0.55	0
2	MES	10-B	401	-	11,12,12	0.81	0	14,16,16	2.32	6 (42%)
3	GOL	10-B	402	-	5,5,5	0.33	0	5,5,5	0.25	0
3	GOL	10-B	403	-	5,5,5	0.27	0	5,5,5	0.53	0
3	GOL	10-B	404	-	5,5,5	0.29	0	5,5,5	0.50	0
3	GOL	10-B	405	-	5,5,5	0.38	0	5,5,5	0.33	0
3	GOL	10-B	406	-	5,5,5	0.33	0	5,5,5	0.43	0
3	GOL	10-B	407	-	5,5,5	0.39	0	5,5,5	0.38	0
2	MES	10-C	401	-	11,12,12	0.73	0	14,16,16	4.30	5 (35%)
3	GOL	10-C	402	-	5,5,5	0.28	0	5,5,5	0.36	0
3	GOL	10-C	403	-	5,5,5	0.34	0	5,5,5	0.21	0
5	FMT	10-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	10-D	401	-	11,12,12	0.72	0	14,16,16	2.09	5 (35%)
3	GOL	10-D	402	-	5,5,5	0.43	0	5,5,5	0.50	0
3	GOL	10-D	403	-	5,5,5	0.28	0	5,5,5	0.45	0
3	GOL	10-D	404	-	5,5,5	0.27	0	5,5,5	0.21	0
2	MES	10-E	401	-	11,12,12	0.64	0	14,16,16	2.67	6 (42%)
3	GOL	10-E	402	-	5,5,5	0.23	0	5,5,5	0.83	0
3	GOL	10-E	403	-	5,5,5	0.34	0	5,5,5	0.48	0
2	MES	10-F	401	-	11,12,12	0.82	0	14,16,16	2.99	8 (57%)
3	GOL	10-F	402	-	5,5,5	0.36	0	5,5,5	0.27	0
3	GOL	10-F	403	-	5,5,5	0.38	0	5,5,5	0.44	0
3	GOL	10-F	404	-	5,5,5	0.38	0	5,5,5	0.22	0
3	GOL	10-F	405	-	5,5,5	0.39	0	5,5,5	0.38	0
3	GOL	10-F	406	-	5,5,5	0.30	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FMT	10-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	10-G	401	-	11,12,12	0.66	0	14,16,16	3.06	8 (57%)
3	GOL	10-G	402	-	5,5,5	0.34	0	5,5,5	0.86	0
3	GOL	10-G	403	-	5,5,5	0.37	0	5,5,5	0.42	0
3	GOL	10-G	404	-	5,5,5	0.35	0	5,5,5	0.32	0
5	FMT	10-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	10-H	401	-	11,12,12	0.65	0	14,16,16	2.48	4 (28%)
3	GOL	10-H	402	-	5,5,5	0.38	0	5,5,5	0.34	0
3	GOL	10-H	403	-	5,5,5	0.39	0	5,5,5	0.68	0
3	GOL	10-H	404	-	5,5,5	0.21	0	5,5,5	0.36	0
3	GOL	10-H	405	-	5,5,5	0.33	0	5,5,5	0.40	0
2	MES	2-A	401	-	11,12,12	0.66	0	14,16,16	1.82	3 (21%)
3	GOL	2-A	402	-	5,5,5	0.39	0	5,5,5	0.31	0
3	GOL	2-A	403	-	5,5,5	0.32	0	5,5,5	0.45	0
3	GOL	2-A	404	-	5,5,5	0.35	0	5,5,5	0.32	0
2	MES	2-B	401	-	11,12,12	0.82	0	14,16,16	2.14	5 (35%)
3	GOL	2-B	402	-	5,5,5	0.31	0	5,5,5	0.39	0
3	GOL	2-B	403	-	5,5,5	1.03	0	5,5,5	2.63	3 (60%)
3	GOL	2-B	404	-	5,5,5	0.40	0	5,5,5	0.39	0
3	GOL	2-B	405	-	5,5,5	0.33	0	5,5,5	0.27	0
3	GOL	2-B	406	-	5,5,5	0.42	0	5,5,5	0.26	0
3	GOL	2-B	407	-	5,5,5	0.38	0	5,5,5	0.34	0
2	MES	2-C	401	-	11,12,12	0.71	0	14,16,16	2.30	6 (42%)
3	GOL	2-C	402	-	5,5,5	0.35	0	5,5,5	0.45	0
3	GOL	2-C	403	-	5,5,5	0.43	0	5,5,5	0.21	0
5	GOL	2-C	404	-	5,5,5	0.36	0	5,5,5	0.24	0
4	FMT	2-C	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	2-D	401	-	11,12,12	0.75	0	14,16,16	3.03	7 (50%)
3	GOL	2-D	402	-	5,5,5	0.40	0	5,5,5	0.43	0
3	GOL	2-D	403	-	5,5,5	0.33	0	5,5,5	0.31	0
2	MES	2-E	401	-	11,12,12	0.59	0	14,16,16	3.12	5 (35%)
3	GOL	2-E	402	-	5,5,5	0.25	0	5,5,5	0.31	0
3	GOL	2-E	403	-	5,5,5	0.36	0	5,5,5	0.41	0
4	GOL	2-E	404	-	5,5,5	0.32	0	5,5,5	0.32	0
2	MES	2-F	401	-	11,12,12	0.79	0	14,16,16	3.19	7 (50%)
3	GOL	2-F	402	-	5,5,5	0.36	0	5,5,5	0.64	0
3	GOL	2-F	403	-	5,5,5	0.44	0	5,5,5	0.36	0
3	GOL	2-F	404	-	5,5,5	0.43	0	5,5,5	0.12	0
3	GOL	2-F	405	-	5,5,5	0.35	0	5,5,5	0.22	0
3	FMT	2-F	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	2-G	401	-	11,12,12	0.76	0	14,16,16	2.53	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	2-G	402	-	5,5,5	0.34	0	5,5,5	0.41	0
3	GOL	2-G	403	-	5,5,5	0.33	0	5,5,5	0.54	0
3	GOL	2-G	404	-	5,5,5	1.23	0	5,5,5	0.87	0
5	FMT	2-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	2-H	401	-	11,12,12	0.72	0	14,16,16	2.15	5 (35%)
3	GOL	2-H	402	-	5,5,5	0.36	0	5,5,5	0.20	0
3	GOL	2-H	403	-	5,5,5	1.15	1 (20%)	5,5,5	1.04	0
3	GOL	2-H	404	-	5,5,5	0.23	0	5,5,5	0.50	0
2	MES	3-A	401	-	11,12,12	0.67	0	14,16,16	2.27	5 (35%)
3	GOL	3-A	402	-	5,5,5	0.23	0	5,5,5	0.21	0
3	GOL	3-A	403	-	5,5,5	0.33	0	5,5,5	0.31	0
3	GOL	3-A	404	-	5,5,5	0.32	0	5,5,5	0.35	0
4	GOL	3-A	405	-	5,5,5	0.36	0	5,5,5	0.22	0
2	MES	3-B	401	-	11,12,12	0.54	0	14,16,16	4.80	7 (50%)
3	GOL	3-B	402	-	5,5,5	0.39	0	5,5,5	0.35	0
3	GOL	3-B	403	-	5,5,5	0.35	0	5,5,5	0.49	0
3	GOL	3-B	404	-	5,5,5	0.31	0	5,5,5	0.17	0
3	GOL	3-B	405	-	5,5,5	0.38	0	5,5,5	0.39	0
3	GOL	3-B	406	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	3-B	407	-	5,5,5	0.26	0	5,5,5	0.43	0
2	MES	3-C	401	-	11,12,12	0.62	0	14,16,16	4.73	7 (50%)
3	GOL	3-C	402	-	5,5,5	0.40	0	5,5,5	0.30	0
3	GOL	3-C	403	-	5,5,5	0.26	0	5,5,5	0.64	0
5	FMT	3-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	3-D	401	-	11,12,12	0.53	0	14,16,16	3.03	7 (50%)
3	GOL	3-D	402	-	5,5,5	0.40	0	5,5,5	0.62	0
3	GOL	3-D	403	-	5,5,5	0.35	0	5,5,5	0.20	0
2	MES	3-E	401	-	11,12,12	0.67	0	14,16,16	4.32	9 (64%)
3	GOL	3-E	402	-	5,5,5	0.40	0	5,5,5	0.41	0
3	GOL	3-E	403	-	5,5,5	0.32	0	5,5,5	0.74	0
4	GOL	3-E	404	-	5,5,5	0.42	0	5,5,5	0.22	0
2	MES	3-F	401	-	11,12,12	0.77	0	14,16,16	3.46	5 (35%)
3	GOL	3-F	402	-	5,5,5	0.32	0	5,5,5	0.19	0
3	GOL	3-F	403	-	5,5,5	0.34	0	5,5,5	0.40	0
3	GOL	3-F	404	-	5,5,5	0.40	0	5,5,5	0.48	0
3	GOL	3-F	405	-	5,5,5	0.26	0	5,5,5	0.88	0
3	GOL	3-F	406	-	5,5,5	0.37	0	5,5,5	0.29	0
5	FMT	3-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	3-G	401	-	11,12,12	0.66	0	14,16,16	2.10	5 (35%)
3	GOL	3-G	402	-	5,5,5	0.41	0	5,5,5	0.39	0
3	GOL	3-G	403	-	5,5,5	0.30	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	3-G	404	-	5,5,5	0.34	0	5,5,5	0.31	0
5	GOL	3-G	405	-	5,5,5	0.28	0	5,5,5	0.34	0
4	FMT	3-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	3-H	401	-	11,12,12	0.61	0	14,16,16	3.86	7 (50%)
3	GOL	3-H	402	-	5,5,5	0.37	0	5,5,5	0.45	0
3	GOL	3-H	403	-	5,5,5	0.38	0	5,5,5	0.30	0
2	MES	4-A	401	-	11,12,12	0.68	0	14,16,16	2.54	6 (42%)
3	GOL	4-A	402	-	5,5,5	0.31	0	5,5,5	0.30	0
3	GOL	4-A	403	-	5,5,5	0.34	0	5,5,5	0.55	0
3	GOL	4-A	404	-	5,5,5	0.38	0	5,5,5	0.52	0
2	MES	4-B	401	-	11,12,12	0.75	0	14,16,16	2.26	6 (42%)
3	GOL	4-B	402	-	5,5,5	0.34	0	5,5,5	0.37	0
3	GOL	4-B	403	-	5,5,5	0.49	0	5,5,5	0.79	0
3	GOL	4-B	404	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	4-B	405	-	5,5,5	0.35	0	5,5,5	0.30	0
3	GOL	4-B	406	-	5,5,5	0.34	0	5,5,5	0.51	0
3	GOL	4-B	407	-	5,5,5	0.44	0	5,5,5	0.38	0
2	MES	4-C	401	-	11,12,12	0.57	0	14,16,16	3.96	5 (35%)
3	GOL	4-C	402	-	5,5,5	0.37	0	5,5,5	0.22	0
3	GOL	4-C	403	-	5,5,5	0.38	0	5,5,5	0.33	0
5	GOL	4-C	404	-	5,5,5	0.43	0	5,5,5	0.66	0
4	FMT	4-C	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	4-D	401	-	11,12,12	0.79	0	14,16,16	2.97	5 (35%)
3	GOL	4-D	402	-	5,5,5	0.35	0	5,5,5	0.40	0
3	GOL	4-D	403	-	5,5,5	0.27	0	5,5,5	0.51	0
2	MES	4-E	401	-	11,12,12	0.77	0	14,16,16	1.81	4 (28%)
3	GOL	4-E	402	-	5,5,5	0.28	0	5,5,5	0.33	0
3	GOL	4-E	403	-	5,5,5	0.44	0	5,5,5	0.57	0
4	GOL	4-E	404	-	5,5,5	0.56	0	5,5,5	0.41	0
2	MES	4-F	401	-	11,12,12	0.82	0	14,16,16	2.37	5 (35%)
3	GOL	4-F	402	-	5,5,5	0.37	0	5,5,5	0.34	0
3	GOL	4-F	403	-	5,5,5	0.42	0	5,5,5	0.25	0
3	GOL	4-F	404	-	5,5,5	0.28	0	5,5,5	0.62	0
3	FMT	4-F	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	4-G	401	-	11,12,12	0.64	0	14,16,16	2.92	4 (28%)
3	GOL	4-G	402	-	5,5,5	0.38	0	5,5,5	0.28	0
3	GOL	4-G	403	-	5,5,5	0.35	0	5,5,5	0.35	0
3	GOL	4-G	404	-	5,5,5	0.38	0	5,5,5	0.65	0
5	GOL	4-G	405	-	5,5,5	0.44	0	5,5,5	0.28	0
4	GOL	4-G	406	-	5,5,5	0.38	0	5,5,5	0.22	0
4	FMT	4-G	407	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MES	4-H	401	-	11,12,12	0.61	0	14,16,16	2.38	7 (50%)
3	GOL	4-H	402	-	5,5,5	0.44	0	5,5,5	0.26	0
3	GOL	4-H	403	-	5,5,5	0.31	0	5,5,5	0.40	0
3	GOL	4-H	404	-	5,5,5	0.32	0	5,5,5	0.26	0
2	MES	5-A	401	-	11,12,12	0.65	0	14,16,16	2.37	5 (35%)
3	GOL	5-A	402	-	5,5,5	0.28	0	5,5,5	0.34	0
3	GOL	5-A	403	-	5,5,5	0.39	0	5,5,5	0.44	0
3	GOL	5-A	404	-	5,5,5	0.36	0	5,5,5	0.42	0
4	GOL	5-A	405	-	5,5,5	0.35	0	5,5,5	0.29	0
2	MES	5-B	401	-	11,12,12	0.90	0	14,16,16	2.53	7 (50%)
3	GOL	5-B	402	-	5,5,5	0.34	0	5,5,5	0.31	0
3	GOL	5-B	403	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	5-B	404	-	5,5,5	0.33	0	5,5,5	0.43	0
3	GOL	5-B	405	-	5,5,5	0.46	0	5,5,5	0.53	0
3	GOL	5-B	406	-	5,5,5	0.43	0	5,5,5	0.22	0
3	GOL	5-B	407	-	5,5,5	0.20	0	5,5,5	0.45	0
2	MES	5-C	401	-	11,12,12	0.86	0	14,16,16	2.38	6 (42%)
3	GOL	5-C	402	-	5,5,5	0.30	0	5,5,5	0.31	0
3	FMT	5-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	5-D	401	-	11,12,12	0.54	0	14,16,16	3.79	5 (35%)
3	GOL	5-D	402	-	5,5,5	0.31	0	5,5,5	0.33	0
3	GOL	5-D	403	-	5,5,5	0.34	0	5,5,5	0.56	0
3	GOL	5-D	404	-	5,5,5	0.37	0	5,5,5	0.62	0
2	MES	5-E	401	-	11,12,12	0.83	0	14,16,16	2.68	8 (57%)
3	GOL	5-E	402	-	5,5,5	0.47	0	5,5,5	0.27	0
3	GOL	5-E	403	-	5,5,5	0.35	0	5,5,5	0.25	0
4	GOL	5-E	404	-	5,5,5	0.36	0	5,5,5	0.28	0
2	MES	5-F	401	-	11,12,12	0.63	0	14,16,16	2.69	4 (28%)
