



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:23 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 Full wwPDB X-ray Structure Validation 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

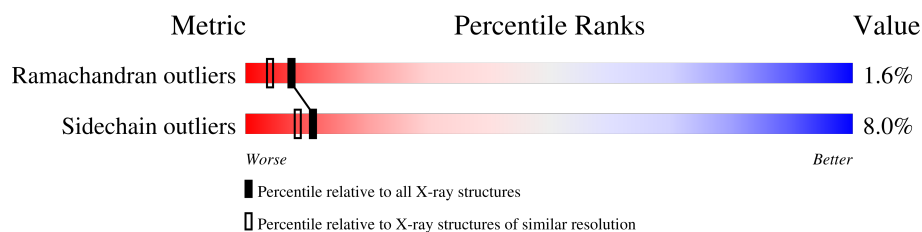
1 Overall quality at a glance

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)

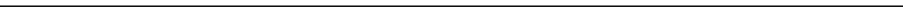
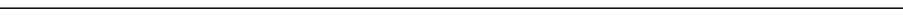
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	

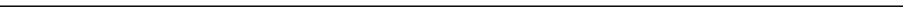
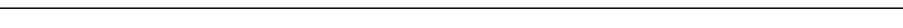
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Mol	Chain	Length	Quality of chain
1	10-B	384	 89% 9% .
1	10-C	384	 91% 8% .
1	10-D	384	 90% 8% .
1	10-E	384	 91% 7% ..
1	10-F	384	 89% 9% ..
1	10-G	384	 91% 8% .
1	10-H	384	 91% 7% .
1	2-A	384	 91% 6% ..
1	2-B	384	 90% 8% ..
1	2-C	384	 91% 7% .
1	2-D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

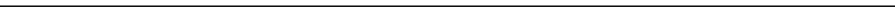
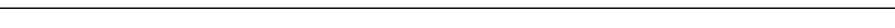
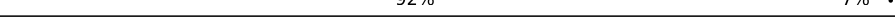
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Mol	Chain	Length	Quality of chain
1	4-C	384	 91% 7% ..
1	4-D	384	 91% 6% .
1	4-E	384	 90% 8% .
1	4-F	384	 89% 9% ..
1	4-G	384	 91% 7% .
1	4-H	384	 92% 7% .
1	5-A	384	 90% 7% ..
1	5-B	384	 90% 8% .
1	5-C	384	 92% 7% .
1	5-D	384	 91% 7% .
1	5-E	384	 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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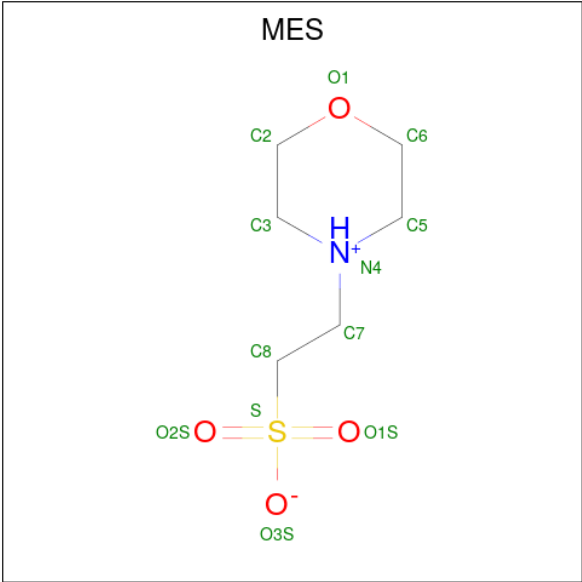
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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	10-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			

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: C₆H₁₃NO₄S).



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

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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: C1).

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

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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	C	O	0	0
			6	3	3		
3	7-A	1	Total	C	O	0	0
			6	3	3		
3	8-A	1	Total	C	O	0	0
			6	3	3		
3	9-A	1	Total	C	O	0	0
			6	3	3		
3	10-A	1	Total	C	O	0	0
			6	3	3		
3	1-B	1	Total	C	O	0	0
			6	3	3		
3	2-B	1	Total	C	O	0	0
			6	3	3		
3	4-B	1	Total	C	O	0	0
			6	3	3		
3	6-B	1	Total	C	O	0	0
			6	3	3		
3	8-B	1	Total	C	O	0	0
			6	3	3		
3	10-B	1	Total	C	O	0	0
			6	3	3		
3	1-B	1	Total	C	O	0	0
			6	3	3		
3	2-B	1	Total	C	O	0	0
			6	3	3		
3	3-B	1	Total	C	O	0	0
			6	3	3		
3	4-B	1	Total	C	O	0	0
			6	3	3		
3	5-B	1	Total	C	O	0	0
			6	3	3		
3	6-B	1	Total	C	O	0	0
			6	3	3		
3	7-B	1	Total	C	O	0	0
			6	3	3		
3	8-B	1	Total	C	O	0	0
			6	3	3		
3	9-B	1	Total	C	O	0	0
			6	3	3		
3	10-B	1	Total	C	O	0	0
			6	3	3		

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

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

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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 6	C 3	O 3	0	0
3	3-G	1	Total 6	C 3	O 3	0	0
3	1-H	1	Total 6	C 3	O 3	0	0
3	2-H	1	Total 6	C 3	O 3	0	0
3	3-H	1	Total 6	C 3	O 3	0	0
3	4-H	1	Total 6	C 3	O 3	0	0
3	5-H	1	Total 6	C 3	O 3	0	0
3	6-H	1	Total 6	C 3	O 3	0	0
3	7-H	1	Total 6	C 3	O 3	0	0
3	8-H	1	Total 6	C 3	O 3	0	0
3	9-H	1	Total 6	C 3	O 3	0	0
3	10-H	1	Total 6	C 3	O 3	0	0
3	1-H	1	Total 6	C 3	O 3	0	0
3	2-H	1	Total 6	C 3	O 3	0	0
3	3-H	1	Total 6	C 3	O 3	0	0
3	4-H	1	Total 6	C 3	O 3	0	0
3	5-H	1	Total 6	C 3	O 3	0	0
3	6-H	1	Total 6	C 3	O 3	0	0
3	7-H	1	Total 6	C 3	O 3	0	0
3	8-H	1	Total 6	C 3	O 3	0	0
3	9-H	1	Total 6	C 3	O 3	0	0

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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 O 183 183	0	0
6	9-A	188	Total O 188 188	0	0
6	10-A	173	Total O 173 173	0	0
6	1-B	198	Total O 198 198	0	0
6	2-B	189	Total O 189 189	0	0
6	3-B	183	Total O 183 183	0	0
6	4-B	189	Total O 189 189	0	0
6	5-B	189	Total O 189 189	0	0
6	6-B	195	Total O 195 195	0	0
6	7-B	196	Total O 196 196	0	0
6	8-B	185	Total O 185 185	0	0
6	9-B	198	Total O 198 198	0	0
6	10-B	195	Total O 195 195	0	0
6	1-C	178	Total O 178 178	0	0
6	2-C	178	Total O 178 178	0	0
6	3-C	181	Total O 181 181	0	0
6	4-C	176	Total O 176 176	0	0
6	5-C	178	Total O 178 178	0	0
6	6-C	174	Total O 174 174	0	0
6	7-C	196	Total O 196 196	0	0
6	8-C	183	Total O 183 183	0	0

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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 O 182 182	0	0
6	1-F	178	Total O 178 178	0	0
6	2-F	175	Total O 175 175	0	0
6	3-F	159	Total O 159 159	0	0
6	4-F	177	Total O 177 177	0	0
6	5-F	166	Total O 166 166	0	0
6	6-F	189	Total O 189 189	0	0
6	7-F	179	Total O 179 179	0	0
6	8-F	162	Total O 162 162	0	0
6	9-F	176	Total O 176 176	0	0
6	10-F	167	Total O 167 167	0	0
6	1-G	186	Total O 186 186	0	0
6	2-G	175	Total O 175 175	0	0
6	3-G	183	Total O 183 183	0	0
6	4-G	185	Total O 185 185	0	0
6	5-G	172	Total O 172 172	0	0
6	6-G	176	Total O 176 176	0	0
6	7-G	187	Total O 187 187	0	0
6	8-G	179	Total O 179 179	0	0
6	9-G	197	Total O 197 197	0	0
6	10-G	182	Total O 182 182	0	0

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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.

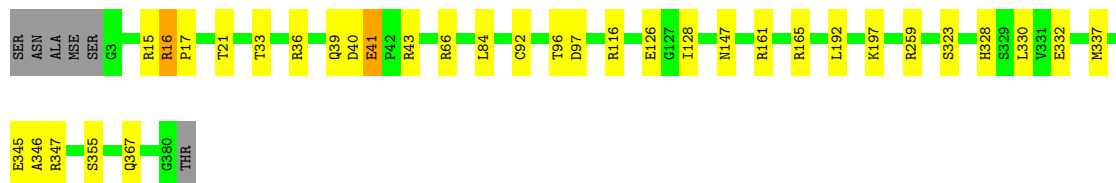
• Molecule 1: CalE6

Chain 1-A:  91% 7% ..



• Molecule 1: CalE6

Chain 1-B:  90% 8% ..



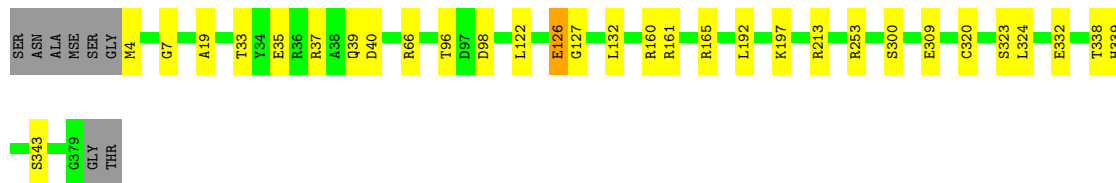
• Molecule 1: CalE6

Chain 1-C:  91% 8% .



• Molecule 1: CalE6

Chain 1-D:  90% 8% .



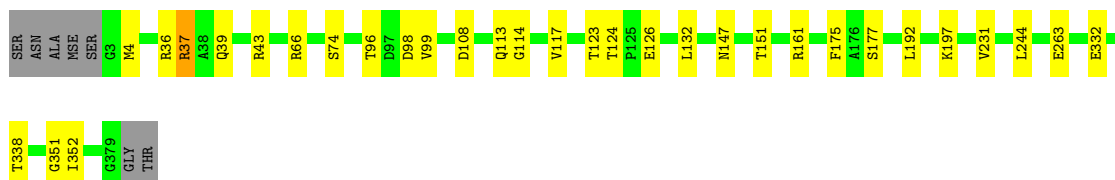
• Molecule 1: CalE6

Chain 1-E:  92% 5% ..



• Molecule 1: CalE6

Chain 1-F:  90% 8% .



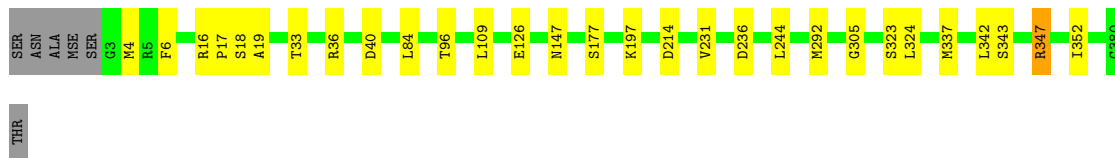
• Molecule 1: CalE6

Chain 1-G:  92% 6% ..



• Molecule 1: CalE6

Chain 1-H:  91% 7% .



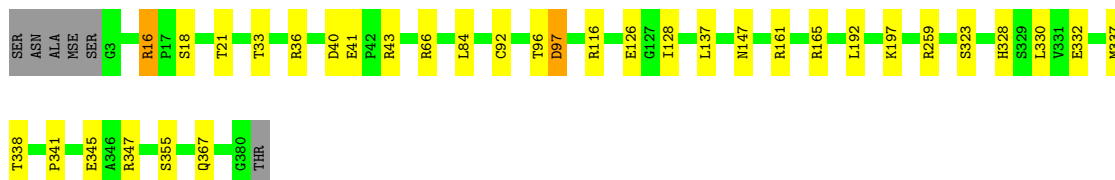
• Molecule 1: CalE6

Chain 2-A:  91% 6% ..

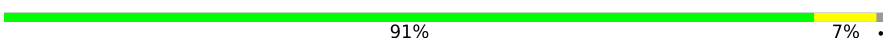


• Molecule 1: CalE6

Chain 2-B:  90% 8% ..



• Molecule 1: CalE6

Chain 2-C:  91% 7% .



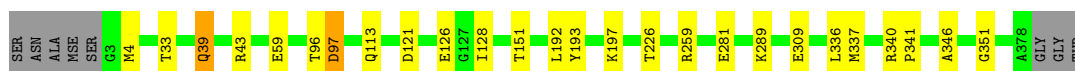
• Molecule 1: CalE6

Chain 2-D:  91% 7% ..



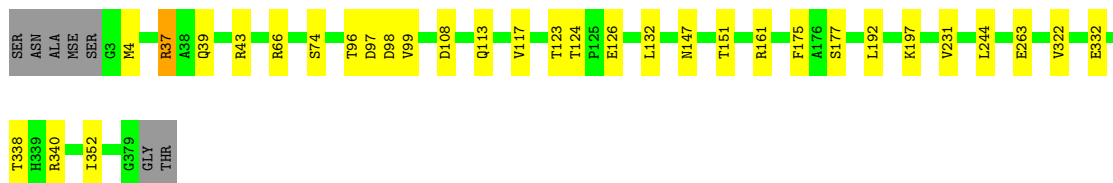
• Molecule 1: CalE6

Chain 2-E:  91% 6% ..

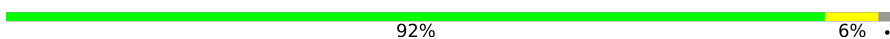


• Molecule 1: CalE6

Chain 2-F:  90% 8% .



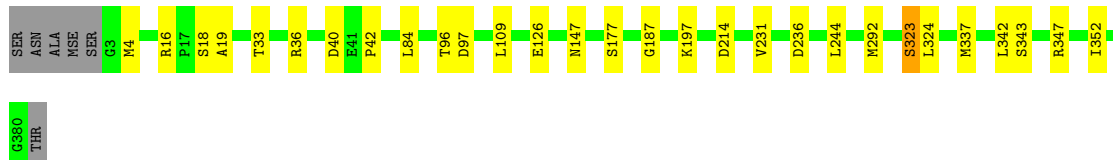
• Molecule 1: CalE6

Chain 2-G:  92% 6% .



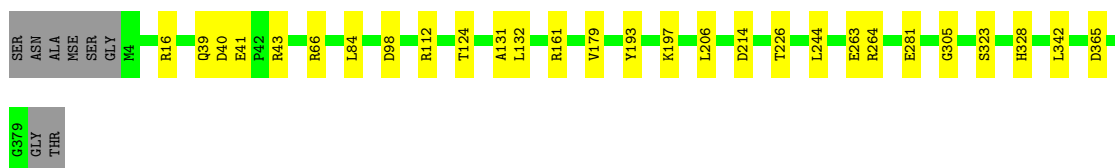
• Molecule 1: CalE6

Chain 2-H:  91% 7% .



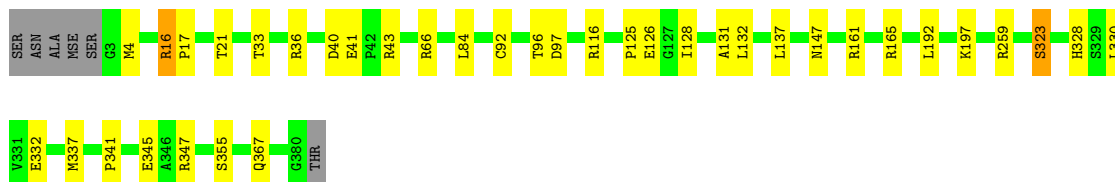
• Molecule 1: CalE6

Chain 3-A:  91% 7% .



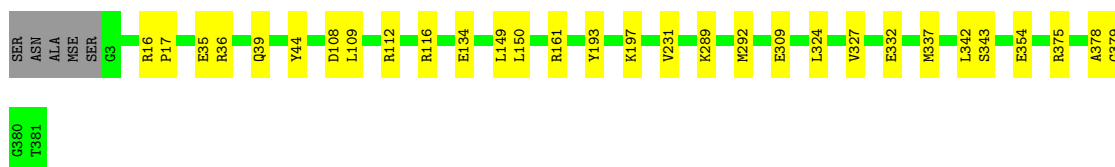
- Molecule 1: CalE6

Chain 3-B: 89% 9%



- Molecule 1: CalE6

Chain 3-C: 91% 8%



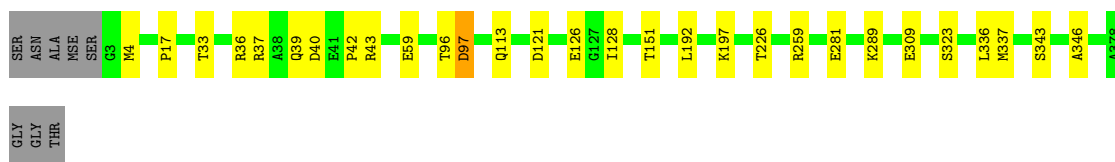
- Molecule 1: CalE6

Chain 3-D: 91% 7%



- Molecule 1: CalE6

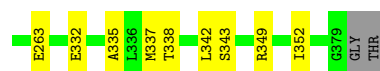
Chain 3-E: 90% 7%



- Molecule 1: CalE6

Chain 3-F: 88% 10%





- Molecule 1: CalE6



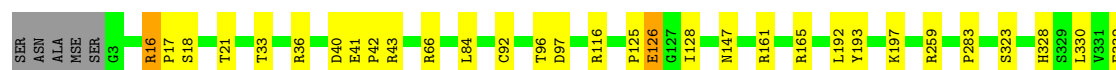
- Molecule 1: CalE6



- Molecule 1: CalE6



- Molecule 1: CalE6



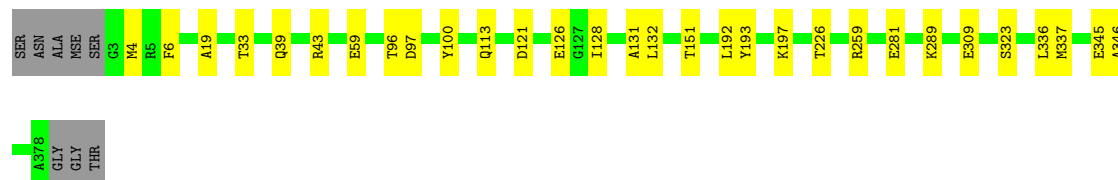
- Molecule 1: CalE6



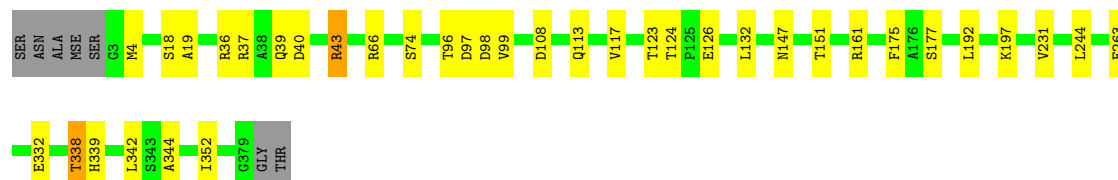
- Molecule 1: CalE6



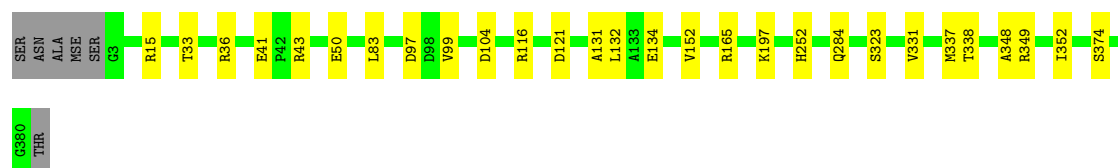
• Molecule 1: CalE6

Chain 4-E:  90% 8% .

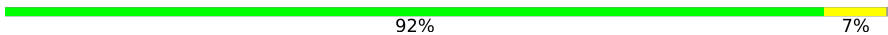
• Molecule 1: CalE6

Chain 4-F:  89% 9% ..

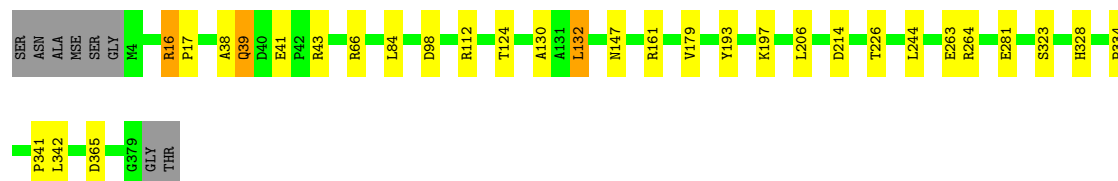
• Molecule 1: CalE6

Chain 4-G:  91% 7% .

• Molecule 1: CalE6

Chain 4-H:  92% 7% .

• Molecule 1: CalE6

Chain 5-A:  90% 7% ..

• Molecule 1: CalE6

Chain 5-B:  90% 8% .



- Molecule 1: CalE6

Chain 5-C: 92% 7% .



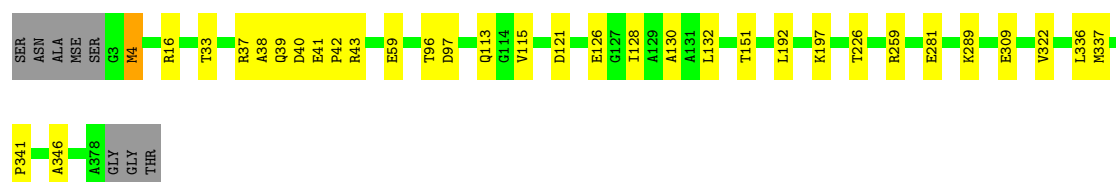
- Molecule 1: CalE6

Chain 5-D: 91% 7% .



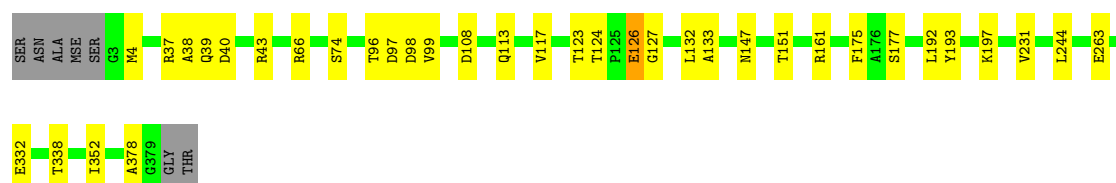
- Molecule 1: CalE6

Chain 5-E: 89% 8% .



- Molecule 1: CalE6

Chain 5-F: 89% 9% .

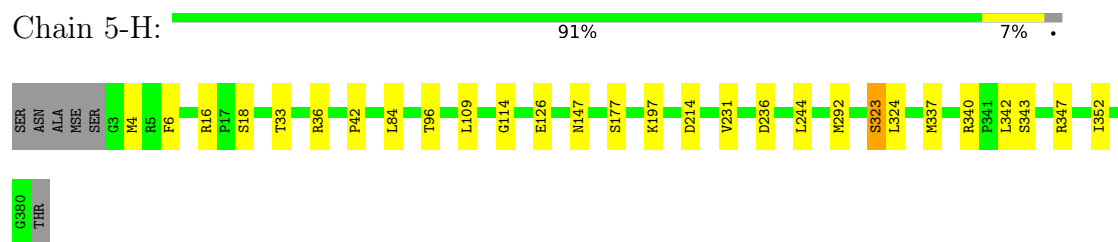


- Molecule 1: CalE6

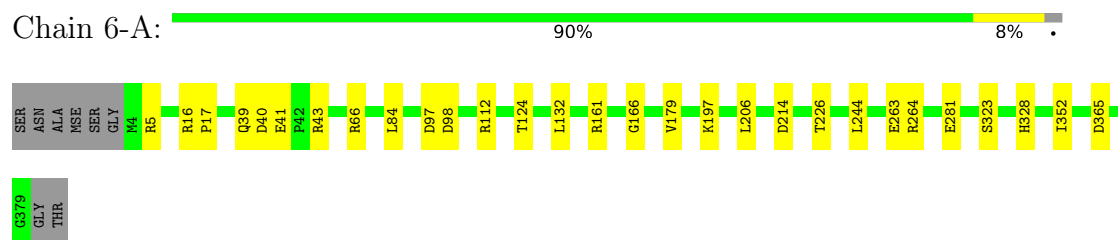
Chain 5-G: 91% 8% .



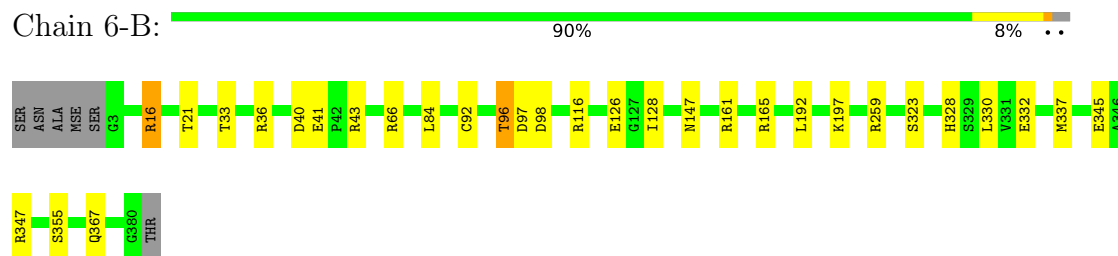
• Molecule 1: CalE6



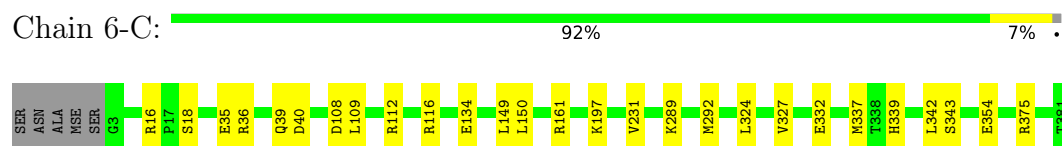
• Molecule 1: CalE6



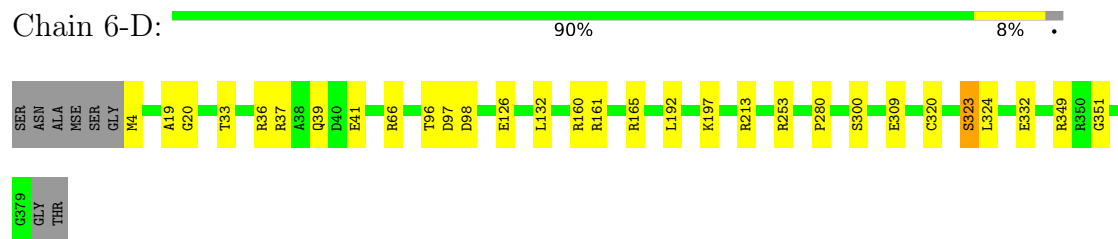
• Molecule 1: CalE6



• Molecule 1: CalE6



• Molecule 1: CalE6



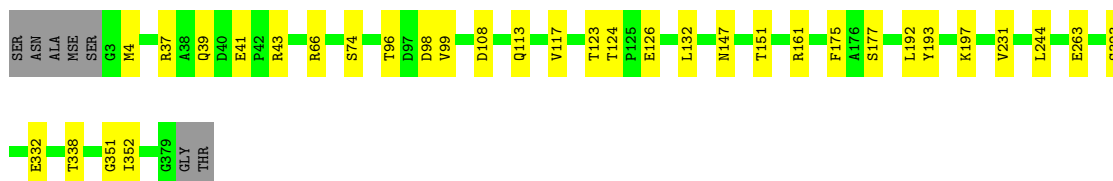
• Molecule 1: CalE6





- 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% .

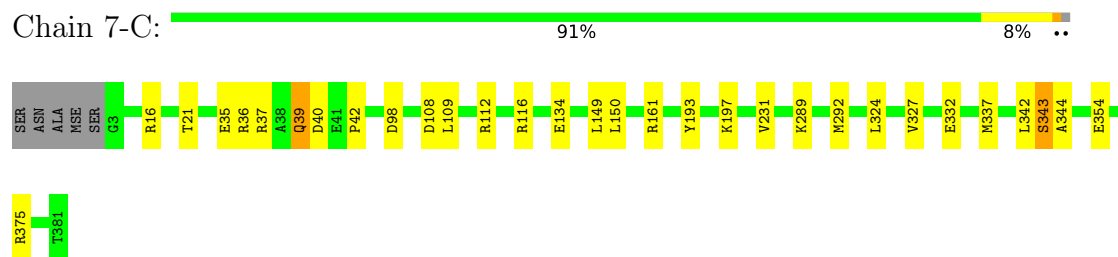


- Molecule 1: CalE6

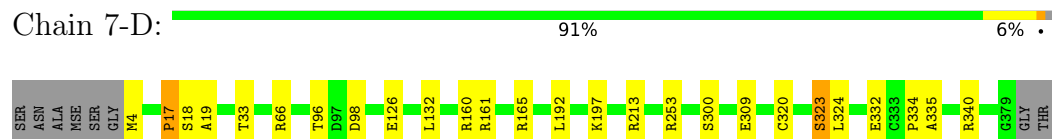
Chain 7-B: 90% 9% .



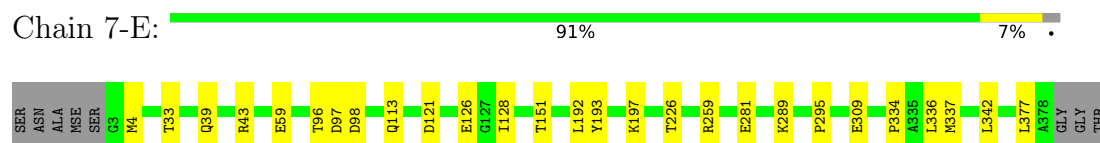
- Molecule 1: CalE6



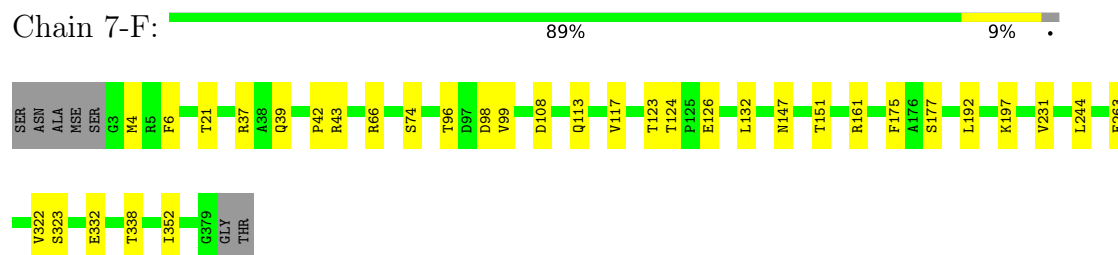
- Molecule 1: CalE6



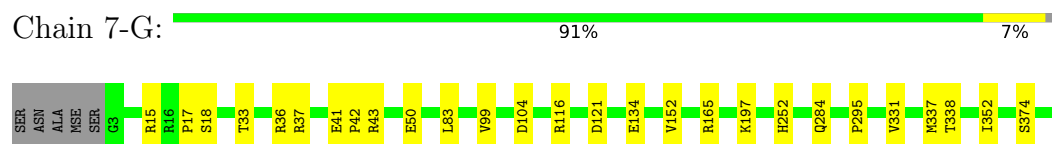
- Molecule 1: CalE6



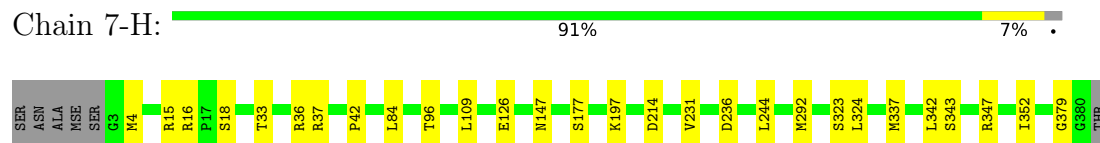
- Molecule 1: CalE6



- Molecule 1: CalE6

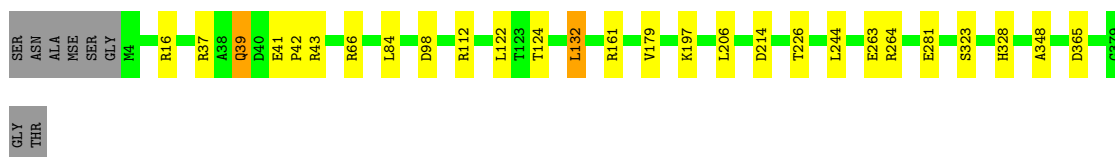


- Molecule 1: CalE6



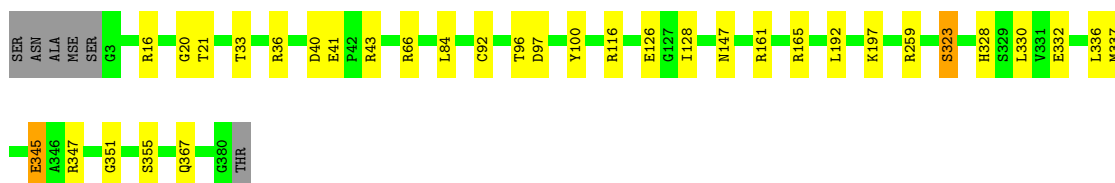
- Molecule 1: CalE6





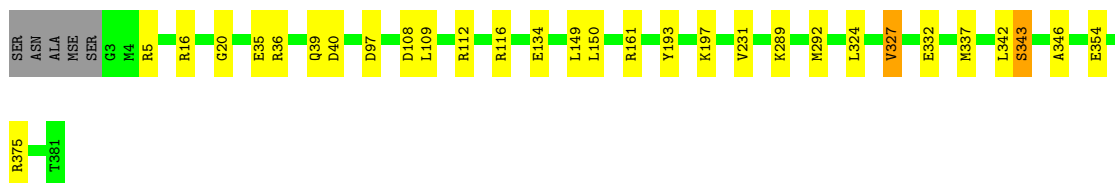
- Molecule 1: CalE6

Chain 8-B: 90% 8% ..



- Molecule 1: CalE6

Chain 8-C: 91% 7% ..



- Molecule 1: CalE6

Chain 8-D: 91% 7% .



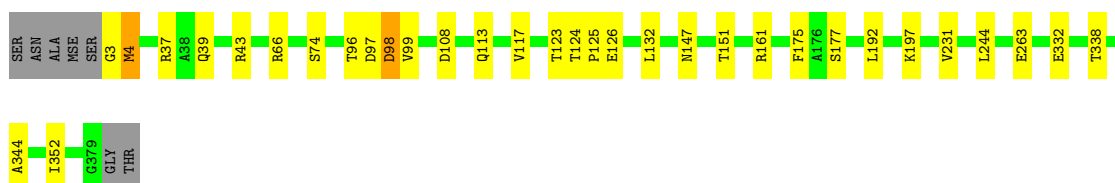
- Molecule 1: CalE6

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% ..



