



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 10:18 AM EDT

PDB ID : 7YP3 / pdb_00007yp3
Title : Crystal structure of elaiophylin glycosyltransferase in complex with elaiophylin
Authors : Xu, T.; Liu, Q.; Gan, Q.; Liu, J.
Deposited on : 2022-08-02
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 : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

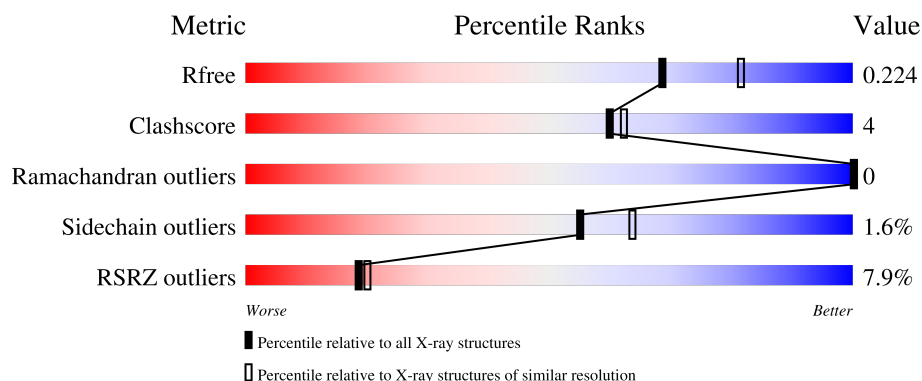
1 Overall quality at a glance

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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	437	3% 83% 10% 6%
1	B	437	10% 83% 9% 7%
1	C	437	9% 82% 10% 7%
1	D	437	6% 84% 8% 7%
1	E	437	10% 82% 10% 7%

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Mol	Chain	Length	Quality of chain
1	F	437	6% 85% 10%
1	G	437	7% 82% 10% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24066 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3225	2052	565	595	13			
1	B	408	Total	C	N	O	S	0	3	0
			3234	2060	564	595	15			
1	C	408	Total	C	N	O	S	0	1	0
			3223	2052	564	593	14			
1	D	408	Total	C	N	O	S	0	0	0
			3218	2048	564	593	13			
1	E	408	Total	C	N	O	S	0	0	0
			3218	2048	564	593	13			
1	F	419	Total	C	N	O	S	0	1	0
			3289	2090	578	608	13			
1	G	408	Total	C	N	O	S	0	0	0
			3218	2048	564	593	13			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E5L4T5
A	-18	GLY	-	expression tag	UNP E5L4T5
A	-17	SER	-	expression tag	UNP E5L4T5
A	-16	SER	-	expression tag	UNP E5L4T5
A	-15	HIS	-	expression tag	UNP E5L4T5
A	-14	HIS	-	expression tag	UNP E5L4T5
A	-13	HIS	-	expression tag	UNP E5L4T5
A	-12	HIS	-	expression tag	UNP E5L4T5
A	-11	HIS	-	expression tag	UNP E5L4T5
A	-10	HIS	-	expression tag	UNP E5L4T5
A	-9	SER	-	expression tag	UNP E5L4T5
A	-8	SER	-	expression tag	UNP E5L4T5
A	-7	GLY	-	expression tag	UNP E5L4T5
A	-6	LEU	-	expression tag	UNP E5L4T5
A	-5	VAL	-	expression tag	UNP E5L4T5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	expression tag	UNP E5L4T5
A	-3	ARG	-	expression tag	UNP E5L4T5
A	-2	GLY	-	expression tag	UNP E5L4T5
A	-1	SER	-	expression tag	UNP E5L4T5
A	0	HIS	-	expression tag	UNP E5L4T5
B	-19	MET	-	initiating methionine	UNP E5L4T5
B	-18	GLY	-	expression tag	UNP E5L4T5
B	-17	SER	-	expression tag	UNP E5L4T5
B	-16	SER	-	expression tag	UNP E5L4T5
B	-15	HIS	-	expression tag	UNP E5L4T5
B	-14	HIS	-	expression tag	UNP E5L4T5
B	-13	HIS	-	expression tag	UNP E5L4T5
B	-12	HIS	-	expression tag	UNP E5L4T5
B	-11	HIS	-	expression tag	UNP E5L4T5
B	-10	HIS	-	expression tag	UNP E5L4T5
B	-9	SER	-	expression tag	UNP E5L4T5
B	-8	SER	-	expression tag	UNP E5L4T5
B	-7	GLY	-	expression tag	UNP E5L4T5
B	-6	LEU	-	expression tag	UNP E5L4T5
B	-5	VAL	-	expression tag	UNP E5L4T5
B	-4	PRO	-	expression tag	UNP E5L4T5
B	-3	ARG	-	expression tag	UNP E5L4T5
B	-2	GLY	-	expression tag	UNP E5L4T5
B	-1	SER	-	expression tag	UNP E5L4T5
B	0	HIS	-	expression tag	UNP E5L4T5
C	-19	MET	-	initiating methionine	UNP E5L4T5
C	-18	GLY	-	expression tag	UNP E5L4T5
C	-17	SER	-	expression tag	UNP E5L4T5
C	-16	SER	-	expression tag	UNP E5L4T5
C	-15	HIS	-	expression tag	UNP E5L4T5
C	-14	HIS	-	expression tag	UNP E5L4T5
C	-13	HIS	-	expression tag	UNP E5L4T5
C	-12	HIS	-	expression tag	UNP E5L4T5
C	-11	HIS	-	expression tag	UNP E5L4T5
C	-10	HIS	-	expression tag	UNP E5L4T5
C	-9	SER	-	expression tag	UNP E5L4T5
C	-8	SER	-	expression tag	UNP E5L4T5
C	-7	GLY	-	expression tag	UNP E5L4T5
C	-6	LEU	-	expression tag	UNP E5L4T5
C	-5	VAL	-	expression tag	UNP E5L4T5
C	-4	PRO	-	expression tag	UNP E5L4T5
C	-3	ARG	-	expression tag	UNP E5L4T5

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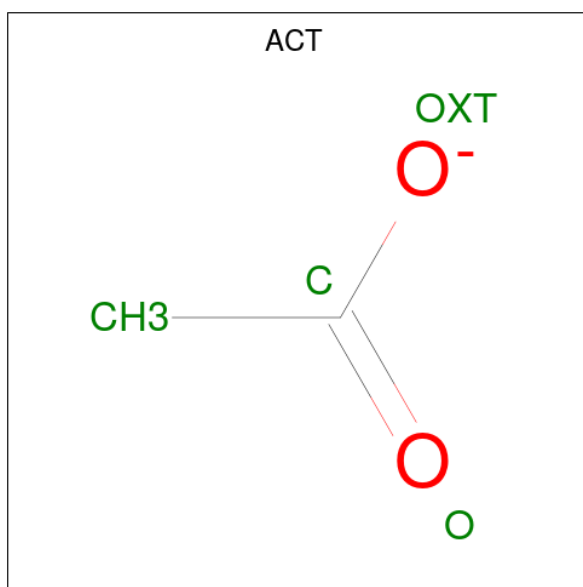
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP E5L4T5
C	-1	SER	-	expression tag	UNP E5L4T5
C	0	HIS	-	expression tag	UNP E5L4T5
D	-19	MET	-	initiating methionine	UNP E5L4T5
D	-18	GLY	-	expression tag	UNP E5L4T5
D	-17	SER	-	expression tag	UNP E5L4T5
D	-16	SER	-	expression tag	UNP E5L4T5
D	-15	HIS	-	expression tag	UNP E5L4T5
D	-14	HIS	-	expression tag	UNP E5L4T5
D	-13	HIS	-	expression tag	UNP E5L4T5
D	-12	HIS	-	expression tag	UNP E5L4T5
D	-11	HIS	-	expression tag	UNP E5L4T5
D	-10	HIS	-	expression tag	UNP E5L4T5
D	-9	SER	-	expression tag	UNP E5L4T5
D	-8	SER	-	expression tag	UNP E5L4T5
D	-7	GLY	-	expression tag	UNP E5L4T5
D	-6	LEU	-	expression tag	UNP E5L4T5
D	-5	VAL	-	expression tag	UNP E5L4T5
D	-4	PRO	-	expression tag	UNP E5L4T5
D	-3	ARG	-	expression tag	UNP E5L4T5
D	-2	GLY	-	expression tag	UNP E5L4T5
D	-1	SER	-	expression tag	UNP E5L4T5
D	0	HIS	-	expression tag	UNP E5L4T5
E	-19	MET	-	initiating methionine	UNP E5L4T5
E	-18	GLY	-	expression tag	UNP E5L4T5
E	-17	SER	-	expression tag	UNP E5L4T5
E	-16	SER	-	expression tag	UNP E5L4T5
E	-15	HIS	-	expression tag	UNP E5L4T5
E	-14	HIS	-	expression tag	UNP E5L4T5
E	-13	HIS	-	expression tag	UNP E5L4T5
E	-12	HIS	-	expression tag	UNP E5L4T5
E	-11	HIS	-	expression tag	UNP E5L4T5
E	-10	HIS	-	expression tag	UNP E5L4T5
E	-9	SER	-	expression tag	UNP E5L4T5
E	-8	SER	-	expression tag	UNP E5L4T5
E	-7	GLY	-	expression tag	UNP E5L4T5
E	-6	LEU	-	expression tag	UNP E5L4T5
E	-5	VAL	-	expression tag	UNP E5L4T5
E	-4	PRO	-	expression tag	UNP E5L4T5
E	-3	ARG	-	expression tag	UNP E5L4T5
E	-2	GLY	-	expression tag	UNP E5L4T5
E	-1	SER	-	expression tag	UNP E5L4T5

