



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 02:55 AM UTC

PDB ID : 4XQ2 / pdb_00004xq2
Title : Ensemble refinement of cystathione gamma lyase (CalE6) D7G from *Micromonospora echinospora*
Authors : Wang, F.; Yennamalli, R.M.; Singh, S.; Tan, K.; Thorson, J.S.; Phillips Jr., G.N.; Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on : 2015-01-18
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

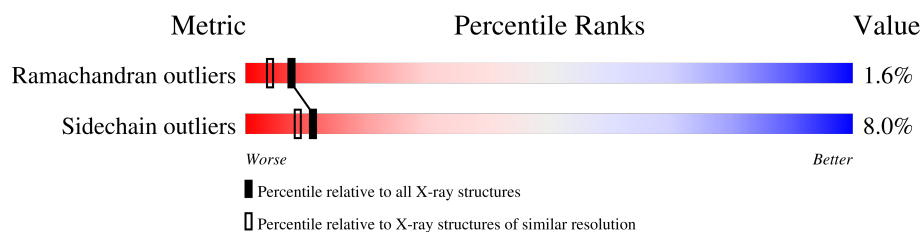
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

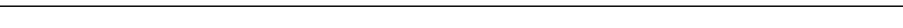
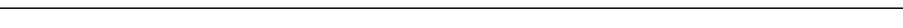
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	384	
1	1-B	384	
1	1-C	384	
1	1-D	384	
1	1-E	384	
1	1-F	384	
1	1-G	384	
1	1-H	384	
1	10-A	384	

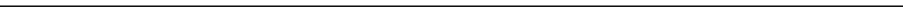
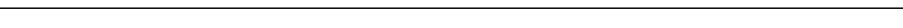
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Mol	Chain	Length	Quality of chain
1	10-B	384	 89% 9% .
1	10-C	384	 91% 8% .
1	10-D	384	 90% 8% .
1	10-E	384	 91% 7% ..
1	10-F	384	 89% 9% ..
1	10-G	384	 91% 8% .
1	10-H	384	 91% 7% .
1	2-A	384	 91% 6% ..
1	2-B	384	 90% 8% ..
1	2-C	384	 91% 7% .
1	2-D	384	 91% 7% ..
1	2-E	384	 91% 6% ..
1	2-F	384	 90% 8% .
1	2-G	384	 92% 6% .
1	2-H	384	 91% 7% .
1	3-A	384	 91% 7% .
1	3-B	384	 89% 9% ..
1	3-C	384	 91% 8% .
1	3-D	384	 91% 7% .
1	3-E	384	 90% 7% .
1	3-F	384	 88% 10% .
1	3-G	384	 92% 7% .
1	3-H	384	 90% 8% ..
1	4-A	384	 91% 7% .
1	4-B	384	 89% 9% ..

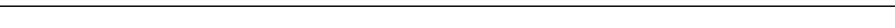
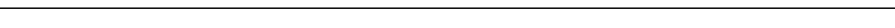
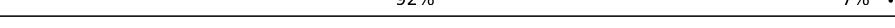
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Mol	Chain	Length	Quality of chain
1	4-C	384	 91% 7% ..
1	4-D	384	 91% 6% .
1	4-E	384	 90% 8% .
1	4-F	384	 89% 9% ..
1	4-G	384	 91% 7% .
1	4-H	384	 92% 7% .
1	5-A	384	 90% 7% ..
1	5-B	384	 90% 8% .
1	5-C	384	 92% 7% .
1	5-D	384	 91% 7% .
1	5-E	384	 89% 8% .
1	5-F	384	 89% 9% .
1	5-G	384	 91% 8% .
1	5-H	384	 91% 7% .
1	6-A	384	 90% 8% .
1	6-B	384	 90% 8% ..
1	6-C	384	 92% 7% .
1	6-D	384	 90% 8% .
1	6-E	384	 91% 7% .
1	6-F	384	 90% 9% .
1	6-G	384	 92% 6% .
1	6-H	384	 91% 8% .
1	7-A	384	 90% 7% .
1	7-B	384	 90% 9% .
1	7-C	384	 91% 8% ..

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Mol	Chain	Length	Quality of chain
1	7-D	384	 91% 6% ..
1	7-E	384	 91% 7% .
1	7-F	384	 89% 9% .
1	7-G	384	 91% 7% .
1	7-H	384	 91% 7% .
1	8-A	384	 91% 7% ..
1	8-B	384	 90% 8% ..
1	8-C	384	 91% 7% ..
1	8-D	384	 91% 7% .
1	8-E	384	 91% 6% ..
1	8-F	384	 90% 8% ..
1	8-G	384	 91% 7% .
1	8-H	384	 91% 7% ..
1	9-A	384	 89% 8% .
1	9-B	384	 90% 8% ..
1	9-C	384	 92% 7% .
1	9-D	384	 91% 6% .
1	9-E	384	 90% 8% .
1	9-F	384	 90% 8% ..
1	9-G	384	 92% 6% .
1	9-H	384	 92% 6% .

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
3	GOL	2-B	403	-	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			

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

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

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

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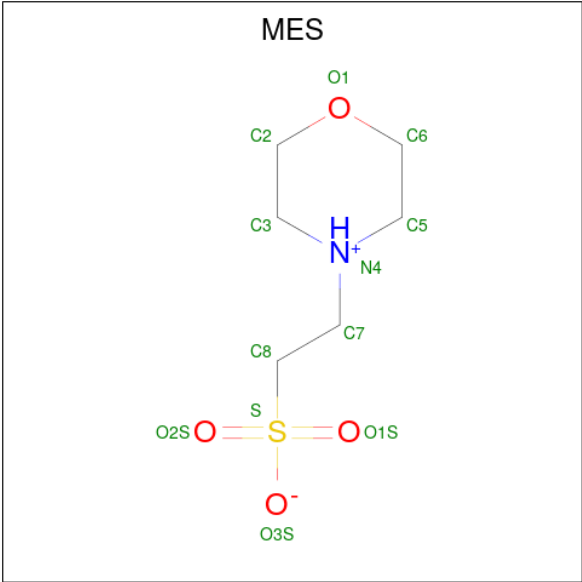
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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	10-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			

There are 32 discrepancies between the modelled and reference sequences:

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

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



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

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

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

- Molecule 3 is GLYCEROL (CCD ID: CL) (formula: C₃H₈O₃).

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

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

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

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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		

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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	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
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		

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

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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-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-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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
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		

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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	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	7-G	1	Total	C	O	0	0
			6	3	3		
3	8-G	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	10-H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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

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

- Molecule 5 is FORMIC ACID (CCD ID: CL) (formula: CL).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	1-C	1	Total 3	C 1	O 2	0	0

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-A	180	Total	O	0	0
			180	180		
6	2-A	190	Total	O	0	0
			190	190		
6	3-A	183	Total	O	0	0
			183	183		
6	4-A	184	Total	O	0	0
			184	184		
6	5-A	197	Total	O	0	0
			197	197		
6	6-A	179	Total	O	0	0
			179	179		
6	7-A	192	Total	O	0	0
			192	192		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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
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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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
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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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
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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

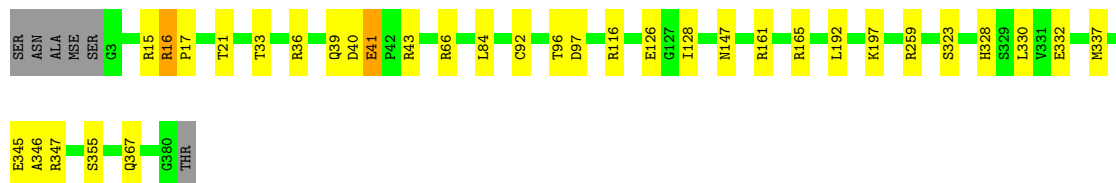
• Molecule 1: CalE6

Chain 1-A:  91% 7% ..



• Molecule 1: CalE6

Chain 1-B:  90% 8% ..



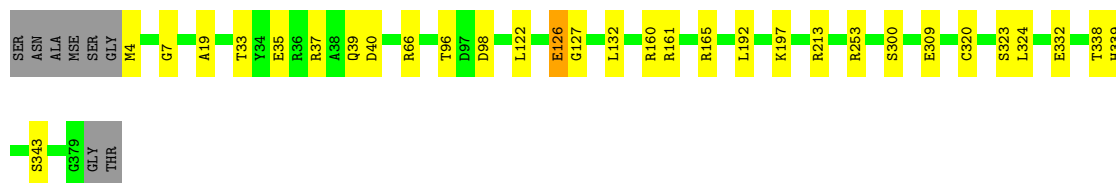
• Molecule 1: CalE6

Chain 1-C:  91% 8% .

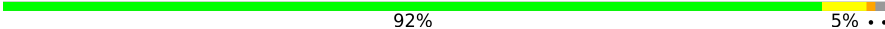


• Molecule 1: CalE6

Chain 1-D:  90% 8% .



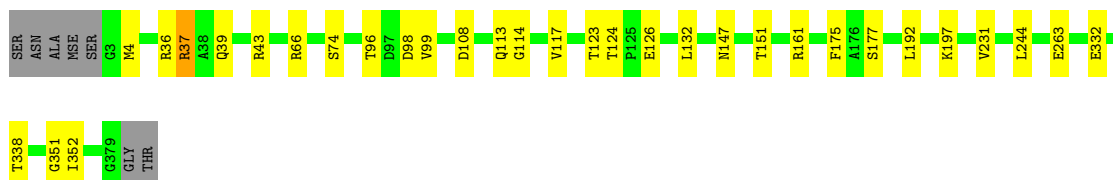
• Molecule 1: CalE6

Chain 1-E:  92% 5% ..



• Molecule 1: CalE6

Chain 1-F:  90% 8% .



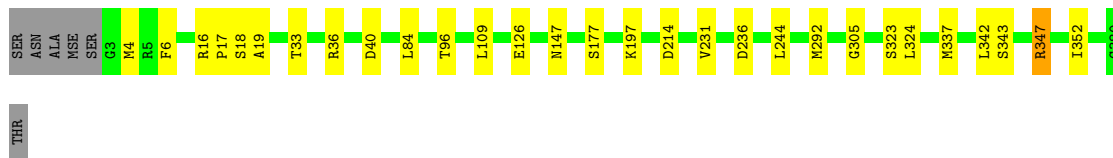
• Molecule 1: CalE6

Chain 1-G:  92% 6% ..



• Molecule 1: CalE6

Chain 1-H:  91% 7% .



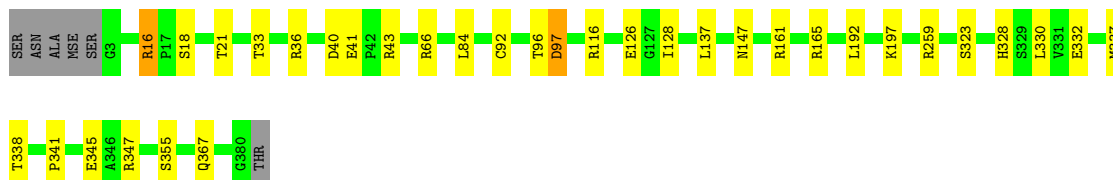
• Molecule 1: CalE6

Chain 2-A:  91% 6% ..

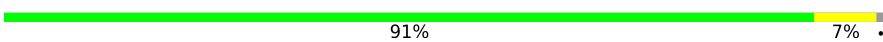


• Molecule 1: CalE6

Chain 2-B:  90% 8% ..



• Molecule 1: CalE6

Chain 2-C:  91% 7% .



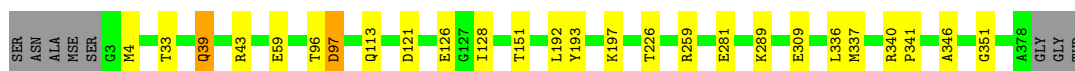
• Molecule 1: CalE6

Chain 2-D:  91% 7% ..



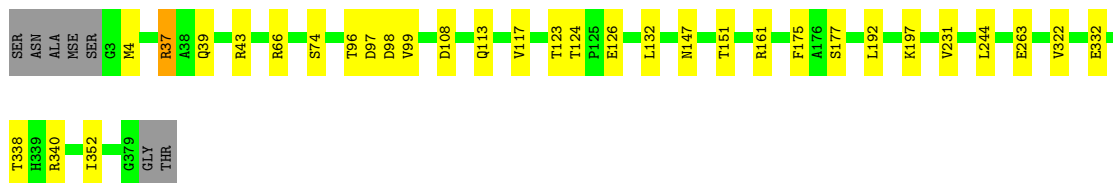
• Molecule 1: CalE6

Chain 2-E:  91% 6% ..

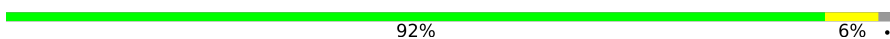


• Molecule 1: CalE6

Chain 2-F:  90% 8% .



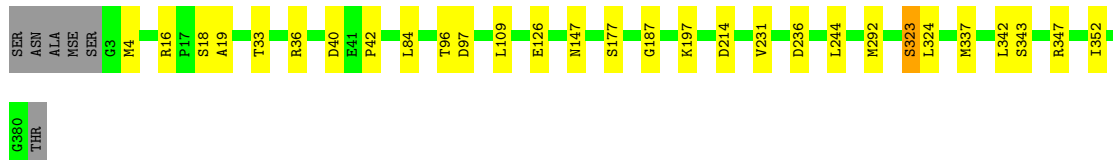
• Molecule 1: CalE6

Chain 2-G:  92% 6% .



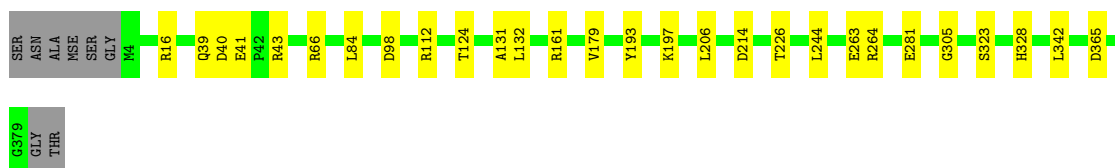
• Molecule 1: CalE6

Chain 2-H:  91% 7% .



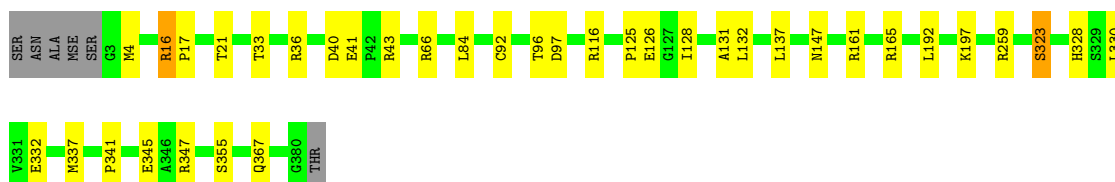
• Molecule 1: CalE6

Chain 3-A:  91% 7% .



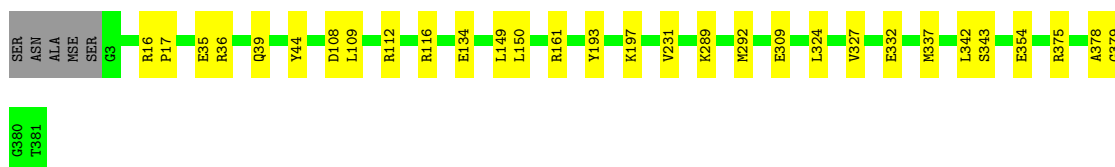
- Molecule 1: CalE6

Chain 3-B: 89% 9% ..



- Molecule 1: CalE6

Chain 3-C: 91% 8% .



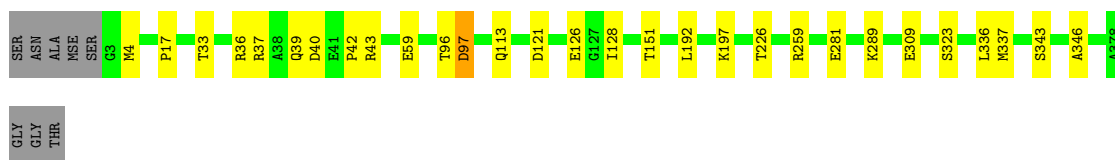
- Molecule 1: CalE6

Chain 3-D: 91% 7% .



- Molecule 1: CalE6

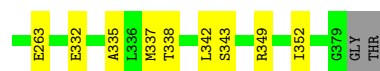
Chain 3-E: 90% 7% .



- Molecule 1: CalE6

Chain 3-F: 88% 10% .





- Molecule 1: CalE6



- Molecule 1: CalE6



- Molecule 1: CalE6



- Molecule 1: CalE6



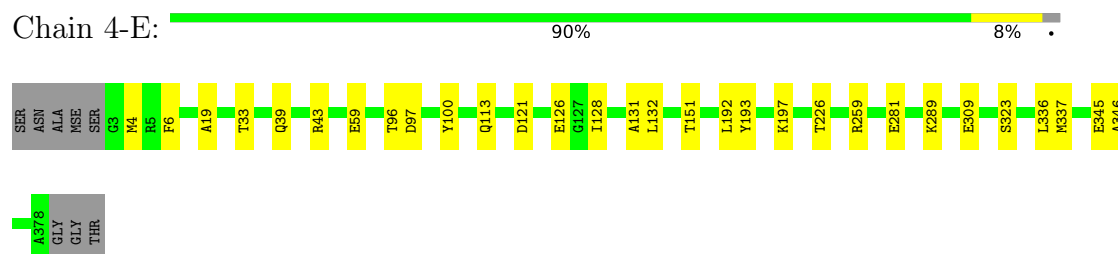
- Molecule 1: CalE6



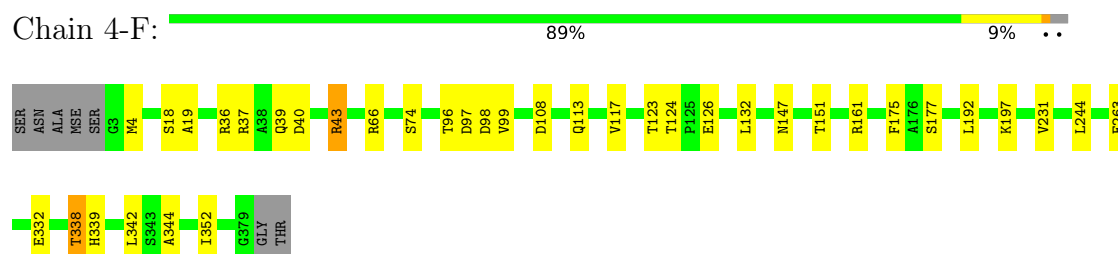
- Molecule 1: CalE6



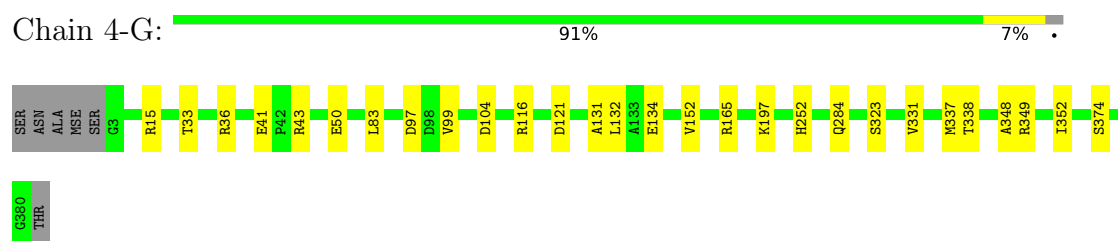
• Molecule 1: CalE6



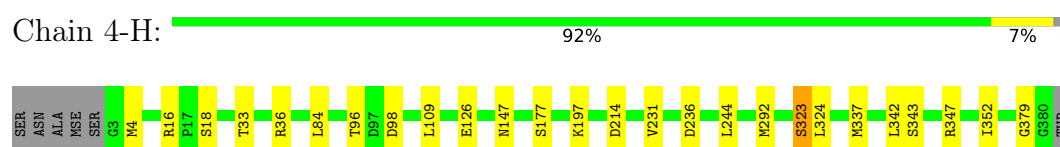
• Molecule 1: CalE6



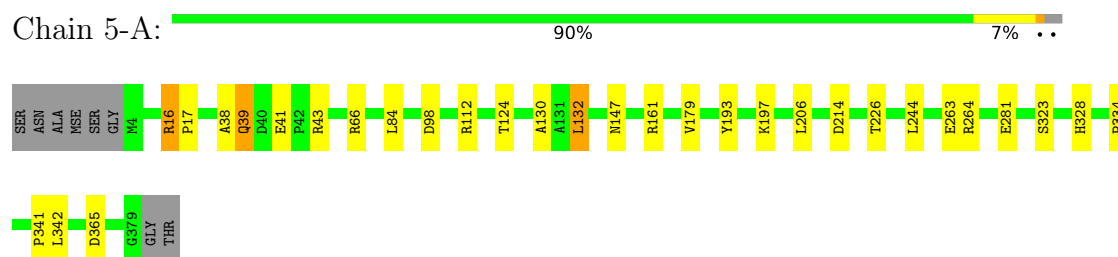
• Molecule 1: CalE6



• Molecule 1: CalE6



• Molecule 1: CalE6



• Molecule 1: CalE6





- Molecule 1: CalE6

Chain 5-C: 92% 7% .