3	GOL	5-F	402	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	5-F	403	-	5,5,5	0.46	0	5,5,5	0.10	0
3	GOL	5-F	404	-	5,5,5	0.33	0	5,5,5	0.40	0
3	FMT	5-F	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	5-G	401	-	11,12,12	0.75	0	14,16,16	3.35	11 (78%)
3	GOL	5-G	402	-	5,5,5	0.27	0	5,5,5	0.66	0
3	GOL	5-G	403	-	5,5,5	0.42	0	5,5,5	0.20	0
3	GOL	5-G	404	-	5,5,5	0.42	0	5,5,5	0.38	0
5	GOL	5-G	405	-	5,5,5	0.37	0	5,5,5	0.32	0
4	FMT	5-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	5-H	401	-	11,12,12	0.69	0	14,16,16	3.40	6 (42%)
3	GOL	5-H	402	-	5,5,5	0.41	0	5,5,5	0.17	0
3	GOL	5-H	403	-	5,5,5	0.51	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	5-H	404	-	5,5,5	0.39	0	5,5,5	0.43	0
2	MES	6-A	401	-	11,12,12	0.73	0	14,16,16	2.41	6 (42%)
3	GOL	6-A	402	-	5,5,5	0.32	0	5,5,5	0.34	0
3	GOL	6-A	403	-	5,5,5	0.39	0	5,5,5	0.68	0
3	GOL	6-A	404	-	5,5,5	0.34	0	5,5,5	0.33	0
4	GOL	6-A	405	-	5,5,5	0.40	0	5,5,5	0.20	0
2	MES	6-B	401	-	11,12,12	0.57	0	14,16,16	2.09	6 (42%)
3	GOL	6-B	402	-	5,5,5	0.32	0	5,5,5	0.27	0
3	GOL	6-B	403	-	5,5,5	0.33	0	5,5,5	0.38	0
3	GOL	6-B	404	-	5,5,5	0.26	0	5,5,5	0.47	0
3	GOL	6-B	405	-	5,5,5	0.40	0	5,5,5	0.37	0
3	GOL	6-B	406	-	5,5,5	0.35	0	5,5,5	0.33	0
3	GOL	6-B	407	-	5,5,5	0.36	0	5,5,5	0.18	0
2	MES	6-C	401	-	11,12,12	0.77	0	14,16,16	3.20	7 (50%)
3	GOL	6-C	402	-	5,5,5	0.27	0	5,5,5	0.41	0
3	FMT	6-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	6-D	401	-	11,12,12	0.72	0	14,16,16	2.97	7 (50%)
3	GOL	6-D	402	-	5,5,5	0.42	0	5,5,5	0.47	0
3	GOL	6-D	403	-	5,5,5	0.22	0	5,5,5	0.61	0
3	GOL	6-D	404	-	5,5,5	0.36	0	5,5,5	0.38	0
2	MES	6-E	401	-	11,12,12	0.70	0	14,16,16	3.56	6 (42%)
3	GOL	6-E	402	-	5,5,5	0.39	0	5,5,5	0.37	0
3	GOL	6-E	403	-	5,5,5	0.36	0	5,5,5	0.18	0
4	GOL	6-E	404	-	5,5,5	0.44	0	5,5,5	0.19	0
2	MES	6-F	401	-	11,12,12	0.68	0	14,16,16	2.40	4 (28%)
3	GOL	6-F	402	-	5,5,5	0.41	0	5,5,5	0.31	0
3	GOL	6-F	403	-	5,5,5	0.38	0	5,5,5	0.56	0
3	GOL	6-F	404	-	5,5,5	0.23	0	5,5,5	0.54	0
3	GOL	6-F	405	-	5,5,5	0.36	0	5,5,5	0.23	0
3	GOL	6-F	406	-	5,5,5	0.33	0	5,5,5	0.23	0
5	FMT	6-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	6-G	401	-	11,12,12	0.69	0	14,16,16	2.81	5 (35%)
3	GOL	6-G	402	-	5,5,5	0.46	0	5,5,5	0.31	0
3	GOL	6-G	403	-	5,5,5	0.35	0	5,5,5	0.53	0
3	FMT	6-G	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	6-H	401	-	11,12,12	0.69	0	14,16,16	1.73	4 (28%)
3	GOL	6-H	402	-	5,5,5	0.84	0	5,5,5	0.39	0
3	GOL	6-H	403	-	5,5,5	0.40	0	5,5,5	0.91	0
3	GOL	6-H	404	-	5,5,5	0.27	0	5,5,5	0.43	0
3	GOL	6-H	405	-	5,5,5	0.53	0	5,5,5	0.31	0
2	MES	7-A	401	-	11,12,12	0.72	0	14,16,16	1.83	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	7-A	402	-	5,5,5	0.34	0	5,5,5	0.20	0
3	GOL	7-A	403	-	5,5,5	0.34	0	5,5,5	0.20	0
3	GOL	7-A	404	-	5,5,5	0.33	0	5,5,5	0.30	0
4	GOL	7-A	405	-	5,5,5	0.36	0	5,5,5	0.28	0
2	MES	7-B	401	-	11,12,12	0.64	0	14,16,16	2.32	5 (35%)
3	GOL	7-B	402	-	5,5,5	0.40	0	5,5,5	0.28	0
3	GOL	7-B	403	-	5,5,5	0.34	0	5,5,5	0.40	0
3	GOL	7-B	404	-	5,5,5	0.28	0	5,5,5	0.73	0
3	GOL	7-B	405	-	5,5,5	0.48	0	5,5,5	0.12	0
3	GOL	7-B	406	-	5,5,5	0.38	0	5,5,5	0.27	0
3	GOL	7-B	407	-	5,5,5	0.35	0	5,5,5	0.24	0
2	MES	7-C	401	-	11,12,12	0.69	0	14,16,16	2.30	4 (28%)
3	GOL	7-C	402	-	5,5,5	0.30	0	5,5,5	0.55	0
3	FMT	7-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	7-D	401	-	11,12,12	0.80	0	14,16,16	3.04	7 (50%)
3	GOL	7-D	402	-	5,5,5	0.33	0	5,5,5	0.69	0
3	GOL	7-D	403	-	5,5,5	0.44	0	5,5,5	0.55	0
3	GOL	7-D	404	-	5,5,5	0.25	0	5,5,5	0.82	0
2	MES	7-E	401	-	11,12,12	0.62	0	14,16,16	3.02	5 (35%)
3	GOL	7-E	402	-	5,5,5	0.67	0	5,5,5	0.67	0
3	GOL	7-E	403	-	5,5,5	0.41	0	5,5,5	0.61	0
4	GOL	7-E	404	-	5,5,5	0.55	0	5,5,5	0.26	0
2	MES	7-F	401	-	11,12,12	0.66	0	14,16,16	2.49	5 (35%)
3	GOL	7-F	402	-	5,5,5	0.37	0	5,5,5	0.25	0
3	GOL	7-F	403	-	5,5,5	0.45	0	5,5,5	0.64	0
3	GOL	7-F	404	-	5,5,5	0.43	0	5,5,5	0.37	0
3	GOL	7-F	405	-	5,5,5	0.32	0	5,5,5	0.27	0
3	GOL	7-F	406	-	5,5,5	0.37	0	5,5,5	0.17	0
5	FMT	7-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	7-G	401	-	11,12,12	0.67	0	14,16,16	2.60	6 (42%)
3	GOL	7-G	402	-	5,5,5	0.42	0	5,5,5	0.36	0
3	GOL	7-G	403	-	5,5,5	0.28	0	5,5,5	0.49	0
3	GOL	7-G	404	-	5,5,5	0.40	0	5,5,5	0.27	0
5	FMT	7-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	7-H	401	-	11,12,12	0.73	0	14,16,16	2.32	5 (35%)
3	GOL	7-H	402	-	5,5,5	0.44	0	5,5,5	0.32	0
3	GOL	7-H	403	-	5,5,5	0.38	0	5,5,5	0.38	0
3	GOL	7-H	404	-	5,5,5	0.32	0	5,5,5	0.23	0
2	MES	8-A	401	-	11,12,12	0.79	0	14,16,16	2.36	6 (42%)
3	GOL	8-A	402	-	5,5,5	0.32	0	5,5,5	0.31	0
3	GOL	8-A	403	-	5,5,5	0.28	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	8-A	404	-	5,5,5	0.40	0	5,5,5	0.22	0
2	MES	8-B	401	-	11,12,12	0.68	0	14,16,16	2.65	4 (28%)
3	GOL	8-B	402	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	8-B	403	-	5,5,5	0.29	0	5,5,5	0.49	0
3	GOL	8-B	404	-	5,5,5	0.32	0	5,5,5	0.59	0
3	GOL	8-B	405	-	5,5,5	0.39	0	5,5,5	0.58	0
3	GOL	8-B	406	-	5,5,5	0.39	0	5,5,5	0.33	0
3	GOL	8-B	407	-	5,5,5	0.68	0	5,5,5	0.64	0
4	GOL	8-B	408	-	5,5,5	0.41	0	5,5,5	0.37	0
2	MES	8-C	401	-	11,12,12	0.79	0	14,16,16	2.94	7 (50%)
3	GOL	8-C	402	-	5,5,5	0.35	0	5,5,5	0.34	0
3	GOL	8-C	403	-	5,5,5	0.37	0	5,5,5	0.27	0
5	FMT	8-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	8-D	401	-	11,12,12	0.77	0	14,16,16	2.37	7 (50%)
3	GOL	8-D	402	-	5,5,5	0.39	0	5,5,5	0.38	0
3	GOL	8-D	403	-	5,5,5	0.41	0	5,5,5	0.31	0
2	MES	8-E	401	-	11,12,12	0.74	0	14,16,16	3.25	6 (42%)
3	GOL	8-E	402	-	5,5,5	0.90	0	5,5,5	1.25	1 (20%)
3	GOL	8-E	403	-	5,5,5	0.60	0	5,5,5	0.84	0
4	GOL	8-E	404	-	5,5,5	0.33	0	5,5,5	0.52	0
2	MES	8-F	401	-	11,12,12	0.79	0	14,16,16	2.44	5 (35%)
3	GOL	8-F	402	-	5,5,5	0.32	0	5,5,5	0.90	0
3	GOL	8-F	403	-	5,5,5	0.47	0	5,5,5	0.26	0
3	GOL	8-F	404	-	5,5,5	0.41	0	5,5,5	0.28	0
3	GOL	8-F	405	-	5,5,5	0.33	0	5,5,5	0.39	0
3	FMT	8-F	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	8-G	401	-	11,12,12	0.65	0	14,16,16	2.59	6 (42%)
3	GOL	8-G	402	-	5,5,5	0.48	0	5,5,5	0.23	0
3	GOL	8-G	403	-	5,5,5	0.38	0	5,5,5	0.19	0
3	GOL	8-G	404	-	5,5,5	0.32	0	5,5,5	0.37	0
5	GOL	8-G	405	-	5,5,5	0.36	0	5,5,5	0.55	0
4	FMT	8-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	8-H	401	-	11,12,12	0.75	0	14,16,16	3.14	5 (35%)
3	GOL	8-H	402	-	5,5,5	0.40	0	5,5,5	0.42	0
3	GOL	8-H	403	-	5,5,5	0.36	0	5,5,5	0.34	0
3	GOL	8-H	404	-	5,5,5	0.26	0	5,5,5	0.71	0
2	MES	9-A	401	-	11,12,12	0.58	0	14,16,16	3.59	10 (71%)
3	GOL	9-A	402	-	5,5,5	0.28	0	5,5,5	0.21	0
3	GOL	9-A	403	-	5,5,5	0.51	0	5,5,5	0.57	0
3	GOL	9-A	404	-	5,5,5	0.35	0	5,5,5	0.40	0
4	GOL	9-A	405	-	5,5,5	0.30	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MES	9-B	401	-	11,12,12	0.75	0	14,16,16	1.77	3 (21%)
3	GOL	9-B	402	-	5,5,5	0.36	0	5,5,5	0.20	0
3	GOL	9-B	403	-	5,5,5	0.41	0	5,5,5	0.39	0
3	GOL	9-B	404	-	5,5,5	0.35	0	5,5,5	0.47	0
3	GOL	9-B	405	-	5,5,5	0.32	0	5,5,5	0.48	0
3	GOL	9-B	406	-	5,5,5	0.32	0	5,5,5	0.23	0
2	MES	9-C	401	-	11,12,12	0.65	0	14,16,16	3.49	5 (35%)
3	GOL	9-C	402	-	5,5,5	0.35	0	5,5,5	0.22	0
3	GOL	9-C	403	-	5,5,5	0.36	0	5,5,5	0.64	0
5	FMT	9-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	9-D	401	-	11,12,12	0.81	0	14,16,16	2.40	6 (42%)
3	GOL	9-D	402	-	5,5,5	0.47	0	5,5,5	0.50	0
3	GOL	9-D	403	-	5,5,5	0.73	0	5,5,5	0.79	0
3	GOL	9-D	404	-	5,5,5	0.30	0	5,5,5	0.33	0
2	MES	9-E	401	-	11,12,12	0.69	0	14,16,16	2.20	3 (21%)
3	GOL	9-E	402	-	5,5,5	0.30	0	5,5,5	0.42	0
3	GOL	9-E	403	-	5,5,5	0.78	0	5,5,5	0.66	0
4	GOL	9-E	404	-	5,5,5	0.40	0	5,5,5	0.34	0
2	MES	9-F	401	-	11,12,12	0.79	0	14,16,16	2.67	5 (35%)
3	GOL	9-F	402	-	5,5,5	0.28	0	5,5,5	0.46	0
3	GOL	9-F	403	-	5,5,5	0.37	0	5,5,5	0.34	0
3	GOL	9-F	404	-	5,5,5	0.33	0	5,5,5	0.35	0
3	FMT	9-F	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	9-G	401	-	11,12,12	0.69	0	14,16,16	3.06	6 (42%)
3	GOL	9-G	402	-	5,5,5	0.49	0	5,5,5	0.65	0
3	GOL	9-G	403	-	5,5,5	0.37	0	5,5,5	0.28	0
3	GOL	9-G	404	-	5,5,5	0.41	0	5,5,5	0.10	0
5	FMT	9-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	9-H	401	-	11,12,12	0.71	0	14,16,16	2.23	4 (28%)
3	GOL	9-H	402	-	5,5,5	0.37	0	5,5,5	0.33	0
3	GOL	9-H	403	-	5,5,5	0.38	0	5,5,5	0.34	0
3	GOL	9-H	404	-	5,5,5	0.40	0	5,5,5	0.38	0
3	GOL	9-H	405	-	5,5,5	0.37	0	5,5,5	0.35	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
2	MES	1-A	401	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	1-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	1-A	404	-	-	0/4/4/4	0/0/0/0
2	MES	1-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	1-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	1-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	1-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	1-B	407	-	-	0/4/4/4	0/0/0/0