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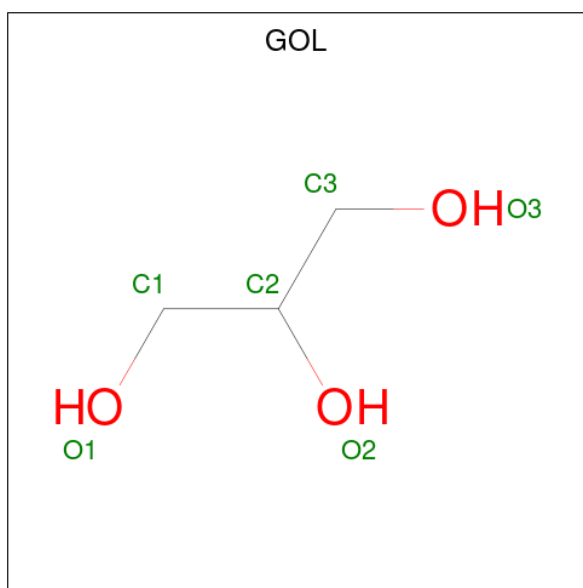
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP E5L4T5
F	-19	MET	-	initiating methionine	UNP E5L4T5
F	-18	GLY	-	expression tag	UNP E5L4T5
F	-17	SER	-	expression tag	UNP E5L4T5
F	-16	SER	-	expression tag	UNP E5L4T5
F	-15	HIS	-	expression tag	UNP E5L4T5
F	-14	HIS	-	expression tag	UNP E5L4T5
F	-13	HIS	-	expression tag	UNP E5L4T5
F	-12	HIS	-	expression tag	UNP E5L4T5
F	-11	HIS	-	expression tag	UNP E5L4T5
F	-10	HIS	-	expression tag	UNP E5L4T5
F	-9	SER	-	expression tag	UNP E5L4T5
F	-8	SER	-	expression tag	UNP E5L4T5
F	-7	GLY	-	expression tag	UNP E5L4T5
F	-6	LEU	-	expression tag	UNP E5L4T5
F	-5	VAL	-	expression tag	UNP E5L4T5
F	-4	PRO	-	expression tag	UNP E5L4T5
F	-3	ARG	-	expression tag	UNP E5L4T5
F	-2	GLY	-	expression tag	UNP E5L4T5
F	-1	SER	-	expression tag	UNP E5L4T5
F	0	HIS	-	expression tag	UNP E5L4T5
G	-19	MET	-	initiating methionine	UNP E5L4T5
G	-18	GLY	-	expression tag	UNP E5L4T5
G	-17	SER	-	expression tag	UNP E5L4T5
G	-16	SER	-	expression tag	UNP E5L4T5
G	-15	HIS	-	expression tag	UNP E5L4T5
G	-14	HIS	-	expression tag	UNP E5L4T5
G	-13	HIS	-	expression tag	UNP E5L4T5
G	-12	HIS	-	expression tag	UNP E5L4T5
G	-11	HIS	-	expression tag	UNP E5L4T5
G	-10	HIS	-	expression tag	UNP E5L4T5
G	-9	SER	-	expression tag	UNP E5L4T5
G	-8	SER	-	expression tag	UNP E5L4T5
G	-7	GLY	-	expression tag	UNP E5L4T5
G	-6	LEU	-	expression tag	UNP E5L4T5
G	-5	VAL	-	expression tag	UNP E5L4T5
G	-4	PRO	-	expression tag	UNP E5L4T5
G	-3	ARG	-	expression tag	UNP E5L4T5
G	-2	GLY	-	expression tag	UNP E5L4T5
G	-1	SER	-	expression tag	UNP E5L4T5
G	0	HIS	-	expression tag	UNP E5L4T5

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



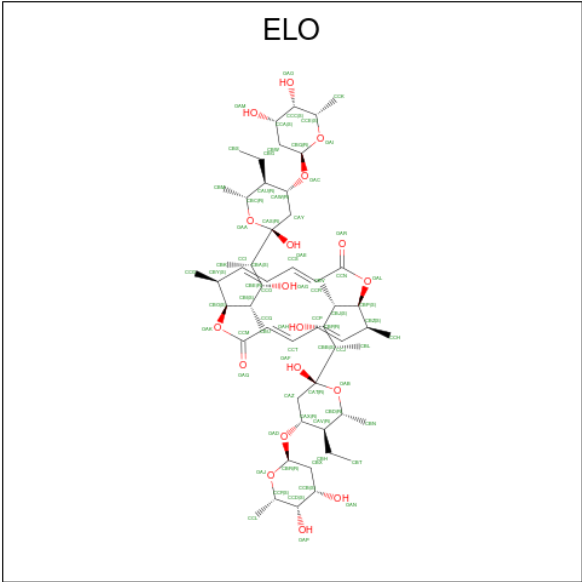
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is Elaiophylin (CCD ID: ELO) (formula: $C_{54}H_{88}O_{18}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	1
			72	54	18		
4	C	1	Total	C	O	0	1
			72	54	18		
4	D	1	Total	C	O	0	1
			72	54	18		
4	E	1	Total	C	O	0	1
			72	54	18		
4	F	1	Total	C	O	0	0
			72	54	18		

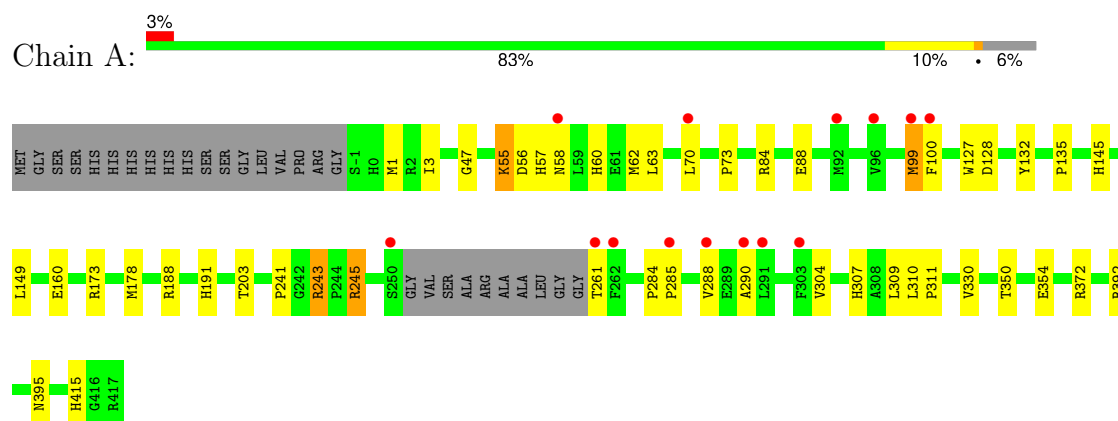
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total	O	0	0
			197	197		
5	B	198	Total	O	0	0
			198	198		
5	C	100	Total	O	0	0
			100	100		
5	D	84	Total	O	0	0
			84	84		
5	E	60	Total	O	0	0
			60	60		
5	F	227	Total	O	0	0
			227	227		
5	G	93	Total	O	0	0
			93	93		

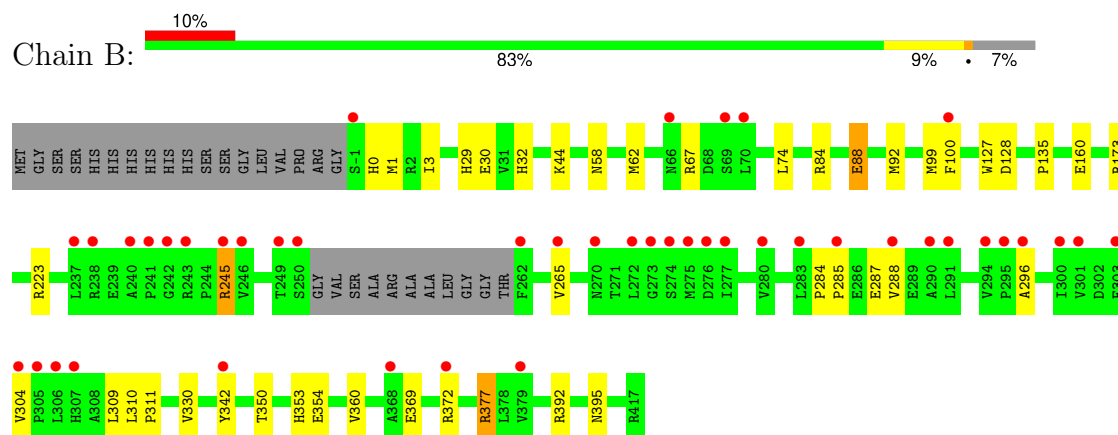
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

