



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 6, 2017 – 09:58 PM EDT

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 : unknown
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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

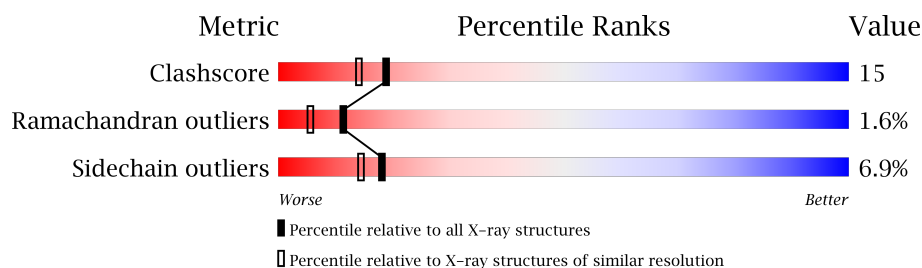
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.




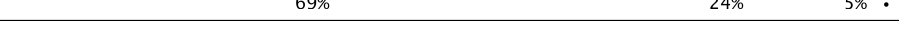
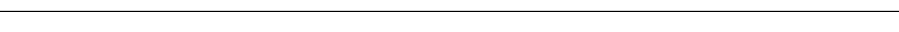


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	384	 71% 23% . .
1	1-B	384	 70% 24% . . .
1	1-C	384	 75% 20% . .
1	1-D	384	 69% 24% 5% .
1	1-E	384	 71% 24% . . .
1	1-F	384	 68% 27% . .
1	1-G	384	 73% 22% . . .


























Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	4-A	384	 71%23% . .
1	4-B	384	 72%21%5% . .
1	4-C	384	 72%23% . .
1	4-D	384	 68%26% . .
1	4-E	384	 67%26%5% .
1	4-F	384	 67%26%5% .
1	4-G	384	 71%23% . .
1	4-H	384	 71%24% . .
1	5-A	384	 71%23% . .
1	5-B	384	 66%28% . .
1	5-C	384	 70%25% . .
1	5-D	384	 74%20% . .
1	5-E	384	 66%25%6% . .
1	5-F	384	 73%23% . .
1	5-G	384	 75%19% . .
1	5-H	384	 72%22% . .
1	6-A	384	 75%20% . .
1	6-B	384	 69%24% . .
1	6-C	384	 71%24% . .
1	6-D	384	 69%25% . .
1	6-E	384	 75%18% . .
1	6-F	384	 70%23%5% .
1	6-G	384	 72%23% . .
1	6-H	384	 74%21% . .
1	7-A	384	 67%24%5% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	7-B	384	
1	7-C	384	
1	7-D	384	
1	7-E	384	
1	7-F	384	
1	7-G	384	
1	7-H	384	
1	8-A	384	
1	8-B	384	
1	8-C	384	
1	8-D	384	
1	8-E	384	
1	8-F	384	
1	8-G	384	
1	8-H	384	
1	9-A	384	
1	9-B	384	
1	9-C	384	
1	9-D	384	
1	9-E	384	
1	9-F	384	
1	9-G	384	
1	9-H	384	

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	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-B	401	-	-	X	-
2	MES	7-H	401	-	-	X	-
2	MES	8-C	401	-	-	X	-
3	GOL	10-A	403	-	-	X	-
3	GOL	5-B	405	-	-	X	-
3	GOL	7-A	402	-	-	X	-
3	GOL	8-E	402	-	-	X	-
3	GOL	8-H	404	-	-	X	-
4	CL	10-E	404	-	-	X	-
4	CL	10-H	407	-	-	X	-
4	CL	2-H	406	-	-	X	-
4	CL	4-A	406	-	-	X	-
4	CL	5-D	405	-	-	X	-
4	CL	6-B	409	-	-	X	-
4	CL	6-D	405	-	-	X	-
4	CL	6-F	408	-	-	X	-
4	CL	7-F	408	-	-	X	-
5	FMT	3-F	407	-	-	X	-
5	FMT	7-F	407	-	-	X	-

2 Entry composition

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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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: C₆H₁₃NO₄S).



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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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	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-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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
3	1-B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

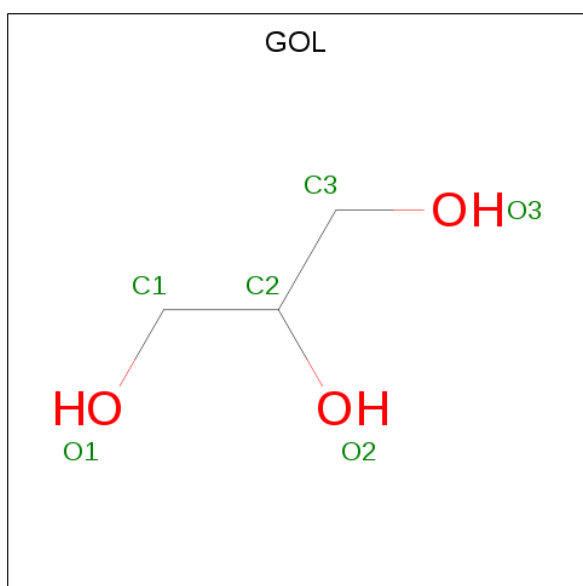
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	7-G	1	Total	C	O	0	0
			6	3	3		
3	8-G	1	Total	C	O	0	0
			6	3	3		
3	9-G	1	Total	C	O	0	0
			6	3	3		
3	10-G	1	Total	C	O	0	0
			6	3	3		
3	1-G	1	Total	C	O	0	0
			6	3	3		
3	2-G	1	Total	C	O	0	0
			6	3	3		
3	3-G	1	Total	C	O	0	0
			6	3	3		
3	4-G	1	Total	C	O	0	0
			6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

Continued on next page...

Continued from previous page...

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

- 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is FORMIC ACID (three-letter code: GOL, FMT, CL) (formula: $\text{C}_3\text{H}_8\text{O}_3$, 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 180	O 180	0	0
6	2-A	190	Total 190	O 190	0	0
6	3-A	183	Total 183	O 183	0	0
6	4-A	184	Total 184	O 184	0	0
6	5-A	197	Total 197	O 197	0	0
6	6-A	179	Total 179	O 179	0	0
6	7-A	192	Total 192	O 192	0	0
6	8-A	183	Total 183	O 183	0	0
6	9-A	188	Total 188	O 188	0	0
6	10-A	173	Total 173	O 173	0	0
6	1-B	198	Total 198	O 198	0	0
6	2-B	189	Total 189	O 189	0	0
6	3-B	183	Total 183	O 183	0	0
6	4-B	189	Total 189	O 189	0	0
6	5-B	189	Total 189	O 189	0	0
6	6-B	195	Total 195	O 195	0	0
6	7-B	196	Total 196	O 196	0	0
6	8-B	185	Total 185	O 185	0	0
6	9-B	198	Total 198	O 198	0	0
6	10-B	195	Total 195	O 195	0	0
6	1-C	178	Total 178	O 178	0	0
6	2-C	178	Total 178	O 178	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

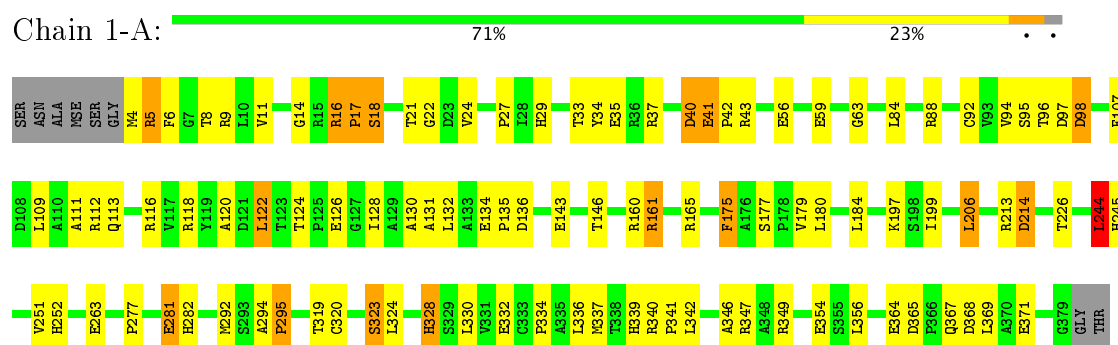
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	5-G	172	Total 172	O 172	0	0
6	6-G	176	Total 176	O 176	0	0
6	7-G	187	Total 187	O 187	0	0
6	8-G	179	Total 179	O 179	0	0
6	9-G	197	Total 197	O 197	0	0
6	10-G	182	Total 182	O 182	0	0
6	1-H	172	Total 172	O 172	0	0
6	2-H	185	Total 185	O 185	0	0
6	3-H	163	Total 163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

3 Residue-property plots [i](#)

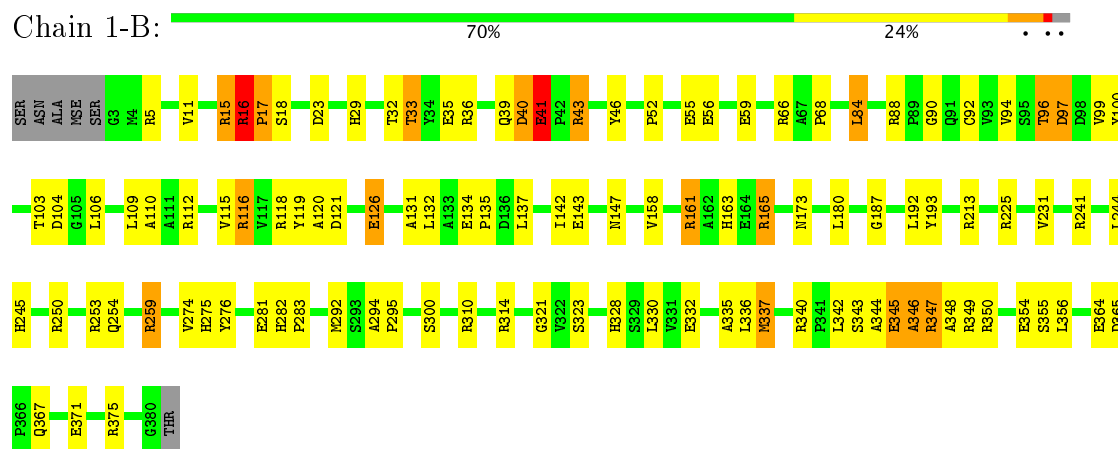
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS failed to run properly.

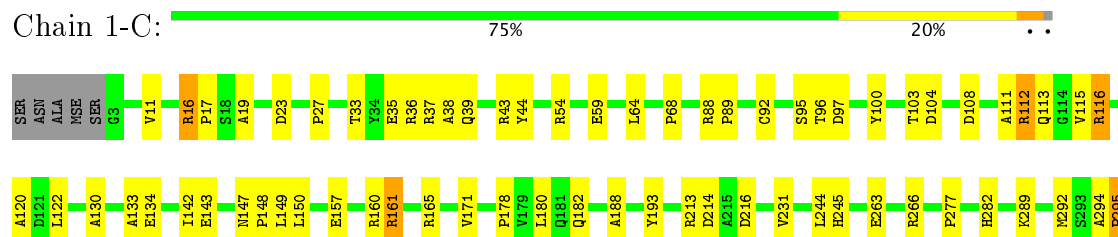
• Molecule 1: CalE6

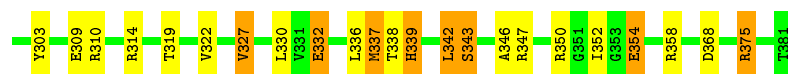


• Molecule 1: CalE6



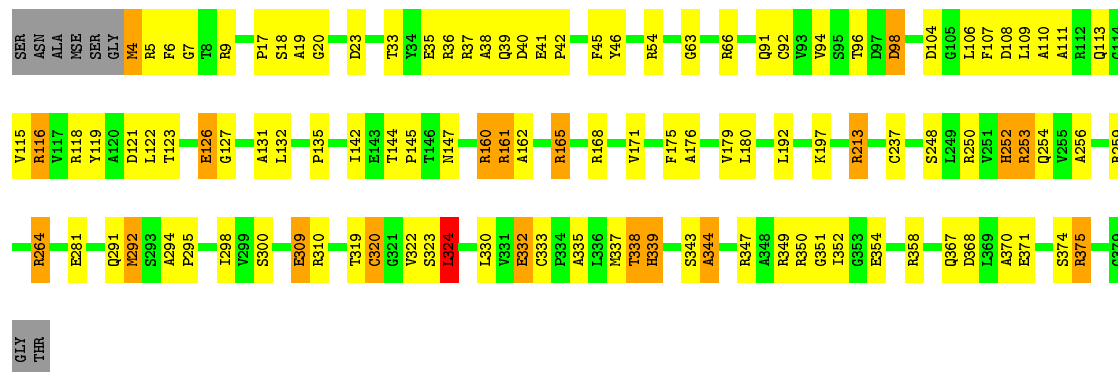
• Molecule 1: CalE6





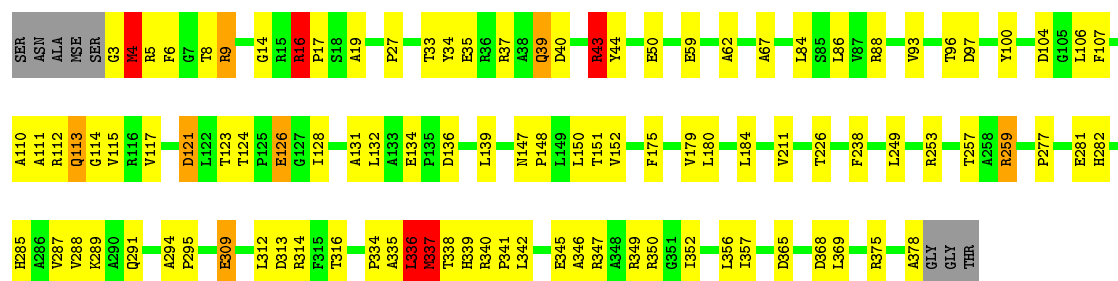
• Molecule 1: CalE6

Chain 1-D: 69% 24% 5%



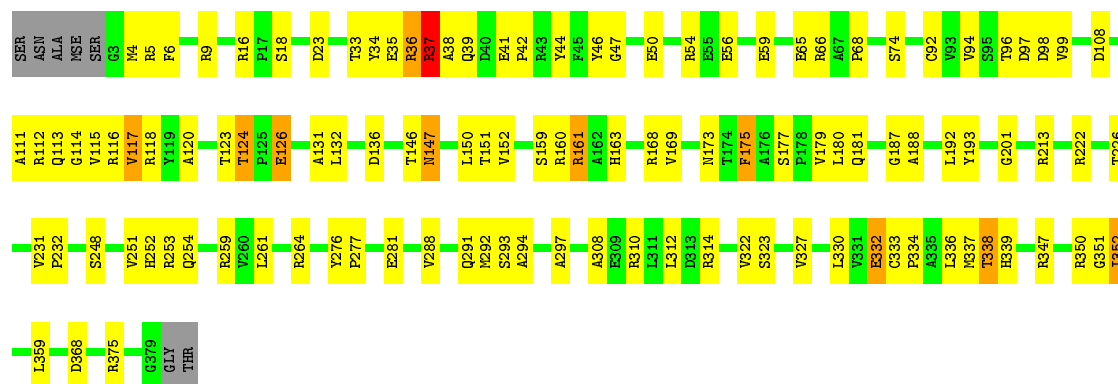
• Molecule 1: CalE6

Chain 1-E: 71% 24% ...



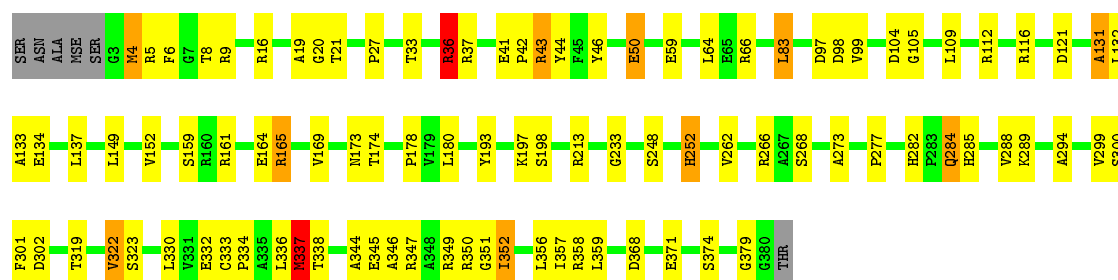
• Molecule 1: CalE6

Chain 1-F: 68% 27% ..



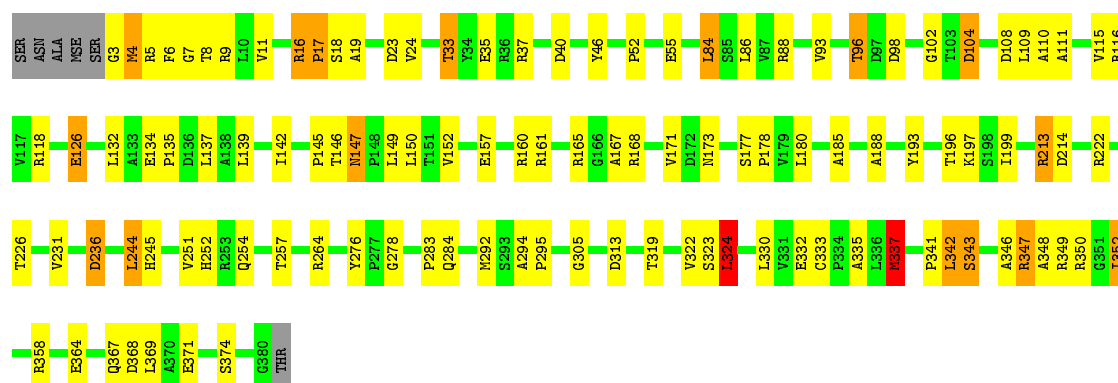
• Molecule 1: CalE6

Chain 1-G: 73% 22% ...



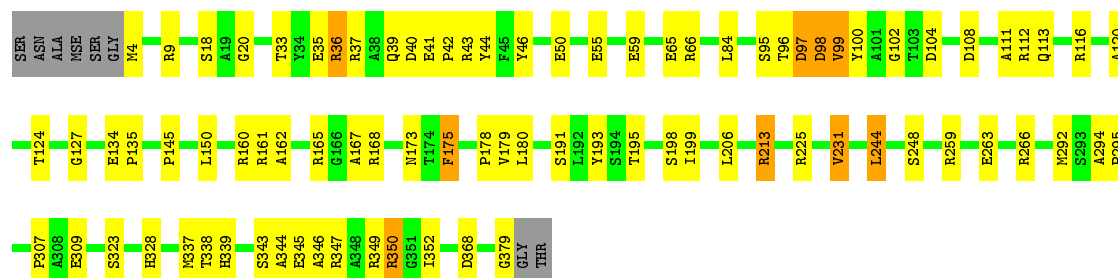
- Molecule 1: CalE6

Chain 1-H: 69% 25% . . .