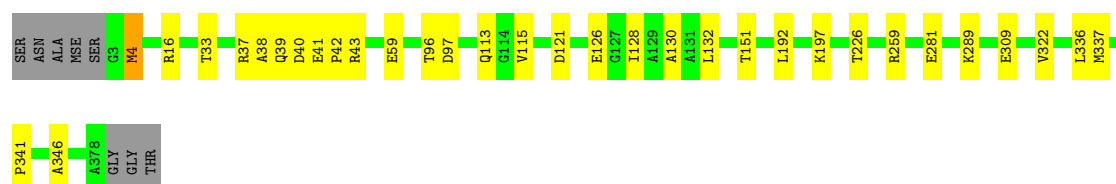
- Molecule 1: CalE6

Chain 5-D: 91% 7% .



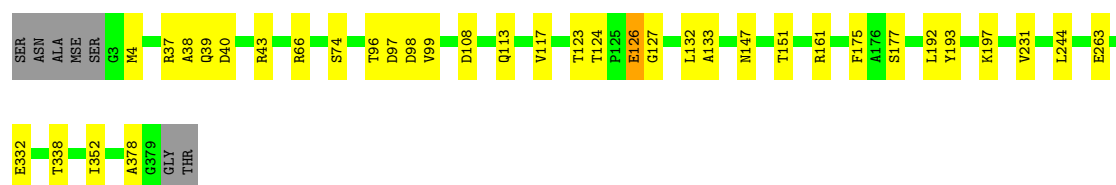
- Molecule 1: CalE6

Chain 5-E: 89% 8% .



- Molecule 1: CalE6

Chain 5-F: 89% 9% .

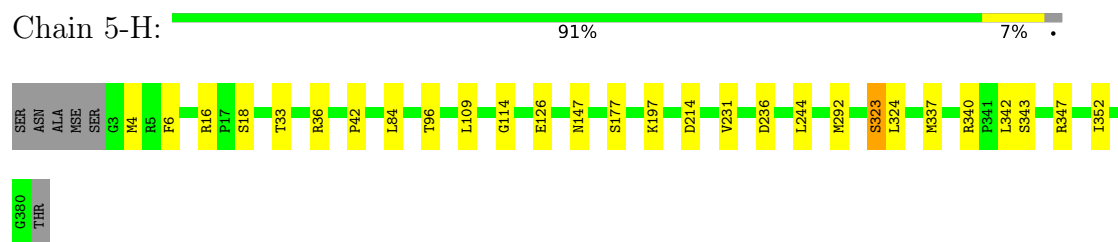


- Molecule 1: CalE6

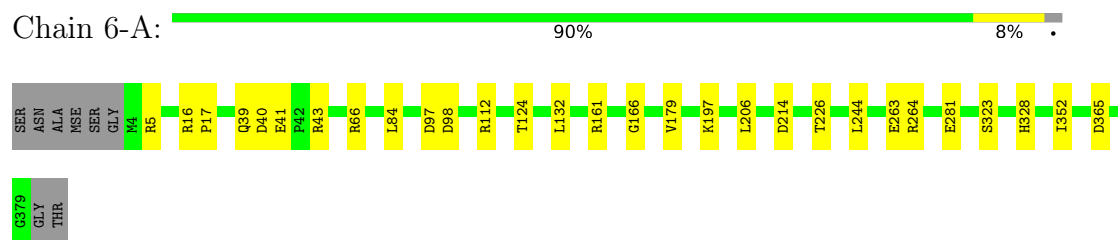
Chain 5-G: 91% 8% .



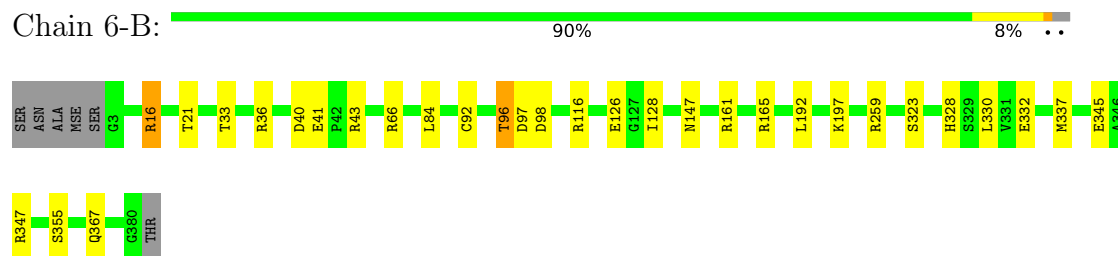
• Molecule 1: CalE6



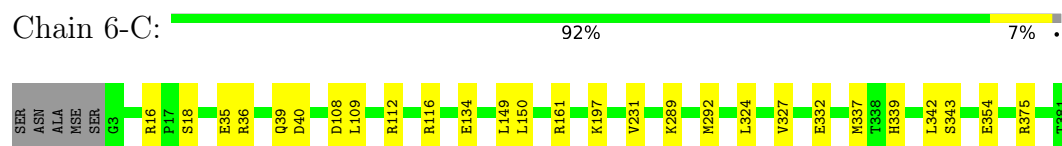
• Molecule 1: CalE6



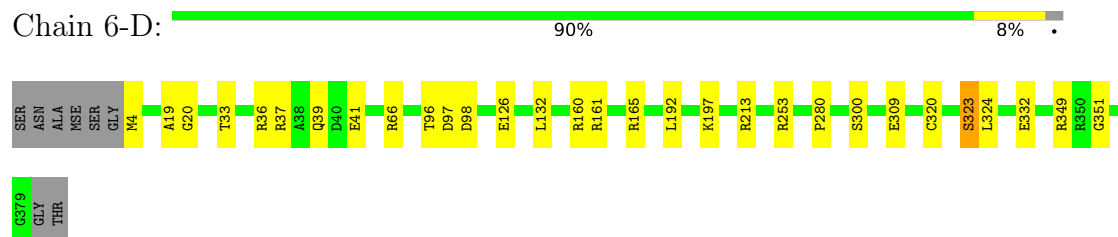
• Molecule 1: CalE6



• Molecule 1: CalE6



• Molecule 1: CalE6



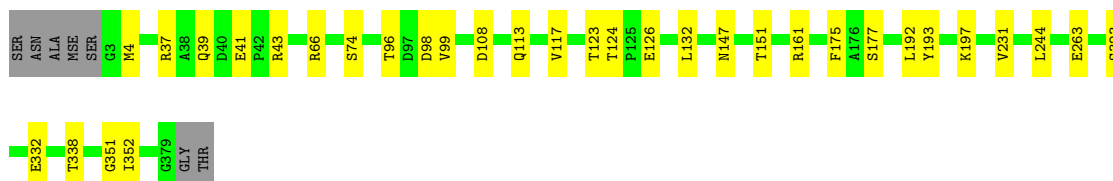
• Molecule 1: CalE6





- Molecule 1: CalE6

Chain 6-F: 90% 9% .



- Molecule 1: CalE6

Chain 6-G: 92% 6% .



- Molecule 1: CalE6

Chain 6-H: 91% 8% .



- Molecule 1: CalE6

Chain 7-A: 90% 7% .

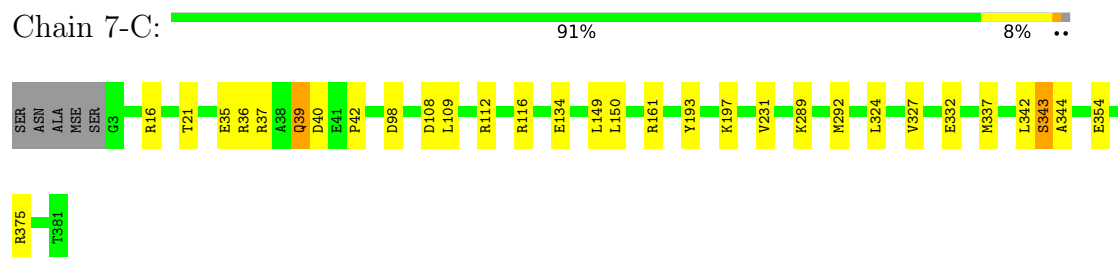


- Molecule 1: CalE6

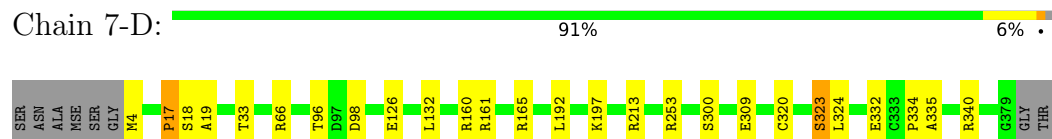
Chain 7-B: 90% 9% .



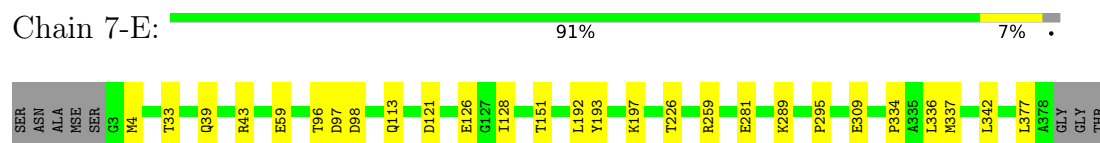
- Molecule 1: CalE6



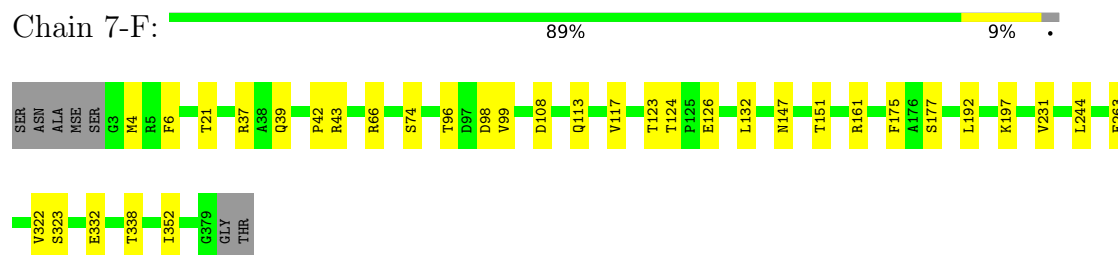
- Molecule 1: CalE6



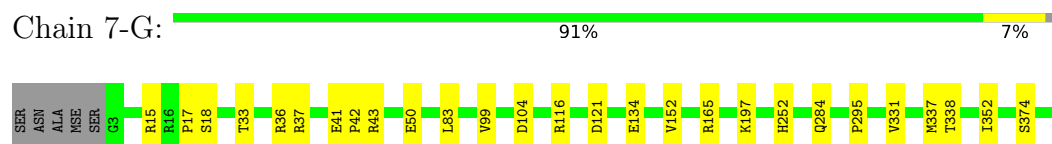
- Molecule 1: CalE6



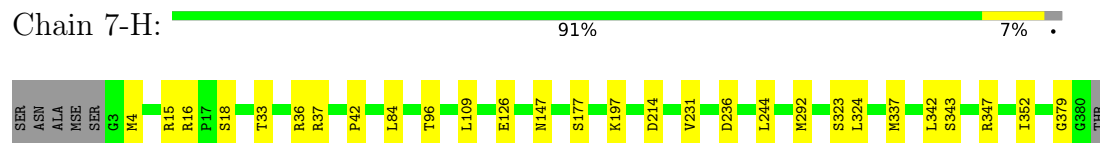
- Molecule 1: CalE6



- Molecule 1: CalE6

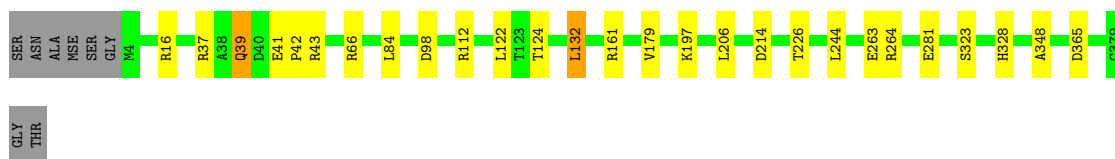


- Molecule 1: CalE6



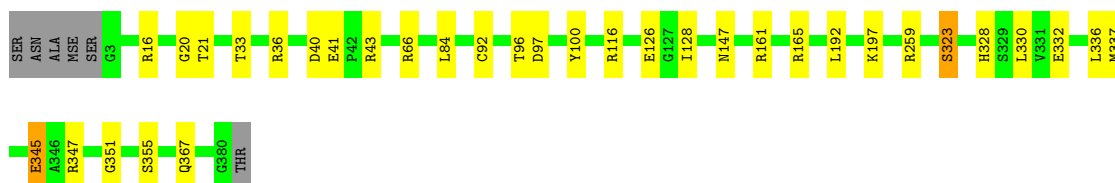
- Molecule 1: CalE6





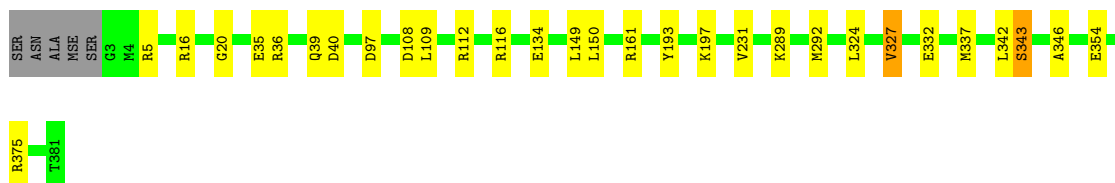
- Molecule 1: CalE6

Chain 8-B: 90% 8% ..



- Molecule 1: CalE6

Chain 8-C: 91% 7% ..



- Molecule 1: CalE6

Chain 8-D: 91% 7% .



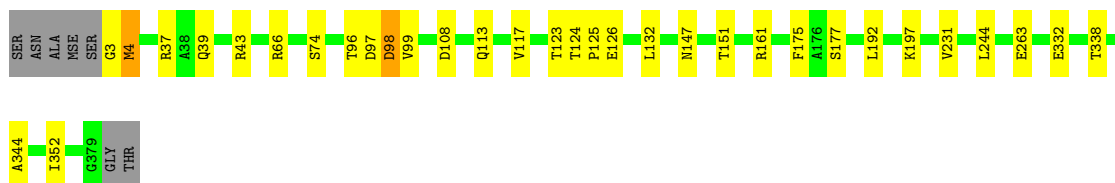
- Molecule 1: CalE6

Chain 8-E: 91% 6% ..



- Molecule 1: CalE6

Chain 8-F: 90% 8% ..



- Molecule 1: CalE6

Chain 8-G:  91% 7% .



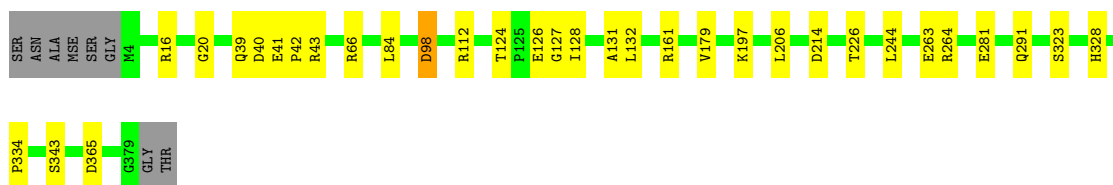
• Molecule 1: CalE6

Chain 8-H:  91% 7% ..



• Molecule 1: CalE6

Chain 9-A:  89% 8% .



• Molecule 1: CalE6

Chain 9-B:  90% 8% ..



• Molecule 1: CalE6

Chain 9-C:  92% 7% .



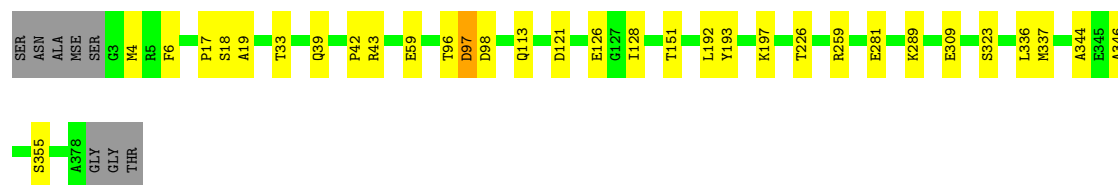
• Molecule 1: CalE6

Chain 9-D:  91% 6% .