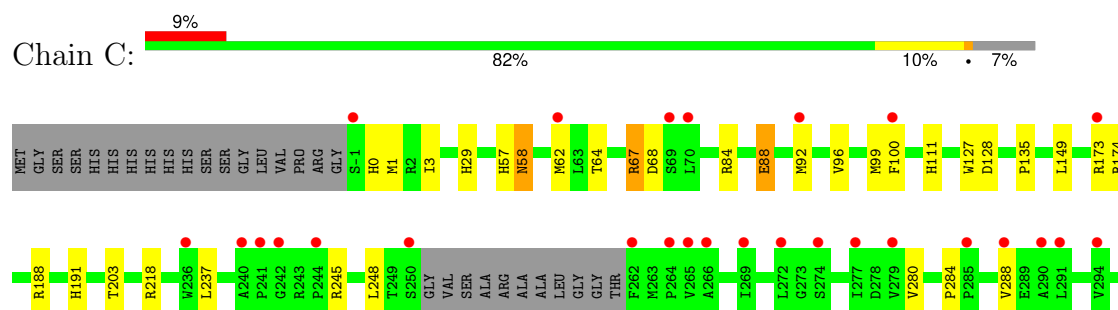
• Molecule 1: Glycosyltransferase



• Molecule 1: Glycosyltransferase

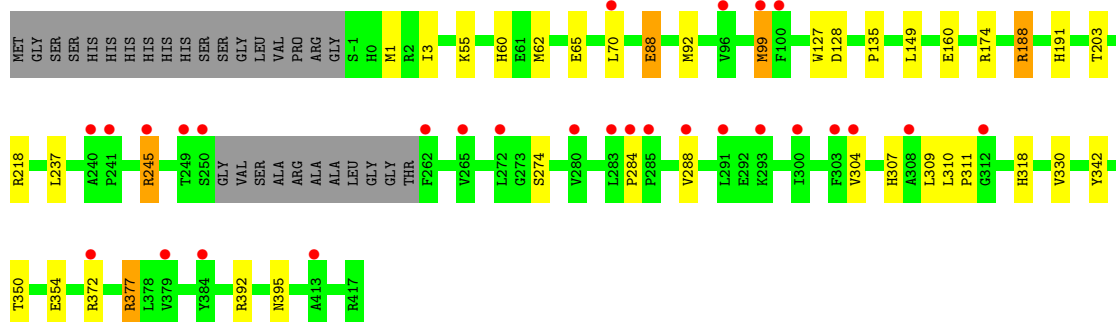
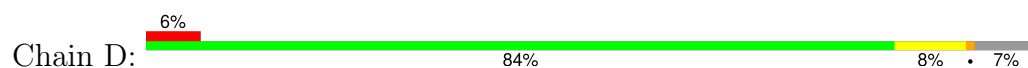


• Molecule 1: Glycosyltransferase

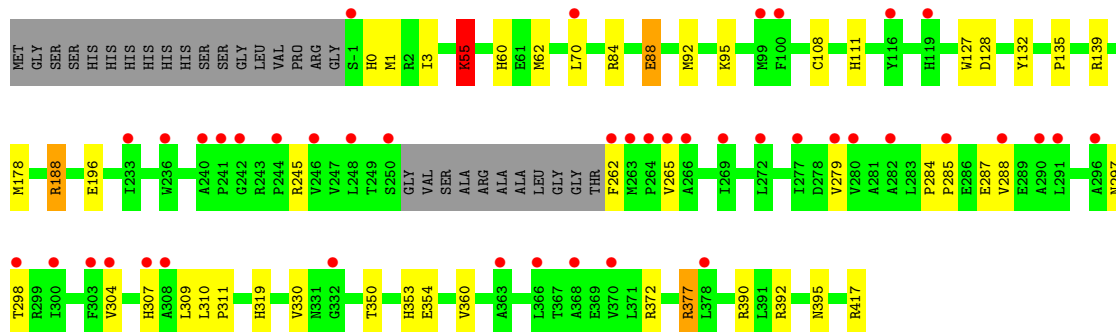
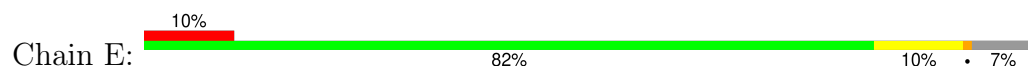




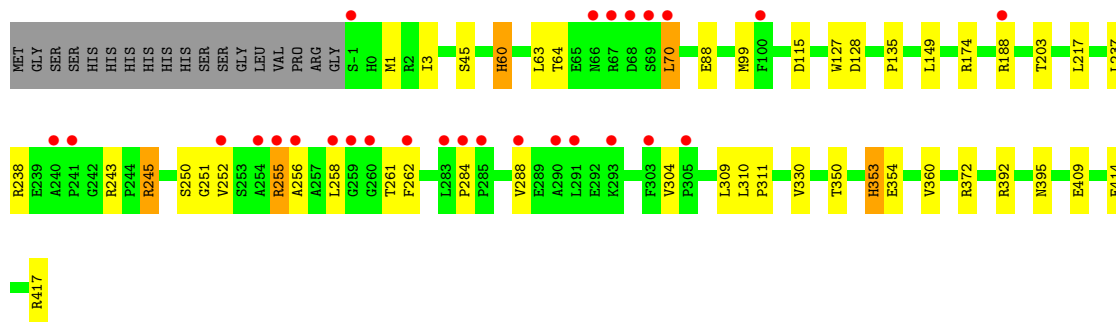
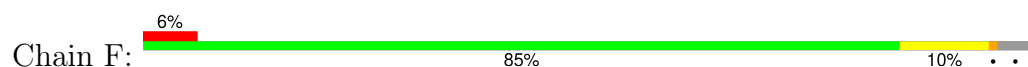
• Molecule 1: Glycosyltransferase



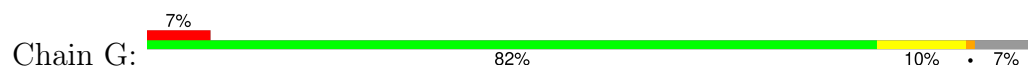
• Molecule 1: Glycosyltransferase

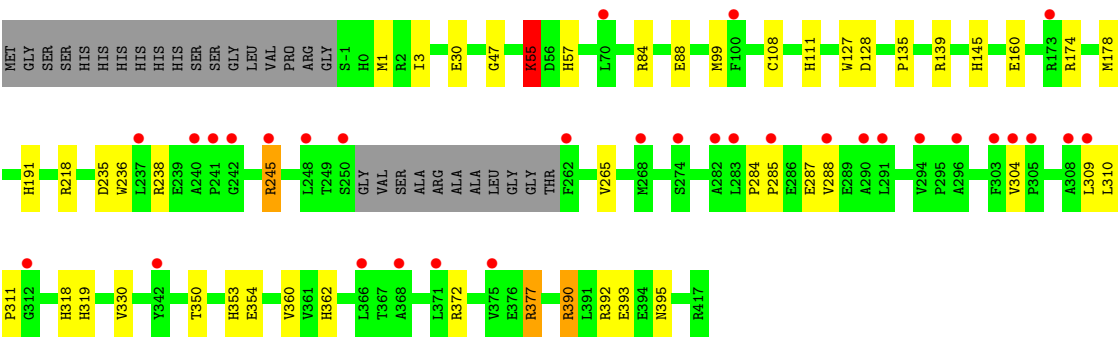


• Molecule 1: Glycosyltransferase



• Molecule 1: Glycosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.10Å 98.13Å 176.51Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	76.01 – 2.10 76.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (76.01-2.10) 98.6 (76.01-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.188 , 0.217 0.197 , 0.224	Depositor DCC
R_{free} test set	10990 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24066	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	A	0.68	6/3314 (0.2%)	0.92	2/4531 (0.0%)
1	B	0.67	2/3332 (0.1%)	0.91	0/4553
1	C	0.64	6/3315 (0.2%)	0.88	0/4531
1	D	0.65	4/3307 (0.1%)	0.89	0/4521
1	E	0.64	5/3307 (0.2%)	0.90	1/4521 (0.0%)
1	F	0.70	2/3382 (0.1%)	0.93	1/4624 (0.0%)
1	G	0.68	7/3307 (0.2%)	0.90	1/4521 (0.0%)
All	All	0.67	32/23264 (0.1%)	0.90	5/31802 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	7
1	D	0	7
1	E	0	8
1	F	0	8
1	G	0	9
All	All	0	53

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	57	HIS	CE1-NE2	7.18	1.39	1.32
1	G	191	HIS	CE1-NE2	6.72	1.39	1.32
1	B	32	HIS	CE1-NE2	6.62	1.39	1.32
1	A	307	HIS	CE1-NE2	6.52	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	HIS	CE1-NE2	6.32	1.38	1.32
1	G	111	HIS	CE1-NE2	6.24	1.38	1.32
1	E	307	HIS	CE1-NE2	6.09	1.38	1.32
1	A	191	HIS	CE1-NE2	6.06	1.38	1.32
1	G	362	HIS	CE1-NE2	6.00	1.38	1.32
1	G	319	HIS	CE1-NE2	5.98	1.38	1.32
1	F	353	HIS	CE1-NE2	5.86	1.38	1.32
1	D	191	HIS	CE1-NE2	5.71	1.38	1.32
1	F	60	HIS	CE1-NE2	5.65	1.38	1.32
1	A	57	HIS	CE1-NE2	5.57	1.38	1.32
1	A	60	HIS	CE1-NE2	5.55	1.38	1.32
1	E	0	HIS	CE1-NE2	5.54	1.38	1.32
1	E	60	HIS	CE1-NE2	5.46	1.38	1.32
1	G	145	HIS	CE1-NE2	5.40	1.38	1.32
1	G	318	HIS	CE1-NE2	5.37	1.38	1.32
1	A	145	HIS	CE1-NE2	5.33	1.37	1.32
1	C	57	HIS	CE1-NE2	5.33	1.37	1.32
1	C	29	HIS	CE1-NE2	5.27	1.37	1.32
1	D	60	HIS	CE1-NE2	5.26	1.37	1.32
1	D	318	HIS	CE1-NE2	5.25	1.37	1.32
1	D	307	HIS	CE1-NE2	5.21	1.37	1.32
1	E	111	HIS	CE1-NE2	5.21	1.37	1.32
1	C	307	HIS	CE1-NE2	5.20	1.37	1.32
1	A	415	HIS	CE1-NE2	5.19	1.37	1.32
1	C	319	HIS	CE1-NE2	5.11	1.37	1.32
1	C	191	HIS	CE1-NE2	5.10	1.37	1.32
1	E	319	HIS	CE1-NE2	5.01	1.37	1.32
1	B	29	HIS	CE1-NE2	5.00	1.37	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ARG	CB-CG-CD	5.81	124.66	111.30
1	F	88	GLU	CB-CG-CD	5.64	122.18	112.60
1	G	55	LYS	CB-CG-CD	5.31	123.52	111.30
1	E	55	LYS	CB-CG-CD	5.19	123.24	111.30
1	A	243	ARG	O-C-N	-5.04	118.48	121.71

There are no chirality outliers.