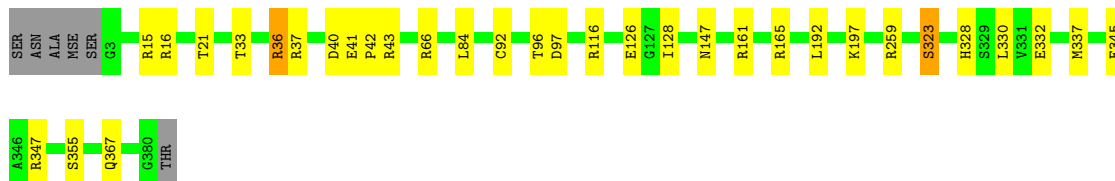
- Molecule 1: CalE6

Chain 9-A:  89% 8% .



- Molecule 1: CalE6

Chain 9-B:  90% 8% ..



- Molecule 1: CalE6

Chain 9-C:  92% 7% .



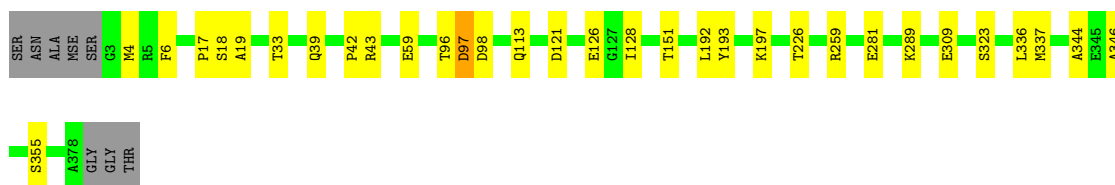
- Molecule 1: CalE6

Chain 9-D:  91% 6% .



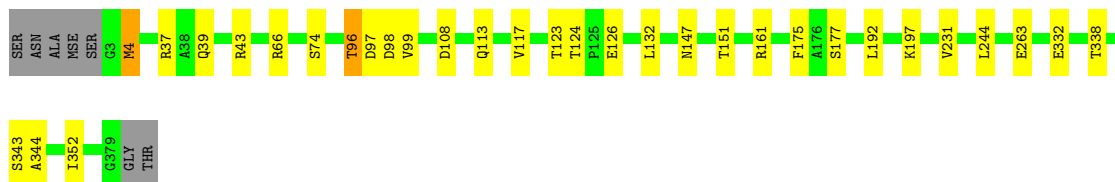
- Molecule 1: CalE6

Chain 9-E:  90% 8% .



- Molecule 1: CalE6

Chain 9-F: 90% 8% ..



- Molecule 1: CalE6

Chain 9-G: 92% 6% .



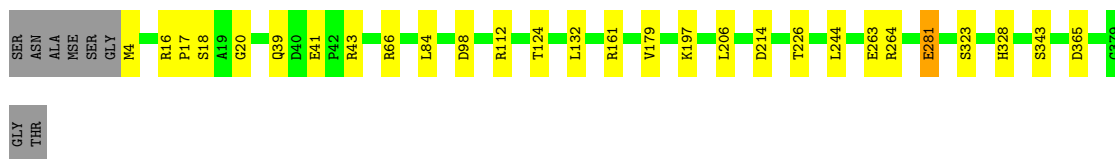
- Molecule 1: CalE6

Chain 9-H: 92% 6% .



- Molecule 1: CalE6

Chain 10-A: 91% 7% .



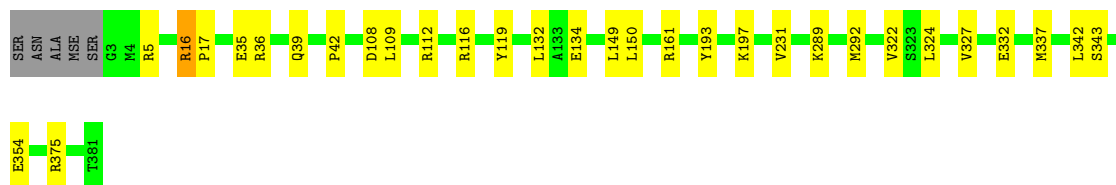
- Molecule 1: CalE6

Chain 10-B: 89% 9% .



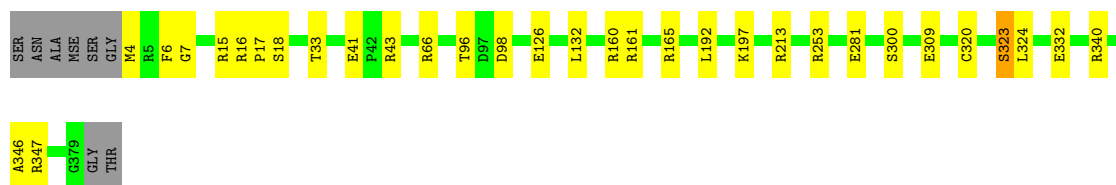
- Molecule 1: CalE6

Chain 10-C:  91% 8% .



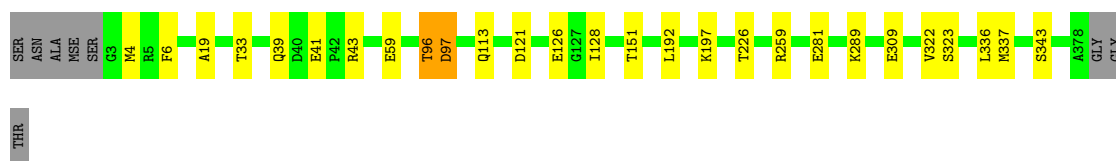
• Molecule 1: CalE6

Chain 10-D:  90% 8% .



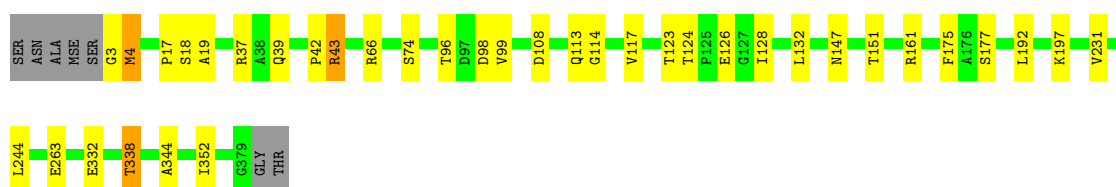
• Molecule 1: CalE6

Chain 10-E:  91% 7% ..



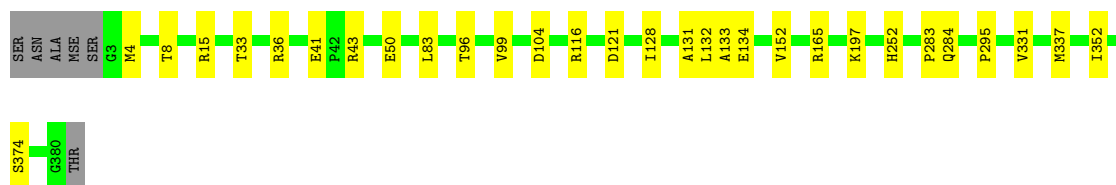
• Molecule 1: CalE6

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.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	10-A	4	MSE	Peptide
1	10-C	193	TYR	Peptide
1	10-D	15	ARG	Peptide
1	10-E	96	THR	Peptide
1	10-F	3	GLY	Peptide
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
1	3-A	193	TYR	Peptide
1	3-B	4	MSE	Peptide
1	3-C	193	TYR	Peptide
1	3-H	193	TYR	Peptide
1	4-B	193	TYR	Peptide
1	4-C	291	GLN	Peptide
1	4-C	4	MSE	Peptide
1	4-E	193	TYR	Peptide
1	5-A	147	ASN	Peptide
1	5-A	193	TYR	Peptide
1	5-A	342	LEU	Peptide
1	5-D	17	PRO	Peptide
1	5-F	193	TYR	Peptide
1	5-G	193	TYR	Peptide
1	6-E	341	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	6-F	193	TYR	Peptide
1	6-G	336	LEU	Peptide
1	7-A	193	TYR	Peptide
1	7-B	193	TYR	Peptide
1	7-C	193	TYR	Peptide
1	7-D	17	PRO	Peptide
1	7-D	340	ARG	Peptide
1	7-E	193	TYR	Peptide
1	7-H	15	ARG	Peptide
1	8-B	336	LEU	Peptide
1	8-C	193	TYR	Peptide
1	8-C	5	ARG	Peptide
1	8-E	193	TYR	Peptide
1	8-E	97	ASP	Peptide
1	8-F	3	GLY	Peptide
1	8-F	97	ASP	Peptide
1	8-H	193	TYR	Peptide
1	9-C	193	TYR	Peptide
1	9-E	193	TYR	Peptide
1	9-F	4	MSE	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
1	2-C	2837	0	2819	0	0
1	2-D	2812	0	2791	0	0
1	2-E	2815	0	2794	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
1	7-E	2815	0	2794	0	0
1	7-F	2812	0	2787	0	0
1	7-G	2814	0	2786	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
2	2-G	12	0	12	0	0
2	2-H	12	0	12	0	0
2	3-A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
2	8-A	12	0	12	0	0
2	8-B	12	0	12	0	0
2	8-C	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	3-C	12	0	16	0	0
3	3-D	12	0	16	0	0
3	3-E	18	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	8-E	18	0	16	0	0
3	8-F	24	0	33	0	0
3	8-G	24	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
4	3-G	1	0	1	0	0
4	3-H	2	0	0	0	0
4	4-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
4	9-A	2	0	8	0	0
4	9-B	1	0	0	0	0
4	9-C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
5	9-G	3	0	1	0	0
5	10-C	3	0	1	0	0
5	10-F	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	5-G	172	0	0	0	0
6	5-H	183	0	0	0	0
6	6-A	179	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
1	1-B	39	GLN
1	1-D	19	ALA
1	1-D	39	GLN
1	1-D	40	ASP
1	1-D	122	LEU
1	1-D	339	HIS
1	1-E	40	ASP
1	1-E	337	MSE
1	1-F	36	ARG
1	1-G	337	MSE
1	1-H	6	PHE
1	1-H	40	ASP
1	1-H	347	ARG
1	2-B	16	ARG
1	2-B	97	ASP
1	2-B	341	PRO
1	2-C	342	LEU
1	2-D	40	ASP
1	2-D	347	ARG
1	2-E	341	PRO
1	3-A	40	ASP
1	3-B	16	ARG
1	3-B	17	PRO
1	3-B	132	LEU
1	3-D	19	ALA
1	3-D	39	GLN
1	3-D	323	SER
1	3-D	348	ALA
1	3-E	36	ARG
1	3-E	37	ARG
1	3-E	40	ASP
1	3-E	97	ASP
1	3-E	343	SER
1	3-F	18	SER
1	3-F	40	ASP
1	3-F	42	PRO
1	3-F	342	LEU
1	3-G	19	ALA

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Mol	Chain	Res	Type
1	3-G	344	ALA
1	3-H	16	ARG
1	3-H	19	ALA
1	3-H	42	PRO
1	3-H	343	SER
1	3-H	344	ALA
1	4-A	5	ARG
1	4-A	6	PHE
1	4-A	323	SER
1	4-B	17	PRO
1	4-B	18	SER
1	4-C	16	ARG
1	4-C	323	SER
1	4-C	342	LEU
1	4-D	6	PHE
1	4-D	18	SER
1	4-D	352	ILE
1	4-E	131	ALA
1	4-E	132	LEU
1	4-E	323	SER
1	4-E	346	ALA
1	4-F	36	ARG
1	4-F	338	THR
1	4-F	342	LEU
1	4-G	131	ALA
1	4-G	132	LEU
1	4-G	323	SER
1	4-G	348	ALA
1	4-G	349	ARG
1	4-H	98	ASP
1	5-A	16	ARG
1	5-A	17	PRO
1	5-A	334	PRO
1	5-A	341	PRO
1	5-B	322	VAL
1	5-B	323	SER
1	5-D	17	PRO
1	5-D	18	SER
1	5-D	41	GLU
1	5-D	295	PRO
1	5-D	338	THR
1	5-D	378	ALA

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Mol	Chain	Res	Type
1	5-E	4	MSE
1	5-E	16	ARG
1	5-E	37	ARG
1	5-E	38	ALA
1	5-E	41	GLU
1	5-E	130	ALA
1	5-F	40	ASP
1	5-F	126	GLU
1	5-F	378	ALA
1	5-G	131	ALA
1	5-G	132	LEU
1	5-G	133	ALA
1	5-H	6	PHE
1	5-H	42	PRO
1	6-A	40	ASP
1	6-B	98	ASP
1	6-C	339	HIS
1	6-D	19	ALA
1	6-D	37	ARG
1	6-D	97	ASP
1	6-D	351	GLY
1	6-E	342	LEU
1	6-E	343	SER
1	6-E	346	ALA
1	6-G	323	SER
1	6-H	322	VAL
1	7-B	20	GLY
1	7-C	21	THR
1	7-C	39	GLN
1	7-C	40	ASP
1	7-D	323	SER
1	7-E	295	PRO
1	7-E	377	LEU
1	7-F	21	THR
1	7-G	17	PRO
1	7-G	18	SER
1	7-G	295	PRO
1	8-C	40	ASP
1	8-C	343	SER
1	8-C	346	ALA
1	8-D	18	SER
1	8-D	42	PRO

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Mol	Chain	Res	Type
1	8-D	342	LEU
1	8-D	343	SER
1	8-E	323	SER
1	8-G	20	GLY
1	8-G	338	THR
1	8-G	343	SER
1	8-H	4	MSE
1	8-H	38	ALA
1	8-H	323	SER
1	9-A	98	ASP
1	9-A	131	ALA
1	9-B	37	ARG
1	9-C	119	TYR
1	9-D	17	PRO
1	9-D	43	ARG
1	9-D	98	ASP
1	9-D	343	SER
1	9-D	347	ARG
1	9-E	17	PRO
1	9-E	18	SER
1	9-E	42	PRO
1	9-E	97	ASP
1	9-E	98	ASP
1	9-E	355	SER
1	9-F	344	ALA
1	9-G	337	MSE
1	9-H	40	ASP
1	10-A	17	PRO
1	10-A	281	GLU
1	10-B	18	SER
1	10-C	16	ARG
1	10-C	17	PRO
1	10-C	132	LEU
1	10-D	6	PHE
1	10-D	7	GLY
1	10-D	323	SER
1	10-D	347	ARG
1	10-E	41	GLU
1	10-E	323	SER
1	10-F	4	MSE
1	10-F	42	PRO
1	10-F	344	ALA

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Mol	Chain	Res	Type
1	10-G	131	ALA
1	10-G	132	LEU
1	10-G	295	PRO
1	10-H	97	ASP
1	1-A	5	ARG
1	1-B	41	GLU
1	1-B	346	ALA
1	1-D	37	ARG
1	1-D	338	THR
1	1-E	19	ALA
1	1-E	43	ARG
1	1-E	126	GLU
1	1-F	37	ARG
1	1-G	99	VAL
1	1-G	132	LEU
1	2-D	41	GLU
1	2-D	42	PRO
1	2-D	323	SER
1	2-D	346	ALA
1	2-E	97	ASP
1	2-E	346	ALA
1	2-F	37	ARG
1	2-H	19	ALA
1	2-H	42	PRO
1	2-H	97	ASP
1	2-H	323	SER
1	3-C	44	TYR
1	3-E	346	ALA
1	3-F	343	SER
1	3-F	349	ARG
1	3-G	5	ARG
1	4-B	16	ARG
1	4-C	20	GLY
1	4-C	42	PRO
1	4-D	323	SER
1	4-E	19	ALA
1	4-E	345	GLU
1	4-F	43	ARG
1	4-G	97	ASP
1	4-G	338	THR
1	4-H	323	SER
1	4-H	379	GLY

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Mol	Chain	Res	Type
1	5-A	38	ALA
1	5-A	132	LEU
1	5-B	290	ALA
1	5-C	96	THR
1	5-E	40	ASP
1	5-E	346	ALA
1	5-G	323	SER
1	5-H	323	SER
1	6-B	96	THR
1	6-D	36	ARG
1	6-D	349	ARG
1	6-E	20	GLY
1	6-E	97	ASP
1	6-G	122	LEU
1	6-H	37	ARG
1	7-A	99	VAL
1	7-B	5	ARG
1	7-D	19	ALA
1	7-F	322	VAL
1	7-G	37	ARG
1	7-H	379	GLY
1	8-A	39	GLN
1	8-B	100	TYR
1	8-B	345	GLU
1	8-B	351	GLY
1	8-C	20	GLY
1	8-D	17	PRO
1	8-E	40	ASP
1	8-E	42	PRO
1	8-F	98	ASP
1	8-F	344	ALA
1	8-H	5	ARG
1	9-A	128	ILE
1	9-A	343	SER
1	9-D	352	ILE
1	9-E	19	ALA
1	9-E	323	SER
1	9-G	101	ALA
1	9-H	343	SER
1	10-A	18	SER
1	10-A	20	GLY
1	10-B	137	LEU

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Mol	Chain	Res	Type
1	10-B	343	SER
1	10-C	119	TYR
1	10-D	17	PRO
1	10-F	17	PRO
1	10-F	43	ARG
1	10-F	338	THR
1	10-G	8	THR
1	10-H	40	ASP
1	10-H	98	ASP
1	1-C	17	PRO
1	1-C	19	ALA
1	1-C	339	HIS
1	1-C	342	LEU
1	1-D	343	SER
1	1-G	20	GLY
1	2-A	42	PRO
1	2-A	98	ASP
1	2-A	323	SER
1	2-B	137	LEU
1	2-B	338	THR
1	2-C	40	ASP
1	2-C	119	TYR
1	2-C	349	ARG
1	2-D	97	ASP
1	2-D	337	MSE
1	2-E	340	ARG
1	2-E	351	GLY
1	2-G	43	ARG
1	2-G	323	SER
1	3-A	342	LEU
1	3-B	131	ALA
1	3-B	341	PRO
1	3-C	379	GLY
1	3-F	121	ASP
1	3-F	125	PRO
1	3-F	335	ALA
1	3-H	6	PHE
1	4-B	283	PRO
1	4-C	17	PRO
1	4-E	6	PHE
1	4-F	19	ALA
1	4-F	97	ASP

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Mol	Chain	Res	Type
1	4-F	339	HIS
1	4-F	344	ALA
1	5-A	39	GLN
1	5-B	175	PHE
1	5-E	132	LEU
1	5-E	341	PRO
1	5-F	97	ASP
1	5-G	283	PRO
1	5-G	350	ARG
1	6-A	5	ARG
1	6-D	41	GLU
1	6-D	323	SER
1	6-G	43	ARG
1	7-A	338	THR
1	7-B	137	LEU
1	7-C	98	ASP
1	7-C	343	SER
1	7-C	344	ALA
1	7-D	18	SER
1	7-D	335	ALA
1	7-E	98	ASP
1	7-E	342	LEU
1	7-G	338	THR
1	7-H	37	ARG
1	7-H	42	PRO
1	8-A	132	LEU
1	8-B	323	SER
1	8-D	340	ARG
1	8-F	4	MSE
1	8-F	125	PRO
1	8-G	341	PRO
1	9-A	20	GLY
1	9-A	40	ASP
1	9-A	126	GLU
1	9-A	291	GLN
1	9-B	42	PRO
1	9-E	344	ALA
1	9-F	343	SER
1	9-G	349	ARG
1	10-A	343	SER
1	10-C	5	ARG
1	10-D	18	SER

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Mol	Chain	Res	Type
1	10-E	6	PHE
1	10-E	97	ASP
1	10-F	18	SER
1	10-F	19	ALA
1	1-D	7	GLY
1	1-D	127	GLY
1	1-E	336	LEU
1	1-F	114	GLY
1	1-F	351	GLY
1	2-E	39	GLN
1	2-H	40	ASP
1	3-A	131	ALA
1	3-C	309	GLU
1	3-F	337	MSE
1	3-G	98	ASP
1	4-B	126	GLU
1	5-F	133	ALA
1	5-G	349	ARG
1	6-A	17	PRO
1	6-C	40	ASP
1	6-D	20	GLY
1	6-D	39	GLN
1	6-F	41	GLU
1	6-F	323	SER
1	6-H	5	ARG
1	6-H	42	PRO
1	7-A	6	PHE
1	7-A	42	PRO
1	7-C	37	ARG
1	7-C	42	PRO
1	7-D	334	PRO
1	7-F	323	SER
1	8-A	42	PRO
1	8-A	122	LEU
1	8-G	16	ARG
1	8-G	19	ALA
1	9-B	15	ARG
1	9-B	323	SER
1	9-E	6	PHE
1	9-E	346	ALA
1	10-B	125	PRO
1	10-C	42	PRO

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Mol	Chain	Res	Type
1	10-D	346	ALA
1	10-E	19	ALA
1	10-F	114	GLY
1	10-G	4	MSE
1	10-G	96	THR
1	10-G	133	ALA
1	1-C	338	THR
1	1-D	35	GLU
1	1-D	126	GLU
1	1-G	42	PRO
1	1-G	131	ALA
1	1-H	19	ALA
1	2-B	18	SER
1	2-F	97	ASP
1	2-F	340	ARG
1	3-B	125	PRO
1	3-B	137	LEU
1	3-C	378	ALA
1	3-D	38	ALA
1	3-E	323	SER
1	3-G	335	ALA
1	4-D	42	PRO
1	4-E	100	TYR
1	4-F	18	SER
1	4-F	40	ASP
1	5-A	130	ALA
1	5-E	42	PRO
1	6-A	352	ILE
1	6-D	280	PRO
1	7-B	323	SER
1	7-D	17	PRO
1	8-A	37	ARG
1	8-E	96	THR
1	9-A	42	PRO
1	9-A	127	GLY
1	9-B	36	ARG
1	9-F	97	ASP
1	9-G	340	ARG
1	10-B	97	ASP
1	10-B	338	THR
1	10-D	43	ARG
1	10-D	340	ARG

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Mol	Chain	Res	Type
1	10-E	343	SER
1	1-A	244	LEU
1	1-B	16	ARG
1	1-G	322	VAL
1	2-H	187	GLY
1	3-B	323	SER
1	3-C	17	PRO
1	3-H	306	GLY
1	4-A	37	ARG
1	5-E	115	VAL
1	5-F	38	ALA
1	6-A	97	ASP
1	6-B	16	ARG
1	6-C	18	SER
1	6-F	351	GLY
1	6-G	18	SER
1	6-H	89	PRO
1	7-F	6	PHE
1	7-F	42	PRO
1	7-G	42	PRO
1	8-A	348	ALA
1	8-C	97	ASP
1	8-E	6	PHE
1	9-F	96	THR
1	10-D	41	GLU
1	10-D	281	GLU
1	1-H	305	GLY
1	3-A	305	GLY
1	3-F	17	PRO
1	5-E	322	VAL
1	6-A	166	GLY
1	8-B	20	GLY
1	10-D	16	ARG
1	10-E	322	VAL
1	10-G	283	PRO
1	1-A	41	GLU
1	1-H	17	PRO
1	3-E	17	PRO
1	4-D	99	VAL
1	5-H	114	GLY
1	2-G	115	VAL
1	3-D	283	PRO

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Mol	Chain	Res	Type
1	3-E	42	PRO
1	5-D	280	PRO
1	5-F	127	GLY
1	7-A	322	VAL
1	8-C	327	VAL
1	10-F	128	ILE
1	1-C	295	PRO
1	2-F	322	VAL
1	3-D	17	PRO
1	3-D	334	PRO
1	4-B	125	PRO
1	8-D	199	ILE
1	9-A	334	PRO
1	10-C	322	VAL
1	10-G	128	ILE
1	1-C	322	VAL
1	2-A	99	VAL
1	3-H	20	GLY
1	4-B	42	PRO
1	5-H	340	ARG
1	7-A	16	ARG
1	7-E	334	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (1839) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	16	ARG
1	1-A	39	GLN
1	1-A	41	GLU
1	1-A	43	ARG
1	1-A	66	ARG
1	1-A	84	LEU
1	1-A	98	ASP
1	1-A	112	ARG
1	1-A	124	THR
1	1-A	132	LEU
1	1-A	161	ARG
1	1-A	179	VAL
1	1-A	206	LEU
1	1-A	214	ASP
1	1-A	226	THR
1	1-A	244	LEU
1	1-A	263	GLU
1	1-A	264	ARG
1	1-A	281	GLU
1	1-A	323	SER
1	1-A	328	HIS
1	1-A	365	ASP

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Mol	Chain	Res	Type
1	1-B	16	ARG
1	1-B	21	THR
1	1-B	33	THR
1	1-B	36	ARG
1	1-B	40	ASP
1	1-B	41	GLU
1	1-B	43	ARG
1	1-B	66	ARG
1	1-B	84	LEU
1	1-B	92	CYS
1	1-B	96	THR
1	1-B	97	ASP
1	1-B	116	ARG
1	1-B	126	GLU
1	1-B	128	ILE
1	1-B	147	ASN
1	1-B	161	ARG
1	1-B	165	ARG
1	1-B	192	LEU
1	1-B	259	ARG
1	1-B	323	SER
1	1-B	328	HIS
1	1-B	330	LEU
1	1-B	332	GLU
1	1-B	337	MSE
1	1-B	345	GLU
1	1-B	347	ARG
1	1-B	355	SER
1	1-B	367	GLN
1	1-C	16	ARG
1	1-C	35	GLU
1	1-C	36	ARG
1	1-C	39	GLN
1	1-C	108	ASP
1	1-C	109	LEU
1	1-C	112	ARG
1	1-C	116	ARG
1	1-C	134	GLU
1	1-C	149	LEU
1	1-C	150	LEU
1	1-C	161	ARG
1	1-C	231	VAL

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Mol	Chain	Res	Type
1	1-C	289	LYS
1	1-C	292	MSE
1	1-C	324	LEU
1	1-C	327	VAL
1	1-C	332	GLU
1	1-C	337	MSE
1	1-C	342	LEU
1	1-C	343	SER
1	1-C	354	GLU
1	1-C	375	ARG
1	1-D	4	MSE
1	1-D	33	THR
1	1-D	66	ARG
1	1-D	96	THR
1	1-D	98	ASP
1	1-D	126	GLU
1	1-D	132	LEU
1	1-D	160	ARG
1	1-D	161	ARG
1	1-D	165	ARG
1	1-D	192	LEU
1	1-D	213	ARG
1	1-D	253	ARG
1	1-D	300	SER
1	1-D	309	GLU
1	1-D	320	CYS
1	1-D	323	SER
1	1-D	324	LEU
1	1-D	332	GLU
1	1-E	4	MSE
1	1-E	33	THR
1	1-E	39	GLN
1	1-E	43	ARG
1	1-E	59	GLU
1	1-E	96	THR
1	1-E	97	ASP
1	1-E	121	ASP
1	1-E	126	GLU
1	1-E	128	ILE
1	1-E	151	THR
1	1-E	192	LEU
1	1-E	226	THR

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Mol	Chain	Res	Type
1	1-E	259	ARG
1	1-E	281	GLU
1	1-E	289	LYS
1	1-E	309	GLU
1	1-E	336	LEU
1	1-E	337	MSE
1	1-F	4	MSE
1	1-F	37	ARG
1	1-F	39	GLN
1	1-F	43	ARG
1	1-F	66	ARG
1	1-F	74	SER
1	1-F	96	THR
1	1-F	98	ASP
1	1-F	99	VAL
1	1-F	108	ASP
1	1-F	113	GLN
1	1-F	117	VAL
1	1-F	123	THR
1	1-F	124	THR
1	1-F	126	GLU
1	1-F	132	LEU
1	1-F	147	ASN
1	1-F	151	THR
1	1-F	161	ARG
1	1-F	175	PHE
1	1-F	177	SER
1	1-F	192	LEU
1	1-F	231	VAL
1	1-F	244	LEU
1	1-F	263	GLU
1	1-F	332	GLU
1	1-F	338	THR
1	1-F	352	ILE
1	1-G	15	ARG
1	1-G	33	THR
1	1-G	36	ARG
1	1-G	41	GLU
1	1-G	43	ARG
1	1-G	50	GLU
1	1-G	83	LEU
1	1-G	99	VAL

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Mol	Chain	Res	Type
1	1-G	104	ASP
1	1-G	116	ARG
1	1-G	121	ASP
1	1-G	134	GLU
1	1-G	152	VAL
1	1-G	165	ARG
1	1-G	252	HIS
1	1-G	284	GLN
1	1-G	331	VAL
1	1-G	337	MSE
1	1-G	352	ILE
1	1-G	374	SER
1	1-H	4	MSE
1	1-H	16	ARG
1	1-H	18	SER
1	1-H	33	THR
1	1-H	36	ARG
1	1-H	84	LEU
1	1-H	96	THR
1	1-H	109	LEU
1	1-H	126	GLU
1	1-H	147	ASN
1	1-H	177	SER
1	1-H	214	ASP
1	1-H	231	VAL
1	1-H	236	ASP
1	1-H	244	LEU
1	1-H	292	MSE
1	1-H	323	SER
1	1-H	324	LEU
1	1-H	337	MSE
1	1-H	342	LEU
1	1-H	343	SER
1	1-H	347	ARG
1	1-H	352	ILE
1	2-A	16	ARG
1	2-A	39	GLN
1	2-A	41	GLU
1	2-A	43	ARG
1	2-A	66	ARG
1	2-A	84	LEU
1	2-A	98	ASP

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Mol	Chain	Res	Type
1	2-A	112	ARG
1	2-A	124	THR
1	2-A	132	LEU
1	2-A	161	ARG
1	2-A	179	VAL
1	2-A	206	LEU
1	2-A	214	ASP
1	2-A	226	THR
1	2-A	244	LEU
1	2-A	263	GLU
1	2-A	264	ARG
1	2-A	281	GLU
1	2-A	323	SER
1	2-A	328	HIS
1	2-A	365	ASP
1	2-B	16	ARG
1	2-B	21	THR
1	2-B	33	THR
1	2-B	36	ARG
1	2-B	40	ASP
1	2-B	41	GLU
1	2-B	43	ARG
1	2-B	66	ARG
1	2-B	84	LEU
1	2-B	92	CYS
1	2-B	96	THR
1	2-B	97	ASP
1	2-B	116	ARG
1	2-B	126	GLU
1	2-B	128	ILE
1	2-B	147	ASN
1	2-B	161	ARG
1	2-B	165	ARG
1	2-B	192	LEU
1	2-B	259	ARG
1	2-B	323	SER
1	2-B	328	HIS
1	2-B	330	LEU
1	2-B	332	GLU
1	2-B	337	MSE
1	2-B	345	GLU
1	2-B	347	ARG

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Mol	Chain	Res	Type
1	2-B	355	SER
1	2-B	367	GLN
1	2-C	16	ARG
1	2-C	35	GLU
1	2-C	36	ARG
1	2-C	39	GLN
1	2-C	108	ASP
1	2-C	109	LEU
1	2-C	112	ARG
1	2-C	116	ARG
1	2-C	134	GLU
1	2-C	149	LEU
1	2-C	150	LEU
1	2-C	161	ARG
1	2-C	231	VAL
1	2-C	289	LYS
1	2-C	292	MSE
1	2-C	324	LEU
1	2-C	327	VAL
1	2-C	332	GLU
1	2-C	337	MSE
1	2-C	342	LEU
1	2-C	343	SER
1	2-C	354	GLU
1	2-C	375	ARG
1	2-D	4	MSE
1	2-D	33	THR
1	2-D	66	ARG
1	2-D	96	THR
1	2-D	98	ASP
1	2-D	126	GLU
1	2-D	132	LEU
1	2-D	160	ARG
1	2-D	161	ARG
1	2-D	165	ARG
1	2-D	192	LEU
1	2-D	213	ARG
1	2-D	253	ARG
1	2-D	300	SER
1	2-D	309	GLU
1	2-D	320	CYS
1	2-D	323	SER

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Mol	Chain	Res	Type
1	2-D	324	LEU
1	2-D	332	GLU
1	2-E	4	MSE
1	2-E	33	THR
1	2-E	39	GLN
1	2-E	43	ARG
1	2-E	59	GLU
1	2-E	96	THR
1	2-E	97	ASP
1	2-E	113	GLN
1	2-E	121	ASP
1	2-E	126	GLU
1	2-E	128	ILE
1	2-E	151	THR
1	2-E	192	LEU
1	2-E	226	THR
1	2-E	259	ARG
1	2-E	281	GLU
1	2-E	289	LYS
1	2-E	309	GLU
1	2-E	336	LEU
1	2-E	337	MSE
1	2-F	4	MSE
1	2-F	37	ARG
1	2-F	39	GLN
1	2-F	43	ARG
1	2-F	66	ARG
1	2-F	74	SER
1	2-F	96	THR
1	2-F	98	ASP
1	2-F	99	VAL
1	2-F	108	ASP
1	2-F	113	GLN
1	2-F	117	VAL
1	2-F	123	THR
1	2-F	124	THR
1	2-F	126	GLU
1	2-F	132	LEU
1	2-F	147	ASN
1	2-F	151	THR
1	2-F	161	ARG
1	2-F	175	PHE

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Mol	Chain	Res	Type
1	2-F	177	SER
1	2-F	192	LEU
1	2-F	231	VAL
1	2-F	244	LEU
1	2-F	263	GLU
1	2-F	332	GLU
1	2-F	338	THR
1	2-F	352	ILE
1	2-G	15	ARG
1	2-G	33	THR
1	2-G	36	ARG
1	2-G	41	GLU
1	2-G	43	ARG
1	2-G	50	GLU
1	2-G	83	LEU
1	2-G	99	VAL
1	2-G	104	ASP
1	2-G	116	ARG
1	2-G	121	ASP
1	2-G	134	GLU
1	2-G	152	VAL
1	2-G	165	ARG
1	2-G	252	HIS
1	2-G	284	GLN
1	2-G	331	VAL
1	2-G	337	MSE
1	2-G	352	ILE
1	2-G	374	SER
1	2-H	4	MSE
1	2-H	16	ARG
1	2-H	18	SER
1	2-H	33	THR
1	2-H	36	ARG
1	2-H	84	LEU
1	2-H	96	THR
1	2-H	109	LEU
1	2-H	126	GLU
1	2-H	147	ASN
1	2-H	177	SER
1	2-H	214	ASP
1	2-H	231	VAL
1	2-H	236	ASP

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Mol	Chain	Res	Type
1	2-H	244	LEU
1	2-H	292	MSE
1	2-H	323	SER
1	2-H	324	LEU
1	2-H	337	MSE
1	2-H	342	LEU
1	2-H	343	SER
1	2-H	347	ARG
1	2-H	352	ILE
1	3-A	16	ARG
1	3-A	39	GLN
1	3-A	41	GLU
1	3-A	43	ARG
1	3-A	66	ARG
1	3-A	84	LEU
1	3-A	98	ASP
1	3-A	112	ARG
1	3-A	124	THR
1	3-A	132	LEU
1	3-A	161	ARG
1	3-A	179	VAL
1	3-A	206	LEU
1	3-A	214	ASP
1	3-A	226	THR
1	3-A	244	LEU
1	3-A	263	GLU
1	3-A	264	ARG
1	3-A	281	GLU
1	3-A	323	SER
1	3-A	328	HIS
1	3-A	365	ASP
1	3-B	16	ARG
1	3-B	21	THR
1	3-B	33	THR
1	3-B	36	ARG
1	3-B	40	ASP
1	3-B	41	GLU
1	3-B	43	ARG
1	3-B	66	ARG
1	3-B	84	LEU
1	3-B	92	CYS
1	3-B	96	THR