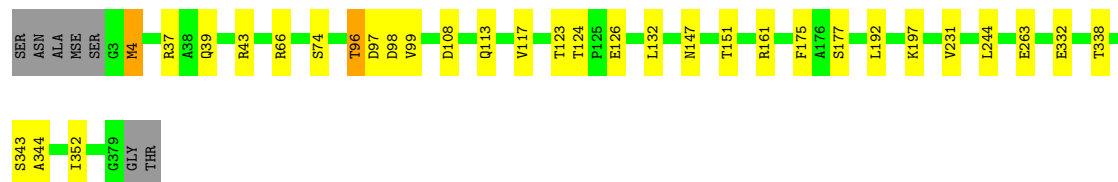
• Molecule 1: CalE6

Chain 9-E:  90% 8% .



- Molecule 1: CalE6

Chain 9-F: 90% 8% ..



- Molecule 1: CalE6

Chain 9-G: 92% 6% .



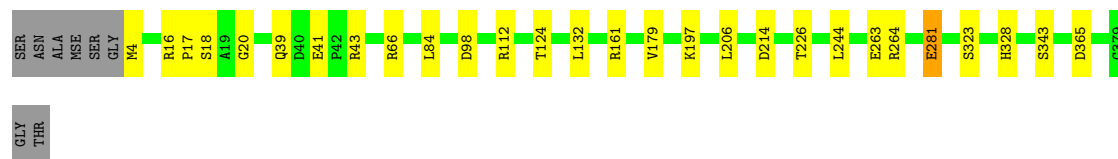
- Molecule 1: CalE6

Chain 9-H: 92% 6% .



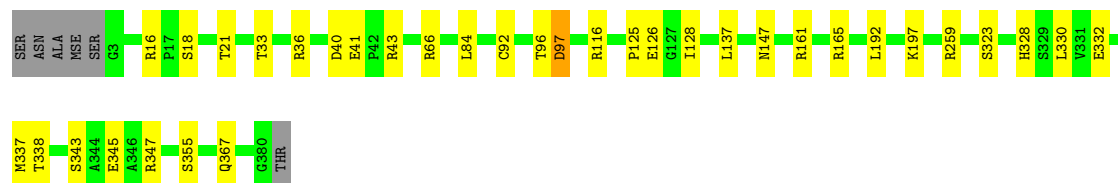
- Molecule 1: CalE6

Chain 10-A: 91% 7% .



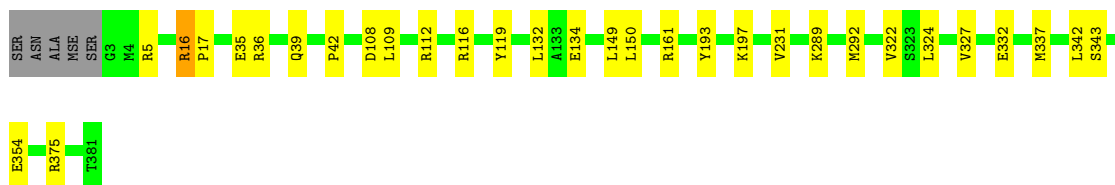
- Molecule 1: CalE6

Chain 10-B: 89% 9% .



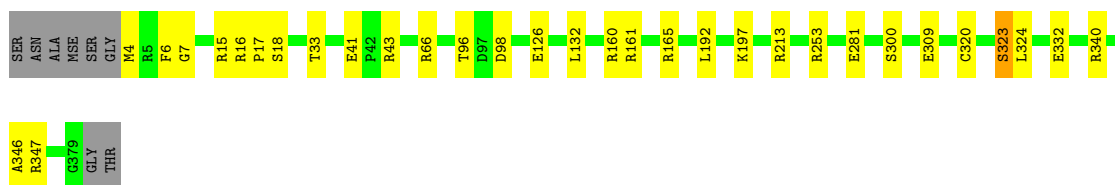
- Molecule 1: CalE6

Chain 10-C:  91% 8% .



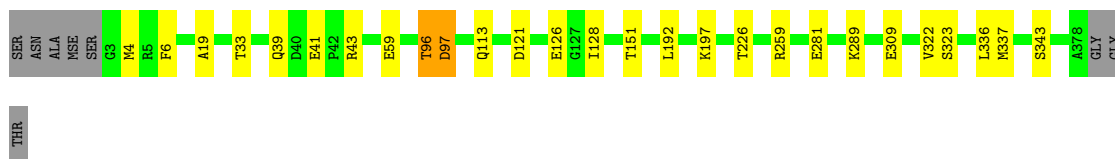
• Molecule 1: CalE6

Chain 10-D:  90% 8% .



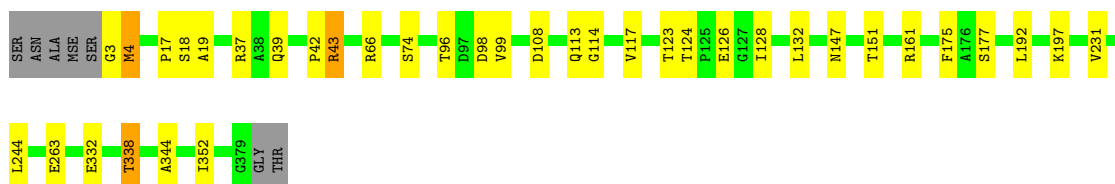
• Molecule 1: CalE6

Chain 10-E:  91% 7% ..



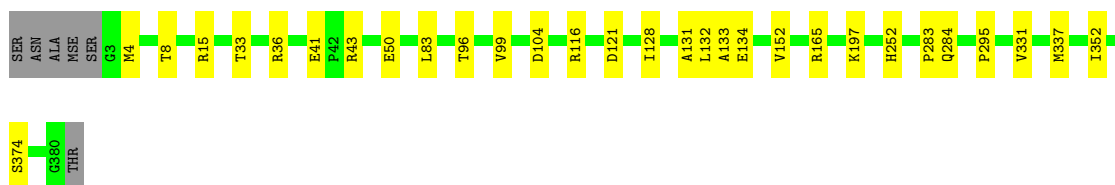
• Molecule 1: CalE6

Chain 10-F:  89% 9% ..



• Molecule 1: CalE6

Chain 10-G:  91% 8% .



• Molecule 1: CalE6

Chain 10-H:

91%

7%

SER	ASN	ALA	NSE	SER	G3	M4	R16	P17	S18	T33	R36	D40	L84	T96	D97	D98	L109	E126	N147	S177	K197	D214	V231	D236	L244	M292	S323	L324	N337	L342	S343	R347	I352	G386	THR
-----	-----	-----	-----	-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

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	2.88 (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)	23.1	Xtriage
Anisotropy	0.187	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.056 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 10.34% 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: CL, FMT, LLP, MES, GOL

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	0.23	0/2790	0.34	0/3799
1	1-B	0.23	0/2845	0.36	0/3871
1	1-C	0.23	0/2863	0.35	0/3900
1	1-D	0.21	0/2841	0.32	0/3874
1	1-E	0.23	0/2722	0.33	0/3704
1	1-F	0.23	0/2840	0.34	0/3871
1	1-G	0.22	0/2842	0.34	0/3874
1	1-H	0.23	0/2859	0.35	0/3893
1	2-A	0.24	0/2868	0.35	0/3906
1	2-B	0.22	0/2874	0.36	0/3912
1	2-C	0.23	0/2865	0.35	0/3903
1	2-D	0.21	0/2841	0.32	0/3874
1	2-E	0.23	0/2843	0.33	0/3874
1	2-F	0.23	0/2840	0.34	0/3871
1	2-G	0.22	0/2842	0.34	0/3874
1	2-H	0.23	0/2859	0.35	0/3893
1	3-A	0.24	0/2868	0.35	0/3906
1	3-B	0.22	0/2874	0.36	0/3912
1	3-C	0.23	0/2865	0.35	0/3903
1	3-D	0.21	0/2841	0.32	0/3874
1	3-E	0.23	0/2843	0.33	0/3874
1	3-F	0.23	0/2840	0.34	0/3871
1	3-G	0.22	0/2842	0.34	0/3874
1	3-H	0.23	0/2859	0.35	0/3893
1	4-A	0.24	0/2868	0.35	0/3906
1	4-B	0.22	0/2874	0.36	0/3912
1	4-C	0.23	0/2865	0.35	0/3903
1	4-D	0.21	0/2841	0.32	0/3874
1	4-E	0.23	0/2843	0.33	0/3874
1	4-F	0.23	0/2840	0.34	0/3871
1	4-G	0.22	0/2842	0.34	0/3874
1	4-H	0.23	0/2859	0.35	0/3893

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	5-A	0.24	0/2868	0.35	0/3906
1	5-B	0.22	0/2874	0.36	0/3912
1	5-C	0.23	0/2865	0.35	0/3903
1	5-D	0.21	0/2841	0.32	0/3874
1	5-E	0.23	0/2843	0.33	0/3874
1	5-F	0.23	0/2840	0.34	0/3871
1	5-G	0.22	0/2842	0.34	0/3874
1	5-H	0.23	0/2859	0.35	0/3893
1	6-A	0.24	0/2868	0.35	0/3906
1	6-B	0.22	0/2874	0.36	0/3912
1	6-C	0.23	0/2865	0.35	0/3903
1	6-D	0.21	0/2841	0.32	0/3874
1	6-E	0.23	0/2843	0.33	0/3874
1	6-F	0.23	0/2840	0.34	0/3871
1	6-G	0.22	0/2842	0.34	0/3874
1	6-H	0.23	0/2859	0.35	0/3893
1	7-A	0.24	0/2868	0.35	0/3906
1	7-B	0.22	0/2874	0.36	0/3912
1	7-C	0.23	0/2865	0.35	0/3903
1	7-D	0.21	0/2841	0.32	0/3874
1	7-E	0.23	0/2843	0.33	0/3874
1	7-F	0.23	0/2840	0.34	0/3871
1	7-G	0.22	0/2842	0.34	0/3874
1	7-H	0.23	0/2859	0.35	0/3893
1	8-A	0.24	0/2868	0.35	0/3906
1	8-B	0.22	0/2874	0.36	0/3912
1	8-C	0.23	0/2865	0.35	0/3903
1	8-D	0.21	0/2841	0.32	0/3874
1	8-E	0.23	0/2843	0.33	0/3874
1	8-F	0.23	0/2840	0.34	0/3871
1	8-G	0.22	0/2842	0.34	0/3874
1	8-H	0.23	0/2859	0.35	0/3893
1	9-A	0.24	0/2868	0.35	0/3906
1	9-B	0.22	0/2874	0.36	0/3912
1	9-C	0.23	0/2865	0.35	0/3903
1	9-D	0.21	0/2841	0.32	0/3874
1	9-E	0.23	0/2843	0.33	0/3874
1	9-F	0.23	0/2840	0.34	0/3871
1	9-G	0.22	0/2842	0.34	0/3874
1	9-H	0.23	0/2859	0.35	0/3893
1	10-A	0.24	0/2868	0.35	0/3906
1	10-B	0.22	0/2874	0.36	0/3912
1	10-C	0.23	0/2865	0.35	0/3903

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	10-D	0.21	0/2841	0.32	0/3874
1	10-E	0.23	0/2843	0.33	0/3874
1	10-F	0.23	0/2840	0.34	0/3871
1	10-G	0.22	0/2842	0.34	0/3874
1	10-H	0.23	0/2859	0.35	0/3893
All	All	0.23	0/228090	0.34	0/310749

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

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	0	0	0
1	1-B	2846	0	0	0	0
1	1-C	2837	0	0	0	0
1	1-D	2812	0	0	0	0
1	1-E	2815	0	0	0	0
1	1-F	2812	0	0	0	0
1	1-G	2814	0	0	0	0
1	1-H	2831	0	0	0	0
1	2-A	2839	0	2834	0	0
1	2-B	2846	0	2838	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2-C	2837	0	2819	0	0
1	2-D	2812	0	2791	0	0
1	2-E	2815	0	2794	0	0
1	2-F	2812	0	2786	0	0
1	2-G	2814	0	2786	0	0
1	2-H	2831	0	2817	0	0
1	3-A	2839	0	2834	0	0
1	3-B	2846	0	2838	0	0
1	3-C	2837	0	2819	0	0
1	3-D	2812	0	2791	0	0
1	3-E	2815	0	2794	0	0
1	3-F	2812	0	2787	0	0
1	3-G	2814	0	2786	0	0
1	3-H	2831	0	2818	0	0
1	4-A	2839	0	2834	0	0
1	4-B	2846	0	2838	0	0
1	4-C	2837	0	2819	0	0
1	4-D	2812	0	2791	0	0
1	4-E	2815	0	2794	0	0
1	4-F	2812	0	2787	0	0
1	4-G	2814	0	2786	0	0
1	4-H	2831	0	2818	0	0
1	5-A	2839	0	2834	0	0
1	5-B	2846	0	2838	0	0
1	5-C	2837	0	2819	0	0
1	5-D	2812	0	2791	0	0
1	5-E	2815	0	2794	0	0
1	5-F	2812	0	2787	0	0
1	5-G	2814	0	2786	0	0
1	5-H	2831	0	2818	0	0
1	6-A	2839	0	2834	0	0
1	6-B	2846	0	2838	0	0
1	6-C	2837	0	2819	0	0
1	6-D	2812	0	2791	0	0
1	6-E	2815	0	2794	0	0
1	6-F	2812	0	2787	0	0
1	6-G	2814	0	2786	0	0
1	6-H	2831	0	2818	0	0
1	7-A	2839	0	2834	0	0
1	7-B	2846	0	2838	0	0
1	7-C	2837	0	2819	0	0
1	7-D	2812	0	2790	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7-E	2815	0	2794	0	0
1	7-F	2812	0	2787	0	0
1	7-G	2814	0	2786	0	0
1	7-H	2831	0	2818	0	0
1	8-A	2839	0	2834	0	0
1	8-B	2846	0	2838	0	0
1	8-C	2837	0	2819	0	0
1	8-D	2812	0	2791	0	0
1	8-E	2815	0	2794	0	0
1	8-F	2812	0	2787	0	0
1	8-G	2814	0	2786	0	0
1	8-H	2831	0	2818	0	0
1	9-A	2839	0	2834	0	0
1	9-B	2846	0	2838	0	0
1	9-C	2837	0	2819	0	0
1	9-D	2812	0	2791	0	0
1	9-E	2815	0	2794	0	0
1	9-F	2812	0	2787	0	0
1	9-G	2814	0	2786	0	0
1	9-H	2831	0	2818	0	0
1	10-A	2839	0	2834	0	0
1	10-B	2846	0	2838	0	0
1	10-C	2837	0	2819	0	0
1	10-D	2812	0	2791	0	0
1	10-E	2815	0	2794	0	0
1	10-F	2812	0	2787	0	0
1	10-G	2814	0	2786	0	0
1	10-H	2831	0	2818	0	0
2	1-A	12	0	0	0	0
2	1-B	12	0	0	0	0
2	1-C	12	0	0	0	0
2	1-D	12	0	0	0	0
2	1-E	12	0	0	0	0
2	1-F	12	0	0	0	0
2	1-G	12	0	0	0	0
2	1-H	12	0	0	0	0
2	2-A	12	0	13	0	0
2	2-B	12	0	12	0	0
2	2-C	12	0	12	0	0
2	2-D	12	0	12	0	0
2	2-E	12	0	12	0	0
2	2-F	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2-G	12	0	12	0	0
2	2-H	12	0	12	0	0
2	3-A	12	0	12	0	0
2	3-B	12	0	12	0	0
2	3-C	12	0	12	0	0
2	3-D	12	0	12	0	0
2	3-E	12	0	12	0	0
2	3-F	12	0	12	0	0
2	3-G	12	0	12	0	0
2	3-H	12	0	12	0	0
2	4-A	12	0	12	0	0
2	4-B	12	0	12	0	0
2	4-C	12	0	12	0	0
2	4-D	12	0	12	0	0
2	4-E	12	0	12	0	0
2	4-F	12	0	12	0	0
2	4-G	12	0	12	0	0
2	4-H	12	0	12	0	0
2	5-A	12	0	12	0	0
2	5-B	12	0	12	0	0
2	5-C	12	0	12	0	0
2	5-D	12	0	12	0	0
2	5-E	12	0	12	0	0
2	5-F	12	0	12	0	0
2	5-G	12	0	12	0	0
2	5-H	12	0	12	0	0
2	6-A	12	0	12	0	0
2	6-B	12	0	12	0	0
2	6-C	12	0	12	0	0
2	6-D	12	0	12	0	0
2	6-E	12	0	12	0	0
2	6-F	12	0	12	0	0
2	6-G	12	0	12	0	0
2	6-H	12	0	12	0	0
2	7-A	12	0	12	0	0
2	7-B	12	0	12	0	0
2	7-C	12	0	12	0	0
2	7-D	12	0	12	0	0
2	7-E	12	0	12	0	0
2	7-F	12	0	12	0	0
2	7-G	12	0	12	0	0
2	7-H	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	8-A	12	0	12	0	0
2	8-B	12	0	12	0	0
2	8-C	12	0	12	0	0
2	8-D	12	0	12	0	0
2	8-E	12	0	12	0	0
2	8-F	12	0	12	0	0
2	8-G	12	0	12	0	0
2	8-H	12	0	12	0	0
2	9-A	12	0	12	0	0
2	9-B	12	0	12	0	0
2	9-C	12	0	12	0	0
2	9-D	12	0	12	0	0
2	9-E	12	0	12	0	0
2	9-F	12	0	12	0	0
2	9-G	12	0	12	0	0
2	9-H	12	0	12	0	0
2	10-A	12	0	12	0	0
2	10-B	12	0	12	0	0
2	10-C	12	0	12	0	0
2	10-D	12	0	12	0	0
2	10-E	12	0	12	0	0
2	10-F	12	0	12	0	0
2	10-G	12	0	12	0	0
2	10-H	12	0	12	0	0
3	1-A	18	0	0	0	0
3	1-B	42	0	0	0	0
3	1-C	6	0	0	0	0
3	1-D	18	0	0	0	0
3	1-E	12	0	0	0	0
3	1-F	36	0	0	0	0
3	1-G	24	0	0	0	0
3	1-H	12	0	0	0	0
3	2-A	18	0	24	0	0
3	2-B	36	0	47	0	0
3	2-C	18	0	16	0	0
3	2-D	12	0	16	0	0
3	2-E	24	0	24	0	0
3	2-F	24	0	33	0	0
3	2-G	18	0	24	0	0
3	2-H	18	0	24	0	0
3	3-A	24	0	24	0	0
3	3-B	36	0	48	0	0