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	ARG	Sidechain
1	A	188	ARG	Sidechain
1	A	243	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	372	ARG	Sidechain
1	A	392	ARG	Sidechain
1	A	84	ARG	Sidechain
1	B	173	ARG	Sidechain
1	B	245	ARG	Sidechain
1	B	372	ARG	Sidechain
1	B	377	ARG	Sidechain
1	B	392	ARG	Sidechain
1	B	67	ARG	Sidechain
1	B	84	ARG	Sidechain
1	C	174	ARG	Sidechain
1	C	188	ARG	Sidechain
1	C	218	ARG	Sidechain
1	C	372	ARG	Sidechain
1	C	377	ARG	Sidechain
1	C	392	ARG	Sidechain
1	C	84	ARG	Sidechain
1	D	174	ARG	Sidechain
1	D	188	ARG	Sidechain
1	D	218	ARG	Sidechain
1	D	245	ARG	Sidechain
1	D	372	ARG	Sidechain
1	D	377	ARG	Sidechain
1	D	392	ARG	Sidechain
1	E	188	ARG	Sidechain
1	E	245	ARG	Sidechain
1	E	372	ARG	Sidechain
1	E	377	ARG	Sidechain
1	E	390	ARG	Sidechain
1	E	392	ARG	Sidechain
1	E	417	ARG	Sidechain
1	E	84	ARG	Sidechain
1	F	174	ARG	Sidechain
1	F	188	ARG	Sidechain
1	F	243	ARG	Sidechain
1	F	245	ARG	Sidechain
1	F	255	ARG	Sidechain
1	F	372	ARG	Sidechain
1	F	392	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	417	ARG	Sidechain
1	G	174	ARG	Sidechain
1	G	218	ARG	Sidechain
1	G	238	ARG	Sidechain
1	G	245	ARG	Sidechain
1	G	372	ARG	Sidechain
1	G	377	ARG	Sidechain
1	G	390	ARG	Sidechain
1	G	392	ARG	Sidechain
1	G	84	ARG	Sidechain