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Mol	Chain	Res	Type
1	3-B	97	ASP
1	3-B	116	ARG
1	3-B	126	GLU
1	3-B	128	ILE
1	3-B	147	ASN
1	3-B	161	ARG
1	3-B	165	ARG
1	3-B	192	LEU
1	3-B	259	ARG
1	3-B	323	SER
1	3-B	328	HIS
1	3-B	330	LEU
1	3-B	332	GLU
1	3-B	337	MSE
1	3-B	345	GLU
1	3-B	347	ARG
1	3-B	355	SER
1	3-B	367	GLN
1	3-C	16	ARG
1	3-C	35	GLU
1	3-C	36	ARG
1	3-C	39	GLN
1	3-C	108	ASP
1	3-C	109	LEU
1	3-C	112	ARG
1	3-C	116	ARG
1	3-C	134	GLU
1	3-C	149	LEU
1	3-C	150	LEU
1	3-C	161	ARG
1	3-C	231	VAL
1	3-C	289	LYS
1	3-C	292	MSE
1	3-C	324	LEU
1	3-C	327	VAL
1	3-C	332	GLU
1	3-C	337	MSE
1	3-C	342	LEU
1	3-C	343	SER
1	3-C	354	GLU
1	3-C	375	ARG
1	3-D	4	MSE

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Mol	Chain	Res	Type
1	3-D	33	THR
1	3-D	66	ARG
1	3-D	96	THR
1	3-D	98	ASP
1	3-D	126	GLU
1	3-D	132	LEU
1	3-D	160	ARG
1	3-D	161	ARG
1	3-D	165	ARG
1	3-D	192	LEU
1	3-D	213	ARG
1	3-D	253	ARG
1	3-D	300	SER
1	3-D	309	GLU
1	3-D	320	CYS
1	3-D	323	SER
1	3-D	324	LEU
1	3-D	332	GLU
1	3-E	4	MSE
1	3-E	33	THR
1	3-E	39	GLN
1	3-E	43	ARG
1	3-E	59	GLU
1	3-E	96	THR
1	3-E	97	ASP
1	3-E	113	GLN
1	3-E	121	ASP
1	3-E	126	GLU
1	3-E	128	ILE
1	3-E	151	THR
1	3-E	192	LEU
1	3-E	226	THR
1	3-E	259	ARG
1	3-E	281	GLU
1	3-E	289	LYS
1	3-E	309	GLU
1	3-E	336	LEU
1	3-E	337	MSE
1	3-F	4	MSE
1	3-F	37	ARG
1	3-F	39	GLN
1	3-F	43	ARG

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Mol	Chain	Res	Type
1	3-F	66	ARG
1	3-F	74	SER
1	3-F	96	THR
1	3-F	98	ASP
1	3-F	99	VAL
1	3-F	108	ASP
1	3-F	113	GLN
1	3-F	117	VAL
1	3-F	123	THR
1	3-F	124	THR
1	3-F	126	GLU
1	3-F	132	LEU
1	3-F	147	ASN
1	3-F	151	THR
1	3-F	161	ARG
1	3-F	175	PHE
1	3-F	177	SER
1	3-F	192	LEU
1	3-F	231	VAL
1	3-F	244	LEU
1	3-F	263	GLU
1	3-F	332	GLU
1	3-F	338	THR
1	3-F	352	ILE
1	3-G	15	ARG
1	3-G	33	THR
1	3-G	36	ARG
1	3-G	41	GLU
1	3-G	43	ARG
1	3-G	50	GLU
1	3-G	83	LEU
1	3-G	99	VAL
1	3-G	104	ASP
1	3-G	116	ARG
1	3-G	121	ASP
1	3-G	134	GLU
1	3-G	152	VAL
1	3-G	165	ARG
1	3-G	252	HIS
1	3-G	284	GLN
1	3-G	331	VAL
1	3-G	337	MSE

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Mol	Chain	Res	Type
1	3-G	352	ILE
1	3-G	374	SER
1	3-H	4	MSE
1	3-H	16	ARG
1	3-H	18	SER
1	3-H	33	THR
1	3-H	36	ARG
1	3-H	84	LEU
1	3-H	96	THR
1	3-H	109	LEU
1	3-H	126	GLU
1	3-H	147	ASN
1	3-H	177	SER
1	3-H	214	ASP
1	3-H	231	VAL
1	3-H	236	ASP
1	3-H	244	LEU
1	3-H	292	MSE
1	3-H	323	SER
1	3-H	324	LEU
1	3-H	337	MSE
1	3-H	342	LEU
1	3-H	343	SER
1	3-H	347	ARG
1	3-H	352	ILE
1	4-A	16	ARG
1	4-A	39	GLN
1	4-A	41	GLU
1	4-A	43	ARG
1	4-A	66	ARG
1	4-A	84	LEU
1	4-A	98	ASP
1	4-A	112	ARG
1	4-A	124	THR
1	4-A	132	LEU
1	4-A	161	ARG
1	4-A	179	VAL
1	4-A	206	LEU
1	4-A	214	ASP
1	4-A	226	THR
1	4-A	244	LEU
1	4-A	263	GLU

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Mol	Chain	Res	Type
1	4-A	264	ARG
1	4-A	281	GLU
1	4-A	323	SER
1	4-A	328	HIS
1	4-A	365	ASP
1	4-B	16	ARG
1	4-B	21	THR
1	4-B	33	THR
1	4-B	36	ARG
1	4-B	40	ASP
1	4-B	41	GLU
1	4-B	43	ARG
1	4-B	66	ARG
1	4-B	84	LEU
1	4-B	92	CYS
1	4-B	96	THR
1	4-B	97	ASP
1	4-B	116	ARG
1	4-B	126	GLU
1	4-B	128	ILE
1	4-B	147	ASN
1	4-B	161	ARG
1	4-B	165	ARG
1	4-B	192	LEU
1	4-B	259	ARG
1	4-B	323	SER
1	4-B	328	HIS
1	4-B	330	LEU
1	4-B	332	GLU
1	4-B	337	MSE
1	4-B	345	GLU
1	4-B	347	ARG
1	4-B	355	SER
1	4-B	367	GLN
1	4-C	16	ARG
1	4-C	35	GLU
1	4-C	36	ARG
1	4-C	39	GLN
1	4-C	108	ASP
1	4-C	109	LEU
1	4-C	112	ARG
1	4-C	116	ARG

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Mol	Chain	Res	Type
1	4-C	134	GLU
1	4-C	149	LEU
1	4-C	150	LEU
1	4-C	161	ARG
1	4-C	231	VAL
1	4-C	289	LYS
1	4-C	292	MSE
1	4-C	324	LEU
1	4-C	327	VAL
1	4-C	332	GLU
1	4-C	337	MSE
1	4-C	342	LEU
1	4-C	343	SER
1	4-C	354	GLU
1	4-C	375	ARG
1	4-D	4	MSE
1	4-D	33	THR
1	4-D	66	ARG
1	4-D	96	THR
1	4-D	98	ASP
1	4-D	126	GLU
1	4-D	132	LEU
1	4-D	160	ARG
1	4-D	161	ARG
1	4-D	165	ARG
1	4-D	192	LEU
1	4-D	213	ARG
1	4-D	253	ARG
1	4-D	300	SER
1	4-D	309	GLU
1	4-D	320	CYS
1	4-D	323	SER
1	4-D	324	LEU
1	4-D	332	GLU
1	4-E	4	MSE
1	4-E	33	THR
1	4-E	39	GLN
1	4-E	43	ARG
1	4-E	59	GLU
1	4-E	96	THR
1	4-E	97	ASP
1	4-E	113	GLN

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Mol	Chain	Res	Type
1	4-E	121	ASP
1	4-E	126	GLU
1	4-E	128	ILE
1	4-E	151	THR
1	4-E	192	LEU
1	4-E	226	THR
1	4-E	259	ARG
1	4-E	281	GLU
1	4-E	289	LYS
1	4-E	309	GLU
1	4-E	336	LEU
1	4-E	337	MSE
1	4-F	4	MSE
1	4-F	37	ARG
1	4-F	39	GLN
1	4-F	43	ARG
1	4-F	66	ARG
1	4-F	74	SER
1	4-F	96	THR
1	4-F	98	ASP
1	4-F	99	VAL
1	4-F	108	ASP
1	4-F	113	GLN
1	4-F	117	VAL
1	4-F	123	THR
1	4-F	124	THR
1	4-F	126	GLU
1	4-F	132	LEU
1	4-F	147	ASN
1	4-F	151	THR
1	4-F	161	ARG
1	4-F	175	PHE
1	4-F	177	SER
1	4-F	192	LEU
1	4-F	231	VAL
1	4-F	244	LEU
1	4-F	263	GLU
1	4-F	332	GLU
1	4-F	338	THR
1	4-F	352	ILE
1	4-G	15	ARG
1	4-G	33	THR

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Mol	Chain	Res	Type
1	4-G	36	ARG
1	4-G	41	GLU
1	4-G	43	ARG
1	4-G	50	GLU
1	4-G	83	LEU
1	4-G	99	VAL
1	4-G	104	ASP
1	4-G	116	ARG
1	4-G	121	ASP
1	4-G	134	GLU
1	4-G	152	VAL
1	4-G	165	ARG
1	4-G	252	HIS
1	4-G	284	GLN
1	4-G	331	VAL
1	4-G	337	MSE
1	4-G	352	ILE
1	4-G	374	SER
1	4-H	4	MSE
1	4-H	16	ARG
1	4-H	18	SER
1	4-H	33	THR
1	4-H	36	ARG
1	4-H	84	LEU
1	4-H	96	THR
1	4-H	109	LEU
1	4-H	126	GLU
1	4-H	147	ASN
1	4-H	177	SER
1	4-H	214	ASP
1	4-H	231	VAL
1	4-H	236	ASP
1	4-H	244	LEU
1	4-H	292	MSE
1	4-H	323	SER
1	4-H	324	LEU
1	4-H	337	MSE
1	4-H	342	LEU
1	4-H	343	SER
1	4-H	347	ARG
1	4-H	352	ILE
1	5-A	16	ARG

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Mol	Chain	Res	Type
1	5-A	39	GLN
1	5-A	41	GLU
1	5-A	43	ARG
1	5-A	66	ARG
1	5-A	84	LEU
1	5-A	98	ASP
1	5-A	112	ARG
1	5-A	124	THR
1	5-A	132	LEU
1	5-A	161	ARG
1	5-A	179	VAL
1	5-A	206	LEU
1	5-A	214	ASP
1	5-A	226	THR
1	5-A	244	LEU
1	5-A	263	GLU
1	5-A	264	ARG
1	5-A	281	GLU
1	5-A	323	SER
1	5-A	328	HIS
1	5-A	365	ASP
1	5-B	16	ARG
1	5-B	21	THR
1	5-B	33	THR
1	5-B	36	ARG
1	5-B	40	ASP
1	5-B	41	GLU
1	5-B	43	ARG
1	5-B	66	ARG
1	5-B	84	LEU
1	5-B	92	CYS
1	5-B	96	THR
1	5-B	97	ASP
1	5-B	116	ARG
1	5-B	126	GLU
1	5-B	128	ILE
1	5-B	147	ASN
1	5-B	161	ARG
1	5-B	165	ARG
1	5-B	192	LEU
1	5-B	259	ARG
1	5-B	323	SER

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Mol	Chain	Res	Type
1	5-B	328	HIS
1	5-B	330	LEU
1	5-B	332	GLU
1	5-B	337	MSE
1	5-B	345	GLU
1	5-B	347	ARG
1	5-B	355	SER
1	5-B	367	GLN
1	5-C	16	ARG
1	5-C	35	GLU
1	5-C	36	ARG
1	5-C	39	GLN
1	5-C	108	ASP
1	5-C	109	LEU
1	5-C	112	ARG
1	5-C	116	ARG
1	5-C	134	GLU
1	5-C	149	LEU
1	5-C	150	LEU
1	5-C	161	ARG
1	5-C	231	VAL
1	5-C	289	LYS
1	5-C	292	MSE
1	5-C	324	LEU
1	5-C	327	VAL
1	5-C	332	GLU
1	5-C	337	MSE
1	5-C	342	LEU
1	5-C	343	SER
1	5-C	354	GLU
1	5-C	375	ARG
1	5-D	4	MSE
1	5-D	33	THR
1	5-D	66	ARG
1	5-D	96	THR
1	5-D	98	ASP
1	5-D	126	GLU
1	5-D	132	LEU
1	5-D	160	ARG
1	5-D	161	ARG
1	5-D	165	ARG
1	5-D	192	LEU

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Mol	Chain	Res	Type
1	5-D	213	ARG
1	5-D	253	ARG
1	5-D	300	SER
1	5-D	309	GLU
1	5-D	320	CYS
1	5-D	323	SER
1	5-D	324	LEU
1	5-D	332	GLU
1	5-E	4	MSE
1	5-E	33	THR
1	5-E	39	GLN
1	5-E	43	ARG
1	5-E	59	GLU
1	5-E	96	THR
1	5-E	97	ASP
1	5-E	113	GLN
1	5-E	121	ASP
1	5-E	126	GLU
1	5-E	128	ILE
1	5-E	151	THR
1	5-E	192	LEU
1	5-E	226	THR
1	5-E	259	ARG
1	5-E	281	GLU
1	5-E	289	LYS
1	5-E	309	GLU
1	5-E	336	LEU
1	5-E	337	MSE
1	5-F	4	MSE
1	5-F	37	ARG
1	5-F	39	GLN
1	5-F	43	ARG
1	5-F	66	ARG
1	5-F	74	SER
1	5-F	96	THR
1	5-F	98	ASP
1	5-F	99	VAL
1	5-F	108	ASP
1	5-F	113	GLN
1	5-F	117	VAL
1	5-F	123	THR
1	5-F	124	THR

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Mol	Chain	Res	Type
1	5-F	126	GLU
1	5-F	132	LEU
1	5-F	147	ASN
1	5-F	151	THR
1	5-F	161	ARG
1	5-F	175	PHE
1	5-F	177	SER
1	5-F	192	LEU
1	5-F	231	VAL
1	5-F	244	LEU
1	5-F	263	GLU
1	5-F	332	GLU
1	5-F	338	THR
1	5-F	352	ILE
1	5-G	15	ARG
1	5-G	33	THR
1	5-G	36	ARG
1	5-G	41	GLU
1	5-G	43	ARG
1	5-G	50	GLU
1	5-G	83	LEU
1	5-G	99	VAL
1	5-G	104	ASP
1	5-G	116	ARG
1	5-G	121	ASP
1	5-G	134	GLU
1	5-G	152	VAL
1	5-G	165	ARG
1	5-G	252	HIS
1	5-G	284	GLN
1	5-G	331	VAL
1	5-G	337	MSE
1	5-G	352	ILE
1	5-G	374	SER
1	5-H	4	MSE
1	5-H	16	ARG
1	5-H	18	SER
1	5-H	33	THR
1	5-H	36	ARG
1	5-H	84	LEU
1	5-H	96	THR
1	5-H	109	LEU

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Mol	Chain	Res	Type
1	5-H	126	GLU
1	5-H	147	ASN
1	5-H	177	SER
1	5-H	214	ASP
1	5-H	231	VAL
1	5-H	236	ASP
1	5-H	244	LEU
1	5-H	292	MSE
1	5-H	323	SER
1	5-H	324	LEU
1	5-H	337	MSE
1	5-H	342	LEU
1	5-H	343	SER
1	5-H	347	ARG
1	5-H	352	ILE
1	6-A	16	ARG
1	6-A	39	GLN
1	6-A	41	GLU
1	6-A	43	ARG
1	6-A	66	ARG
1	6-A	84	LEU
1	6-A	98	ASP
1	6-A	112	ARG
1	6-A	124	THR
1	6-A	132	LEU
1	6-A	161	ARG
1	6-A	179	VAL
1	6-A	206	LEU
1	6-A	214	ASP
1	6-A	226	THR
1	6-A	244	LEU
1	6-A	263	GLU
1	6-A	264	ARG
1	6-A	281	GLU
1	6-A	323	SER
1	6-A	328	HIS
1	6-A	365	ASP
1	6-B	16	ARG
1	6-B	21	THR
1	6-B	33	THR
1	6-B	36	ARG
1	6-B	40	ASP

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Mol	Chain	Res	Type
1	6-B	41	GLU
1	6-B	43	ARG
1	6-B	66	ARG
1	6-B	84	LEU
1	6-B	92	CYS
1	6-B	96	THR
1	6-B	97	ASP
1	6-B	116	ARG
1	6-B	126	GLU
1	6-B	128	ILE
1	6-B	147	ASN
1	6-B	161	ARG
1	6-B	165	ARG
1	6-B	192	LEU
1	6-B	259	ARG
1	6-B	323	SER
1	6-B	328	HIS
1	6-B	330	LEU
1	6-B	332	GLU
1	6-B	337	MSE
1	6-B	345	GLU
1	6-B	347	ARG
1	6-B	355	SER
1	6-B	367	GLN
1	6-C	16	ARG
1	6-C	35	GLU
1	6-C	36	ARG
1	6-C	39	GLN
1	6-C	108	ASP
1	6-C	109	LEU
1	6-C	112	ARG
1	6-C	116	ARG
1	6-C	134	GLU
1	6-C	149	LEU
1	6-C	150	LEU
1	6-C	161	ARG
1	6-C	231	VAL
1	6-C	289	LYS
1	6-C	292	MSE
1	6-C	324	LEU
1	6-C	327	VAL
1	6-C	332	GLU

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Mol	Chain	Res	Type
1	6-C	337	MSE
1	6-C	342	LEU
1	6-C	343	SER
1	6-C	354	GLU
1	6-C	375	ARG
1	6-D	4	MSE
1	6-D	33	THR
1	6-D	66	ARG
1	6-D	96	THR
1	6-D	98	ASP
1	6-D	126	GLU
1	6-D	132	LEU
1	6-D	160	ARG
1	6-D	161	ARG
1	6-D	165	ARG
1	6-D	192	LEU
1	6-D	213	ARG
1	6-D	253	ARG
1	6-D	300	SER
1	6-D	309	GLU
1	6-D	320	CYS
1	6-D	323	SER
1	6-D	324	LEU
1	6-D	332	GLU
1	6-E	4	MSE
1	6-E	33	THR
1	6-E	39	GLN
1	6-E	43	ARG
1	6-E	59	GLU
1	6-E	96	THR
1	6-E	97	ASP
1	6-E	113	GLN
1	6-E	121	ASP
1	6-E	126	GLU
1	6-E	128	ILE
1	6-E	151	THR
1	6-E	192	LEU
1	6-E	226	THR
1	6-E	259	ARG
1	6-E	281	GLU
1	6-E	289	LYS
1	6-E	309	GLU

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Mol	Chain	Res	Type
1	6-E	336	LEU
1	6-E	337	MSE
1	6-F	4	MSE
1	6-F	37	ARG
1	6-F	39	GLN
1	6-F	43	ARG
1	6-F	66	ARG
1	6-F	74	SER
1	6-F	96	THR
1	6-F	98	ASP
1	6-F	99	VAL
1	6-F	108	ASP
1	6-F	113	GLN
1	6-F	117	VAL
1	6-F	123	THR
1	6-F	124	THR
1	6-F	126	GLU
1	6-F	132	LEU
1	6-F	147	ASN
1	6-F	151	THR
1	6-F	161	ARG
1	6-F	175	PHE
1	6-F	177	SER
1	6-F	192	LEU
1	6-F	231	VAL
1	6-F	244	LEU
1	6-F	263	GLU
1	6-F	332	GLU
1	6-F	338	THR
1	6-F	352	ILE
1	6-G	15	ARG
1	6-G	33	THR
1	6-G	36	ARG
1	6-G	41	GLU
1	6-G	43	ARG
1	6-G	50	GLU
1	6-G	83	LEU
1	6-G	99	VAL
1	6-G	104	ASP
1	6-G	116	ARG
1	6-G	121	ASP
1	6-G	134	GLU

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Mol	Chain	Res	Type
1	6-G	152	VAL
1	6-G	165	ARG
1	6-G	252	HIS
1	6-G	284	GLN
1	6-G	331	VAL
1	6-G	337	MSE
1	6-G	352	ILE
1	6-G	374	SER
1	6-H	4	MSE
1	6-H	16	ARG
1	6-H	18	SER
1	6-H	33	THR
1	6-H	36	ARG
1	6-H	84	LEU
1	6-H	96	THR
1	6-H	109	LEU
1	6-H	126	GLU
1	6-H	147	ASN
1	6-H	177	SER
1	6-H	214	ASP
1	6-H	231	VAL
1	6-H	236	ASP
1	6-H	244	LEU
1	6-H	292	MSE
1	6-H	323	SER
1	6-H	324	LEU
1	6-H	337	MSE
1	6-H	342	LEU
1	6-H	343	SER
1	6-H	347	ARG
1	6-H	352	ILE
1	7-A	16	ARG
1	7-A	39	GLN
1	7-A	41	GLU
1	7-A	43	ARG
1	7-A	66	ARG
1	7-A	84	LEU
1	7-A	98	ASP
1	7-A	112	ARG
1	7-A	124	THR
1	7-A	132	LEU
1	7-A	161	ARG

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Mol	Chain	Res	Type
1	7-A	179	VAL
1	7-A	206	LEU
1	7-A	214	ASP
1	7-A	226	THR
1	7-A	244	LEU
1	7-A	263	GLU
1	7-A	264	ARG
1	7-A	281	GLU
1	7-A	323	SER
1	7-A	328	HIS
1	7-A	365	ASP
1	7-B	16	ARG
1	7-B	21	THR
1	7-B	33	THR
1	7-B	36	ARG
1	7-B	40	ASP
1	7-B	41	GLU
1	7-B	43	ARG
1	7-B	66	ARG
1	7-B	84	LEU
1	7-B	92	CYS
1	7-B	96	THR
1	7-B	97	ASP
1	7-B	116	ARG
1	7-B	126	GLU
1	7-B	128	ILE
1	7-B	147	ASN
1	7-B	161	ARG
1	7-B	165	ARG
1	7-B	192	LEU
1	7-B	259	ARG
1	7-B	323	SER
1	7-B	328	HIS
1	7-B	330	LEU
1	7-B	332	GLU
1	7-B	337	MSE
1	7-B	345	GLU
1	7-B	347	ARG
1	7-B	355	SER
1	7-B	367	GLN
1	7-C	16	ARG
1	7-C	35	GLU

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Mol	Chain	Res	Type
1	7-C	36	ARG
1	7-C	39	GLN
1	7-C	108	ASP
1	7-C	109	LEU
1	7-C	112	ARG
1	7-C	116	ARG
1	7-C	134	GLU
1	7-C	149	LEU
1	7-C	150	LEU
1	7-C	161	ARG
1	7-C	231	VAL
1	7-C	289	LYS
1	7-C	292	MSE
1	7-C	324	LEU
1	7-C	327	VAL
1	7-C	332	GLU
1	7-C	337	MSE
1	7-C	342	LEU
1	7-C	343	SER
1	7-C	354	GLU
1	7-C	375	ARG
1	7-D	4	MSE
1	7-D	33	THR
1	7-D	66	ARG
1	7-D	96	THR
1	7-D	98	ASP
1	7-D	126	GLU
1	7-D	132	LEU
1	7-D	160	ARG
1	7-D	161	ARG
1	7-D	165	ARG
1	7-D	192	LEU
1	7-D	213	ARG
1	7-D	253	ARG
1	7-D	300	SER
1	7-D	309	GLU
1	7-D	320	CYS
1	7-D	323	SER
1	7-D	324	LEU
1	7-D	332	GLU
1	7-E	4	MSE
1	7-E	33	THR

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Mol	Chain	Res	Type
1	7-E	39	GLN
1	7-E	43	ARG
1	7-E	59	GLU
1	7-E	96	THR
1	7-E	97	ASP
1	7-E	113	GLN
1	7-E	121	ASP
1	7-E	126	GLU
1	7-E	128	ILE
1	7-E	151	THR
1	7-E	192	LEU
1	7-E	226	THR
1	7-E	259	ARG
1	7-E	281	GLU
1	7-E	289	LYS
1	7-E	309	GLU
1	7-E	336	LEU
1	7-E	337	MSE
1	7-F	4	MSE
1	7-F	37	ARG
1	7-F	39	GLN
1	7-F	43	ARG
1	7-F	66	ARG
1	7-F	74	SER
1	7-F	96	THR
1	7-F	98	ASP
1	7-F	99	VAL
1	7-F	108	ASP
1	7-F	113	GLN
1	7-F	117	VAL
1	7-F	123	THR
1	7-F	124	THR
1	7-F	126	GLU
1	7-F	132	LEU
1	7-F	147	ASN
1	7-F	151	THR
1	7-F	161	ARG
1	7-F	175	PHE
1	7-F	177	SER
1	7-F	192	LEU
1	7-F	231	VAL
1	7-F	244	LEU

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Mol	Chain	Res	Type
1	7-F	263	GLU
1	7-F	332	GLU
1	7-F	338	THR
1	7-F	352	ILE
1	7-G	15	ARG
1	7-G	33	THR
1	7-G	36	ARG
1	7-G	41	GLU
1	7-G	43	ARG
1	7-G	50	GLU
1	7-G	83	LEU
1	7-G	99	VAL
1	7-G	104	ASP
1	7-G	116	ARG
1	7-G	121	ASP
1	7-G	134	GLU
1	7-G	152	VAL
1	7-G	165	ARG
1	7-G	252	HIS
1	7-G	284	GLN
1	7-G	331	VAL
1	7-G	337	MSE
1	7-G	352	ILE
1	7-G	374	SER
1	7-H	4	MSE
1	7-H	16	ARG
1	7-H	18	SER
1	7-H	33	THR
1	7-H	36	ARG
1	7-H	84	LEU
1	7-H	96	THR
1	7-H	109	LEU
1	7-H	126	GLU
1	7-H	147	ASN
1	7-H	177	SER
1	7-H	214	ASP
1	7-H	231	VAL
1	7-H	236	ASP
1	7-H	244	LEU
1	7-H	292	MSE
1	7-H	323	SER
1	7-H	324	LEU

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Mol	Chain	Res	Type
1	7-H	337	MSE
1	7-H	342	LEU
1	7-H	343	SER
1	7-H	347	ARG
1	7-H	352	ILE
1	8-A	16	ARG
1	8-A	39	GLN
1	8-A	41	GLU
1	8-A	43	ARG
1	8-A	66	ARG
1	8-A	84	LEU
1	8-A	98	ASP
1	8-A	112	ARG
1	8-A	124	THR
1	8-A	132	LEU
1	8-A	161	ARG
1	8-A	179	VAL
1	8-A	206	LEU
1	8-A	214	ASP
1	8-A	226	THR
1	8-A	244	LEU
1	8-A	263	GLU
1	8-A	264	ARG
1	8-A	281	GLU
1	8-A	323	SER
1	8-A	328	HIS
1	8-A	365	ASP
1	8-B	16	ARG
1	8-B	21	THR
1	8-B	33	THR
1	8-B	36	ARG
1	8-B	40	ASP
1	8-B	41	GLU
1	8-B	43	ARG
1	8-B	66	ARG
1	8-B	84	LEU
1	8-B	92	CYS
1	8-B	96	THR
1	8-B	97	ASP
1	8-B	116	ARG
1	8-B	126	GLU
1	8-B	128	ILE

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Mol	Chain	Res	Type
1	8-B	147	ASN
1	8-B	161	ARG
1	8-B	165	ARG
1	8-B	192	LEU
1	8-B	259	ARG
1	8-B	323	SER
1	8-B	328	HIS
1	8-B	330	LEU
1	8-B	332	GLU
1	8-B	337	MSE
1	8-B	345	GLU
1	8-B	347	ARG
1	8-B	355	SER
1	8-B	367	GLN
1	8-C	16	ARG
1	8-C	35	GLU
1	8-C	36	ARG
1	8-C	39	GLN
1	8-C	108	ASP
1	8-C	109	LEU
1	8-C	112	ARG
1	8-C	116	ARG
1	8-C	134	GLU
1	8-C	149	LEU
1	8-C	150	LEU
1	8-C	161	ARG
1	8-C	231	VAL
1	8-C	289	LYS
1	8-C	292	MSE
1	8-C	324	LEU
1	8-C	327	VAL
1	8-C	332	GLU
1	8-C	337	MSE
1	8-C	342	LEU
1	8-C	343	SER
1	8-C	354	GLU
1	8-C	375	ARG
1	8-D	4	MSE
1	8-D	33	THR
1	8-D	66	ARG
1	8-D	96	THR
1	8-D	98	ASP

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Mol	Chain	Res	Type
1	8-D	126	GLU
1	8-D	132	LEU
1	8-D	160	ARG
1	8-D	161	ARG
1	8-D	165	ARG
1	8-D	192	LEU
1	8-D	213	ARG
1	8-D	253	ARG
1	8-D	300	SER
1	8-D	309	GLU
1	8-D	320	CYS
1	8-D	323	SER
1	8-D	324	LEU
1	8-D	332	GLU
1	8-E	4	MSE
1	8-E	33	THR
1	8-E	39	GLN
1	8-E	43	ARG
1	8-E	59	GLU
1	8-E	96	THR
1	8-E	97	ASP
1	8-E	113	GLN
1	8-E	121	ASP
1	8-E	126	GLU
1	8-E	128	ILE
1	8-E	151	THR
1	8-E	192	LEU
1	8-E	226	THR
1	8-E	259	ARG
1	8-E	281	GLU
1	8-E	289	LYS
1	8-E	309	GLU
1	8-E	336	LEU
1	8-E	337	MSE
1	8-F	4	MSE
1	8-F	37	ARG
1	8-F	39	GLN
1	8-F	43	ARG
1	8-F	66	ARG
1	8-F	74	SER
1	8-F	96	THR
1	8-F	98	ASP

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Mol	Chain	Res	Type
1	8-F	99	VAL
1	8-F	108	ASP
1	8-F	113	GLN
1	8-F	117	VAL
1	8-F	123	THR
1	8-F	124	THR
1	8-F	126	GLU
1	8-F	132	LEU
1	8-F	147	ASN
1	8-F	151	THR
1	8-F	161	ARG
1	8-F	175	PHE
1	8-F	177	SER
1	8-F	192	LEU
1	8-F	231	VAL
1	8-F	244	LEU
1	8-F	263	GLU
1	8-F	332	GLU
1	8-F	338	THR
1	8-F	352	ILE
1	8-G	15	ARG
1	8-G	33	THR
1	8-G	36	ARG
1	8-G	41	GLU
1	8-G	43	ARG
1	8-G	50	GLU
1	8-G	83	LEU
1	8-G	99	VAL
1	8-G	104	ASP
1	8-G	116	ARG
1	8-G	121	ASP
1	8-G	134	GLU
1	8-G	152	VAL
1	8-G	165	ARG
1	8-G	252	HIS
1	8-G	284	GLN
1	8-G	331	VAL
1	8-G	337	MSE
1	8-G	352	ILE
1	8-G	374	SER
1	8-H	4	MSE
1	8-H	16	ARG

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Mol	Chain	Res	Type
1	8-H	18	SER
1	8-H	33	THR
1	8-H	36	ARG
1	8-H	84	LEU
1	8-H	96	THR
1	8-H	109	LEU
1	8-H	126	GLU
1	8-H	147	ASN
1	8-H	177	SER
1	8-H	214	ASP
1	8-H	231	VAL
1	8-H	236	ASP
1	8-H	244	LEU
1	8-H	292	MSE
1	8-H	323	SER
1	8-H	324	LEU
1	8-H	337	MSE
1	8-H	342	LEU
1	8-H	343	SER
1	8-H	347	ARG
1	8-H	352	ILE
1	9-A	16	ARG
1	9-A	39	GLN
1	9-A	41	GLU
1	9-A	43	ARG
1	9-A	66	ARG
1	9-A	84	LEU
1	9-A	98	ASP
1	9-A	112	ARG
1	9-A	124	THR
1	9-A	132	LEU
1	9-A	161	ARG
1	9-A	179	VAL
1	9-A	206	LEU
1	9-A	214	ASP
1	9-A	226	THR
1	9-A	244	LEU
1	9-A	263	GLU
1	9-A	264	ARG
1	9-A	281	GLU
1	9-A	323	SER
1	9-A	328	HIS

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Mol	Chain	Res	Type
1	9-A	365	ASP
1	9-B	16	ARG
1	9-B	21	THR
1	9-B	33	THR
1	9-B	36	ARG
1	9-B	40	ASP
1	9-B	41	GLU
1	9-B	43	ARG
1	9-B	66	ARG
1	9-B	84	LEU
1	9-B	92	CYS
1	9-B	96	THR
1	9-B	97	ASP
1	9-B	116	ARG
1	9-B	126	GLU
1	9-B	128	ILE
1	9-B	147	ASN
1	9-B	161	ARG
1	9-B	165	ARG
1	9-B	192	LEU
1	9-B	259	ARG
1	9-B	323	SER
1	9-B	328	HIS
1	9-B	330	LEU
1	9-B	332	GLU
1	9-B	337	MSE
1	9-B	345	GLU
1	9-B	347	ARG
1	9-B	355	SER
1	9-B	367	GLN
1	9-C	16	ARG
1	9-C	35	GLU
1	9-C	36	ARG
1	9-C	39	GLN
1	9-C	108	ASP
1	9-C	109	LEU
1	9-C	112	ARG
1	9-C	116	ARG
1	9-C	134	GLU
1	9-C	149	LEU
1	9-C	150	LEU
1	9-C	161	ARG

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Mol	Chain	Res	Type
1	9-C	231	VAL
1	9-C	289	LYS
1	9-C	292	MSE
1	9-C	324	LEU
1	9-C	327	VAL
1	9-C	332	GLU
1	9-C	337	MSE
1	9-C	342	LEU
1	9-C	343	SER
1	9-C	354	GLU
1	9-C	375	ARG
1	9-D	4	MSE
1	9-D	33	THR
1	9-D	66	ARG
1	9-D	96	THR
1	9-D	98	ASP
1	9-D	126	GLU
1	9-D	132	LEU
1	9-D	160	ARG
1	9-D	161	ARG
1	9-D	165	ARG
1	9-D	192	LEU
1	9-D	213	ARG
1	9-D	253	ARG
1	9-D	300	SER
1	9-D	309	GLU
1	9-D	320	CYS
1	9-D	323	SER
1	9-D	324	LEU
1	9-D	332	GLU
1	9-E	4	MSE
1	9-E	33	THR
1	9-E	39	GLN
1	9-E	43	ARG
1	9-E	59	GLU
1	9-E	96	THR
1	9-E	97	ASP
1	9-E	113	GLN
1	9-E	121	ASP
1	9-E	126	GLU
1	9-E	128	ILE
1	9-E	151	THR

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Mol	Chain	Res	Type
1	9-E	192	LEU
1	9-E	226	THR
1	9-E	259	ARG
1	9-E	281	GLU
1	9-E	289	LYS
1	9-E	309	GLU
1	9-E	336	LEU
1	9-E	337	MSE
1	9-F	4	MSE
1	9-F	37	ARG
1	9-F	39	GLN
1	9-F	43	ARG
1	9-F	66	ARG
1	9-F	74	SER
1	9-F	96	THR
1	9-F	98	ASP
1	9-F	99	VAL
1	9-F	108	ASP
1	9-F	113	GLN
1	9-F	117	VAL
1	9-F	123	THR
1	9-F	124	THR
1	9-F	126	GLU
1	9-F	132	LEU
1	9-F	147	ASN
1	9-F	151	THR
1	9-F	161	ARG
1	9-F	175	PHE
1	9-F	177	SER
1	9-F	192	LEU
1	9-F	231	VAL
1	9-F	244	LEU
1	9-F	263	GLU
1	9-F	332	GLU
1	9-F	338	THR
1	9-F	352	ILE
1	9-G	15	ARG
1	9-G	33	THR
1	9-G	36	ARG
1	9-G	41	GLU
1	9-G	43	ARG
1	9-G	50	GLU