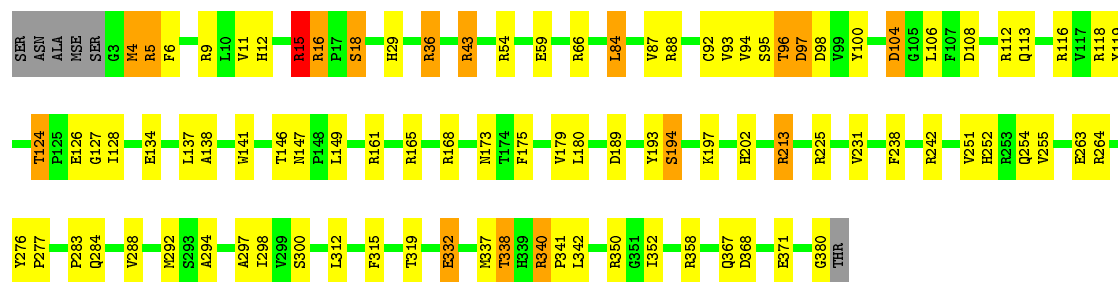
- Molecule 1: CalE6

Chain 2-A: 76% 20% . . .



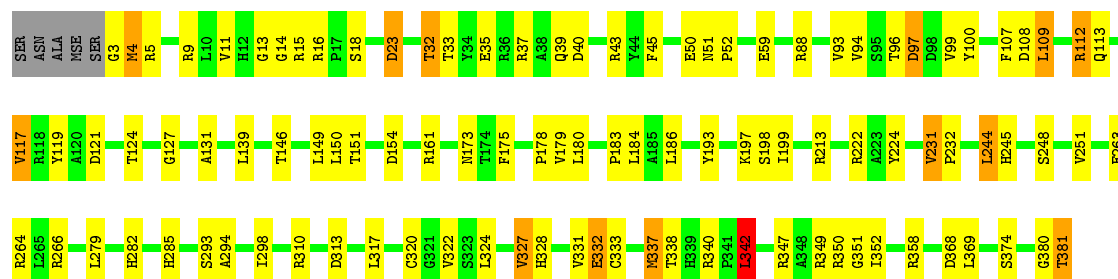
- Molecule 1: CalE6

Chain 2-B: 74% 20% . . .



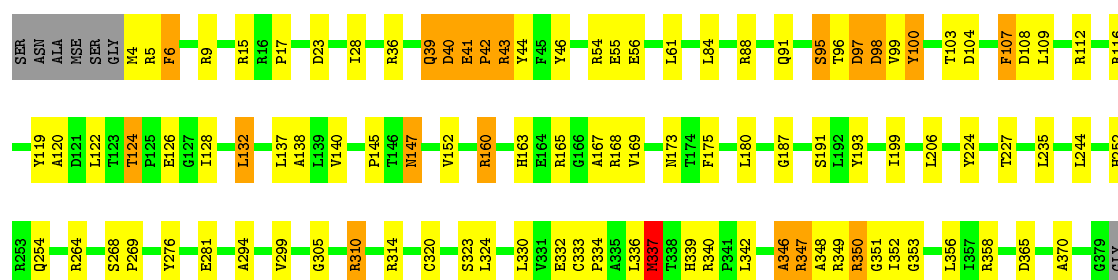
- Molecule 1: CalE6

Chain 2-C:  72% 23% ..



• Molecule 1: CalE6

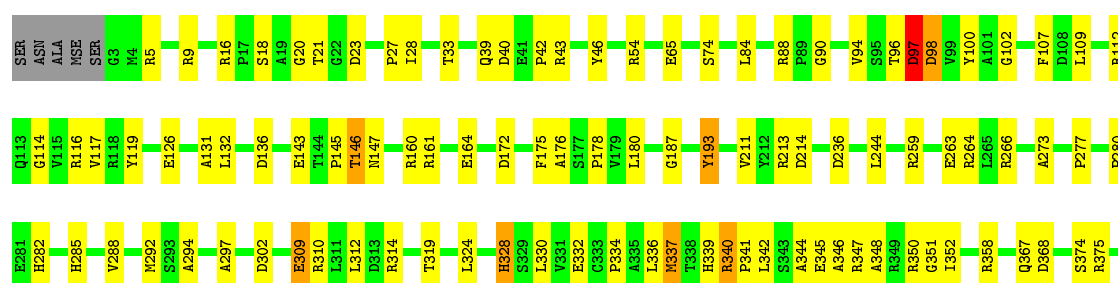
Chain 2-D:  71% 22% 5% .



THR


• Molecule 1: CalE6

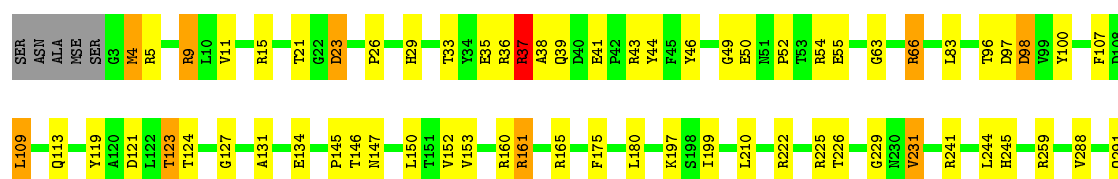
Chain 2-E:  72% 24% ..



A378
GLY
GLY
THR

• Molecule 1: CalE6

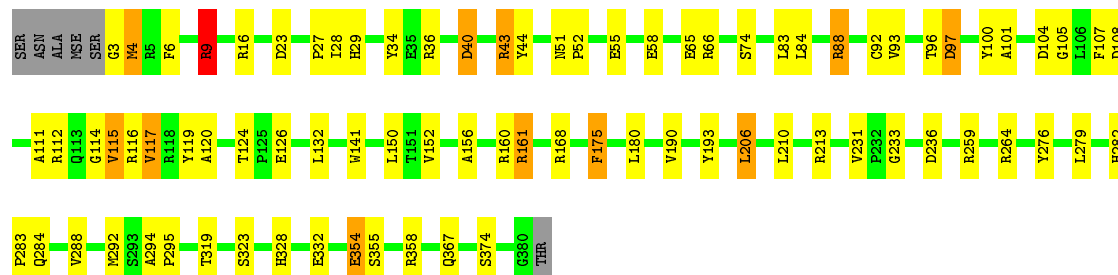
Chain 2-F:  75% 21% ..





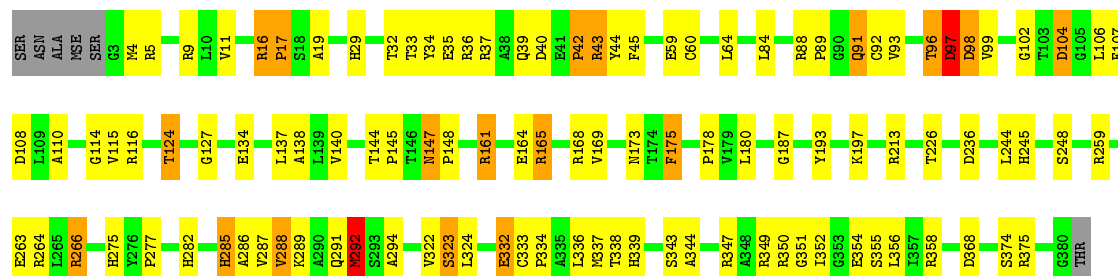
• Molecule 1: CalE6

Chain 2-G: 77% 18% . .



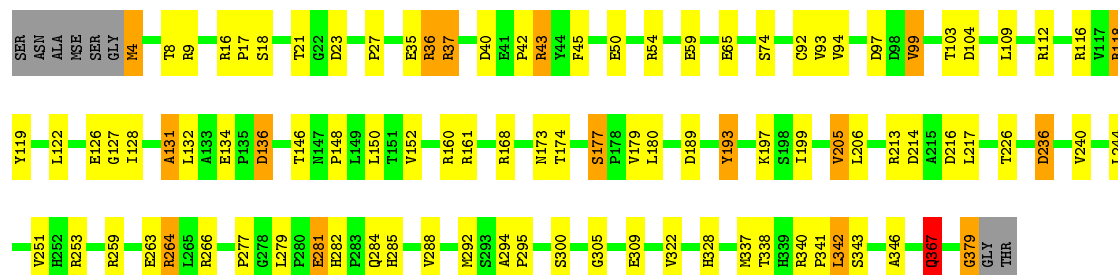
• Molecule 1: CalE6

Chain 2-H: 70% 23% 5% . .



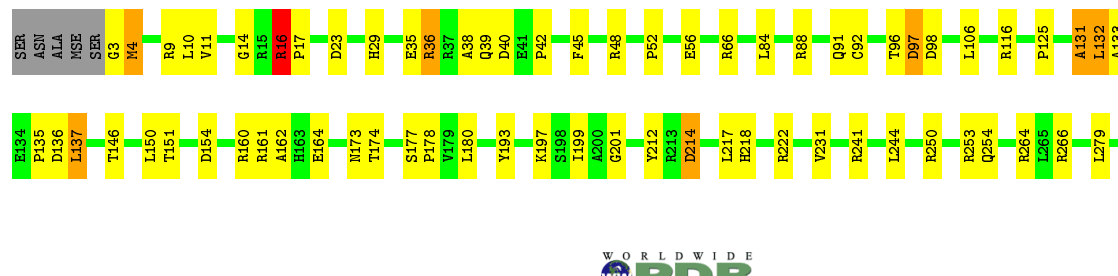
• Molecule 1: CalE6

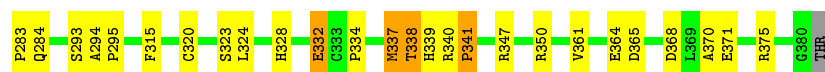
Chain 3-A: 73% 21% . .



• Molecule 1: CalE6

Chain 3-B: 74% 21% . .





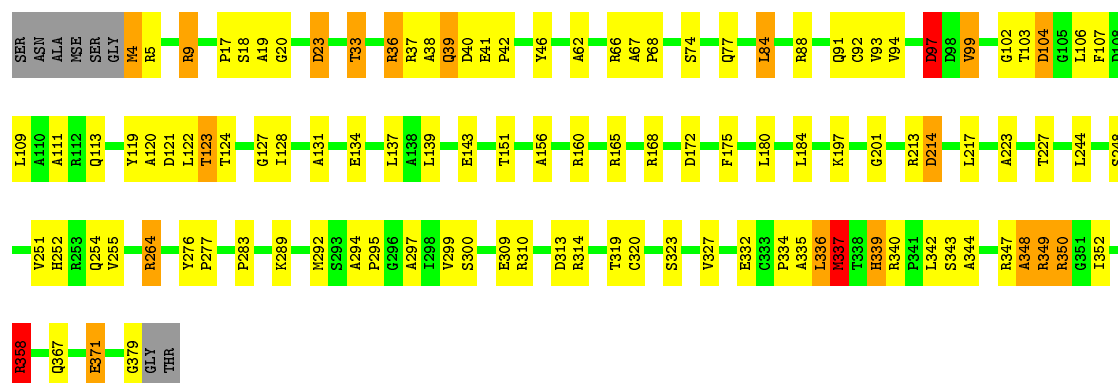
- Molecule 1: CalE6

Chain 3-C: 70% 23% 5%



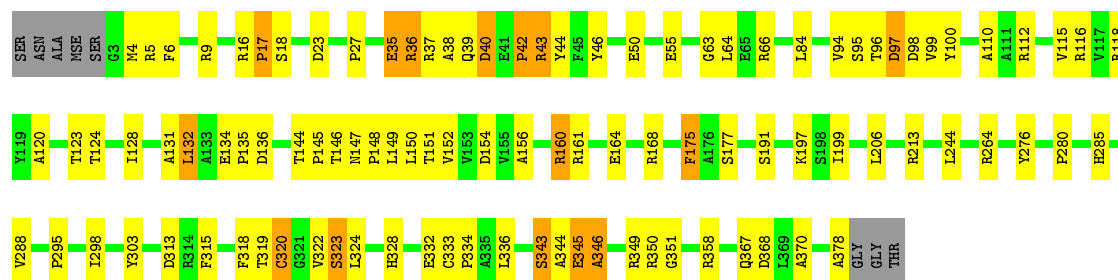
- Molecule 1: CalE6

Chain 3-D: 69% 24% 5%



- Molecule 1: CalE6

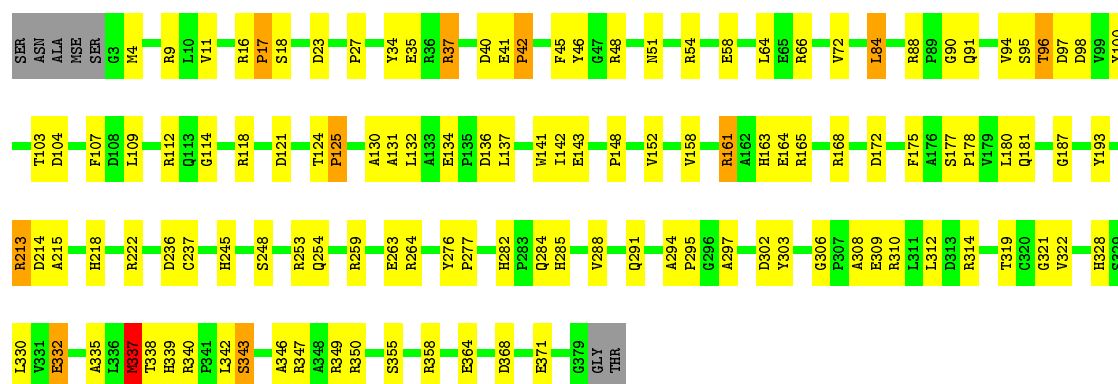
Chain 3-E: 71% 23%



- Molecule 1: CalE6

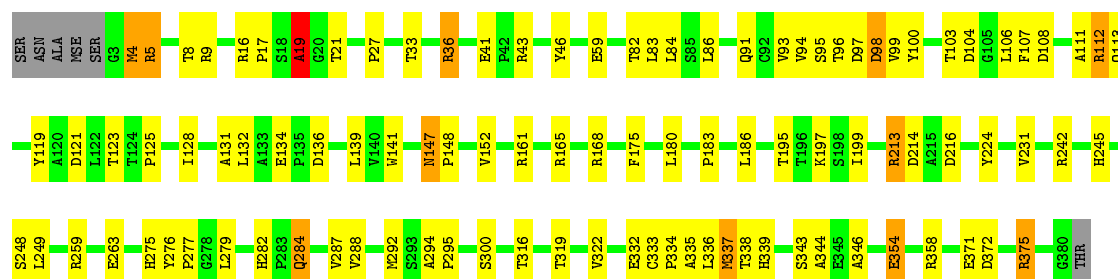
Chain 3-F: 66% 29%





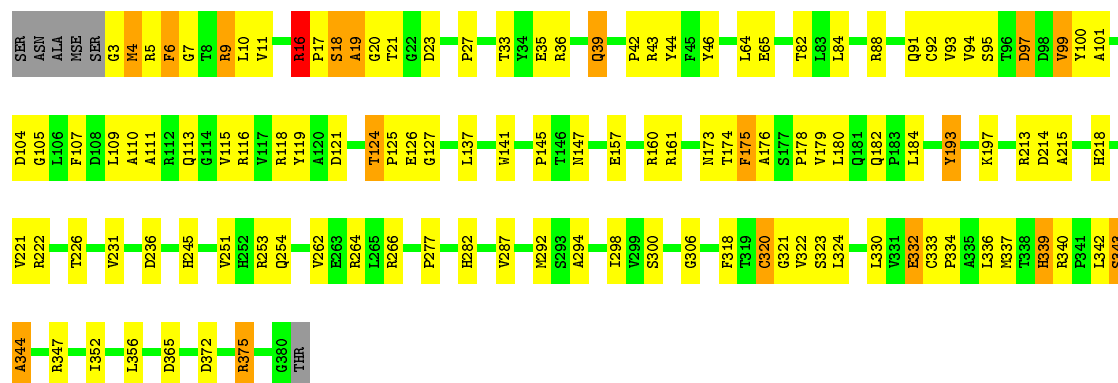
• Molecule 1: CalE6

Chain 3-G: 72% 23%



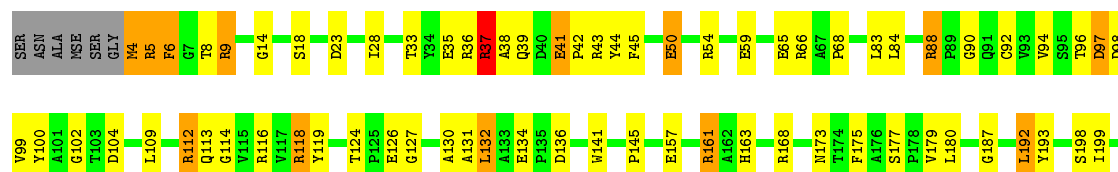
• Molecule 1: CalE6

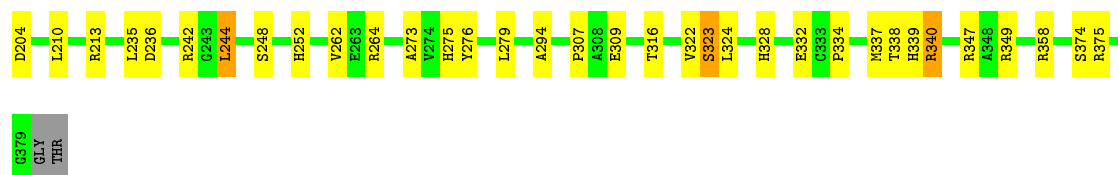
Chain 3-H: 67% 26%



• Molecule 1: CalE6

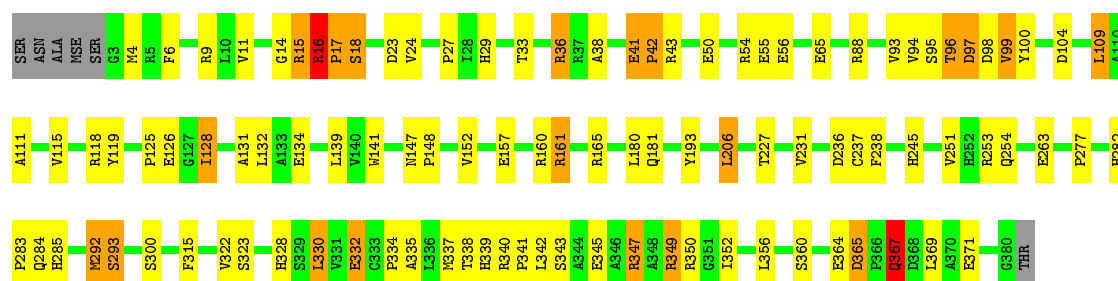
Chain 4-A: 71% 23%





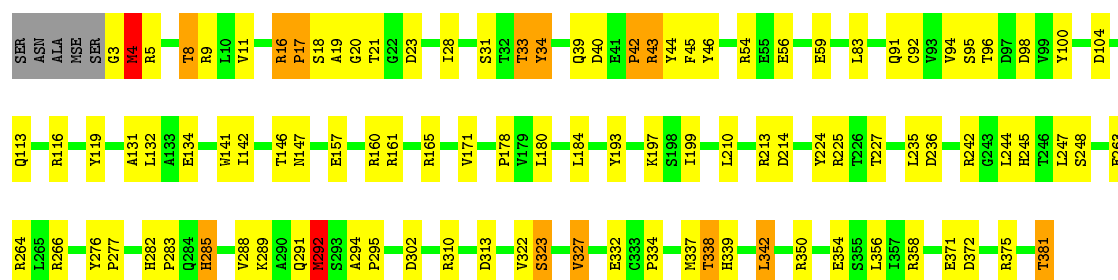
- Molecule 1: CalE6

Chain 4-B: 72% 21% 5% ..