4	GOL	1-B	408	-	-	0/4/4/4	0/0/0/0
2	MES	1-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-C	402	-	-	0/4/4/4	0/0/0/0
3	FMT	1-C	403	-	-	0/0/0/0	0/0/0/0
2	MES	1-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	1-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	1-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-E	403	-	-	0/4/4/4	0/0/0/0
2	MES	1-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	1-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	1-F	405	-	-	0/4/4/4	0/0/0/0
3	GOL	1-F	406	-	-	0/4/4/4	0/0/0/0
5	GOL	1-F	407	-	-	0/4/4/4	0/0/0/0
4	FMT	1-F	408	-	-	0/0/0/0	0/0/0/0
2	MES	1-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	1-G	404	-	-	0/4/4/4	0/0/0/0
5	GOL	1-G	405	-	-	0/4/4/4	0/0/0/0
4	FMT	1-G	406	-	-	0/0/0/0	0/0/0/0
2	MES	1-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-H	403	-	-	0/4/4/4	0/0/0/0
2	MES	10-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-A	404	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	10-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	10-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	10-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	10-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	10-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-C	403	-	-	0/4/4/4	0/0/0/0
5	FMT	10-C	404	-	-	0/0/0/0	0/0/0/0
2	MES	10-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	10-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-E	403	-	-	0/4/4/4	0/0/0/0
2	MES	10-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	10-F	405	-	-	0/4/4/4	0/0/0/0
3	GOL	10-F	406	-	-	0/4/4/4	0/0/0/0
5	FMT	10-F	407	-	-	0/0/0/0	0/0/0/0
2	MES	10-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-G	404	-	-	0/4/4/4	0/0/0/0
5	FMT	10-G	405	-	-	0/0/0/0	0/0/0/0
2	MES	10-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-H	404	-	-	0/4/4/4	0/0/0/0
3	GOL	10-H	405	-	-	0/4/4/4	0/0/0/0
2	MES	2-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	2-A	404	-	-	0/4/4/4	0/0/0/0
2	MES	2-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-B	403	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	2-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	2-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	2-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	2-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	2-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-C	403	-	-	0/4/4/4	0/0/0/0
5	GOL	2-C	404	-	-	0/4/4/4	0/0/0/0
4	FMT	2-C	405	-	-	0/0/0/0	0/0/0/0
2	MES	2-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-D	403	-	-	0/4/4/4	0/0/0/0
2	MES	2-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	2-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	2-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	2-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	2-F	405	-	-	0/4/4/4	0/0/0/0
3	FMT	2-F	406	-	-	0/0/0/0	0/0/0/0
2	MES	2-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	2-G	404	-	-	0/4/4/4	0/0/0/0
5	FMT	2-G	405	-	-	0/0/0/0	0/0/0/0
2	MES	2-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	2-H	404	-	-	0/4/4/4	0/0/0/0
2	MES	3-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	3-A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	3-A	405	-	-	0/4/4/4	0/0/0/0
2	MES	3-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	3-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	3-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	3-B	406	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	3-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	3-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-C	403	-	-	0/4/4/4	0/0/0/0
5	FMT	3-C	404	-	-	0/0/0/0	0/0/0/0
2	MES	3-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-D	403	-	-	0/4/4/4	0/0/0/0
2	MES	3-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	3-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	3-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	3-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	3-F	405	-	-	0/4/4/4	0/0/0/0
3	GOL	3-F	406	-	-	0/4/4/4	0/0/0/0
5	FMT	3-F	407	-	-	0/0/0/0	0/0/0/0
2	MES	3-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	3-G	404	-	-	0/4/4/4	0/0/0/0
5	GOL	3-G	405	-	-	0/4/4/4	0/0/0/0
4	FMT	3-G	406	-	-	0/0/0/0	0/0/0/0
2	MES	3-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-H	403	-	-	0/4/4/4	0/0/0/0
2	MES	4-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	4-A	404	-	-	0/4/4/4	0/0/0/0
2	MES	4-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	4-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	4-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	4-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	4-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	4-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-C	403	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	4-C	404	-	-	0/4/4/4	0/0/0/0
4	FMT	4-C	405	-	-	0/0/0/0	0/0/0/0
2	MES	4-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-D	403	-	-	0/4/4/4	0/0/0/0
2	MES	4-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	4-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	4-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	4-F	404	-	-	0/4/4/4	0/0/0/0
3	FMT	4-F	405	-	-	0/0/0/0	0/0/0/0
2	MES	4-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	4-G	404	-	-	0/4/4/4	0/0/0/0
5	GOL	4-G	405	-	-	0/4/4/4	0/0/0/0
4	GOL	4-G	406	-	-	0/4/4/4	0/0/0/0
4	FMT	4-G	407	-	-	0/0/0/0	0/0/0/0
2	MES	4-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	4-H	404	-	-	0/4/4/4	0/0/0/0
2	MES	5-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	5-A	405	-	-	0/4/4/4	0/0/0/0
2	MES	5-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	5-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	5-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	5-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	5-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-C	402	-	-	0/4/4/4	0/0/0/0
3	FMT	5-C	403	-	-	0/0/0/0	0/0/0/0
2	MES	5-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-D	402	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	5-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	5-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	5-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	5-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-F	404	-	-	0/4/4/4	0/0/0/0
3	FMT	5-F	405	-	-	0/0/0/0	0/0/0/0
2	MES	5-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-G	404	-	-	0/4/4/4	0/0/0/0
5	GOL	5-G	405	-	-	0/4/4/4	0/0/0/0
4	FMT	5-G	406	-	-	0/0/0/0	0/0/0/0
2	MES	5-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-H	404	-	-	0/4/4/4	0/0/0/0
2	MES	6-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	6-A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	6-A	405	-	-	0/4/4/4	0/0/0/0
2	MES	6-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	6-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	6-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	6-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	6-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	6-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-C	402	-	-	0/4/4/4	0/0/0/0
3	FMT	6-C	403	-	-	0/0/0/0	0/0/0/0
2	MES	6-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	6-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	6-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-E	402	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	6-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	6-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	6-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	6-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	6-F	405	-	-	0/4/4/4	0/0/0/0
3	GOL	6-F	406	-	-	0/4/4/4	0/0/0/0
5	FMT	6-F	407	-	-	0/0/0/0	0/0/0/0
2	MES	6-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-G	403	-	-	0/4/4/4	0/0/0/0
3	FMT	6-G	404	-	-	0/0/0/0	0/0/0/0
2	MES	6-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	6-H	404	-	-	0/4/4/4	0/0/0/0
3	GOL	6-H	405	-	-	0/4/4/4	0/0/0/0
2	MES	7-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	7-A	405	-	-	0/4/4/4	0/0/0/0
2	MES	7-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	7-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	7-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	7-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	7-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-C	402	-	-	0/4/4/4	0/0/0/0