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

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

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	9-G	3	0	1	0	0
5	10-C	3	0	1	0	0
5	10-F	3	0	1	0	0
5	10-G	3	0	1	0	0
6	1-A	180	0	0	0	0
6	1-B	198	0	0	0	0
6	1-C	178	0	0	0	0
6	1-D	183	0	0	0	0
6	1-E	178	0	0	0	0
6	1-F	178	0	0	0	0
6	1-G	186	0	0	0	0
6	1-H	172	0	0	0	0
6	2-A	190	0	0	0	0
6	2-B	189	0	0	0	0
6	2-C	178	0	0	0	0
6	2-D	159	0	0	0	0
6	2-E	177	0	0	0	0
6	2-F	175	0	0	0	0
6	2-G	175	0	0	0	0
6	2-H	185	0	0	0	0
6	3-A	183	0	0	0	0
6	3-B	183	0	0	0	0
6	3-C	181	0	0	0	0
6	3-D	188	0	0	0	0
6	3-E	196	0	0	0	0
6	3-F	159	0	0	0	0
6	3-G	183	0	0	0	0
6	3-H	163	0	0	0	0
6	4-A	184	0	0	0	0
6	4-B	189	0	0	0	0
6	4-C	176	0	0	0	0
6	4-D	179	0	0	0	0
6	4-E	197	0	0	0	0
6	4-F	177	0	0	0	0
6	4-G	185	0	0	0	0
6	4-H	184	0	0	0	0
6	5-A	197	0	0	0	0
6	5-B	189	0	0	0	0
6	5-C	178	0	0	0	0
6	5-D	179	0	0	0	0
6	5-E	173	0	0	0	0
6	5-F	166	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	5-G	172	0	0	0	0
6	5-H	183	0	0	0	0
6	6-A	179	0	0	0	0
6	6-B	195	0	0	0	0
6	6-C	174	0	0	0	0
6	6-D	161	0	0	0	0
6	6-E	191	0	0	0	0
6	6-F	189	0	0	0	0
6	6-G	176	0	0	0	0
6	6-H	184	0	0	0	0
6	7-A	192	0	0	0	0
6	7-B	196	0	0	0	0
6	7-C	196	0	0	0	0
6	7-D	177	0	0	0	0
6	7-E	180	0	0	0	0
6	7-F	179	0	0	0	0
6	7-G	187	0	0	0	0
6	7-H	183	0	0	0	0
6	8-A	183	0	0	0	0
6	8-B	185	0	0	0	0
6	8-C	183	0	0	0	0
6	8-D	179	0	0	0	0
6	8-E	194	0	0	0	0
6	8-F	162	0	0	0	0
6	8-G	179	0	0	0	0
6	8-H	191	0	0	0	0
6	9-A	188	0	0	0	0
6	9-B	198	0	0	0	0
6	9-C	178	0	0	0	0
6	9-D	179	0	0	0	0
6	9-E	181	0	0	0	0
6	9-F	176	0	0	0	0
6	9-G	197	0	0	0	0
6	9-H	168	0	0	0	0
6	10-A	173	0	0	0	0
6	10-B	195	0	0	0	0
6	10-C	188	0	0	0	0
6	10-D	177	0	0	0	0
6	10-E	182	0	0	0	0
6	10-F	167	0	0	0	0
6	10-G	182	0	0	0	0
6	10-H	194	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	243453	0	205107	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	361/384 (94%)	335 (93%)	20 (6%)	6 (2%)	7	3
1	1-B	370/384 (96%)	345 (93%)	19 (5%)	6 (2%)	7	4
1	1-C	374/384 (97%)	344 (92%)	23 (6%)	7 (2%)	6	3
1	1-D	373/384 (97%)	338 (91%)	23 (6%)	12 (3%)	3	1
1	1-E	352/384 (92%)	328 (93%)	18 (5%)	6 (2%)	7	3
1	1-F	374/384 (97%)	352 (94%)	18 (5%)	4 (1%)	11	8
1	1-G	375/384 (98%)	341 (91%)	27 (7%)	7 (2%)	6	3
1	1-H	375/384 (98%)	341 (91%)	28 (8%)	6 (2%)	7	4
1	2-A	373/384 (97%)	348 (93%)	21 (6%)	4 (1%)	11	8
1	2-B	375/384 (98%)	345 (92%)	24 (6%)	6 (2%)	7	4
1	2-C	376/384 (98%)	348 (93%)	24 (6%)	4 (1%)	11	8
1	2-D	373/384 (97%)	350 (94%)	15 (4%)	8 (2%)	5	2
1	2-E	373/384 (97%)	350 (94%)	17 (5%)	6 (2%)	7	4
1	2-F	374/384 (97%)	345 (92%)	25 (7%)	4 (1%)	11	8
1	2-G	375/384 (98%)	344 (92%)	28 (8%)	3 (1%)	16	12
1	2-H	375/384 (98%)	345 (92%)	24 (6%)	6 (2%)	7	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-A	373/384 (97%)	341 (91%)	28 (8%)	4 (1%)	11	8
1	3-B	375/384 (98%)	347 (92%)	20 (5%)	8 (2%)	5	2
1	3-C	376/384 (98%)	341 (91%)	30 (8%)	5 (1%)	9	6
1	3-D	373/384 (97%)	342 (92%)	23 (6%)	8 (2%)	5	2
1	3-E	373/384 (97%)	345 (92%)	19 (5%)	9 (2%)	4	2
1	3-F	374/384 (97%)	346 (92%)	17 (4%)	11 (3%)	3	1
1	3-G	375/384 (98%)	339 (90%)	31 (8%)	5 (1%)	9	6
1	3-H	375/384 (98%)	346 (92%)	21 (6%)	8 (2%)	5	2
1	4-A	373/384 (97%)	348 (93%)	21 (6%)	4 (1%)	11	8
1	4-B	375/384 (98%)	350 (93%)	18 (5%)	7 (2%)	6	3
1	4-C	376/384 (98%)	353 (94%)	17 (4%)	6 (2%)	7	4
1	4-D	373/384 (97%)	342 (92%)	25 (7%)	6 (2%)	7	4
1	4-E	373/384 (97%)	347 (93%)	18 (5%)	8 (2%)	5	2
1	4-F	374/384 (97%)	340 (91%)	24 (6%)	10 (3%)	4	1
1	4-G	375/384 (98%)	344 (92%)	24 (6%)	7 (2%)	6	3
1	4-H	375/384 (98%)	348 (93%)	24 (6%)	3 (1%)	16	12
1	5-A	373/384 (97%)	333 (89%)	32 (9%)	8 (2%)	5	2
1	5-B	375/384 (98%)	352 (94%)	19 (5%)	4 (1%)	11	8
1	5-C	376/384 (98%)	347 (92%)	28 (7%)	1 (0%)	36	36
1	5-D	373/384 (97%)	345 (92%)	21 (6%)	7 (2%)	6	3
1	5-E	373/384 (97%)	343 (92%)	17 (5%)	13 (4%)	3	1
1	5-F	374/384 (97%)	349 (93%)	18 (5%)	7 (2%)	6	3
1	5-G	375/384 (98%)	339 (90%)	29 (8%)	7 (2%)	6	3
1	5-H	375/384 (98%)	345 (92%)	25 (7%)	5 (1%)	9	6
1	6-A	373/384 (97%)	342 (92%)	25 (7%)	6 (2%)	7	4
1	6-B	375/384 (98%)	343 (92%)	29 (8%)	3 (1%)	16	12
1	6-C	376/384 (98%)	345 (92%)	28 (7%)	3 (1%)	16	12
1	6-D	373/384 (97%)	340 (91%)	22 (6%)	11 (3%)	3	1
1	6-E	373/384 (97%)	351 (94%)	17 (5%)	5 (1%)	9	6
1	6-F	374/384 (97%)	347 (93%)	24 (6%)	3 (1%)	16	12
1	6-G	375/384 (98%)	351 (94%)	20 (5%)	4 (1%)	11	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6-H	375/384 (98%)	347 (92%)	23 (6%)	5 (1%)	9	6
1	7-A	373/384 (97%)	345 (92%)	22 (6%)	6 (2%)	7	4
1	7-B	375/384 (98%)	349 (93%)	22 (6%)	4 (1%)	11	8
1	7-C	376/384 (98%)	340 (90%)	28 (7%)	8 (2%)	5	2
1	7-D	373/384 (97%)	343 (92%)	24 (6%)	6 (2%)	7	4
1	7-E	373/384 (97%)	344 (92%)	24 (6%)	5 (1%)	9	6
1	7-F	374/384 (97%)	344 (92%)	25 (7%)	5 (1%)	9	6
1	7-G	375/384 (98%)	339 (90%)	30 (8%)	6 (2%)	7	4
1	7-H	375/384 (98%)	349 (93%)	23 (6%)	3 (1%)	16	12
1	8-A	373/384 (97%)	344 (92%)	23 (6%)	6 (2%)	7	4
1	8-B	375/384 (98%)	347 (92%)	23 (6%)	5 (1%)	9	6
1	8-C	376/384 (98%)	347 (92%)	23 (6%)	6 (2%)	7	4
1	8-D	373/384 (97%)	345 (92%)	21 (6%)	7 (2%)	6	3
1	8-E	373/384 (97%)	353 (95%)	15 (4%)	5 (1%)	9	6
1	8-F	374/384 (97%)	341 (91%)	29 (8%)	4 (1%)	11	8
1	8-G	375/384 (98%)	347 (92%)	22 (6%)	6 (2%)	7	4
1	8-H	375/384 (98%)	346 (92%)	25 (7%)	4 (1%)	11	8
1	9-A	373/384 (97%)	344 (92%)	18 (5%)	11 (3%)	3	1
1	9-B	375/384 (98%)	345 (92%)	25 (7%)	5 (1%)	9	6
1	9-C	376/384 (98%)	349 (93%)	26 (7%)	1 (0%)	36	36
1	9-D	373/384 (97%)	335 (90%)	32 (9%)	6 (2%)	7	4
1	9-E	373/384 (97%)	342 (92%)	20 (5%)	11 (3%)	3	1
1	9-F	374/384 (97%)	351 (94%)	19 (5%)	4 (1%)	11	8
1	9-G	375/384 (98%)	347 (92%)	24 (6%)	4 (1%)	11	8
1	9-H	375/384 (98%)	350 (93%)	23 (6%)	2 (0%)	24	22
1	10-A	373/384 (97%)	343 (92%)	25 (7%)	5 (1%)	9	6
1	10-B	375/384 (98%)	342 (91%)	27 (7%)	6 (2%)	7	4
1	10-C	376/384 (98%)	340 (90%)	29 (8%)	7 (2%)	6	3
1	10-D	373/384 (97%)	345 (92%)	16 (4%)	12 (3%)	3	1
1	10-E	373/384 (97%)	346 (93%)	20 (5%)	7 (2%)	6	3
1	10-F	374/384 (97%)	347 (93%)	17 (4%)	10 (3%)	4	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	10-G	375/384 (98%)	341 (91%)	25 (7%)	9 (2%)	4	2
1	10-H	375/384 (98%)	349 (93%)	23 (6%)	3 (1%)	16	12
All	All	29900/30720 (97%)	27576 (92%)	1839 (6%)	485 (2%)	7	4

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	284/293 (97%)	262 (92%)	22 (8%)	12	9
1	1-B	288/293 (98%)	259 (90%)	29 (10%)	7	5
1	1-C	288/293 (98%)	265 (92%)	23 (8%)	11	8
1	1-D	285/293 (97%)	266 (93%)	19 (7%)	15	12
1	1-E	272/293 (93%)	253 (93%)	19 (7%)	14	11
1	1-F	284/293 (97%)	256 (90%)	28 (10%)	7	5
1	1-G	285/293 (97%)	265 (93%)	20 (7%)	14	11
1	1-H	287/293 (98%)	264 (92%)	23 (8%)	11	8
1	2-A	291/293 (99%)	269 (92%)	22 (8%)	12	9
1	2-B	291/293 (99%)	262 (90%)	29 (10%)	7	5
1	2-C	289/293 (99%)	266 (92%)	23 (8%)	11	8
1	2-D	285/293 (97%)	266 (93%)	19 (7%)	15	12
1	2-E	286/293 (98%)	266 (93%)	20 (7%)	14	11
1	2-F	284/293 (97%)	256 (90%)	28 (10%)	7	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-G	285/293 (97%)	265 (93%)	20 (7%)	14	11
1	2-H	287/293 (98%)	264 (92%)	23 (8%)	11	8
1	3-A	291/293 (99%)	269 (92%)	22 (8%)	12	9
1	3-B	291/293 (99%)	262 (90%)	29 (10%)	7	5
1	3-C	289/293 (99%)	266 (92%)	23 (8%)	11	8
1	3-D	285/293 (97%)	266 (93%)	19 (7%)	15	12
1	3-E	286/293 (98%)	266 (93%)	20 (7%)	14	11
1	3-F	284/293 (97%)	256 (90%)	28 (10%)	7	5
1	3-G	285/293 (97%)	265 (93%)	20 (7%)	14	11
1	3-H	287/293 (98%)	264 (92%)	23 (8%)	11	8
1	4-A	291/293 (99%)	269 (92%)	22 (8%)	12	9
1	4-B	291/293 (99%)	262 (90%)	29 (10%)	7	5
1	4-C	289/293 (99%)	266 (92%)	23 (8%)	11	8
1	4-D	285/293 (97%)	266 (93%)	19 (7%)	15	12
1	4-E	286/293 (98%)	266 (93%)	20 (7%)	14	11
1	4-F	284/293 (97%)	256 (90%)	28 (10%)	7	5
1	4-G	285/293 (97%)	265 (93%)	20 (7%)	14	11
1	4-H	287/293 (98%)	264 (92%)	23 (8%)	11	8
1	5-A	291/293 (99%)	269 (92%)	22 (8%)	12	9
1	5-B	291/293 (99%)	262 (90%)	29 (10%)	7	5
1	5-C	289/293 (99%)	266 (92%)	23 (8%)	11	8
1	5-D	285/293 (97%)	266 (93%)	19 (7%)	15	12
1	5-E	286/293 (98%)	266 (93%)	20 (7%)	14	11
1	5-F	284/293 (97%)	256 (90%)	28 (10%)	7	5
1	5-G	285/293 (97%)	265 (93%)	20 (7%)	14	11
1	5-H	287/293 (98%)	264 (92%)	23 (8%)	11	8
1	6-A	291/293 (99%)	269 (92%)	22 (8%)	12	9
1	6-B	291/293 (99%)	262 (90%)	29 (10%)	7	5
1	6-C	289/293 (99%)	266 (92%)	23 (8%)	11	8
1	6-D	285/293 (97%)	266 (93%)	19 (7%)	15	12
1	6-E	286/293 (98%)	266 (93%)	20 (7%)	14	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-F	284/293 (97%)	256 (90%)	28 (10%)	7	5
1	6-G	285/293 (97%)	265 (93%)	20 (7%)	14	11
1	6-H	287/293 (98%)	264 (92%)	23 (8%)	11	8
1	7-A	291/293 (99%)	269 (92%)	22 (8%)	12	9
1	7-B	291/293 (99%)	262 (90%)	29 (10%)	7	5
1	7-C	289/293 (99%)	266 (92%)	23 (8%)	11	8
1	7-D	285/293 (97%)	266 (93%)	19 (7%)	15	12
1	7-E	286/293 (98%)	266 (93%)	20 (7%)	14	11
1	7-F	284/293 (97%)	256 (90%)	28 (10%)	7	5
1	7-G	285/293 (97%)	265 (93%)	20 (7%)	14	11
1	7-H	287/293 (98%)	264 (92%)	23 (8%)	11	8
1	8-A	291/293 (99%)	269 (92%)	22 (8%)	12	9
1	8-B	291/293 (99%)	262 (90%)	29 (10%)	7	5
1	8-C	289/293 (99%)	266 (92%)	23 (8%)	11	8
1	8-D	285/293 (97%)	266 (93%)	19 (7%)	15	12
1	8-E	286/293 (98%)	266 (93%)	20 (7%)	14	11
1	8-F	284/293 (97%)	256 (90%)	28 (10%)	7	5
1	8-G	285/293 (97%)	265 (93%)	20 (7%)	14	11
1	8-H	287/293 (98%)	264 (92%)	23 (8%)	11	8
1	9-A	291/293 (99%)	269 (92%)	22 (8%)	12	9
1	9-B	291/293 (99%)	262 (90%)	29 (10%)	7	5
1	9-C	289/293 (99%)	266 (92%)	23 (8%)	11	8
1	9-D	285/293 (97%)	266 (93%)	19 (7%)	15	12
1	9-E	286/293 (98%)	266 (93%)	20 (7%)	14	11
1	9-F	284/293 (97%)	256 (90%)	28 (10%)	7	5
1	9-G	285/293 (97%)	265 (93%)	20 (7%)	14	11
1	9-H	287/293 (98%)	264 (92%)	23 (8%)	11	8
1	10-A	291/293 (99%)	269 (92%)	22 (8%)	12	9
1	10-B	291/293 (99%)	262 (90%)	29 (10%)	7	5
1	10-C	289/293 (99%)	266 (92%)	23 (8%)	11	8
1	10-D	285/293 (97%)	266 (93%)	19 (7%)	15	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	10-E	286/293 (98%)	266 (93%)	20 (7%)	14	11
1	10-F	284/293 (97%)	256 (90%)	28 (10%)	7	5
1	10-G	285/293 (97%)	265 (93%)	20 (7%)	14	11
1	10-H	287/293 (98%)	264 (92%)	23 (8%)	11	8
All	All	22955/23440 (98%)	21116 (92%)	1839 (8%)	11	8

5 of 1839 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	6-A	112	ARG
1	10-F	74	SER
1	7-B	328	HIS
1	10-E	97	ASP
1	9-F	132	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 221 such sidechains are listed below:

Mol	Chain	Res	Type
1	6-H	147	ASN
1	8-B	113	GLN
1	10-H	245	HIS
1	10-B	285	HIS
1	7-A	163	HIS