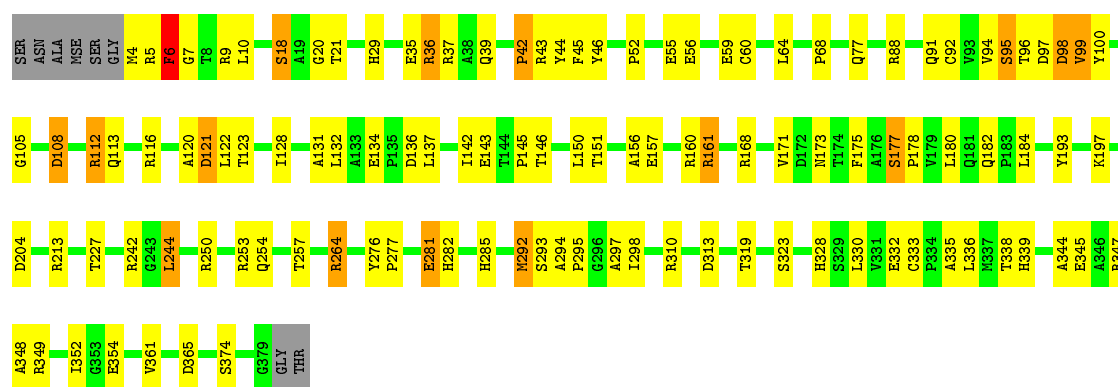
- Molecule 1: CalE6

Chain 4-C: 72% 23% ..



- Molecule 1: CalE6

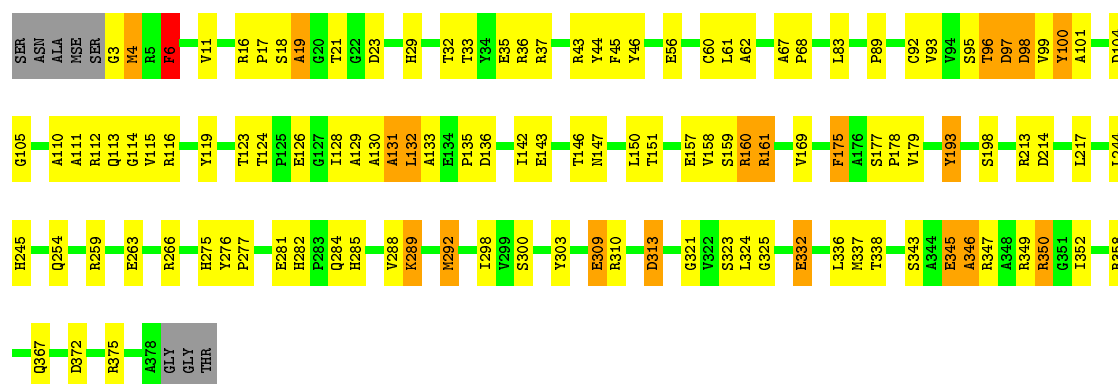
Chain 4-D: 68% 26% ..



- Molecule 1: CalE6

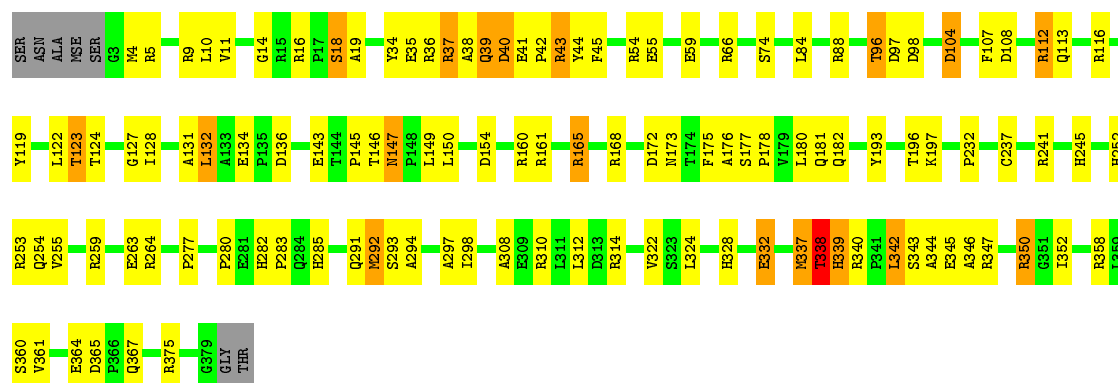
Chain 4-E: 67% 26% 5% ..





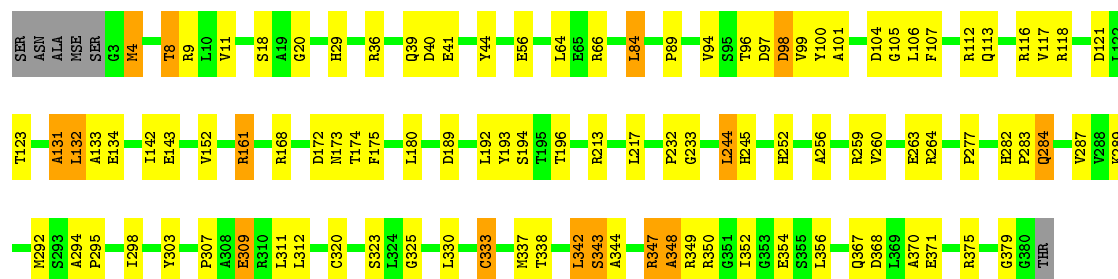
• Molecule 1: CalE6

Chain 4-F: 67% 26% 5% .



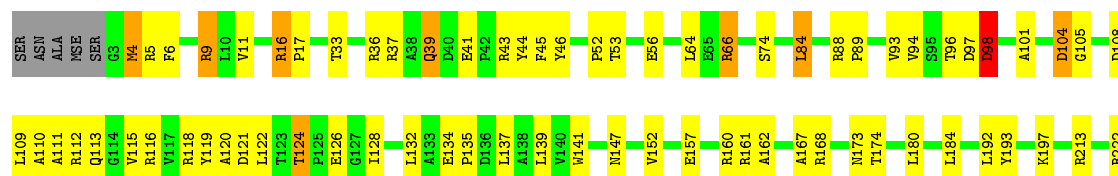
• Molecule 1: CalE6

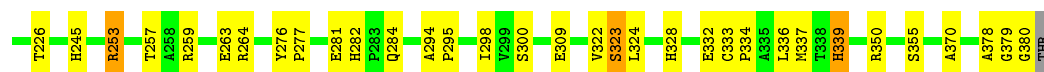
Chain 4-G: 71% 23% . .



• Molecule 1: CalE6

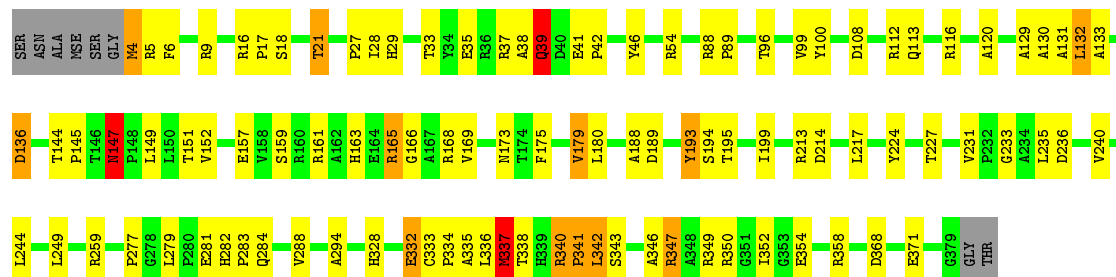
Chain 4-H: 71% 24% . .





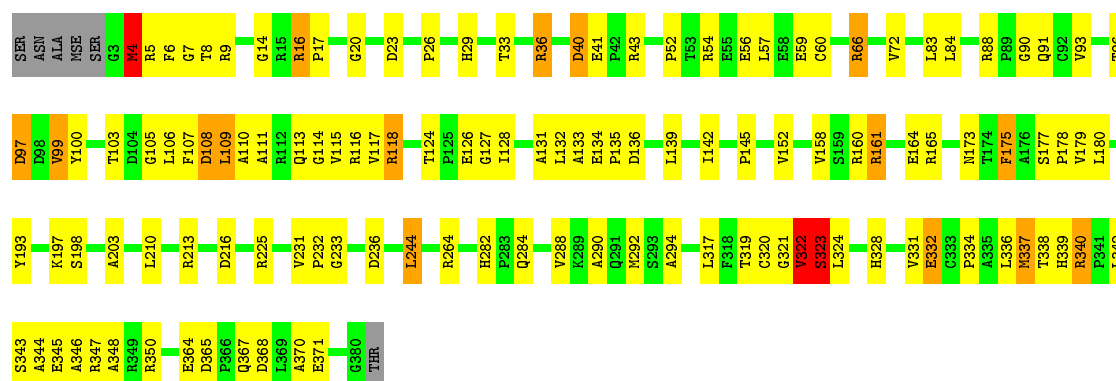
- Molecule 1: CalE6

Chain 5-A: 71% 23% . . .



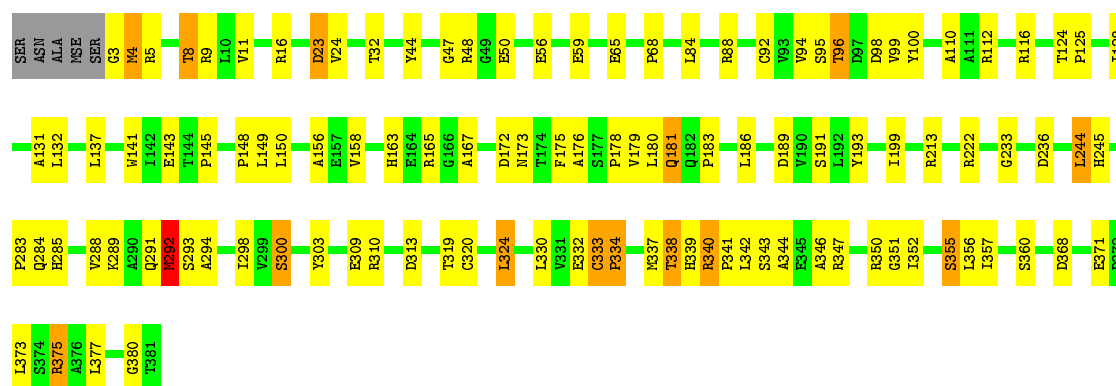
- Molecule 1: CalE6

Chain 5-B: 66% 28% . . .



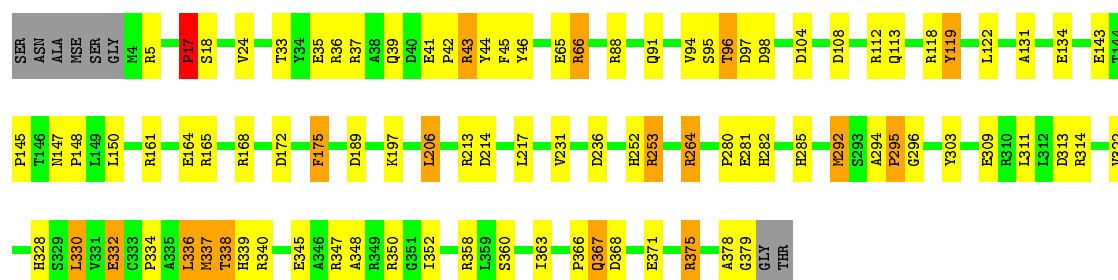
- Molecule 1: CalE6

Chain 5-C: 70% 25% . .



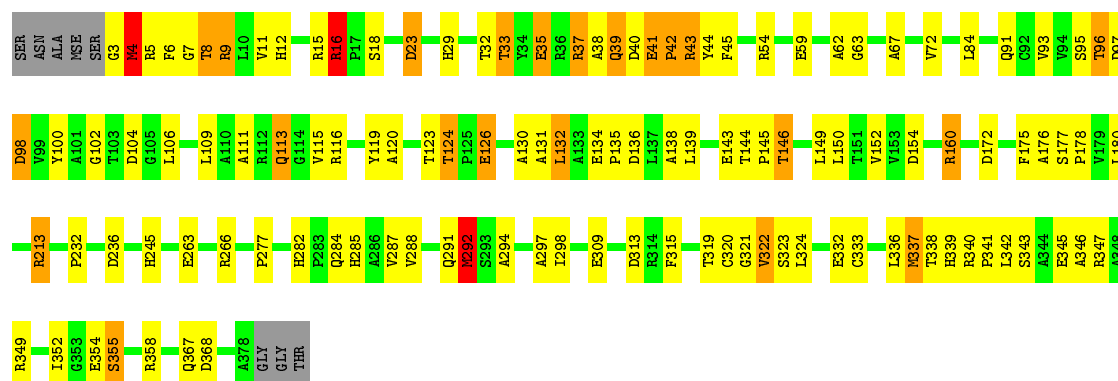
- Molecule 1: CalE6

Chain 5-D: 74% 20% . .



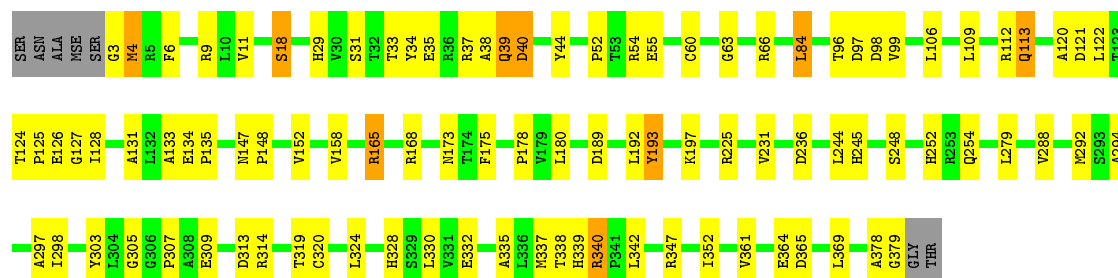
• Molecule 1: CalE6

Chain 5-E: 66% 25% 6% ..



• Molecule 1: CalE6

Chain 5-F: 73% 23% ..

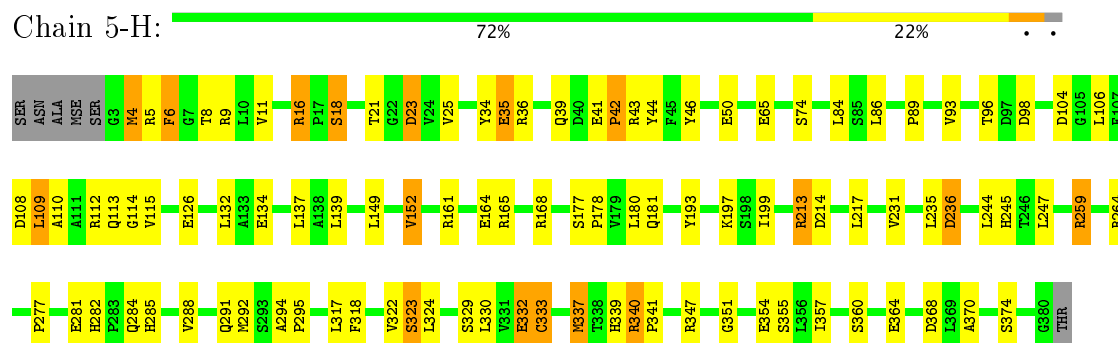


• Molecule 1: CalE6

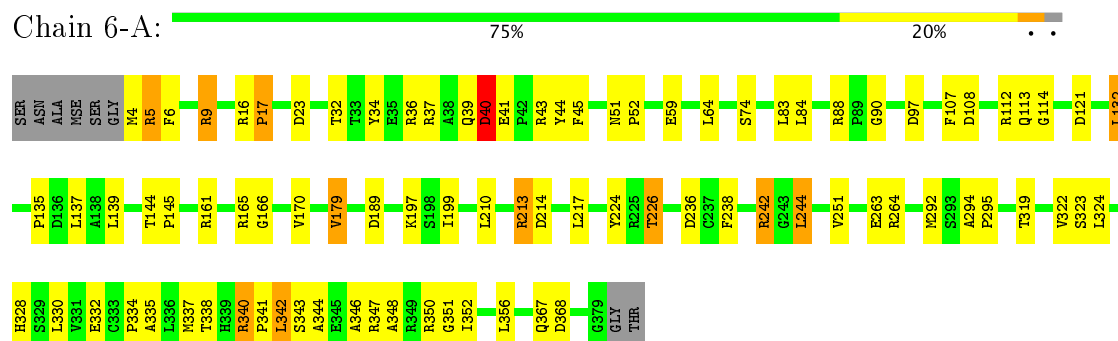
Chain 5-G: 75% 19% ..