3	FMT	7-C	403	-	-	0/0/0/0	0/0/0/0
2	MES	7-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	7-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	7-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	7-F	401	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	7-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	7-F	405	-	-	0/4/4/4	0/0/0/0
3	GOL	7-F	406	-	-	0/4/4/4	0/0/0/0
5	FMT	7-F	407	-	-	0/0/0/0	0/0/0/0
2	MES	7-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-G	404	-	-	0/4/4/4	0/0/0/0
5	FMT	7-G	405	-	-	0/0/0/0	0/0/0/0
2	MES	7-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-H	404	-	-	0/4/4/4	0/0/0/0
2	MES	8-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	8-A	404	-	-	0/4/4/4	0/0/0/0
2	MES	8-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	8-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	8-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	8-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	8-B	407	-	-	0/4/4/4	0/0/0/0
4	GOL	8-B	408	-	-	0/4/4/4	0/0/0/0
2	MES	8-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-C	403	-	-	0/4/4/4	0/0/0/0
5	FMT	8-C	404	-	-	0/0/0/0	0/0/0/0
2	MES	8-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-D	403	-	-	0/4/4/4	0/0/0/0
2	MES	8-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	8-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	8-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	8-F	404	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	8-F	405	-	-	0/4/4/4	0/0/0/0
3	FMT	8-F	406	-	-	0/0/0/0	0/0/0/0
2	MES	8-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	8-G	404	-	-	0/4/4/4	0/0/0/0
5	GOL	8-G	405	-	-	0/4/4/4	0/0/0/0
4	FMT	8-G	406	-	-	0/0/0/0	0/0/0/0
2	MES	8-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	8-H	404	-	-	0/4/4/4	0/0/0/0
2	MES	9-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	9-A	405	-	-	0/4/4/4	0/0/0/0
2	MES	9-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	9-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	9-B	406	-	-	0/4/4/4	0/0/0/0
2	MES	9-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-C	403	-	-	0/4/4/4	0/0/0/0
5	FMT	9-C	404	-	-	0/0/0/0	0/0/0/0
2	MES	9-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	9-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	9-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	9-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-F	404	-	-	0/4/4/4	0/0/0/0
3	FMT	9-F	405	-	-	0/0/0/0	0/0/0/0
2	MES	9-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-G	402	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	9-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-G	404	-	-	0/4/4/4	0/0/0/0
5	FMT	9-G	405	-	-	0/0/0/0	0/0/0/0
2	MES	9-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-H	404	-	-	0/4/4/4	0/0/0/0
3	GOL	9-H	405	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-F	406	GOL	O2-C2	-3.03	1.34	1.43
3	2-H	403	GOL	C3-C2	-2.13	1.44	1.52

The worst 5 of 461 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3-B	401	MES	O2S-S-C8	-9.26	99.00	106.91
2	5-G	401	MES	O1S-S-C8	-8.37	99.77	106.91
2	3-H	401	MES	O2S-S-C8	-7.39	100.60	106.91
2	6-E	401	MES	O2S-S-C8	-6.47	101.38	106.91
2	10-C	401	MES	O2S-S-C8	-6.09	101.71	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

213 monomers are involved in 426 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1-A	401	MES	1	0
3	1-A	404	GOL	2	0
3	1-B	402	GOL	2	0
3	1-B	405	GOL	1	0
3	1-B	406	GOL	2	0
2	1-C	401	MES	1	0
2	1-D	401	MES	3	0
2	1-E	401	MES	2	0
3	1-E	402	GOL	1	0
3	1-E	403	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1-F	401	MES	2	0
3	1-F	404	GOL	1	0
3	1-F	405	GOL	2	0
2	1-G	401	MES	3	0
3	1-G	402	GOL	2	0
3	1-G	403	GOL	2	0
2	1-H	401	MES	2	0
3	1-H	402	GOL	2	0
3	1-H	403	GOL	1	0
2	10-A	401	MES	2	0
3	10-A	403	GOL	4	0
3	10-A	404	GOL	1	0
2	10-B	401	MES	6	0
3	10-B	404	GOL	3	0
2	10-C	401	MES	2	0
3	10-C	402	GOL	1	0
3	10-D	403	GOL	1	0
3	10-D	404	GOL	2	0
2	10-E	401	MES	2	0
3	10-E	402	GOL	1	0
2	10-F	401	MES	5	0
3	10-F	403	GOL	1	0
3	10-F	406	GOL	1	0
5	10-F	407	FMT	1	0
3	10-G	402	GOL	3	0
3	10-G	404	GOL	1	0
2	10-H	401	MES	5	0
3	10-H	402	GOL	1	0
3	10-H	403	GOL	1	0
3	10-H	404	GOL	1	0
3	10-H	405	GOL	1	0
3	2-A	402	GOL	1	0
3	2-A	404	GOL	1	0
2	2-B	401	MES	3	0
3	2-B	402	GOL	1	0
3	2-B	403	GOL	1	0
2	2-C	401	MES	5	0
3	2-C	403	GOL	2	0
5	2-C	404	GOL	1	0
2	2-D	401	MES	2	0
3	2-D	403	GOL	1	0
2	2-E	401	MES	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2-E	402	GOL	1	0
2	2-F	401	MES	3	0
2	2-G	401	MES	2	0
3	2-G	402	GOL	1	0
3	2-G	403	GOL	1	0
2	2-H	401	MES	2	0
3	2-H	402	GOL	2	0
3	2-H	404	GOL	2	0
3	3-A	402	GOL	1	0
3	3-A	403	GOL	1	0
4	3-A	405	GOL	1	0
2	3-B	401	MES	1	0
3	3-B	402	GOL	2	0
3	3-B	404	GOL	1	0
3	3-B	405	GOL	2	0
2	3-C	401	MES	2	0
2	3-D	401	MES	1	0
3	3-D	403	GOL	1	0
2	3-E	401	MES	6	0
3	3-E	402	GOL	3	0
3	3-E	403	GOL	2	0
2	3-F	401	MES	2	0
3	3-F	403	GOL	1	0
3	3-F	405	GOL	2	0
3	3-F	406	GOL	1	0
5	3-F	407	FMT	2	0
2	3-G	401	MES	3	0
3	3-G	402	GOL	1	0
3	3-G	404	GOL	3	0
4	3-G	406	FMT	1	0
2	3-H	401	MES	5	0
3	3-H	402	GOL	1	0
2	4-A	401	MES	4	0
3	4-A	402	GOL	2	0
3	4-A	403	GOL	1	0
2	4-B	401	MES	5	0
3	4-B	404	GOL	2	0
3	4-B	405	GOL	1	0
3	4-B	406	GOL	1	0
2	4-C	401	MES	8	0
3	4-C	402	GOL	1	0
3	4-C	403	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	4-C	404	GOL	1	0
2	4-D	401	MES	2	0
3	4-D	403	GOL	3	0
2	4-E	401	MES	4	0
3	4-E	402	GOL	1	0
4	4-E	404	GOL	1	0
2	4-F	401	MES	2	0
3	4-F	403	GOL	1	0
2	4-G	401	MES	1	0
3	4-G	402	GOL	1	0
3	4-G	404	GOL	2	0
4	4-G	407	FMT	1	0
2	4-H	401	MES	2	0
3	4-H	402	GOL	2	0
3	4-H	404	GOL	2	0
3	5-A	402	GOL	2	0
3	5-A	403	GOL	3	0
4	5-A	405	GOL	3	0
2	5-B	401	MES	3	0
3	5-B	402	GOL	1	0
3	5-B	403	GOL	1	0
3	5-B	405	GOL	4	0
3	5-B	406	GOL	1	0
2	5-C	401	MES	3	0
2	5-D	401	MES	2	0
3	5-D	402	GOL	2	0
3	5-D	404	GOL	1	0
2	5-E	401	MES	5	0
3	5-E	402	GOL	2	0
2	5-F	401	MES	2	0
3	5-F	402	GOL	2	0
2	5-G	401	MES	7	0
3	5-G	402	GOL	2	0
5	5-G	405	GOL	1	0
2	5-H	401	MES	1	0
3	5-H	402	GOL	2	0
3	5-H	404	GOL	2	0
3	6-A	403	GOL	1	0
3	6-A	404	GOL	1	0
4	6-A	405	GOL	1	0
2	6-B	401	MES	3	0
3	6-B	402	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	6-B	405	GOL	1	0
2	6-C	401	MES	1	0
3	6-C	402	GOL	1	0
2	6-D	401	MES	3	0
3	6-D	403	GOL	1	0
3	6-D	404	GOL	3	0
2	6-E	401	MES	3	0
3	6-E	402	GOL	2	0
2	6-F	401	MES	8	0
3	6-F	402	GOL	1	0
3	6-F	403	GOL	2	0
3	6-F	404	GOL	3	0
3	6-F	405	GOL	1	0
2	6-G	401	MES	1	0
3	6-G	402	GOL	1	0
3	6-G	403	GOL	1	0
3	6-G	404	FMT	1	0
2	6-H	401	MES	4	0
3	7-A	402	GOL	4	0
3	7-A	403	GOL	1	0
3	7-A	404	GOL	1	0
2	7-B	401	MES	5	0
3	7-B	405	GOL	1	0
2	7-C	401	MES	2	0
2	7-D	401	MES	2	0
3	7-D	404	GOL	2	0
2	7-E	401	MES	2	0
3	7-E	402	GOL	3	0
3	7-E	403	GOL	1	0
2	7-F	401	MES	1	0
3	7-F	402	GOL	1	0
3	7-F	404	GOL	2	0
3	7-F	405	GOL	2	0
5	7-F	407	FMT	2	0
2	7-G	401	MES	3	0
3	7-G	404	GOL	2	0
2	7-H	401	MES	6	0
3	7-H	404	GOL	1	0
2	8-A	401	MES	2	0
3	8-A	402	GOL	1	0
3	8-A	403	GOL	1	0
2	8-B	401	MES	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	8-B	404	GOL	1	0
3	8-B	405	GOL	1	0
3	8-B	407	GOL	2	0
2	8-C	401	MES	8	0
3	8-C	402	GOL	1	0
2	8-D	401	MES	3	0
3	8-D	403	GOL	1	0
3	8-E	402	GOL	5	0
3	8-E	403	GOL	1	0
4	8-E	404	GOL	2	0
2	8-F	401	MES	1	0
3	8-F	402	GOL	2	0
3	8-F	403	GOL	1	0
3	8-F	405	GOL	2	0
2	8-G	401	MES	1	0
3	8-G	402	GOL	1	0
3	8-G	403	GOL	1	0
2	8-H	401	MES	2	0
3	8-H	404	GOL	4	0
2	9-A	401	MES	1	0
2	9-B	401	MES	1	0
2	9-C	401	MES	2	0
3	9-C	403	GOL	2	0
2	9-D	401	MES	3	0
3	9-D	402	GOL	2	0
3	9-D	403	GOL	1	0
3	9-D	404	GOL	2	0
2	9-E	401	MES	2	0
3	9-F	403	GOL	1	0
3	9-G	402	GOL	2	0
3	9-G	404	GOL	1	0
2	9-H	401	MES	3	0
3	9-H	403	GOL	1	0
3	9-H	404	GOL	1	0
3	9-H	405	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1-A	372/384 (96%)	0.20	40 (10%) 8 10	15, 24, 36, 41	372 (100%)
1	1-B	374/384 (97%)	0.18	32 (8%) 13 18	15, 23, 38, 45	374 (100%)
1	1-C	375/384 (97%)	0.26	36 (9%) 10 14	15, 24, 37, 43	375 (100%)
1	1-D	372/384 (96%)	0.31	37 (9%) 9 13	16, 23, 37, 45	372 (100%)
1	1-E	372/384 (96%)	0.15	29 (7%) 16 22	16, 23, 35, 41	372 (100%)
1	1-F	373/384 (97%)	0.33	34 (9%) 11 16	16, 24, 39, 46	373 (100%)
1	1-G	374/384 (97%)	0.29	37 (9%) 9 13	15, 25, 40, 47	374 (100%)
1	1-H	374/384 (97%)	0.28	39 (10%) 8 12	15, 23, 41, 50	374 (100%)
1	2-A	372/384 (96%)	0.20	40 (10%) 8 10	15, 24, 36, 41	372 (100%)
1	2-B	374/384 (97%)	0.18	32 (8%) 13 18	15, 23, 38, 45	374 (100%)
1	2-C	375/384 (97%)	0.26	36 (9%) 10 14	15, 24, 37, 43	375 (100%)
1	2-D	372/384 (96%)	0.31	37 (9%) 9 13	16, 23, 37, 45	372 (100%)