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Mol	Chain	Res	Type
1	9-G	83	LEU
1	9-G	99	VAL
1	9-G	104	ASP
1	9-G	116	ARG
1	9-G	121	ASP
1	9-G	134	GLU
1	9-G	152	VAL
1	9-G	165	ARG
1	9-G	252	HIS
1	9-G	284	GLN
1	9-G	331	VAL
1	9-G	337	MSE
1	9-G	352	ILE
1	9-G	374	SER
1	9-H	4	MSE
1	9-H	16	ARG
1	9-H	18	SER
1	9-H	33	THR
1	9-H	36	ARG
1	9-H	84	LEU
1	9-H	96	THR
1	9-H	109	LEU
1	9-H	126	GLU
1	9-H	147	ASN
1	9-H	177	SER
1	9-H	214	ASP
1	9-H	231	VAL
1	9-H	236	ASP
1	9-H	244	LEU
1	9-H	292	MSE
1	9-H	323	SER
1	9-H	324	LEU
1	9-H	337	MSE
1	9-H	342	LEU
1	9-H	343	SER
1	9-H	347	ARG
1	9-H	352	ILE
1	10-A	16	ARG
1	10-A	39	GLN
1	10-A	41	GLU
1	10-A	43	ARG
1	10-A	66	ARG

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Mol	Chain	Res	Type
1	10-A	84	LEU
1	10-A	98	ASP
1	10-A	112	ARG
1	10-A	124	THR
1	10-A	132	LEU
1	10-A	161	ARG
1	10-A	179	VAL
1	10-A	206	LEU
1	10-A	214	ASP
1	10-A	226	THR
1	10-A	244	LEU
1	10-A	263	GLU
1	10-A	264	ARG
1	10-A	281	GLU
1	10-A	323	SER
1	10-A	328	HIS
1	10-A	365	ASP
1	10-B	16	ARG
1	10-B	21	THR
1	10-B	33	THR
1	10-B	36	ARG
1	10-B	40	ASP
1	10-B	41	GLU
1	10-B	43	ARG
1	10-B	66	ARG
1	10-B	84	LEU
1	10-B	92	CYS
1	10-B	96	THR
1	10-B	97	ASP
1	10-B	116	ARG
1	10-B	126	GLU
1	10-B	128	ILE
1	10-B	147	ASN
1	10-B	161	ARG
1	10-B	165	ARG
1	10-B	192	LEU
1	10-B	259	ARG
1	10-B	323	SER
1	10-B	328	HIS
1	10-B	330	LEU
1	10-B	332	GLU
1	10-B	337	MSE

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Mol	Chain	Res	Type
1	10-B	345	GLU
1	10-B	347	ARG
1	10-B	355	SER
1	10-B	367	GLN
1	10-C	16	ARG
1	10-C	35	GLU
1	10-C	36	ARG
1	10-C	39	GLN
1	10-C	108	ASP
1	10-C	109	LEU
1	10-C	112	ARG
1	10-C	116	ARG
1	10-C	134	GLU
1	10-C	149	LEU
1	10-C	150	LEU
1	10-C	161	ARG
1	10-C	231	VAL
1	10-C	289	LYS
1	10-C	292	MSE
1	10-C	324	LEU
1	10-C	327	VAL
1	10-C	332	GLU
1	10-C	337	MSE
1	10-C	342	LEU
1	10-C	343	SER
1	10-C	354	GLU
1	10-C	375	ARG
1	10-D	4	MSE
1	10-D	33	THR
1	10-D	66	ARG
1	10-D	96	THR
1	10-D	98	ASP
1	10-D	126	GLU
1	10-D	132	LEU
1	10-D	160	ARG
1	10-D	161	ARG
1	10-D	165	ARG
1	10-D	192	LEU
1	10-D	213	ARG
1	10-D	253	ARG
1	10-D	300	SER
1	10-D	309	GLU

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Mol	Chain	Res	Type
1	10-D	320	CYS
1	10-D	323	SER
1	10-D	324	LEU
1	10-D	332	GLU
1	10-E	4	MSE
1	10-E	33	THR
1	10-E	39	GLN
1	10-E	43	ARG
1	10-E	59	GLU
1	10-E	96	THR
1	10-E	97	ASP
1	10-E	113	GLN
1	10-E	121	ASP
1	10-E	126	GLU
1	10-E	128	ILE
1	10-E	151	THR
1	10-E	192	LEU
1	10-E	226	THR
1	10-E	259	ARG
1	10-E	281	GLU
1	10-E	289	LYS
1	10-E	309	GLU
1	10-E	336	LEU
1	10-E	337	MSE
1	10-F	4	MSE
1	10-F	37	ARG
1	10-F	39	GLN
1	10-F	43	ARG
1	10-F	66	ARG
1	10-F	74	SER
1	10-F	96	THR
1	10-F	98	ASP
1	10-F	99	VAL
1	10-F	108	ASP
1	10-F	113	GLN
1	10-F	117	VAL
1	10-F	123	THR
1	10-F	124	THR
1	10-F	126	GLU
1	10-F	132	LEU
1	10-F	147	ASN
1	10-F	151	THR

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Mol	Chain	Res	Type
1	10-F	161	ARG
1	10-F	175	PHE
1	10-F	177	SER
1	10-F	192	LEU
1	10-F	231	VAL
1	10-F	244	LEU
1	10-F	263	GLU
1	10-F	332	GLU
1	10-F	338	THR
1	10-F	352	ILE
1	10-G	15	ARG
1	10-G	33	THR
1	10-G	36	ARG
1	10-G	41	GLU
1	10-G	43	ARG
1	10-G	50	GLU
1	10-G	83	LEU
1	10-G	99	VAL
1	10-G	104	ASP
1	10-G	116	ARG
1	10-G	121	ASP
1	10-G	134	GLU
1	10-G	152	VAL
1	10-G	165	ARG
1	10-G	252	HIS
1	10-G	284	GLN
1	10-G	331	VAL
1	10-G	337	MSE
1	10-G	352	ILE
1	10-G	374	SER
1	10-H	4	MSE
1	10-H	16	ARG
1	10-H	18	SER
1	10-H	33	THR
1	10-H	36	ARG
1	10-H	84	LEU
1	10-H	96	THR
1	10-H	109	LEU
1	10-H	126	GLU
1	10-H	147	ASN
1	10-H	177	SER
1	10-H	214	ASP

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Mol	Chain	Res	Type
1	10-H	231	VAL
1	10-H	236	ASP
1	10-H	244	LEU
1	10-H	292	MSE
1	10-H	323	SER
1	10-H	324	LEU
1	10-H	337	MSE
1	10-H	342	LEU
1	10-H	343	SER
1	10-H	347	ARG
1	10-H	352	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (221) such sidechains are listed below:

Mol	Chain	Res	Type
1	2-A	163	HIS
1	2-A	181	GLN
1	2-A	252	HIS
1	2-A	339	HIS
1	2-B	252	HIS
1	2-B	284	GLN
1	2-C	147	ASN
1	2-C	163	HIS
1	2-C	285	HIS
1	2-C	339	HIS
1	2-C	367	GLN
1	2-D	39	GLN
1	2-D	77	GLN
1	2-D	254	GLN
1	2-D	275	HIS
1	2-E	181	GLN
1	2-E	285	HIS
1	2-F	252	HIS
1	2-F	367	GLN
1	2-G	284	GLN
1	2-H	113	GLN
1	2-H	147	ASN
1	2-H	245	HIS
1	2-H	254	GLN
1	2-H	282	HIS
1	3-A	163	HIS
1	3-A	181	GLN

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Mol	Chain	Res	Type
1	3-A	252	HIS
1	3-A	367	GLN
1	3-B	252	HIS
1	3-C	39	GLN
1	3-C	147	ASN
1	3-D	91	GLN
1	3-D	254	GLN
1	3-D	339	HIS
1	3-E	163	HIS
1	3-E	285	HIS
1	3-F	181	GLN
1	3-F	285	HIS
1	3-G	147	ASN
1	3-G	284	GLN
1	3-H	245	HIS
1	3-H	252	HIS
1	3-H	254	GLN
1	4-A	275	HIS
1	4-A	339	HIS
1	4-A	367	GLN
1	4-B	181	GLN
1	4-B	284	GLN
1	4-B	285	HIS
1	4-C	39	GLN
1	4-C	147	ASN
1	4-C	275	HIS
1	4-C	367	GLN
1	4-D	91	GLN
1	4-D	113	GLN
1	4-D	252	HIS
1	4-D	254	GLN
1	4-D	285	HIS
1	4-D	367	GLN
1	4-E	147	ASN
1	4-E	181	GLN
1	4-F	181	GLN
1	4-F	285	HIS
1	4-F	367	GLN
1	4-G	252	HIS
1	4-G	367	GLN
1	4-H	29	HIS
1	4-H	245	HIS

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Mol	Chain	Res	Type
1	4-H	284	GLN
1	5-A	252	HIS
1	5-B	113	GLN
1	5-B	284	GLN
1	5-C	39	GLN
1	5-C	113	GLN
1	5-C	181	GLN
1	5-C	254	GLN
1	5-D	39	GLN
1	5-D	91	GLN
1	5-D	113	GLN
1	5-D	147	ASN
1	5-D	339	HIS
1	5-E	39	GLN
1	5-E	113	GLN
1	5-E	181	GLN
1	5-E	339	HIS
1	5-E	367	GLN
1	5-F	39	GLN
1	5-F	77	GLN
1	5-F	181	GLN
1	5-F	252	HIS
1	5-F	285	HIS
1	5-G	113	GLN
1	5-G	147	ASN
1	5-G	275	HIS
1	5-H	245	HIS
1	5-H	284	GLN
1	6-B	284	GLN
1	6-B	285	HIS
1	6-C	29	HIS
1	6-C	39	GLN
1	6-C	113	GLN
1	6-C	147	ASN
1	6-D	91	GLN
1	6-D	113	GLN
1	6-D	147	ASN
1	6-D	275	HIS
1	6-D	285	HIS
1	6-D	339	HIS
1	6-E	113	GLN
1	6-F	285	HIS

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Mol	Chain	Res	Type
1	6-F	367	GLN
1	6-G	77	GLN
1	6-G	252	HIS
1	6-H	91	GLN
1	6-H	147	ASN
1	6-H	245	HIS
1	6-H	285	HIS
1	6-H	367	GLN
1	7-A	163	HIS
1	7-B	113	GLN
1	7-B	284	GLN
1	7-B	339	HIS
1	7-C	29	HIS
1	7-C	39	GLN
1	7-C	113	GLN
1	7-C	147	ASN
1	7-C	252	HIS
1	7-C	275	HIS
1	7-D	91	GLN
1	7-D	147	ASN
1	7-D	275	HIS
1	7-E	39	GLN
1	7-E	252	HIS
1	7-E	275	HIS
1	7-F	275	HIS
1	7-F	367	GLN
1	7-G	181	GLN
1	7-H	147	ASN
1	7-H	245	HIS
1	7-H	339	HIS
1	7-H	367	GLN
1	8-A	39	GLN
1	8-B	113	GLN
1	8-B	147	ASN
1	8-B	367	GLN
1	8-C	39	GLN
1	8-C	113	GLN
1	8-C	339	HIS
1	8-D	29	HIS
1	8-D	91	GLN
1	8-D	181	GLN
1	8-E	147	ASN

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Mol	Chain	Res	Type
1	8-E	252	HIS
1	8-E	285	HIS
1	8-E	367	GLN
1	8-G	147	ASN
1	8-H	39	GLN
1	8-H	113	GLN
1	8-H	147	ASN
1	8-H	245	HIS
1	8-H	254	GLN
1	8-H	339	HIS
1	9-A	39	GLN
1	9-A	163	HIS
1	9-A	252	HIS
1	9-B	77	GLN
1	9-B	113	GLN
1	9-B	284	GLN
1	9-B	285	HIS
1	9-C	275	HIS
1	9-D	77	GLN
1	9-D	91	GLN
1	9-D	113	GLN
1	9-D	181	GLN
1	9-D	252	HIS
1	9-D	275	HIS
1	9-E	39	GLN
1	9-E	285	HIS
1	9-E	367	GLN
1	9-F	39	GLN
1	9-F	113	GLN
1	9-F	147	ASN
1	9-F	181	GLN
1	9-F	252	HIS
1	9-F	275	HIS
1	9-F	285	HIS
1	9-G	147	ASN
1	9-G	163	HIS
1	9-G	275	HIS
1	9-G	339	HIS
1	9-H	245	HIS
1	9-H	367	GLN
1	10-A	181	GLN
1	10-A	252	HIS

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Mol	Chain	Res	Type
1	10-B	163	HIS
1	10-B	181	GLN
1	10-B	252	HIS
1	10-B	284	GLN
1	10-B	285	HIS
1	10-C	113	GLN
1	10-C	339	HIS
1	10-C	367	GLN
1	10-D	91	GLN
1	10-D	113	GLN
1	10-D	367	GLN
1	10-E	39	GLN
1	10-E	113	GLN
1	10-E	147	ASN
1	10-E	163	HIS
1	10-E	252	HIS
1	10-E	275	HIS
1	10-F	147	ASN
1	10-F	252	HIS
1	10-F	275	HIS
1	10-F	339	HIS
1	10-G	328	HIS
1	10-H	29	HIS
1	10-H	91	GLN
1	10-H	245	HIS
1	10-H	254	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

80 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-B	197	LLP	C4-C4'	7.90	1.63	1.46
1	5-A	197	LLP	C4-C4'	7.90	1.63	1.46
1	2-E	197	LLP	C4-C4'	7.89	1.63	1.46
1	7-A	197	LLP	C4-C4'	7.89	1.63	1.46
1	3-B	197	LLP	C4-C4'	7.85	1.63	1.46
1	7-D	197	LLP	C4-C4'	7.84	1.63	1.46
1	3-H	197	LLP	C4-C4'	7.83	1.63	1.46
1	3-E	197	LLP	C4-C4'	7.83	1.63	1.46
1	2-B	197	LLP	C4-C4'	7.82	1.63	1.46
1	9-G	197	LLP	C4-C4'	7.81	1.63	1.46
1	4-B	197	LLP	C4-C4'	7.80	1.63	1.46
1	4-C	197	LLP	C4-C4'	7.77	1.63	1.46
1	1-G	197	LLP	C4-C4'	7.73	1.63	1.46
1	8-E	197	LLP	C4-C4'	7.71	1.63	1.46
1	3-D	197	LLP	C4-C4'	7.71	1.63	1.46
1	5-C	197	LLP	C4-C4'	7.70	1.63	1.46
1	8-A	197	LLP	C4-C4'	7.69	1.63	1.46
1	9-C	197	LLP	C4-C4'	7.69	1.63	1.46
1	10-D	197	LLP	C4-C4'	7.69	1.63	1.46
1	7-E	197	LLP	C4-C4'	7.68	1.63	1.46
1	5-G	197	LLP	C4-C4'	7.68	1.63	1.46
1	10-C	197	LLP	C4-C4'	7.68	1.63	1.46
1	1-D	197	LLP	C4-C4'	7.66	1.63	1.46
1	6-D	197	LLP	C4-C4'	7.65	1.62	1.46
1	10-A	197	LLP	C4-C4'	7.65	1.62	1.46
1	4-E	197	LLP	C4-C4'	7.65	1.62	1.46
1	6-G	197	LLP	C4-C4'	7.65	1.62	1.46
1	10-G	197	LLP	C4-C4'	7.65	1.62	1.46
1	4-G	197	LLP	C4-C4'	7.64	1.62	1.46
1	1-B	197	LLP	C4-C4'	7.63	1.62	1.46
1	3-A	197	LLP	C4-C4'	7.63	1.62	1.46
1	3-C	197	LLP	C4-C4'	7.63	1.62	1.46
1	8-C	197	LLP	C4-C4'	7.62	1.62	1.46
1	2-C	197	LLP	C4-C4'	7.61	1.62	1.46
1	3-G	197	LLP	C4-C4'	7.59	1.62	1.46
1	10-B	197	LLP	C4-C4'	7.59	1.62	1.46
1	10-F	197	LLP	C4-C4'	7.58	1.62	1.46
1	10-H	197	LLP	C4-C4'	7.58	1.62	1.46
1	5-E	197	LLP	C4-C4'	7.56	1.62	1.46
1	7-B	197	LLP	C4-C4'	7.56	1.62	1.46
1	8-H	197	LLP	C4-C4'	7.55	1.62	1.46
1	4-D	197	LLP	C4-C4'	7.55	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-B	197	LLP	C4-C4'	7.54	1.62	1.46
1	2-D	197	LLP	C4-C4'	7.52	1.62	1.46
1	7-F	197	LLP	C4-C4'	7.51	1.62	1.46
1	1-F	197	LLP	C4-C4'	7.49	1.62	1.46
1	7-H	197	LLP	C4-C4'	7.49	1.62	1.46
1	6-F	197	LLP	C4-C4'	7.49	1.62	1.46
1	10-E	197	LLP	C4-C4'	7.49	1.62	1.46
1	5-D	197	LLP	C4-C4'	7.48	1.62	1.46
1	6-E	197	LLP	C4-C4'	7.48	1.62	1.46
1	3-F	197	LLP	C4-C4'	7.48	1.62	1.46
1	8-G	197	LLP	C4-C4'	7.46	1.62	1.46
1	7-C	197	LLP	C4-C4'	7.45	1.62	1.46
1	8-B	197	LLP	C4-C4'	7.44	1.62	1.46
1	9-D	197	LLP	C4-C4'	7.44	1.62	1.46
1	9-F	197	LLP	C4-C4'	7.43	1.62	1.46
1	4-A	197	LLP	C4-C4'	7.42	1.62	1.46
1	1-C	197	LLP	C4-C4'	7.41	1.62	1.46
1	5-H	197	LLP	C4-C4'	7.41	1.62	1.46
1	2-F	197	LLP	C4-C4'	7.41	1.62	1.46
1	1-E	197	LLP	C4-C4'	7.40	1.62	1.46
1	1-H	197	LLP	C4-C4'	7.37	1.62	1.46
1	6-H	197	LLP	C4-C4'	7.37	1.62	1.46
1	8-F	197	LLP	C4-C4'	7.35	1.62	1.46
1	6-A	197	LLP	C4-C4'	7.35	1.62	1.46
1	4-F	197	LLP	C4-C4'	7.35	1.62	1.46
1	9-E	197	LLP	C4-C4'	7.34	1.62	1.46
1	9-H	197	LLP	C4-C4'	7.31	1.62	1.46
1	8-D	197	LLP	C4-C4'	7.21	1.62	1.46
1	9-A	197	LLP	C4-C4'	7.20	1.62	1.46
1	1-A	197	LLP	C4-C4'	7.17	1.61	1.46
1	2-H	197	LLP	C4-C4'	7.10	1.61	1.46
1	9-B	197	LLP	C4-C4'	7.01	1.61	1.46
1	5-F	197	LLP	C4-C4'	6.97	1.61	1.46
1	4-H	197	LLP	C4'-NZ	5.54	1.45	1.27
1	3-H	197	LLP	C4'-NZ	5.49	1.45	1.27
1	5-B	197	LLP	C4'-NZ	5.33	1.45	1.27
1	10-H	197	LLP	C4'-NZ	5.30	1.44	1.27
1	3-B	197	LLP	C4'-NZ	5.30	1.44	1.27
1	6-C	197	LLP	C4'-NZ	5.28	1.44	1.27
1	8-C	197	LLP	C4'-NZ	5.27	1.44	1.27
1	10-B	197	LLP	C4'-NZ	5.25	1.44	1.27
1	6-H	197	LLP	C4'-NZ	5.24	1.44	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-B	197	LLP	C4'-NZ	5.21	1.44	1.27
1	8-B	197	LLP	C4'-NZ	5.20	1.44	1.27
1	10-A	197	LLP	C4'-NZ	5.19	1.44	1.27
1	2-G	197	LLP	C4'-NZ	5.18	1.44	1.27
1	1-H	197	LLP	C4'-NZ	5.17	1.44	1.27
1	10-G	197	LLP	C4'-NZ	5.17	1.44	1.27
1	2-E	197	LLP	C4'-NZ	5.17	1.44	1.27
1	8-H	197	LLP	C4'-NZ	5.16	1.44	1.27
1	6-A	197	LLP	C4'-NZ	5.16	1.44	1.27
1	8-F	197	LLP	C4'-NZ	5.16	1.44	1.27
1	5-H	197	LLP	C4'-NZ	5.14	1.44	1.27
1	1-B	197	LLP	C4'-NZ	5.14	1.44	1.27
1	3-F	197	LLP	C4'-NZ	5.13	1.44	1.27
1	8-D	197	LLP	C4'-NZ	5.12	1.44	1.27
1	8-A	197	LLP	C4'-NZ	5.12	1.44	1.27
1	4-C	197	LLP	C4'-NZ	5.12	1.44	1.27
1	7-H	197	LLP	C4'-NZ	5.12	1.44	1.27
1	6-F	197	LLP	C4'-NZ	5.11	1.44	1.27
1	2-F	197	LLP	C4'-NZ	5.11	1.44	1.27
1	2-B	197	LLP	C4'-NZ	5.11	1.44	1.27
1	7-C	197	LLP	C4'-NZ	5.10	1.44	1.27
1	9-H	197	LLP	C4'-NZ	5.10	1.44	1.27
1	2-C	197	LLP	C4'-NZ	5.10	1.44	1.27
1	3-C	197	LLP	C4'-NZ	5.08	1.44	1.27
1	3-G	197	LLP	C4'-NZ	5.07	1.44	1.27
1	7-B	197	LLP	C4'-NZ	5.06	1.44	1.27
1	9-G	197	LLP	C4'-NZ	5.06	1.44	1.27
1	4-E	197	LLP	C4'-NZ	5.05	1.44	1.27
1	7-G	197	LLP	C4'-NZ	5.05	1.44	1.27
1	1-G	197	LLP	C4'-NZ	5.05	1.44	1.27
1	3-A	197	LLP	C4'-NZ	5.04	1.44	1.27
1	6-G	197	LLP	C4'-NZ	5.04	1.44	1.27
1	7-F	197	LLP	C4'-NZ	5.03	1.44	1.27
1	7-E	197	LLP	C4'-NZ	5.02	1.44	1.27
1	5-C	197	LLP	C4'-NZ	5.02	1.44	1.27
1	6-B	197	LLP	C4'-NZ	5.01	1.43	1.27
1	5-G	197	LLP	C4'-NZ	5.01	1.43	1.27
1	10-F	197	LLP	C4'-NZ	5.00	1.43	1.27
1	8-E	197	LLP	C4'-NZ	5.00	1.43	1.27
1	4-F	197	LLP	C4'-NZ	5.00	1.43	1.27
1	9-C	197	LLP	C4'-NZ	4.99	1.43	1.27
1	7-A	197	LLP	C4'-NZ	4.99	1.43	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-D	197	LLP	C4'-NZ	4.98	1.43	1.27
1	5-A	197	LLP	C4'-NZ	4.98	1.43	1.27
1	1-F	197	LLP	C4'-NZ	4.97	1.43	1.27
1	1-E	197	LLP	C4'-NZ	4.97	1.43	1.27
1	5-E	197	LLP	C4'-NZ	4.97	1.43	1.27
1	4-G	197	LLP	C4'-NZ	4.95	1.43	1.27
1	9-F	197	LLP	C4'-NZ	4.95	1.43	1.27
1	9-A	197	LLP	C4'-NZ	4.91	1.43	1.27
1	2-H	197	LLP	C4'-NZ	4.91	1.43	1.27
1	10-C	197	LLP	C4'-NZ	4.91	1.43	1.27
1	1-A	197	LLP	C4'-NZ	4.90	1.43	1.27
1	3-D	197	LLP	C4'-NZ	4.90	1.43	1.27
1	4-A	197	LLP	C4'-NZ	4.90	1.43	1.27
1	9-E	197	LLP	C4'-NZ	4.90	1.43	1.27
1	5-D	197	LLP	C4'-NZ	4.90	1.43	1.27
1	2-A	197	LLP	C4'-NZ	4.89	1.43	1.27
1	3-E	197	LLP	C4'-NZ	4.88	1.43	1.27
1	1-C	197	LLP	C4'-NZ	4.86	1.43	1.27
1	2-D	197	LLP	C4'-NZ	4.86	1.43	1.27
1	6-E	197	LLP	C4'-NZ	4.84	1.43	1.27
1	10-E	197	LLP	C4'-NZ	4.83	1.43	1.27
1	7-D	197	LLP	C4'-NZ	4.83	1.43	1.27
1	6-D	197	LLP	C4'-NZ	4.82	1.43	1.27
1	1-D	197	LLP	C4'-NZ	4.82	1.43	1.27
1	8-G	197	LLP	C4'-NZ	4.76	1.43	1.27
1	9-D	197	LLP	C4'-NZ	4.72	1.43	1.27
1	4-D	197	LLP	C4'-NZ	4.65	1.42	1.27
1	5-F	197	LLP	C4'-NZ	4.60	1.42	1.27
1	7-E	197	LLP	C2'-C2	4.24	1.57	1.50
1	9-B	197	LLP	C4'-NZ	4.23	1.41	1.27
1	5-C	197	LLP	C2'-C2	4.19	1.57	1.50
1	2-E	197	LLP	C2'-C2	4.16	1.57	1.50
1	9-E	197	LLP	C2'-C2	4.16	1.57	1.50
1	5-E	197	LLP	C2'-C2	4.15	1.57	1.50
1	8-E	197	LLP	C2'-C2	4.15	1.57	1.50
1	2-H	197	LLP	C2'-C2	4.13	1.56	1.50
1	10-E	197	LLP	C2'-C2	4.11	1.56	1.50
1	8-G	197	LLP	C2'-C2	4.11	1.56	1.50
1	4-E	197	LLP	C2'-C2	4.10	1.56	1.50
1	10-H	197	LLP	C2'-C2	4.09	1.56	1.50
1	1-E	197	LLP	C2'-C2	4.07	1.56	1.50
1	1-A	197	LLP	C2'-C2	4.05	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-E	197	LLP	C2'-C2	4.05	1.56	1.50
1	1-C	197	LLP	C2'-C2	4.04	1.56	1.50
1	2-C	197	LLP	C2'-C2	4.03	1.56	1.50
1	8-C	197	LLP	C2'-C2	4.03	1.56	1.50
1	8-H	197	LLP	C2'-C2	3.99	1.56	1.50
1	9-H	197	LLP	C2'-C2	3.98	1.56	1.50
1	1-H	197	LLP	C2'-C2	3.98	1.56	1.50
1	6-G	197	LLP	C2'-C2	3.96	1.56	1.50
1	10-A	197	LLP	C2'-C2	3.96	1.56	1.50
1	6-A	197	LLP	C2'-C2	3.96	1.56	1.50
1	5-H	197	LLP	C2'-C2	3.95	1.56	1.50
1	7-H	197	LLP	C2'-C2	3.95	1.56	1.50
1	1-G	197	LLP	C2'-C2	3.94	1.56	1.50
1	4-H	197	LLP	C2'-C2	3.93	1.56	1.50
1	3-C	197	LLP	C2'-C2	3.93	1.56	1.50
1	1-D	197	LLP	C2'-C2	3.93	1.56	1.50
1	6-C	197	LLP	C2'-C2	3.92	1.56	1.50
1	9-C	197	LLP	C2'-C2	3.92	1.56	1.50
1	4-C	197	LLP	C2'-C2	3.90	1.56	1.50
1	6-E	197	LLP	C2'-C2	3.90	1.56	1.50
1	9-A	197	LLP	C2'-C2	3.90	1.56	1.50
1	10-C	197	LLP	C2'-C2	3.89	1.56	1.50
1	5-G	197	LLP	C2'-C2	3.86	1.56	1.50
1	8-A	197	LLP	C2'-C2	3.86	1.56	1.50
1	3-H	197	LLP	C2'-C2	3.86	1.56	1.50
1	7-C	197	LLP	C2'-C2	3.86	1.56	1.50
1	7-A	197	LLP	C2'-C2	3.85	1.56	1.50
1	5-A	197	LLP	C2'-C2	3.84	1.56	1.50
1	2-A	197	LLP	C2'-C2	3.82	1.56	1.50
1	9-C	197	LLP	C4-C5	-3.81	1.36	1.42
1	8-D	197	LLP	C2'-C2	3.80	1.56	1.50
1	7-G	197	LLP	C2'-C2	3.79	1.56	1.50
1	6-H	197	LLP	C2'-C2	3.79	1.56	1.50
1	2-D	197	LLP	C2'-C2	3.78	1.56	1.50
1	9-D	197	LLP	C2'-C2	3.76	1.56	1.50
1	9-G	197	LLP	C2'-C2	3.75	1.56	1.50
1	4-C	197	LLP	C4-C5	-3.74	1.36	1.42
1	4-A	197	LLP	C4-C5	-3.73	1.36	1.42
1	4-A	197	LLP	C2'-C2	3.73	1.56	1.50
1	10-D	197	LLP	C2'-C2	3.71	1.56	1.50
1	2-G	197	LLP	C2'-C2	3.68	1.56	1.50
1	5-A	197	LLP	C4-C5	-3.67	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-D	197	LLP	C2'-C2	3.66	1.56	1.50
1	6-D	197	LLP	C2'-C2	3.66	1.56	1.50
1	3-D	197	LLP	C2'-C2	3.65	1.56	1.50
1	10-G	197	LLP	C2'-C2	3.62	1.56	1.50
1	4-G	197	LLP	C2'-C2	3.62	1.56	1.50
1	3-A	197	LLP	C2'-C2	3.60	1.56	1.50
1	4-D	197	LLP	C2'-C2	3.60	1.56	1.50
1	9-A	197	LLP	C4-C5	-3.57	1.37	1.42
1	5-D	197	LLP	C4-C5	-3.57	1.37	1.42
1	7-C	197	LLP	C4-C5	-3.56	1.37	1.42
1	1-F	197	LLP	C2'-C2	3.54	1.56	1.50
1	5-D	197	LLP	C2'-C2	3.52	1.56	1.50
1	3-G	197	LLP	C2'-C2	3.52	1.56	1.50
1	10-F	197	LLP	C2'-C2	3.51	1.56	1.50
1	5-F	197	LLP	C2'-C2	3.45	1.55	1.50
1	3-B	197	LLP	C2'-C2	3.45	1.55	1.50
1	7-F	197	LLP	C6-N1	3.44	1.41	1.34
1	7-A	197	LLP	C4-C5	-3.44	1.37	1.42
1	1-D	197	LLP	C4-C5	-3.43	1.37	1.42
1	3-A	197	LLP	C4-C5	-3.42	1.37	1.42
1	2-A	197	LLP	C4-C5	-3.42	1.37	1.42
1	10-B	197	LLP	C2'-C2	3.42	1.55	1.50
1	3-B	197	LLP	C4-C5	-3.41	1.37	1.42
1	7-F	197	LLP	C2'-C2	3.41	1.55	1.50
1	10-E	197	LLP	C4-C5	-3.40	1.37	1.42
1	7-D	197	LLP	C4-C5	-3.40	1.37	1.42
1	10-A	197	LLP	C4-C5	-3.40	1.37	1.42
1	2-C	197	LLP	C4-C5	-3.39	1.37	1.42
1	7-B	197	LLP	C2'-C2	3.39	1.55	1.50
1	6-D	197	LLP	C4-C5	-3.39	1.37	1.42
1	1-F	197	LLP	C6-N1	3.37	1.41	1.34
1	10-C	197	LLP	C4-C5	-3.36	1.37	1.42
1	7-B	197	LLP	C4-C5	-3.35	1.37	1.42
1	9-F	197	LLP	C2'-C2	3.33	1.55	1.50
1	8-D	197	LLP	C4-C5	-3.33	1.37	1.42
1	2-B	197	LLP	C2'-C2	3.33	1.55	1.50
1	4-F	197	LLP	C2'-C2	3.32	1.55	1.50
1	2-F	197	LLP	C2'-C2	3.30	1.55	1.50
1	8-A	197	LLP	C4-C5	-3.30	1.37	1.42
1	4-B	197	LLP	C2'-C2	3.30	1.55	1.50
1	4-F	197	LLP	C6-N1	3.29	1.41	1.34
1	6-F	197	LLP	C2'-C2	3.29	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-B	197	LLP	C2'-C2	3.28	1.55	1.50
1	9-F	197	LLP	C6-N1	3.28	1.41	1.34
1	9-D	197	LLP	C4-C5	-3.27	1.37	1.42
1	6-B	197	LLP	C4-C5	-3.26	1.37	1.42
1	9-B	197	LLP	C2'-C2	3.26	1.55	1.50
1	3-F	197	LLP	C2'-C2	3.24	1.55	1.50
1	5-F	197	LLP	C4-C5	-3.23	1.37	1.42
1	2-F	197	LLP	C4-C5	-3.22	1.37	1.42
1	2-D	197	LLP	C4-C5	-3.21	1.37	1.42
1	1-A	197	LLP	C4-C5	-3.19	1.37	1.42
1	6-A	197	LLP	C4-C5	-3.19	1.37	1.42
1	2-F	197	LLP	C6-N1	3.17	1.40	1.34
1	8-E	197	LLP	C4-C5	-3.17	1.37	1.42
1	1-C	197	LLP	C4-C5	-3.17	1.37	1.42
1	8-F	197	LLP	C2'-C2	3.15	1.55	1.50
1	7-F	197	LLP	C4-C5	-3.14	1.37	1.42
1	6-E	197	LLP	C4-C5	-3.14	1.37	1.42
1	8-F	197	LLP	C6-N1	3.14	1.40	1.34
1	8-B	197	LLP	C2'-C2	3.13	1.55	1.50
1	9-F	197	LLP	C4-C5	-3.11	1.37	1.42
1	10-D	197	LLP	C4-C5	-3.10	1.37	1.42
1	3-F	197	LLP	C6-N1	3.09	1.40	1.34
1	8-B	197	LLP	C4-C5	-3.06	1.37	1.42
1	4-F	197	LLP	C4-C5	-3.06	1.37	1.42
1	6-B	197	LLP	C2'-C2	3.05	1.55	1.50
1	6-F	197	LLP	C6-N1	3.05	1.40	1.34
1	3-D	197	LLP	C4-C5	-3.05	1.37	1.42
1	3-B	197	LLP	C6-N1	3.04	1.40	1.34
1	6-F	197	LLP	C4-C5	-3.03	1.37	1.42
1	8-C	197	LLP	C4-C5	-3.02	1.37	1.42
1	3-A	197	LLP	C6-N1	3.02	1.40	1.34
1	8-F	197	LLP	C4-C5	-3.01	1.37	1.42
1	9-B	197	LLP	C4-C5	-3.00	1.37	1.42
1	9-E	197	LLP	C4-C5	-2.99	1.37	1.42
1	3-F	197	LLP	C4-C5	-2.98	1.37	1.42
1	10-B	197	LLP	C4-C5	-2.98	1.37	1.42
1	5-F	197	LLP	C6-N1	2.97	1.40	1.34
1	5-B	197	LLP	C2'-C2	2.96	1.55	1.50
1	9-G	197	LLP	C4-C5	-2.96	1.37	1.42
1	4-D	197	LLP	C4-C5	-2.95	1.37	1.42
1	1-E	197	LLP	C6-N1	2.94	1.40	1.34
1	6-G	197	LLP	C4-C5	-2.94	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-F	197	LLP	C6-N1	2.93	1.40	1.34
1	3-E	197	LLP	C6-N1	2.93	1.40	1.34
1	4-A	197	LLP	C6-N1	2.93	1.40	1.34
1	3-G	197	LLP	C4-C5	-2.92	1.37	1.42
1	8-D	197	LLP	C6-N1	2.92	1.40	1.34
1	2-E	197	LLP	C6-N1	2.92	1.40	1.34
1	5-C	197	LLP	C4-C5	-2.92	1.37	1.42
1	2-E	197	LLP	C4-C5	-2.91	1.37	1.42
1	1-F	197	LLP	C4-C5	-2.90	1.37	1.42
1	6-A	197	LLP	C6-N1	2.89	1.40	1.34
1	9-A	197	LLP	C6-N1	2.89	1.40	1.34
1	3-E	197	LLP	C4-C5	-2.88	1.38	1.42
1	2-B	197	LLP	C4-C5	-2.88	1.38	1.42
1	7-C	197	LLP	C6-N1	2.88	1.40	1.34
1	3-C	197	LLP	C6-N1	2.87	1.40	1.34
1	5-E	197	LLP	C4-C5	-2.86	1.38	1.42
1	3-H	197	LLP	C4-C5	-2.86	1.38	1.42
1	7-H	197	LLP	C4-C5	-2.86	1.38	1.42
1	5-H	197	LLP	C6-N1	2.85	1.40	1.34
1	8-A	197	LLP	C6-N1	2.84	1.40	1.34
1	7-E	197	LLP	C4-C5	-2.84	1.38	1.42
1	10-F	197	LLP	C4-C5	-2.84	1.38	1.42
1	1-E	197	LLP	C4-C5	-2.84	1.38	1.42
1	8-G	197	LLP	C4-C5	-2.83	1.38	1.42
1	10-B	197	LLP	C6-N1	2.83	1.40	1.34
1	10-A	197	LLP	C6-N1	2.82	1.40	1.34
1	1-B	197	LLP	C4-C5	-2.82	1.38	1.42
1	6-E	197	LLP	C6-N1	2.82	1.40	1.34
1	7-A	197	LLP	C6-N1	2.81	1.40	1.34
1	4-B	197	LLP	C6-N1	2.79	1.40	1.34
1	2-A	197	LLP	C6-N1	2.78	1.40	1.34
1	9-C	197	LLP	C6-N1	2.78	1.40	1.34
1	4-C	197	LLP	C3-C2	2.77	1.43	1.41
1	5-A	197	LLP	C6-N1	2.77	1.40	1.34
1	6-H	197	LLP	C6-N1	2.76	1.40	1.34
1	5-B	197	LLP	C6-N1	2.76	1.40	1.34
1	4-C	197	LLP	C6-N1	2.75	1.40	1.34
1	4-H	197	LLP	C6-N1	2.75	1.40	1.34
1	6-C	197	LLP	C4-C5	-2.75	1.38	1.42
1	1-A	197	LLP	C6-N1	2.73	1.40	1.34
1	10-C	197	LLP	C6-N1	2.73	1.40	1.34
1	2-G	197	LLP	C4-C5	-2.72	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-B	197	LLP	C6-N1	2.72	1.40	1.34
1	4-E	197	LLP	C6-N1	2.72	1.40	1.34
1	9-H	197	LLP	C6-N1	2.72	1.40	1.34
1	3-E	197	LLP	C3-C2	2.72	1.43	1.41
1	7-E	197	LLP	C6-N1	2.71	1.39	1.34
1	6-C	197	LLP	C6-N1	2.71	1.39	1.34
1	5-G	197	LLP	C4-C5	-2.70	1.38	1.42
1	2-C	197	LLP	C6-N1	2.70	1.39	1.34
1	4-G	197	LLP	C4-C5	-2.70	1.38	1.42
1	5-B	197	LLP	C4-C5	-2.69	1.38	1.42
1	8-B	197	LLP	C6-N1	2.69	1.39	1.34
1	1-G	197	LLP	C4-C5	-2.69	1.38	1.42
1	8-E	197	LLP	C6-N1	2.69	1.39	1.34
1	8-C	197	LLP	C6-N1	2.69	1.39	1.34
1	10-H	197	LLP	C6-N1	2.68	1.39	1.34
1	2-B	197	LLP	C6-N1	2.68	1.39	1.34
1	8-H	197	LLP	C6-N1	2.68	1.39	1.34
1	8-G	197	LLP	C5'-C5	2.68	1.57	1.50
1	2-H	197	LLP	C4-C5	-2.68	1.38	1.42
1	3-H	197	LLP	C6-N1	2.67	1.39	1.34
1	3-C	197	LLP	C5'-C5	2.66	1.57	1.50
1	1-B	197	LLP	C6-N1	2.66	1.39	1.34
1	4-D	197	LLP	C6-N1	2.66	1.39	1.34
1	8-G	197	LLP	C6-N1	2.66	1.39	1.34
1	6-D	197	LLP	C6-N1	2.65	1.39	1.34
1	9-D	197	LLP	C6-N1	2.64	1.39	1.34
1	1-D	197	LLP	C6-N1	2.64	1.39	1.34
1	5-H	197	LLP	C4-C5	-2.63	1.38	1.42
1	9-B	197	LLP	C6-N1	2.63	1.39	1.34
1	1-C	197	LLP	C6-N1	2.63	1.39	1.34
1	9-E	197	LLP	C6-N1	2.62	1.39	1.34
1	2-H	197	LLP	C6-N1	2.62	1.39	1.34
1	1-H	197	LLP	C6-N1	2.61	1.39	1.34
1	4-H	197	LLP	C5'-C5	2.61	1.57	1.50
1	2-D	197	LLP	C6-N1	2.61	1.39	1.34
1	3-G	197	LLP	C6-N1	2.61	1.39	1.34
1	1-H	197	LLP	C4-C5	-2.59	1.38	1.42
1	5-E	197	LLP	C6-N1	2.59	1.39	1.34
1	9-H	197	LLP	C4-C5	-2.59	1.38	1.42
1	6-C	197	LLP	C3-C2	2.58	1.43	1.41
1	7-H	197	LLP	C6-N1	2.58	1.39	1.34
1	9-H	197	LLP	C5'-C5	2.57	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-G	197	LLP	C6-N1	2.57	1.39	1.34
1	5-C	197	LLP	C6-N1	2.56	1.39	1.34
1	10-D	197	LLP	C6-N1	2.56	1.39	1.34
1	3-H	197	LLP	C5'-C5	2.55	1.57	1.50
1	10-H	197	LLP	C5'-C5	2.55	1.57	1.50
1	5-D	197	LLP	C6-N1	2.55	1.39	1.34
1	10-E	197	LLP	C6-N1	2.55	1.39	1.34
1	1-C	197	LLP	C5'-C5	2.53	1.57	1.50
1	6-G	197	LLP	C6-N1	2.53	1.39	1.34
1	7-D	197	LLP	C6-N1	2.53	1.39	1.34
1	7-G	197	LLP	C4-C5	-2.53	1.38	1.42
1	9-G	197	LLP	C6-N1	2.53	1.39	1.34
1	3-C	197	LLP	C4-C5	-2.52	1.38	1.42
1	1-F	197	LLP	C5'-C5	2.51	1.57	1.50
1	5-C	197	LLP	C5'-C5	2.51	1.57	1.50
1	2-G	197	LLP	C6-N1	2.50	1.39	1.34
1	6-C	197	LLP	C5'-C5	2.50	1.57	1.50
1	10-G	197	LLP	C6-N1	2.50	1.39	1.34
1	3-D	197	LLP	C6-N1	2.50	1.39	1.34
1	1-A	197	LLP	C5'-C5	2.49	1.57	1.50
1	4-H	197	LLP	C4-C5	-2.48	1.38	1.42
1	4-B	197	LLP	C5'-C5	2.47	1.57	1.50
1	8-H	197	LLP	C4-C5	-2.46	1.38	1.42
1	4-B	197	LLP	C4-C5	-2.46	1.38	1.42
1	4-F	197	LLP	C5'-C5	2.46	1.57	1.50
1	2-G	197	LLP	C3-C2	2.45	1.43	1.41
1	5-F	197	LLP	C5'-C5	2.45	1.57	1.50
1	10-H	197	LLP	C4-C5	-2.45	1.38	1.42
1	2-F	197	LLP	C5'-C5	2.45	1.57	1.50
1	10-G	197	LLP	C4-C5	-2.45	1.38	1.42
1	1-G	197	LLP	C3-C2	2.44	1.43	1.41
1	6-A	197	LLP	C5'-C5	2.44	1.57	1.50
1	1-G	197	LLP	C6-N1	2.43	1.39	1.34
1	2-E	197	LLP	C5'-C5	2.43	1.57	1.50
1	6-H	197	LLP	C5'-C5	2.43	1.57	1.50
1	6-B	197	LLP	C6-N1	2.42	1.39	1.34
1	8-F	197	LLP	C5'-C5	2.42	1.57	1.50
1	4-E	197	LLP	C4-C5	-2.41	1.38	1.42
1	1-B	197	LLP	C3-C2	2.41	1.43	1.41
1	7-E	197	LLP	C5'-C5	2.39	1.57	1.50
1	8-C	197	LLP	C5'-C5	2.39	1.57	1.50
1	2-C	197	LLP	C5'-C5	2.39	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-F	197	LLP	C5'-C5	2.39	1.57	1.50
1	2-G	197	LLP	C5'-C5	2.38	1.57	1.50
1	2-H	197	LLP	C5'-C5	2.38	1.57	1.50
1	8-A	197	LLP	C5'-C5	2.38	1.57	1.50
1	3-E	197	LLP	C5'-C5	2.37	1.57	1.50
1	7-F	197	LLP	C5'-C5	2.36	1.57	1.50
1	7-G	197	LLP	C5'-C5	2.35	1.57	1.50
1	9-A	197	LLP	C5'-C5	2.35	1.57	1.50
1	4-G	197	LLP	C5'-C5	2.35	1.57	1.50
1	10-F	197	LLP	C5'-C5	2.34	1.57	1.50
1	7-G	197	LLP	C6-N1	2.33	1.39	1.34
1	1-G	197	LLP	C5'-C5	2.33	1.57	1.50
1	1-B	197	LLP	C5'-C5	2.33	1.57	1.50
1	2-A	197	LLP	C5'-C5	2.33	1.57	1.50
1	4-E	197	LLP	C5'-C5	2.33	1.57	1.50
1	6-G	197	LLP	C5'-C5	2.33	1.57	1.50
1	7-H	197	LLP	C5'-C5	2.33	1.57	1.50
1	6-G	197	LLP	C3-C2	2.33	1.43	1.41
1	4-D	197	LLP	C5'-C5	2.31	1.56	1.50
1	3-A	197	LLP	C5'-C5	2.31	1.56	1.50
1	3-F	197	LLP	C5'-C5	2.31	1.56	1.50
1	3-G	197	LLP	C5'-C5	2.31	1.56	1.50
1	2-B	197	LLP	C3-C2	2.30	1.43	1.41
1	8-H	197	LLP	C5'-C5	2.30	1.56	1.50
1	1-E	197	LLP	C5'-C5	2.30	1.56	1.50
1	8-D	197	LLP	C5'-C5	2.28	1.56	1.50
1	6-H	197	LLP	C4-C5	-2.27	1.38	1.42
1	5-G	197	LLP	C5'-C5	2.27	1.56	1.50
1	10-A	197	LLP	C5'-C5	2.27	1.56	1.50
1	10-C	197	LLP	C5'-C5	2.26	1.56	1.50
1	7-C	197	LLP	C5'-C5	2.24	1.56	1.50
1	5-E	197	LLP	C5'-C5	2.24	1.56	1.50
1	4-C	197	LLP	C5'-C5	2.23	1.56	1.50
1	9-E	197	LLP	C5'-C5	2.22	1.56	1.50
1	9-F	197	LLP	C5'-C5	2.21	1.56	1.50
1	5-G	197	LLP	C6-N1	2.21	1.38	1.34
1	9-G	197	LLP	C5'-C5	2.21	1.56	1.50
1	4-A	197	LLP	C5'-C5	2.20	1.56	1.50
1	6-D	197	LLP	C5'-C5	2.20	1.56	1.50
1	5-H	197	LLP	C5'-C5	2.19	1.56	1.50
1	7-A	197	LLP	C5'-C5	2.19	1.56	1.50
1	7-G	197	LLP	C3-C2	2.18	1.43	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-E	197	LLP	C5'-C5	2.18	1.56	1.50
1	10-G	197	LLP	C5'-C5	2.17	1.56	1.50
1	9-C	197	LLP	C5'-C5	2.17	1.56	1.50
1	5-B	197	LLP	C5'-C5	2.17	1.56	1.50
1	5-A	197	LLP	C5'-C5	2.15	1.56	1.50
1	2-A	197	LLP	C3-C2	2.14	1.43	1.41
1	6-E	197	LLP	C5'-C5	2.14	1.56	1.50
1	3-B	197	LLP	C5'-C5	2.13	1.56	1.50
1	9-B	197	LLP	C5'-C5	2.13	1.56	1.50
1	7-B	197	LLP	C5'-C5	2.13	1.56	1.50
1	3-D	197	LLP	C5'-C5	2.11	1.56	1.50
1	2-B	197	LLP	C5'-C5	2.11	1.56	1.50
1	2-D	197	LLP	C5'-C5	2.10	1.56	1.50
1	6-A	197	LLP	C3-C2	2.10	1.43	1.41
1	10-G	197	LLP	C3-C2	2.09	1.43	1.41
1	10-D	197	LLP	C5'-C5	2.09	1.56	1.50
1	5-E	197	LLP	O3-C3	2.09	1.41	1.36
1	1-H	197	LLP	C5'-C5	2.09	1.56	1.50
1	10-E	197	LLP	C5'-C5	2.07	1.56	1.50
1	3-G	197	LLP	C3-C2	2.05	1.43	1.41
1	7-E	197	LLP	C3-C2	2.05	1.43	1.41
1	1-D	197	LLP	C5'-C5	2.05	1.56	1.50
1	7-D	197	LLP	C5'-C5	2.05	1.56	1.50
1	9-B	197	LLP	C4-C3	-2.04	1.37	1.41
1	4-E	197	LLP	C3-C2	2.02	1.43	1.41
1	10-E	197	LLP	C3-C2	2.02	1.43	1.41
1	10-B	197	LLP	C4-C3	-2.01	1.37	1.41
1	10-C	197	LLP	C3-C2	2.00	1.43	1.41
1	9-D	197	LLP	C5'-C5	2.00	1.56	1.50