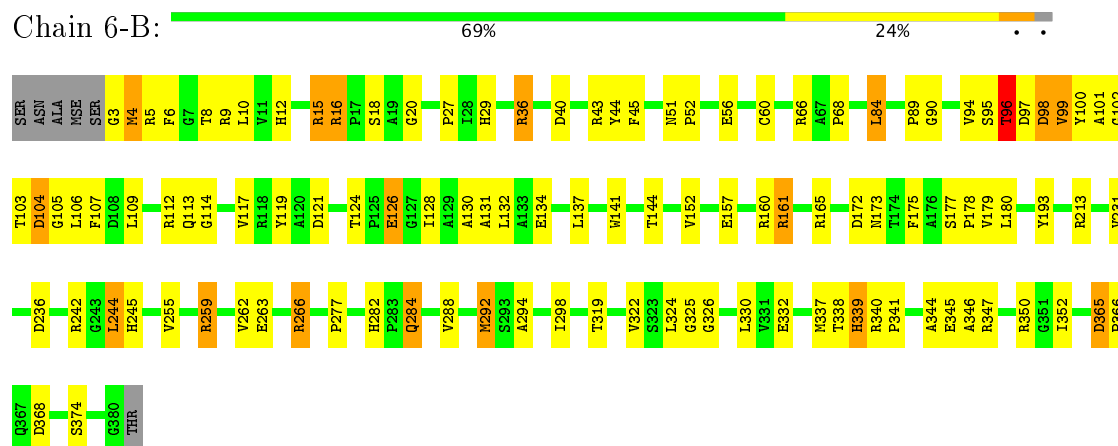
• Molecule 1: CalE6



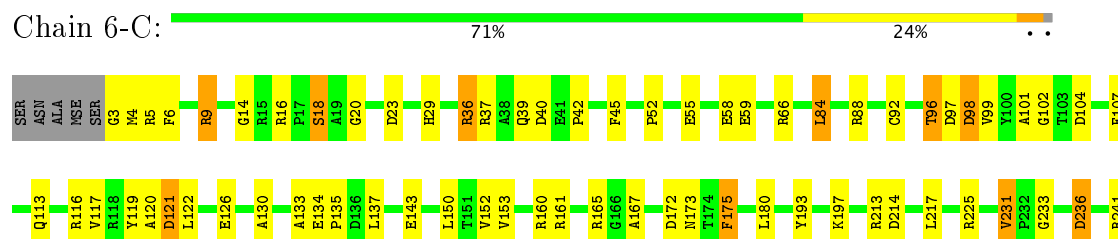
- Molecule 1: CalE6

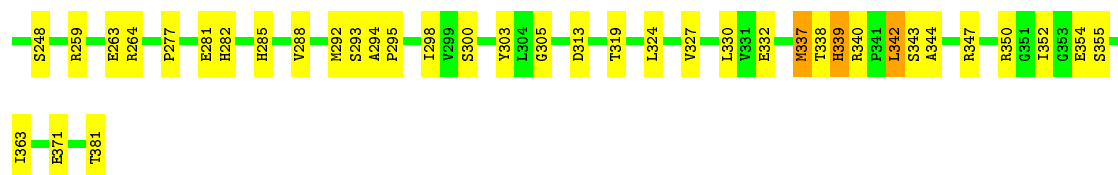


- Molecule 1: CalE6



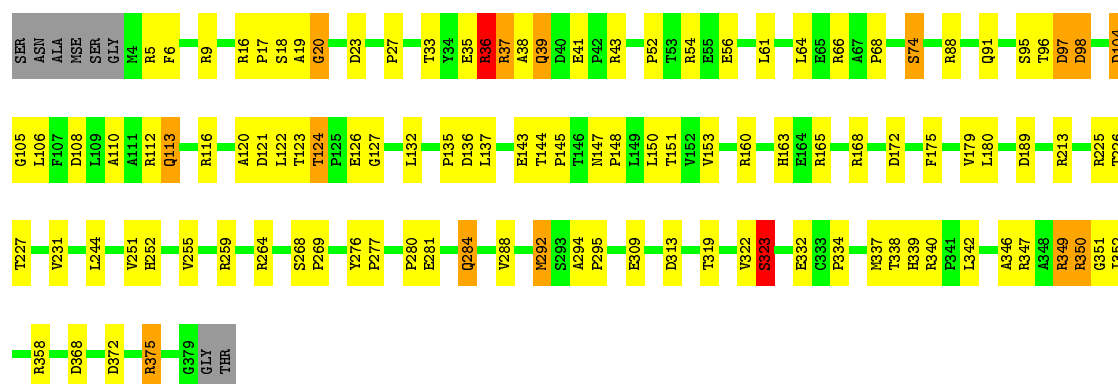
- Molecule 1: CalE6





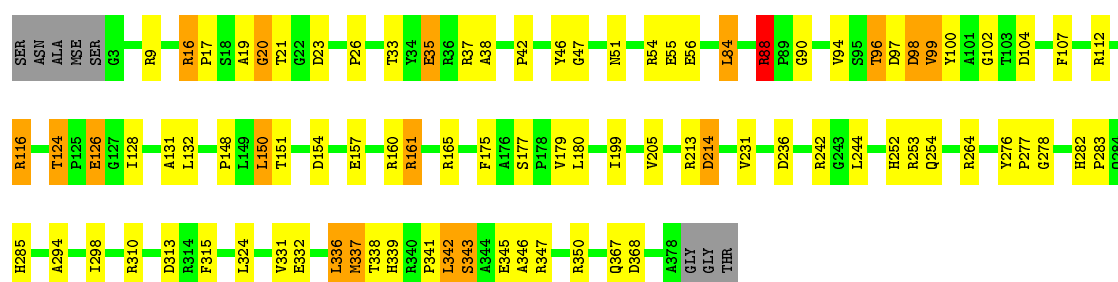
- Molecule 1: CalE6

Chain 6-D: 69% 25% . .



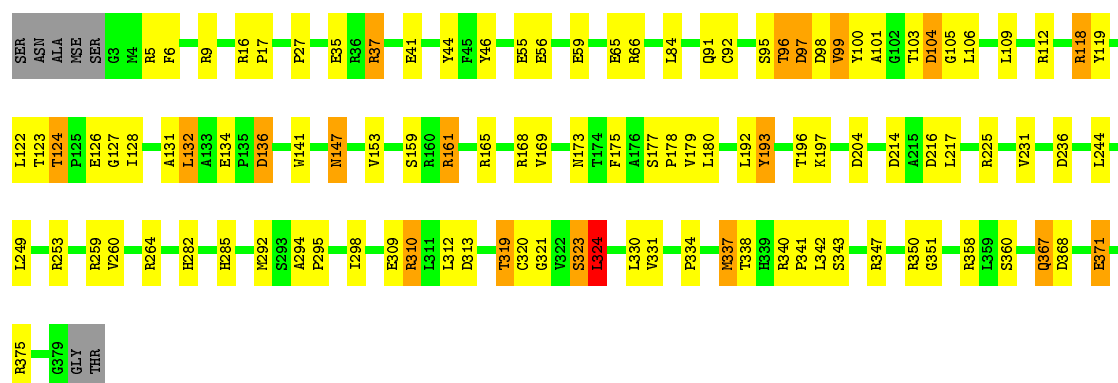
- Molecule 1: CalE6

Chain 6-E: 75% 18% . .



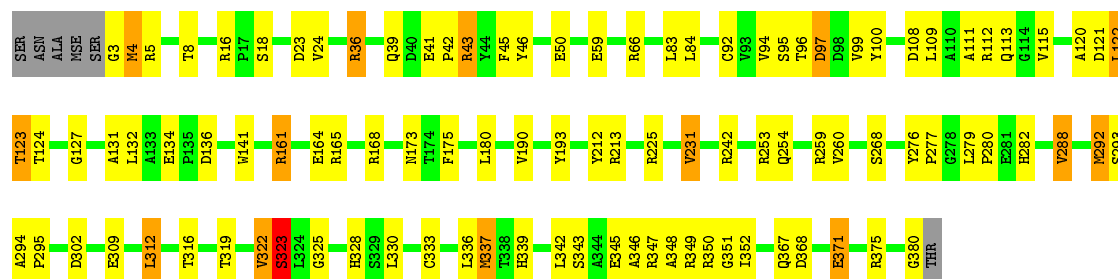
- Molecule 1: CalE6

Chain 6-F: 70% 23% 5% .




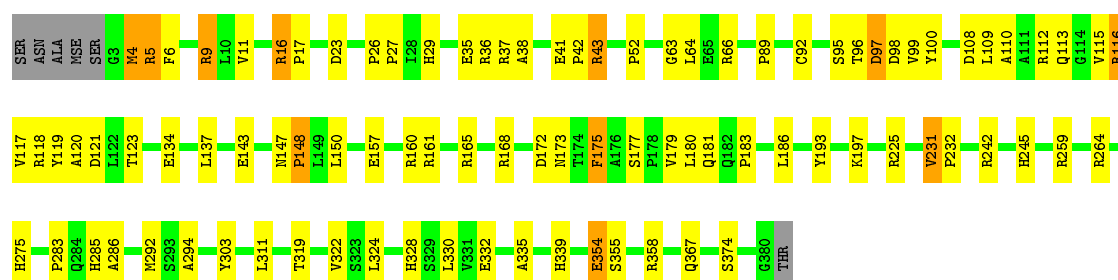
- Molecule 1: CalE6

Chain 6-G:  72% 23% . .



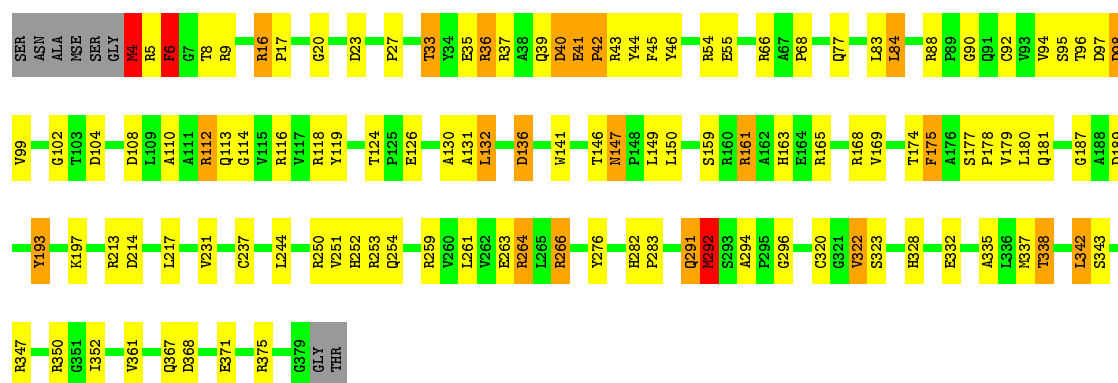
• Molecule 1: CalE6

Chain 6-H:  74% 21% . .



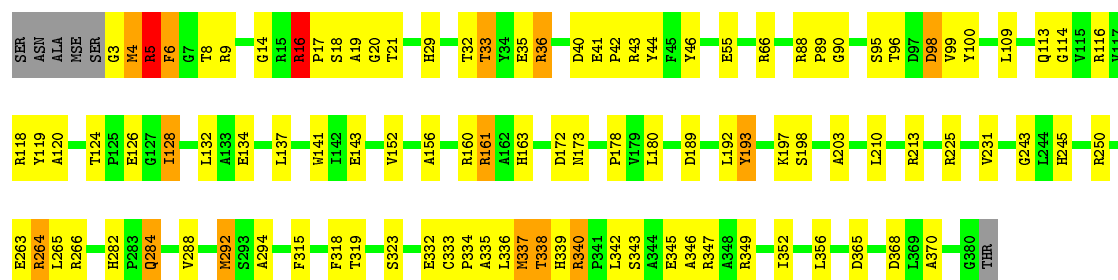
• Molecule 1: CalE6

Chain 7-A:  67% 24% 5% . .

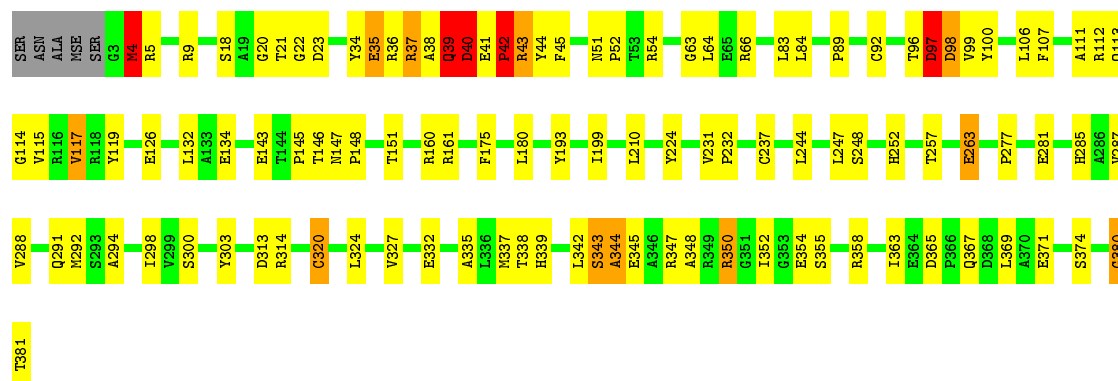


• Molecule 1: CalE6

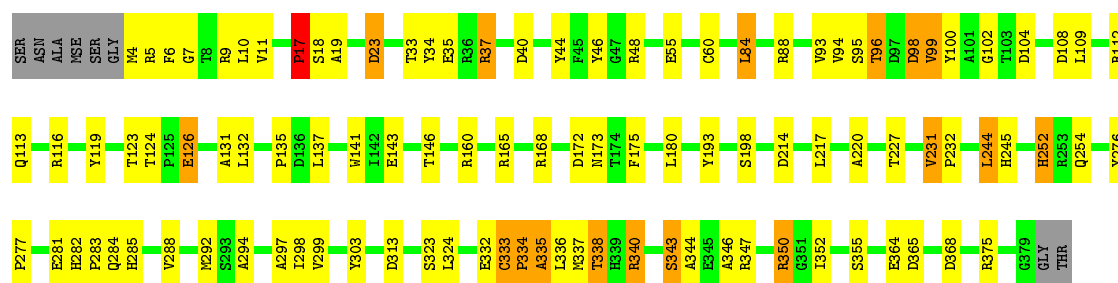
Chain 7-B:  71% 23% . . .



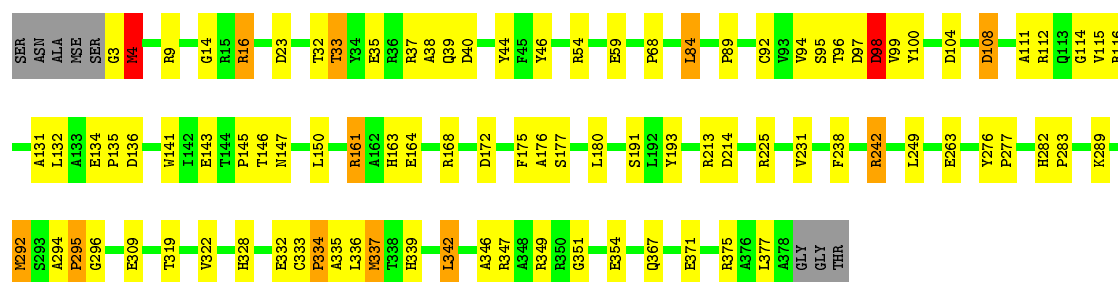
- Molecule 1: CalE6

Chain 7-C: 

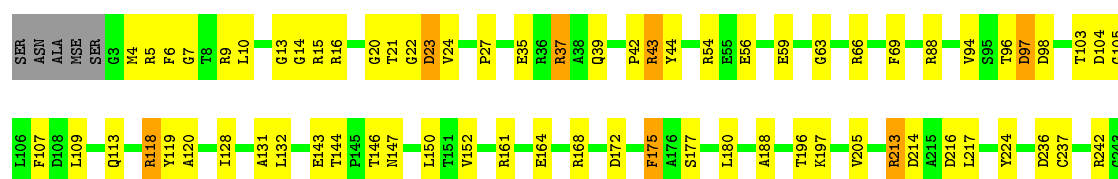
- Molecule 1: CalE6

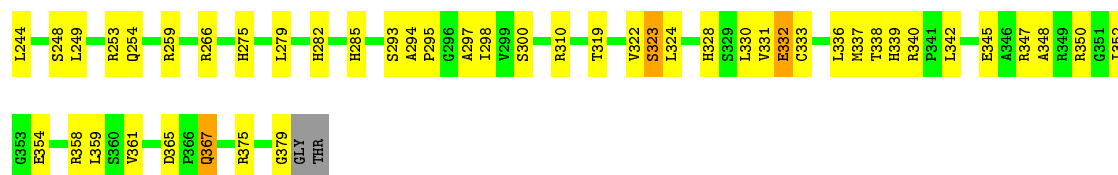
Chain 7-D: 

- Molecule 1: CalE6

Chain 7-E: 

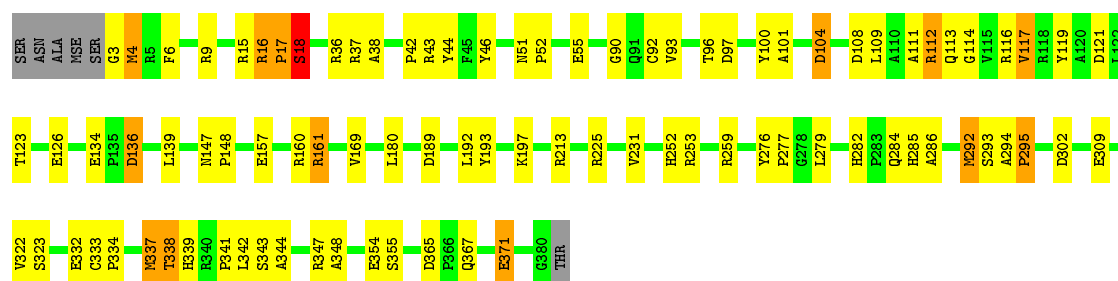
- Molecule 1: CalE6

Chain 7-F: 