1	2-E	372/384 (96%)	0.15	29 (7%) 16 22	16, 23, 35, 41	372 (100%)
1	2-F	373/384 (97%)	0.33	34 (9%) 11 16	16, 24, 39, 46	373 (100%)
1	2-G	374/384 (97%)	0.29	37 (9%) 9 13	15, 25, 40, 47	374 (100%)
1	2-H	374/384 (97%)	0.28	39 (10%) 8 12	15, 23, 41, 50	374 (100%)
1	3-A	372/384 (96%)	0.20	40 (10%) 8 10	15, 24, 36, 41	372 (100%)
1	3-B	374/384 (97%)	0.18	32 (8%) 13 18	15, 23, 38, 45	374 (100%)
1	3-C	375/384 (97%)	0.26	36 (9%) 10 14	15, 24, 37, 43	375 (100%)
1	3-D	372/384 (96%)	0.31	37 (9%) 9 13	16, 23, 37, 45	372 (100%)
1	3-E	372/384 (96%)	0.15	29 (7%) 16 22	16, 23, 35, 41	372 (100%)
1	3-F	373/384 (97%)	0.33	34 (9%) 11 16	16, 24, 39, 46	373 (100%)
1	3-G	374/384 (97%)	0.29	37 (9%) 9 13	15, 25, 40, 47	374 (100%)
1	3-H	374/384 (97%)	0.28	39 (10%) 8 12	15, 23, 41, 50	374 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	4-A	372/384 (96%)	0.20	40 (10%) 8 10	15, 24, 36, 41	372 (100%)
1	4-B	374/384 (97%)	0.18	32 (8%) 13 18	15, 23, 38, 45	374 (100%)
1	4-C	375/384 (97%)	0.26	36 (9%) 10 14	15, 24, 37, 43	375 (100%)
1	4-D	372/384 (96%)	0.31	37 (9%) 9 13	16, 23, 37, 45	372 (100%)
1	4-E	372/384 (96%)	0.15	29 (7%) 16 22	16, 23, 35, 41	372 (100%)
1	4-F	373/384 (97%)	0.33	34 (9%) 11 16	16, 24, 39, 46	373 (100%)
1	4-G	374/384 (97%)	0.29	37 (9%) 9 13	15, 25, 40, 47	374 (100%)
1	4-H	374/384 (97%)	0.28	39 (10%) 8 12	15, 23, 41, 50	374 (100%)
1	5-A	372/384 (96%)	0.20	40 (10%) 8 10	15, 24, 36, 41	372 (100%)
1	5-B	374/384 (97%)	0.18	32 (8%) 13 18	15, 23, 38, 45	374 (100%)
1	5-C	375/384 (97%)	0.26	36 (9%) 10 14	15, 24, 37, 43	375 (100%)
1	5-D	372/384 (96%)	0.31	37 (9%) 9 13	16, 23, 37, 45	372 (100%)
1	5-E	372/384 (96%)	0.15	29 (7%) 16 22	16, 23, 35, 41	372 (100%)
1	5-F	373/384 (97%)	0.33	34 (9%) 11 16	16, 24, 39, 46	373 (100%)
1	5-G	374/384 (97%)	0.29	37 (9%) 9 13	15, 25, 40, 47	374 (100%)
1	5-H	374/384 (97%)	0.28	39 (10%) 8 12	15, 23, 41, 50	374 (100%)
1	6-A	372/384 (96%)	0.20	40 (10%) 8 10	15, 24, 36, 41	372 (100%)
1	6-B	374/384 (97%)	0.18	32 (8%) 13 18	15, 23, 38, 45	374 (100%)
1	6-C	375/384 (97%)	0.26	36 (9%) 10 14	15, 24, 37, 43	375 (100%)
1	6-D	372/384 (96%)	0.31	37 (9%) 9 13	16, 23, 37, 45	372 (100%)
1	6-E	372/384 (96%)	0.15	29 (7%) 16 22	16, 23, 35, 41	372 (100%)
1	6-F	373/384 (97%)	0.33	34 (9%) 11 16	16, 24, 39, 46	373 (100%)
1	6-G	374/384 (97%)	0.29	37 (9%) 9 13	15, 25, 40, 47	374 (100%)
1	6-H	374/384 (97%)	0.28	39 (10%) 8 12	15, 23, 41, 50	374 (100%)
1	7-A	372/384 (96%)	0.20	40 (10%) 8 10	15, 24, 36, 41	372 (100%)
1	7-B	374/384 (97%)	0.18	32 (8%) 13 18	15, 23, 38, 45	374 (100%)
1	7-C	375/384 (97%)	0.26	36 (9%) 10 14	15, 24, 37, 43	375 (100%)
1	7-D	372/384 (96%)	0.31	37 (9%) 9 13	16, 23, 37, 45	372 (100%)
1	7-E	372/384 (96%)	0.15	29 (7%) 16 22	16, 23, 35, 41	372 (100%)
1	7-F	373/384 (97%)	0.33	34 (9%) 11 16	16, 24, 39, 46	373 (100%)
1	7-G	374/384 (97%)	0.29	37 (9%) 9 13	15, 25, 40, 47	374 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	7-H	374/384 (97%)	0.28	39 (10%) 8 12	15, 23, 41, 50	374 (100%)
1	8-A	372/384 (96%)	0.20	40 (10%) 8 10	15, 24, 36, 41	372 (100%)
1	8-B	374/384 (97%)	0.18	32 (8%) 13 18	15, 23, 38, 45	374 (100%)
1	8-C	375/384 (97%)	0.26	36 (9%) 10 14	15, 24, 37, 43	375 (100%)
1	8-D	372/384 (96%)	0.31	37 (9%) 9 13	16, 23, 37, 45	372 (100%)
1	8-E	372/384 (96%)	0.15	29 (7%) 16 22	16, 23, 35, 41	372 (100%)
1	8-F	373/384 (97%)	0.33	34 (9%) 11 16	16, 24, 39, 46	373 (100%)
1	8-G	374/384 (97%)	0.29	37 (9%) 9 13	15, 25, 40, 47	374 (100%)
1	8-H	374/384 (97%)	0.28	39 (10%) 8 12	15, 23, 41, 50	374 (100%)
1	9-A	372/384 (96%)	0.20	40 (10%) 8 10	15, 24, 36, 41	372 (100%)
1	9-B	374/384 (97%)	0.18	32 (8%) 13 18	15, 23, 38, 45	374 (100%)
1	9-C	375/384 (97%)	0.26	36 (9%) 10 14	15, 24, 37, 43	375 (100%)
1	9-D	372/384 (96%)	0.31	37 (9%) 9 13	16, 23, 37, 45	372 (100%)
1	9-E	372/384 (96%)	0.15	29 (7%) 16 22	16, 23, 35, 41	372 (100%)
1	9-F	373/384 (97%)	0.33	34 (9%) 11 16	16, 24, 39, 46	373 (100%)
1	9-G	374/384 (97%)	0.29	37 (9%) 9 13	15, 25, 40, 47	374 (100%)
1	9-H	374/384 (97%)	0.28	39 (10%) 8 12	15, 23, 41, 50	374 (100%)
1	10-A	372/384 (96%)	0.20	40 (10%) 8 10	15, 24, 36, 41	372 (100%)
1	10-B	374/384 (97%)	0.18	32 (8%) 13 18	15, 23, 38, 45	374 (100%)
1	10-C	375/384 (97%)	0.26	36 (9%) 10 14	15, 24, 37, 43	375 (100%)
1	10-D	372/384 (96%)	0.31	37 (9%) 9 13	16, 23, 37, 45	372 (100%)
1	10-E	372/384 (96%)	0.15	29 (7%) 16 22	16, 23, 35, 41	372 (100%)
1	10-F	373/384 (97%)	0.33	34 (9%) 11 16	16, 24, 39, 46	373 (100%)
1	10-G	374/384 (97%)	0.29	37 (9%) 9 13	15, 25, 40, 47	374 (100%)
1	10-H	374/384 (97%)	0.28	39 (10%) 8 12	15, 23, 41, 50	374 (100%)
All	All	29860/30720 (97%)	0.25	2840 (9%) 10 14	15, 24, 38, 50	29860 (100%)

The worst 5 of 2840 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-G	3	GLY	18.2
1	2-G	3	GLY	18.2
1	3-G	3	GLY	18.2

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Mol	Chain	Res	Type	RSRZ
1	4-G	3	GLY	18.2
1	5-G	3	GLY	18.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
1	LLP	3-C	197	24/25	0.97	0.16	-	15,17,19,19	24
1	LLP	7-D	197	24/25	0.98	0.12	-	16,19,19,20	24
1	LLP	2-F	197	24/25	0.98	0.16	-	16,19,20,20	24
1	LLP	7-B	197	24/25	0.98	0.13	-	15,18,19,19	24
1	LLP	8-C	197	24/25	0.97	0.16	-	15,17,18,19	24
1	LLP	4-G	197	24/25	0.97	0.14	-	16,19,21,21	24
1	LLP	10-D	197	24/25	0.98	0.12	-	16,19,19,20	24
1	LLP	4-E	197	24/25	0.96	0.13	-	15,18,19,19	24
1	LLP	4-D	197	24/25	0.98	0.12	-	16,19,19,20	24
1	LLP	6-H	197	24/25	0.97	0.14	-	15,18,20,20	24
1	LLP	8-D	197	24/25	0.98	0.12	-	16,19,19,20	24
1	LLP	1-B	197	24/25	0.98	0.13	-	15,18,19,19	24
1	LLP	1-C	197	24/25	0.97	0.16	-	15,17,18,19	24
1	LLP	1-D	197	24/25	0.98	0.12	-	16,19,19,20	24
1	LLP	2-H	197	24/25	0.97	0.14	-	15,18,20,20	24
1	LLP	6-G	197	24/25	0.97	0.14	-	16,19,21,21	24
1	LLP	3-B	197	24/25	0.98	0.13	-	15,18,19,19	24
1	LLP	3-H	197	24/25	0.97	0.14	-	15,18,20,20	24
1	LLP	6-B	197	24/25	0.98	0.13	-	15,18,19,19	24
1	LLP	7-A	197	24/25	0.98	0.11	-	15,17,19,19	24
1	LLP	4-H	197	24/25	0.97	0.14	-	15,18,20,20	24
1	LLP	2-D	197	24/25	0.98	0.12	-	16,18,19,20	24
1	LLP	10-A	197	24/25	0.98	0.11	-	15,17,19,19	24
1	LLP	3-F	197	24/25	0.98	0.16	-	16,19,20,20	24
1	LLP	4-B	197	24/25	0.98	0.13	-	15,18,19,19	24
1	LLP	4-A	197	24/25	0.98	0.11	-	15,17,19,19	24
1	LLP	6-C	197	24/25	0.97	0.16	-	15,17,18,18	24
1	LLP	4-C	197	24/25	0.97	0.16	-	15,17,18,18	24
1	LLP	1-G	197	24/25	0.97	0.14	-	16,19,21,21	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	LLP	8-A	197	24/25	0.98	0.11	-	15,17,19,19	24
1	LLP	2-E	197	24/25	0.96	0.13	-	15,18,19,19	24
1	LLP	9-A	197	24/25	0.98	0.11	-	15,17,19,19	24
1	LLP	3-D	197	24/25	0.98	0.12	-	16,19,19,20	24
1	LLP	3-E	197	24/25	0.96	0.13	-	15,18,19,19	24
1	LLP	1-H	197	24/25	0.97	0.14	-	15,18,20,20	24
1	LLP	2-G	197	24/25	0.97	0.14	-	16,19,21,21	24
1	LLP	7-E	197	24/25	0.96	0.13	-	15,18,19,19	24
1	LLP	2-A	197	24/25	0.98	0.11	-	15,18,19,19	24
1	LLP	10-E	197	24/25	0.96	0.13	-	15,18,19,19	24
1	LLP	10-F	197	24/25	0.98	0.16	-	16,19,20,20	24
1	LLP	4-F	197	24/25	0.98	0.16	-	16,19,20,20	24
1	LLP	9-F	197	24/25	0.98	0.16	-	16,19,20,20	24
1	LLP	8-F	197	24/25	0.98	0.16	-	16,19,20,20	24
1	LLP	8-E	197	24/25	0.96	0.13	-	15,18,19,19	24
1	LLP	10-C	197	24/25	0.97	0.16	-	15,17,18,18	24
1	LLP	8-B	197	24/25	0.98	0.13	-	15,18,19,19	24
1	LLP	5-A	197	24/25	0.98	0.11	-	15,17,19,19	24
1	LLP	9-E	197	24/25	0.96	0.13	-	15,18,19,19	24
1	LLP	7-F	197	24/25	0.98	0.16	-	16,19,20,20	24
1	LLP	9-G	197	24/25	0.97	0.14	-	16,19,21,21	24
1	LLP	3-A	197	24/25	0.98	0.11	-	15,17,19,19	24
1	LLP	10-B	197	24/25	0.98	0.13	-	15,18,19,19	24
1	LLP	5-B	197	24/25	0.98	0.13	-	15,18,19,19	24
1	LLP	9-D	197	24/25	0.98	0.12	-	16,19,19,20	24
1	LLP	7-C	197	24/25	0.97	0.16	-	15,17,18,19	24
1	LLP	2-C	197	24/25	0.97	0.16	-	15,17,18,19	24
1	LLP	2-B	197	24/25	0.98	0.13	-	15,18,19,19	24
1	LLP	5-C	197	24/25	0.97	0.16	-	15,17,19,19	24
1	LLP	7-G	197	24/25	0.97	0.14	-	16,19,21,21	24
1	LLP	10-H	197	24/25	0.97	0.14	-	15,18,20,20	24
1	LLP	5-H	197	24/25	0.97	0.14	-	15,18,20,20	24
1	LLP	6-A	197	24/25	0.98	0.11	-	15,17,19,19	24
1	LLP	5-D	197	24/25	0.98	0.12	-	16,19,19,20	24
1	LLP	8-H	197	24/25	0.97	0.14	-	15,18,20,20	24
1	LLP	5-E	197	24/25	0.96	0.13	-	15,18,19,19	24
1	LLP	1-E	197	24/25	0.96	0.13	-	15,18,19,19	24
1	LLP	6-E	197	24/25	0.96	0.13	-	15,18,19,19	24
1	LLP	1-A	197	24/25	0.98	0.11	-	15,17,19,19	24
1	LLP	5-F	197	24/25	0.98	0.16	-	16,19,20,20	24
1	LLP	5-G	197	24/25	0.97	0.14	-	16,19,21,21	24