All (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
1	3-G	197	LLP	C4-C4'-NZ	-3.48	107.96	124.04
1	5-D	197	LLP	C4-C4'-NZ	-3.46	108.07	124.04
1	4-D	197	LLP	C4-C4'-NZ	-3.43	108.21	124.04
1	7-C	197	LLP	C4-C4'-NZ	-3.43	108.23	124.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-G	197	LLP	CE-NZ-C4'	-3.38	107.91	118.72
1	9-B	197	LLP	CE-NZ-C4'	-3.33	108.05	118.72
1	1-C	197	LLP	C4-C4'-NZ	-3.32	108.70	124.04
1	4-C	197	LLP	OP4-C5'-C5	3.32	115.57	109.36
1	10-G	197	LLP	CE-NZ-C4'	-3.32	108.09	118.72
1	3-A	197	LLP	OP4-C5'-C5	3.30	115.54	109.36
1	6-E	197	LLP	C4-C4'-NZ	-3.24	109.09	124.04
1	6-B	197	LLP	CE-NZ-C4'	-3.18	108.52	118.72
1	5-F	197	LLP	C4-C4'-NZ	-3.18	109.38	124.04
1	10-C	197	LLP	C4-C4'-NZ	-3.13	109.58	124.04
1	8-B	197	LLP	CE-NZ-C4'	-3.12	108.73	118.72
1	2-C	197	LLP	CE-NZ-C4'	-3.10	108.79	118.72
1	2-A	197	LLP	OP4-C5'-C5	3.10	115.16	109.36
1	2-H	197	LLP	CE-NZ-C4'	-3.07	108.89	118.72
1	9-A	197	LLP	C4-C4'-NZ	-3.04	110.02	124.04
1	1-D	197	LLP	C4-C4'-NZ	-3.04	110.02	124.04
1	6-C	197	LLP	CE-NZ-C4'	-3.04	108.99	118.72
1	5-G	197	LLP	CE-NZ-C4'	-3.02	109.04	118.72
1	7-A	197	LLP	OP4-C5'-C5	3.01	114.99	109.36
1	9-E	197	LLP	C4-C4'-NZ	-2.95	110.44	124.04
1	2-F	197	LLP	C4-C4'-NZ	-2.91	110.62	124.04
1	1-E	197	LLP	C4-C4'-NZ	-2.89	110.69	124.04
1	1-A	197	LLP	C4-C4'-NZ	-2.89	110.72	124.04
1	2-D	197	LLP	C4-C4'-NZ	-2.86	110.84	124.04
1	4-A	197	LLP	CE-NZ-C4'	-2.85	109.61	118.72
1	10-D	197	LLP	C4-C4'-NZ	-2.84	110.94	124.04
1	10-H	197	LLP	CE-NZ-C4'	-2.84	109.63	118.72
1	3-C	197	LLP	C4-C4'-NZ	-2.83	110.96	124.04
1	6-C	197	LLP	OP4-C5'-C5	2.83	114.66	109.36
1	5-C	197	LLP	C5'-C5-C6	-2.83	114.75	119.36
1	9-C	197	LLP	C4-C4'-NZ	-2.83	111.00	124.04
1	4-A	197	LLP	OP4-C5'-C5	2.82	114.65	109.36
1	6-D	197	LLP	C4-C4'-NZ	-2.82	111.03	124.04
1	9-B	197	LLP	C4-C4'-NZ	-2.82	111.04	124.04
1	8-F	197	LLP	C4-C4'-NZ	-2.82	111.04	124.04
1	5-A	197	LLP	C4-C4'-NZ	-2.80	111.10	124.04
1	6-A	197	LLP	C4-C4'-NZ	-2.80	111.13	124.04
1	5-H	197	LLP	C4-C4'-NZ	-2.79	111.16	124.04
1	9-B	197	LLP	C5-C6-N1	-2.78	119.31	123.83
1	9-F	197	LLP	C5-C6-N1	-2.78	119.31	123.83
1	5-F	197	LLP	C3-C4-C5	2.78	120.50	118.28
1	3-D	197	LLP	C4-C4'-NZ	-2.77	111.26	124.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-G	197	LLP	CE-NZ-C4'	-2.77	109.85	118.72
1	4-H	197	LLP	OP4-C5'-C5	2.76	114.53	109.36
1	6-C	197	LLP	C5'-C5-C6	-2.74	114.89	119.36
1	4-A	197	LLP	C4-C4'-NZ	-2.74	111.42	124.04
1	4-H	197	LLP	C4-C4'-NZ	-2.73	111.46	124.04
1	3-A	197	LLP	C4-C4'-NZ	-2.72	111.50	124.04
1	1-A	197	LLP	CE-NZ-C4'	-2.71	110.04	118.72
1	7-H	197	LLP	C5-C6-N1	-2.70	119.43	123.83
1	2-G	197	LLP	CE-NZ-C4'	-2.70	110.06	118.72
1	9-H	197	LLP	CE-NZ-C4'	-2.70	110.06	118.72
1	9-D	197	LLP	CE-NZ-C4'	-2.69	110.09	118.72
1	7-F	197	LLP	OP4-C5'-C5	2.69	114.41	109.36
1	6-H	197	LLP	CE-NZ-C4'	-2.69	110.11	118.72
1	1-B	197	LLP	CE-NZ-C4'	-2.68	110.12	118.72
1	1-G	197	LLP	C4-C4'-NZ	-2.68	111.67	124.04
1	7-B	197	LLP	CE-NZ-C4'	-2.68	110.13	118.72
1	7-F	197	LLP	C4-C4'-NZ	-2.67	111.74	124.04
1	1-F	197	LLP	C4-C4'-NZ	-2.66	111.78	124.04
1	7-H	197	LLP	C4-C4'-NZ	-2.65	111.82	124.04
1	1-H	197	LLP	C5-C6-N1	-2.64	119.53	123.83
1	8-A	197	LLP	C4-C4'-NZ	-2.64	111.87	124.04
1	8-C	197	LLP	C4-C4'-NZ	-2.63	111.88	124.04
1	6-F	197	LLP	CE-NZ-C4'	-2.63	110.28	118.72
1	4-F	197	LLP	C4-C4'-NZ	-2.63	111.89	124.04
1	9-D	197	LLP	C5-C6-N1	-2.63	119.55	123.83
1	7-H	197	LLP	CE-NZ-C4'	-2.63	110.30	118.72
1	9-B	197	LLP	C3-C4-C5	2.61	120.37	118.28
1	3-B	197	LLP	OP4-C5'-C5	2.60	114.24	109.36
1	5-D	197	LLP	C5-C6-N1	-2.60	119.61	123.83
1	10-E	197	LLP	C4-C4'-NZ	-2.58	112.13	124.04
1	9-F	197	LLP	C4-C4'-NZ	-2.58	112.14	124.04
1	7-D	197	LLP	C4-C4'-NZ	-2.58	112.15	124.04
1	5-F	197	LLP	C5-C6-N1	-2.58	119.64	123.83
1	2-H	197	LLP	C5-C6-N1	-2.57	119.64	123.83
1	2-H	197	LLP	C4-C4'-NZ	-2.57	112.19	124.04
1	10-C	197	LLP	OP4-C5'-C5	2.56	114.15	109.36
1	6-D	197	LLP	CE-NZ-C4'	-2.55	110.54	118.72
1	10-F	197	LLP	C4-C4'-NZ	-2.54	112.31	124.04
1	5-E	197	LLP	CE-NZ-C4'	-2.54	110.58	118.72
1	8-C	197	LLP	CE-NZ-C4'	-2.54	110.59	118.72
1	9-G	197	LLP	CE-NZ-C4'	-2.53	110.62	118.72
1	5-H	197	LLP	CE-NZ-C4'	-2.53	110.62	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-H	197	LLP	C4-C4'-NZ	-2.53	112.37	124.04
1	6-F	197	LLP	C5-C6-N1	-2.53	119.72	123.83
1	8-H	197	LLP	CE-NZ-C4'	-2.52	110.64	118.72
1	9-C	197	LLP	CE-NZ-C4'	-2.52	110.65	118.72
1	7-A	197	LLP	C4-C4'-NZ	-2.52	112.42	124.04
1	7-D	197	LLP	C5-C6-N1	-2.51	119.74	123.83
1	1-F	197	LLP	OP4-C5'-C5	2.51	114.06	109.36
1	9-H	197	LLP	C5-C6-N1	-2.50	119.77	123.83
1	10-H	197	LLP	C5-C6-N1	-2.50	119.77	123.83
1	6-B	197	LLP	C5-C6-N1	-2.49	119.79	123.83
1	8-H	197	LLP	C5-C6-N1	-2.49	119.79	123.83
1	7-B	197	LLP	C5-C6-N1	-2.48	119.79	123.83
1	9-D	197	LLP	C4-C4'-NZ	-2.48	112.61	124.04
1	8-D	197	LLP	CE-NZ-C4'	-2.47	110.80	118.72
1	3-F	197	LLP	C5-C6-N1	-2.47	119.81	123.83
1	2-F	197	LLP	OP4-C5'-C5	2.47	113.98	109.36
1	2-D	197	LLP	C5-C6-N1	-2.46	119.83	123.83
1	9-B	197	LLP	C2'-C2-N1	2.46	122.27	117.64
1	10-A	197	LLP	C4-C4'-NZ	-2.46	112.71	124.04
1	8-D	197	LLP	CG-CD-CE	-2.46	104.82	113.38
1	2-B	197	LLP	C4-C4'-NZ	-2.45	112.72	124.04
1	2-F	197	LLP	C5-C6-N1	-2.45	119.85	123.83
1	10-F	197	LLP	OP4-C5'-C5	2.44	113.93	109.36
1	8-F	197	LLP	CE-NZ-C4'	-2.44	110.92	118.72
1	10-B	197	LLP	CE-NZ-C4'	-2.44	110.92	118.72
1	5-E	197	LLP	C4-C4'-NZ	-2.43	112.81	124.04
1	8-G	197	LLP	C3-C4-C5	2.42	120.22	118.28
1	3-H	197	LLP	OP4-C5'-C5	2.42	113.89	109.36
1	8-F	197	LLP	OP4-C5'-C5	2.42	113.89	109.36
1	7-D	197	LLP	CE-NZ-C4'	-2.41	110.99	118.72
1	5-H	197	LLP	C5-C6-N1	-2.41	119.91	123.83
1	8-A	197	LLP	CE-NZ-C4'	-2.41	111.01	118.72
1	5-D	197	LLP	CE-NZ-C4'	-2.41	111.01	118.72
1	4-C	197	LLP	C4-C4'-NZ	-2.40	112.96	124.04
1	1-D	197	LLP	C5-C6-N1	-2.40	119.92	123.83
1	2-C	197	LLP	C4-C4'-NZ	-2.40	112.97	124.04
1	10-B	197	LLP	C2'-C2-C3	-2.39	118.00	120.80
1	9-B	197	LLP	C2'-C2-C3	-2.38	118.01	120.80
1	7-E	197	LLP	CE-NZ-C4'	-2.38	111.09	118.72
1	6-F	197	LLP	C4-C4'-NZ	-2.38	113.08	124.04
1	1-H	197	LLP	CE-NZ-C4'	-2.37	111.13	118.72
1	3-A	197	LLP	CE-NZ-C4'	-2.37	111.13	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-H	197	LLP	C4-C4'-NZ	-2.37	113.11	124.04
1	3-E	197	LLP	CE-NZ-C4'	-2.37	111.13	118.72
1	10-B	197	LLP	C4-C4'-NZ	-2.35	113.20	124.04
1	6-D	197	LLP	C5-C6-N1	-2.35	120.01	123.83
1	2-B	197	LLP	CE-NZ-C4'	-2.35	111.20	118.72
1	8-D	197	LLP	C4-C4'-NZ	-2.35	113.22	124.04
1	10-D	197	LLP	CE-NZ-C4'	-2.34	111.23	118.72
1	4-F	197	LLP	OP4-C5'-C5	2.34	113.74	109.36
1	10-A	197	LLP	CE-NZ-C4'	-2.34	111.24	118.72
1	6-H	197	LLP	C5-C6-N1	-2.33	120.04	123.83
1	6-H	197	LLP	C4-C4'-NZ	-2.33	113.28	124.04
1	10-D	197	LLP	C5-C6-N1	-2.33	120.04	123.83
1	4-C	197	LLP	CE-NZ-C4'	-2.33	111.25	118.72
1	2-C	197	LLP	C5-C6-N1	-2.33	120.04	123.83
1	3-B	197	LLP	CD-CE-NZ	2.33	116.99	110.83
1	3-D	197	LLP	C5-C6-N1	-2.33	120.04	123.83
1	10-E	197	LLP	C5-C6-N1	-2.33	120.05	123.83
1	8-A	197	LLP	OP4-C5'-C5	2.33	113.72	109.36
1	1-G	197	LLP	CE-NZ-C4'	-2.32	111.29	118.72
1	4-F	197	LLP	CE-NZ-C4'	-2.32	111.29	118.72
1	1-E	197	LLP	C5-C6-N1	-2.31	120.07	123.83
1	4-B	197	LLP	CE-NZ-C4'	-2.30	111.36	118.72
1	2-E	197	LLP	CD-CE-NZ	2.30	116.91	110.83
1	8-E	197	LLP	C5-C6-N1	-2.29	120.11	123.83
1	8-B	197	LLP	C5-C6-N1	-2.29	120.11	123.83
1	8-F	197	LLP	C5-C6-N1	-2.29	120.11	123.83
1	10-E	197	LLP	CE-NZ-C4'	-2.28	111.41	118.72
1	9-E	197	LLP	CE-NZ-C4'	-2.28	111.42	118.72
1	1-H	197	LLP	C4-C4'-NZ	-2.28	113.52	124.04
1	8-D	197	LLP	C5-C6-N1	-2.28	120.13	123.83
1	6-G	197	LLP	C4-C4'-NZ	-2.27	113.56	124.04
1	10-F	197	LLP	C5-C6-N1	-2.27	120.14	123.83
1	4-F	197	LLP	C5-C6-N1	-2.27	120.14	123.83
1	3-C	197	LLP	CE-NZ-C4'	-2.27	111.46	118.72
1	1-F	197	LLP	C5-C6-N1	-2.27	120.15	123.83
1	4-E	197	LLP	C5-C6-N1	-2.26	120.16	123.83
1	8-E	197	LLP	CE-NZ-C4'	-2.26	111.49	118.72
1	1-D	197	LLP	CE-NZ-C4'	-2.25	111.51	118.72
1	9-G	197	LLP	C5-C6-N1	-2.25	120.17	123.83
1	2-B	197	LLP	C5-C6-N1	-2.25	120.17	123.83
1	3-B	197	LLP	C5-C6-N1	-2.25	120.18	123.83
1	8-E	197	LLP	C4-C4'-NZ	-2.24	113.68	124.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-C	197	LLP	OP4-C5'-C5	2.24	113.56	109.36
1	9-E	197	LLP	C5-C6-N1	-2.23	120.20	123.83
1	1-C	197	LLP	C5'-C5-C6	-2.23	115.72	119.36
1	7-C	197	LLP	C5-C6-N1	-2.23	120.20	123.83
1	2-D	197	LLP	CE-NZ-C4'	-2.22	111.60	118.72
1	1-F	197	LLP	CE-NZ-C4'	-2.22	111.61	118.72
1	3-C	197	LLP	C4-C3-C2	2.21	121.39	120.14
1	3-A	197	LLP	C5-C6-N1	-2.20	120.25	123.83
1	5-E	197	LLP	C5-C6-N1	-2.20	120.25	123.83
1	5-G	197	LLP	C5-C6-N1	-2.20	120.25	123.83
1	10-B	197	LLP	C5-C6-N1	-2.20	120.26	123.83
1	10-B	197	LLP	C2'-C2-N1	2.20	121.78	117.64
1	1-E	197	LLP	CE-NZ-C4'	-2.19	111.69	118.72
1	5-A	197	LLP	CE-NZ-C4'	-2.19	111.70	118.72
1	9-A	197	LLP	C5-C6-N1	-2.19	120.27	123.83
1	10-C	197	LLP	CE-NZ-C4'	-2.19	111.72	118.72
1	2-E	197	LLP	C4-C3-C2	2.19	121.37	120.14
1	8-C	197	LLP	C5'-C5-C6	-2.18	115.81	119.36
1	6-B	197	LLP	C4-C4'-NZ	-2.18	113.99	124.04
1	9-A	197	LLP	CE-NZ-C4'	-2.18	111.75	118.72
1	7-F	197	LLP	C5-C6-N1	-2.18	120.29	123.83
1	1-C	197	LLP	OP4-C5'-C5	2.18	113.43	109.36
1	5-B	197	LLP	C4-C4'-NZ	-2.17	114.03	124.04
1	3-B	197	LLP	CE-NZ-C4'	-2.17	111.78	118.72
1	4-G	197	LLP	C5-C6-N1	-2.16	120.32	123.83
1	2-G	197	LLP	C4-C4'-NZ	-2.16	114.09	124.04
1	9-H	197	LLP	C4-C4'-NZ	-2.15	114.10	124.04
1	10-G	197	LLP	C4-C4'-NZ	-2.15	114.11	124.04
1	5-C	197	LLP	OP4-C5'-C5	2.15	113.39	109.36
1	3-C	197	LLP	C5'-C5-C6	-2.15	115.86	119.36
1	7-E	197	LLP	C4-C4'-NZ	-2.15	114.14	124.04
1	10-B	197	LLP	OP4-C5'-C5	2.14	113.37	109.36
1	7-A	197	LLP	C5-C6-N1	-2.14	120.35	123.83
1	7-C	197	LLP	CE-NZ-C4'	-2.14	111.86	118.72
1	7-A	197	LLP	CE-NZ-C4'	-2.14	111.87	118.72
1	4-C	197	LLP	C5-C6-N1	-2.14	120.36	123.83
1	1-B	197	LLP	C4-C4'-NZ	-2.13	114.22	124.04
1	1-A	197	LLP	C5-C6-N1	-2.13	120.37	123.83
1	7-G	197	LLP	C5'-C5-C6	-2.13	115.89	119.36
1	2-E	197	LLP	OP3-P-OP4	2.12	112.19	106.67
1	4-A	197	LLP	C5-C6-N1	-2.11	120.39	123.83
1	5-B	197	LLP	CE-NZ-C4'	-2.11	111.95	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-B	197	LLP	C4-C4'-NZ	-2.11	114.31	124.04
1	3-H	197	LLP	C5-C6-N1	-2.11	120.40	123.83
1	5-B	197	LLP	OP4-C5'-C5	2.10	113.30	109.36
1	5-A	197	LLP	C5-C6-N1	-2.10	120.42	123.83
1	6-A	197	LLP	CE-NZ-C4'	-2.10	112.00	118.72
1	9-F	197	LLP	CE-NZ-C4'	-2.10	112.00	118.72
1	5-F	197	LLP	CE-NZ-C4'	-2.10	112.01	118.72
1	9-E	197	LLP	C3-C4-C5	2.09	119.96	118.28
1	7-G	197	LLP	CE-NZ-C4'	-2.09	112.03	118.72
1	4-D	197	LLP	C5-C6-N1	-2.09	120.44	123.83
1	4-H	197	LLP	C5-C6-N1	-2.09	120.44	123.83
1	7-G	197	LLP	C5-C6-N1	-2.08	120.45	123.83
1	5-C	197	LLP	C5-C6-N1	-2.08	120.45	123.83
1	2-E	197	LLP	CE-NZ-C4'	-2.07	112.09	118.72
1	7-F	197	LLP	CE-NZ-C4'	-2.07	112.10	118.72
1	3-D	197	LLP	CE-NZ-C4'	-2.06	112.12	118.72
1	9-A	197	LLP	C3-C4-C5	2.06	119.93	118.28
1	2-A	197	LLP	C4-C4'-NZ	-2.05	114.58	124.04
1	3-E	197	LLP	C5-C6-N1	-2.05	120.50	123.83
1	10-C	197	LLP	C5-C6-N1	-2.05	120.50	123.83
1	7-C	197	LLP	C2'-C2-N1	2.04	121.49	117.64
1	5-G	197	LLP	C5'-C5-C6	-2.03	116.05	119.36
1	3-B	197	LLP	C4-C4'-NZ	-2.03	114.67	124.04
1	5-B	197	LLP	C5-C6-N1	-2.03	120.53	123.83
1	5-D	197	LLP	C2'-C2-N1	2.03	121.47	117.64
1	6-G	197	LLP	C5-C6-N1	-2.03	120.54	123.83
1	6-E	197	LLP	C5-C6-N1	-2.03	120.54	123.83
1	1-B	197	LLP	C5-C6-N1	-2.02	120.55	123.83
1	10-F	197	LLP	CE-NZ-C4'	-2.02	112.26	118.72
1	7-E	197	LLP	C5-C6-N1	-2.01	120.56	123.83
1	9-C	197	LLP	C5-C6-N1	-2.01	120.57	123.83

There are no chirality outliers.