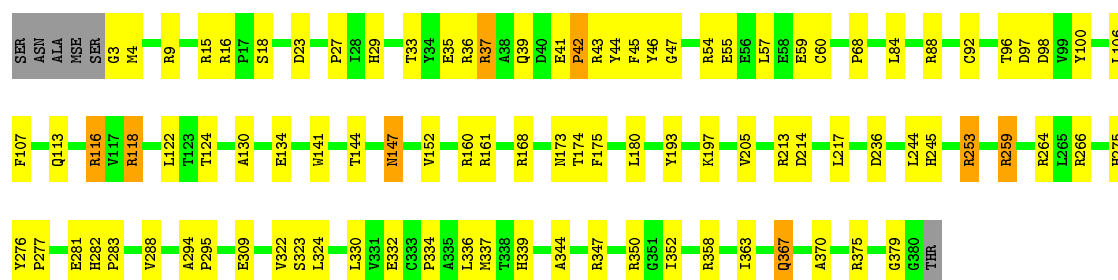
- Molecule 1: CalE6

Chain 7-G: 75% 20%



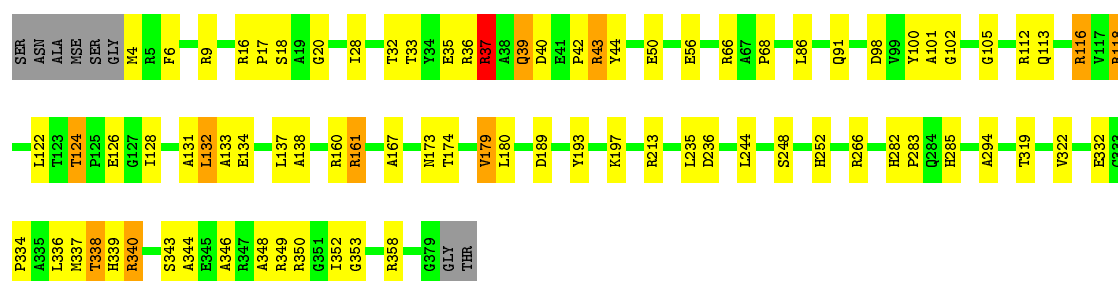
- Molecule 1: CalE6

Chain 7-H: 73% 23%



- Molecule 1: CalE6

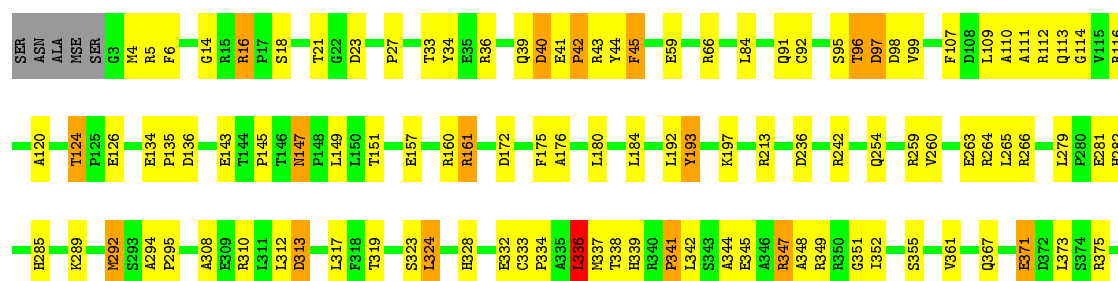
Chain 8-A: 77% 18%



- Molecule 1: CalE6

Chain 8-B: 68% 28%

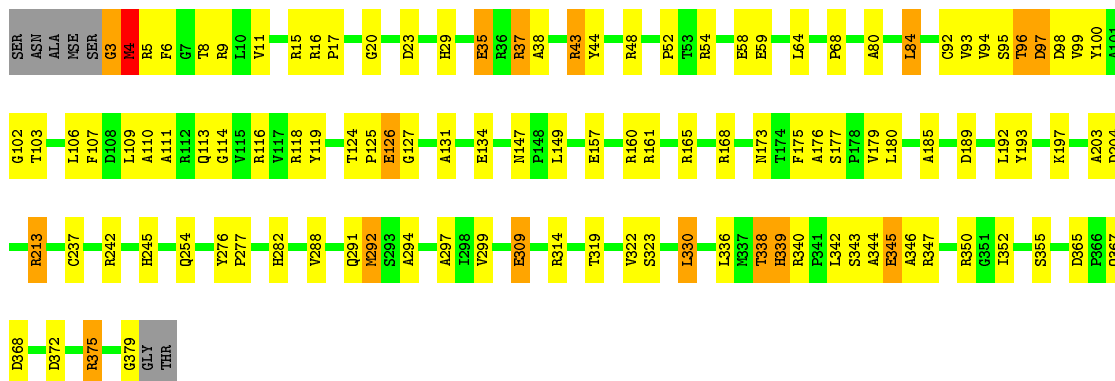







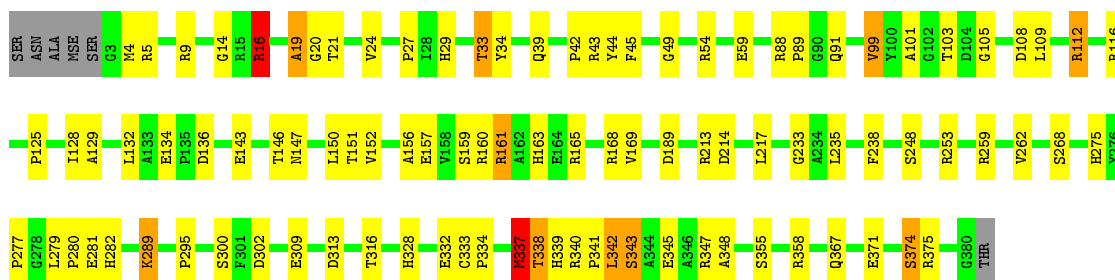
• Molecule 1: CalE6

Chain 8-F:  69% 25% ..




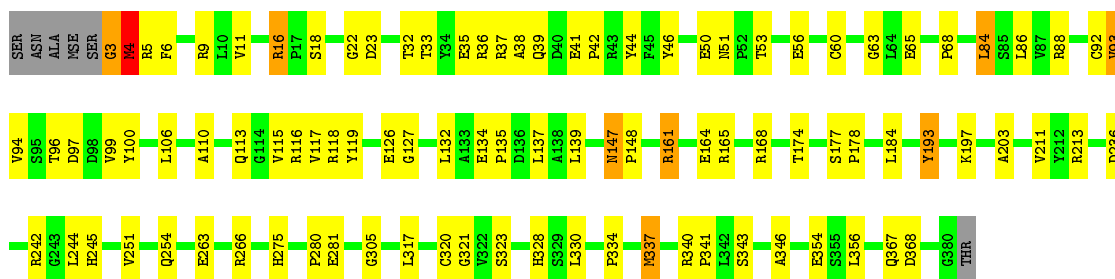
• Molecule 1: CalE6

Chain 8-G:  73% 22% ..



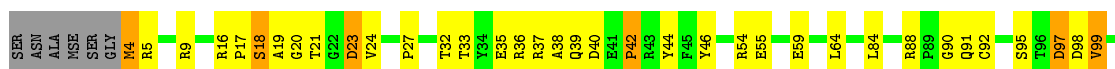
• Molecule 1: CalE6

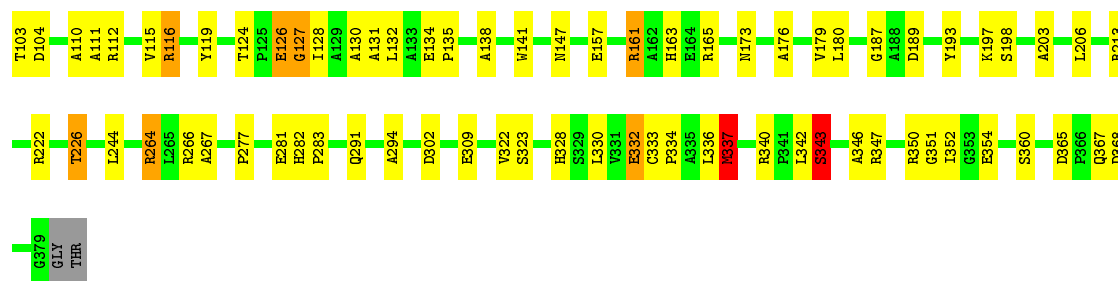
Chain 8-H:  73% 23% ..



• Molecule 1: CalE6

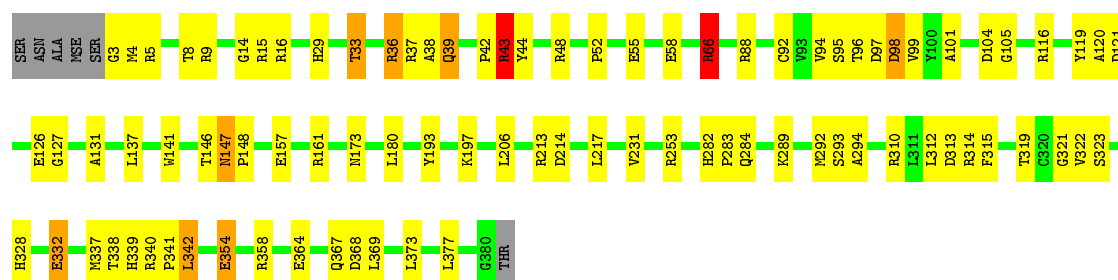
Chain 9-A:  70% 24% ..





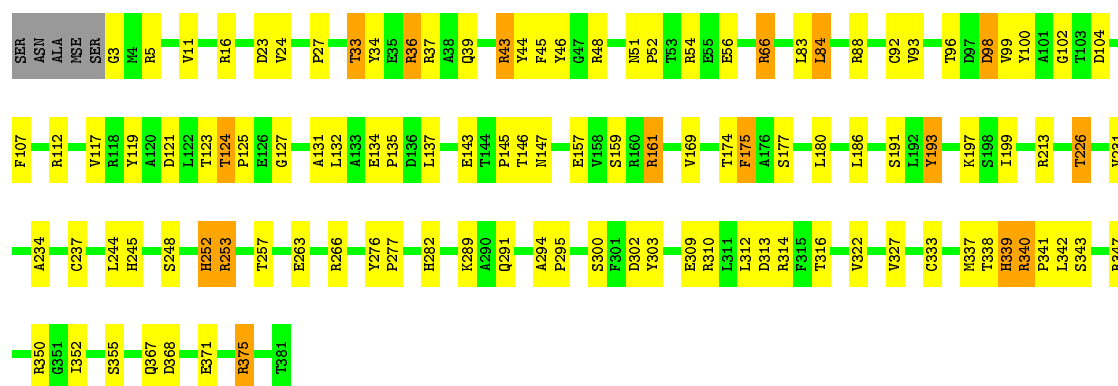
- Molecule 1: CalE6

Chain 9-B: 75% 21% ...



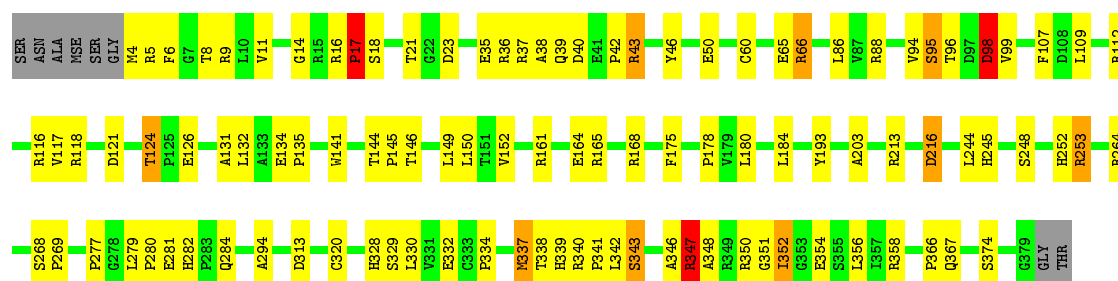
- Molecule 1: CalE6

Chain 9-C: 70% 25% ..



- Molecule 1: CalE6

Chain 9-D: 71% 24% ...



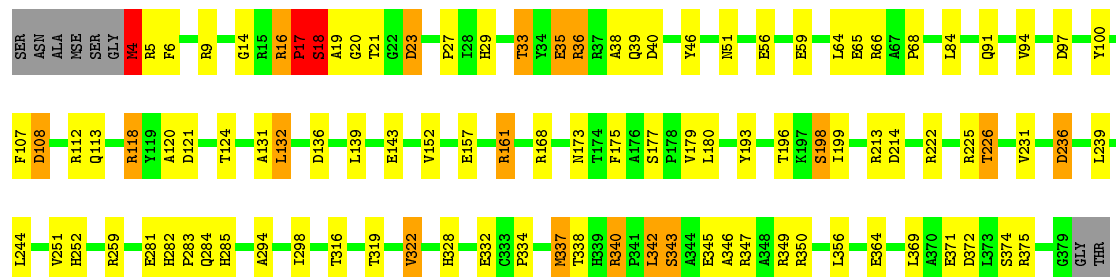
- Molecule 1: CalE6

SER	ASN	MSE	ALA	SER	G3	F6	M4	G7	R16	T8	P17	L10	R16	P17	T21	G22	D23	E29	Y34	E35	R36	R37	D40	E41	P42	R43	Y44	F45	Y46	E50	N51	P52	E55	E59	E65	L84	V87	R88	P89	G90	C92	V93	V94	S95	Y100	E103														
	G102		G105		L109		R112		Q113		R116		R118		Y119		A120		T124		L132		A133		E134		P135		D136		L137		L149		E157		Y158		S159		R161		A162		E163		R165	G166	A167	R168	N173	L180	L192	Y193	T196	I199	L210	R213	V231	L235



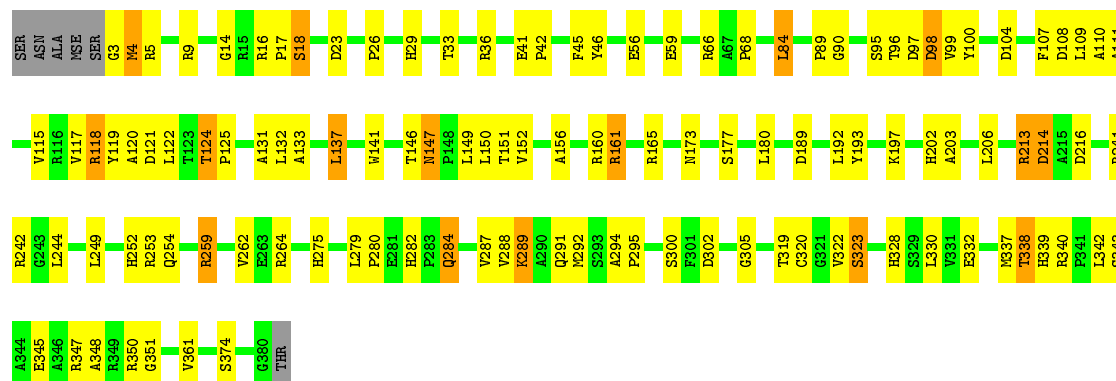
• Molecule 1: CalE6

Chain 10-A: 72% 21% . .



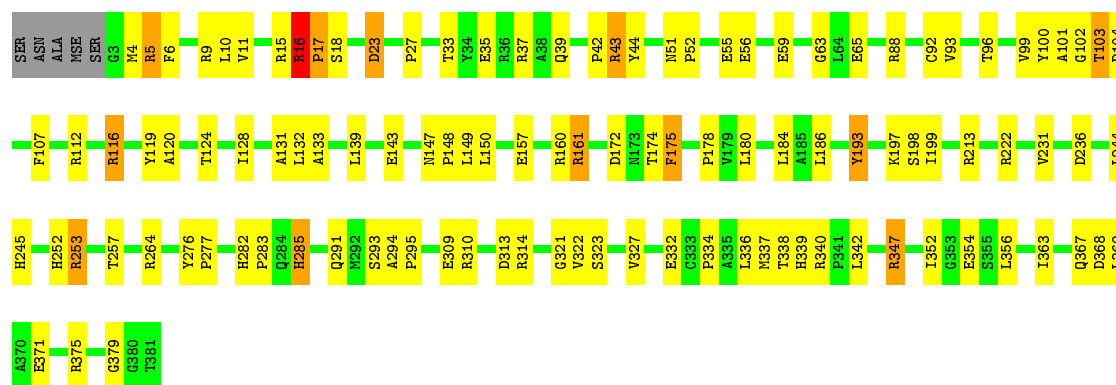
• Molecule 1: CalE6

Chain 10-B: 68% 27% . .



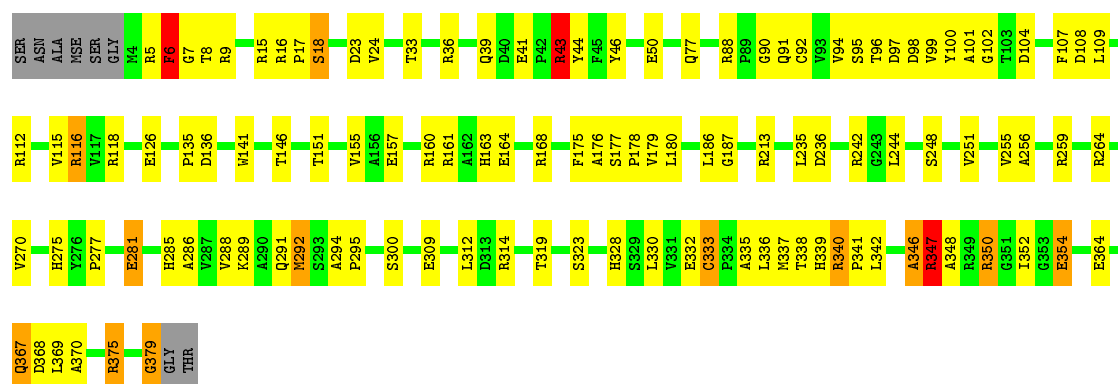
• Molecule 1: CalE6

Chain 10-C: 70% 26% . .



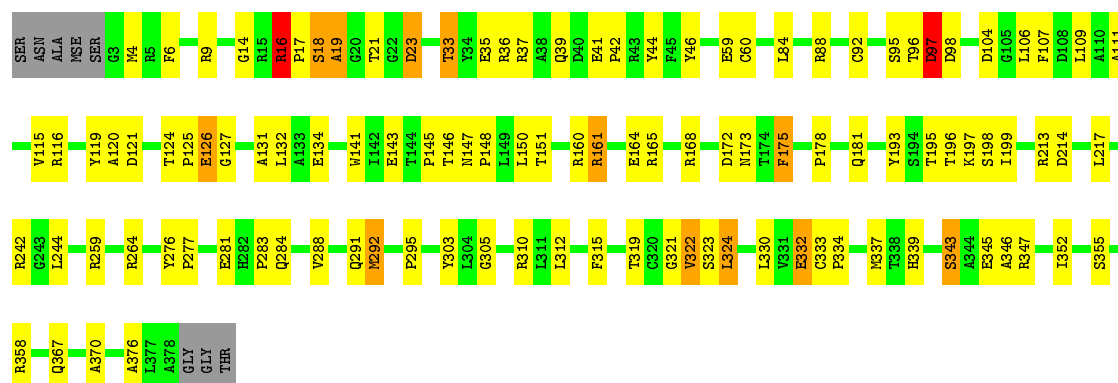
• Molecule 1: CalE6

Chain 10-D: 68% 26% . .



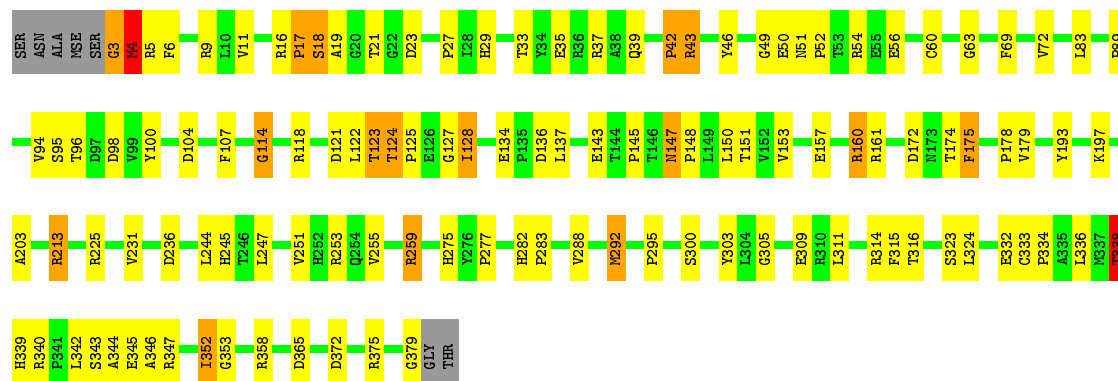
• Molecule 1: CalE6

Chain 10-E: 69% 25% ..



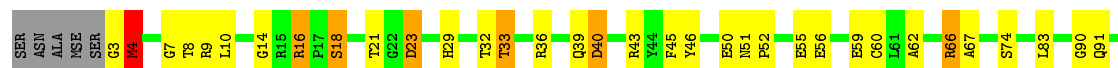
• Molecule 1: CalE6

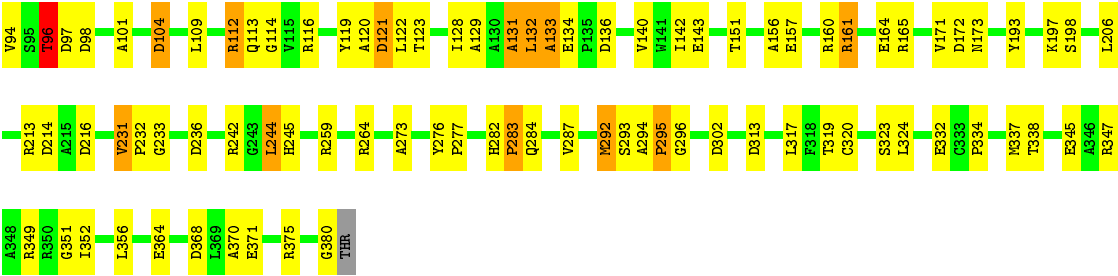
Chain 10-F: 67% 26% ..