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	9-H	197	1	23,24,25	2.47	6 (26%)	25,32,34	1.18	3 (12%)
1	LLP	1-A	197	1	23,24,25	2.41	6 (26%)	25,32,34	1.34	3 (12%)
1	LLP	2-F	197	1	23,24,25	2.49	6 (26%)	25,32,34	1.27	3 (12%)
1	LLP	4-G	197	1	23,24,25	2.46	6 (26%)	25,32,34	1.20	2 (8%)
1	LLP	3-A	197	1	23,24,25	2.50	6 (26%)	25,32,34	1.31	4 (16%)
1	LLP	3-C	197	1	23,24,25	2.48	6 (26%)	25,32,34	1.37	5 (20%)
1	LLP	1-G	197	1	23,24,25	2.51	7 (30%)	25,32,34	1.12	2 (8%)
1	LLP	5-B	197	1	23,24,25	2.49	6 (26%)	25,32,34	1.08	4 (16%)
1	LLP	5-G	197	1	23,24,25	2.45	6 (26%)	25,32,34	1.22	3 (12%)
1	LLP	1-B	197	1	23,24,25	2.47	7 (30%)	25,32,34	1.17	3 (12%)
1	LLP	9-C	197	1	23,24,25	2.54	6 (26%)	25,32,34	1.10	3 (12%)
1	LLP	3-B	197	1	23,24,25	2.56	6 (26%)	25,32,34	1.30	5 (20%)
1	LLP	10-B	197	1	23,24,25	2.47	6 (26%)	25,32,34	1.31	6 (24%)
1	LLP	10-F	197	1	23,24,25	2.46	6 (26%)	25,32,34	1.17	4 (16%)
1	LLP	6-B	197	1	23,24,25	2.40	5 (21%)	25,32,34	1.23	3 (12%)
1	LLP	8-G	197	1	23,24,25	2.46	6 (26%)	25,32,34	1.36	2 (8%)
1	LLP	6-F	197	1	23,24,25	2.47	6 (26%)	25,32,34	1.16	3 (12%)
1	LLP	7-H	197	1	23,24,25	2.48	6 (26%)	25,32,34	1.25	3 (12%)
1	LLP	8-D	197	1	23,24,25	2.43	6 (26%)	25,32,34	1.35	4 (16%)
1	LLP	4-H	197	1	23,24,25	2.60	6 (26%)	25,32,34	1.25	3 (12%)
1	LLP	1-H	197	1	23,24,25	2.44	6 (26%)	25,32,34	1.18	3 (12%)
1	LLP	6-E	197	1	23,24,25	2.45	6 (26%)	25,32,34	1.14	2 (8%)
1	LLP	4-F	197	1	23,24,25	2.46	6 (26%)	25,32,34	1.19	4 (16%)
1	LLP	2-B	197	1	23,24,25	2.48	7 (30%)	25,32,34	1.09	3 (12%)
1	LLP	8-C	197	1	23,24,25	2.52	6 (26%)	25,32,34	1.22	3 (12%)
1	LLP	8-E	197	1	23,24,25	2.50	6 (26%)	25,32,34	1.11	3 (12%)
1	LLP	6-H	197	1	23,24,25	2.46	6 (26%)	25,32,34	1.20	3 (12%)
1	LLP	4-C	197	1	23,24,25	2.58	7 (30%)	25,32,34	1.34	4 (16%)
1	LLP	9-E	197	1	23,24,25	2.47	6 (26%)	25,32,34	1.21	4 (16%)
1	LLP	5-A	197	1	23,24,25	2.56	6 (26%)	25,32,34	1.20	3 (12%)
1	LLP	3-D	197	1	23,24,25	2.42	6 (26%)	25,32,34	1.14	3 (12%)
1	LLP	10-D	197	1	23,24,25	2.44	6 (26%)	25,32,34	1.09	3 (12%)
1	LLP	7-F	197	1	23,24,25	2.50	6 (26%)	25,32,34	1.21	4 (16%)
1	LLP	6-A	197	1	23,24,25	2.49	7 (30%)	25,32,34	1.23	2 (8%)
1	LLP	7-A	197	1	23,24,25	2.54	6 (26%)	25,32,34	1.25	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	6-G	197	1	23,24,25	2.51	7 (30%)	25,32,34	1.18	3 (12%)
1	LLP	10-E	197	1	23,24,25	2.47	7 (30%)	25,32,34	1.13	3 (12%)
1	LLP	7-B	197	1	23,24,25	2.45	6 (26%)	25,32,34	1.23	3 (12%)
1	LLP	5-D	197	1	23,24,25	2.40	5 (21%)	25,32,34	1.31	4 (16%)
1	LLP	3-F	197	1	23,24,25	2.47	6 (26%)	25,32,34	1.26	2 (8%)
1	LLP	6-C	197	1	23,24,25	2.60	7 (30%)	25,32,34	1.32	3 (12%)
1	LLP	3-H	197	1	23,24,25	2.58	6 (26%)	25,32,34	1.12	3 (12%)
1	LLP	2-H	197	1	23,24,25	2.43	6 (26%)	25,32,34	1.33	3 (12%)
1	LLP	1-E	197	1	23,24,25	2.46	6 (26%)	25,32,34	1.14	3 (12%)
1	LLP	9-B	197	1	23,24,25	2.26	7 (30%)	25,32,34	1.52	6 (24%)
1	LLP	8-F	197	1	23,24,25	2.44	6 (26%)	25,32,34	1.27	4 (16%)
1	LLP	9-F	197	1	23,24,25	2.47	6 (26%)	25,32,34	1.21	3 (12%)
1	LLP	6-D	197	1	23,24,25	2.43	6 (26%)	25,32,34	1.16	3 (12%)
1	LLP	3-E	197	1	23,24,25	2.55	7 (30%)	25,32,34	1.09	2 (8%)
1	LLP	4-B	197	1	23,24,25	2.48	6 (26%)	25,32,34	1.12	1 (4%)
1	LLP	2-C	197	1	23,24,25	2.52	6 (26%)	25,32,34	1.30	3 (12%)
1	LLP	8-A	197	1	23,24,25	2.52	6 (26%)	25,32,34	1.22	3 (12%)
1	LLP	2-A	197	1	23,24,25	2.55	7 (30%)	25,32,34	1.38	3 (12%)
1	LLP	2-E	197	1	23,24,25	2.57	6 (26%)	25,32,34	1.24	4 (16%)
1	LLP	4-E	197	1	23,24,25	2.49	7 (30%)	25,32,34	1.21	2 (8%)
1	LLP	7-E	197	1	23,24,25	2.50	7 (30%)	25,32,34	1.05	3 (12%)
1	LLP	5-C	197	1	23,24,25	2.52	6 (26%)	25,32,34	1.40	4 (16%)
1	LLP	10-A	197	1	23,24,25	2.54	6 (26%)	25,32,34	1.19	2 (8%)
1	LLP	1-C	197	1	23,24,25	2.45	6 (26%)	25,32,34	1.35	3 (12%)
1	LLP	7-G	197	1	23,24,25	2.51	7 (30%)	25,32,34	1.13	3 (12%)
1	LLP	7-D	197	1	23,24,25	2.45	6 (26%)	25,32,34	1.21	3 (12%)
1	LLP	1-F	197	1	23,24,25	2.48	6 (26%)	25,32,34	1.23	4 (16%)
1	LLP	2-D	197	1	23,24,25	2.41	6 (26%)	25,32,34	1.12	3 (12%)
1	LLP	7-C	197	1	23,24,25	2.49	6 (26%)	25,32,34	1.34	4 (16%)
1	LLP	3-G	197	1	23,24,25	2.48	7 (30%)	25,32,34	1.21	1 (4%)
1	LLP	2-G	197	1	23,24,25	2.54	7 (30%)	25,32,34	1.13	2 (8%)
1	LLP	5-E	197	1	23,24,25	2.46	7 (30%)	25,32,34	1.15	3 (12%)
1	LLP	1-D	197	1	23,24,25	2.44	6 (26%)	25,32,34	1.14	3 (12%)
1	LLP	4-D	197	1	23,24,25	2.38	6 (26%)	25,32,34	1.23	2 (8%)
1	LLP	10-C	197	1	23,24,25	2.52	7 (30%)	25,32,34	1.27	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	9-A	197	1	23,24,25	2.46	6 (26%)	25,32,34	1.23	4 (16%)
1	LLP	10-H	197	1	23,24,25	2.51	6 (26%)	25,32,34	1.19	2 (8%)
1	LLP	9-G	197	1	23,24,25	2.50	6 (26%)	25,32,34	1.09	2 (8%)
1	LLP	8-B	197	1	23,24,25	2.44	5 (21%)	25,32,34	1.14	2 (8%)
1	LLP	10-G	197	1	23,24,25	2.48	7 (30%)	25,32,34	1.23	2 (8%)
1	LLP	4-A	197	1	23,24,25	2.48	6 (26%)	25,32,34	1.31	4 (16%)
1	LLP	5-H	197	1	23,24,25	2.46	6 (26%)	25,32,34	1.24	3 (12%)
1	LLP	9-D	197	1	23,24,25	2.38	6 (26%)	25,32,34	1.18	3 (12%)
1	LLP	8-H	197	1	23,24,25	2.50	6 (26%)	25,32,34	1.24	3 (12%)
1	LLP	5-F	197	1	23,24,25	2.35	6 (26%)	25,32,34	1.35	4 (16%)

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	9-H	197	1	-	4/16/17/19	0/1/1/1
1	LLP	1-A	197	1	-	2/16/17/19	0/1/1/1
1	LLP	2-F	197	1	-	4/16/17/19	0/1/1/1
1	LLP	4-G	197	1	-	2/16/17/19	0/1/1/1
1	LLP	3-A	197	1	-	9/16/17/19	0/1/1/1
1	LLP	3-C	197	1	-	5/16/17/19	0/1/1/1
1	LLP	1-G	197	1	-	2/16/17/19	0/1/1/1
1	LLP	5-B	197	1	-	6/16/17/19	0/1/1/1
1	LLP	5-G	197	1	-	4/16/17/19	0/1/1/1
1	LLP	1-B	197	1	-	4/16/17/19	0/1/1/1
1	LLP	9-C	197	1	-	6/16/17/19	0/1/1/1
1	LLP	3-B	197	1	-	11/16/17/19	0/1/1/1
1	LLP	10-B	197	1	-	9/16/17/19	0/1/1/1
1	LLP	10-F	197	1	-	2/16/17/19	0/1/1/1
1	LLP	6-B	197	1	-	3/16/17/19	0/1/1/1
1	LLP	8-G	197	1	-	5/16/17/19	0/1/1/1
1	LLP	6-F	197	1	-	2/16/17/19	0/1/1/1
1	LLP	7-H	197	1	-	3/16/17/19	0/1/1/1
1	LLP	8-D	197	1	-	6/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	4-H	197	1	-	6/16/17/19	0/1/1/1
1	LLP	1-H	197	1	-	4/16/17/19	0/1/1/1
1	LLP	6-E	197	1	-	3/16/17/19	0/1/1/1
1	LLP	4-F	197	1	-	2/16/17/19	0/1/1/1
1	LLP	2-B	197	1	-	4/16/17/19	0/1/1/1
1	LLP	8-C	197	1	-	5/16/17/19	0/1/1/1
1	LLP	8-E	197	1	-	2/16/17/19	0/1/1/1
1	LLP	6-H	197	1	-	3/16/17/19	0/1/1/1
1	LLP	4-C	197	1	-	6/16/17/19	0/1/1/1
1	LLP	9-E	197	1	-	5/16/17/19	0/1/1/1
1	LLP	5-A	197	1	-	5/16/17/19	0/1/1/1
1	LLP	3-D	197	1	-	4/16/17/19	0/1/1/1
1	LLP	10-D	197	1	-	4/16/17/19	0/1/1/1
1	LLP	7-F	197	1	-	2/16/17/19	0/1/1/1
1	LLP	6-A	197	1	-	3/16/17/19	0/1/1/1
1	LLP	7-A	197	1	-	5/16/17/19	0/1/1/1
1	LLP	6-G	197	1	-	3/16/17/19	0/1/1/1
1	LLP	10-E	197	1	-	3/16/17/19	0/1/1/1
1	LLP	7-B	197	1	-	4/16/17/19	0/1/1/1
1	LLP	5-D	197	1	-	6/16/17/19	0/1/1/1
1	LLP	3-F	197	1	-	4/16/17/19	0/1/1/1
1	LLP	6-C	197	1	-	4/16/17/19	0/1/1/1
1	LLP	3-H	197	1	-	10/16/17/19	0/1/1/1
1	LLP	2-H	197	1	-	5/16/17/19	0/1/1/1
1	LLP	1-E	197	1	-	4/16/17/19	0/1/1/1
1	LLP	9-B	197	1	-	5/16/17/19	0/1/1/1
1	LLP	8-F	197	1	-	4/16/17/19	0/1/1/1
1	LLP	9-F	197	1	-	6/16/17/19	0/1/1/1
1	LLP	6-D	197	1	-	5/16/17/19	0/1/1/1
1	LLP	3-E	197	1	-	2/16/17/19	0/1/1/1
1	LLP	4-B	197	1	-	5/16/17/19	0/1/1/1
1	LLP	2-C	197	1	-	2/16/17/19	0/1/1/1
1	LLP	8-A	197	1	-	4/16/17/19	0/1/1/1
1	LLP	2-A	197	1	-	6/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	2-E	197	1	-	5/16/17/19	0/1/1/1
1	LLP	4-E	197	1	-	4/16/17/19	0/1/1/1
1	LLP	7-E	197	1	-	3/16/17/19	0/1/1/1
1	LLP	5-C	197	1	-	5/16/17/19	0/1/1/1
1	LLP	10-A	197	1	-	5/16/17/19	0/1/1/1
1	LLP	1-C	197	1	-	4/16/17/19	0/1/1/1
1	LLP	7-G	197	1	-	3/16/17/19	0/1/1/1
1	LLP	7-D	197	1	-	2/16/17/19	0/1/1/1
1	LLP	1-F	197	1	-	3/16/17/19	0/1/1/1
1	LLP	2-D	197	1	-	6/16/17/19	0/1/1/1
1	LLP	7-C	197	1	-	4/16/17/19	0/1/1/1
1	LLP	3-G	197	1	-	4/16/17/19	0/1/1/1
1	LLP	2-G	197	1	-	2/16/17/19	0/1/1/1
1	LLP	5-E	197	1	-	2/16/17/19	0/1/1/1
1	LLP	1-D	197	1	-	3/16/17/19	0/1/1/1
1	LLP	4-D	197	1	-	7/16/17/19	0/1/1/1
1	LLP	10-C	197	1	-	6/16/17/19	0/1/1/1
1	LLP	9-A	197	1	-	3/16/17/19	0/1/1/1
1	LLP	10-H	197	1	-	2/16/17/19	0/1/1/1
1	LLP	9-G	197	1	-	3/16/17/19	0/1/1/1
1	LLP	8-B	197	1	-	4/16/17/19	0/1/1/1
1	LLP	10-G	197	1	-	3/16/17/19	0/1/1/1
1	LLP	4-A	197	1	-	10/16/17/19	0/1/1/1
1	LLP	5-H	197	1	-	4/16/17/19	0/1/1/1
1	LLP	9-D	197	1	-	5/16/17/19	0/1/1/1
1	LLP	8-H	197	1	-	2/16/17/19	0/1/1/1
1	LLP	5-F	197	1	-	6/16/17/19	0/1/1/1

The worst 5 of 496 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-G	197	LLP	C4-C4'	8.10	1.63	1.46
1	6-C	197	LLP	C4-C4'	8.07	1.63	1.46
1	2-A	197	LLP	C4-C4'	8.01	1.63	1.46
1	2-G	197	LLP	C4-C4'	7.96	1.63	1.46
1	4-H	197	LLP	C4-C4'	7.95	1.63	1.46

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-G	197	LLP	C4-C4'-NZ	-3.89	106.08	124.04
1	3-F	197	LLP	C4-C4'-NZ	-3.70	106.98	124.04
1	2-A	197	LLP	CE-NZ-C4'	-3.57	107.28	118.72
1	4-E	197	LLP	C4-C4'-NZ	-3.57	107.57	124.04
1	5-C	197	LLP	C4-C4'-NZ	-3.52	107.78	124.04

There are no chirality outliers.

5 of 344 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1-A	197	LLP	O-C-CA-CB
1	2-A	197	LLP	C4-C4'-NZ-CE
1	2-A	197	LLP	O-C-CA-CB
1	3-A	197	LLP	C5'-OP4-P-OP2
1	3-A	197	LLP	C5'-OP4-P-OP3