All (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
1	3-A	197	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	4-A	197	LLP	O-C-CA-CB
1	5-A	197	LLP	O-C-CA-CB
1	6-A	197	LLP	O-C-CA-CB
1	7-A	197	LLP	O-C-CA-CB
1	8-A	197	LLP	O-C-CA-CB
1	9-A	197	LLP	O-C-CA-CB
1	10-A	197	LLP	O-C-CA-CB
1	1-B	197	LLP	O-C-CA-CB
1	2-B	197	LLP	O-C-CA-CB
1	3-B	197	LLP	C4-C4'-NZ-CE
1	3-B	197	LLP	C5'-OP4-P-OP2
1	3-B	197	LLP	C5'-OP4-P-OP3
1	3-B	197	LLP	O-C-CA-CB
1	4-B	197	LLP	O-C-CA-CB
1	5-B	197	LLP	O-C-CA-CB
1	6-B	197	LLP	O-C-CA-CB
1	7-B	197	LLP	O-C-CA-CB
1	8-B	197	LLP	O-C-CA-CB
1	9-B	197	LLP	C-CA-CB-CG
1	9-B	197	LLP	O-C-CA-CB
1	10-B	197	LLP	C4-C4'-NZ-CE
1	10-B	197	LLP	C5'-OP4-P-OP2
1	10-B	197	LLP	O-C-CA-CB
1	1-C	197	LLP	O-C-CA-CB
1	3-C	197	LLP	C4-C5-C5'-OP4
1	3-C	197	LLP	C6-C5-C5'-OP4
1	3-C	197	LLP	O-C-CA-CB
1	4-C	197	LLP	C4-C4'-NZ-CE
1	4-C	197	LLP	O-C-CA-CB
1	5-C	197	LLP	O-C-CA-CB
1	6-C	197	LLP	C4-C4'-NZ-CE
1	6-C	197	LLP	O-C-CA-CB
1	7-C	197	LLP	O-C-CA-CB
1	8-C	197	LLP	O-C-CA-CB
1	9-C	197	LLP	C4-C4'-NZ-CE
1	9-C	197	LLP	O-C-CA-CB
1	10-C	197	LLP	C4-C4'-NZ-CE
1	10-C	197	LLP	O-C-CA-CB
1	1-D	197	LLP	O-C-CA-CB
1	2-D	197	LLP	C-CA-CB-CG
1	2-D	197	LLP	O-C-CA-CB
1	3-D	197	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	5-D	197	LLP	O-C-CA-CB
1	6-D	197	LLP	O-C-CA-CB
1	7-D	197	LLP	C4-C4'-NZ-CE
1	7-D	197	LLP	O-C-CA-CB
1	8-D	197	LLP	C4-C4'-NZ-CE
1	8-D	197	LLP	O-C-CA-CB
1	9-D	197	LLP	O-C-CA-CB
1	10-D	197	LLP	O-C-CA-CB
1	1-E	197	LLP	O-C-CA-CB
1	2-E	197	LLP	O-C-CA-CB
1	2-E	197	LLP	CA-CB-CG-CD
1	3-E	197	LLP	O-C-CA-CB
1	4-E	197	LLP	O-C-CA-CB
1	5-E	197	LLP	O-C-CA-CB
1	6-E	197	LLP	O-C-CA-CB
1	7-E	197	LLP	O-C-CA-CB
1	8-E	197	LLP	O-C-CA-CB
1	9-E	197	LLP	O-C-CA-CB
1	10-E	197	LLP	O-C-CA-CB
1	1-F	197	LLP	O-C-CA-CB
1	2-F	197	LLP	O-C-CA-CB
1	3-F	197	LLP	O-C-CA-CB
1	4-F	197	LLP	O-C-CA-CB
1	5-F	197	LLP	O-C-CA-CB
1	6-F	197	LLP	O-C-CA-CB
1	7-F	197	LLP	O-C-CA-CB
1	8-F	197	LLP	O-C-CA-CB
1	9-F	197	LLP	O-C-CA-CB
1	10-F	197	LLP	O-C-CA-CB
1	1-G	197	LLP	O-C-CA-CB
1	2-G	197	LLP	O-C-CA-CB
1	3-G	197	LLP	O-C-CA-CB
1	4-G	197	LLP	O-C-CA-CB
1	5-G	197	LLP	O-C-CA-CB
1	7-G	197	LLP	O-C-CA-CB
1	8-G	197	LLP	O-C-CA-CB
1	9-G	197	LLP	O-C-CA-CB
1	10-G	197	LLP	C4-C4'-NZ-CE
1	10-G	197	LLP	O-C-CA-CB
1	1-H	197	LLP	O-C-CA-CB
1	2-H	197	LLP	O-C-CA-CB
1	3-H	197	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	3-H	197	LLP	C4-C5-C5'-OP4
1	3-H	197	LLP	O-C-CA-CB
1	4-H	197	LLP	C4-C4'-NZ-CE
1	4-H	197	LLP	O-C-CA-CB
1	5-H	197	LLP	O-C-CA-CB
1	6-H	197	LLP	O-C-CA-CB
1	7-H	197	LLP	C4-C4'-NZ-CE
1	7-H	197	LLP	O-C-CA-CB
1	8-H	197	LLP	O-C-CA-CB
1	9-H	197	LLP	O-C-CA-CB
1	10-H	197	LLP	O-C-CA-CB
1	3-A	197	LLP	C4-C4'-NZ-CE
1	4-A	197	LLP	C4-C4'-NZ-CE
1	5-A	197	LLP	C4-C4'-NZ-CE
1	4-B	197	LLP	C4-C4'-NZ-CE
1	8-B	197	LLP	C4-C4'-NZ-CE
1	9-G	197	LLP	C4-C4'-NZ-CE
1	3-B	197	LLP	CA-CB-CG-CD
1	7-A	197	LLP	C4-C4'-NZ-CE
1	8-A	197	LLP	C4-C4'-NZ-CE
1	10-A	197	LLP	C4-C4'-NZ-CE
1	1-B	197	LLP	C4-C4'-NZ-CE
1	2-B	197	LLP	C4-C4'-NZ-CE
1	5-B	197	LLP	C4-C4'-NZ-CE
1	7-B	197	LLP	C4-C4'-NZ-CE
1	9-B	197	LLP	C4-C4'-NZ-CE
1	8-C	197	LLP	C4-C4'-NZ-CE
1	2-D	197	LLP	C4-C4'-NZ-CE
1	8-E	197	LLP	C4-C4'-NZ-CE
1	1-F	197	LLP	C4-C4'-NZ-CE
1	2-F	197	LLP	C4-C4'-NZ-CE
1	9-F	197	LLP	C4-C4'-NZ-CE
1	1-G	197	LLP	C4-C4'-NZ-CE
1	2-G	197	LLP	C4-C4'-NZ-CE
1	5-G	197	LLP	C4-C4'-NZ-CE
1	1-E	197	LLP	CA-CB-CG-CD
1	9-D	197	LLP	C4-C4'-NZ-CE
1	3-E	197	LLP	C4-C4'-NZ-CE
1	8-F	197	LLP	C4-C4'-NZ-CE
1	1-H	197	LLP	C4-C4'-NZ-CE
1	8-D	197	LLP	CA-CB-CG-CD
1	6-D	197	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	6-B	197	LLP	C4-C4'-NZ-CE
1	2-C	197	LLP	C4-C4'-NZ-CE
1	1-D	197	LLP	C4-C4'-NZ-CE
1	3-D	197	LLP	C4-C4'-NZ-CE
1	4-D	197	LLP	C4-C4'-NZ-CE
1	5-D	197	LLP	C4-C4'-NZ-CE
1	5-E	197	LLP	C4-C4'-NZ-CE
1	7-E	197	LLP	C4-C4'-NZ-CE
1	7-F	197	LLP	C4-C4'-NZ-CE
1	6-G	197	LLP	C4-C4'-NZ-CE
1	9-H	197	LLP	C4-C4'-NZ-CE
1	10-H	197	LLP	C4-C4'-NZ-CE
1	6-F	197	LLP	C4-C4'-NZ-CE
1	2-H	197	LLP	C4-C4'-NZ-CE
1	6-H	197	LLP	C4-C4'-NZ-CE
1	2-A	197	LLP	CG-CD-CE-NZ
1	9-A	197	LLP	CG-CD-CE-NZ
1	9-B	197	LLP	CG-CD-CE-NZ
1	10-B	197	LLP	CG-CD-CE-NZ
1	1-C	197	LLP	CG-CD-CE-NZ
1	5-C	197	LLP	CG-CD-CE-NZ
1	7-C	197	LLP	CG-CD-CE-NZ
1	9-C	197	LLP	CG-CD-CE-NZ
1	2-D	197	LLP	CG-CD-CE-NZ
1	6-D	197	LLP	CG-CD-CE-NZ
1	8-D	197	LLP	CG-CD-CE-NZ
1	1-E	197	LLP	CG-CD-CE-NZ
1	2-E	197	LLP	CG-CD-CE-NZ
1	5-F	197	LLP	CG-CD-CE-NZ
1	8-G	197	LLP	CG-CD-CE-NZ
1	3-H	197	LLP	CG-CD-CE-NZ
1	6-G	197	LLP	CA-CB-CG-CD
1	5-B	197	LLP	CA-CB-CG-CD
1	9-E	197	LLP	CA-CB-CG-CD
1	9-B	197	LLP	C3-C4-C4'-NZ
1	10-C	197	LLP	C3-C4-C4'-NZ
1	4-D	197	LLP	C3-C4-C4'-NZ
1	9-F	197	LLP	C3-C4-C4'-NZ
1	3-A	197	LLP	CA-CB-CG-CD
1	6-A	197	LLP	CA-CB-CG-CD
1	5-H	197	LLP	C4-C4'-NZ-CE
1	1-A	197	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	10-D	197	LLP	C4-C4'-NZ-CE
1	2-E	197	LLP	C4-C4'-NZ-CE
1	9-E	197	LLP	C4-C4'-NZ-CE
1	10-F	197	LLP	C4-C4'-NZ-CE
1	3-G	197	LLP	CG-CD-CE-NZ
1	8-G	197	LLP	C5-C4-C4'-NZ
1	6-D	197	LLP	CA-CB-CG-CD
1	5-H	197	LLP	CA-CB-CG-CD
1	8-G	197	LLP	C3-C4-C4'-NZ
1	4-D	197	LLP	CA-CB-CG-CD
1	7-B	197	LLP	CG-CD-CE-NZ
1	10-C	197	LLP	CG-CD-CE-NZ
1	10-D	197	LLP	CG-CD-CE-NZ
1	3-F	197	LLP	CG-CD-CE-NZ
1	9-F	197	LLP	CG-CD-CE-NZ
1	6-G	197	LLP	CG-CD-CE-NZ
1	7-G	197	LLP	CG-CD-CE-NZ
1	7-H	197	LLP	CG-CD-CE-NZ
1	7-B	197	LLP	CA-CB-CG-CD
1	8-F	197	LLP	CA-CB-CG-CD
1	2-A	197	LLP	CA-CB-CG-CD
1	5-D	197	LLP	CA-CB-CG-CD
1	3-A	197	LLP	C5'-OP4-P-OP1
1	3-B	197	LLP	C5'-OP4-P-OP1
1	3-B	197	LLP	CG-CD-CE-NZ
1	8-B	197	LLP	CA-CB-CG-CD
1	5-F	197	LLP	CA-CB-CG-CD
1	9-C	197	LLP	CA-CB-CG-CD
1	3-H	197	LLP	CA-CB-CG-CD
1	4-A	197	LLP	CG-CD-CE-NZ
1	5-A	197	LLP	CG-CD-CE-NZ
1	4-B	197	LLP	CG-CD-CE-NZ
1	6-C	197	LLP	CG-CD-CE-NZ
1	5-G	197	LLP	CG-CD-CE-NZ
1	5-F	197	LLP	C3-C4-C4'-NZ
1	2-D	197	LLP	CD-CE-NZ-C4'
1	4-G	197	LLP	C4-C4'-NZ-CE
1	3-H	197	LLP	C6-C5-C5'-OP4
1	10-E	197	LLP	C4-C4'-NZ-CE
1	5-A	197	LLP	CA-CB-CG-CD
1	6-C	197	LLP	CA-CB-CG-CD
1	8-D	197	LLP	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	5-F	197	LLP	CD-CE-NZ-C4'
1	4-A	197	LLP	C5'-OP4-P-OP2
1	10-B	197	LLP	C5'-OP4-P-OP3
1	8-C	197	LLP	CG-CD-CE-NZ
1	4-E	197	LLP	CG-CD-CE-NZ
1	10-E	197	LLP	CG-CD-CE-NZ
1	8-F	197	LLP	CG-CD-CE-NZ
1	5-H	197	LLP	CG-CD-CE-NZ
1	1-C	197	LLP	CD-CE-NZ-C4'
1	8-G	197	LLP	CD-CE-NZ-C4'
1	9-D	197	LLP	CA-CB-CG-CD
1	3-A	197	LLP	CD-CE-NZ-C4'
1	7-C	197	LLP	CD-CE-NZ-C4'
1	4-D	197	LLP	CD-CE-NZ-C4'
1	4-E	197	LLP	CD-CE-NZ-C4'
1	2-A	197	LLP	C4-C5-C5'-OP4
1	4-A	197	LLP	C4-C5-C5'-OP4
1	4-C	197	LLP	C4-C5-C5'-OP4
1	9-C	197	LLP	C4-C5-C5'-OP4
1	4-D	197	LLP	C4-C5-C5'-OP4
1	4-H	197	LLP	C4-C5-C5'-OP4
1	8-C	197	LLP	CA-CB-CG-CD
1	6-A	197	LLP	C-CA-CB-CG
1	3-B	197	LLP	C-CA-CB-CG
1	4-D	197	LLP	CG-CD-CE-NZ
1	9-D	197	LLP	CG-CD-CE-NZ
1	6-E	197	LLP	CG-CD-CE-NZ
1	2-H	197	LLP	CG-CD-CE-NZ
1	3-B	197	LLP	CD-CE-NZ-C4'
1	2-H	197	LLP	CE-CD-CG-CB
1	7-A	197	LLP	CD-CE-NZ-C4'
1	5-C	197	LLP	CD-CE-NZ-C4'
1	8-D	197	LLP	CD-CE-NZ-C4'
1	3-F	197	LLP	CD-CE-NZ-C4'
1	9-F	197	LLP	CD-CE-NZ-C4'
1	3-G	197	LLP	CD-CE-NZ-C4'
1	3-A	197	LLP	C3-C4-C4'-NZ
1	10-B	197	LLP	C5'-OP4-P-OP1
1	10-A	197	LLP	CD-CE-NZ-C4'
1	2-B	197	LLP	CD-CE-NZ-C4'
1	5-B	197	LLP	CD-CE-NZ-C4'
1	10-B	197	LLP	CD-CE-NZ-C4'

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Mol	Chain	Res	Type	Atoms
1	10-C	197	LLP	CD-CE-NZ-C4'
1	3-B	197	LLP	C3-C4-C4'-NZ
1	1-C	197	LLP	C3-C4-C4'-NZ
1	5-C	197	LLP	C3-C4-C4'-NZ
1	7-C	197	LLP	C3-C4-C4'-NZ
1	3-F	197	LLP	C3-C4-C4'-NZ
1	3-G	197	LLP	C3-C4-C4'-NZ
1	3-B	197	LLP	CE-CD-CG-CB
1	2-D	197	LLP	CA-CB-CG-CD
1	5-B	197	LLP	CE-CD-CG-CB
1	4-A	197	LLP	CA-CB-CG-CD
1	4-B	197	LLP	CA-CB-CG-CD
1	9-A	197	LLP	CA-CB-CG-CD
1	7-G	197	LLP	CA-CB-CG-CD
1	9-E	197	LLP	CG-CD-CE-NZ
1	5-F	197	LLP	C5-C4-C4'-NZ
1	2-A	197	LLP	C6-C5-C5'-OP4
1	4-A	197	LLP	C6-C5-C5'-OP4
1	4-C	197	LLP	C6-C5-C5'-OP4
1	4-H	197	LLP	C6-C5-C5'-OP4
1	3-D	197	LLP	CA-CB-CG-CD
1	6-E	197	LLP	CD-CE-NZ-C4'
1	4-A	197	LLP	CD-CE-NZ-C4'
1	1-B	197	LLP	CD-CE-NZ-C4'
1	6-B	197	LLP	CD-CE-NZ-C4'
1	9-H	197	LLP	CD-CE-NZ-C4'
1	4-E	197	LLP	C3-C4-C4'-NZ
1	4-H	197	LLP	C3-C4-C4'-NZ
1	4-A	197	LLP	C5'-OP4-P-OP3
1	5-B	197	LLP	C5'-OP4-P-OP3
1	2-E	197	LLP	C5'-OP4-P-OP3
1	9-G	197	LLP	CG-CD-CE-NZ
1	10-G	197	LLP	CG-CD-CE-NZ
1	3-H	197	LLP	C5'-OP4-P-OP1
1	3-H	197	LLP	C5'-OP4-P-OP3
1	10-D	197	LLP	CD-CE-NZ-C4'
1	2-F	197	LLP	CD-CE-NZ-C4'
1	4-D	197	LLP	C5-C4-C4'-NZ
1	7-A	197	LLP	C3-C4-C4'-NZ
1	4-C	197	LLP	C3-C4-C4'-NZ
1	1-E	197	LLP	C3-C4-C4'-NZ
1	2-F	197	LLP	C3-C4-C4'-NZ

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Mol	Chain	Res	Type	Atoms
1	3-H	197	LLP	C3-C4-C4'-NZ
1	8-A	197	LLP	CG-CD-CE-NZ
1	4-C	197	LLP	CG-CD-CE-NZ
1	10-A	197	LLP	CA-CB-CG-CD
1	2-C	197	LLP	CA-CB-CG-CD
1	8-B	197	LLP	CD-CE-NZ-C4'
1	5-D	197	LLP	CD-CE-NZ-C4'
1	10-B	197	LLP	C4-C5-C5'-OP4
1	5-C	197	LLP	C4-C5-C5'-OP4
1	10-C	197	LLP	C4-C5-C5'-OP4
1	9-E	197	LLP	C-CA-CB-CG
1	2-H	197	LLP	C-CA-CB-CG
1	8-A	197	LLP	CD-CE-NZ-C4'
1	4-H	197	LLP	CD-CE-NZ-C4'
1	3-A	197	LLP	CG-CD-CE-NZ
1	10-B	197	LLP	C3-C4-C4'-NZ
1	8-H	197	LLP	CA-CB-CG-CD
1	5-D	197	LLP	CG-CD-CE-NZ
1	1-H	197	LLP	CG-CD-CE-NZ
1	3-C	197	LLP	CD-CE-NZ-C4'
1	1-F	197	LLP	CD-CE-NZ-C4'
1	4-F	197	LLP	C4-C4'-NZ-CE
1	4-A	197	LLP	N-CA-CB-CG
1	5-A	197	LLP	N-CA-CB-CG
1	7-A	197	LLP	N-CA-CB-CG
1	1-B	197	LLP	N-CA-CB-CG
1	4-B	197	LLP	N-CA-CB-CG
1	3-C	197	LLP	N-CA-CB-CG
1	8-C	197	LLP	N-CA-CB-CG
1	9-C	197	LLP	N-CA-CB-CG
1	1-D	197	LLP	N-CA-CB-CG
1	3-D	197	LLP	N-CA-CB-CG
1	5-D	197	LLP	N-CA-CB-CG
1	6-D	197	LLP	N-CA-CB-CG
1	9-D	197	LLP	N-CA-CB-CG
1	7-E	197	LLP	N-CA-CB-CG
1	9-F	197	LLP	N-CA-CB-CG
1	5-G	197	LLP	N-CA-CB-CG
1	1-H	197	LLP	N-CA-CB-CG
1	3-H	197	LLP	N-CA-CB-CG
1	6-H	197	LLP	N-CA-CB-CG
1	9-H	197	LLP	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	10-A	197	LLP	C3-C4-C4'-NZ
1	2-B	197	LLP	C3-C4-C4'-NZ

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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
2	8-E	401	MES	C8-S	-8.67	1.65	1.77
2	9-D	401	MES	C8-S	-8.65	1.65	1.77
2	5-G	401	MES	C8-S	-8.62	1.65	1.77
2	8-D	401	MES	C8-S	-8.35	1.65	1.77
2	8-G	401	MES	C8-S	-8.30	1.66	1.77
2	10-F	401	MES	C8-S	-8.29	1.66	1.77
2	6-H	401	MES	C8-S	-8.18	1.66	1.77
2	7-H	401	MES	C8-S	-8.13	1.66	1.77
2	9-C	401	MES	C8-S	-8.07	1.66	1.77
2	8-C	401	MES	C8-S	-7.77	1.66	1.77
2	6-B	401	MES	C8-S	-7.76	1.66	1.77
2	1-C	401	MES	C8-S	-7.75	1.66	1.77
2	8-B	401	MES	C8-S	-7.70	1.66	1.77
2	3-B	401	MES	C8-S	-7.60	1.66	1.77
2	8-A	401	MES	C8-S	-7.55	1.67	1.77
2	1-A	401	MES	C8-S	-7.53	1.67	1.77
2	10-A	401	MES	C8-S	-7.51	1.67	1.77
2	2-G	401	MES	C8-S	-7.50	1.67	1.77
2	9-H	401	MES	C8-S	-7.50	1.67	1.77
2	10-H	401	MES	C8-S	-7.49	1.67	1.77
2	1-D	401	MES	C8-S	-7.46	1.67	1.77
2	4-A	401	MES	C8-S	-7.46	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-D	401	MES	C8-S	-7.44	1.67	1.77
2	4-G	401	MES	C8-S	-7.26	1.67	1.77
2	8-F	401	MES	C8-S	-7.21	1.67	1.77
2	1-G	401	MES	C8-S	-7.15	1.67	1.77
2	7-G	401	MES	C8-S	-7.13	1.67	1.77
2	4-D	401	MES	C8-S	-7.13	1.67	1.77
2	9-B	401	MES	C8-S	-7.12	1.67	1.77
2	5-E	401	MES	C8-S	-7.09	1.67	1.77
2	4-H	401	MES	C8-S	-7.03	1.67	1.77
2	9-G	401	MES	C8-S	-6.99	1.67	1.77
2	1-E	401	MES	C8-S	-6.98	1.67	1.77
2	5-B	401	MES	C8-S	-6.93	1.67	1.77
2	5-H	401	MES	C8-S	-6.92	1.67	1.77
2	2-A	401	MES	C8-S	-6.89	1.67	1.77
2	3-C	401	MES	C8-S	-6.89	1.67	1.77
2	5-C	401	MES	C8-S	-6.89	1.67	1.77
2	2-B	401	MES	C8-S	-6.89	1.67	1.77
2	5-F	401	MES	C8-S	-6.87	1.68	1.77
2	7-B	401	MES	C8-S	-6.85	1.68	1.77
2	2-D	401	MES	C8-S	-6.73	1.68	1.77
2	10-D	401	MES	C8-S	-6.66	1.68	1.77
2	7-C	401	MES	C8-S	-6.62	1.68	1.77
2	6-D	401	MES	C8-S	-6.61	1.68	1.77
2	10-E	401	MES	C8-S	-6.61	1.68	1.77
2	9-E	401	MES	C8-S	-6.52	1.68	1.77
2	7-F	401	MES	C8-S	-6.50	1.68	1.77
2	3-E	401	MES	C8-S	-6.50	1.68	1.77
2	4-B	401	MES	C8-S	-6.47	1.68	1.77
2	10-G	401	MES	C8-S	-6.46	1.68	1.77
2	7-E	401	MES	C8-S	-6.46	1.68	1.77
2	10-B	401	MES	C8-S	-6.46	1.68	1.77
2	9-F	401	MES	C8-S	-6.43	1.68	1.77
2	7-A	401	MES	C8-S	-6.43	1.68	1.77
2	3-F	401	MES	C8-S	-6.40	1.68	1.77
2	1-B	401	MES	C8-S	-6.39	1.68	1.77
2	6-E	401	MES	C8-S	-6.37	1.68	1.77
2	6-G	401	MES	C8-S	-6.34	1.68	1.77
2	4-F	401	MES	C8-S	-6.33	1.68	1.77
2	5-A	401	MES	C8-S	-6.29	1.68	1.77
2	2-E	401	MES	C8-S	-6.17	1.68	1.77
2	2-F	401	MES	C8-S	-6.14	1.69	1.77
2	3-D	401	MES	C8-S	-6.10	1.69	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-H	401	MES	C8-S	-6.09	1.69	1.77
2	6-F	401	MES	C8-S	-6.05	1.69	1.77
2	2-C	401	MES	C8-S	-5.94	1.69	1.77
2	1-F	401	MES	C8-S	-5.87	1.69	1.77
2	9-A	401	MES	C8-S	-5.83	1.69	1.77
2	8-H	401	MES	C8-S	-5.23	1.70	1.77
2	3-G	401	MES	C8-S	-5.23	1.70	1.77
2	10-C	401	MES	C8-S	-5.22	1.70	1.77
2	3-A	401	MES	C8-S	-5.22	1.70	1.77
2	6-A	401	MES	C8-S	-4.75	1.70	1.77
2	4-E	401	MES	C8-S	-4.26	1.71	1.77
3	1-F	406	GOL	O2-C2	-3.07	1.34	1.43
2	8-D	401	MES	O2S-S	2.26	1.51	1.45
2	5-B	401	MES	O1S-S	2.17	1.51	1.45