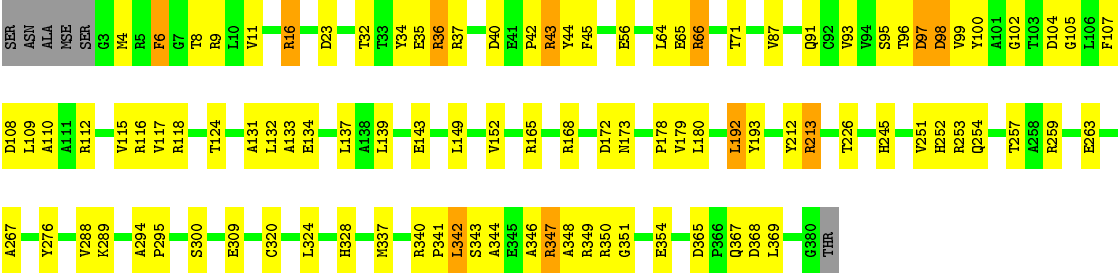
• Molecule 1: CalE6

Chain 10-G: 67% 26% 5% ..





● Molecule 1: CalE6



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	146.85Å 146.98Å 349.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.97 – 2.10	Depositor
% Data completeness (in resolution range)	100.0 (33.97-2.10)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.ENSEMBLE_REFINEMENT: DEV_1839)	Depositor
R, R_{free}	0.143 , 0.183	Depositor
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.192	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
Total number of atoms	243453	wwPDB-V
Average B, all atoms (Å ²)	25.0	wwPDB-V

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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Continued on next page...

Continued from previous page...

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(°)	Ideal(°)
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 ⓘ

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	2834	78	0
1	1-B	2846	0	2838	83	0
1	1-C	2837	0	2819	68	0
1	1-D	2812	0	2791	100	0
1	1-E	2815	0	2794	90	0
1	1-F	2812	0	2787	92	0
1	1-G	2814	0	2786	86	0
1	1-H	2831	0	2818	91	0
1	2-A	2839	0	2834	67	0
1	2-B	2846	0	2837	89	0
1	2-C	2837	0	2818	86	0
1	2-D	2812	0	2791	87	0
1	2-E	2815	0	2794	84	0
1	2-F	2812	0	2786	75	0
1	2-G	2814	0	2786	58	0
1	2-H	2831	0	2817	93	0
1	3-A	2839	0	2833	85	0
1	3-B	2846	0	2838	80	0
1	3-C	2837	0	2818	100	0
1	3-D	2812	0	2791	90	0
1	3-E	2815	0	2793	84	0
1	3-F	2812	0	2786	88	0
1	3-G	2814	0	2786	86	0
1	3-H	2831	0	2817	97	0
1	4-A	2839	0	2833	98	0
1	4-B	2846	0	2837	95	0
1	4-C	2837	0	2819	87	0
1	4-D	2812	0	2791	85	0
1	4-E	2815	0	2794	104	0
1	4-F	2812	0	2786	95	0
1	4-G	2814	0	2786	87	0
1	4-H	2831	0	2818	89	0
1	5-A	2839	0	2833	102	0
1	5-B	2846	0	2838	115	0
1	5-C	2837	0	2818	102	0
1	5-D	2812	0	2790	79	0
1	5-E	2815	0	2794	117	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5-F	2812	0	2787	84	0
1	5-G	2814	0	2786	79	0
1	5-H	2831	0	2817	100	0
1	6-A	2839	0	2834	68	0
1	6-B	2846	0	2837	90	0
1	6-C	2837	0	2818	91	0
1	6-D	2812	0	2790	91	0
1	6-E	2815	0	2794	79	0
1	6-F	2812	0	2786	87	0
1	6-G	2814	0	2785	81	0
1	6-H	2831	0	2817	70	0
1	7-A	2839	0	2833	110	0
1	7-B	2846	0	2837	99	0
1	7-C	2837	0	2818	90	0
1	7-D	2812	0	2790	85	0
1	7-E	2815	0	2793	87	0
1	7-F	2812	0	2786	94	0
1	7-G	2814	0	2786	87	0
1	7-H	2831	0	2817	75	0
1	8-A	2839	0	2834	75	0
1	8-B	2846	0	2838	94	0
1	8-C	2837	0	2818	85	0
1	8-D	2812	0	2791	92	0
1	8-E	2815	0	2793	100	0
1	8-F	2812	0	2787	100	0
1	8-G	2814	0	2786	79	0
1	8-H	2831	0	2817	79	0
1	9-A	2839	0	2834	85	0
1	9-B	2846	0	2837	78	0
1	9-C	2837	0	2818	99	0
1	9-D	2812	0	2790	92	0
1	9-E	2815	0	2794	96	0
1	9-F	2812	0	2786	104	0
1	9-G	2814	0	2785	79	0
1	9-H	2831	0	2817	75	0
1	10-A	2839	0	2833	86	0
1	10-B	2846	0	2837	113	0
1	10-C	2837	0	2818	90	0
1	10-D	2812	0	2790	92	0
1	10-E	2815	0	2794	97	0
1	10-F	2812	0	2787	86	0
1	10-G	2814	0	2786	92	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10-H	2831	0	2818	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	2	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	3	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	6	0
2	5-H	12	0	12	1	0
2	6-A	12	0	12	0	0

Continued on next page...

Continued from previous page...

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	6	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	2	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	5	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	19	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

Continued on next page...

Continued from previous page...

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	22	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	227856	6730	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 6730 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%)	11	5
1	1-B	375/384 (98%)	350 (93%)	19 (5%)	6 (2%)	11	5
1	1-C	376/384 (98%)	346 (92%)	23 (6%)	7 (2%)	9	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%)	11	5
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%)	9	4
1	1-H	375/384 (98%)	341 (91%)	28 (8%)	6 (2%)	11	5
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%)	11	5
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%)	8	3
1	2-E	373/384 (97%)	350 (94%)	17 (5%)	6 (2%)	11	5
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%)	22	17
1	2-H	375/384 (98%)	345 (92%)	24 (6%)	6 (2%)	11	5
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%)	8	3
1	3-C	376/384 (98%)	341 (91%)	30 (8%)	5 (1%)	14	8
1	3-D	373/384 (97%)	342 (92%)	23 (6%)	8 (2%)	8	3
1	3-E	373/384 (97%)	345 (92%)	19 (5%)	9 (2%)	7	2
1	3-F	374/384 (97%)	346 (92%)	17 (4%)	11 (3%)	5	2
1	3-G	375/384 (98%)	339 (90%)	31 (8%)	5 (1%)	14	8
1	3-H	375/384 (98%)	346 (92%)	21 (6%)	8 (2%)	8	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%)	9	4
1	4-C	376/384 (98%)	353 (94%)	17 (4%)	6 (2%)	11	5
1	4-D	373/384 (97%)	342 (92%)	25 (7%)	6 (2%)	11	5
1	4-E	373/384 (97%)	347 (93%)	18 (5%)	8 (2%)	8	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%)	9	4
1	4-H	375/384 (98%)	348 (93%)	24 (6%)	3 (1%)	22	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-A	373/384 (97%)	333 (89%)	32 (9%)	8 (2%)	8	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%)	44	44
1	5-D	373/384 (97%)	345 (92%)	21 (6%)	7 (2%)	9	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%)	9	4
1	5-G	375/384 (98%)	339 (90%)	29 (8%)	7 (2%)	9	4
1	5-H	375/384 (98%)	345 (92%)	25 (7%)	5 (1%)	14	8
1	6-A	373/384 (97%)	342 (92%)	25 (7%)	6 (2%)	11	5
1	6-B	375/384 (98%)	343 (92%)	29 (8%)	3 (1%)	22	17
1	6-C	376/384 (98%)	345 (92%)	28 (7%)	3 (1%)	22	17
1	6-D	373/384 (97%)	340 (91%)	22 (6%)	11 (3%)	5	2
1	6-E	373/384 (97%)	351 (94%)	17 (5%)	5 (1%)	14	8
1	6-F	374/384 (97%)	347 (93%)	24 (6%)	3 (1%)	22	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%)	14	8
1	7-A	373/384 (97%)	345 (92%)	22 (6%)	6 (2%)	11	5
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%)	8	3
1	7-D	373/384 (97%)	343 (92%)	24 (6%)	6 (2%)	11	5
1	7-E	373/384 (97%)	344 (92%)	24 (6%)	5 (1%)	14	8
1	7-F	374/384 (97%)	344 (92%)	25 (7%)	5 (1%)	14	8
1	7-G	375/384 (98%)	339 (90%)	30 (8%)	6 (2%)	11	5
1	7-H	375/384 (98%)	349 (93%)	23 (6%)	3 (1%)	22	17
1	8-A	373/384 (97%)	344 (92%)	23 (6%)	6 (2%)	11	5
1	8-B	375/384 (98%)	347 (92%)	23 (6%)	5 (1%)	14	8
1	8-C	376/384 (98%)	347 (92%)	23 (6%)	6 (2%)	11	5
1	8-D	373/384 (97%)	345 (92%)	21 (6%)	7 (2%)	9	4
1	8-E	373/384 (97%)	353 (95%)	15 (4%)	5 (1%)	14	8
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%)	11	5

Continued on next page...

Continued from previous page...

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%)	5	2
1	9-B	375/384 (98%)	345 (92%)	25 (7%)	5 (1%)	14	8
1	9-C	376/384 (98%)	349 (93%)	26 (7%)	1 (0%)	44	44
1	9-D	373/384 (97%)	335 (90%)	32 (9%)	6 (2%)	11	5
1	9-E	373/384 (97%)	342 (92%)	20 (5%)	11 (3%)	5	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%)	32	28
1	10-A	373/384 (97%)	343 (92%)	25 (7%)	5 (1%)	14	8
1	10-B	375/384 (98%)	342 (91%)	27 (7%)	6 (2%)	11	5
1	10-C	376/384 (98%)	340 (90%)	29 (8%)	7 (2%)	9	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%)	9	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	2
1	10-H	375/384 (98%)	349 (93%)	23 (6%)	3 (1%)	22	17
All	All	29940/30720 (98%)	27614 (92%)	1841 (6%)	485 (2%)	11	5

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 ⓘ

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%)	15	11
1	1-B	291/293 (99%)	263 (90%)	28 (10%)	10	6
1	1-C	289/293 (99%)	268 (93%)	21 (7%)	16	13
1	1-D	285/293 (97%)	261 (92%)	24 (8%)	13	8
1	1-E	286/293 (98%)	268 (94%)	18 (6%)	21	17
1	1-F	284/293 (97%)	261 (92%)	23 (8%)	14	9
1	1-G	285/293 (97%)	267 (94%)	18 (6%)	21	17
1	1-H	287/293 (98%)	263 (92%)	24 (8%)	13	8
1	2-A	291/293 (99%)	274 (94%)	17 (6%)	23	20
1	2-B	291/293 (99%)	270 (93%)	21 (7%)	17	13
1	2-C	289/293 (99%)	274 (95%)	15 (5%)	27	24
1	2-D	285/293 (97%)	263 (92%)	22 (8%)	15	11
1	2-E	286/293 (98%)	271 (95%)	15 (5%)	27	24
1	2-F	284/293 (97%)	266 (94%)	18 (6%)	21	17
1	2-G	285/293 (97%)	265 (93%)	20 (7%)	18	14
1	2-H	287/293 (98%)	263 (92%)	24 (8%)	13	8
1	3-A	291/293 (99%)	267 (92%)	24 (8%)	13	9
1	3-B	291/293 (99%)	281 (97%)	10 (3%)	42	43
1	3-C	289/293 (99%)	264 (91%)	25 (9%)	12	8
1	3-D	285/293 (97%)	260 (91%)	25 (9%)	12	8
1	3-E	286/293 (98%)	273 (96%)	13 (4%)	32	30
1	3-F	284/293 (97%)	264 (93%)	20 (7%)	18	14
1	3-G	285/293 (97%)	267 (94%)	18 (6%)	21	17
1	3-H	287/293 (98%)	267 (93%)	20 (7%)	18	14
1	4-A	291/293 (99%)	270 (93%)	21 (7%)	17	13
1	4-B	291/293 (99%)	268 (92%)	23 (8%)	14	10
1	4-C	289/293 (99%)	273 (94%)	16 (6%)	25	22
1	4-D	285/293 (97%)	263 (92%)	22 (8%)	15	11
1	4-E	286/293 (98%)	266 (93%)	20 (7%)	18	14
1	4-F	284/293 (97%)	261 (92%)	23 (8%)	14	9
1	4-G	285/293 (97%)	269 (94%)	16 (6%)	25	21
1	4-H	287/293 (98%)	265 (92%)	22 (8%)	15	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5-A	291/293 (99%)	275 (94%)	16 (6%)	25	22
1	5-B	291/293 (99%)	269 (92%)	22 (8%)	15	11
1	5-C	289/293 (99%)	269 (93%)	20 (7%)	18	14
1	5-D	285/293 (97%)	260 (91%)	25 (9%)	12	8
1	5-E	286/293 (98%)	261 (91%)	25 (9%)	12	8
1	5-F	284/293 (97%)	273 (96%)	11 (4%)	37	37
1	5-G	285/293 (97%)	272 (95%)	13 (5%)	31	29
1	5-H	287/293 (98%)	266 (93%)	21 (7%)	16	13
1	6-A	291/293 (99%)	274 (94%)	17 (6%)	23	20
1	6-B	291/293 (99%)	270 (93%)	21 (7%)	17	13
1	6-C	289/293 (99%)	271 (94%)	18 (6%)	21	18
1	6-D	285/293 (97%)	260 (91%)	25 (9%)	12	8
1	6-E	286/293 (98%)	264 (92%)	22 (8%)	15	11
1	6-F	284/293 (97%)	259 (91%)	25 (9%)	12	8
1	6-G	285/293 (97%)	261 (92%)	24 (8%)	13	8
1	6-H	287/293 (98%)	269 (94%)	18 (6%)	21	17
1	7-A	291/293 (99%)	258 (89%)	33 (11%)	7	3
1	7-B	291/293 (99%)	267 (92%)	24 (8%)	13	9
1	7-C	289/293 (99%)	269 (93%)	20 (7%)	18	14
1	7-D	285/293 (97%)	261 (92%)	24 (8%)	13	8
1	7-E	286/293 (98%)	268 (94%)	18 (6%)	21	17
1	7-F	284/293 (97%)	265 (93%)	19 (7%)	19	15
1	7-G	285/293 (97%)	272 (95%)	13 (5%)	31	29
1	7-H	287/293 (98%)	269 (94%)	18 (6%)	21	17
1	8-A	291/293 (99%)	276 (95%)	15 (5%)	27	24
1	8-B	291/293 (99%)	277 (95%)	14 (5%)	30	27
1	8-C	289/293 (99%)	271 (94%)	18 (6%)	21	18
1	8-D	285/293 (97%)	267 (94%)	18 (6%)	21	17
1	8-E	286/293 (98%)	267 (93%)	19 (7%)	19	16
1	8-F	284/293 (97%)	265 (93%)	19 (7%)	19	15
1	8-G	285/293 (97%)	269 (94%)	16 (6%)	25	21