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
3	GOL	3-B	406	-	5,5,5	0.40	0	5,5,5	0.40	0
2	MES	3-E	401	-	12,12,12	2.00	1 (8%)	15,16,16	3.32	11 (73%)
3	GOL	1-H	402	-	5,5,5	0.42	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	9-H	401	-	12,12,12	2.27	1 (8%)	15,16,16	1.67	4 (26%)
3	FMT	9-F	405	-	2,2,2	0.73	0	1,1,1	0.15	0
3	GOL	5-D	403	-	5,5,5	0.34	0	5,5,5	0.64	0
5	FMT	9-C	404	-	2,2,2	0.75	0	1,1,1	0.27	0
3	GOL	10-B	403	-	5,5,5	0.34	0	5,5,5	0.60	0
3	GOL	8-F	403	-	5,5,5	0.47	0	5,5,5	0.36	0
2	MES	2-D	401	-	12,12,12	2.05	1 (8%)	15,16,16	2.40	6 (40%)
3	GOL	8-F	405	-	5,5,5	0.34	0	5,5,5	0.50	0
3	GOL	2-G	403	-	5,5,5	0.37	0	5,5,5	0.56	0
2	MES	2-B	401	-	12,12,12	2.14	1 (8%)	15,16,16	2.00	4 (26%)
3	GOL	8-A	403	-	5,5,5	0.32	0	5,5,5	0.34	0
3	GOL	6-B	404	-	5,5,5	0.32	0	5,5,5	0.48	0
3	GOL	6-F	404	-	5,5,5	0.26	0	5,5,5	0.60	0
2	MES	9-C	401	-	12,12,12	2.41	1 (8%)	15,16,16	2.49	4 (26%)
3	GOL	3-B	403	-	5,5,5	0.38	0	5,5,5	0.58	0
3	GOL	5-E	402	-	5,5,5	0.50	0	5,5,5	0.30	0
3	GOL	6-B	407	-	5,5,5	0.38	0	5,5,5	0.25	0
2	MES	3-D	401	-	12,12,12	1.82	1 (8%)	15,16,16	2.56	8 (53%)
3	GOL	2-B	406	-	5,5,5	0.45	0	5,5,5	0.37	0
3	GOL	8-B	407	-	5,5,5	0.67	0	5,5,5	0.69	0
2	MES	5-F	401	-	12,12,12	2.09	1 (8%)	15,16,16	2.20	4 (26%)
3	GOL	8-C	402	-	5,5,5	0.41	0	5,5,5	0.30	0
3	GOL	3-E	402	-	5,5,5	0.40	0	5,5,5	0.42	0
3	GOL	2-C	402	-	5,5,5	0.37	0	5,5,5	0.52	0
3	GOL	2-E	403	-	5,5,5	0.37	0	5,5,5	0.53	0
3	GOL	10-C	402	-	5,5,5	0.31	0	5,5,5	0.37	0
3	GOL	6-E	402	-	5,5,5	0.41	0	5,5,5	0.37	0
3	GOL	7-H	402	-	5,5,5	0.47	0	5,5,5	0.25	0
3	GOL	9-B	406	-	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	8-G	403	-	5,5,5	0.42	0	5,5,5	0.24	0
3	GOL	9-H	403	-	5,5,5	0.39	0	5,5,5	0.44	0
3	GOL	10-D	403	-	5,5,5	0.32	0	5,5,5	0.52	0
3	GOL	3-C	402	-	5,5,5	0.42	0	5,5,5	0.37	0
3	GOL	10-H	403	-	5,5,5	0.41	0	5,5,5	0.74	0
3	GOL	7-F	404	-	5,5,5	0.45	0	5,5,5	0.42	0
3	GOL	10-G	402	-	5,5,5	0.32	0	5,5,5	0.93	0
2	MES	2-A	401	-	12,12,12	2.10	1 (8%)	15,16,16	1.62	3 (20%)
3	GOL	3-D	403	-	5,5,5	0.39	0	5,5,5	0.23	0
5	FMT	10-F	407	-	2,2,2	0.60	0	1,1,1	0.33	0
3	GOL	9-B	402	-	5,5,5	0.39	0	5,5,5	0.31	0
3	GOL	2-G	404	-	5,5,5	1.18	0	5,5,5	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	9-C	402	-	5,5,5	0.37	0	5,5,5	0.26	0
2	MES	5-G	401	-	12,12,12	2.60	1 (8%)	15,16,16	2.98	9 (60%)
3	GOL	4-B	405	-	5,5,5	0.36	0	5,5,5	0.37	0
3	GOL	8-E	403	-	5,5,5	0.56	0	5,5,5	0.93	0
4	GOL	5-A	405	-	5,5,5	0.36	0	5,5,5	0.36	0
5	GOL	2-C	404	-	5,5,5	0.37	0	5,5,5	0.36	0
3	GOL	4-E	403	-	5,5,5	0.45	0	5,5,5	0.71	0
4	FMT	1-G	406	-	2,2,2	0.73	0	1,1,1	0.22	0
3	GOL	6-H	403	-	5,5,5	0.43	0	5,5,5	0.97	0
3	GOL	3-A	402	-	5,5,5	0.26	0	5,5,5	0.29	0
3	GOL	8-H	403	-	5,5,5	0.39	0	5,5,5	0.44	0
3	GOL	5-D	402	-	5,5,5	0.33	0	5,5,5	0.43	0
5	FMT	3-F	407	-	2,2,2	0.89	0	1,1,1	0.46	0
3	GOL	10-B	402	-	5,5,5	0.35	0	5,5,5	0.37	0
3	GOL	3-G	403	-	5,5,5	0.28	0	5,5,5	0.71	0
2	MES	8-C	401	-	12,12,12	2.36	1 (8%)	15,16,16	2.60	8 (53%)
3	GOL	2-H	402	-	5,5,5	0.39	0	5,5,5	0.27	0
3	GOL	6-G	403	-	5,5,5	0.39	0	5,5,5	0.65	0
3	GOL	8-F	402	-	5,5,5	0.37	0	5,5,5	0.89	0
3	GOL	3-B	402	-	5,5,5	0.41	0	5,5,5	0.40	0
3	GOL	10-A	404	-	5,5,5	0.36	0	5,5,5	0.68	0
3	GOL	4-C	402	-	5,5,5	0.40	0	5,5,5	0.31	0
3	GOL	5-B	405	-	5,5,5	0.48	0	5,5,5	0.68	0
3	GOL	1-F	404	-	5,5,5	0.38	0	5,5,5	0.66	0
3	GOL	2-A	402	-	5,5,5	0.41	0	5,5,5	0.36	0
5	FMT	9-G	405	-	2,2,2	0.78	0	1,1,1	0.15	0
4	GOL	9-E	404	-	5,5,5	0.44	0	5,5,5	0.39	0
2	MES	7-H	401	-	12,12,12	2.45	1 (8%)	15,16,16	2.15	4 (26%)
3	GOL	6-B	406	-	5,5,5	0.37	0	5,5,5	0.45	0
5	GOL	8-G	405	-	5,5,5	0.39	0	5,5,5	0.67	0
2	MES	10-D	401	-	12,12,12	2.06	1 (8%)	15,16,16	1.75	4 (26%)
3	GOL	7-A	404	-	5,5,5	0.34	0	5,5,5	0.40	0
3	GOL	1-D	404	-	5,5,5	0.46	0	5,5,5	0.17	0
3	GOL	7-G	404	-	5,5,5	0.41	0	5,5,5	0.38	0
3	GOL	2-E	402	-	5,5,5	0.28	0	5,5,5	0.38	0
3	GOL	8-C	403	-	5,5,5	0.40	0	5,5,5	0.33	0
2	MES	3-F	401	-	12,12,12	2.00	1 (8%)	15,16,16	2.57	5 (33%)
3	GOL	10-D	402	-	5,5,5	0.44	0	5,5,5	0.64	0
4	FMT	3-G	406	-	2,2,2	0.76	0	1,1,1	0.27	0
3	GOL	9-A	403	-	5,5,5	0.48	0	5,5,5	0.53	0
3	GOL	7-B	404	-	5,5,5	0.35	0	5,5,5	0.73	0
2	MES	6-C	401	-	12,12,12	2.93	1 (8%)	15,16,16	2.83	8 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	6-F	401	-	12,12,12	1.89	1 (8%)	15,16,16	2.09	4 (26%)
3	GOL	8-D	402	-	5,5,5	0.40	0	5,5,5	0.49	0
2	MES	6-E	401	-	12,12,12	1.99	1 (8%)	15,16,16	2.73	8 (53%)
4	FMT	1-F	408	-	2,2,2	0.71	0	1,1,1	0.29	0
3	GOL	1-F	406	-	5,5,5	1.42	1 (20%)	5,5,5	1.53	1 (20%)
3	GOL	3-B	404	-	5,5,5	0.35	0	5,5,5	0.14	0
2	MES	7-D	401	-	12,12,12	2.77	1 (8%)	15,16,16	2.81	5 (33%)
3	GOL	5-A	402	-	5,5,5	0.31	0	5,5,5	0.39	0
3	FMT	2-F	406	-	2,2,2	0.75	0	1,1,1	0.00	0
3	GOL	6-F	406	-	5,5,5	0.36	0	5,5,5	0.30	0
3	GOL	1-G	404	-	5,5,5	0.43	0	5,5,5	0.35	0
3	GOL	2-C	403	-	5,5,5	0.46	0	5,5,5	0.17	0
3	GOL	10-E	403	-	5,5,5	0.36	0	5,5,5	0.56	0
3	GOL	10-C	403	-	5,5,5	0.36	0	5,5,5	0.16	0
5	GOL	3-G	405	-	5,5,5	0.29	0	5,5,5	0.47	0
3	GOL	10-F	404	-	5,5,5	0.42	0	5,5,5	0.23	0
2	MES	3-A	401	-	12,12,12	1.65	1 (8%)	15,16,16	2.26	4 (26%)
3	GOL	4-E	402	-	5,5,5	0.31	0	5,5,5	0.41	0
2	MES	1-F	401	-	12,12,12	1.86	1 (8%)	15,16,16	2.45	7 (46%)
3	GOL	5-C	402	-	5,5,5	0.34	0	5,5,5	0.33	0
3	GOL	4-B	407	-	5,5,5	0.47	0	5,5,5	0.42	0
3	GOL	1-C	402	-	5,5,5	0.34	0	5,5,5	0.37	0
2	MES	1-D	401	-	12,12,12	2.27	1 (8%)	15,16,16	2.59	8 (53%)
3	GOL	9-H	404	-	5,5,5	0.44	0	5,5,5	0.48	0
3	GOL	4-F	403	-	5,5,5	0.43	0	5,5,5	0.27	0
2	MES	1-B	401	-	12,12,12	1.98	1 (8%)	15,16,16	2.06	4 (26%)
2	MES	7-G	401	-	12,12,12	2.17	1 (8%)	15,16,16	2.59	6 (40%)
3	GOL	7-B	406	-	5,5,5	0.40	0	5,5,5	0.33	0
3	FMT	6-C	403	-	2,2,2	0.75	0	1,1,1	0.16	0
3	GOL	3-F	405	-	5,5,5	0.33	0	5,5,5	0.93	0
3	GOL	9-F	403	-	5,5,5	0.39	0	5,5,5	0.38	0
2	MES	2-H	401	-	12,12,12	2.73	1 (8%)	15,16,16	1.87	5 (33%)
2	MES	4-C	401	-	12,12,12	2.74	1 (8%)	15,16,16	2.71	4 (26%)
3	GOL	3-G	402	-	5,5,5	0.43	0	5,5,5	0.45	0
2	MES	9-B	401	-	12,12,12	2.18	1 (8%)	15,16,16	1.72	3 (20%)
2	MES	7-C	401	-	12,12,12	2.04	1 (8%)	15,16,16	1.75	4 (26%)
3	GOL	3-B	405	-	5,5,5	0.41	0	5,5,5	0.49	0
3	GOL	1-B	406	-	5,5,5	0.37	0	5,5,5	0.38	0
2	MES	4-D	401	-	12,12,12	2.18	1 (8%)	15,16,16	2.36	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	7-B	401	-	12,12,12	2.07	1 (8%)	15,16,16	2.37	5 (33%)
3	GOL	10-H	402	-	5,5,5	0.41	0	5,5,5	0.34	0
2	MES	1-C	401	-	12,12,12	2.35	1 (8%)	15,16,16	2.35	6 (40%)
2	MES	5-A	401	-	12,12,12	1.92	1 (8%)	15,16,16	2.24	6 (40%)
3	GOL	6-H	404	-	5,5,5	0.32	0	5,5,5	0.51	0
3	GOL	7-F	406	-	5,5,5	0.39	0	5,5,5	0.25	0
3	GOL	1-F	402	-	5,5,5	0.43	0	5,5,5	0.23	0
5	FMT	10-G	405	-	2,2,2	0.73	0	1,1,1	0.25	0
2	MES	4-B	401	-	12,12,12	2.02	1 (8%)	15,16,16	2.13	5 (33%)
2	MES	5-C	401	-	12,12,12	2.17	1 (8%)	15,16,16	2.08	4 (26%)
3	GOL	2-D	403	-	5,5,5	0.39	0	5,5,5	0.34	0
2	MES	1-E	401	-	12,12,12	2.14	1 (8%)	15,16,16	2.11	4 (26%)
5	FMT	10-C	404	-	2,2,2	0.75	0	1,1,1	0.25	0
2	MES	6-H	401	-	12,12,12	2.46	1 (8%)	15,16,16	2.07	4 (26%)
3	GOL	7-C	402	-	5,5,5	0.31	0	5,5,5	0.64	0
3	GOL	9-D	403	-	5,5,5	0.72	0	5,5,5	0.84	0
4	GOL	9-A	405	-	5,5,5	0.34	0	5,5,5	0.42	0
3	GOL	5-F	404	-	5,5,5	0.35	0	5,5,5	0.48	0
3	FMT	4-F	405	-	2,2,2	0.72	0	1,1,1	0.37	0
3	GOL	6-D	404	-	5,5,5	0.37	0	5,5,5	0.48	0
3	GOL	2-B	405	-	5,5,5	0.36	0	5,5,5	0.35	0
2	MES	6-D	401	-	12,12,12	2.05	1 (8%)	15,16,16	2.38	7 (46%)
2	MES	7-E	401	-	12,12,12	1.97	1 (8%)	15,16,16	2.50	6 (40%)
2	MES	5-D	401	-	12,12,12	2.22	1 (8%)	15,16,16	2.81	4 (26%)
2	MES	4-H	401	-	12,12,12	2.13	1 (8%)	15,16,16	2.21	7 (46%)
3	GOL	3-H	402	-	5,5,5	0.39	0	5,5,5	0.49	0
3	GOL	9-H	402	-	5,5,5	0.40	0	5,5,5	0.36	0
3	FMT	8-F	406	-	2,2,2	0.77	0	1,1,1	0.17	0
3	GOL	9-B	405	-	5,5,5	0.36	0	5,5,5	0.56	0
2	MES	4-F	401	-	12,12,12	1.99	1 (8%)	15,16,16	2.22	5 (33%)
3	GOL	4-F	402	-	5,5,5	0.40	0	5,5,5	0.41	0
4	FMT	8-G	406	-	2,2,2	0.73	0	1,1,1	0.28	0
3	GOL	5-B	406	-	5,5,5	0.45	0	5,5,5	0.29	0
3	GOL	9-F	402	-	5,5,5	0.32	0	5,5,5	0.50	0
3	GOL	6-C	402	-	5,5,5	0.31	0	5,5,5	0.48	0
3	GOL	7-F	403	-	5,5,5	0.46	0	5,5,5	0.73	0
3	GOL	1-H	403	-	5,5,5	0.40	0	5,5,5	0.32	0
2	MES	10-H	401	-	12,12,12	2.26	1 (8%)	15,16,16	2.23	6 (40%)
2	MES	4-G	401	-	12,12,12	2.19	1 (8%)	15,16,16	2.06	4 (26%)
3	GOL	9-A	402	-	5,5,5	0.31	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	7-H	403	-	5,5,5	0.40	0	5,5,5	0.48	0
3	FMT	1-C	403	-	2,2,2	0.77	0	1,1,1	0.31	0
3	GOL	5-G	404	-	5,5,5	0.43	0	5,5,5	0.47	0
3	GOL	6-D	402	-	5,5,5	0.43	0	5,5,5	0.61	0
3	GOL	1-F	403	-	5,5,5	0.36	0	5,5,5	0.55	0
3	GOL	5-F	402	-	5,5,5	0.40	0	5,5,5	0.37	0
2	MES	1-G	401	-	12,12,12	2.15	1 (8%)	15,16,16	2.22	6 (40%)
3	GOL	3-H	403	-	5,5,5	0.41	0	5,5,5	0.39	0
3	GOL	1-A	403	-	5,5,5	0.41	0	5,5,5	0.39	0
3	GOL	10-A	402	-	5,5,5	0.36	0	5,5,5	0.19	0
5	FMT	3-C	404	-	2,2,2	0.73	0	1,1,1	0.23	0
3	GOL	5-B	407	-	5,5,5	0.26	0	5,5,5	0.50	0
3	GOL	1-B	402	-	5,5,5	0.40	0	5,5,5	0.49	0
3	GOL	8-H	402	-	5,5,5	0.35	0	5,5,5	0.40	0
3	GOL	10-D	404	-	5,5,5	0.32	0	5,5,5	0.25	0
2	MES	8-G	401	-	12,12,12	2.46	1 (8%)	15,16,16	2.49	8 (53%)
3	GOL	10-E	402	-	5,5,5	0.25	0	5,5,5	0.97	1 (20%)
4	FMT	2-C	405	-	2,2,2	0.75	0	1,1,1	0.31	0
3	GOL	8-A	402	-	5,5,5	0.36	0	5,5,5	0.23	0
3	GOL	3-F	404	-	5,5,5	0.44	0	5,5,5	0.48	0
3	GOL	9-G	402	-	5,5,5	0.49	0	5,5,5	0.80	0
3	GOL	10-H	405	-	5,5,5	0.38	0	5,5,5	0.43	0
3	GOL	7-D	403	-	5,5,5	0.45	0	5,5,5	0.61	0
4	GOL	6-E	404	-	5,5,5	0.47	0	5,5,5	0.27	0
3	GOL	7-B	407	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	9-D	402	-	5,5,5	0.47	0	5,5,5	0.65	0
3	GOL	6-E	403	-	5,5,5	0.38	0	5,5,5	0.25	0
3	GOL	1-G	403	-	5,5,5	0.43	0	5,5,5	0.59	0
2	MES	4-E	401	-	12,12,12	1.44	1 (8%)	15,16,16	1.60	4 (26%)
3	FMT	7-C	403	-	2,2,2	1.52	0	1,1,1	0.03	0
2	MES	5-B	401	-	12,12,12	2.19	2 (16%)	15,16,16	2.43	7 (46%)
2	MES	2-F	401	-	12,12,12	1.96	1 (8%)	15,16,16	2.35	6 (40%)
3	GOL	7-H	404	-	5,5,5	0.36	0	5,5,5	0.32	0
3	GOL	6-H	402	-	5,5,5	0.80	0	5,5,5	0.40	0
3	GOL	2-D	402	-	5,5,5	0.40	0	5,5,5	0.56	0
3	GOL	7-A	403	-	5,5,5	0.38	0	5,5,5	0.25	0
2	MES	9-G	401	-	12,12,12	2.12	1 (8%)	15,16,16	2.44	6 (40%)
3	GOL	4-H	404	-	5,5,5	0.34	0	5,5,5	0.31	0
3	GOL	3-A	404	-	5,5,5	0.36	0	5,5,5	0.42	0
5	FMT	7-F	407	-	2,2,2	0.72	0	1,1,1	0.20	0
2	MES	3-G	401	-	12,12,12	1.65	1 (8%)	15,16,16	1.84	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	6-A	401	-	12,12,12	1.54	1 (8%)	15,16,16	2.40	6 (40%)
3	GOL	10-G	403	-	5,5,5	0.39	0	5,5,5	0.46	0
2	MES	3-C	401	-	12,12,12	2.10	1 (8%)	15,16,16	3.04	7 (46%)
3	GOL	8-G	402	-	5,5,5	0.50	0	5,5,5	0.27	0
3	GOL	6-F	402	-	5,5,5	0.42	0	5,5,5	0.40	0