All (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
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
2	5-D	401	MES	C5-N4-C3	7.09	124.11	108.84
2	3-E	401	MES	O1S-S-C8	6.85	117.08	106.73
2	7-G	401	MES	C5-N4-C3	6.39	122.61	108.84
2	1-A	401	MES	C5-N4-C3	6.39	122.60	108.84
2	9-C	401	MES	C5-N4-C3	6.33	122.47	108.84
2	7-D	401	MES	C5-N4-C3	6.32	122.45	108.84
2	5-D	401	MES	O2S-S-C8	6.30	116.25	106.73
2	5-F	401	MES	C5-N4-C3	6.07	121.92	108.84
2	10-F	401	MES	C5-N4-C3	6.04	121.86	108.84
2	7-B	401	MES	C5-N4-C3	5.98	121.72	108.84
2	6-C	401	MES	C2-C3-N4	-5.93	101.11	110.12
2	5-G	401	MES	O3S-S-C8	5.86	117.47	106.00
2	9-C	401	MES	O1S-S-C8	5.84	115.55	106.73
2	9-E	401	MES	C5-N4-C3	5.82	121.39	108.84
2	5-H	401	MES	O1S-S-C8	5.80	115.49	106.73
2	3-A	401	MES	C5-N4-C3	5.78	121.28	108.84
2	1-C	401	MES	C5-N4-C3	5.72	121.15	108.84
2	5-A	401	MES	C5-N4-C3	5.68	121.07	108.84
2	8-F	401	MES	C5-N4-C3	5.67	121.06	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-G	401	MES	C5-N4-C3	5.65	121.02	108.84
2	4-D	401	MES	C5-N4-C3	5.62	120.95	108.84
2	6-G	401	MES	C5-N4-C3	5.58	120.85	108.84
2	8-A	401	MES	C5-N4-C3	5.53	120.75	108.84
2	4-F	401	MES	C5-N4-C3	5.52	120.74	108.84
2	9-A	401	MES	C5-N4-C3	5.47	120.62	108.84
2	3-H	401	MES	O1S-S-C8	5.46	114.98	106.73
2	1-D	401	MES	C5-N4-C3	5.46	120.61	108.84
2	2-E	401	MES	C5-N4-C3	5.46	120.61	108.84
2	7-E	401	MES	C5-N4-C3	5.45	120.58	108.84
2	8-H	401	MES	O1S-S-C8	5.43	114.93	106.73
2	6-E	401	MES	O1S-S-C8	5.41	114.90	106.73
2	7-H	401	MES	C2-C3-N4	-5.34	102.00	110.12
2	6-A	401	MES	C5-N4-C3	5.30	120.26	108.84
2	10-E	401	MES	C5-N4-C3	5.30	120.25	108.84
2	1-G	401	MES	C5-N4-C3	5.26	120.18	108.84
2	8-D	401	MES	C5-N4-C3	5.23	120.10	108.84
2	3-B	401	MES	C7-N4-C5	5.22	125.14	111.24
2	8-C	401	MES	C6-C5-N4	-5.21	102.20	110.12
2	2-B	401	MES	C5-N4-C3	5.20	120.05	108.84
2	6-H	401	MES	O3S-S-C8	5.20	116.17	106.00
2	5-B	401	MES	C5-N4-C3	5.19	120.03	108.84
2	7-A	401	MES	C5-N4-C3	5.18	119.99	108.84
2	4-H	401	MES	C5-N4-C3	5.17	119.98	108.84
2	4-G	401	MES	O1S-S-C8	5.17	114.54	106.73
2	10-C	401	MES	C6-C5-N4	-5.16	102.28	110.12
2	3-B	401	MES	O2S-S-C8	-5.11	99.00	106.73
2	6-F	401	MES	C5-N4-C3	5.11	119.85	108.84
2	4-A	401	MES	C5-N4-C3	5.11	119.84	108.84
2	7-F	401	MES	C5-N4-C3	5.05	119.72	108.84
2	1-F	401	MES	C5-N4-C3	5.01	119.63	108.84
2	1-E	401	MES	C5-N4-C3	5.01	119.63	108.84
2	3-E	401	MES	C6-C5-N4	-4.98	102.55	110.12
2	2-E	401	MES	O2S-S-C8	4.94	114.19	106.73
2	9-A	401	MES	O2S-S-C8	4.89	114.11	106.73
2	9-D	401	MES	C5-N4-C3	4.87	119.33	108.84
2	3-B	401	MES	C5-N4-C3	4.85	119.29	108.84
2	3-F	401	MES	C5-N4-C3	4.85	119.28	108.84
2	10-B	401	MES	C5-N4-C3	4.84	119.28	108.84
2	8-G	401	MES	C6-C5-N4	-4.79	102.84	110.12
2	3-D	401	MES	C5-N4-C3	4.78	119.13	108.84
2	8-G	401	MES	C5-N4-C3	4.77	119.11	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-G	401	MES	C5-N4-C3	4.75	119.08	108.84
2	2-C	401	MES	C5-N4-C3	4.68	118.93	108.84
2	6-C	401	MES	C5-N4-C3	4.66	118.87	108.84
2	2-D	401	MES	C5-N4-C3	4.65	118.85	108.84
3	2-B	403	GOL	C3-C2-C1	4.64	128.83	111.80
2	3-G	401	MES	C5-N4-C3	4.63	118.82	108.84
2	7-D	401	MES	C6-C5-N4	-4.62	103.09	110.12
2	5-G	401	MES	O1S-S-C8	-4.61	99.77	106.73
2	10-F	401	MES	C6-C5-N4	-4.59	103.14	110.12
2	6-E	401	MES	O3S-S-C8	4.57	114.95	106.00
2	10-H	401	MES	C5-N4-C3	4.56	118.67	108.84
2	3-B	401	MES	O3S-S-C8	4.56	114.92	106.00
2	1-B	401	MES	C5-N4-C3	4.52	118.58	108.84
2	6-D	401	MES	O1S-S-C8	4.52	113.55	106.73
2	7-G	401	MES	O3S-S-C8	4.50	114.80	106.00
2	10-A	401	MES	C5-N4-C3	4.47	118.47	108.84
2	5-G	401	MES	C2-C3-N4	-4.46	103.34	110.12
2	5-C	401	MES	C5-N4-C3	4.44	118.42	108.84
2	2-G	401	MES	O1S-S-C8	4.44	113.44	106.73
2	8-E	401	MES	O2S-S-C8	4.42	113.41	106.73
2	4-C	401	MES	C5-N4-C3	4.41	118.35	108.84
2	2-A	401	MES	C5-N4-C3	4.41	118.34	108.84
2	4-B	401	MES	C5-N4-C3	4.41	118.33	108.84
2	3-H	401	MES	C5-N4-C3	4.40	118.32	108.84
2	7-E	401	MES	O2S-S-C8	4.37	113.34	106.73
2	9-F	401	MES	C5-N4-C3	4.32	118.15	108.84
2	7-D	401	MES	O1-C6-C5	-4.32	102.46	111.77
2	8-C	401	MES	C5-N4-C3	4.31	118.13	108.84
2	4-G	401	MES	C5-N4-C3	4.31	118.12	108.84
2	2-D	401	MES	O1S-S-C8	4.31	113.24	106.73
2	4-D	401	MES	O1S-S-C8	4.30	113.22	106.73
2	8-B	401	MES	O1S-S-C8	4.28	113.20	106.73
2	2-F	401	MES	C5-N4-C3	4.27	118.05	108.84
2	9-B	401	MES	C5-N4-C3	4.24	117.98	108.84
2	3-F	401	MES	O1S-S-C8	4.22	113.11	106.73
2	2-F	401	MES	O1S-S-C8	4.22	113.10	106.73
2	10-G	401	MES	C6-C5-N4	-4.19	103.76	110.12
2	3-F	401	MES	O2S-S-C8	4.17	113.03	106.73
2	5-E	401	MES	C7-N4-C3	4.15	122.29	111.24
2	9-G	401	MES	O1S-S-C8	4.14	112.99	106.73
2	2-H	401	MES	C5-N4-C3	4.09	117.65	108.84
2	2-G	401	MES	C5-N4-C3	4.07	117.60	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-H	401	MES	O2S-S-C8	-4.05	100.60	106.73
2	1-F	401	MES	O2S-S-C8	4.05	112.84	106.73
2	1-E	401	MES	C7-N4-C3	4.04	122.02	111.24
2	3-E	401	MES	O3S-S-C8	4.04	113.92	106.00
2	5-E	401	MES	C5-N4-C3	4.01	117.47	108.84
2	3-D	401	MES	O2S-S-C8	4.00	112.78	106.73
2	9-F	401	MES	O1S-S-C8	3.99	112.76	106.73
2	3-E	401	MES	C5-N4-C3	3.97	117.39	108.84
2	8-H	401	MES	C5-N4-C3	3.97	117.39	108.84
2	3-D	401	MES	O2S-S-O1S	-3.93	101.04	113.82
2	10-C	401	MES	C5-N4-C3	3.92	117.29	108.84
2	1-H	401	MES	O3S-S-C8	3.88	113.59	106.00
2	6-B	401	MES	C5-N4-C3	3.87	117.17	108.84
2	10-D	401	MES	C5-N4-C3	3.83	117.09	108.84
2	4-D	401	MES	C7-N4-C3	3.82	121.42	111.24
2	1-D	401	MES	O3S-S-C8	3.82	113.47	106.00
2	5-B	401	MES	C7-N4-C5	3.78	121.32	111.24
2	7-D	401	MES	C7-N4-C3	3.76	121.26	111.24
2	6-C	401	MES	O2S-S-C8	3.76	112.40	106.73
2	6-A	401	MES	O3S-S-C8	3.76	113.35	106.00
2	4-C	401	MES	O2S-S-O1S	-3.74	101.66	113.82
2	6-D	401	MES	C5-N4-C3	3.73	116.88	108.84
2	6-G	401	MES	O1S-S-C8	3.73	112.36	106.73
2	8-C	401	MES	C2-C3-N4	-3.71	104.48	110.12
2	5-C	401	MES	C7-N4-C5	3.71	121.12	111.24
2	6-E	401	MES	C7-N4-C5	3.68	121.06	111.24
2	3-D	401	MES	C7-N4-C5	3.68	121.05	111.24
2	4-B	401	MES	C7-N4-C5	3.68	121.04	111.24
2	9-A	401	MES	O3S-S-O1S	-3.66	102.24	111.40
2	6-E	401	MES	C5-N4-C3	3.63	116.66	108.84
2	7-C	401	MES	O1S-S-C8	3.63	112.21	106.73
2	3-F	401	MES	C7-N4-C3	3.62	120.89	111.24
2	5-B	401	MES	O3S-S-C8	3.61	113.06	106.00
2	1-H	401	MES	C6-C5-N4	-3.59	104.67	110.12
2	6-C	401	MES	C7-N4-C5	3.55	120.69	111.24
2	1-B	401	MES	O3S-S-C8	3.54	112.94	106.00
2	6-E	401	MES	O2S-S-C8	-3.54	101.38	106.73
2	7-H	401	MES	C5-N4-C3	3.54	116.46	108.84
2	10-E	401	MES	C2-C3-N4	3.53	115.49	110.12
2	3-H	401	MES	C7-N4-C3	3.53	120.65	111.24
2	3-C	401	MES	C5-N4-C3	3.52	116.43	108.84
2	6-C	401	MES	C6-C5-N4	-3.49	104.81	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-H	401	MES	O1S-S-C8	3.49	112.01	106.73
2	3-C	401	MES	O3S-S-O2S	-3.49	102.66	111.40
2	5-G	401	MES	C5-N4-C3	3.46	116.30	108.84
2	5-E	401	MES	O3S-S-C8	3.44	112.74	106.00
2	10-H	401	MES	O2S-S-C8	3.42	111.90	106.73
2	7-D	401	MES	C2-C3-N4	-3.41	104.93	110.12
2	10-H	401	MES	C6-C5-N4	-3.41	104.94	110.12
2	3-E	401	MES	O2S-S-O1S	-3.41	102.74	113.82
2	2-E	401	MES	C7-N4-C5	3.41	120.31	111.24
2	2-F	401	MES	O2S-S-C8	3.40	111.86	106.73
2	8-D	401	MES	O3S-S-C8	3.39	112.64	106.00
2	1-C	401	MES	C6-C5-N4	-3.36	105.02	110.12
2	1-F	401	MES	C7-N4-C5	3.35	120.18	111.24
2	7-C	401	MES	C5-N4-C3	3.35	116.05	108.84
2	1-A	401	MES	C6-C5-N4	-3.34	105.04	110.12
2	2-D	401	MES	O3S-S-O1S	-3.32	103.08	111.40
2	1-D	401	MES	C7-N4-C5	3.32	120.10	111.24
2	10-C	401	MES	O2S-S-C8	-3.32	101.71	106.73
2	2-F	401	MES	C7-N4-C5	3.32	120.08	111.24
2	4-A	401	MES	C6-C5-N4	-3.32	105.08	110.12
2	5-C	401	MES	C6-C5-N4	-3.30	105.11	110.12
2	6-G	401	MES	C7-N4-C5	3.29	120.02	111.24
2	7-A	401	MES	O3S-S-C8	3.29	112.44	106.00
2	1-B	401	MES	C7-N4-C3	3.29	120.01	111.24
2	8-B	401	MES	C5-N4-C3	3.29	115.92	108.84
2	1-H	401	MES	C5-N4-C3	3.29	115.92	108.84
2	1-G	401	MES	C6-C5-N4	-3.28	105.13	110.12
2	8-D	401	MES	C7-N4-C3	3.28	119.98	111.24
2	9-H	401	MES	C5-N4-C3	3.27	115.88	108.84
2	1-E	401	MES	O1S-S-C8	3.26	111.65	106.73
2	9-G	401	MES	C7-N4-C3	3.25	119.91	111.24
2	6-D	401	MES	C7-N4-C5	3.24	119.88	111.24
2	6-H	401	MES	C6-C5-N4	-3.23	105.21	110.12
2	6-D	401	MES	C7-N4-C3	3.23	119.83	111.24
2	8-A	401	MES	C2-C3-N4	-3.22	105.23	110.12
2	5-F	401	MES	O2S-S-O1S	-3.21	103.38	113.82
2	5-E	401	MES	O1-C6-C5	-3.21	104.86	111.77
2	2-C	401	MES	O2S-S-O1S	-3.21	103.39	113.82
2	3-E	401	MES	C7-N4-C3	3.21	119.78	111.24
2	9-B	401	MES	O3S-S-C8	3.20	112.26	106.00
2	1-D	401	MES	C2-C3-N4	-3.19	105.28	110.12
2	6-A	401	MES	C7-N4-C5	3.17	119.69	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-C	401	MES	O3S-S-C8	3.16	112.18	106.00
2	5-H	401	MES	C5-N4-C3	3.16	115.64	108.84
2	10-G	401	MES	C7-N4-C5	3.15	119.63	111.24
2	3-A	401	MES	O3S-S-C8	3.14	112.15	106.00
2	6-A	401	MES	C7-N4-C3	3.13	119.57	111.24
2	10-G	401	MES	O1S-S-C8	3.12	111.45	106.73
2	4-H	401	MES	C7-N4-C5	3.11	119.54	111.24
2	7-F	401	MES	O2S-S-C8	3.11	111.43	106.73
2	9-A	401	MES	C6-C5-N4	3.11	114.85	110.12
2	6-G	401	MES	C6-C5-N4	-3.10	105.40	110.12
2	3-A	401	MES	C7-N4-C3	3.10	119.50	111.24
2	7-F	401	MES	C2-C3-N4	3.09	114.82	110.12
2	6-C	401	MES	C8-C7-N4	-3.09	100.67	112.36
2	7-B	401	MES	O3S-S-C8	3.09	112.05	106.00
2	2-C	401	MES	C7-N4-C5	3.08	119.45	111.24
2	4-F	401	MES	C7-N4-C3	3.08	119.44	111.24
2	8-F	401	MES	C7-N4-C3	3.07	119.42	111.24
2	6-D	401	MES	O3S-S-C8	3.07	112.01	106.00
2	1-C	401	MES	C7-N4-C5	3.07	119.41	111.24
2	10-E	401	MES	O2S-S-C8	3.06	111.36	106.73
2	8-G	401	MES	C7-N4-C5	3.06	119.39	111.24
2	4-B	401	MES	C6-C5-N4	-3.05	105.48	110.12
2	2-H	401	MES	C7-N4-C3	3.03	119.31	111.24
2	7-E	401	MES	C7-N4-C3	3.03	119.31	111.24
2	5-F	401	MES	O2S-S-C8	3.02	111.30	106.73
2	7-B	401	MES	O2S-S-O1S	-2.99	104.10	113.82
2	5-H	401	MES	C7-N4-C3	2.99	119.21	111.24
2	10-G	401	MES	O2S-S-C8	2.99	111.24	106.73
2	10-E	401	MES	C6-C5-N4	-2.99	105.58	110.12
2	1-F	401	MES	O2S-S-O1S	-2.98	104.13	113.82
2	10-F	401	MES	O2S-S-O1S	-2.98	104.14	113.82
2	7-E	401	MES	C6-C5-N4	-2.98	105.60	110.12
2	3-A	401	MES	C7-N4-C5	2.98	119.17	111.24
2	7-B	401	MES	C7-N4-C3	2.97	119.16	111.24
2	1-H	401	MES	O3S-S-O2S	-2.96	104.00	111.40
2	3-H	401	MES	C7-N4-C5	2.95	119.11	111.24
2	9-A	401	MES	O1S-S-C8	2.95	111.18	106.73
2	5-F	401	MES	O1S-S-C8	2.94	111.17	106.73
2	4-A	401	MES	C7-N4-C3	2.92	119.03	111.24
2	2-D	401	MES	C6-C5-N4	-2.92	105.69	110.12
2	10-F	401	MES	C7-N4-C5	2.92	119.02	111.24
2	6-F	401	MES	O1S-S-C8	2.91	111.12	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-C	401	MES	O3S-S-C8	2.90	111.68	106.00
2	5-G	401	MES	O1-C6-C5	-2.90	105.52	111.77
2	3-C	401	MES	C7-N4-C3	2.90	118.97	111.24
2	3-E	401	MES	O3S-S-O1S	-2.89	104.16	111.40
2	5-H	401	MES	O2S-S-C8	-2.88	102.38	106.73
2	8-F	401	MES	O1S-S-C8	2.87	111.07	106.73
2	4-B	401	MES	C7-N4-C3	2.87	118.90	111.24
2	5-D	401	MES	C7-N4-C3	2.86	118.85	111.24
2	10-B	401	MES	O2S-S-C8	2.85	111.04	106.73
2	2-H	401	MES	C6-C5-N4	-2.85	105.79	110.12
2	7-B	401	MES	C7-N4-C5	2.85	118.83	111.24
2	1-F	401	MES	O1S-S-C8	2.84	111.03	106.73
2	8-G	401	MES	O3S-S-C8	2.83	111.55	106.00
2	4-C	401	MES	C6-C5-N4	-2.83	105.82	110.12
2	3-H	401	MES	O3S-S-C8	2.83	111.54	106.00
2	1-D	401	MES	C7-N4-C3	2.82	118.76	111.24
2	2-D	401	MES	C7-N4-C5	2.82	118.76	111.24
2	1-G	401	MES	O3S-S-C8	2.82	111.52	106.00
2	8-C	401	MES	O1S-S-C8	2.82	110.98	106.73
2	3-G	401	MES	C7-N4-C3	2.81	118.73	111.24
2	10-G	401	MES	O1-C2-C3	2.80	117.81	111.77
2	6-H	401	MES	C7-N4-C5	2.80	118.69	111.24
2	2-A	401	MES	O3S-S-C8	2.79	111.47	106.00
2	4-A	401	MES	C7-N4-C5	2.79	118.68	111.24
2	2-E	401	MES	C7-N4-C3	2.79	118.67	111.24
2	10-C	401	MES	C7-N4-C5	2.79	118.67	111.24
2	9-D	401	MES	C6-C5-N4	-2.78	105.89	110.12
2	5-G	401	MES	C6-C5-N4	-2.78	105.89	110.12
2	2-B	401	MES	O3S-S-C8	2.78	111.45	106.00
2	4-E	401	MES	O3S-S-C8	2.76	111.41	106.00
2	8-H	401	MES	C7-N4-C5	2.76	118.60	111.24
2	3-F	401	MES	O1-C2-C3	2.76	117.71	111.77
2	8-C	401	MES	C7-N4-C3	2.76	118.58	111.24
2	9-E	401	MES	C7-N4-C5	2.75	118.58	111.24
2	7-C	401	MES	C7-N4-C5	2.74	118.55	111.24
2	8-C	401	MES	O2S-S-O1S	-2.74	104.91	113.82
2	6-F	401	MES	C7-N4-C5	2.73	118.50	111.24
2	10-A	401	MES	O3S-S-C8	2.72	111.33	106.00
2	7-G	401	MES	C7-N4-C5	2.72	118.50	111.24
2	2-G	401	MES	C7-N4-C3	2.72	118.49	111.24
2	2-F	401	MES	C7-N4-C3	2.72	118.49	111.24
2	6-H	401	MES	C5-N4-C3	2.72	114.69	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-E	401	MES	C5-N4-C3	2.72	114.69	108.84
2	5-E	401	MES	C7-N4-C5	2.71	118.47	111.24
2	1-D	401	MES	O3S-S-O2S	-2.70	104.64	111.40
2	7-E	401	MES	O3S-S-C8	2.69	111.27	106.00
2	7-G	401	MES	O2S-S-O1S	-2.69	105.07	113.82
2	3-H	401	MES	O3S-S-O1S	-2.68	104.69	111.40
2	8-A	401	MES	C7-N4-C5	2.68	118.38	111.24
2	8-H	401	MES	O3S-S-O1S	-2.68	104.69	111.40
2	4-H	401	MES	C7-N4-C3	2.68	118.38	111.24
2	8-B	401	MES	O2S-S-C8	2.66	110.75	106.73
2	3-E	401	MES	C7-N4-C5	2.66	118.34	111.24
2	5-E	401	MES	O2S-S-O1S	-2.66	105.17	113.82
2	5-B	401	MES	C7-N4-C3	2.66	118.32	111.24
2	3-E	401	MES	O2S-S-C8	-2.66	102.72	106.73
2	1-G	401	MES	O3S-S-O2S	-2.65	104.76	111.40
2	4-E	401	MES	C7-N4-C5	2.65	118.31	111.24
2	9-G	401	MES	C7-N4-C5	2.65	118.29	111.24
2	3-G	401	MES	O3S-S-O2S	-2.62	104.84	111.40
2	5-B	401	MES	C6-C5-N4	-2.62	106.14	110.12
2	6-G	401	MES	C7-N4-C3	2.62	118.21	111.24
2	2-C	401	MES	C6-C5-N4	-2.60	106.16	110.12
2	3-D	401	MES	O3S-S-C8	2.60	111.09	106.00
2	8-G	401	MES	O1S-S-C8	2.59	110.65	106.73
2	9-C	401	MES	C7-N4-C5	2.59	118.14	111.24
2	3-D	401	MES	C6-C5-N4	-2.59	106.19	110.12
3	1-D	403	GOL	C3-C2-C1	-2.59	102.31	111.80
2	4-F	401	MES	C7-N4-C5	2.58	118.12	111.24
2	8-A	401	MES	C7-N4-C3	2.58	118.12	111.24
2	8-G	401	MES	C2-C3-N4	-2.56	106.22	110.12
2	6-D	401	MES	O2S-S-O1S	-2.56	105.49	113.82
2	5-A	401	MES	C2-C3-N4	-2.56	106.23	110.12
2	7-E	401	MES	C7-N4-C5	2.56	118.05	111.24
2	10-H	401	MES	C7-N4-C3	2.55	118.03	111.24
2	3-E	401	MES	C2-C3-N4	2.55	113.99	110.12
2	10-D	401	MES	O2S-S-C8	2.53	110.56	106.73
2	6-B	401	MES	C7-N4-C3	2.53	117.97	111.24
2	8-E	401	MES	C7-N4-C3	2.52	117.97	111.24
2	1-F	401	MES	C6-C5-N4	-2.52	106.28	110.12
2	10-H	401	MES	O3S-S-C8	2.52	110.94	106.00
3	2-B	403	GOL	O3-C3-C2	-2.52	99.04	110.38
2	4-B	401	MES	O3S-S-C8	2.52	110.93	106.00
2	2-H	401	MES	O3S-S-C8	2.52	110.93	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-C	401	MES	O1S-S-C8	2.51	110.52	106.73
2	5-E	401	MES	O2S-S-C8	2.51	110.51	106.73
2	7-G	401	MES	C6-C5-N4	-2.49	106.33	110.12
2	2-F	401	MES	C6-C5-N4	-2.49	106.34	110.12
2	10-F	401	MES	C2-C3-N4	-2.49	106.34	110.12
2	10-G	401	MES	C2-C3-N4	2.49	113.90	110.12
2	10-H	401	MES	C8-C7-N4	-2.48	102.97	112.36
3	8-E	402	GOL	O2-C2-C3	-2.48	98.91	109.18
2	3-D	401	MES	C7-N4-C3	2.48	117.84	111.24
2	1-C	401	MES	O2S-S-O1S	-2.47	105.78	113.82
2	10-F	401	MES	O1S-S-C8	2.47	110.46	106.73
2	9-A	401	MES	O1-C2-C3	-2.47	106.46	111.77
2	5-G	401	MES	O3S-S-O1S	-2.46	105.23	111.40
2	7-C	401	MES	C6-C5-N4	-2.46	106.38	110.12
2	9-H	401	MES	C7-N4-C3	2.46	117.79	111.24
2	5-A	401	MES	C7-N4-C3	2.44	117.73	111.24
2	10-B	401	MES	C6-O1-C2	2.43	117.73	109.88
2	8-C	401	MES	O2S-S-C8	2.42	110.38	106.73
2	10-E	401	MES	O1-C2-C3	2.41	116.97	111.77
2	7-F	401	MES	C6-C5-N4	-2.41	106.45	110.12
2	2-E	401	MES	O2S-S-O1S	-2.40	106.01	113.82
3	1-F	406	GOL	O2-C2-C3	2.39	119.08	109.18
2	3-B	401	MES	O2S-S-O1S	-2.37	106.10	113.82
2	10-D	401	MES	C7-N4-C5	2.37	117.56	111.24
2	8-H	401	MES	C7-N4-C3	2.37	117.56	111.24
2	10-D	401	MES	C7-N4-C3	2.37	117.55	111.24
2	5-A	401	MES	C7-N4-C5	2.37	117.55	111.24
2	2-B	401	MES	C7-N4-C3	2.36	117.53	111.24
2	4-H	401	MES	C8-C7-N4	-2.35	103.46	112.36
2	5-G	401	MES	C7-N4-C5	2.35	117.50	111.24
2	1-A	401	MES	C7-N4-C3	2.35	117.49	111.24
2	5-G	401	MES	C7-N4-C3	2.34	117.48	111.24
2	8-D	401	MES	C6-C5-N4	-2.34	106.57	110.12
2	9-E	401	MES	C7-N4-C3	2.34	117.46	111.24
2	10-B	401	MES	O1-C2-C3	2.34	116.80	111.77
2	1-F	401	MES	C7-N4-C3	2.34	117.46	111.24
2	8-D	401	MES	C2-C3-N4	-2.33	106.58	110.12
2	5-E	401	MES	C2-C3-N4	-2.33	106.58	110.12
2	9-A	401	MES	O1-C6-C5	2.32	116.77	111.77
2	4-F	401	MES	C6-C5-N4	-2.32	106.59	110.12
2	3-D	401	MES	O1S-S-C8	2.32	110.23	106.73
2	1-E	401	MES	C7-N4-C5	2.31	117.41	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-D	401	MES	C8-C7-N4	-2.31	103.61	112.36
2	6-A	401	MES	O1-C2-C3	2.31	116.75	111.77
2	4-E	401	MES	O1S-S-C8	2.31	110.22	106.73
2	1-A	401	MES	C7-N4-C5	2.31	117.39	111.24
2	5-C	401	MES	O2S-S-C8	2.30	110.21	106.73
2	4-G	401	MES	C7-N4-C3	2.30	117.37	111.24
2	5-D	401	MES	C6-C5-N4	2.30	113.61	110.12
2	1-H	401	MES	C7-N4-C5	2.28	117.32	111.24
2	6-C	401	MES	O2S-S-O1S	-2.28	106.40	113.82
3	2-B	403	GOL	O1-C1-C2	-2.27	100.14	110.38
2	9-F	401	MES	C6-C5-N4	-2.27	106.66	110.12
2	5-A	401	MES	O3S-S-C8	2.27	110.45	106.00
2	4-F	401	MES	O2S-S-C8	2.27	110.16	106.73
2	6-E	401	MES	C2-C3-N4	-2.27	106.67	110.12
2	8-E	401	MES	C2-C3-N4	2.26	113.56	110.12
2	6-A	401	MES	C2-C3-N4	2.26	113.56	110.12
2	4-H	401	MES	C6-C5-N4	-2.26	106.69	110.12
2	9-F	401	MES	C7-N4-C5	2.24	117.22	111.24
2	4-D	401	MES	O2S-S-O1S	-2.24	106.53	113.82
2	9-C	401	MES	O1-C2-C3	-2.24	106.94	111.77
2	4-H	401	MES	C2-C3-N4	-2.24	106.71	110.12
2	5-E	401	MES	O1S-S-C8	2.23	110.10	106.73
2	6-D	401	MES	C2-C3-N4	-2.22	106.74	110.12
2	2-A	401	MES	O2S-S-C8	2.22	110.08	106.73
2	2-H	401	MES	C2-C3-N4	-2.22	106.75	110.12
2	7-H	401	MES	O1-C6-C5	2.21	116.54	111.77
2	2-D	401	MES	C7-N4-C3	2.21	117.14	111.24
2	4-H	401	MES	O2S-S-C8	2.21	110.07	106.73
2	6-B	401	MES	O2S-S-C8	2.21	110.07	106.73
2	8-B	401	MES	C7-N4-C3	2.21	117.13	111.24
2	3-B	401	MES	O1-C6-C5	2.21	116.53	111.77
2	8-D	401	MES	C8-C7-N4	-2.20	104.03	112.36
2	4-A	401	MES	O2S-S-C8	2.20	110.05	106.73
2	3-C	401	MES	C6-C5-N4	-2.19	106.78	110.12
2	8-D	401	MES	O1-C6-C5	-2.19	107.05	111.77
2	8-G	401	MES	C8-C7-N4	-2.18	104.11	112.36
2	1-G	401	MES	C7-N4-C3	2.18	117.04	111.24
2	10-C	401	MES	O2S-S-O1S	-2.17	106.77	113.82
2	10-B	401	MES	C2-C3-N4	2.17	113.41	110.12
2	6-E	401	MES	C7-N4-C3	2.16	116.99	111.24
2	10-G	401	MES	C6-O1-C2	2.15	116.85	109.88
2	9-D	401	MES	C7-N4-C3	2.15	116.97	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-B	401	MES	O2S-S-C8	2.15	109.97	106.73
2	10-A	401	MES	C6-C5-N4	-2.14	106.86	110.12
2	7-H	401	MES	C7-N4-C5	2.14	116.94	111.24
2	3-E	401	MES	O1-C2-C3	2.14	116.38	111.77
2	3-C	401	MES	C7-N4-C5	2.14	116.93	111.24
2	10-E	401	MES	O3S-S-C8	2.13	110.17	106.00
2	6-E	401	MES	O2S-S-O1S	-2.13	106.91	113.82
2	6-B	401	MES	C6-O1-C2	2.13	116.76	109.88
2	9-G	401	MES	O2S-S-C8	2.13	109.94	106.73
2	1-D	401	MES	C6-C5-N4	-2.13	106.89	110.12
2	1-B	401	MES	O3S-S-O1S	-2.12	106.09	111.40
2	8-F	401	MES	O3S-S-C8	2.12	110.14	106.00
2	9-A	401	MES	C2-C3-N4	-2.11	106.91	110.12
2	8-C	401	MES	C8-C7-N4	-2.11	104.38	112.36
2	6-F	401	MES	O1-C6-C5	2.11	116.31	111.77
2	10-B	401	MES	O3S-S-C8	2.10	110.11	106.00
2	9-D	401	MES	O2S-S-C8	2.10	109.90	106.73
2	10-F	401	MES	O1-C6-C5	-2.09	107.26	111.77
2	1-G	401	MES	C7-N4-C5	2.09	116.81	111.24
2	7-G	401	MES	O1S-S-C8	2.09	109.88	106.73
2	9-D	401	MES	O1-C6-C5	-2.08	107.28	111.77
2	9-A	401	MES	C7-N4-C5	2.08	116.79	111.24
2	7-A	401	MES	C2-C3-N4	2.07	113.27	110.12
2	3-B	401	MES	C8-C7-N4	2.07	120.19	112.36
2	8-G	401	MES	C7-N4-C3	2.07	116.75	111.24
2	10-B	401	MES	C7-N4-C5	2.06	116.74	111.24
2	2-B	401	MES	O2S-S-C8	2.06	109.83	106.73
2	9-H	401	MES	O3S-S-C8	2.05	110.02	106.00
2	5-B	401	MES	O3S-S-O1S	-2.05	106.28	111.40
2	5-A	401	MES	O2S-S-C8	2.04	109.82	106.73
3	10-E	402	GOL	C3-C2-C1	-2.04	104.31	111.80
2	9-E	401	MES	O1-C2-C3	2.04	116.17	111.77
2	6-C	401	MES	C7-N4-C3	2.04	116.67	111.24
2	8-H	401	MES	O3S-S-C8	2.04	109.99	106.00
2	8-E	401	MES	O3S-S-C8	2.03	109.98	106.00
3	2-B	403	GOL	O2-C2-C3	2.03	117.59	109.18
2	9-B	401	MES	O2S-S-C8	2.03	109.80	106.73
2	3-C	401	MES	O1S-S-C8	2.03	109.79	106.73
2	8-D	401	MES	O2S-S-C8	2.02	109.78	106.73
2	4-A	401	MES	O1S-S-C8	2.02	109.78	106.73
2	9-G	401	MES	O3S-S-O2S	-2.01	106.36	111.40
2	10-A	401	MES	O2S-S-C8	2.01	109.77	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-G	401	MES	O2S-S-O1S	-2.00	107.31	113.82

There are no chirality outliers.