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

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	24,24,25	2.57	7 (29%)	28,32,34	1.34	4 (14%)
1	LLP	1-B	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.19	2 (7%)
1	LLP	1-C	197	1	24,24,25	2.63	7 (29%)	28,32,34	1.37	5 (17%)
1	LLP	1-D	197	1	24,24,25	2.63	6 (25%)	28,32,34	1.16	4 (14%)
1	LLP	1-E	197	1	24,24,25	2.64	7 (29%)	28,32,34	1.15	4 (14%)
1	LLP	1-F	197	1	24,24,25	2.65	7 (29%)	28,32,34	1.29	6 (21%)
1	LLP	1-G	197	1	24,24,25	2.73	7 (29%)	28,32,34	1.14	2 (7%)
1	LLP	1-H	197	1	24,24,25	2.60	5 (20%)	28,32,34	1.19	3 (10%)
1	LLP	10-A	197	1	24,24,25	2.74	7 (29%)	28,32,34	1.29	4 (14%)
1	LLP	10-B	197	1	24,24,25	2.67	6 (25%)	28,32,34	1.52	7 (25%)
1	LLP	10-C	197	1	24,24,25	2.72	7 (29%)	28,32,34	1.29	4 (14%)
1	LLP	10-D	197	1	24,24,25	2.62	5 (20%)	28,32,34	1.10	3 (10%)
1	LLP	10-E	197	1	24,24,25	2.67	6 (25%)	28,32,34	1.07	3 (10%)
1	LLP	10-F	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.24	5 (17%)
1	LLP	10-G	197	1	24,24,25	2.70	7 (29%)	28,32,34	1.43	5 (17%)
1	LLP	10-H	197	1	24,24,25	2.69	7 (29%)	28,32,34	1.25	3 (10%)
1	LLP	2-A	197	1	24,24,25	2.77	7 (29%)	28,32,34	1.32	3 (10%)
1	LLP	2-B	197	1	24,24,25	2.72	6 (25%)	28,32,34	1.13	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	24,24,25	2.70	7 (29%)	28,32,34	1.30	3 (10%)
1	LLP	2-D	197	1	24,24,25	2.60	6 (25%)	28,32,34	1.13	3 (10%)
1	LLP	2-E	197	1	24,24,25	2.79	7 (29%)	28,32,34	1.26	3 (10%)
1	LLP	2-F	197	1	24,24,25	2.67	7 (29%)	28,32,34	1.40	6 (21%)
1	LLP	2-G	197	1	24,24,25	2.78	7 (29%)	28,32,34	1.19	2 (7%)
1	LLP	2-H	197	1	24,24,25	2.60	7 (29%)	28,32,34	1.67	6 (21%)
1	LLP	3-A	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.31	5 (17%)
1	LLP	3-B	197	1	24,24,25	2.75	6 (25%)	28,32,34	1.34	6 (21%)
1	LLP	3-C	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.38	5 (17%)
1	LLP	3-D	197	1	24,24,25	2.60	5 (20%)	28,32,34	1.16	4 (14%)
1	LLP	3-E	197	1	24,24,25	2.79	7 (29%)	28,32,34	1.14	2 (7%)
1	LLP	3-F	197	1	24,24,25	2.64	6 (25%)	28,32,34	1.28	3 (10%)
1	LLP	3-G	197	1	24,24,25	2.69	7 (29%)	28,32,34	1.25	3 (10%)
1	LLP	3-H	197	1	24,24,25	2.80	7 (29%)	28,32,34	1.37	5 (17%)
1	LLP	4-A	197	1	24,24,25	2.67	7 (29%)	28,32,34	1.32	5 (17%)
1	LLP	4-B	197	1	24,24,25	2.69	7 (29%)	28,32,34	1.28	3 (10%)
1	LLP	4-C	197	1	24,24,25	2.83	7 (29%)	28,32,34	1.38	6 (21%)
1	LLP	4-D	197	1	24,24,25	2.56	6 (25%)	28,32,34	1.25	3 (10%)
1	LLP	4-E	197	1	24,24,25	2.70	7 (29%)	28,32,34	1.30	4 (14%)
1	LLP	4-F	197	1	24,24,25	2.65	7 (29%)	28,32,34	1.29	6 (21%)
1	LLP	4-G	197	1	24,24,25	2.67	7 (29%)	28,32,34	1.33	4 (14%)
1	LLP	4-H	197	1	24,24,25	2.80	7 (29%)	28,32,34	1.26	3 (10%)
1	LLP	5-A	197	1	24,24,25	2.78	7 (29%)	28,32,34	1.34	5 (17%)
1	LLP	5-B	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.11	3 (10%)
1	LLP	5-C	197	1	24,24,25	2.69	7 (29%)	28,32,34	1.46	6 (21%)
1	LLP	5-D	197	1	24,24,25	2.57	5 (20%)	28,32,34	1.33	4 (14%)
1	LLP	5-E	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.18	3 (10%)
1	LLP	5-F	197	1	24,24,25	2.49	6 (25%)	28,32,34	1.32	4 (14%)
1	LLP	5-G	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.36	4 (14%)
1	LLP	5-H	197	1	24,24,25	2.63	7 (29%)	28,32,34	1.45	5 (17%)
1	LLP	6-A	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.32	4 (14%)
1	LLP	6-B	197	1	24,24,25	2.62	6 (25%)	28,32,34	1.26	4 (14%)
1	LLP	6-C	197	1	24,24,25	2.84	7 (29%)	28,32,34	1.47	6 (21%)
1	LLP	6-D	197	1	24,24,25	2.60	6 (25%)	28,32,34	1.23	4 (14%)
1	LLP	6-E	197	1	24,24,25	2.63	7 (29%)	28,32,34	1.19	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	24,24,25	2.66	7 (29%)	28,32,34	1.23	4 (14%)
1	LLP	6-G	197	1	24,24,25	2.73	7 (29%)	28,32,34	1.26	4 (14%)
1	LLP	6-H	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.23	3 (10%)
1	LLP	7-A	197	1	24,24,25	2.76	7 (29%)	28,32,34	1.28	5 (17%)
1	LLP	7-B	197	1	24,24,25	2.64	6 (25%)	28,32,34	1.34	5 (17%)
1	LLP	7-C	197	1	24,24,25	2.65	6 (25%)	28,32,34	1.36	4 (14%)
1	LLP	7-D	197	1	24,24,25	2.65	6 (25%)	28,32,34	1.60	5 (17%)
1	LLP	7-E	197	1	24,24,25	2.73	7 (29%)	28,32,34	1.12	3 (10%)
1	LLP	7-F	197	1	24,24,25	2.70	7 (29%)	28,32,34	1.34	6 (21%)
1	LLP	7-G	197	1	24,24,25	2.75	7 (29%)	28,32,34	1.33	5 (17%)
1	LLP	7-H	197	1	24,24,25	2.65	7 (29%)	28,32,34	1.64	5 (17%)
1	LLP	8-A	197	1	24,24,25	2.73	7 (29%)	28,32,34	1.27	4 (14%)
1	LLP	8-B	197	1	24,24,25	2.65	6 (25%)	28,32,34	1.19	3 (10%)
1	LLP	8-C	197	1	24,24,25	2.72	7 (29%)	28,32,34	1.40	5 (17%)
1	LLP	8-D	197	1	24,24,25	2.60	6 (25%)	28,32,34	1.52	6 (21%)
1	LLP	8-E	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.18	4 (14%)
1	LLP	8-F	197	1	24,24,25	2.62	7 (29%)	28,32,34	1.37	6 (21%)
1	LLP	8-G	197	1	24,24,25	2.62	7 (29%)	28,32,34	1.34	2 (7%)
1	LLP	8-H	197	1	24,24,25	2.69	7 (29%)	28,32,34	1.29	4 (14%)
1	LLP	9-A	197	1	24,24,25	2.64	7 (29%)	28,32,34	1.22	4 (14%)
1	LLP	9-B	197	1	24,24,25	2.40	5 (20%)	28,32,34	1.60	8 (28%)
1	LLP	9-C	197	1	24,24,25	2.74	7 (29%)	28,32,34	1.26	4 (14%)
1	LLP	9-D	197	1	24,24,25	2.55	5 (20%)	28,32,34	1.20	3 (10%)
1	LLP	9-E	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.25	4 (14%)
1	LLP	9-F	197	1	24,24,25	2.65	7 (29%)	28,32,34	1.36	5 (17%)
1	LLP	9-G	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.14	2 (7%)
1	LLP	9-H	197	1	24,24,25	2.65	7 (29%)	28,32,34	1.20	3 (10%)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 532 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-C	197	LLP	C4-C5	-4.12	1.36	1.42
1	4-C	197	LLP	C4-C5	-4.04	1.36	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	197	LLP	C4-C5	-4.03	1.36	1.42
1	5-A	197	LLP	C4-C5	-3.97	1.36	1.42
1	9-A	197	LLP	C4-C5	-3.86	1.37	1.42

The worst 5 of 331 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	197	LLP	CE-NZ-C4'	-4.05	107.28	119.03
1	8-D	197	LLP	CB-CA-C	-3.94	105.16	111.65
1	4-G	197	LLP	CE-NZ-C4'	-3.83	107.91	119.03
1	8-G	197	LLP	C4-C4'-NZ	-3.82	106.08	124.66
1	9-B	197	LLP	CE-NZ-C4'	-3.78	108.05	119.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