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	A	3225	0	3161	20	0
1	B	3234	0	3178	29	0
1	C	3223	0	3163	33	0
1	D	3218	0	3154	26	0
1	E	3218	0	3154	30	0
1	F	3289	0	3228	26	0
1	G	3218	0	3154	23	0
2	A	12	0	9	0	0
2	B	8	0	6	0	0
2	D	8	0	6	0	0
2	E	4	0	3	0	0
2	F	12	0	9	1	0
2	G	12	0	9	1	0
3	A	12	0	16	1	0
3	B	12	0	16	0	0
3	C	6	0	8	0	0
3	E	6	0	8	0	0
3	F	18	0	24	1	0
3	G	12	0	16	1	0
4	B	72	0	0	7	0
4	C	72	0	0	9	0
4	D	72	0	0	11	0
4	E	72	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	72	0	0	0	0
5	A	197	0	0	5	0
5	B	198	0	0	3	0
5	C	100	0	0	3	0
5	D	84	0	0	2	0
5	E	60	0	0	3	0
5	F	227	0	0	3	0
5	G	93	0	0	7	0
All	All	24066	0	22322	197	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:501[B]:ELO:CCR	4:D:501[B]:ELO:CCP	2.46	0.92
4:D:501[B]:ELO:CCQ	4:D:501[B]:ELO:CCO	2.49	0.91
1:D:99:MET:HE3	1:E:95:LYS:HE3	1.55	0.89
1:B:99[A]:MET:HE2	1:C:99[A]:MET:HE2	1.55	0.88
4:E:501[A]:ELO:CCQ	4:E:501[A]:ELO:CCO	2.53	0.87
4:E:501[A]:ELO:CCR	4:E:501[A]:ELO:CCP	2.56	0.83
4:E:501[A]:ELO:CCO	4:E:501[A]:ELO:CCM	2.61	0.78
1:A:73:PRO:O	5:A:601:HOH:O	2.03	0.76
1:B:100:PHE:CE1	1:C:92:MET:HE1	2.20	0.75
1:G:30:GLU:OE1	5:G:601:HOH:O	2.04	0.75
1:A:160:GLU:OE1	5:A:602:HOH:O	2.07	0.72
1:B:160:GLU:OE1	5:B:601:HOH:O	2.08	0.71
1:B:99[A]:MET:CE	1:C:99[A]:MET:HE2	2.19	0.71
1:B:304:VAL:HG21	1:B:309:LEU:HD22	1.72	0.71
1:D:160:GLU:OE1	5:D:601:HOH:O	2.09	0.71
1:D:304:VAL:HG21	1:D:309:LEU:HD22	1.73	0.71
1:F:414:GLU:OE1	5:F:601:HOH:O	2.06	0.71
4:D:501[B]:ELO:CCO	4:D:501[B]:ELO:CCM	2.68	0.71
1:C:304:VAL:HG21	1:C:309:LEU:HD22	1.74	0.70
1:F:115[B]:ASP:OD2	5:F:602:HOH:O	2.09	0.69
1:F:304:VAL:HG21	1:F:309:LEU:HD22	1.75	0.69
1:E:297:ASN:OD1	1:E:298:THR:HG23	1.94	0.67
1:E:304:VAL:HG21	1:E:309:LEU:HD22	1.74	0.67
1:G:304:VAL:HG21	1:G:309:LEU:HD22	1.76	0.67
1:B:99[A]:MET:HE2	1:C:99[A]:MET:CE	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:GLU:OE1	5:E:601:HOH:O	2.11	0.67
4:C:501[B]:ELO:CCN	4:C:501[B]:ELO:CCP	2.74	0.67
1:A:58:ASN:HD21	1:A:62:MET:HE3	1.61	0.66
4:E:501[A]:ELO:CCP	4:E:501[A]:ELO:CCN	2.74	0.66
1:B:58:ASN:HB3	1:C:173:ARG:HH12	1.60	0.66
3:A:505:GOL:H32	1:B:223:ARG:HH12	1.62	0.65
4:C:501[B]:ELO:CCP	4:C:501[B]:ELO:CCR	2.74	0.65
1:E:139:ARG:HA	5:E:643:HOH:O	1.96	0.65
1:A:304:VAL:HG21	1:A:309:LEU:HD22	1.78	0.64
1:C:173:ARG:NH1	5:C:601:HOH:O	2.30	0.64
1:D:70:LEU:HD12	4:E:501[A]:ELO:CCL	2.28	0.64
4:C:501[B]:ELO:CCS	4:C:501[B]:ELO:CCQ	2.75	0.64
4:E:501[A]:ELO:CCQ	4:E:501[A]:ELO:CCS	2.75	0.64
1:E:55:LYS:HD2	1:E:108:CYS:O	1.97	0.64
1:G:55:LYS:HD2	1:G:108:CYS:O	1.99	0.62
1:A:58:ASN:ND2	1:A:62:MET:HE3	2.13	0.62
4:D:501[B]:ELO:CCP	4:D:501[B]:ELO:CCN	2.77	0.62
1:C:342:TYR:CE2	4:C:501[B]:ELO:OAE	2.53	0.62
4:D:501[B]:ELO:CCR	4:D:501[B]:ELO:CCT	2.78	0.61
4:B:501[A]:ELO:CCQ	4:B:501[A]:ELO:CCO	2.78	0.60
4:B:501[A]:ELO:CCR	4:B:501[A]:ELO:CCP	2.79	0.60
1:G:235:ASP:HA	3:G:505:GOL:H31	1.84	0.60
1:B:74:LEU:HD12	4:C:501[B]:ELO:CBL	2.33	0.59
4:C:501[B]:ELO:CCQ	4:C:501[B]:ELO:CCO	2.81	0.58
1:F:63:LEU:HD22	1:F:70:LEU:HD23	1.85	0.58
4:D:501[B]:ELO:CCM	4:D:501[B]:ELO:CCI	2.82	0.57
1:C:248:LEU:C	1:C:248:LEU:HD23	2.29	0.57
4:E:501[A]:ELO:CCM	4:E:501[A]:ELO:CCI	2.82	0.57
1:A:330:VAL:HG12	1:A:395:ASN:ND2	2.19	0.57
1:E:330:VAL:HG12	1:E:395:ASN:ND2	2.20	0.57
1:C:330:VAL:HG12	1:C:395:ASN:ND2	2.20	0.56
4:D:501[B]:ELO:CCN	4:D:501[B]:ELO:CCJ	2.83	0.56
4:D:501[B]:ELO:CCT	4:D:501[B]:ELO:CCS	2.83	0.56
1:G:330:VAL:HG12	1:G:395:ASN:ND2	2.20	0.56
1:A:99:MET:HE3	1:A:100:PHE:HB2	1.88	0.56
1:B:0:HIS:NE2	1:B:30[B]:GLU:HG2	2.20	0.56
1:D:92:MET:CE	1:E:62:MET:HE2	2.36	0.55
4:E:501[A]:ELO:CCR	4:E:501[A]:ELO:CCT	2.85	0.55
4:C:501[B]:ELO:CCN	4:C:501[B]:ELO:CCJ	2.85	0.54
1:C:67:ARG:O	1:C:68:ASP:HB2	2.08	0.54
1:G:245:ARG:NH1	1:G:309:LEU:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:VAL:HG12	1:B:395:ASN:ND2	2.23	0.54
1:D:92:MET:HE2	1:E:62:MET:HE2	1.90	0.54
1:C:353:HIS:HD2	1:C:360:VAL:H	1.55	0.54
1:D:330:VAL:HG12	1:D:395:ASN:ND2	2.21	0.54
1:B:296:ALA:N	5:B:606:HOH:O	2.40	0.54
1:D:245:ARG:NH1	1:D:309:LEU:O	2.41	0.54
1:B:62[A]:MET:SD	1:C:88:GLU:CB	2.95	0.53
1:D:62:MET:CE	1:E:92:MET:HE2	2.38	0.53
1:F:330:VAL:HG12	1:F:395:ASN:ND2	2.22	0.53
1:A:47:GLY:HA2	5:A:603:HOH:O	2.08	0.53
1:E:353:HIS:HD2	1:E:360:VAL:H	1.56	0.53
1:F:245:ARG:HH21	1:F:309:LEU:HD12	1.72	0.53
1:B:353:HIS:HD2	1:B:360:VAL:H	1.56	0.53
1:F:1:MET:HE3	1:F:3:ILE:HD11	1.91	0.53
1:B:350:THR:O	1:B:354:GLU:HG2	2.09	0.53
4:D:501[B]:ELO:CCQ	4:D:501[B]:ELO:CCS	2.87	0.53
1:F:353:HIS:HD2	1:F:360:VAL:H	1.55	0.53
1:G:1:MET:HE3	1:G:3:ILE:HD11	1.91	0.53
1:E:350:THR:O	1:E:354:GLU:HG2	2.09	0.53
4:E:501[A]:ELO:OAC	4:E:501[A]:ELO:CBS	2.57	0.52
1:D:65:GLU:HG3	1:E:88:GLU:CG	2.39	0.52
1:D:350:THR:O	1:D:354:GLU:HG2	2.09	0.52
1:F:350:THR:O	1:F:354:GLU:HG2	2.10	0.52
1:A:350:THR:O	1:A:354:GLU:HG2	2.10	0.52
1:B:88:GLU:HB3	1:C:62:MET:SD	2.50	0.52
1:C:350:THR:O	1:C:354:GLU:HG2	2.10	0.52
1:G:353:HIS:HD2	1:G:360:VAL:H	1.56	0.52
1:G:350:THR:O	1:G:354:GLU:HG2	2.10	0.52
4:C:501[B]:ELO:CCM	4:C:501[B]:ELO:CCI	2.88	0.52
1:D:92:MET:HE2	1:E:62:MET:CE	2.40	0.52
1:D:1:MET:HE3	1:D:3:ILE:HD11	1.90	0.51
1:E:1:MET:HE3	1:E:3:ILE:HD11	1.91	0.51