All (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
2	6-A	401	MES	C7-C8-S-O2S
2	6-A	401	MES	C7-C8-S-O3S
2	7-A	401	MES	C7-C8-S-O1S
2	7-A	401	MES	C7-C8-S-O2S
2	8-A	401	MES	C7-C8-S-O1S
2	8-A	401	MES	C7-C8-S-O3S
2	10-A	401	MES	C8-C7-N4-C5
2	1-B	401	MES	C8-C7-N4-C3
2	3-B	401	MES	C8-C7-N4-C5
2	4-B	401	MES	C8-C7-N4-C3
2	5-B	401	MES	C7-C8-S-O1S
2	5-B	401	MES	C7-C8-S-O2S
2	6-B	401	MES	C8-C7-N4-C3
2	4-C	401	MES	C7-C8-S-O3S
2	6-C	401	MES	N4-C7-C8-S
2	9-C	401	MES	C7-C8-S-O2S
2	1-D	401	MES	C8-C7-N4-C3
2	2-D	401	MES	C7-C8-S-O2S
2	3-D	401	MES	C8-C7-N4-C5
2	3-D	401	MES	C7-C8-S-O2S
2	3-D	401	MES	C7-C8-S-O3S
2	4-D	401	MES	C7-C8-S-O2S
2	4-D	401	MES	C7-C8-S-O3S
2	5-D	401	MES	C8-C7-N4-C3
2	6-D	401	MES	C8-C7-N4-C3
2	7-D	401	MES	C8-C7-N4-C3
2	8-D	401	MES	C8-C7-N4-C3
2	8-D	401	MES	C8-C7-N4-C5
2	9-D	401	MES	C8-C7-N4-C3
2	9-D	401	MES	C7-C8-S-O2S
2	10-D	401	MES	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
2	10-D	401	MES	C7-C8-S-O1S
2	10-D	401	MES	C7-C8-S-O2S
2	10-D	401	MES	C7-C8-S-O3S
2	1-E	401	MES	C8-C7-N4-C3
2	2-E	401	MES	C7-C8-S-O1S
2	2-E	401	MES	C7-C8-S-O3S
2	4-E	401	MES	C7-C8-S-O2S
2	5-E	401	MES	N4-C7-C8-S
2	5-E	401	MES	C7-C8-S-O1S
2	5-E	401	MES	C7-C8-S-O3S
2	6-E	401	MES	N4-C7-C8-S
2	7-E	401	MES	C8-C7-N4-C3
2	8-E	401	MES	N4-C7-C8-S
2	8-E	401	MES	C7-C8-S-O2S
2	8-E	401	MES	C7-C8-S-O3S
2	10-E	401	MES	C8-C7-N4-C3
2	1-F	401	MES	C8-C7-N4-C3
2	4-F	401	MES	C8-C7-N4-C5
2	5-F	401	MES	C7-C8-S-O1S
2	5-F	401	MES	C7-C8-S-O3S
2	6-F	401	MES	C8-C7-N4-C3
2	8-F	401	MES	C8-C7-N4-C5
2	8-F	401	MES	C7-C8-S-O1S
2	8-F	401	MES	C7-C8-S-O3S
2	9-F	401	MES	C8-C7-N4-C3
2	9-F	401	MES	C7-C8-S-O1S
2	9-F	401	MES	C7-C8-S-O3S
2	10-F	401	MES	C8-C7-N4-C5
2	3-G	401	MES	C8-C7-N4-C3
2	3-G	401	MES	C7-C8-S-O2S
2	3-G	401	MES	C7-C8-S-O3S
2	4-G	401	MES	C8-C7-N4-C3
2	5-G	401	MES	C8-C7-N4-C3
2	5-G	401	MES	N4-C7-C8-S
2	5-G	401	MES	C7-C8-S-O2S
2	5-G	401	MES	C7-C8-S-O3S
2	6-G	401	MES	C8-C7-N4-C3
2	7-G	401	MES	C7-C8-S-O1S
2	7-G	401	MES	C7-C8-S-O3S
2	8-G	401	MES	C8-C7-N4-C5
2	9-G	401	MES	C8-C7-N4-C5
2	9-G	401	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
2	9-G	401	MES	C7-C8-S-O3S
2	3-H	401	MES	C8-C7-N4-C3
2	3-H	401	MES	C7-C8-S-O1S
2	4-H	401	MES	C8-C7-N4-C3
2	5-H	401	MES	C8-C7-N4-C3
2	5-H	401	MES	C7-C8-S-O2S
2	5-H	401	MES	C7-C8-S-O3S
2	6-H	401	MES	C8-C7-N4-C5
2	6-H	401	MES	C7-C8-S-O2S
2	6-H	401	MES	C7-C8-S-O3S
2	7-H	401	MES	C7-C8-S-O1S
2	7-H	401	MES	C7-C8-S-O2S
2	7-H	401	MES	C7-C8-S-O3S
2	8-H	401	MES	N4-C7-C8-S
2	8-H	401	MES	C7-C8-S-O1S
2	8-H	401	MES	C7-C8-S-O3S
2	10-H	401	MES	N4-C7-C8-S
3	1-A	402	GOL	O1-C1-C2-C3
3	3-A	402	GOL	O1-C1-C2-C3
3	4-A	402	GOL	O1-C1-C2-C3
3	5-A	402	GOL	O1-C1-C2-O2
3	5-A	402	GOL	O1-C1-C2-C3
3	6-A	402	GOL	O1-C1-C2-C3
3	7-A	402	GOL	O1-C1-C2-C3
3	8-A	402	GOL	O1-C1-C2-C3
3	8-A	402	GOL	C1-C2-C3-O3
3	4-A	403	GOL	O1-C1-C2-C3
3	5-A	403	GOL	O1-C1-C2-C3
3	6-A	403	GOL	O1-C1-C2-C3
3	10-A	403	GOL	C1-C2-C3-O3
3	10-A	403	GOL	O2-C2-C3-O3
3	1-A	404	GOL	O1-C1-C2-C3
3	2-A	404	GOL	O1-C1-C2-C3
3	4-A	404	GOL	O1-C1-C2-C3
3	9-A	404	GOL	O1-C1-C2-C3
3	10-A	404	GOL	O1-C1-C2-C3
3	1-B	402	GOL	C1-C2-C3-O3
3	4-B	402	GOL	O1-C1-C2-C3
3	6-B	402	GOL	O1-C1-C2-O2
3	6-B	402	GOL	O1-C1-C2-C3
3	8-B	402	GOL	O1-C1-C2-C3
3	9-B	402	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	10-B	402	GOL	O1-C1-C2-C3
3	1-B	403	GOL	O1-C1-C2-C3
3	2-B	403	GOL	O2-C2-C3-O3
3	4-B	403	GOL	O1-C1-C2-C3
3	6-B	403	GOL	O1-C1-C2-C3
3	10-B	403	GOL	O1-C1-C2-C3
3	1-B	404	GOL	O1-C1-C2-C3
3	4-B	404	GOL	C1-C2-C3-O3
3	5-B	404	GOL	O1-C1-C2-C3
3	6-B	404	GOL	O1-C1-C2-C3
3	7-B	404	GOL	O1-C1-C2-C3
3	8-B	404	GOL	O1-C1-C2-C3
3	10-B	404	GOL	O1-C1-C2-O2
3	10-B	404	GOL	O1-C1-C2-C3
3	1-B	405	GOL	O1-C1-C2-C3
3	2-B	405	GOL	O1-C1-C2-C3
3	5-B	405	GOL	C1-C2-C3-O3
3	6-B	405	GOL	O1-C1-C2-C3
3	9-B	405	GOL	O1-C1-C2-C3
3	9-B	405	GOL	C1-C2-C3-O3
3	9-B	405	GOL	O2-C2-C3-O3
3	10-B	405	GOL	C1-C2-C3-O3
3	1-B	406	GOL	O1-C1-C2-C3
3	2-B	406	GOL	O1-C1-C2-O2
3	2-B	406	GOL	O1-C1-C2-C3
3	6-B	406	GOL	O1-C1-C2-C3
3	7-B	406	GOL	O1-C1-C2-C3
3	8-B	406	GOL	O1-C1-C2-C3
3	9-B	406	GOL	O1-C1-C2-O2
3	9-B	406	GOL	O1-C1-C2-C3
3	10-B	406	GOL	O1-C1-C2-C3
3	1-B	407	GOL	O1-C1-C2-C3
3	2-B	407	GOL	O1-C1-C2-C3
3	4-B	407	GOL	O1-C1-C2-C3
3	10-B	407	GOL	O1-C1-C2-C3
4	1-B	408	GOL	O1-C1-C2-C3
4	8-B	408	GOL	O1-C1-C2-C3
3	1-C	402	GOL	O1-C1-C2-C3
3	3-C	402	GOL	O1-C1-C2-C3
3	4-C	402	GOL	O2-C2-C3-O3
3	5-C	402	GOL	O1-C1-C2-C3
3	6-C	402	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	6-C	402	GOL	O1-C1-C2-C3
3	7-C	402	GOL	O1-C1-C2-C3
3	7-C	402	GOL	C1-C2-C3-O3
3	8-C	402	GOL	O1-C1-C2-C3
3	9-C	402	GOL	O1-C1-C2-C3
3	10-C	402	GOL	O1-C1-C2-C3
3	2-C	403	GOL	C1-C2-C3-O3
3	3-C	403	GOL	O1-C1-C2-C3
3	4-C	403	GOL	O1-C1-C2-C3
3	8-C	403	GOL	O1-C1-C2-C3
3	9-C	403	GOL	O1-C1-C2-C3
3	9-C	403	GOL	C1-C2-C3-O3
3	10-C	403	GOL	O1-C1-C2-C3
3	1-D	402	GOL	O1-C1-C2-C3
3	2-D	402	GOL	O1-C1-C2-C3
3	3-D	402	GOL	O1-C1-C2-C3
3	4-D	402	GOL	O1-C1-C2-C3
3	5-D	402	GOL	O1-C1-C2-C3
3	7-D	402	GOL	O1-C1-C2-C3
3	8-D	402	GOL	O1-C1-C2-C3
3	10-D	402	GOL	O1-C1-C2-C3
3	10-D	402	GOL	C1-C2-C3-O3
3	10-D	402	GOL	O2-C2-C3-O3
3	1-D	403	GOL	O1-C1-C2-O2
3	1-D	403	GOL	O1-C1-C2-C3
3	1-D	403	GOL	C1-C2-C3-O3
3	2-D	403	GOL	O1-C1-C2-C3
3	5-D	403	GOL	O1-C1-C2-O2
3	7-D	403	GOL	C1-C2-C3-O3
3	7-D	403	GOL	O2-C2-C3-O3
3	8-D	403	GOL	O1-C1-C2-C3
3	8-D	403	GOL	C1-C2-C3-O3
3	9-D	403	GOL	O1-C1-C2-C3
3	5-D	404	GOL	O1-C1-C2-C3
3	7-D	404	GOL	O1-C1-C2-C3
3	7-D	404	GOL	C1-C2-C3-O3
3	10-D	404	GOL	O1-C1-C2-C3
3	2-E	402	GOL	O1-C1-C2-C3
3	5-E	402	GOL	O1-C1-C2-C3
3	6-E	402	GOL	O1-C1-C2-O2
3	6-E	402	GOL	O1-C1-C2-C3
3	7-E	402	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	7-E	402	GOL	O1-C1-C2-C3
3	2-E	403	GOL	O1-C1-C2-C3
3	3-E	403	GOL	O1-C1-C2-C3
3	4-E	403	GOL	O1-C1-C2-C3
3	5-E	403	GOL	O1-C1-C2-C3
3	6-E	403	GOL	O1-C1-C2-C3
3	7-E	403	GOL	O1-C1-C2-O2
3	7-E	403	GOL	O1-C1-C2-C3
3	9-E	403	GOL	O1-C1-C2-O2
3	9-E	403	GOL	O1-C1-C2-C3
3	10-E	403	GOL	O1-C1-C2-C3
3	1-F	402	GOL	O1-C1-C2-C3
3	2-F	402	GOL	O1-C1-C2-C3
3	3-F	402	GOL	C1-C2-C3-O3
3	4-F	402	GOL	O1-C1-C2-O2
3	4-F	402	GOL	O1-C1-C2-C3
3	6-F	402	GOL	O1-C1-C2-O2
3	6-F	402	GOL	O1-C1-C2-C3
3	7-F	402	GOL	O1-C1-C2-C3
3	8-F	402	GOL	O1-C1-C2-C3
3	10-F	402	GOL	O1-C1-C2-C3
3	1-F	403	GOL	O1-C1-C2-C3
3	8-F	403	GOL	O1-C1-C2-C3
3	9-F	403	GOL	O1-C1-C2-O2
3	9-F	403	GOL	O1-C1-C2-C3
3	10-F	403	GOL	O1-C1-C2-C3
3	10-F	403	GOL	C1-C2-C3-O3
3	2-F	404	GOL	O1-C1-C2-C3
3	4-F	404	GOL	O1-C1-C2-C3
3	6-F	404	GOL	O1-C1-C2-C3
3	7-F	404	GOL	O1-C1-C2-C3
3	7-F	404	GOL	C1-C2-C3-O3
3	8-F	404	GOL	O1-C1-C2-C3
3	9-F	404	GOL	O1-C1-C2-C3
3	10-F	404	GOL	O1-C1-C2-O2
3	1-F	405	GOL	O1-C1-C2-C3
3	2-F	405	GOL	O1-C1-C2-C3
3	7-F	405	GOL	O1-C1-C2-C3
3	8-F	405	GOL	O1-C1-C2-C3
3	10-F	405	GOL	C1-C2-C3-O3
3	1-F	406	GOL	O1-C1-C2-C3
3	7-F	406	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	10-F	406	GOL	O1-C1-C2-C3
5	1-F	407	GOL	O1-C1-C2-C3
3	1-G	402	GOL	O1-C1-C2-O2
3	3-G	402	GOL	O1-C1-C2-C3
3	5-G	402	GOL	O1-C1-C2-C3
3	7-G	402	GOL	O1-C1-C2-C3
3	10-G	402	GOL	O1-C1-C2-C3
3	1-G	404	GOL	O1-C1-C2-C3
3	4-G	404	GOL	O1-C1-C2-C3
3	10-G	404	GOL	C1-C2-C3-O3
3	1-G	403	GOL	O1-C1-C2-C3
3	2-G	403	GOL	O1-C1-C2-C3
3	8-G	403	GOL	O1-C1-C2-C3
5	4-G	405	GOL	O1-C1-C2-C3
5	5-G	405	GOL	O1-C1-C2-C3
4	4-G	406	GOL	O1-C1-C2-C3
3	1-H	402	GOL	O1-C1-C2-O2
3	1-H	402	GOL	O1-C1-C2-C3
3	4-H	402	GOL	O1-C1-C2-C3
3	5-H	402	GOL	C1-C2-C3-O3
3	5-H	402	GOL	O2-C2-C3-O3
3	6-H	402	GOL	O1-C1-C2-C3
3	6-H	402	GOL	C1-C2-C3-O3
3	7-H	402	GOL	O1-C1-C2-C3
3	8-H	402	GOL	C1-C2-C3-O3
3	9-H	402	GOL	O1-C1-C2-C3
3	3-H	403	GOL	O1-C1-C2-C3
3	10-H	403	GOL	O1-C1-C2-C3
3	4-H	404	GOL	O1-C1-C2-C3
3	9-H	404	GOL	O1-C1-C2-C3
3	9-H	405	GOL	C1-C2-C3-O3
3	9-H	405	GOL	O2-C2-C3-O3
3	10-H	405	GOL	O1-C1-C2-C3
4	3-A	405	GOL	O1-C1-C2-C3
4	5-A	405	GOL	O1-C1-C2-O2
4	5-A	405	GOL	O1-C1-C2-C3
4	6-A	405	GOL	O1-C1-C2-C3
4	6-A	405	GOL	C1-C2-C3-O3
4	6-A	405	GOL	O2-C2-C3-O3
4	7-A	405	GOL	O1-C1-C2-C3
4	9-A	405	GOL	O1-C1-C2-C3
5	4-C	404	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	4-C	404	GOL	O2-C2-C3-O3
4	4-E	404	GOL	O1-C1-C2-O2
4	4-E	404	GOL	O1-C1-C2-C3
4	5-E	404	GOL	C1-C2-C3-O3
4	6-E	404	GOL	O1-C1-C2-O2
4	6-E	404	GOL	O1-C1-C2-C3
4	6-E	404	GOL	C1-C2-C3-O3
4	8-E	404	GOL	O1-C1-C2-O2
4	8-E	404	GOL	O1-C1-C2-C3
4	9-E	404	GOL	O1-C1-C2-C3
3	4-A	402	GOL	O1-C1-C2-O2
3	7-A	402	GOL	O1-C1-C2-O2
3	9-A	402	GOL	O1-C1-C2-O2
3	8-A	403	GOL	O1-C1-C2-O2
3	4-B	402	GOL	O1-C1-C2-O2
3	10-B	402	GOL	O1-C1-C2-O2
3	4-B	404	GOL	O2-C2-C3-O3
3	5-B	404	GOL	O1-C1-C2-O2
3	8-B	404	GOL	O1-C1-C2-O2
3	1-B	405	GOL	O1-C1-C2-O2
3	1-B	405	GOL	O2-C2-C3-O3
3	10-B	405	GOL	O2-C2-C3-O3
3	6-B	406	GOL	O1-C1-C2-O2
3	7-C	402	GOL	O1-C1-C2-O2
3	8-C	402	GOL	O1-C1-C2-O2
3	2-C	403	GOL	O2-C2-C3-O3
3	9-C	403	GOL	O1-C1-C2-O2
3	10-C	403	GOL	O1-C1-C2-O2
3	4-D	402	GOL	O1-C1-C2-O2
3	7-D	402	GOL	O1-C1-C2-O2
3	1-D	403	GOL	O2-C2-C3-O3
3	8-D	403	GOL	O2-C2-C3-O3
3	2-E	403	GOL	O1-C1-C2-O2
3	4-E	403	GOL	O1-C1-C2-O2
3	5-E	403	GOL	O1-C1-C2-O2
3	3-F	402	GOL	O1-C1-C2-O2
3	3-F	402	GOL	O2-C2-C3-O3
3	7-F	402	GOL	O1-C1-C2-O2
3	5-F	403	GOL	O1-C1-C2-O2
3	7-F	403	GOL	O1-C1-C2-O2
3	10-F	403	GOL	O2-C2-C3-O3
3	10-F	405	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	10-G	404	GOL	O2-C2-C3-O3
3	2-G	403	GOL	O1-C1-C2-O2
3	9-G	403	GOL	O1-C1-C2-O2
5	4-G	405	GOL	O1-C1-C2-O2
3	6-H	402	GOL	O1-C1-C2-O2
2	2-A	401	MES	C7-C8-S-O3S
2	3-A	401	MES	C7-C8-S-O3S
2	5-B	401	MES	C7-C8-S-O3S
2	9-B	401	MES	C7-C8-S-O3S
2	10-B	401	MES	C7-C8-S-O3S
2	1-C	401	MES	C7-C8-S-O3S
2	3-C	401	MES	C7-C8-S-O3S
2	8-C	401	MES	C7-C8-S-O3S
2	9-C	401	MES	C7-C8-S-O3S
2	10-C	401	MES	C7-C8-S-O3S
2	2-D	401	MES	C7-C8-S-O3S
2	6-D	401	MES	C7-C8-S-O3S
2	9-D	401	MES	C7-C8-S-O3S
2	10-E	401	MES	C7-C8-S-O3S
3	4-A	402	GOL	C1-C2-C3-O3
3	7-A	402	GOL	C1-C2-C3-O3
3	9-A	402	GOL	O1-C1-C2-C3
3	9-A	402	GOL	C1-C2-C3-O3
3	10-A	402	GOL	O1-C1-C2-C3
3	3-A	403	GOL	O1-C1-C2-C3
3	7-A	403	GOL	O1-C1-C2-C3
3	8-A	403	GOL	O1-C1-C2-C3
3	9-A	403	GOL	O1-C1-C2-C3
3	5-A	404	GOL	O1-C1-C2-C3
3	8-A	404	GOL	O1-C1-C2-C3
3	1-B	402	GOL	O1-C1-C2-C3
3	2-B	402	GOL	O1-C1-C2-C3
3	3-B	402	GOL	C1-C2-C3-O3
3	5-B	402	GOL	C1-C2-C3-O3
3	2-B	403	GOL	O1-C1-C2-C3
3	3-B	403	GOL	O1-C1-C2-C3
3	7-B	403	GOL	O1-C1-C2-C3
3	8-B	403	GOL	O1-C1-C2-C3
3	2-B	404	GOL	C1-C2-C3-O3
3	9-B	404	GOL	C1-C2-C3-O3
3	1-B	405	GOL	C1-C2-C3-O3
3	4-B	405	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	4-B	405	GOL	C1-C2-C3-O3
3	6-B	405	GOL	C1-C2-C3-O3
3	7-B	405	GOL	O1-C1-C2-C3
3	7-B	405	GOL	C1-C2-C3-O3
3	8-B	405	GOL	C1-C2-C3-O3
3	10-B	405	GOL	O1-C1-C2-C3
3	3-B	406	GOL	O1-C1-C2-C3
3	3-B	406	GOL	C1-C2-C3-O3
3	5-B	406	GOL	O1-C1-C2-C3
3	6-B	406	GOL	C1-C2-C3-O3
3	1-B	407	GOL	C1-C2-C3-O3
3	8-B	407	GOL	O1-C1-C2-C3
3	4-C	402	GOL	C1-C2-C3-O3
3	8-C	402	GOL	C1-C2-C3-O3
3	10-C	402	GOL	C1-C2-C3-O3
3	2-C	403	GOL	O1-C1-C2-C3
3	6-D	402	GOL	O1-C1-C2-C3
3	9-D	402	GOL	O1-C1-C2-C3
3	4-D	403	GOL	O1-C1-C2-C3
3	4-D	403	GOL	C1-C2-C3-O3
3	5-D	403	GOL	O1-C1-C2-C3
3	9-D	403	GOL	C1-C2-C3-O3
3	5-D	404	GOL	C1-C2-C3-O3
3	9-D	404	GOL	O1-C1-C2-C3
3	9-D	404	GOL	C1-C2-C3-O3
3	9-E	402	GOL	O1-C1-C2-C3
3	1-E	403	GOL	C1-C2-C3-O3
3	4-E	403	GOL	C1-C2-C3-O3
3	3-F	402	GOL	O1-C1-C2-C3
3	10-F	402	GOL	C1-C2-C3-O3
3	5-F	403	GOL	O1-C1-C2-C3
3	7-F	403	GOL	O1-C1-C2-C3
3	5-F	404	GOL	O1-C1-C2-C3
3	10-F	404	GOL	O1-C1-C2-C3
3	3-F	405	GOL	O1-C1-C2-C3
3	3-F	405	GOL	C1-C2-C3-O3
3	6-F	405	GOL	O1-C1-C2-C3
3	10-F	405	GOL	O1-C1-C2-C3
3	1-G	402	GOL	O1-C1-C2-C3
3	8-G	402	GOL	C1-C2-C3-O3
3	9-G	402	GOL	O1-C1-C2-C3
3	2-G	404	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	3-G	404	GOL	C1-C2-C3-O3
3	5-G	404	GOL	O1-C1-C2-C3
3	7-G	404	GOL	C1-C2-C3-O3
3	8-G	404	GOL	O1-C1-C2-C3
3	10-G	404	GOL	O1-C1-C2-C3
3	4-G	403	GOL	O1-C1-C2-C3
3	6-G	403	GOL	O1-C1-C2-C3
3	7-G	403	GOL	O1-C1-C2-C3
3	9-G	403	GOL	O1-C1-C2-C3
3	10-G	403	GOL	C1-C2-C3-O3
5	8-G	405	GOL	O1-C1-C2-C3
3	2-H	402	GOL	C1-C2-C3-O3
3	3-H	402	GOL	O1-C1-C2-C3
3	3-H	402	GOL	C1-C2-C3-O3
3	9-H	402	GOL	C1-C2-C3-O3
3	10-H	402	GOL	O1-C1-C2-C3
3	1-H	403	GOL	O1-C1-C2-C3
3	2-H	403	GOL	C1-C2-C3-O3
3	3-H	403	GOL	C1-C2-C3-O3
3	6-H	403	GOL	O1-C1-C2-C3
3	7-H	403	GOL	O1-C1-C2-C3
3	2-H	404	GOL	O1-C1-C2-C3
3	6-H	404	GOL	O1-C1-C2-C3
3	8-H	404	GOL	C1-C2-C3-O3
3	10-H	404	GOL	O1-C1-C2-C3
3	6-H	405	GOL	C1-C2-C3-O3
3	10-H	405	GOL	C1-C2-C3-O3
4	5-A	405	GOL	C1-C2-C3-O3
5	2-C	404	GOL	O1-C1-C2-C3
4	7-E	404	GOL	O1-C1-C2-C3
4	7-E	404	GOL	C1-C2-C3-O3
4	8-E	404	GOL	C1-C2-C3-O3
3	1-A	402	GOL	O1-C1-C2-O2
3	3-A	402	GOL	O1-C1-C2-O2
3	6-A	402	GOL	O1-C1-C2-O2
3	8-A	402	GOL	O1-C1-C2-O2
3	4-A	403	GOL	O1-C1-C2-O2
3	5-A	403	GOL	O1-C1-C2-O2
3	6-A	403	GOL	O1-C1-C2-O2
3	1-A	404	GOL	O1-C1-C2-O2
3	2-A	404	GOL	O1-C1-C2-O2
3	5-A	404	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	9-A	404	GOL	O1-C1-C2-O2
3	10-A	404	GOL	O1-C1-C2-O2
3	1-B	402	GOL	O2-C2-C3-O3
3	3-B	402	GOL	O2-C2-C3-O3
3	8-B	402	GOL	O1-C1-C2-O2
3	9-B	402	GOL	O1-C1-C2-O2
3	2-B	403	GOL	O1-C1-C2-O2
3	4-B	403	GOL	O1-C1-C2-O2
3	6-B	403	GOL	O1-C1-C2-O2
3	10-B	403	GOL	O1-C1-C2-O2
3	1-B	404	GOL	O1-C1-C2-O2
3	6-B	404	GOL	O1-C1-C2-O2
3	7-B	404	GOL	O1-C1-C2-O2
3	2-B	405	GOL	O1-C1-C2-O2
3	4-B	405	GOL	O1-C1-C2-O2
3	4-B	405	GOL	O2-C2-C3-O3
3	5-B	405	GOL	O2-C2-C3-O3
3	6-B	405	GOL	O1-C1-C2-O2
3	7-B	405	GOL	O1-C1-C2-O2
3	9-B	405	GOL	O1-C1-C2-O2
3	1-B	406	GOL	O1-C1-C2-O2
3	3-B	406	GOL	O1-C1-C2-O2
3	5-B	406	GOL	O1-C1-C2-O2
3	10-B	406	GOL	O1-C1-C2-O2
3	1-B	407	GOL	O1-C1-C2-O2
3	2-B	407	GOL	O1-C1-C2-O2
3	4-B	407	GOL	O1-C1-C2-O2
3	10-B	407	GOL	O1-C1-C2-O2
4	1-B	408	GOL	O1-C1-C2-O2
3	3-C	402	GOL	O1-C1-C2-O2
3	8-C	402	GOL	O2-C2-C3-O3
3	9-C	402	GOL	O1-C1-C2-O2
3	3-C	403	GOL	O1-C1-C2-O2
3	4-C	403	GOL	O1-C1-C2-O2
3	8-C	403	GOL	O1-C1-C2-O2
3	1-D	402	GOL	O1-C1-C2-O2
3	2-D	402	GOL	O1-C1-C2-O2
3	3-D	402	GOL	O1-C1-C2-O2
3	5-D	402	GOL	O1-C1-C2-O2
3	9-D	402	GOL	O1-C1-C2-O2
3	10-D	402	GOL	O1-C1-C2-O2
3	2-D	403	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	4-D	403	GOL	O1-C1-C2-O2
3	4-D	403	GOL	O2-C2-C3-O3
3	8-D	403	GOL	O1-C1-C2-O2
3	9-D	403	GOL	O2-C2-C3-O3
3	5-D	404	GOL	O1-C1-C2-O2
3	7-D	404	GOL	O1-C1-C2-O2
3	7-D	404	GOL	O2-C2-C3-O3
3	2-E	402	GOL	O1-C1-C2-O2
3	6-E	403	GOL	O1-C1-C2-O2
3	1-F	402	GOL	O1-C1-C2-O2
3	2-F	402	GOL	O1-C1-C2-O2
3	10-F	402	GOL	O1-C1-C2-O2
3	1-F	403	GOL	O1-C1-C2-O2
3	8-F	403	GOL	O1-C1-C2-O2
3	10-F	403	GOL	O1-C1-C2-O2
3	6-F	404	GOL	O1-C1-C2-O2
3	7-F	404	GOL	O2-C2-C3-O3
3	9-F	404	GOL	O1-C1-C2-O2
3	7-F	405	GOL	O1-C1-C2-O2
3	8-F	405	GOL	O1-C1-C2-O2
3	10-F	405	GOL	O2-C2-C3-O3
3	1-F	406	GOL	O1-C1-C2-O2
3	1-F	406	GOL	O2-C2-C3-O3
3	5-G	402	GOL	O1-C1-C2-O2
3	10-G	402	GOL	O1-C1-C2-O2
3	1-G	404	GOL	O1-C1-C2-O2
3	8-G	404	GOL	O1-C1-C2-O2
3	8-G	403	GOL	O1-C1-C2-O2
5	5-G	405	GOL	O1-C1-C2-O2
5	8-G	405	GOL	O1-C1-C2-O2
4	4-G	406	GOL	O1-C1-C2-O2
3	3-H	402	GOL	O1-C1-C2-O2
3	3-H	402	GOL	O2-C2-C3-O3
3	4-H	402	GOL	O1-C1-C2-O2
3	7-H	402	GOL	O1-C1-C2-O2
3	8-H	402	GOL	O2-C2-C3-O3
3	9-H	402	GOL	O1-C1-C2-O2
3	10-H	402	GOL	O1-C1-C2-O2
3	3-H	403	GOL	O1-C1-C2-O2
3	10-H	403	GOL	O1-C1-C2-O2
3	2-H	404	GOL	O1-C1-C2-O2
3	4-H	404	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	9-H	404	GOL	O1-C1-C2-O2
4	3-A	405	GOL	O1-C1-C2-O2
4	6-A	405	GOL	O1-C1-C2-O2
4	9-A	405	GOL	O1-C1-C2-O2
4	7-E	404	GOL	O1-C1-C2-O2
4	7-E	404	GOL	O2-C2-C3-O3
2	4-A	401	MES	C7-C8-S-O3S
2	7-A	401	MES	C7-C8-S-O3S
2	7-E	401	MES	C7-C8-S-O3S
2	8-B	401	MES	N4-C7-C8-S
2	2-E	401	MES	N4-C7-C8-S
2	7-G	401	MES	N4-C7-C8-S
3	8-A	402	GOL	O2-C2-C3-O3
3	3-A	403	GOL	O1-C1-C2-O2
3	4-A	404	GOL	O1-C1-C2-O2
3	1-B	402	GOL	O1-C1-C2-O2
3	1-B	403	GOL	O1-C1-C2-O2
3	2-B	404	GOL	O2-C2-C3-O3
3	7-B	406	GOL	O1-C1-C2-O2
3	8-B	406	GOL	O1-C1-C2-O2
4	8-B	408	GOL	O1-C1-C2-O2
3	7-C	402	GOL	O2-C2-C3-O3
3	10-C	402	GOL	O1-C1-C2-O2
3	9-C	403	GOL	O2-C2-C3-O3
3	6-D	402	GOL	O1-C1-C2-O2
3	8-D	402	GOL	O1-C1-C2-O2
3	9-D	403	GOL	O1-C1-C2-O2
3	9-D	404	GOL	O1-C1-C2-O2
3	10-D	404	GOL	O1-C1-C2-O2
3	5-E	402	GOL	O1-C1-C2-O2
3	3-E	403	GOL	O1-C1-C2-O2
3	4-E	403	GOL	O2-C2-C3-O3
3	10-E	403	GOL	O1-C1-C2-O2
3	2-F	404	GOL	O1-C1-C2-O2
3	4-F	404	GOL	O1-C1-C2-O2
3	7-F	404	GOL	O1-C1-C2-O2
3	8-F	404	GOL	O1-C1-C2-O2
3	2-F	405	GOL	O1-C1-C2-O2
3	6-F	405	GOL	O1-C1-C2-O2
3	7-F	406	GOL	O1-C1-C2-O2
5	1-F	407	GOL	O1-C1-C2-O2
3	3-G	402	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	7-G	402	GOL	O1-C1-C2-O2
3	4-G	403	GOL	O1-C1-C2-O2
3	9-H	402	GOL	O2-C2-C3-O3
3	2-H	403	GOL	O2-C2-C3-O3
3	3-H	403	GOL	O2-C2-C3-O3
3	6-H	403	GOL	O1-C1-C2-O2
3	6-H	404	GOL	O1-C1-C2-O2
3	8-H	404	GOL	O2-C2-C3-O3
3	10-H	404	GOL	O1-C1-C2-O2
3	10-H	405	GOL	O1-C1-C2-O2
4	5-A	405	GOL	O2-C2-C3-O3
4	7-A	405	GOL	O1-C1-C2-O2
4	5-E	404	GOL	O2-C2-C3-O3
4	6-E	404	GOL	O2-C2-C3-O3
4	9-E	404	GOL	O1-C1-C2-O2
2	1-A	401	MES	C8-C7-N4-C3
2	2-A	401	MES	C8-C7-N4-C3
2	5-A	401	MES	C8-C7-N4-C5
2	6-A	401	MES	C8-C7-N4-C3
2	8-A	401	MES	C8-C7-N4-C3
2	2-B	401	MES	C8-C7-N4-C5
2	3-B	401	MES	C8-C7-N4-C3
2	5-B	401	MES	C8-C7-N4-C5
2	7-B	401	MES	C8-C7-N4-C3
2	10-B	401	MES	C8-C7-N4-C3
2	1-C	401	MES	C8-C7-N4-C3
2	2-C	401	MES	C8-C7-N4-C3
2	2-C	401	MES	C8-C7-N4-C5
2	3-C	401	MES	C8-C7-N4-C3
2	5-C	401	MES	C8-C7-N4-C3
2	10-C	401	MES	C8-C7-N4-C5
2	2-D	401	MES	C8-C7-N4-C3
2	6-D	401	MES	C8-C7-N4-C5
2	10-D	401	MES	C8-C7-N4-C5
2	5-E	401	MES	C8-C7-N4-C3
2	6-E	401	MES	C8-C7-N4-C3
2	6-E	401	MES	C8-C7-N4-C5
2	8-E	401	MES	C8-C7-N4-C3
2	9-E	401	MES	C8-C7-N4-C3
2	9-E	401	MES	C8-C7-N4-C5
2	5-F	401	MES	C8-C7-N4-C3
2	5-F	401	MES	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
2	9-F	401	MES	C8-C7-N4-C5
2	7-G	401	MES	C8-C7-N4-C5
2	10-G	401	MES	C8-C7-N4-C3
2	3-H	401	MES	C8-C7-N4-C5
2	5-H	401	MES	C8-C7-N4-C5
2	6-H	401	MES	C8-C7-N4-C3
2	7-H	401	MES	C8-C7-N4-C3
2	1-A	401	MES	C7-C8-S-O3S
2	4-B	401	MES	C7-C8-S-O3S
2	4-E	401	MES	C7-C8-S-O3S
2	3-H	401	MES	C7-C8-S-O3S
3	1-A	402	GOL	O2-C2-C3-O3
3	4-A	402	GOL	O2-C2-C3-O3
3	9-A	402	GOL	O2-C2-C3-O3
3	9-A	403	GOL	O1-C1-C2-O2
3	3-A	404	GOL	O1-C1-C2-O2
3	6-B	405	GOL	O2-C2-C3-O3
3	7-B	405	GOL	O2-C2-C3-O3
3	5-C	402	GOL	O1-C1-C2-O2
3	7-E	402	GOL	O2-C2-C3-O3
3	8-E	402	GOL	O1-C1-C2-O2
3	3-F	404	GOL	O1-C1-C2-O2
3	5-F	404	GOL	O1-C1-C2-O2
3	1-F	405	GOL	O1-C1-C2-O2
3	3-F	405	GOL	O1-C1-C2-O2
3	10-F	406	GOL	O1-C1-C2-O2
3	8-G	402	GOL	O2-C2-C3-O3
3	9-G	402	GOL	O1-C1-C2-O2
3	4-G	404	GOL	O1-C1-C2-O2
3	10-G	403	GOL	O1-C1-C2-O2
3	2-H	402	GOL	O2-C2-C3-O3
3	7-B	403	GOL	O1-C1-C2-O2
3	2-B	404	GOL	O1-C1-C2-O2
3	9-B	404	GOL	O2-C2-C3-O3
3	2-C	403	GOL	O1-C1-C2-O2
3	3-C	403	GOL	O2-C2-C3-O3
3	5-D	403	GOL	O2-C2-C3-O3
3	5-D	404	GOL	O2-C2-C3-O3
3	1-E	403	GOL	O2-C2-C3-O3
3	10-F	402	GOL	O2-C2-C3-O3
3	6-F	404	GOL	O2-C2-C3-O3
3	3-F	406	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	6-F	406	GOL	O1-C1-C2-O2
3	5-G	402	GOL	O2-C2-C3-O3
3	3-G	404	GOL	O2-C2-C3-O3
3	1-G	403	GOL	O1-C1-C2-O2
3	6-G	403	GOL	O1-C1-C2-O2
3	1-H	403	GOL	O1-C1-C2-O2
3	5-H	403	GOL	O1-C1-C2-O2
3	6-H	404	GOL	O2-C2-C3-O3
3	10-H	405	GOL	O2-C2-C3-O3
5	4-C	404	GOL	O1-C1-C2-O2
4	8-E	404	GOL	O2-C2-C3-O3
2	1-A	401	MES	C7-C8-S-O1S
2	1-A	401	MES	C7-C8-S-O2S
2	2-A	401	MES	C7-C8-S-O1S
2	3-A	401	MES	C7-C8-S-O1S
2	3-A	401	MES	C7-C8-S-O2S
2	4-A	401	MES	C7-C8-S-O1S
2	4-A	401	MES	C7-C8-S-O2S
2	8-A	401	MES	C7-C8-S-O2S
2	4-B	401	MES	C7-C8-S-O1S
2	4-B	401	MES	C7-C8-S-O2S
2	9-B	401	MES	C7-C8-S-O1S
2	9-B	401	MES	C7-C8-S-O2S
2	10-B	401	MES	C7-C8-S-O1S
2	10-B	401	MES	C7-C8-S-O2S
2	1-C	401	MES	C7-C8-S-O1S
2	1-C	401	MES	C7-C8-S-O2S
2	2-C	401	MES	C7-C8-S-O2S
2	3-C	401	MES	C7-C8-S-O1S
2	3-C	401	MES	C7-C8-S-O2S
2	4-C	401	MES	C7-C8-S-O1S
2	4-C	401	MES	C7-C8-S-O2S
2	8-C	401	MES	C7-C8-S-O1S
2	8-C	401	MES	C7-C8-S-O2S
2	9-C	401	MES	C7-C8-S-O1S
2	10-C	401	MES	C7-C8-S-O1S
2	10-C	401	MES	C7-C8-S-O2S
2	2-D	401	MES	C7-C8-S-O1S
2	3-D	401	MES	C7-C8-S-O1S
2	4-D	401	MES	C7-C8-S-O1S
2	6-D	401	MES	C7-C8-S-O1S
2	6-D	401	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
2	9-D	401	MES	C7-C8-S-O1S
2	2-E	401	MES	C7-C8-S-O2S
2	4-E	401	MES	C7-C8-S-O1S
2	5-E	401	MES	C7-C8-S-O2S
2	7-E	401	MES	C7-C8-S-O1S
2	7-E	401	MES	C7-C8-S-O2S
2	8-E	401	MES	C7-C8-S-O1S
2	10-E	401	MES	C7-C8-S-O1S
2	10-E	401	MES	C7-C8-S-O2S
2	5-F	401	MES	C7-C8-S-O2S
2	8-F	401	MES	C7-C8-S-O2S
2	9-F	401	MES	C7-C8-S-O2S
2	3-G	401	MES	C7-C8-S-O1S
2	5-G	401	MES	C7-C8-S-O1S
2	7-G	401	MES	C7-C8-S-O2S
2	8-G	401	MES	C7-C8-S-O1S
2	9-G	401	MES	C7-C8-S-O1S
2	3-H	401	MES	C7-C8-S-O2S
2	5-H	401	MES	C7-C8-S-O1S
2	6-H	401	MES	C7-C8-S-O1S
2	8-H	401	MES	C7-C8-S-O2S
3	5-A	404	GOL	C1-C2-C3-O3
3	9-B	403	GOL	O1-C1-C2-C3
3	1-E	403	GOL	O1-C1-C2-C3
3	3-F	406	GOL	O1-C1-C2-C3
3	6-F	406	GOL	O1-C1-C2-C3
3	2-H	402	GOL	O1-C1-C2-C3
2	4-A	401	MES	N4-C7-C8-S
2	3-B	401	MES	N4-C7-C8-S
2	8-C	401	MES	N4-C7-C8-S
2	9-C	401	MES	N4-C7-C8-S
2	5-D	401	MES	N4-C7-C8-S
2	8-D	401	MES	N4-C7-C8-S
2	9-D	401	MES	N4-C7-C8-S
2	4-E	401	MES	N4-C7-C8-S
2	5-F	401	MES	N4-C7-C8-S
2	6-F	401	MES	N4-C7-C8-S
2	8-F	401	MES	N4-C7-C8-S
2	8-G	401	MES	N4-C7-C8-S
2	2-H	401	MES	N4-C7-C8-S
2	3-H	401	MES	N4-C7-C8-S
2	4-H	401	MES	N4-C7-C8-S

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Mol	Chain	Res	Type	Atoms
2	7-H	401	MES	N4-C7-C8-S
3	6-B	403	GOL	O2-C2-C3-O3
3	9-B	403	GOL	O1-C1-C2-O2
3	1-C	402	GOL	O1-C1-C2-O2
3	9-E	402	GOL	O1-C1-C2-O2
3	5-G	404	GOL	O1-C1-C2-O2
3	6-H	402	GOL	O2-C2-C3-O3
3	4-H	403	GOL	O2-C2-C3-O3
2	8-G	401	MES	C7-C8-S-O3S
3	10-A	402	GOL	O1-C1-C2-O2
3	2-B	402	GOL	O1-C1-C2-O2
3	5-B	405	GOL	O1-C1-C2-O2
3	3-B	406	GOL	O2-C2-C3-O3
3	6-B	406	GOL	O2-C2-C3-O3
3	1-B	407	GOL	O2-C2-C3-O3
3	6-D	404	GOL	O1-C1-C2-O2
3	6-F	405	GOL	O2-C2-C3-O3
3	10-G	403	GOL	O2-C2-C3-O3
2	6-A	401	MES	C8-C7-N4-C5
2	10-A	401	MES	C8-C7-N4-C3
2	5-B	401	MES	C8-C7-N4-C3
2	9-B	401	MES	C8-C7-N4-C3
2	4-C	401	MES	C8-C7-N4-C5
2	8-C	401	MES	C8-C7-N4-C3
2	8-C	401	MES	C8-C7-N4-C5
2	2-E	401	MES	C8-C7-N4-C3
2	4-E	401	MES	C8-C7-N4-C3
2	10-E	401	MES	C8-C7-N4-C5
2	3-F	401	MES	C8-C7-N4-C5
2	6-F	401	MES	C8-C7-N4-C5
3	7-F	402	GOL	C1-C2-C3-O3
5	1-G	405	GOL	C1-C2-C3-O3
4	2-E	404	GOL	O1-C1-C2-C3
2	1-E	401	MES	C7-C8-S-O3S
2	10-G	401	MES	C7-C8-S-O3S
3	5-A	402	GOL	C1-C2-C3-O3
3	2-A	403	GOL	O1-C1-C2-C3
3	4-E	402	GOL	O1-C1-C2-C3
3	8-E	402	GOL	O1-C1-C2-C3
3	3-F	404	GOL	O1-C1-C2-C3
5	8-G	405	GOL	C1-C2-C3-O3
3	5-B	402	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	5-F	402	GOL	O1-C1-C2-O2
3	9-H	404	GOL	O2-C2-C3-O3
3	6-H	405	GOL	O2-C2-C3-O3
3	7-A	403	GOL	O1-C1-C2-O2
3	9-A	403	GOL	O2-C2-C3-O3
3	8-A	404	GOL	O1-C1-C2-O2
3	8-A	404	GOL	O2-C2-C3-O3
3	8-B	403	GOL	O1-C1-C2-O2
3	10-B	406	GOL	O2-C2-C3-O3
3	8-B	407	GOL	O1-C1-C2-O2
3	8-F	405	GOL	O2-C2-C3-O3
3	2-G	404	GOL	O1-C1-C2-O2
3	3-G	404	GOL	O1-C1-C2-O2
2	2-C	401	MES	C7-C8-S-O3S
2	2-C	401	MES	C7-C8-S-O1S
2	5-C	401	MES	C7-C8-S-O1S
2	1-E	401	MES	C7-C8-S-O1S
2	8-G	401	MES	C7-C8-S-O2S
2	10-G	401	MES	C7-C8-S-O2S
2	1-H	401	MES	C7-C8-S-O1S
2	2-F	401	MES	C8-C7-N4-C3
2	4-F	401	MES	C8-C7-N4-C3
2	2-H	401	MES	C8-C7-N4-C3
3	2-B	404	GOL	O1-C1-C2-C3
3	6-H	404	GOL	C1-C2-C3-O3
3	7-A	404	GOL	O1-C1-C2-O2
5	8-G	405	GOL	O2-C2-C3-O3
2	5-C	401	MES	C7-C8-S-O3S
2	6-C	401	MES	C7-C8-S-O3S
3	10-C	402	GOL	O2-C2-C3-O3
3	8-F	402	GOL	O1-C1-C2-O2
3	5-A	404	GOL	O2-C2-C3-O3
3	8-B	402	GOL	O2-C2-C3-O3
3	3-B	403	GOL	O1-C1-C2-O2
3	10-G	404	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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.