1	LLP	8-G	197	24/25	0.97	0.14	-	16,19,21,21	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	LLP	6-D	197	24/25	0.98	0.12	-	16,19,19,20	24
1	LLP	7-H	197	24/25	0.97	0.14	-	15,18,20,20	24
1	LLP	6-F	197	24/25	0.98	0.16	-	16,19,20,20	24
1	LLP	9-H	197	24/25	0.97	0.14	-	15,18,20,20	24
1	LLP	9-B	197	24/25	0.98	0.13	-	15,18,19,19	24
1	LLP	9-C	197	24/25	0.97	0.16	-	15,17,18,18	24
1	LLP	10-G	197	24/25	0.97	0.14	-	16,19,21,21	24
1	LLP	3-G	197	24/25	0.97	0.14	-	16,19,21,21	24
1	LLP	1-F	197	24/25	0.98	0.16	-	16,19,20,20	24

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
3	GOL	3-B	404	6/6	0.92	0.32	32.15	23,94,96,97	6
3	GOL	6-D	403	6/6	0.75	0.49	18.38	24,36,252,269	6
3	GOL	10-D	403	6/6	0.75	0.49	18.38	24,36,252,269	6
3	GOL	6-F	403	6/6	0.80	0.30	18.28	35,117,202,207	6
3	GOL	7-D	403	6/6	0.75	0.49	17.04	24,36,252,269	6
5	GOL	2-C	404	6/6	0.68	0.45	17.03	19,35,37,177	6
3	GOL	5-D	403	6/6	0.75	0.49	16.36	24,36,252,269	6
5	GOL	4-C	404	6/6	0.68	0.45	16.34	19,35,37,177	6
3	GOL	9-D	403	6/6	0.75	0.49	16.14	24,36,252,269	6
3	GOL	9-H	403	6/6	0.75	0.29	14.00	22,34,195,229	6
3	GOL	9-B	403	6/6	0.58	0.39	13.08	23,94,96,97	6
3	GOL	2-G	403	6/6	0.76	0.27	12.25	22,34,195,229	6
3	GOL	7-G	403	6/6	0.76	0.27	11.72	22,34,195,229	6
5	GOL	4-G	405	6/6	0.69	0.26	11.53	22,34,195,229	6
3	GOL	2-B	407	6/6	0.81	0.29	11.43	24,75,77,98	6
3	GOL	6-F	405	6/6	0.67	0.38	10.92	24,33,50,86	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	8-G	404	6/6	0.75	0.24	10.62	22,34,195,229	6
3	GOL	10-H	403	6/6	0.75	0.29	10.58	22,34,195,229	6
3	GOL	5-H	403	6/6	0.75	0.29	10.58	22,34,195,229	6
3	GOL	6-H	403	6/6	0.75	0.29	10.58	22,34,195,229	6
3	GOL	10-F	405	6/6	0.67	0.38	10.49	24,33,50,86	6
3	GOL	1-B	404	6/6	0.92	0.32	10.31	23,94,96,97	6
3	GOL	3-G	403	6/6	0.76	0.27	10.25	22,34,195,229	6
3	GOL	4-B	403	6/6	0.58	0.39	10.08	23,94,96,97	6
3	GOL	10-C	403	6/6	0.80	0.31	9.94	19,35,37,177	6
3	GOL	4-F	402	6/6	0.76	0.33	9.85	34,68,106,111	6
3	GOL	3-F	402	6/6	0.76	0.33	9.85	34,68,106,111	6
3	GOL	1-F	402	6/6	0.76	0.33	9.85	34,68,106,111	6
3	GOL	5-B	404	6/6	0.92	0.32	9.82	23,94,96,97	6
3	GOL	8-F	402	6/6	0.76	0.33	9.75	34,68,106,111	6
3	GOL	7-F	402	6/6	0.76	0.33	9.75	34,68,106,111	6
3	GOL	10-F	402	6/6	0.76	0.33	9.75	34,68,106,111	6
3	GOL	10-B	403	6/6	0.58	0.39	9.67	23,94,96,97	6
3	GOL	2-B	403	6/6	0.58	0.39	9.45	23,94,96,97	6
3	GOL	8-B	404	6/6	0.92	0.32	9.43	23,94,96,97	6
3	GOL	1-G	403	6/6	0.76	0.27	9.40	22,34,195,229	6
3	GOL	1-F	405	6/6	0.67	0.38	9.04	20,31,173,206	6
3	GOL	7-F	405	6/6	0.67	0.38	9.04	20,31,173,206	6
3	GOL	9-C	403	6/6	0.80	0.31	8.93	19,35,37,177	6
3	GOL	5-G	403	6/6	0.76	0.27	8.48	35,117,202,207	6
4	FMT	1-G	406	3/3	0.81	0.47	8.00	38,38,218,325	3
3	GOL	7-B	404	6/6	0.92	0.32	7.78	23,94,96,97	6
3	GOL	10-B	407	6/6	0.81	0.29	7.76	24,75,77,98	6
3	GOL	4-B	407	6/6	0.81	0.29	7.76	24,75,77,98	6
3	GOL	2-D	403	6/6	0.75	0.49	7.58	30,35,49,275	6
3	GOL	5-F	403	6/6	0.80	0.30	7.42	20,31,173,206	6
3	GOL	5-B	402	6/6	0.77	0.25	7.41	19,35,37,177	6
3	GOL	6-B	404	6/6	0.92	0.32	7.19	23,94,96,97	6
3	GOL	10-F	404	6/6	0.83	0.29	7.08	20,31,173,206	6
3	GOL	5-E	403	6/6	0.76	0.26	7.07	34,68,106,111	6
3	GOL	8-B	402	6/6	0.77	0.25	7.07	19,35,37,177	6
3	GOL	9-E	403	6/6	0.76	0.26	7.07	34,68,106,111	6
3	GOL	6-E	403	6/6	0.76	0.26	7.02	34,68,106,111	6
3	GOL	2-E	403	6/6	0.76	0.26	7.00	34,68,106,111	6
3	GOL	1-B	402	6/6	0.77	0.25	6.90	19,35,37,177	6
3	GOL	3-B	402	6/6	0.77	0.25	6.79	19,35,37,177	6
3	GOL	6-B	402	6/6	0.77	0.25	6.74	19,35,37,177	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	7-B	402	6/6	0.77	0.25	6.74	19,35,37,177	6
3	GOL	6-F	404	6/6	0.83	0.29	6.56	20,31,173,206	6
3	GOL	8-F	404	6/6	0.83	0.29	6.56	20,31,173,206	6
3	GOL	2-F	404	6/6	0.83	0.29	6.56	20,31,173,206	6
3	GOL	8-D	402	6/6	0.50	0.44	6.35	25,194,233,275	6
3	GOL	7-D	402	6/6	0.50	0.44	6.35	25,194,233,275	6
3	GOL	5-D	402	6/6	0.50	0.44	6.35	25,194,233,275	6
3	GOL	4-D	402	6/6	0.50	0.44	6.35	25,194,233,275	6
3	GOL	2-D	402	6/6	0.50	0.44	6.35	25,194,233,275	6
3	GOL	3-D	402	6/6	0.50	0.44	6.35	25,194,233,275	6
3	GOL	10-D	402	6/6	0.50	0.44	6.35	25,194,233,275	6
3	GOL	6-D	402	6/6	0.50	0.44	6.35	25,194,233,275	6
3	GOL	9-D	402	6/6	0.50	0.44	6.35	25,194,233,275	6
3	GOL	1-D	402	6/6	0.50	0.44	6.35	25,194,233,275	6
3	GOL	10-E	403	6/6	0.76	0.26	6.30	29,57,83,86	6
3	GOL	9-F	402	6/6	0.76	0.33	6.29	29,35,59,94	6
3	GOL	6-F	402	6/6	0.76	0.33	6.29	29,35,59,94	6
3	GOL	5-F	402	6/6	0.76	0.33	6.29	29,35,59,94	6
4	GOL	8-B	408	6/6	0.77	0.25	6.28	24,75,77,98	6
4	GOL	1-B	408	6/6	0.77	0.25	6.28	24,75,77,98	6
5	FMT	3-C	404	3/3	0.87	0.41	5.97	29,29,276,319	3
3	GOL	1-F	406	6/6	0.74	0.27	5.91	24,33,50,86	6
3	GOL	3-C	402	6/6	0.94	0.23	5.83	24,36,252,269	6
3	GOL	3-F	403	6/6	0.80	0.30	5.48	29,35,59,94	6
3	GOL	4-F	403	6/6	0.80	0.30	5.48	29,35,59,94	6
3	GOL	1-F	403	6/6	0.80	0.30	5.48	29,35,59,94	6
3	GOL	8-F	403	6/6	0.80	0.30	5.48	29,35,59,94	6
4	FMT	4-G	407	3/3	0.95	0.35	5.38	38,38,218,325	3
3	GOL	4-C	402	6/6	0.94	0.23	5.32	24,36,252,269	6
3	GOL	2-C	402	6/6	0.94	0.23	5.32	24,36,252,269	6
4	GOL	3-A	405	6/6	0.81	0.22	5.26	24,75,77,98	6
4	GOL	6-A	405	6/6	0.81	0.22	5.19	24,75,77,98	6
4	GOL	9-A	405	6/6	0.81	0.22	5.19	24,75,77,98	6
4	GOL	7-A	405	6/6	0.81	0.22	5.19	24,75,77,98	6
3	GOL	8-C	402	6/6	0.94	0.23	4.97	24,36,252,269	6
3	FMT	5-F	405	3/3	0.92	0.37	4.91	23,23,31,80	3
3	GOL	8-E	403	6/6	0.76	0.26	4.85	29,57,83,86	6
3	FMT	9-F	405	3/3	0.92	0.37	4.75	23,23,31,80	3
3	FMT	2-F	406	3/3	0.66	0.37	4.71	23,23,31,80	3
5	FMT	7-F	407	3/3	0.79	0.36	4.66	23,23,31,80	3
5	FMT	6-F	407	3/3	0.79	0.36	4.66	23,23,31,80	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	FMT	3-F	407	3/3	0.79	0.36	4.66	23,23,31,80	3
3	GOL	2-B	406	6/6	0.67	0.33	4.65	40,79,89,91	6
3	GOL	9-B	406	6/6	0.67	0.33	4.65	40,79,89,91	6
3	FMT	4-F	405	3/3	0.92	0.37	4.57	23,23,31,80	3
3	FMT	8-F	406	3/3	0.66	0.37	4.48	23,23,31,80	3
5	FMT	10-F	407	3/3	0.79	0.36	4.40	23,23,31,80	3
3	GOL	2-F	405	6/6	0.67	0.38	4.40	72,110,114,139	6
3	GOL	8-F	405	6/6	0.67	0.38	4.40	72,110,114,139	6
4	GOL	9-E	404	6/6	0.87	0.19	4.21	29,57,83,86	6
3	GOL	10-H	405	6/6	0.79	0.32	4.20	32,37,218,314	6
3	GOL	6-H	405	6/6	0.79	0.32	4.20	32,37,218,314	6
3	GOL	2-A	403	6/6	0.70	0.40	4.15	21,23,174,178	6
3	GOL	1-B	406	6/6	0.67	0.33	4.05	60,112,120,132	6
3	GOL	10-B	405	6/6	0.69	0.34	4.01	60,112,120,132	6
3	GOL	7-B	406	6/6	0.67	0.33	3.88	60,112,120,132	6
3	GOL	8-B	406	6/6	0.67	0.33	3.88	60,112,120,132	6
4	GOL	5-A	405	6/6	0.81	0.22	3.87	24,75,77,98	6
3	GOL	1-B	403	6/6	0.58	0.39	3.78	24,117,121,122	6
3	GOL	9-B	405	6/6	0.69	0.34	3.78	60,112,120,132	6
3	GOL	8-B	403	6/6	0.58	0.39	3.78	24,117,121,122	6
3	GOL	4-B	405	6/6	0.69	0.34	3.78	60,112,120,132	6
3	GOL	6-B	403	6/6	0.58	0.39	3.78	24,117,121,122	6
3	GOL	5-B	403	6/6	0.58	0.39	3.78	24,117,121,122	6
3	GOL	2-B	405	6/6	0.69	0.34	3.78	60,112,120,132	6
4	GOL	8-E	404	6/6	0.87	0.19	3.68	24,33,50,86	6
4	GOL	5-E	404	6/6	0.87	0.19	3.66	29,57,83,86	6
3	GOL	3-B	406	6/6	0.67	0.33	3.65	60,112,120,132	6
3	GOL	6-B	406	6/6	0.67	0.33	3.65	60,112,120,132	6
3	GOL	8-B	407	6/6	0.81	0.29	3.62	40,79,89,91	6
3	GOL	3-B	407	6/6	0.81	0.29	3.62	40,79,89,91	6
4	GOL	4-E	404	6/6	0.87	0.19	3.52	24,33,50,86	6
3	GOL	3-B	403	6/6	0.58	0.39	3.49	24,117,121,122	6
4	FMT	1-F	408	3/3	0.86	0.30	3.49	23,23,31,80	3
3	GOL	5-B	406	6/6	0.67	0.33	3.44	60,112,120,132	6
4	GOL	7-E	404	6/6	0.87	0.19	3.43	24,33,50,86	6
3	GOL	3-H	403	6/6	0.75	0.29	3.42	32,37,218,314	6
3	GOL	3-H	402	6/6	0.68	0.30	3.38	27,213,267,270	6
3	GOL	1-H	402	6/6	0.68	0.30	3.38	27,213,267,270	6
3	GOL	7-H	403	6/6	0.75	0.29	3.22	30,50,233,252	6
4	GOL	3-E	404	6/6	0.87	0.19	3.21	24,33,50,86	6
3	GOL	8-H	402	6/6	0.68	0.30	3.17	27,213,267,270	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	9-H	402	6/6	0.68	0.30	3.15	27,213,267,270	6
3	GOL	7-H	402	6/6	0.68	0.30	3.15	27,213,267,270	6
3	GOL	2-H	402	6/6	0.68	0.30	3.15	27,213,267,270	6
3	GOL	10-H	402	6/6	0.68	0.30	3.15	27,213,267,270	6
3	GOL	7-A	403	6/6	0.70	0.40	3.12	21,23,174,178	6
3	GOL	10-A	403	6/6	0.70	0.40	3.02	21,23,174,178	6
5	GOL	5-G	405	6/6	0.69	0.26	2.93	26,41,231,232	6
5	GOL	3-G	405	6/6	0.69	0.26	2.93	26,41,231,232	6
3	GOL	6-H	402	6/6	0.68	0.30	2.92	27,213,267,270	6
3	GOL	4-C	403	6/6	0.80	0.31	2.77	26,44,244,271	6
3	GOL	2-C	403	6/6	0.80	0.31	2.77	26,44,244,271	6
3	GOL	3-C	403	6/6	0.80	0.31	2.77	26,44,244,271	6
3	GOL	8-C	403	6/6	0.80	0.31	2.77	26,44,244,271	6
3	GOL	6-H	404	6/6	0.76	0.39	2.73	30,50,233,252	6
3	GOL	9-H	404	6/6	0.76	0.39	2.72	30,50,233,252	6
3	GOL	2-G	404	6/6	0.75	0.24	2.64	26,41,231,232	6