1:G:393:GLU:HB3	5:G:665:HOH:O	2.09	0.51
1:A:290:ALA:HB3	5:A:604:HOH:O	2.10	0.51
1:C:64:THR:HA	1:C:67:ARG:NH1	2.26	0.51
1:C:0:HIS:HB2	5:C:682:HOH:O	2.09	0.51
1:C:58:ASN:H	1:C:58:ASN:HD22	1.58	0.51
1:B:245:ARG:NH1	1:B:309:LEU:O	2.43	0.51
1:D:92:MET:CE	1:E:62:MET:CE	2.90	0.50
1:A:63:LEU:HD22	1:A:70:LEU:CD1	2.41	0.50
1:C:1:MET:HE3	1:C:3:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:ARG:HD3	1:F:262:PHE:HE2	1.75	0.50
1:A:1:MET:HE3	1:A:3:ILE:HD11	1.92	0.50
1:F:238:ARG:NH2	5:F:604:HOH:O	2.21	0.50
1:B:62[A]:MET:SD	1:C:88:GLU:HB3	2.51	0.49
1:C:245:ARG:NH1	1:C:280:VAL:HG21	2.27	0.49
1:B:44:LYS:NZ	5:B:611:HOH:O	2.45	0.49
4:D:501[B]:ELO:CCL	1:E:70:LEU:HD12	2.43	0.49
1:D:62:MET:CE	1:E:92:MET:CE	2.90	0.49
1:G:139:ARG:HA	5:G:675:HOH:O	2.13	0.48
1:G:127:TRP:CD2	1:G:135:PRO:HD3	2.48	0.48
1:B:1:MET:HE3	1:B:3:ILE:HD11	1.95	0.48
1:B:62[A]:MET:SD	1:C:88:GLU:HB2	2.54	0.48
1:C:58:ASN:ND2	5:C:606:HOH:O	2.47	0.48
1:D:127:TRP:CD2	1:D:135:PRO:HD3	2.48	0.48
1:E:127:TRP:CD2	1:E:135:PRO:HD3	2.49	0.48
1:D:62:MET:HE2	1:E:92:MET:HE2	1.96	0.48
4:E:501[A]:ELO:CCN	4:E:501[A]:ELO:CCJ	2.92	0.48
1:F:217:LEU:O	3:F:506:GOL:H2	2.14	0.47
1:F:250:SER:OG	1:F:251:GLY:N	2.46	0.47
1:F:127:TRP:CD2	1:F:135:PRO:HD3	2.50	0.47
1:F:245:ARG:NH2	1:F:309:LEU:O	2.46	0.47
1:B:127:TRP:CD2	1:B:135:PRO:HD3	2.50	0.47
1:G:390:ARG:HH11	1:G:390:ARG:CG	2.26	0.47
1:B:310:LEU:N	1:B:311:PRO:CD	2.78	0.47
1:C:127:TRP:CD2	1:C:135:PRO:HD3	2.49	0.47
1:F:255:ARG:HD3	1:F:262:PHE:CE2	2.50	0.47
1:A:55:LYS:HD3	1:A:56:ASP:O	2.15	0.47
1:G:310:LEU:N	1:G:311:PRO:CD	2.78	0.47
1:C:310:LEU:N	1:C:311:PRO:CD	2.78	0.46
4:B:501[A]:ELO:CCD	1:C:100:PHE:HD2	2.27	0.46
1:G:390:ARG:NH1	1:G:390:ARG:HB3	2.30	0.46
1:D:62:MET:HE2	1:E:92:MET:CE	2.45	0.46
1:G:236:TRP:N	5:G:612:HOH:O	2.46	0.46
1:G:390:ARG:HH11	1:G:390:ARG:HB3	1.81	0.46
2:G:502:ACT:H1	5:G:645:HOH:O	2.15	0.46
1:B:92:MET:CE	1:C:62:MET:HE2	2.45	0.46
1:A:310:LEU:N	1:A:311:PRO:CD	2.79	0.46
1:A:127:TRP:CD2	1:A:135:PRO:HD3	2.50	0.46
1:D:88:GLU:HB3	1:E:62:MET:SD	2.56	0.46
1:D:310:LEU:N	1:D:311:PRO:CD	2.79	0.46
1:E:310:LEU:N	1:E:311:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:SER:HB2	1:F:255:ARG:CG	2.47	0.45
1:G:160:GLU:OE1	5:G:602:HOH:O	2.21	0.45
1:F:310:LEU:N	1:F:311:PRO:CD	2.80	0.44
1:G:390:ARG:HH11	1:G:390:ARG:CB	2.30	0.44
4:B:501[A]:ELO:CCO	4:B:501[A]:ELO:CCM	2.95	0.44
1:F:255:ARG:HH21	1:F:258:LEU:HD11	1.83	0.44
1:D:342:TYR:CE2	4:D:501[B]:ELO:OAE	2.70	0.44
4:B:501[A]:ELO:CCP	4:B:501[A]:ELO:CCN	2.96	0.43
1:F:250:SER:HB2	1:F:255:ARG:HG3	2.00	0.43
1:F:149:LEU:HD22	1:F:203:THR:CG2	2.48	0.43
1:A:241:PRO:HD2	5:A:628:HOH:O	2.17	0.43
1:C:99[B]:MET:HE3	1:C:99[B]:MET:HB2	1.83	0.43
4:C:501[B]:ELO:CCO	4:C:501[B]:ELO:CCM	2.96	0.43
1:E:279:VAL:HB	1:E:298:THR:HG22	2.01	0.43
1:D:149:LEU:HD22	1:D:203:THR:CG2	2.48	0.43
1:F:252:VAL:O	1:F:256:ALA:HB3	2.19	0.43
4:E:501[A]:ELO:CCQ	4:E:501[A]:ELO:CCR	2.96	0.43
1:B:284:PRO:O	1:B:288:VAL:HG23	2.19	0.43
1:C:284:PRO:O	1:C:288:VAL:HG23	2.19	0.43
1:D:284:PRO:O	1:D:288:VAL:HG23	2.19	0.43
1:E:132:TYR:CZ	1:E:178:MET:HE1	2.54	0.43
1:A:284:PRO:O	1:A:288:VAL:HG23	2.18	0.43
4:E:501[A]:ELO:CCS	4:E:501[A]:ELO:CCT	2.97	0.43
1:G:265:VAL:HG21	1:G:287:GLU:OE2	2.19	0.43
1:E:284:PRO:O	1:E:288:VAL:HG23	2.19	0.42
1:D:65:GLU:HG3	1:E:88:GLU:HG3	2.00	0.42
1:F:284:PRO:O	1:F:288:VAL:HG23	2.18	0.42
1:D:188:ARG:O	1:D:188:ARG:HG2	2.19	0.42
1:A:132:TYR:CZ	1:A:178:MET:HE1	2.54	0.42
1:D:395:ASN:OD1	5:D:602:HOH:O	2.22	0.42
1:A:149:LEU:HD22	1:A:203:THR:CG2	2.49	0.42
1:F:409:GLU:OE2	2:F:504:ACT:H1	2.20	0.41
1:B:265:VAL:HG21	1:B:287:GLU:OE2	2.21	0.41
1:C:245:ARG:NH1	1:C:280:VAL:CG2	2.84	0.41
1:F:60:HIS:O	1:F:64:THR:HG23	2.21	0.41
1:C:149:LEU:HD22	1:C:203:THR:CG2	2.51	0.41
4:E:501[A]:ELO:OAD	4:E:501[A]:ELO:CBT	2.68	0.41
1:G:284:PRO:O	1:G:288:VAL:HG23	2.20	0.41
1:E:188:ARG:HD2	5:E:657:HOH:O	2.20	0.41
1:E:265:VAL:HG21	1:E:287:GLU:OE2	2.21	0.41
1:E:285:PRO:O	1:E:288:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:PRO:O	1:B:288:VAL:HB	2.21	0.41
4:B:501[A]:ELO:CAZ	1:C:96:VAL:HG21	2.51	0.41
1:B:342:TYR:CE2	4:B:501[A]:ELO:OAE	2.73	0.40
1:G:285:PRO:O	1:G:288:VAL:HB	2.21	0.40
1:A:285:PRO:O	1:A:288:VAL:HB	2.21	0.40
1:G:47:GLY:HA2	5:G:607:HOH:O	2.21	0.40
1:B:88:GLU:CB	1:C:62:MET:SD	3.10	0.40
1:F:252:VAL:O	1:F:256:ALA:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	405/437 (93%)	396 (98%)	9 (2%)	0	100	100
1	B	407/437 (93%)	398 (98%)	9 (2%)	0	100	100
1	C	405/437 (93%)	396 (98%)	9 (2%)	0	100	100
1	D	404/437 (92%)	395 (98%)	9 (2%)	0	100	100
1	E	404/437 (92%)	396 (98%)	8 (2%)	0	100	100
1	F	418/437 (96%)	407 (97%)	11 (3%)	0	100	100
1	G	404/437 (92%)	396 (98%)	8 (2%)	0	100	100
All	All	2847/3059 (93%)	2784 (98%)	63 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/366 (95%)	342 (99%)	5 (1%)	59	67
1	B	349/366 (95%)	345 (99%)	4 (1%)	65	74
1	C	347/366 (95%)	341 (98%)	6 (2%)	53	62
1	D	346/366 (94%)	339 (98%)	7 (2%)	48	56
1	E	346/366 (94%)	341 (99%)	5 (1%)	59	67
1	F	352/366 (96%)	346 (98%)	6 (2%)	53	62
1	G	346/366 (94%)	340 (98%)	6 (2%)	53	62
All	All	2433/2562 (95%)	2394 (98%)	39 (2%)	55	64