2	MES	6-G	401	-	12,12,12	1.96	1 (8%)	15,16,16	2.39	5 (33%)
5	FMT	8-C	404	-	2,2,2	0.75	0	1,1,1	0.27	0
3	GOL	6-A	402	-	5,5,5	0.35	0	5,5,5	0.44	0
3	GOL	10-F	406	-	5,5,5	0.33	0	5,5,5	0.29	0
2	MES	1-H	401	-	12,12,12	1.88	1 (8%)	15,16,16	2.14	5 (33%)
3	GOL	4-B	403	-	5,5,5	0.51	0	5,5,5	0.86	0
2	MES	5-H	401	-	12,12,12	2.10	1 (8%)	15,16,16	2.19	4 (26%)
3	GOL	8-B	402	-	5,5,5	0.40	0	5,5,5	0.42	0
5	GOL	4-C	404	-	5,5,5	0.48	0	5,5,5	0.65	0
4	GOL	4-G	406	-	5,5,5	0.40	0	5,5,5	0.29	0
3	GOL	5-F	403	-	5,5,5	0.51	0	5,5,5	0.13	0
3	GOL	10-A	403	-	5,5,5	0.43	0	5,5,5	0.32	0
3	GOL	10-B	406	-	5,5,5	0.34	0	5,5,5	0.55	0
2	MES	8-H	401	-	12,12,12	1.70	1 (8%)	15,16,16	2.29	6 (40%)
3	GOL	1-F	405	-	5,5,5	0.40	0	5,5,5	0.34	0
3	GOL	7-B	402	-	5,5,5	0.42	0	5,5,5	0.41	0
3	GOL	7-E	403	-	5,5,5	0.45	0	5,5,5	0.56	0
3	GOL	3-F	406	-	5,5,5	0.38	0	5,5,5	0.40	0
2	MES	1-A	401	-	12,12,12	2.31	1 (8%)	15,16,16	2.30	4 (26%)
3	GOL	2-B	404	-	5,5,5	0.43	0	5,5,5	0.49	0
3	GOL	8-E	402	-	5,5,5	0.87	0	5,5,5	1.38	1 (20%)
4	GOL	1-B	408	-	5,5,5	0.38	0	5,5,5	0.33	0
3	GOL	3-A	403	-	5,5,5	0.36	0	5,5,5	0.41	0
4	GOL	3-A	405	-	5,5,5	0.39	0	5,5,5	0.30	0
2	MES	8-F	401	-	12,12,12	2.22	1 (8%)	15,16,16	2.13	4 (26%)
2	MES	2-E	401	-	12,12,12	1.87	1 (8%)	15,16,16	2.42	5 (33%)
4	FMT	4-G	407	-	2,2,2	0.76	0	1,1,1	0.21	0
2	MES	10-E	401	-	12,12,12	2.01	1 (8%)	15,16,16	2.38	6 (40%)
3	GOL	1-D	403	-	5,5,5	1.03	0	5,5,5	1.39	1 (20%)
2	MES	8-A	401	-	12,12,12	2.32	1 (8%)	15,16,16	2.19	4 (26%)
3	GOL	6-A	403	-	5,5,5	0.40	0	5,5,5	0.76	0
3	GOL	9-A	404	-	5,5,5	0.39	0	5,5,5	0.47	0
3	GOL	9-G	403	-	5,5,5	0.40	0	5,5,5	0.34	0
2	MES	7-A	401	-	12,12,12	1.99	1 (8%)	15,16,16	1.88	3 (20%)
3	GOL	6-B	402	-	5,5,5	0.34	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	1-F	407	-	5,5,5	0.40	0	5,5,5	0.31	0
3	GOL	7-F	402	-	5,5,5	0.40	0	5,5,5	0.30	0
3	GOL	7-B	405	-	5,5,5	0.52	0	5,5,5	0.13	0
3	GOL	9-B	404	-	5,5,5	0.39	0	5,5,5	0.61	0
3	GOL	9-C	403	-	5,5,5	0.40	0	5,5,5	0.61	0
3	GOL	9-F	404	-	5,5,5	0.35	0	5,5,5	0.43	0
3	GOL	7-A	402	-	5,5,5	0.37	0	5,5,5	0.23	0
2	MES	9-D	401	-	12,12,12	2.62	1 (8%)	15,16,16	1.95	5 (33%)
2	MES	10-G	401	-	12,12,12	1.97	1 (8%)	15,16,16	2.52	8 (53%)
2	MES	4-A	401	-	12,12,12	2.25	1 (8%)	15,16,16	2.24	6 (40%)
3	GOL	4-D	403	-	5,5,5	0.30	0	5,5,5	0.56	0
5	FMT	7-G	405	-	2,2,2	0.74	0	1,1,1	0.24	0
3	GOL	5-A	404	-	5,5,5	0.39	0	5,5,5	0.50	0
3	GOL	6-D	403	-	5,5,5	0.28	0	5,5,5	0.67	0
3	GOL	1-B	405	-	5,5,5	0.40	0	5,5,5	0.56	0
3	GOL	1-A	402	-	5,5,5	0.36	0	5,5,5	0.28	0
3	GOL	2-F	402	-	5,5,5	0.39	0	5,5,5	0.74	0
3	GOL	7-F	405	-	5,5,5	0.37	0	5,5,5	0.34	0
3	GOL	4-B	404	-	5,5,5	0.37	0	5,5,5	0.32	0
3	GOL	1-B	403	-	5,5,5	0.40	0	5,5,5	0.34	0
3	GOL	7-G	403	-	5,5,5	0.31	0	5,5,5	0.58	0
3	GOL	9-E	402	-	5,5,5	0.33	0	5,5,5	0.53	0
4	GOL	7-A	405	-	5,5,5	0.40	0	5,5,5	0.37	0
3	GOL	4-H	402	-	5,5,5	0.46	0	5,5,5	0.34	0
3	GOL	1-E	403	-	5,5,5	0.41	0	5,5,5	0.28	0
3	GOL	2-H	403	-	5,5,5	1.10	0	5,5,5	1.18	0
3	GOL	8-D	403	-	5,5,5	0.43	0	5,5,5	0.40	0
2	MES	6-B	401	-	12,12,12	2.31	1 (8%)	15,16,16	1.84	4 (26%)
2	MES	8-B	401	-	12,12,12	2.33	1 (8%)	15,16,16	1.82	4 (26%)
2	MES	9-A	401	-	12,12,12	1.80	1 (8%)	15,16,16	2.78	9 (60%)
3	GOL	4-F	404	-	5,5,5	0.31	0	5,5,5	0.68	0
3	GOL	4-C	403	-	5,5,5	0.41	0	5,5,5	0.35	0
4	GOL	8-B	408	-	5,5,5	0.44	0	5,5,5	0.43	0
3	GOL	5-A	403	-	5,5,5	0.39	0	5,5,5	0.56	0
3	GOL	2-A	403	-	5,5,5	0.35	0	5,5,5	0.54	0
3	GOL	10-H	404	-	5,5,5	0.25	0	5,5,5	0.41	0
4	FMT	5-G	406	-	2,2,2	0.74	0	1,1,1	0.29	0
3	GOL	5-G	403	-	5,5,5	0.45	0	5,5,5	0.32	0
3	GOL	9-H	405	-	5,5,5	0.40	0	5,5,5	0.41	0
4	GOL	7-E	404	-	5,5,5	0.58	0	5,5,5	0.37	0
3	GOL	6-H	405	-	5,5,5	0.55	0	5,5,5	0.26	0
3	GOL	2-F	405	-	5,5,5	0.37	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	2-B	402	-	5,5,5	0.34	0	5,5,5	0.47	0
3	GOL	5-E	403	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	4-G	403	-	5,5,5	0.36	0	5,5,5	0.46	0
3	FMT	5-F	405	-	2,2,2	0.70	0	1,1,1	0.02	0
3	GOL	4-B	406	-	5,5,5	0.37	0	5,5,5	0.56	0
3	GOL	6-F	405	-	5,5,5	0.41	0	5,5,5	0.33	0
3	GOL	4-G	404	-	5,5,5	0.44	0	5,5,5	0.62	0
3	GOL	5-H	402	-	5,5,5	0.45	0	5,5,5	0.22	0
3	GOL	10-B	407	-	5,5,5	0.43	0	5,5,5	0.46	0
3	GOL	8-B	405	-	5,5,5	0.44	0	5,5,5	0.65	0
3	GOL	2-B	407	-	5,5,5	0.42	0	5,5,5	0.45	0
3	GOL	6-F	403	-	5,5,5	0.40	0	5,5,5	0.56	0
2	MES	2-G	401	-	12,12,12	2.29	1 (8%)	15,16,16	1.86	3 (20%)
3	GOL	7-B	403	-	5,5,5	0.37	0	5,5,5	0.49	0
2	MES	8-D	401	-	12,12,12	2.54	2 (16%)	15,16,16	2.39	8 (53%)
3	GOL	3-F	403	-	5,5,5	0.34	0	5,5,5	0.50	0
3	GOL	6-B	403	-	5,5,5	0.32	0	5,5,5	0.49	0
2	MES	2-C	401	-	12,12,12	1.85	1 (8%)	15,16,16	2.24	5 (33%)
3	GOL	7-E	402	-	5,5,5	0.71	0	5,5,5	0.62	0
3	FMT	6-G	404	-	2,2,2	0.75	0	1,1,1	0.25	0
4	FMT	4-C	405	-	2,2,2	0.75	0	1,1,1	0.20	0
3	GOL	5-D	404	-	5,5,5	0.39	0	5,5,5	0.72	0
3	GOL	4-B	402	-	5,5,5	0.37	0	5,5,5	0.48	0
3	GOL	5-B	402	-	5,5,5	0.36	0	5,5,5	0.39	0
5	GOL	4-G	405	-	5,5,5	0.46	0	5,5,5	0.39	0
3	GOL	1-D	402	-	5,5,5	0.42	0	5,5,5	0.48	0
3	GOL	8-G	404	-	5,5,5	0.36	0	5,5,5	0.38	0
3	GOL	5-B	404	-	5,5,5	0.35	0	5,5,5	0.54	0
2	MES	3-H	401	-	12,12,12	2.60	1 (8%)	15,16,16	2.74	7 (46%)
3	GOL	6-B	405	-	5,5,5	0.44	0	5,5,5	0.31	0
5	FMT	6-F	407	-	2,2,2	0.75	0	1,1,1	0.03	0
3	GOL	2-F	404	-	5,5,5	0.49	0	5,5,5	0.18	0
3	GOL	7-G	402	-	5,5,5	0.40	0	5,5,5	0.44	0
4	GOL	5-E	404	-	5,5,5	0.39	0	5,5,5	0.32	0
2	MES	5-E	401	-	12,12,12	2.22	1 (8%)	15,16,16	2.49	9 (60%)
3	GOL	9-G	404	-	5,5,5	0.45	0	5,5,5	0.17	0
3	GOL	4-A	404	-	5,5,5	0.40	0	5,5,5	0.64	0
5	GOL	1-G	405	-	5,5,5	0.36	0	5,5,5	0.64	0
5	GOL	5-G	405	-	5,5,5	0.42	0	5,5,5	0.33	0
2	MES	8-E	401	-	12,12,12	2.61	1 (8%)	15,16,16	2.61	5 (33%)
4	GOL	4-E	404	-	5,5,5	0.60	0	5,5,5	0.49	0
3	GOL	4-D	402	-	5,5,5	0.37	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	8-E	404	-	5,5,5	0.38	0	5,5,5	0.47	0
3	GOL	3-B	407	-	5,5,5	0.31	0	5,5,5	0.46	0
3	GOL	8-B	406	-	5,5,5	0.42	0	5,5,5	0.40	0
3	GOL	5-B	403	-	5,5,5	0.41	0	5,5,5	0.39	0
3	GOL	3-E	403	-	5,5,5	0.32	0	5,5,5	0.90	0
3	GOL	1-G	402	-	5,5,5	0.44	0	5,5,5	0.69	0
3	GOL	1-A	404	-	5,5,5	0.42	0	5,5,5	0.45	0
2	MES	10-F	401	-	12,12,12	2.54	1 (8%)	15,16,16	2.57	7 (46%)
2	MES	10-A	401	-	12,12,12	2.28	1 (8%)	15,16,16	1.72	4 (26%)
3	GOL	5-G	402	-	5,5,5	0.33	0	5,5,5	0.72	0
2	MES	10-C	401	-	12,12,12	1.71	1 (8%)	15,16,16	2.94	6 (40%)
3	GOL	1-B	404	-	5,5,5	0.38	0	5,5,5	0.72	0
3	GOL	2-F	403	-	5,5,5	0.47	0	5,5,5	0.40	0
3	GOL	8-B	403	-	5,5,5	0.32	0	5,5,5	0.54	0
3	GOL	10-B	404	-	5,5,5	0.32	0	5,5,5	0.63	0
3	GOL	2-H	404	-	5,5,5	0.28	0	5,5,5	0.61	0
3	GOL	10-F	402	-	5,5,5	0.38	0	5,5,5	0.39	0
3	GOL	4-A	403	-	5,5,5	0.36	0	5,5,5	0.60	0
2	MES	10-B	401	-	12,12,12	2.02	1 (8%)	15,16,16	2.09	7 (46%)
3	GOL	4-G	402	-	5,5,5	0.42	0	5,5,5	0.24	0
2	MES	7-F	401	-	12,12,12	2.00	1 (8%)	15,16,16	2.03	4 (26%)
3	GOL	8-F	404	-	5,5,5	0.45	0	5,5,5	0.20	0
3	GOL	3-G	404	-	5,5,5	0.35	0	5,5,5	0.40	0
3	GOL	4-H	403	-	5,5,5	0.34	0	5,5,5	0.47	0
3	GOL	4-A	402	-	5,5,5	0.34	0	5,5,5	0.38	0
3	GOL	2-A	404	-	5,5,5	0.37	0	5,5,5	0.37	0
3	GOL	5-H	404	-	5,5,5	0.41	0	5,5,5	0.50	0
3	GOL	1-E	402	-	5,5,5	0.29	0	5,5,5	0.78	0
2	MES	9-E	401	-	12,12,12	2.01	1 (8%)	15,16,16	2.14	4 (26%)
3	GOL	10-F	405	-	5,5,5	0.42	0	5,5,5	0.51	0
5	FMT	2-G	405	-	2,2,2	0.74	0	1,1,1	0.26	0
3	GOL	7-D	404	-	5,5,5	0.30	0	5,5,5	0.95	0
4	GOL	6-A	405	-	5,5,5	0.43	0	5,5,5	0.24	0
3	GOL	10-F	403	-	5,5,5	0.41	0	5,5,5	0.47	0
3	GOL	10-B	405	-	5,5,5	0.40	0	5,5,5	0.43	0
3	GOL	2-B	403	-	5,5,5	1.01	0	5,5,5	2.76	4 (80%)
3	GOL	8-H	404	-	5,5,5	0.28	0	5,5,5	0.83	0
4	GOL	2-E	404	-	5,5,5	0.35	0	5,5,5	0.39	0
3	GOL	1-B	407	-	5,5,5	0.41	0	5,5,5	0.45	0
3	GOL	3-C	403	-	5,5,5	0.30	0	5,5,5	0.72	0
3	GOL	8-A	404	-	5,5,5	0.43	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	9-B	403	-	5,5,5	0.43	0	5,5,5	0.47	0
3	GOL	6-G	402	-	5,5,5	0.48	0	5,5,5	0.28	0
3	GOL	6-A	404	-	5,5,5	0.35	0	5,5,5	0.37	0
3	GOL	3-F	402	-	5,5,5	0.34	0	5,5,5	0.23	0
2	MES	3-B	401	-	12,12,12	2.26	1 (8%)	15,16,16	3.41	8 (53%)
3	GOL	8-B	404	-	5,5,5	0.34	0	5,5,5	0.69	0
3	GOL	10-G	404	-	5,5,5	0.40	0	5,5,5	0.33	0
3	FMT	5-C	403	-	2,2,2	0.72	0	1,1,1	0.18	0
3	GOL	9-E	403	-	5,5,5	0.78	0	5,5,5	0.69	0
3	GOL	5-H	403	-	5,5,5	0.55	0	5,5,5	0.44	0
3	GOL	7-D	402	-	5,5,5	0.34	0	5,5,5	0.83	0
3	GOL	2-G	402	-	5,5,5	0.36	0	5,5,5	0.45	0
3	GOL	3-D	402	-	5,5,5	0.41	0	5,5,5	0.74	0
2	MES	9-F	401	-	12,12,12	2.02	1 (8%)	15,16,16	2.04	4 (26%)
3	GOL	9-D	404	-	5,5,5	0.33	0	5,5,5	0.44	0
4	GOL	3-E	404	-	5,5,5	0.46	0	5,5,5	0.25	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
3	GOL	3-B	406	-	-	4/4/4/4	-
2	MES	3-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-H	402	-	-	2/4/4/4	-
2	MES	9-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-D	403	-	-	3/4/4/4	-
3	GOL	10-B	403	-	-	2/4/4/4	-
3	GOL	8-F	403	-	-	2/4/4/4	-
2	MES	2-D	401	-	-	4/6/14/14	0/1/1/1
3	GOL	8-F	405	-	-	3/4/4/4	-
3	GOL	2-G	403	-	-	2/4/4/4	-
2	MES	2-B	401	-	-	1/6/14/14	0/1/1/1
3	GOL	8-A	403	-	-	2/4/4/4	-
3	GOL	6-B	404	-	-	2/4/4/4	-
3	GOL	6-F	404	-	-	3/4/4/4	-
2	MES	9-C	401	-	-	4/6/14/14	0/1/1/1
3	GOL	3-B	403	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	5-E	402	-	-	2/4/4/4	-
3	GOL	6-B	407	-	-	0/4/4/4	-
2	MES	3-D	401	-	-	4/6/14/14	0/1/1/1
3	GOL	2-B	406	-	-	2/4/4/4	-
3	GOL	8-B	407	-	-	2/4/4/4	-
2	MES	5-F	401	-	-	6/6/14/14	0/1/1/1
3	GOL	8-C	402	-	-	4/4/4/4	-
3	GOL	3-E	402	-	-	0/4/4/4	-
3	GOL	2-C	402	-	-	0/4/4/4	-
3	GOL	2-E	403	-	-	2/4/4/4	-
3	GOL	10-C	402	-	-	4/4/4/4	-
3	GOL	6-E	402	-	-	2/4/4/4	-
3	GOL	7-H	402	-	-	2/4/4/4	-
3	GOL	9-B	406	-	-	2/4/4/4	-
3	GOL	8-G	403	-	-	2/4/4/4	-
3	GOL	9-H	403	-	-	0/4/4/4	-
3	GOL	10-D	403	-	-	0/4/4/4	-
3	GOL	3-C	402	-	-	2/4/4/4	-
3	GOL	10-H	403	-	-	2/4/4/4	-
3	GOL	7-F	404	-	-	4/4/4/4	-
3	GOL	10-G	402	-	-	2/4/4/4	-
2	MES	2-A	401	-	-	5/6/14/14	0/1/1/1
3	GOL	3-D	403	-	-	0/4/4/4	-
3	GOL	9-B	402	-	-	2/4/4/4	-
3	GOL	2-G	404	-	-	2/4/4/4	-
3	GOL	9-C	402	-	-	2/4/4/4	-
2	MES	5-G	401	-	-	5/6/14/14	0/1/1/1
3	GOL	4-B	405	-	-	4/4/4/4	-
3	GOL	8-E	403	-	-	0/4/4/4	-
4	GOL	5-A	405	-	-	4/4/4/4	-
5	GOL	2-C	404	-	-	1/4/4/4	-
3	GOL	4-E	403	-	-	4/4/4/4	-
3	GOL	6-H	403	-	-	2/4/4/4	-
3	GOL	3-A	402	-	-	2/4/4/4	-
3	GOL	8-H	403	-	-	0/4/4/4	-
3	GOL	5-D	402	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	10-B	402	-	-	2/4/4/4	-
3	GOL	3-G	403	-	-	0/4/4/4	-
2	MES	8-C	401	-	-	6/6/14/14	0/1/1/1
3	GOL	2-H	402	-	-	3/4/4/4	-
3	GOL	6-G	403	-	-	2/4/4/4	-
3	GOL	8-F	402	-	-	2/4/4/4	-
3	GOL	3-B	402	-	-	2/4/4/4	-
3	GOL	10-A	404	-	-	2/4/4/4	-
3	GOL	4-C	402	-	-	2/4/4/4	-
3	GOL	5-B	405	-	-	3/4/4/4	-