3	GOL	4-F	404	6/6	0.83	0.29	2.61	72,110,114,139	6
3	GOL	9-F	404	6/6	0.83	0.29	2.61	72,110,114,139	6
3	GOL	5-F	404	6/6	0.83	0.29	2.61	72,110,114,139	6
3	GOL	10-H	404	6/6	0.76	0.39	2.56	30,50,233,252	6
2	MES	8-D	401	12/12	0.95	0.15	2.37	18,20,22,22	12
3	GOL	3-F	406	6/6	0.74	0.27	2.26	72,110,114,139	6
3	GOL	10-F	406	6/6	0.74	0.27	2.26	72,110,114,139	6
3	GOL	7-F	406	6/6	0.74	0.27	2.26	72,110,114,139	6
3	GOL	6-F	406	6/6	0.74	0.27	2.26	72,110,114,139	6
3	GOL	5-A	403	6/6	0.70	0.40	2.16	21,23,174,178	6
3	GOL	6-A	403	6/6	0.70	0.40	2.15	21,23,174,178	6
3	GOL	1-A	403	6/6	0.70	0.40	2.12	21,23,174,178	6
3	GOL	4-A	403	6/6	0.70	0.40	2.10	21,23,174,178	6
3	GOL	9-A	403	6/6	0.70	0.40	2.02	21,23,174,178	6
3	GOL	3-A	403	6/6	0.70	0.40	1.90	21,23,174,178	6
3	GOL	8-A	403	6/6	0.70	0.40	1.90	21,23,174,178	6
3	GOL	2-H	403	6/6	0.75	0.29	1.85	30,50,233,252	6
3	GOL	10-B	402	6/6	0.77	0.25	1.82	24,117,121,122	6
3	GOL	7-C	402	6/6	0.94	0.23	1.82	26,44,244,271	6
5	GOL	1-F	407	6/6	0.69	0.25	1.82	72,110,114,139	6
3	GOL	9-B	402	6/6	0.77	0.25	1.82	24,117,121,122	6
3	GOL	4-B	402	6/6	0.77	0.25	1.82	24,117,121,122	6
3	GOL	8-E	402	6/6	0.91	0.21	1.76	29,44,81,118	6
3	GOL	6-E	402	6/6	0.91	0.21	1.76	29,44,81,118	6
3	GOL	7-E	402	6/6	0.91	0.21	1.76	29,44,81,118	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	5-E	402	6/6	0.91	0.21	1.76	29,44,81,118	6
3	GOL	10-E	402	6/6	0.91	0.21	1.76	29,44,81,118	6
3	GOL	3-E	402	6/6	0.91	0.21	1.76	29,44,81,118	6
3	GOL	3-B	405	6/6	0.69	0.34	1.70	19,20,117,167	6
3	GOL	8-B	405	6/6	0.69	0.34	1.68	19,20,117,167	6
3	GOL	9-E	402	6/6	0.91	0.21	1.60	29,44,81,118	6
3	GOL	1-E	402	6/6	0.91	0.21	1.60	29,44,81,118	6
3	GOL	4-E	402	6/6	0.91	0.21	1.60	29,44,81,118	6
3	GOL	2-E	402	6/6	0.91	0.21	1.60	29,44,81,118	6
3	GOL	6-B	405	6/6	0.69	0.34	1.57	19,20,117,167	6
3	GOL	1-B	405	6/6	0.69	0.34	1.57	19,20,117,167	6
3	GOL	7-B	405	6/6	0.69	0.34	1.49	19,20,117,167	6
3	GOL	5-B	405	6/6	0.69	0.34	1.49	19,20,117,167	6
3	GOL	6-D	404	6/6	0.92	0.19	1.48	30,35,49,275	6
3	GOL	7-D	404	6/6	0.92	0.19	1.48	30,35,49,275	6
3	GOL	6-C	402	6/6	0.94	0.23	1.45	26,44,244,271	6
3	GOL	10-C	402	6/6	0.94	0.23	1.45	26,44,244,271	6
3	GOL	9-C	402	6/6	0.94	0.23	1.45	26,44,244,271	6
3	GOL	1-C	402	6/6	0.94	0.23	1.45	26,44,244,271	6
3	GOL	2-B	404	6/6	0.92	0.32	1.45	19,20,117,167	6
3	GOL	5-C	402	6/6	0.94	0.23	1.45	26,44,244,271	6
3	GOL	4-B	404	6/6	0.92	0.32	1.37	19,20,117,167	6
2	MES	10-D	401	12/12	0.95	0.15	1.36	19,20,22,22	12
3	GOL	10-B	404	6/6	0.92	0.32	1.36	19,20,117,167	6
3	GOL	8-H	403	6/6	0.75	0.29	1.32	30,50,233,252	6
3	GOL	9-B	404	6/6	0.92	0.32	1.27	19,20,117,167	6
3	GOL	5-G	404	6/6	0.75	0.24	1.15	30,50,233,252	6
3	GOL	3-G	404	6/6	0.75	0.24	1.12	30,50,233,252	6
3	GOL	5-A	404	6/6	0.91	0.20	1.10	25,45,91,117	6
3	GOL	8-A	404	6/6	0.91	0.20	1.10	25,45,91,117	6
3	GOL	9-A	404	6/6	0.91	0.20	1.10	25,45,91,117	6
3	GOL	6-A	404	6/6	0.91	0.20	1.10	25,45,91,117	6
3	GOL	10-A	404	6/6	0.91	0.20	1.10	25,45,91,117	6
3	GOL	1-A	404	6/6	0.91	0.20	1.10	25,45,91,117	6
3	GOL	7-A	404	6/6	0.91	0.20	1.10	25,45,91,117	6
3	GOL	3-A	404	6/6	0.91	0.20	1.10	25,45,91,117	6
3	GOL	10-G	402	6/6	0.96	0.19	1.06	35,40,182,227	6
3	GOL	4-H	403	6/6	0.75	0.29	1.05	30,50,233,252	6
3	GOL	2-A	404	6/6	0.91	0.20	0.98	25,45,91,117	6
3	GOL	4-A	404	6/6	0.91	0.20	0.98	25,45,91,117	6
3	GOL	6-G	402	6/6	0.96	0.19	0.94	35,40,182,227	6
3	GOL	5-G	402	6/6	0.96	0.19	0.94	35,40,182,227	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	7-G	402	6/6	0.96	0.19	0.94	35,40,182,227	6
3	GOL	3-G	402	6/6	0.96	0.19	0.94	35,40,182,227	6
3	GOL	4-G	402	6/6	0.96	0.19	0.94	35,40,182,227	6
3	GOL	8-G	402	6/6	0.96	0.19	0.94	35,40,182,227	6
3	GOL	1-G	402	6/6	0.96	0.19	0.94	35,40,182,227	6
3	GOL	2-G	402	6/6	0.96	0.19	0.94	35,40,182,227	6
3	GOL	9-G	402	6/6	0.96	0.19	0.94	35,40,182,227	6
3	GOL	10-A	402	6/6	0.84	0.20	0.88	39,51,59,85	6
3	GOL	2-A	402	6/6	0.84	0.20	0.88	39,51,59,85	6
3	GOL	4-A	402	6/6	0.84	0.20	0.88	39,51,59,85	6
3	GOL	5-A	402	6/6	0.84	0.20	0.88	39,51,59,85	6
3	GOL	9-A	402	6/6	0.84	0.20	0.88	39,51,59,85	6
3	GOL	6-A	402	6/6	0.84	0.20	0.88	39,51,59,85	6
3	GOL	3-A	402	6/6	0.84	0.20	0.88	39,51,59,85	6
2	MES	3-D	401	12/12	0.95	0.15	0.87	18,20,22,22	12
3	GOL	1-G	404	6/6	0.75	0.24	0.84	30,50,233,252	6
2	MES	6-D	401	12/12	0.95	0.15	0.76	19,20,22,23	12
2	MES	9-D	401	12/12	0.95	0.15	0.66	19,20,21,21	12
2	MES	1-D	401	12/12	0.95	0.15	0.66	19,20,22,22	12
2	MES	5-D	401	12/12	0.95	0.15	0.61	19,20,22,22	12
2	MES	2-D	401	12/12	0.95	0.15	0.61	19,20,22,22	12
2	MES	4-D	401	12/12	0.95	0.15	0.61	19,20,22,22	12
2	MES	7-D	401	12/12	0.95	0.15	0.61	19,20,21,21	12
2	MES	6-C	401	12/12	0.94	0.15	0.54	19,20,22,22	12
2	MES	8-C	401	12/12	0.94	0.15	0.44	19,20,20,20	12
2	MES	7-C	401	12/12	0.94	0.15	0.33	18,19,21,21	12
2	MES	4-C	401	12/12	0.94	0.15	0.31	18,19,20,20	12
2	MES	5-C	401	12/12	0.94	0.15	0.31	18,19,21,21	12
2	MES	1-C	401	12/12	0.94	0.15	0.31	17,19,20,20	12
2	MES	9-C	401	12/12	0.94	0.15	0.31	18,19,20,21	12
2	MES	10-C	401	12/12	0.94	0.15	0.31	18,19,21,21	12
2	MES	3-C	401	12/12	0.94	0.15	0.29	18,19,21,21	12
2	MES	2-C	401	12/12	0.94	0.15	0.09	19,19,20,21	12
2	MES	7-F	401	12/12	0.96	0.14	0.04	19,21,23,23	12
2	MES	9-F	401	12/12	0.96	0.14	0.04	19,21,23,23	12
2	MES	5-F	401	12/12	0.96	0.14	0.04	19,20,23,23	12
2	MES	6-F	401	12/12	0.96	0.14	0.03	20,20,22,22	12
2	MES	8-F	401	12/12	0.96	0.14	0.03	19,21,23,23	12
2	MES	2-F	401	12/12	0.96	0.14	0.03	19,21,23,23	12
2	MES	3-F	401	12/12	0.96	0.14	0.03	19,21,23,23	12
2	MES	4-F	401	12/12	0.96	0.14	-0.01	19,21,23,24	12
2	MES	10-F	401	12/12	0.96	0.14	-0.01	19,21,22,23	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MES	1-F	401	12/12	0.96	0.14	-0.01	19,21,24,24	12
2	MES	8-H	401	12/12	0.96	0.12	-0.05	19,19,20,21	12
2	MES	7-H	401	12/12	0.96	0.12	-0.05	18,19,20,20	12
2	MES	9-H	401	12/12	0.96	0.12	-0.05	18,19,21,21	12
2	MES	3-H	401	12/12	0.96	0.12	-0.05	18,19,20,20	12
2	MES	1-H	401	12/12	0.96	0.12	-0.05	18,19,21,21	12
2	MES	4-H	401	12/12	0.96	0.12	-0.05	18,19,20,20	12
2	MES	3-B	401	12/12	0.95	0.12	-0.12	18,19,21,21	12
2	MES	2-B	401	12/12	0.95	0.12	-0.12	18,19,21,21	12
2	MES	7-B	401	12/12	0.95	0.12	-0.12	18,19,21,21	12
2	MES	8-B	401	12/12	0.95	0.12	-0.12	18,20,22,22	12
2	MES	4-B	401	12/12	0.95	0.12	-0.12	18,20,22,22	12
2	MES	10-B	401	12/12	0.95	0.12	-0.12	18,19,21,21	12
2	MES	1-B	401	12/12	0.95	0.12	-0.12	18,19,21,21	12
2	MES	9-B	401	12/12	0.95	0.12	-0.12	18,19,21,21	12
2	MES	6-A	401	12/12	0.97	0.12	-0.15	18,19,20,20	12
2	MES	5-A	401	12/12	0.97	0.12	-0.15	18,19,20,20	12
2	MES	1-A	401	12/12	0.97	0.12	-0.15	18,19,20,20	12
2	MES	6-H	401	12/12	0.96	0.12	-0.16	18,19,20,21	12
2	MES	2-H	401	12/12	0.96	0.12	-0.16	18,19,20,20	12
2	MES	10-H	401	12/12	0.96	0.12	-0.16	18,19,20,21	12
2	MES	5-H	401	12/12	0.96	0.12	-0.16	18,19,21,21	12
2	MES	6-B	401	12/12	0.95	0.12	-0.31	18,19,21,21	12
2	MES	5-B	401	12/12	0.95	0.12	-0.31	19,20,21,21	12
2	MES	2-A	401	12/12	0.97	0.12	-0.36	18,19,20,20	12
2	MES	10-A	401	12/12	0.97	0.12	-0.36	18,19,20,20	12
2	MES	7-A	401	12/12	0.97	0.12	-0.43	18,19,20,21	12
2	MES	8-A	401	12/12	0.97	0.12	-0.49	18,19,20,21	12
2	MES	3-A	401	12/12	0.97	0.12	-0.49	18,19,21,21	12
2	MES	9-A	401	12/12	0.97	0.12	-0.49	18,19,21,21	12
2	MES	10-G	401	12/12	0.96	0.12	-0.56	19,21,23,23	12
2	MES	7-G	401	12/12	0.96	0.12	-0.56	20,22,23,23	12
2	MES	6-G	401	12/12	0.96	0.12	-0.56	20,21,23,23	12
2	MES	8-G	401	12/12	0.96	0.12	-0.56	20,21,22,22	12
2	MES	2-G	401	12/12	0.96	0.12	-0.56	20,21,22,23	12
2	MES	4-G	401	12/12	0.96	0.12	-0.56	20,21,22,23	12
2	MES	9-G	401	12/12	0.96	0.12	-0.59	20,21,22,23	12
2	MES	5-G	401	12/12	0.96	0.12	-0.59	19,21,22,22	12
2	MES	1-G	401	12/12	0.96	0.12	-0.59	19,21,22,23	12
2	MES	4-A	401	12/12	0.97	0.12	-0.61	19,19,21,21	12
2	MES	3-G	401	12/12	0.96	0.12	-0.67	21,22,23,23	12
2	MES	6-E	401	12/12	0.96	0.10	-0.71	19,20,21,21	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MES	5-E	401	12/12	0.96	0.10	-0.79	18,19,21,21	12
2	MES	9-E	401	12/12	0.96	0.10	-0.79	19,20,21,22	12
2	MES	3-E	401	12/12	0.96	0.10	-0.84	18,19,21,21	12
2	MES	7-E	401	12/12	0.96	0.10	-0.84	18,19,21,21	12
2	MES	2-E	401	12/12	0.96	0.10	-0.90	18,19,20,21	12
2	MES	8-E	401	12/12	0.96	0.10	-0.90	19,20,21,21	12
2	MES	10-E	401	12/12	0.96	0.10	-0.92	18,19,20,21	12
2	MES	1-E	401	12/12	0.96	0.10	-0.92	18,19,20,21	12
2	MES	4-E	401	12/12	0.96	0.10	-0.98	18,19,21,21	12
4	CL	10-D	405	1/1	0.87	1.22	-	261,261,261,261	1
3	GOL	9-G	403	6/6	0.76	0.27	-	20,31,173,206	6