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	88	GLU
1	A	99	MET
1	A	128	ASP
1	A	261	THR
1	B	88	GLU
1	B	128	ASP
1	B	369	GLU
1	B	377	ARG
1	C	58	ASN
1	C	67	ARG
1	C	88	GLU
1	C	128	ASP
1	C	237	LEU
1	C	377	ARG
1	D	55	LYS
1	D	88	GLU
1	D	99	MET
1	D	128	ASP
1	D	237	LEU
1	D	274	SER
1	D	377	ARG
1	E	55	LYS
1	E	88	GLU

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Mol	Chain	Res	Type
1	E	128	ASP
1	E	262	PHE
1	E	377	ARG
1	F	45	SER
1	F	70	LEU
1	F	99	MET
1	F	128	ASP
1	F	237	LEU
1	F	261	THR
1	G	55	LYS
1	G	88	GLU
1	G	99	MET
1	G	128	ASP
1	G	178	MET
1	G	377	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	66	ASN
1	B	60	HIS
1	B	353	HIS
1	B	395	ASN
1	C	353	HIS
1	D	60	HIS
1	D	119	HIS
1	D	402	HIS
1	E	60	HIS
1	E	353	HIS
1	F	60	HIS
1	F	66	ASN
1	F	228	ASN
1	F	353	HIS
1	G	60	HIS
1	G	66	ASN
1	G	119	HIS
1	G	353	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	E	502	-	3,3,3	1.14	0	3,3,3	0.81	0
2	ACT	A	503	-	3,3,3	1.15	0	3,3,3	0.83	0
3	GOL	G	505	-	5,5,5	0.19	0	5,5,5	0.56	0
3	GOL	C	502	-	5,5,5	0.12	0	5,5,5	0.45	0
4	ELO	B	501[A]	-	72,76,76	2.02	19 (26%)	84,112,112	2.18	28 (33%)
3	GOL	F	505	-	5,5,5	0.27	0	5,5,5	0.45	0
3	GOL	F	506	-	5,5,5	0.14	0	5,5,5	0.35	0
2	ACT	F	503	-	3,3,3	1.04	0	3,3,3	0.81	0
2	ACT	G	503	-	3,3,3	0.90	0	3,3,3	1.02	0
3	GOL	B	505	-	5,5,5	0.25	0	5,5,5	0.60	0
2	ACT	B	503	-	3,3,3	1.20	0	3,3,3	0.77	0
4	ELO	F	501	-	72,76,76	2.27	26 (36%)	84,112,112	2.30	28 (33%)
2	ACT	A	501	-	3,3,3	1.03	0	3,3,3	0.83	0
3	GOL	A	505	-	5,5,5	0.21	0	5,5,5	0.47	0
4	ELO	E	501[A]	-	72,76,76	1.95	17 (23%)	84,112,112	2.22	26 (30%)
2	ACT	F	504	-	3,3,3	1.43	0	3,3,3	0.56	0
4	ELO	C	501[B]	-	72,76,76	1.79	19 (26%)	84,112,112	2.10	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ELO	D	501[B]	-	72,76,76	1.86	21 (29%)	84,112,112	2.22	27 (32%)
2	ACT	G	501	-	3,3,3	1.25	0	3,3,3	0.74	0
2	ACT	A	502	-	3,3,3	1.16	0	3,3,3	0.64	0
2	ACT	D	502	-	3,3,3	1.13	0	3,3,3	0.68	0
3	GOL	G	504	-	5,5,5	0.39	0	5,5,5	0.52	0
3	GOL	B	504	-	5,5,5	0.24	0	5,5,5	0.44	0
2	ACT	F	502	-	3,3,3	0.91	0	3,3,3	0.97	0
3	GOL	E	503	-	5,5,5	0.16	0	5,5,5	0.53	0
2	ACT	G	502	-	3,3,3	0.91	0	3,3,3	0.82	0
2	ACT	B	502	-	3,3,3	1.08	0	3,3,3	0.93	0
3	GOL	F	507	-	5,5,5	0.17	0	5,5,5	0.41	0
3	GOL	A	504	-	5,5,5	0.27	0	5,5,5	0.46	0
2	ACT	D	503	-	3,3,3	1.21	0	3,3,3	0.89	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
4	ELO	B	501[A]	-	-	28/78/146/146	0/4/5/5
3	GOL	F	505	-	-	4/4/4/4	-
3	GOL	F	506	-	-	0/4/4/4	-
4	ELO	E	501[A]	-	-	28/78/146/146	0/4/5/5
4	ELO	C	501[B]	-	-	14/78/146/146	0/4/5/5
4	ELO	D	501[B]	-	-	36/78/146/146	0/4/5/5
3	GOL	B	505	-	-	4/4/4/4	-
3	GOL	F	507	-	-	3/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
3	GOL	G	505	-	-	2/4/4/4	-
4	ELO	F	501	-	-	29/78/146/146	0/4/5/5
3	GOL	G	504	-	-	4/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-
3	GOL	E	503	-	-	2/4/4/4	-
3	GOL	A	505	-	-	4/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	501[A]	ELO	CCA-CCC	-6.56	1.42	1.52
4	F	501	ELO	CBY-CCI	-6.30	1.36	1.51
4	B	501[A]	ELO	CBY-CCI	-6.11	1.36	1.51
4	F	501	ELO	CBW-CBQ	5.59	1.65	1.50
4	B	501[A]	ELO	OAL-CBP	5.24	1.52	1.44
4	C	501[B]	ELO	CBY-CCI	-5.17	1.39	1.51
4	F	501	ELO	CBZ-CCJ	-5.00	1.39	1.51
4	F	501	ELO	CCA-CCC	-4.80	1.45	1.52
4	B	501[A]	ELO	CBZ-CCJ	-4.65	1.40	1.51
4	E	501[A]	ELO	CBY-CCI	-4.62	1.40	1.51
4	E	501[A]	ELO	CBZ-CCJ	-4.50	1.40	1.51
4	C	501[B]	ELO	CBZ-CCJ	-4.45	1.40	1.51
4	B	501[A]	ELO	CCQ-CCM	-4.44	1.38	1.48
4	E	501[A]	ELO	CAY-CAS	4.44	1.58	1.52
4	D	501[B]	ELO	CAZ-CAT	4.44	1.58	1.52
4	C	501[B]	ELO	CCA-CCC	-4.36	1.45	1.52
4	F	501	ELO	OAA-CBC	4.33	1.50	1.44
4	E	501[A]	ELO	CBW-CBQ	4.22	1.61	1.50
4	E	501[A]	ELO	OAA-CBC	4.22	1.49	1.44
4	F	501	ELO	CCQ-CCM	-4.21	1.38	1.48
4	D	501[B]	ELO	CBY-CCI	-4.15	1.41	1.51
4	D	501[B]	ELO	CCA-CCC	-4.15	1.46	1.52
4	B	501[A]	ELO	CBY-CBO	4.03	1.64	1.54
4	D	501[B]	ELO	CBZ-CCJ	-3.96	1.41	1.51
4	B	501[A]	ELO	CCA-CCC	-3.93	1.46	1.52
4	E	501[A]	ELO	OAC-CBQ	3.92	1.52	1.41
4	C	501[B]	ELO	CCQ-CCM	-3.92	1.39	1.48
4	F	501	ELO	OAC-CBQ	3.87	1.52	1.41
4	E	501[A]	ELO	CCQ-CCM	-3.87	1.39	1.48
4	B	501[A]	ELO	OAA-CBC	3.86	1.49	1.44
4	D	501[B]	ELO	OAA-CBC	3.85	1.49	1.44
4	F	501	ELO	CBY-CBO	3.72	1.63	1.54
4	F	501	ELO	CCB-CCD	3.58	1.58	1.52
4	D	501[B]	ELO	CCQ-CCM	-3.58	1.40	1.48
4	F	501	ELO	CBU-CBI	-3.44	1.46	1.53
4	F	501	ELO	OAJ-CCF	3.33	1.52	1.44
4	B	501[A]	ELO	OAA-CAS	3.33	1.48	1.43
4	D	501[B]	ELO	CBW-CBQ	3.22	1.59	1.50
4	B	501[A]	ELO	OAC-CBQ	3.14	1.50	1.41
4	D	501[B]	ELO	OAC-CBQ	3.11	1.49	1.41
4	F	501	ELO	CCS-CCR	3.10	1.42	1.34
4	C	501[B]	ELO	OAL-CBP	3.08	1.49	1.44
4	F	501	ELO	OAA-CAS	2.98	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	501[A]	ELO	CCS-CCR	2.90	1.42	1.34
4	C	501[B]	ELO	CAZ-CAT	2.85	1.56	1.52
4	C	501[B]	ELO	OAC-CBQ	2.84	1.49	1.41
4	D	501[B]	ELO	CCR-CCN	-2.82	1.41	1.48
4	B	501[A]	ELO	CCR-CCN	-2.80	1.41	1.48
4	F	501	ELO	CAU-CBC	-2.80	1.48	1.52
4	C	501[B]	ELO	OAD-CBR	2.78	1.49	1.41
4	B	501[A]	ELO	CBU-CBI	-2.78	1.47	1.53
4	E	501[A]	ELO	CAZ-CAT	2.73	1.56	1.52
4	F	501	ELO	CAY-CAW	2.73	1.58	1.52
4	C	501[B]	ELO	OAA-CBC	2.69	1.48	1.44
4	D	501[B]	ELO	CCS-CCR	2.68	1.41	1.34
4	B	501[A]	ELO	CBW-CBQ	2.67	1.57	1.50
4	C	501[B]	ELO	CCS-CCR	2.66	1.41	1.34
4	F	501	ELO	OAI-CCE	-2.60	1.38	1.44
4	F	501	ELO	OAP-CCD	2.58	1.49	1.43
4	F	501	ELO	OAM-CCA	2.58	1.48	1.43
4	D	501[B]	ELO	OAF-CAT	2.50	1.45	1.40
4	E	501[A]	ELO	CAY-CAW	2.50	1.57	1.52
4	F	501	ELO	OAF-CAT	2.49	1.45	1.40
4	E	501[A]	ELO	CBX-CCB	2.49	1.57	1.52
4	C	501[B]	ELO	OAJ-CBR	2.46	1.48	1.42
4	B	501[A]	ELO	CCK-CCE	2.46	1.57	1.51
4	C	501[B]	ELO	CCO-CCI	2.44	1.42	1.33
4	D	501[B]	ELO	CAV-CBD	-2.42	1.48	1.52
4	D	501[B]	ELO	CCC-CCE	2.40	1.58	1.52
4	C	501[B]	ELO	OAF-CAT	2.36	1.44	1.40
4	B	501[A]	ELO	CCS-CCR	2.36	1.40	1.34
4	D	501[B]	ELO	CCT-CCQ	2.36	1.40	1.34
4	F	501	ELO	CCC-CCE	2.35	1.58	1.52
4	D	501[B]	ELO	CAU-CBC	2.34	1.55	1.52
4	D	501[B]	ELO	CBX-CBR	2.33	1.56	1.50
4	D	501[B]	ELO	OAA-CAS	2.29	1.47	1.43
4	B	501[A]	ELO	OAJ-CBR	2.29	1.48	1.42
4	D	501[B]	ELO	OAL-CCN	2.26	1.39	1.34
4	C	501[B]	ELO	CAY-CAW	2.21	1.57	1.52
4	E	501[A]	ELO	CCT-CCQ	2.21	1.40	1.34
4	E	501[A]	ELO	CBI-CBE	-2.21	1.48	1.54
4	B	501[A]	ELO	OAL-CCN	2.21	1.39	1.34
4	C	501[B]	ELO	CCT-CCQ	2.20	1.40	1.34
4	C	501[B]	ELO	CBY-CBO	2.18	1.59	1.54
4	C	501[B]	ELO	OAP-CCD	2.18	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	501	ELO	CCK-CCE	2.18	1.56	1.51
4	D	501[B]	ELO	CCO-CCI	2.17	1.41	1.33
4	F	501	ELO	OAK-CBO	2.17	1.48	1.44
4	F	501	ELO	OAK-CCM	2.16	1.39	1.34
4	E	501[A]	ELO	CCO-CCI	2.14	1.41	1.33
4	E	501[A]	ELO	CCB-CCD	2.13	1.55	1.52
4	B	501[A]	ELO	CCB-CCD	2.12	1.55	1.52
4	E	501[A]	ELO	CCR-CCN	-2.12	1.43	1.48
4	D	501[B]	ELO	CBX-CCB	2.10	1.56	1.52
4	D	501[B]	ELO	CBU-CBI	-2.10	1.49	1.53
4	F	501	ELO	CCO-CCI	2.09	1.41	1.33
4	C	501[B]	ELO	CCB-CCD	2.09	1.55	1.52
4	B	501[A]	ELO	CCT-CCQ	2.08	1.40	1.34
4	F	501	ELO	OAE-CAS	2.08	1.44	1.40
4	C	501[B]	ELO	CCK-CCE	2.02	1.56	1.51
4	F	501	ELO	CAV-CBD	-2.02	1.49	1.52
4	B	501[A]	ELO	OAF-CAT	2.01	1.44	1.40