3	GOL	1-F	404	-	-	0/4/4/4	-
3	GOL	2-A	402	-	-	0/4/4/4	-
4	GOL	9-E	404	-	-	2/4/4/4	-
2	MES	7-H	401	-	-	5/6/14/14	0/1/1/1
3	GOL	6-B	406	-	-	4/4/4/4	-
5	GOL	8-G	405	-	-	4/4/4/4	-
2	MES	10-D	401	-	-	5/6/14/14	0/1/1/1
3	GOL	7-A	404	-	-	1/4/4/4	-
3	GOL	1-D	404	-	-	0/4/4/4	-
3	GOL	7-G	404	-	-	1/4/4/4	-
3	GOL	2-E	402	-	-	2/4/4/4	-
3	GOL	8-C	403	-	-	2/4/4/4	-
2	MES	3-F	401	-	-	1/6/14/14	0/1/1/1
3	GOL	10-D	402	-	-	4/4/4/4	-
3	GOL	9-A	403	-	-	3/4/4/4	-
3	GOL	7-B	404	-	-	2/4/4/4	-
2	MES	6-C	401	-	-	2/6/14/14	0/1/1/1
2	MES	6-F	401	-	-	3/6/14/14	0/1/1/1
3	GOL	8-D	402	-	-	2/4/4/4	-
2	MES	6-E	401	-	-	3/6/14/14	0/1/1/1
3	GOL	1-F	406	-	-	3/4/4/4	-
3	GOL	3-B	404	-	-	0/4/4/4	-
2	MES	7-D	401	-	-	1/6/14/14	0/1/1/1
3	GOL	5-A	402	-	-	3/4/4/4	-
3	GOL	6-F	406	-	-	2/4/4/4	-
3	GOL	1-G	404	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	2-C	403	-	-	4/4/4/4	-
3	GOL	10-E	403	-	-	2/4/4/4	-
3	GOL	10-C	403	-	-	2/4/4/4	-
5	GOL	3-G	405	-	-	0/4/4/4	-
3	GOL	10-F	404	-	-	2/4/4/4	-
2	MES	3-A	401	-	-	4/6/14/14	0/1/1/1
3	GOL	4-E	402	-	-	1/4/4/4	-
2	MES	1-F	401	-	-	1/6/14/14	0/1/1/1
3	GOL	5-C	402	-	-	2/4/4/4	-
3	GOL	4-B	407	-	-	2/4/4/4	-
3	GOL	1-C	402	-	-	2/4/4/4	-
2	MES	1-D	401	-	-	1/6/14/14	0/1/1/1
3	GOL	9-H	404	-	-	3/4/4/4	-
3	GOL	4-F	403	-	-	0/4/4/4	-
2	MES	1-B	401	-	-	1/6/14/14	0/1/1/1
2	MES	7-G	401	-	-	5/6/14/14	0/1/1/1
3	GOL	7-B	406	-	-	2/4/4/4	-
3	GOL	3-F	405	-	-	3/4/4/4	-
3	GOL	9-F	403	-	-	2/4/4/4	-
2	MES	2-H	401	-	-	2/6/14/14	0/1/1/1
2	MES	4-C	401	-	-	4/6/14/14	0/1/1/1
3	GOL	3-G	402	-	-	2/4/4/4	-
2	MES	9-B	401	-	-	4/6/14/14	0/1/1/1
2	MES	7-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-B	405	-	-	0/4/4/4	-
3	GOL	1-B	406	-	-	2/4/4/4	-
2	MES	4-D	401	-	-	3/6/14/14	0/1/1/1
2	MES	7-B	401	-	-	1/6/14/14	0/1/1/1
3	GOL	10-H	402	-	-	2/4/4/4	-
2	MES	1-C	401	-	-	4/6/14/14	0/1/1/1
2	MES	5-A	401	-	-	1/6/14/14	0/1/1/1
3	GOL	6-H	404	-	-	4/4/4/4	-
3	GOL	7-F	406	-	-	2/4/4/4	-
3	GOL	1-F	402	-	-	2/4/4/4	-
2	MES	4-B	401	-	-	4/6/14/14	0/1/1/1
2	MES	5-C	401	-	-	3/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	2-D	403	-	-	2/4/4/4	-
2	MES	1-E	401	-	-	3/6/14/14	0/1/1/1
2	MES	6-H	401	-	-	5/6/14/14	0/1/1/1
3	GOL	7-C	402	-	-	4/4/4/4	-
3	GOL	9-D	403	-	-	4/4/4/4	-
4	GOL	9-A	405	-	-	2/4/4/4	-
3	GOL	5-F	404	-	-	2/4/4/4	-
3	GOL	6-D	404	-	-	1/4/4/4	-
3	GOL	2-B	405	-	-	2/4/4/4	-
2	MES	6-D	401	-	-	5/6/14/14	0/1/1/1
2	MES	7-E	401	-	-	4/6/14/14	0/1/1/1
2	MES	5-D	401	-	-	2/6/14/14	0/1/1/1
2	MES	4-H	401	-	-	2/6/14/14	0/1/1/1
3	GOL	3-H	402	-	-	4/4/4/4	-
3	GOL	9-H	402	-	-	4/4/4/4	-
3	GOL	9-B	405	-	-	4/4/4/4	-
2	MES	4-F	401	-	-	2/6/14/14	0/1/1/1
3	GOL	4-F	402	-	-	2/4/4/4	-
3	GOL	5-B	406	-	-	2/4/4/4	-
3	GOL	9-F	402	-	-	0/4/4/4	-
3	GOL	6-C	402	-	-	2/4/4/4	-
3	GOL	7-F	403	-	-	2/4/4/4	-
3	GOL	1-H	403	-	-	2/4/4/4	-
2	MES	10-H	401	-	-	1/6/14/14	0/1/1/1
2	MES	4-G	401	-	-	1/6/14/14	0/1/1/1
3	GOL	9-A	402	-	-	4/4/4/4	-
3	GOL	7-H	403	-	-	1/4/4/4	-
3	GOL	5-G	404	-	-	2/4/4/4	-
3	GOL	6-D	402	-	-	2/4/4/4	-
3	GOL	1-F	403	-	-	2/4/4/4	-
3	GOL	5-F	402	-	-	1/4/4/4	-
2	MES	1-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-H	403	-	-	4/4/4/4	-
3	GOL	1-A	403	-	-	0/4/4/4	-
3	GOL	10-A	402	-	-	2/4/4/4	-
3	GOL	5-B	407	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	1-B	402	-	-	4/4/4/4	-
3	GOL	8-H	402	-	-	2/4/4/4	-
3	GOL	10-D	404	-	-	2/4/4/4	-
2	MES	8-G	401	-	-	5/6/14/14	0/1/1/1
3	GOL	10-E	402	-	-	0/4/4/4	-
3	GOL	8-A	402	-	-	4/4/4/4	-
3	GOL	3-F	404	-	-	2/4/4/4	-
3	GOL	9-G	402	-	-	2/4/4/4	-
3	GOL	10-H	405	-	-	4/4/4/4	-
3	GOL	7-D	403	-	-	2/4/4/4	-
4	GOL	6-E	404	-	-	4/4/4/4	-
3	GOL	7-B	407	-	-	0/4/4/4	-
3	GOL	9-D	402	-	-	2/4/4/4	-
3	GOL	6-E	403	-	-	2/4/4/4	-
3	GOL	1-G	403	-	-	2/4/4/4	-
2	MES	4-E	401	-	-	5/6/14/14	0/1/1/1
2	MES	5-B	401	-	-	5/6/14/14	0/1/1/1
2	MES	2-F	401	-	-	1/6/14/14	0/1/1/1
3	GOL	7-H	404	-	-	0/4/4/4	-
3	GOL	6-H	402	-	-	4/4/4/4	-
3	GOL	2-D	402	-	-	2/4/4/4	-
3	GOL	7-A	403	-	-	2/4/4/4	-
2	MES	9-G	401	-	-	4/6/14/14	0/1/1/1
3	GOL	4-H	404	-	-	2/4/4/4	-
3	GOL	3-A	404	-	-	1/4/4/4	-
2	MES	3-G	401	-	-	4/6/14/14	0/1/1/1
2	MES	6-A	401	-	-	5/6/14/14	0/1/1/1
3	GOL	10-G	403	-	-	3/4/4/4	-
2	MES	3-C	401	-	-	4/6/14/14	0/1/1/1
3	GOL	8-G	402	-	-	2/4/4/4	-
3	GOL	6-F	402	-	-	2/4/4/4	-
2	MES	6-G	401	-	-	1/6/14/14	0/1/1/1
3	GOL	6-A	402	-	-	2/4/4/4	-
3	GOL	10-F	406	-	-	2/4/4/4	-
2	MES	1-H	401	-	-	1/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	4-B	403	-	-	2/4/4/4	-
2	MES	5-H	401	-	-	5/6/14/14	0/1/1/1
3	GOL	8-B	402	-	-	3/4/4/4	-
5	GOL	4-C	404	-	-	3/4/4/4	-
4	GOL	4-G	406	-	-	2/4/4/4	-
3	GOL	5-F	403	-	-	2/4/4/4	-
3	GOL	10-A	403	-	-	2/4/4/4	-
3	GOL	10-B	406	-	-	3/4/4/4	-
2	MES	8-H	401	-	-	4/6/14/14	0/1/1/1
3	GOL	1-F	405	-	-	2/4/4/4	-
3	GOL	7-B	402	-	-	0/4/4/4	-
3	GOL	7-E	403	-	-	2/4/4/4	-
3	GOL	3-F	406	-	-	2/4/4/4	-
2	MES	1-A	401	-	-	4/6/14/14	0/1/1/1
3	GOL	2-B	404	-	-	4/4/4/4	-
3	GOL	8-E	402	-	-	2/4/4/4	-
4	GOL	1-B	408	-	-	2/4/4/4	-
3	GOL	3-A	403	-	-	2/4/4/4	-
4	GOL	3-A	405	-	-	2/4/4/4	-
2	MES	8-F	401	-	-	5/6/14/14	0/1/1/1
2	MES	2-E	401	-	-	5/6/14/14	0/1/1/1
2	MES	10-E	401	-	-	5/6/14/14	0/1/1/1
3	GOL	1-D	403	-	-	4/4/4/4	-
2	MES	8-A	401	-	-	4/6/14/14	0/1/1/1
3	GOL	6-A	403	-	-	2/4/4/4	-
3	GOL	9-A	404	-	-	2/4/4/4	-
3	GOL	9-G	403	-	-	2/4/4/4	-
2	MES	7-A	401	-	-	3/6/14/14	0/1/1/1
3	GOL	6-B	402	-	-	2/4/4/4	-
5	GOL	1-F	407	-	-	2/4/4/4	-
3	GOL	7-F	402	-	-	3/4/4/4	-
3	GOL	7-B	405	-	-	4/4/4/4	-
3	GOL	9-B	404	-	-	2/4/4/4	-
3	GOL	9-C	403	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	9-F	404	-	-	2/4/4/4	-
3	GOL	7-A	402	-	-	3/4/4/4	-
2	MES	9-D	401	-	-	5/6/14/14	0/1/1/1
2	MES	10-G	401	-	-	3/6/14/14	0/1/1/1
2	MES	4-A	401	-	-	5/6/14/14	0/1/1/1
3	GOL	4-D	403	-	-	4/4/4/4	-
3	GOL	5-A	404	-	-	4/4/4/4	-
3	GOL	6-D	403	-	-	0/4/4/4	-
3	GOL	1-B	405	-	-	4/4/4/4	-
3	GOL	1-A	402	-	-	3/4/4/4	-
3	GOL	2-F	402	-	-	2/4/4/4	-
3	GOL	7-F	405	-	-	2/4/4/4	-
3	GOL	4-B	404	-	-	2/4/4/4	-
3	GOL	1-B	403	-	-	2/4/4/4	-
3	GOL	7-G	403	-	-	1/4/4/4	-
3	GOL	9-E	402	-	-	2/4/4/4	-
4	GOL	7-A	405	-	-	2/4/4/4	-
3	GOL	4-H	402	-	-	2/4/4/4	-
3	GOL	1-E	403	-	-	3/4/4/4	-
3	GOL	2-H	403	-	-	2/4/4/4	-
3	GOL	8-D	403	-	-	4/4/4/4	-
2	MES	6-B	401	-	-	1/6/14/14	0/1/1/1
2	MES	8-B	401	-	-	1/6/14/14	0/1/1/1
2	MES	9-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-F	404	-	-	2/4/4/4	-
3	GOL	4-C	403	-	-	2/4/4/4	-
4	GOL	8-B	408	-	-	2/4/4/4	-
3	GOL	5-A	403	-	-	2/4/4/4	-
3	GOL	2-A	403	-	-	1/4/4/4	-
3	GOL	10-H	404	-	-	2/4/4/4	-
3	GOL	5-G	403	-	-	0/4/4/4	-
3	GOL	9-H	405	-	-	2/4/4/4	-
4	GOL	7-E	404	-	-	4/4/4/4	-
3	GOL	6-H	405	-	-	2/4/4/4	-
3	GOL	2-F	405	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	2-B	402	-	-	2/4/4/4	-
3	GOL	5-E	403	-	-	2/4/4/4	-
3	GOL	4-G	403	-	-	2/4/4/4	-
3	GOL	4-B	406	-	-	0/4/4/4	-
3	GOL	6-F	405	-	-	3/4/4/4	-
3	GOL	4-G	404	-	-	2/4/4/4	-
3	GOL	5-H	402	-	-	2/4/4/4	-
3	GOL	10-B	407	-	-	2/4/4/4	-
3	GOL	8-B	405	-	-	1/4/4/4	-
3	GOL	2-B	407	-	-	2/4/4/4	-
3	GOL	6-F	403	-	-	0/4/4/4	-
2	MES	2-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-B	403	-	-	2/4/4/4	-
2	MES	8-D	401	-	-	3/6/14/14	0/1/1/1
3	GOL	3-F	403	-	-	0/4/4/4	-
3	GOL	6-B	403	-	-	3/4/4/4	-
2	MES	2-C	401	-	-	5/6/14/14	0/1/1/1
3	GOL	7-E	402	-	-	3/4/4/4	-
3	GOL	5-D	404	-	-	4/4/4/4	-
3	GOL	4-B	402	-	-	2/4/4/4	-
3	GOL	5-B	402	-	-	2/4/4/4	-
5	GOL	4-G	405	-	-	2/4/4/4	-
3	GOL	1-D	402	-	-	2/4/4/4	-
3	GOL	8-G	404	-	-	2/4/4/4	-
3	GOL	5-B	404	-	-	2/4/4/4	-
2	MES	3-H	401	-	-	6/6/14/14	0/1/1/1
3	GOL	6-B	405	-	-	4/4/4/4	-
3	GOL	2-F	404	-	-	2/4/4/4	-
3	GOL	7-G	402	-	-	2/4/4/4	-
4	GOL	5-E	404	-	-	2/4/4/4	-
2	MES	5-E	401	-	-	5/6/14/14	0/1/1/1
3	GOL	9-G	404	-	-	0/4/4/4	-
3	GOL	4-A	404	-	-	2/4/4/4	-
5	GOL	1-G	405	-	-	1/4/4/4	-
5	GOL	5-G	405	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	8-E	401	-	-	5/6/14/14	0/1/1/1
4	GOL	4-E	404	-	-	2/4/4/4	-
3	GOL	4-D	402	-	-	2/4/4/4	-
4	GOL	8-E	404	-	-	4/4/4/4	-
3	GOL	3-B	407	-	-	0/4/4/4	-
3	GOL	8-B	406	-	-	2/4/4/4	-
3	GOL	5-B	403	-	-	0/4/4/4	-
3	GOL	3-E	403	-	-	2/4/4/4	-
3	GOL	1-G	402	-	-	2/4/4/4	-
3	GOL	1-A	404	-	-	2/4/4/4	-
2	MES	10-F	401	-	-	1/6/14/14	0/1/1/1
2	MES	10-A	401	-	-	2/6/14/14	0/1/1/1
3	GOL	5-G	402	-	-	3/4/4/4	-
2	MES	10-C	401	-	-	4/6/14/14	0/1/1/1
3	GOL	1-B	404	-	-	2/4/4/4	-
3	GOL	2-F	403	-	-	0/4/4/4	-
3	GOL	8-B	403	-	-	2/4/4/4	-
3	GOL	10-B	404	-	-	2/4/4/4	-
3	GOL	2-H	404	-	-	2/4/4/4	-
3	GOL	10-F	402	-	-	4/4/4/4	-
3	GOL	4-A	403	-	-	2/4/4/4	-
2	MES	10-B	401	-	-	4/6/14/14	0/1/1/1
3	GOL	4-G	402	-	-	0/4/4/4	-
2	MES	7-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-F	404	-	-	2/4/4/4	-
3	GOL	3-G	404	-	-	3/4/4/4	-
3	GOL	4-H	403	-	-	1/4/4/4	-
3	GOL	4-A	402	-	-	4/4/4/4	-
3	GOL	2-A	404	-	-	2/4/4/4	-
3	GOL	5-H	404	-	-	0/4/4/4	-
3	GOL	1-E	402	-	-	0/4/4/4	-
2	MES	9-E	401	-	-	2/6/14/14	0/1/1/1
3	GOL	10-F	405	-	-	4/4/4/4	-
3	GOL	7-D	404	-	-	4/4/4/4	-
4	GOL	6-A	405	-	-	4/4/4/4	-
3	GOL	10-F	403	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	10-B	405	-	-	3/4/4/4	-
3	GOL	2-B	403	-	-	3/4/4/4	-
3	GOL	8-H	404	-	-	2/4/4/4	-
4	GOL	2-E	404	-	-	1/4/4/4	-
3	GOL	1-B	407	-	-	4/4/4/4	-
3	GOL	3-C	403	-	-	3/4/4/4	-
3	GOL	8-A	404	-	-	3/4/4/4	-
3	GOL	9-B	403	-	-	2/4/4/4	-
3	GOL	6-G	402	-	-	0/4/4/4	-
3	GOL	6-A	404	-	-	0/4/4/4	-
3	GOL	3-F	402	-	-	4/4/4/4	-
2	MES	3-B	401	-	-	3/6/14/14	0/1/1/1
3	GOL	8-B	404	-	-	2/4/4/4	-
3	GOL	10-G	404	-	-	4/4/4/4	-
3	GOL	9-E	403	-	-	2/4/4/4	-
3	GOL	5-H	403	-	-	1/4/4/4	-
3	GOL	7-D	402	-	-	2/4/4/4	-
3	GOL	2-G	402	-	-	0/4/4/4	-
3	GOL	3-D	402	-	-	2/4/4/4	-
2	MES	9-F	401	-	-	5/6/14/14	0/1/1/1
3	GOL	9-D	404	-	-	3/4/4/4	-
4	GOL	3-E	404	-	-	0/4/4/4	-

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-C	401	MES	C8-S	-9.85	1.63	1.77
2	4-C	401	MES	C8-S	-9.27	1.64	1.77
2	7-D	401	MES	C8-S	-9.17	1.64	1.77
2	2-H	401	MES	C8-S	-9.16	1.64	1.77
2	3-H	401	MES	C8-S	-8.78	1.65	1.77

The worst 5 of 445 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-C	401	MES	O2S-S-C8	8.99	120.31	106.73
2	4-C	401	MES	O2S-S-C8	7.30	117.75	106.73
2	10-C	401	MES	O1S-S-C8	7.15	117.54	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-B	401	MES	O1S-S-C8	7.10	117.45	106.73
2	8-E	401	MES	C5-N4-C3	7.09	124.12	108.84

There are no chirality outliers.

5 of 827 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2-A	401	MES	C8-C7-N4-C5
2	2-A	401	MES	C7-C8-S-O2S
2	3-A	401	MES	C8-C7-N4-C3
2	4-A	401	MES	C8-C7-N4-C3
2	6-A	401	MES	C7-C8-S-O1S

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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