5	CL	6-C	404	1/1	0.90	0.17	-	41,41,41,41	1
3	GOL	7-H	404	6/6	0.76	0.39	-	32,37,218,314	6
4	CL	5-B	408	1/1	0.60	0.54	-	97,97,97,97	1
3	GOL	4-B	406	6/6	0.67	0.33	-	40,79,89,91	6
3	GOL	3-F	405	6/6	0.67	0.38	-	20,31,173,206	6
4	CL	8-B	409	1/1	0.83	0.21	-	97,97,97,97	1
5	CL	5-C	404	1/1	0.90	0.17	-	41,41,41,41	1
4	CL	4-A	406	1/1	0.78	0.61	-	122,122,122,122	1
5	GOL	1-G	405	6/6	0.69	0.26	-	26,41,231,232	6
3	GOL	8-A	402	6/6	0.84	0.20	-	39,51,59,85	6
3	CL	4-H	405	1/1	0.29	0.91	-	303,303,303,303	1
3	GOL	7-A	402	6/6	0.84	0.20	-	39,51,59,85	6
3	GOL	1-D	404	6/6	0.92	0.19	-	30,35,49,275	6
4	GOL	2-E	404	6/6	0.87	0.19	-	29,57,83,86	6
3	GOL	6-G	403	6/6	0.76	0.27	-	26,41,231,232	6
4	CL	5-A	406	1/1	0.78	0.61	-	43,43,43,43	1
4	CL	8-A	406	1/1	0.78	0.61	-	122,122,122,122	1
4	CL	6-B	408	1/1	0.60	0.54	-	97,97,97,97	1
4	CL	1-D	405	1/1	0.87	1.22	-	261,261,261,261	1
4	CL	2-B	408	1/1	0.60	0.54	-	97,97,97,97	1
4	CL	5-H	406	1/1	0.29	0.91	-	32,32,32,32	1
3	CL	5-F	406	1/1	0.98	0.26	-	28,28,28,28	1
4	CL	9-A	406	1/1	0.78	0.61	-	43,43,43,43	1
3	GOL	1-E	403	6/6	0.76	0.26	-	29,57,83,86	6
3	GOL	5-D	404	6/6	0.92	0.19	-	30,35,49,275	6
3	CL	8-H	405	1/1	0.29	0.91	-	303,303,303,303	1
3	CL	9-B	407	1/1	0.76	0.90	-	97,97,97,97	1
3	GOL	3-E	403	6/6	0.76	0.26	-	29,57,83,86	6
4	CL	9-D	405	1/1	0.87	1.22	-	261,261,261,261	1
3	GOL	8-G	403	6/6	0.76	0.27	-	35,117,202,207	6
3	GOL	4-E	403	6/6	0.76	0.26	-	29,57,83,86	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CL	2-A	406	1/1	0.78	0.61	-	122,122,122,122	1
5	FMT	9-G	405	3/3	0.95	0.38	-	38,38,218,325	3
4	CL	10-D	406	1/1	0.76	0.82	-	263,263,263,263	1
4	CL	7-D	406	1/1	0.76	0.82	-	245,245,245,245	1
4	CL	3-G	407	1/1	0.82	0.34	-	29,29,29,29	1
4	CL	2-A	405	1/1	0.46	0.88	-	43,43,43,43	1
3	GOL	4-H	402	6/6	0.68	0.30	-	27,213,267,270	6
3	GOL	2-F	403	6/6	0.80	0.30	-	35,117,202,207	6
4	CL	8-A	405	1/1	0.46	0.88	-	43,43,43,43	1
4	CL	8-G	407	1/1	0.82	0.34	-	29,29,29,29	1
4	CL	9-G	406	1/1	0.27	0.89	-	29,29,29,29	1
4	CL	5-D	406	1/1	0.76	0.82	-	263,263,263,263	1
4	CL	10-B	408	1/1	0.60	0.54	-	97,97,97,97	1
4	CL	8-D	406	1/1	0.76	0.82	-	263,263,263,263	1
4	CL	10-F	408	1/1	0.77	0.47	-	28,28,28,28	1
3	GOL	7-G	404	6/6	0.75	0.24	-	26,41,231,232	6
4	CL	8-H	406	1/1	0.29	0.91	-	32,32,32,32	1
3	GOL	9-G	404	6/6	0.75	0.24	-	26,41,231,232	6
4	CL	4-B	408	1/1	0.60	0.54	-	97,97,97,97	1
3	GOL	6-B	407	6/6	0.81	0.29	-	40,79,89,91	6
3	CL	7-H	405	1/1	0.29	0.91	-	303,303,303,303	1
4	CL	7-A	406	1/1	0.78	0.61	-	43,43,43,43	1
3	GOL	7-B	407	6/6	0.81	0.29	-	40,79,89,91	6
3	CL	9-F	406	1/1	0.98	0.26	-	28,28,28,28	1
3	GOL	10-B	406	6/6	0.67	0.33	-	40,79,89,91	6
3	FMT	1-C	403	3/3	0.85	0.46	-	29,29,276,319	3
3	GOL	3-F	404	6/6	0.83	0.29	-	35,117,202,207	6
4	CL	7-G	407	1/1	0.82	0.34	-	32,32,32,32	1
4	CL	2-D	406	1/1	0.76	0.82	-	263,263,263,263	1
3	GOL	9-H	405	6/6	0.79	0.32	-	32,37,218,314	6
3	CL	1-H	404	1/1	0.04	0.84	-	303,303,303,303	1
4	CL	10-C	406	1/1	0.76	0.49	-	245,245,245,245	1
4	CL	3-D	406	1/1	0.76	0.82	-	263,263,263,263	1
4	FMT	4-C	405	3/3	0.86	0.42	-	29,29,276,319	3
4	CL	10-H	407	1/1	0.91	0.30	-	32,32,32,32	1
3	GOL	7-F	403	6/6	0.80	0.30	-	29,35,59,94	6
4	CL	4-C	406	1/1	0.76	0.49	-	41,41,41,41	1
5	GOL	8-G	405	6/6	0.69	0.26	-	26,41,231,232	6
3	CL	2-D	404	1/1	-0.04	0.99	-	261,261,261,261	1
4	CL	10-H	406	1/1	0.29	0.91	-	303,303,303,303	1
5	CL	7-C	404	1/1	0.90	0.17	-	41,41,41,41	1
5	FMT	8-C	404	3/3	0.87	0.41	-	29,29,276,319	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	6-E	404	6/6	0.87	0.19	-	29,57,83,86	6
4	CL	3-F	408	1/1	0.77	0.47	-	28,28,28,28	1
5	FMT	9-C	404	3/3	0.87	0.41	-	29,29,276,319	3
3	GOL	1-A	402	6/6	0.84	0.20	-	39,51,59,85	6
4	CL	8-C	405	1/1	0.57	0.64	-	41,41,41,41	1
3	GOL	9-F	403	6/6	0.80	0.30	-	35,117,202,207	6
4	FMT	5-G	406	3/3	0.81	0.47	-	38,38,218,325	3
3	CL	3-H	404	1/1	0.04	0.84	-	303,303,303,303	1
3	GOL	4-D	403	6/6	0.75	0.49	-	30,35,49,275	6
4	CL	7-D	405	1/1	0.87	1.22	-	261,261,261,261	1
4	CL	6-D	405	1/1	0.87	1.22	-	261,261,261,261	1
4	CL	6-D	407	1/1	0.85	0.86	-	263,263,263,263	1
3	CL	5-H	405	1/1	0.29	0.91	-	303,303,303,303	1
4	CL	4-D	406	1/1	0.76	0.82	-	263,263,263,263	1
4	CL	7-D	407	1/1	0.85	0.86	-	263,263,263,263	1
4	CL	2-H	406	1/1	0.29	0.91	-	32,32,32,32	1
3	GOL	2-B	402	6/6	0.77	0.25	-	24,117,121,122	6
4	CL	4-G	409	1/1	0.94	0.55	-	32,32,32,32	1
4	CL	10-A	405	1/1	0.46	0.88	-	43,43,43,43	1
5	FMT	7-G	405	3/3	0.95	0.38	-	38,38,218,325	3
3	GOL	1-H	403	6/6	0.75	0.29	-	32,37,218,314	6
3	CL	4-F	406	1/1	0.98	0.26	-	28,28,28,28	1
4	CL	10-C	405	1/1	0.57	0.64	-	41,41,41,41	1
4	CL	2-G	406	1/1	0.27	0.89	-	29,29,29,29	1
4	CL	7-G	406	1/1	0.27	0.89	-	29,29,29,29	1
4	CL	3-D	405	1/1	0.87	1.22	-	245,245,245,245	1
3	CL	4-D	404	1/1	-0.04	0.99	-	261,261,261,261	1
4	CL	6-H	407	1/1	0.91	0.30	-	32,32,32,32	1
3	CL	3-D	404	1/1	-0.04	0.99	-	261,261,261,261	1
3	GOL	10-F	403	6/6	0.80	0.30	-	29,35,59,94	6
3	FMT	6-C	403	3/3	0.85	0.46	-	29,29,276,319	3
4	FMT	8-G	406	3/3	0.81	0.47	-	38,38,218,325	3
4	CL	10-E	404	1/1	0.92	0.25	-	38,38,38,38	1
4	CL	6-F	408	1/1	0.77	0.47	-	28,28,28,28	1
4	CL	6-D	406	1/1	0.76	0.82	-	245,245,245,245	1
4	CL	9-H	406	1/1	0.29	0.91	-	303,303,303,303	1
3	GOL	10-D	404	6/6	0.92	0.19	-	30,35,49,275	6
3	GOL	5-H	404	6/6	0.76	0.39	-	32,37,218,314	6
3	GOL	8-H	404	6/6	0.76	0.39	-	32,37,218,314	6
4	CL	3-B	408	1/1	0.60	0.54	-	97,97,97,97	1
3	FMT	7-C	403	3/3	0.85	0.46	-	29,29,276,319	3
4	CL	6-A	406	1/1	0.78	0.61	-	43,43,43,43	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	FMT	2-C	405	3/3	0.86	0.42	-	29,29,276,319	3
3	FMT	5-C	403	3/3	0.85	0.46	-	29,29,276,319	3
3	GOL	4-H	404	6/6	0.76	0.39	-	32,37,218,314	6
4	CL	9-H	407	1/1	0.91	0.30	-	32,32,32,32	1
4	CL	7-B	408	1/1	0.60	0.54	-	97,97,97,97	1
4	CL	6-H	406	1/1	0.29	0.91	-	303,303,303,303	1
4	CL	1-E	404	1/1	0.92	0.25	-	38,38,38,38	1
5	CL	6-G	405	1/1	0.63	0.32	-	29,29,29,29	1
4	CL	1-G	407	1/1	0.82	0.34	-	29,29,29,29	1
3	CL	8-D	404	1/1	-0.04	0.99	-	261,261,261,261	1
3	GOL	4-G	404	6/6	0.75	0.24	-	20,31,173,206	6
3	CL	3-H	405	1/1	0.29	0.91	-	32,32,32,32	1
4	CL	9-C	405	1/1	0.57	0.64	-	41,41,41,41	1
5	FMT	2-G	405	3/3	0.95	0.38	-	38,38,218,325	3
4	CL	8-D	405	1/1	0.87	1.22	-	245,245,245,245	1
3	GOL	3-D	403	6/6	0.75	0.49	-	30,35,49,275	6
3	GOL	1-D	403	6/6	0.75	0.49	-	24,36,252,269	6
4	CL	3-C	405	1/1	0.57	0.64	-	41,41,41,41	1
3	GOL	10-G	404	6/6	0.75	0.24	-	26,41,231,232	6
4	CL	7-F	408	1/1	0.77	0.47	-	28,28,28,28	1
3	GOL	7-B	403	6/6	0.58	0.39	-	24,117,121,122	6
4	FMT	3-G	406	3/3	0.81	0.47	-	38,38,218,325	3
4	CL	1-B	409	1/1	0.83	0.21	-	97,97,97,97	1
3	GOL	9-D	404	6/6	0.92	0.19	-	30,35,49,275	6
4	GOL	4-G	406	6/6	0.67	0.41	-	26,41,231,232	6
4	CL	10-A	406	1/1	0.78	0.61	-	122,122,122,122	1
5	FMT	10-G	405	3/3	0.95	0.38	-	38,38,218,325	3
4	CL	2-D	405	1/1	0.87	1.22	-	245,245,245,245	1
3	CL	1-H	405	1/1	0.29	0.91	-	32,32,32,32	1
3	GOL	1-F	404	6/6	0.83	0.29	-	35,117,202,207	6
3	GOL	10-G	403	6/6	0.76	0.27	-	35,117,202,207	6
4	CL	3-A	406	1/1	0.78	0.61	-	43,43,43,43	1
4	CL	1-D	406	1/1	0.76	0.82	-	263,263,263,263	1
3	GOL	4-G	403	6/6	0.76	0.27	-	35,117,202,207	6
4	CL	9-D	407	1/1	0.85	0.86	-	263,263,263,263	1
3	GOL	2-H	404	6/6	0.76	0.39	-	32,37,218,314	6
5	FMT	10-C	404	3/3	0.87	0.41	-	29,29,276,319	3
3	CL	2-H	405	1/1	0.29	0.91	-	303,303,303,303	1
4	CL	4-D	405	1/1	0.87	1.22	-	245,245,245,245	1
4	CL	10-G	406	1/1	0.27	0.89	-	29,29,29,29	1
4	CL	1-F	409	1/1	0.85	0.20	-	28,28,28,28	1
3	GOL	7-E	403	6/6	0.76	0.26	-	29,57,83,86	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	2-F	402	6/6	0.76	0.33	-	29,35,59,94	6
5	CL	8-F	407	1/1	0.93	0.22	-	28,28,28,28	1
3	GOL	5-B	407	6/6	0.81	0.29	-	40,79,89,91	6
4	CL	4-A	405	1/1	0.46	0.88	-	43,43,43,43	1
3	GOL	1-B	407	6/6	0.81	0.29	-	40,79,89,91	6
4	CL	6-B	409	1/1	0.83	0.21	-	122,122,122,122	1
5	CL	1-C	404	1/1	0.90	0.17	-	41,41,41,41	1
3	GOL	7-F	404	6/6	0.83	0.29	-	35,117,202,207	6
3	FMT	6-G	404	3/3	0.91	0.37	-	38,38,218,325	3
3	GOL	8-D	403	6/6	0.75	0.49	-	30,35,49,275	6
4	CL	5-G	407	1/1	0.82	0.34	-	29,29,29,29	1
4	CL	2-C	406	1/1	0.76	0.49	-	41,41,41,41	1
4	CL	1-A	406	1/1	0.78	0.61	-	122,122,122,122	1
5	CL	2-F	407	1/1	0.93	0.22	-	28,28,28,28	1
4	CL	1-C	405	1/1	0.57	0.64	-	245,245,245,245	1
3	GOL	5-H	402	6/6	0.68	0.30	-	27,213,267,270	6
4	CL	9-D	406	1/1	0.76	0.82	-	245,245,245,245	1
4	CL	1-A	405	1/1	0.46	0.88	-	43,43,43,43	1
4	CL	5-D	405	1/1	0.87	1.22	-	261,261,261,261	1
4	CL	5-C	405	1/1	0.57	0.64	-	245,245,245,245	1

6.5 Other polymers (i)

There are no such residues in this entry.