48 monomers are involved in 74 short contacts:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	4-F	197	LLP	2	0
1	4-H	197	LLP	3	0
1	5-B	197	LLP	1	0
1	5-D	197	LLP	1	0
1	5-F	197	LLP	1	0
1	5-H	197	LLP	1	0
1	6-A	197	LLP	2	0
1	6-C	197	LLP	1	0
1	6-F	197	LLP	1	0
1	6-H	197	LLP	2	0
1	7-A	197	LLP	1	0
1	7-B	197	LLP	2	0
1	7-F	197	LLP	2	0
1	7-G	197	LLP	2	0
1	7-H	197	LLP	2	0
1	8-A	197	LLP	2	0
1	8-B	197	LLP	2	0
1	8-D	197	LLP	2	0
1	8-E	197	LLP	1	0
1	8-F	197	LLP	1	0
1	8-H	197	LLP	1	0
1	9-A	197	LLP	3	0
1	9-B	197	LLP	1	0
1	9-C	197	LLP	2	0
1	9-E	197	LLP	1	0
1	9-F	197	LLP	3	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	-	12,12,12	2.15	1 (8%)	14,16,16	2.44	6 (42%)
3	GOL	1-A	402	-	5,5,5	0.33	0	5,5,5	0.23	0
3	GOL	1-A	403	-	5,5,5	0.36	0	5,5,5	0.40	0
3	GOL	1-A	404	-	5,5,5	0.40	0	5,5,5	0.39	0
2	MES	1-B	401	-	12,12,12	1.84	1 (8%)	14,16,16	2.53	6 (42%)
3	GOL	1-B	402	-	5,5,5	0.37	0	5,5,5	0.41	0
3	GOL	1-B	403	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	1-B	404	-	5,5,5	0.31	0	5,5,5	0.69	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	0.32	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	0.28	0
2	MES	1-C	401	-	12,12,12	2.19	1 (8%)	14,16,16	2.80	7 (50%)
3	GOL	1-C	402	-	5,5,5	0.31	0	5,5,5	0.33	0
3	FMT	1-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	1-D	401	-	12,12,12	2.12	1 (8%)	14,16,16	3.00	8 (57%)
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	1.04	0	5,5,5	1.24	1 (20%)
3	GOL	1-D	404	-	5,5,5	0.42	0	5,5,5	0.13	0
2	MES	1-E	401	-	12,12,12	1.99	1 (8%)	14,16,16	2.51	4 (28%)
3	GOL	1-E	402	-	5,5,5	0.26	0	5,5,5	0.68	0
3	GOL	1-E	403	-	5,5,5	0.39	0	5,5,5	0.21	0
2	MES	1-F	401	-	12,12,12	1.73	1 (8%)	14,16,16	3.17	8 (57%)
3	GOL	1-F	402	-	5,5,5	0.40	0	5,5,5	0.22	0
3	GOL	1-F	403	-	5,5,5	0.34	0	5,5,5	0.45	0
3	GOL	1-F	404	-	5,5,5	0.37	0	5,5,5	0.55	0
3	GOL	1-F	405	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	1-F	406	-	5,5,5	1.40	1 (20%)	5,5,5	1.38	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	-	12,12,12	2.00	1 (8%)	14,16,16	2.56	7 (50%)
3	GOL	1-G	402	-	5,5,5	0.45	0	5,5,5	0.59	0
3	GOL	1-G	403	-	5,5,5	0.41	0	5,5,5	0.50	0
3	GOL	1-G	404	-	5,5,5	0.41	0	5,5,5	0.32	0
5	GOL	1-G	405	-	5,5,5	0.32	0	5,5,5	0.55	0
4	FMT	1-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	1-H	401	-	12,12,12	1.75	1 (8%)	14,16,16	2.75	8 (57%)
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	0.36	0	5,5,5	0.26	0
2	MES	10-A	401	-	12,12,12	2.12	1 (8%)	14,16,16	2.15	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	10-A	402	-	5,5,5	0.33	0	5,5,5	0.17	0
3	GOL	10-A	403	-	5,5,5	0.39	0	5,5,5	0.33	0
3	GOL	10-A	404	-	5,5,5	0.34	0	5,5,5	0.58	0
2	MES	10-B	401	-	12,12,12	1.89	1 (8%)	14,16,16	2.48	7 (50%)
3	GOL	10-B	402	-	5,5,5	0.33	0	5,5,5	0.27	0
3	GOL	10-B	403	-	5,5,5	0.28	0	5,5,5	0.54	0
3	GOL	10-B	404	-	5,5,5	0.29	0	5,5,5	0.54	0
3	GOL	10-B	405	-	5,5,5	0.38	0	5,5,5	0.35	0
3	GOL	10-B	406	-	5,5,5	0.32	0	5,5,5	0.45	0
3	GOL	10-B	407	-	5,5,5	0.39	0	5,5,5	0.41	0
2	MES	10-C	401	-	12,12,12	1.59	1 (8%)	14,16,16	4.37	7 (50%)
3	GOL	10-C	402	-	5,5,5	0.28	0	5,5,5	0.34	0
3	GOL	10-C	403	-	5,5,5	0.34	0	5,5,5	0.17	0
5	FMT	10-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	10-D	401	-	12,12,12	1.92	1 (8%)	14,16,16	2.09	5 (35%)
3	GOL	10-D	402	-	5,5,5	0.43	0	5,5,5	0.51	0
3	GOL	10-D	403	-	5,5,5	0.28	0	5,5,5	0.46	0
3	GOL	10-D	404	-	5,5,5	0.27	0	5,5,5	0.22	0
2	MES	10-E	401	-	12,12,12	1.87	1 (8%)	14,16,16	2.84	7 (50%)
3	GOL	10-E	402	-	5,5,5	0.24	0	5,5,5	0.85	0
3	GOL	10-E	403	-	5,5,5	0.34	0	5,5,5	0.50	0
2	MES	10-F	401	-	12,12,12	2.37	1 (8%)	14,16,16	2.91	8 (57%)
3	GOL	10-F	402	-	5,5,5	0.36	0	5,5,5	0.30	0
3	GOL	10-F	403	-	5,5,5	0.38	0	5,5,5	0.43	0
3	GOL	10-F	404	-	5,5,5	0.38	0	5,5,5	0.20	0
3	GOL	10-F	405	-	5,5,5	0.39	0	5,5,5	0.43	0
3	GOL	10-F	406	-	5,5,5	0.30	0	5,5,5	0.23	0
5	FMT	10-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	10-G	401	-	12,12,12	1.83	1 (8%)	14,16,16	3.12	8 (57%)
3	GOL	10-G	402	-	5,5,5	0.34	0	5,5,5	0.82	0
3	GOL	10-G	403	-	5,5,5	0.37	0	5,5,5	0.40	0
3	GOL	10-G	404	-	5,5,5	0.36	0	5,5,5	0.31	0
5	FMT	10-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	10-H	401	-	12,12,12	2.11	1 (8%)	14,16,16	2.72	5 (35%)
3	GOL	10-H	402	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	10-H	403	-	5,5,5	0.39	0	5,5,5	0.66	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	0.39	0
2	MES	2-A	401	-	12,12,12	1.96	1 (8%)	14,16,16	2.07	3 (21%)
3	GOL	2-A	402	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	2-A	403	-	5,5,5	0.32	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	2-A	404	-	5,5,5	0.35	0	5,5,5	0.32	0
2	MES	2-B	401	-	12,12,12	2.00	1 (8%)	14,16,16	2.36	5 (35%)
3	GOL	2-B	402	-	5,5,5	0.31	0	5,5,5	0.41	0
3	GOL	2-B	403	-	5,5,5	1.06	0	5,5,5	2.52	2 (40%)
3	GOL	2-B	404	-	5,5,5	0.41	0	5,5,5	0.40	0
3	GOL	2-B	405	-	5,5,5	0.34	0	5,5,5	0.28	0
3	GOL	2-B	406	-	5,5,5	0.43	0	5,5,5	0.29	0
3	GOL	2-B	407	-	5,5,5	0.39	0	5,5,5	0.38	0
2	MES	2-C	401	-	12,12,12	1.72	1 (8%)	14,16,16	2.66	7 (50%)
3	GOL	2-C	402	-	5,5,5	0.35	0	5,5,5	0.46	0
3	GOL	2-C	403	-	5,5,5	0.44	0	5,5,5	0.18	0
5	GOL	2-C	404	-	5,5,5	0.36	0	5,5,5	0.27	0
4	FMT	2-C	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	2-D	401	-	12,12,12	1.91	1 (8%)	14,16,16	3.11	8 (57%)
3	GOL	2-D	402	-	5,5,5	0.39	0	5,5,5	0.45	0
3	GOL	2-D	403	-	5,5,5	0.33	0	5,5,5	0.32	0
2	MES	2-E	401	-	12,12,12	1.74	1 (8%)	14,16,16	3.11	5 (35%)
3	GOL	2-E	402	-	5,5,5	0.26	0	5,5,5	0.32	0
3	GOL	2-E	403	-	5,5,5	0.36	0	5,5,5	0.44	0
4	GOL	2-E	404	-	5,5,5	0.32	0	5,5,5	0.32	0
2	MES	2-F	401	-	12,12,12	1.82	1 (8%)	14,16,16	3.20	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	0.32	0
3	GOL	2-F	404	-	5,5,5	0.44	0	5,5,5	0.15	0
3	GOL	2-F	405	-	5,5,5	0.35	0	5,5,5	0.23	0
3	FMT	2-F	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	2-G	401	-	12,12,12	2.14	1 (8%)	14,16,16	2.56	3 (21%)
3	GOL	2-G	402	-	5,5,5	0.34	0	5,5,5	0.38	0
3	GOL	2-G	403	-	5,5,5	0.33	0	5,5,5	0.52	0
3	GOL	2-G	404	-	5,5,5	1.25	0	5,5,5	0.85	0
5	FMT	2-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	2-H	401	-	12,12,12	2.55	1 (8%)	14,16,16	2.11	5 (35%)
3	GOL	2-H	402	-	5,5,5	0.36	0	5,5,5	0.21	0
3	GOL	2-H	403	-	5,5,5	1.17	1 (20%)	5,5,5	1.04	0
3	GOL	2-H	404	-	5,5,5	0.24	0	5,5,5	0.53	0
2	MES	3-A	401	-	12,12,12	1.53	1 (8%)	14,16,16	2.61	6 (42%)
3	GOL	3-A	402	-	5,5,5	0.23	0	5,5,5	0.23	0
3	GOL	3-A	403	-	5,5,5	0.33	0	5,5,5	0.33	0
3	GOL	3-A	404	-	5,5,5	0.32	0	5,5,5	0.37	0
4	GOL	3-A	405	-	5,5,5	0.36	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	3-B	401	-	12,12,12	2.11	1 (8%)	14,16,16	5.08	7 (50%)
3	GOL	3-B	402	-	5,5,5	0.39	0	5,5,5	0.36	0
3	GOL	3-B	403	-	5,5,5	0.35	0	5,5,5	0.51	0
3	GOL	3-B	404	-	5,5,5	0.31	0	5,5,5	0.16	0
3	GOL	3-B	405	-	5,5,5	0.39	0	5,5,5	0.40	0
3	GOL	3-B	406	-	5,5,5	0.39	0	5,5,5	0.32	0
3	GOL	3-B	407	-	5,5,5	0.27	0	5,5,5	0.42	0
2	MES	3-C	401	-	12,12,12	1.95	1 (8%)	14,16,16	4.74	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	0.27	0	5,5,5	0.62	0
5	FMT	3-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	3-D	401	-	12,12,12	1.68	1 (8%)	14,16,16	3.26	8 (57%)
3	GOL	3-D	402	-	5,5,5	0.40	0	5,5,5	0.61	0
3	GOL	3-D	403	-	5,5,5	0.35	0	5,5,5	0.19	0
2	MES	3-E	401	-	12,12,12	1.86	1 (8%)	14,16,16	4.68	12 (85%)
3	GOL	3-E	402	-	5,5,5	0.40	0	5,5,5	0.38	0
3	GOL	3-E	403	-	5,5,5	0.32	0	5,5,5	0.76	0
4	GOL	3-E	404	-	5,5,5	0.43	0	5,5,5	0.23	0
2	MES	3-F	401	-	12,12,12	1.86	1 (8%)	14,16,16	3.49	5 (35%)
3	GOL	3-F	402	-	5,5,5	0.32	0	5,5,5	0.20	0
3	GOL	3-F	403	-	5,5,5	0.34	0	5,5,5	0.42	0
3	GOL	3-F	404	-	5,5,5	0.41	0	5,5,5	0.44	0
3	GOL	3-F	405	-	5,5,5	0.27	0	5,5,5	0.84	0
3	GOL	3-F	406	-	5,5,5	0.37	0	5,5,5	0.30	0
5	FMT	3-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	3-G	401	-	12,12,12	1.53	1 (8%)	14,16,16	2.07	5 (35%)
3	GOL	3-G	402	-	5,5,5	0.41	0	5,5,5	0.40	0
3	GOL	3-G	403	-	5,5,5	0.30	0	5,5,5	0.63	0
3	GOL	3-G	404	-	5,5,5	0.34	0	5,5,5	0.32	0
5	GOL	3-G	405	-	5,5,5	0.28	0	5,5,5	0.37	0
4	FMT	3-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	3-H	401	-	12,12,12	2.42	1 (8%)	14,16,16	3.97	7 (50%)
3	GOL	3-H	402	-	5,5,5	0.37	0	5,5,5	0.44	0
3	GOL	3-H	403	-	5,5,5	0.39	0	5,5,5	0.32	0
2	MES	4-A	401	-	12,12,12	2.09	1 (8%)	14,16,16	2.60	6 (42%)
3	GOL	4-A	402	-	5,5,5	0.31	0	5,5,5	0.31	0
3	GOL	4-A	403	-	5,5,5	0.34	0	5,5,5	0.53	0
3	GOL	4-A	404	-	5,5,5	0.38	0	5,5,5	0.53	0
2	MES	4-B	401	-	12,12,12	1.88	1 (8%)	14,16,16	2.49	7 (50%)
3	GOL	4-B	402	-	5,5,5	0.35	0	5,5,5	0.39	0
3	GOL	4-B	403	-	5,5,5	0.50	0	5,5,5	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.32	0
3	GOL	4-B	406	-	5,5,5	0.34	0	5,5,5	0.50	0
3	GOL	4-B	407	-	5,5,5	0.45	0	5,5,5	0.39	0
2	MES	4-C	401	-	12,12,12	2.56	1 (8%)	14,16,16	3.96	4 (28%)
3	GOL	4-C	402	-	5,5,5	0.37	0	5,5,5	0.25	0
3	GOL	4-C	403	-	5,5,5	0.38	0	5,5,5	0.30	0
5	GOL	4-C	404	-	5,5,5	0.43	0	5,5,5	0.63	0
4	FMT	4-C	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	4-D	401	-	12,12,12	2.04	1 (8%)	14,16,16	2.97	6 (42%)
3	GOL	4-D	402	-	5,5,5	0.35	0	5,5,5	0.39	0
3	GOL	4-D	403	-	5,5,5	0.27	0	5,5,5	0.49	0
2	MES	4-E	401	-	12,12,12	1.33	1 (8%)	14,16,16	2.12	5 (35%)
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	0.57	0	5,5,5	0.41	0
2	MES	4-F	401	-	12,12,12	1.86	1 (8%)	14,16,16	2.48	6 (42%)
3	GOL	4-F	402	-	5,5,5	0.37	0	5,5,5	0.37	0
3	GOL	4-F	403	-	5,5,5	0.42	0	5,5,5	0.22	0
3	GOL	4-F	404	-	5,5,5	0.28	0	5,5,5	0.61	0
3	FMT	4-F	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	4-G	401	-	12,12,12	2.04	1 (8%)	14,16,16	2.95	4 (28%)
3	GOL	4-G	402	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	4-G	403	-	5,5,5	0.35	0	5,5,5	0.37	0
3	GOL	4-G	404	-	5,5,5	0.39	0	5,5,5	0.60	0
5	GOL	4-G	405	-	5,5,5	0.44	0	5,5,5	0.29	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	-
2	MES	4-H	401	-	12,12,12	1.98	1 (8%)	14,16,16	2.40	7 (50%)
3	GOL	4-H	402	-	5,5,5	0.44	0	5,5,5	0.27	0
3	GOL	4-H	403	-	5,5,5	0.31	0	5,5,5	0.41	0
3	GOL	4-H	404	-	5,5,5	0.32	0	5,5,5	0.24	0
2	MES	5-A	401	-	12,12,12	1.78	1 (8%)	14,16,16	2.55	7 (50%)
3	GOL	5-A	402	-	5,5,5	0.28	0	5,5,5	0.33	0
3	GOL	5-A	403	-	5,5,5	0.39	0	5,5,5	0.46	0
3	GOL	5-A	404	-	5,5,5	0.36	0	5,5,5	0.43	0
4	GOL	5-A	405	-	5,5,5	0.35	0	5,5,5	0.32	0
2	MES	5-B	401	-	12,12,12	2.05	2 (16%)	14,16,16	2.87	8 (57%)
3	GOL	5-B	402	-	5,5,5	0.34	0	5,5,5	0.34	0
3	GOL	5-B	403	-	5,5,5	0.39	0	5,5,5	0.32	0
3	GOL	5-B	404	-	5,5,5	0.33	0	5,5,5	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	5-B	405	-	5,5,5	0.46	0	5,5,5	0.55	0
3	GOL	5-B	406	-	5,5,5	0.43	0	5,5,5	0.23	0
3	GOL	5-B	407	-	5,5,5	0.20	0	5,5,5	0.45	0
2	MES	5-C	401	-	12,12,12	2.03	1 (8%)	14,16,16	2.42	6 (42%)
3	GOL	5-C	402	-	5,5,5	0.31	0	5,5,5	0.29	0
3	FMT	5-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	5-D	401	-	12,12,12	2.07	1 (8%)	14,16,16	3.78	5 (35%)
3	GOL	5-D	402	-	5,5,5	0.31	0	5,5,5	0.35	0
3	GOL	5-D	403	-	5,5,5	0.34	0	5,5,5	0.54	0
3	GOL	5-D	404	-	5,5,5	0.37	0	5,5,5	0.61	0
2	MES	5-E	401	-	12,12,12	2.08	1 (8%)	14,16,16	3.07	9 (64%)
3	GOL	5-E	402	-	5,5,5	0.47	0	5,5,5	0.25	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	0.27	0
2	MES	5-F	401	-	12,12,12	1.95	1 (8%)	14,16,16	2.76	5 (35%)
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	0.47	0	5,5,5	0.09	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	-	12,12,12	2.42	1 (8%)	14,16,16	4.11	11 (78%)
3	GOL	5-G	402	-	5,5,5	0.28	0	5,5,5	0.66	0
3	GOL	5-G	403	-	5,5,5	0.42	0	5,5,5	0.22	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	0.38	0	5,5,5	0.31	0
4	FMT	5-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	5-H	401	-	12,12,12	1.95	1 (8%)	14,16,16	3.37	5 (35%)
3	GOL	5-H	402	-	5,5,5	0.41	0	5,5,5	0.19	0
3	GOL	5-H	403	-	5,5,5	0.51	0	5,5,5	0.41	0
3	GOL	5-H	404	-	5,5,5	0.39	0	5,5,5	0.42	0
2	MES	6-A	401	-	12,12,12	1.43	1 (8%)	14,16,16	2.86	7 (50%)
3	GOL	6-A	402	-	5,5,5	0.32	0	5,5,5	0.35	0
3	GOL	6-A	403	-	5,5,5	0.39	0	5,5,5	0.67	0
3	GOL	6-A	404	-	5,5,5	0.34	0	5,5,5	0.34	0
4	GOL	6-A	405	-	5,5,5	0.40	0	5,5,5	0.21	0
2	MES	6-B	401	-	12,12,12	2.15	1 (8%)	14,16,16	2.26	7 (50%)
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	0.32	0	5,5,5	0.41	0
3	GOL	6-B	404	-	5,5,5	0.26	0	5,5,5	0.44	0
3	GOL	6-B	405	-	5,5,5	0.40	0	5,5,5	0.33	0
3	GOL	6-B	406	-	5,5,5	0.36	0	5,5,5	0.36	0
3	GOL	6-B	407	-	5,5,5	0.36	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	6-C	401	-	12,12,12	2.74	1 (8%)	14,16,16	3.28	8 (57%)
3	GOL	6-C	402	-	5,5,5	0.27	0	5,5,5	0.42	0
3	FMT	6-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	6-D	401	-	12,12,12	1.91	1 (8%)	14,16,16	3.17	7 (50%)
3	GOL	6-D	402	-	5,5,5	0.42	0	5,5,5	0.48	0
3	GOL	6-D	403	-	5,5,5	0.23	0	5,5,5	0.61	0
3	GOL	6-D	404	-	5,5,5	0.36	0	5,5,5	0.40	0
2	MES	6-E	401	-	12,12,12	1.85	1 (8%)	14,16,16	4.05	8 (57%)
3	GOL	6-E	402	-	5,5,5	0.39	0	5,5,5	0.33	0
3	GOL	6-E	403	-	5,5,5	0.36	0	5,5,5	0.20	0
4	GOL	6-E	404	-	5,5,5	0.45	0	5,5,5	0.21	0
2	MES	6-F	401	-	12,12,12	1.76	1 (8%)	14,16,16	2.42	6 (42%)
3	GOL	6-F	402	-	5,5,5	0.41	0	5,5,5	0.33	0
3	GOL	6-F	403	-	5,5,5	0.38	0	5,5,5	0.50	0
3	GOL	6-F	404	-	5,5,5	0.24	0	5,5,5	0.52	0
3	GOL	6-F	405	-	5,5,5	0.36	0	5,5,5	0.27	0
3	GOL	6-F	406	-	5,5,5	0.33	0	5,5,5	0.25	0
5	FMT	6-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	6-G	401	-	12,12,12	1.83	1 (8%)	14,16,16	2.89	6 (42%)
3	GOL	6-G	402	-	5,5,5	0.46	0	5,5,5	0.26	0
3	GOL	6-G	403	-	5,5,5	0.35	0	5,5,5	0.56	0
3	FMT	6-G	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	6-H	401	-	12,12,12	2.30	1 (8%)	14,16,16	2.79	5 (35%)
3	GOL	6-H	402	-	5,5,5	0.85	0	5,5,5	0.37	0
3	GOL	6-H	403	-	5,5,5	0.40	0	5,5,5	0.90	0
3	GOL	6-H	404	-	5,5,5	0.28	0	5,5,5	0.44	0
3	GOL	6-H	405	-	5,5,5	0.53	0	5,5,5	0.26	0
2	MES	7-A	401	-	12,12,12	1.85	1 (8%)	14,16,16	2.27	4 (28%)
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	0.23	0
3	GOL	7-A	404	-	5,5,5	0.32	0	5,5,5	0.33	0
4	GOL	7-A	405	-	5,5,5	0.36	0	5,5,5	0.30	0
2	MES	7-B	401	-	12,12,12	1.93	1 (8%)	14,16,16	2.65	6 (42%)
3	GOL	7-B	402	-	5,5,5	0.40	0	5,5,5	0.32	0
3	GOL	7-B	403	-	5,5,5	0.34	0	5,5,5	0.42	0
3	GOL	7-B	404	-	5,5,5	0.29	0	5,5,5	0.69	0
3	GOL	7-B	405	-	5,5,5	0.48	0	5,5,5	0.08	0
3	GOL	7-B	406	-	5,5,5	0.38	0	5,5,5	0.28	0
3	GOL	7-B	407	-	5,5,5	0.35	0	5,5,5	0.23	0
2	MES	7-C	401	-	12,12,12	1.90	1 (8%)	14,16,16	2.34	4 (28%)
3	GOL	7-C	402	-	5,5,5	0.30	0	5,5,5	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMT	7-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	7-D	401	-	12,12,12	2.58	1 (8%)	14,16,16	2.95	6 (42%)
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	0.52	0
3	GOL	7-D	404	-	5,5,5	0.26	0	5,5,5	0.83	0
2	MES	7-E	401	-	12,12,12	1.83	1 (8%)	14,16,16	3.20	6 (42%)
3	GOL	7-E	402	-	5,5,5	0.68	0	5,5,5	0.62	0
3	GOL	7-E	403	-	5,5,5	0.41	0	5,5,5	0.56	0
4	GOL	7-E	404	-	5,5,5	0.55	0	5,5,5	0.28	0
2	MES	7-F	401	-	12,12,12	1.86	1 (8%)	14,16,16	2.52	5 (35%)
3	GOL	7-F	402	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	7-F	403	-	5,5,5	0.45	0	5,5,5	0.63	0
3	GOL	7-F	404	-	5,5,5	0.43	0	5,5,5	0.36	0
3	GOL	7-F	405	-	5,5,5	0.33	0	5,5,5	0.29	0
3	GOL	7-F	406	-	5,5,5	0.37	0	5,5,5	0.18	0
5	FMT	7-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	7-G	401	-	12,12,12	2.02	1 (8%)	14,16,16	3.18	8 (57%)
3	GOL	7-G	402	-	5,5,5	0.42	0	5,5,5	0.35	0
3	GOL	7-G	403	-	5,5,5	0.28	0	5,5,5	0.50	0
3	GOL	7-G	404	-	5,5,5	0.40	0	5,5,5	0.30	0
5	FMT	7-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	7-H	401	-	12,12,12	2.28	1 (8%)	14,16,16	2.41	6 (42%)
3	GOL	7-H	402	-	5,5,5	0.44	0	5,5,5	0.26	0
3	GOL	7-H	403	-	5,5,5	0.38	0	5,5,5	0.41	0
3	GOL	7-H	404	-	5,5,5	0.32	0	5,5,5	0.25	0
2	MES	8-A	401	-	12,12,12	2.16	1 (8%)	14,16,16	2.38	6 (42%)
3	GOL	8-A	402	-	5,5,5	0.32	0	5,5,5	0.27	0
3	GOL	8-A	403	-	5,5,5	0.28	0	5,5,5	0.26	0
3	GOL	8-A	404	-	5,5,5	0.40	0	5,5,5	0.26	0
2	MES	8-B	401	-	12,12,12	2.17	1 (8%)	14,16,16	2.68	4 (28%)
3	GOL	8-B	402	-	5,5,5	0.38	0	5,5,5	0.36	0
3	GOL	8-B	403	-	5,5,5	0.29	0	5,5,5	0.46	0
3	GOL	8-B	404	-	5,5,5	0.32	0	5,5,5	0.60	0
3	GOL	8-B	405	-	5,5,5	0.39	0	5,5,5	0.57	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	0.69	0	5,5,5	0.64	0
4	GOL	8-B	408	-	5,5,5	0.42	0	5,5,5	0.38	0
2	MES	8-C	401	-	12,12,12	2.20	1 (8%)	14,16,16	3.04	7 (50%)
3	GOL	8-C	402	-	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	8-C	403	-	5,5,5	0.38	0	5,5,5	0.27	0
5	FMT	8-C	404	-	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	8-D	401	-	12,12,12	2.37	2 (16%)	14,16,16	2.75	8 (57%)
3	GOL	8-D	402	-	5,5,5	0.39	0	5,5,5	0.39	0
3	GOL	8-D	403	-	5,5,5	0.41	0	5,5,5	0.32	0
2	MES	8-E	401	-	12,12,12	2.43	1 (8%)	14,16,16	3.25	6 (42%)
3	GOL	8-E	402	-	5,5,5	0.92	0	5,5,5	1.22	1 (20%)
3	GOL	8-E	403	-	5,5,5	0.61	0	5,5,5	0.84	0
4	GOL	8-E	404	-	5,5,5	0.34	0	5,5,5	0.48	0
2	MES	8-F	401	-	12,12,12	2.07	1 (8%)	14,16,16	2.53	5 (35%)
3	GOL	8-F	402	-	5,5,5	0.32	0	5,5,5	0.84	0
3	GOL	8-F	403	-	5,5,5	0.47	0	5,5,5	0.28	0
3	GOL	8-F	404	-	5,5,5	0.41	0	5,5,5	0.23	0
3	GOL	8-F	405	-	5,5,5	0.33	0	5,5,5	0.41	0
3	FMT	8-F	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	8-G	401	-	12,12,12	2.30	1 (8%)	14,16,16	2.91	7 (50%)
3	GOL	8-G	402	-	5,5,5	0.48	0	5,5,5	0.24	0
3	GOL	8-G	403	-	5,5,5	0.38	0	5,5,5	0.21	0
3	GOL	8-G	404	-	5,5,5	0.32	0	5,5,5	0.36	0
5	GOL	8-G	405	-	5,5,5	0.36	0	5,5,5	0.56	0
4	FMT	8-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	8-H	401	-	12,12,12	1.57	1 (8%)	14,16,16	3.23	6 (42%)
3	GOL	8-H	402	-	5,5,5	0.41	0	5,5,5	0.37	0
3	GOL	8-H	403	-	5,5,5	0.36	0	5,5,5	0.36	0
3	GOL	8-H	404	-	5,5,5	0.26	0	5,5,5	0.73	0
2	MES	9-A	401	-	12,12,12	1.67	1 (8%)	14,16,16	3.66	10 (71%)
3	GOL	9-A	402	-	5,5,5	0.28	0	5,5,5	0.18	0
3	GOL	9-A	403	-	5,5,5	0.51	0	5,5,5	0.51	0
3	GOL	9-A	404	-	5,5,5	0.35	0	5,5,5	0.43	0
4	GOL	9-A	405	-	5,5,5	0.30	0	5,5,5	0.36	0
2	MES	9-B	401	-	12,12,12	2.03	1 (8%)	14,16,16	2.19	4 (28%)
3	GOL	9-B	402	-	5,5,5	0.36	0	5,5,5	0.24	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	0.51	0
3	GOL	9-B	405	-	5,5,5	0.33	0	5,5,5	0.50	0
3	GOL	9-B	406	-	5,5,5	0.33	0	5,5,5	0.25	0
2	MES	9-C	401	-	12,12,12	2.25	1 (8%)	14,16,16	3.39	4 (28%)
3	GOL	9-C	402	-	5,5,5	0.35	0	5,5,5	0.21	0
3	GOL	9-C	403	-	5,5,5	0.36	0	5,5,5	0.60	0
5	FMT	9-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	9-D	401	-	12,12,12	2.45	1 (8%)	14,16,16	2.24	6 (42%)
3	GOL	9-D	402	-	5,5,5	0.47	0	5,5,5	0.53	0
3	GOL	9-D	403	-	5,5,5	0.75	0	5,5,5	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	9-D	404	-	5,5,5	0.30	0	5,5,5	0.36	0
2	MES	9-E	401	-	12,12,12	1.87	1 (8%)	14,16,16	2.30	5 (35%)
3	GOL	9-E	402	-	5,5,5	0.31	0	5,5,5	0.43	0
3	GOL	9-E	403	-	5,5,5	0.79	0	5,5,5	0.62	0
4	GOL	9-E	404	-	5,5,5	0.41	0	5,5,5	0.35	0
2	MES	9-F	401	-	12,12,12	1.89	1 (8%)	14,16,16	2.72	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	0.32	0
3	GOL	9-F	404	-	5,5,5	0.33	0	5,5,5	0.37	0
3	FMT	9-F	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	9-G	401	-	12,12,12	1.98	1 (8%)	14,16,16	3.13	7 (50%)
3	GOL	9-G	402	-	5,5,5	0.49	0	5,5,5	0.66	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	0.13	0
5	FMT	9-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	9-H	401	-	12,12,12	2.12	1 (8%)	14,16,16	2.36	5 (35%)
3	GOL	9-H	402	-	5,5,5	0.37	0	5,5,5	0.34	0
3	GOL	9-H	403	-	5,5,5	0.38	0	5,5,5	0.36	0
3	GOL	9-H	404	-	5,5,5	0.41	0	5,5,5	0.42	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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-C	401	MES	C8-S	-9.17	1.63	1.77
2	4-C	401	MES	C8-S	-8.62	1.64	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-D	401	MES	C8-S	-8.53	1.64	1.77
2	2-H	401	MES	C8-S	-8.52	1.64	1.77
2	3-H	401	MES	C8-S	-8.16	1.65	1.77

The worst 5 of 505 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-B	401	MES	O2S-S-C8	-9.07	99.00	106.79
2	5-G	401	MES	O1S-S-C8	-8.18	99.77	106.79
2	3-H	401	MES	O2S-S-C8	-7.21	100.60	106.79
2	6-C	401	MES	C2-C3-N4	-6.42	101.11	110.11
2	6-E	401	MES	O2S-S-C8	-6.30	101.38	106.79

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
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	2	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	10-B	401	MES	5	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
5	4-C	404	GOL	1	0
2	4-D	401	MES	3	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	6	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	6	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	2	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.