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501[A]	ELO	OAA-CBC-CBM	7.09	114.57	105.94
4	D	501[B]	ELO	OAO-CCC-CCA	-6.91	95.96	110.05
4	F	501	ELO	OAO-CCC-CCA	-6.80	96.17	110.05
4	F	501	ELO	OAA-CBC-CBM	6.76	114.17	105.94
4	F	501	ELO	OAK-CBO-CBY	6.15	117.28	107.12
4	F	501	ELO	CBW-CCA-CCC	-6.10	101.87	110.67
4	E	501[A]	ELO	OAO-CCC-CCA	-5.53	98.76	110.05
4	E	501[A]	ELO	CBU-CBI-CBE	-5.33	100.94	111.43
4	B	501[A]	ELO	OAK-CBO-CBY	5.33	115.93	107.12
4	B	501[A]	ELO	CBN-CBD-CAV	-5.32	105.32	115.19
4	E	501[A]	ELO	CAS-OAA-CBC	-5.30	106.62	114.31
4	B	501[A]	ELO	CBZ-CCJ-CCP	-5.01	115.76	126.11
4	D	501[B]	ELO	OAA-CBC-CBM	4.90	111.91	105.94
4	D	501[B]	ELO	OAL-CCN-CCR	4.90	122.06	111.39
4	B	501[A]	ELO	CBW-CCA-CCC	-4.76	103.80	110.67
4	B	501[A]	ELO	OAO-CCC-CCA	-4.76	100.34	110.05
4	C	501[B]	ELO	CBP-OAL-CCN	-4.70	109.94	117.42
4	C	501[B]	ELO	CBZ-CCJ-CCP	-4.67	116.45	126.11
4	B	501[A]	ELO	CAY-CAW-CAU	-4.63	106.21	113.47
4	C	501[B]	ELO	CBN-CBD-CAV	-4.63	106.59	115.19
4	D	501[B]	ELO	CAT-OAB-CBD	4.57	120.95	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501[B]	ELO	CBW-CCA-CCC	-4.51	104.17	110.67
4	B	501[A]	ELO	OAA-CBC-CBM	4.39	111.28	105.94
4	E	501[A]	ELO	CBZ-CCJ-CCP	-4.34	117.14	126.11
4	E	501[A]	ELO	CBN-CBD-CAV	-4.29	107.23	115.19
4	D	501[B]	ELO	CBN-CBD-CAV	-4.22	107.36	115.19
4	E	501[A]	ELO	CBW-CCA-CCC	-4.20	104.61	110.67
4	B	501[A]	ELO	CBP-OAL-CCN	-4.18	110.77	117.42
4	E	501[A]	ELO	OAE-CAS-OAA	-4.15	101.93	110.00
4	F	501	ELO	CBN-CBD-CAV	-4.14	107.50	115.19
4	D	501[B]	ELO	CBO-OAK-CCM	-4.12	110.87	117.42
4	F	501	ELO	CCP-CCT-CCQ	-4.07	115.01	124.65
4	C	501[B]	ELO	CCL-CCF-CCD	-4.00	105.76	113.08
4	C	501[B]	ELO	OAK-CBO-CBY	3.99	113.72	107.12
4	B	501[A]	ELO	OAC-CAW-CAU	3.93	112.94	107.42
4	D	501[B]	ELO	OAK-CCM-CCQ	3.92	119.92	111.39
4	C	501[B]	ELO	OAA-CBC-CBM	3.86	110.64	105.94
4	F	501	ELO	CCK-CCE-CCC	3.86	120.13	113.08
4	C	501[B]	ELO	CAY-CAW-CAU	-3.79	107.53	113.47
4	E	501[A]	ELO	OAL-CCN-CCR	3.76	119.58	111.39
4	D	501[B]	ELO	CAS-OAA-CBC	-3.73	108.89	114.31
4	E	501[A]	ELO	CBX-CCB-CCD	3.69	115.98	110.67
4	C	501[B]	ELO	OAJ-CCF-CCD	3.63	116.08	109.55
4	B	501[A]	ELO	OAK-CCM-CCQ	3.59	119.21	111.39
4	C	501[B]	ELO	OAB-CBD-CBN	3.55	110.27	105.94
4	D	501[B]	ELO	OAD-CAX-CAV	-3.51	102.47	107.42
4	F	501	ELO	CBY-CCI-CCO	-3.47	118.93	126.11
4	B	501[A]	ELO	CCP-CCT-CCQ	-3.47	116.44	124.65
4	C	501[B]	ELO	CCP-CCT-CCQ	-3.47	116.45	124.65
4	F	501	ELO	CBM-CBC-CAU	-3.45	108.79	115.19
4	E	501[A]	ELO	CCP-CCT-CCQ	-3.38	116.64	124.65
4	E	501[A]	ELO	OAD-CAX-CAV	-3.37	102.67	107.42
4	C	501[B]	ELO	CBR-OAJ-CCF	3.37	123.05	113.82
4	B	501[A]	ELO	OAL-CCN-CCR	3.35	118.67	111.39
4	F	501	ELO	CCL-CCF-CCD	-3.34	106.96	113.08
4	D	501[B]	ELO	CBP-OAL-CCN	-3.34	112.11	117.42
4	E	501[A]	ELO	CBM-CBC-CAU	-3.33	109.00	115.19
4	D	501[B]	ELO	CBZ-CCJ-CCP	-3.26	119.36	126.11
4	D	501[B]	ELO	CAZ-CAX-CAV	-3.26	108.36	113.47
4	C	501[B]	ELO	CCG-CBY-CCI	3.24	117.23	109.91
4	C	501[B]	ELO	OAO-CCC-CCA	-3.23	103.45	110.05
4	F	501	ELO	OAK-CCM-OAQ	3.23	128.51	123.34
4	D	501[B]	ELO	CBQ-OAC-CAW	3.22	123.50	116.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501[B]	ELO	CBY-CCI-CCO	-3.13	119.64	126.11
4	F	501	ELO	OAB-CBD-CBN	3.11	109.73	105.94
4	F	501	ELO	CBZ-CCJ-CCP	-3.11	119.69	126.11
4	D	501[B]	ELO	CBR-OAD-CAX	3.10	123.25	116.22
4	D	501[B]	ELO	OAL-CBP-CBJ	3.07	114.60	107.52
4	F	501	ELO	CBU-CBI-CBE	-3.03	105.47	111.43
4	C	501[B]	ELO	OAL-CCN-OAR	-3.00	118.54	123.34
4	E	501[A]	ELO	CBS-CBG-CAU	-2.99	107.89	114.15
4	D	501[B]	ELO	CAY-CAW-CAU	-2.97	108.81	113.47
4	C	501[B]	ELO	CBI-CBE-CBA	-2.95	110.36	114.51
4	B	501[A]	ELO	CBJ-CBF-CBB	-2.95	110.36	114.51
4	C	501[B]	ELO	CAS-OAA-CBC	-2.94	110.05	114.31
4	D	501[B]	ELO	CBX-CCB-CCD	2.90	114.84	110.67
4	E	501[A]	ELO	OAG-CBE-CBI	-2.88	103.17	109.56
4	E	501[A]	ELO	CBQ-OAC-CAW	2.87	122.73	116.22
4	D	501[B]	ELO	OAD-CAX-CAZ	2.86	116.51	109.34
4	C	501[B]	ELO	CBO-CBY-CCI	-2.83	100.44	109.46
4	B	501[A]	ELO	OAQ-CCM-CCQ	-2.83	114.07	123.69
4	E	501[A]	ELO	CBI-CBE-CBA	-2.82	110.54	114.51
4	B	501[A]	ELO	OAI-CCE-CCK	2.76	112.87	106.74
4	F	501	ELO	OAO-CCC-CCE	2.76	115.82	109.74
4	D	501[B]	ELO	OAG-CBE-CBI	-2.71	103.54	109.56
4	D	501[B]	ELO	OAO-CCC-CCE	2.68	115.65	109.74
4	B	501[A]	ELO	OAL-CBP-CBZ	2.68	111.55	107.12
4	C	501[B]	ELO	OAI-CCE-CCK	2.67	112.67	106.74
4	C	501[B]	ELO	OAL-CCN-CCR	2.66	117.17	111.39
4	B	501[A]	ELO	OAL-CBP-CBJ	2.65	113.62	107.52
4	B	501[A]	ELO	OAI-CCE-CCC	-2.63	104.81	109.55
4	F	501	ELO	CBQ-OAI-CCE	-2.59	106.73	113.82
4	B	501[A]	ELO	OAG-CBE-CBI	-2.53	103.94	109.56
4	F	501	ELO	OAI-CCE-CCC	-2.49	105.08	109.55
4	D	501[B]	ELO	OAC-CBQ-CBW	2.49	113.06	108.28
4	E	501[A]	ELO	OAK-CBO-CBY	2.48	111.21	107.12
4	F	501	ELO	OAP-CCD-CCB	2.47	115.09	110.05
4	C	501[B]	ELO	OAO-CCC-CCE	2.46	115.16	109.74
4	B	501[A]	ELO	CBR-OAJ-CCF	2.45	120.54	113.82
4	F	501	ELO	CBI-CBE-CBA	2.45	117.95	114.51
4	B	501[A]	ELO	OAJ-CCF-CCD	2.42	113.91	109.55
4	C	501[B]	ELO	CBU-CBI-CBE	-2.42	106.67	111.43
4	B	501[A]	ELO	OAB-CBD-CBN	2.41	108.87	105.94
4	E	501[A]	ELO	CBR-OAD-CAX	2.40	121.65	116.22
4	C	501[B]	ELO	CBE-CBI-CBO	-2.39	106.02	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501[B]	ELO	CBU-CBI-CBE	-2.37	106.78	111.43
4	D	501[B]	ELO	CCK-CCE-CCC	2.36	117.40	113.08
4	B	501[A]	ELO	CBQ-OAC-CAW	2.36	121.56	116.22
4	E	501[A]	ELO	CBE-CBI-CBO	-2.34	106.12	110.58
4	C	501[B]	ELO	CBW-CCA-CCC	-2.31	107.33	110.67
4	E	501[A]	ELO	OAM-CCA-CCC	-2.31	105.37	110.15
4	E	501[A]	ELO	OAK-CCM-CCQ	2.31	116.41	111.39
4	D	501[B]	ELO	CCL-CCF-CCD	-2.29	108.89	113.08
4	F	501	ELO	OAC-CAW-CAU	-2.29	104.20	107.42
4	C	501[B]	ELO	CBM-CBC-CAU	-2.27	110.97	115.19
4	B	501[A]	ELO	CCL-CCF-CCD	-2.21	109.03	113.08
4	D	501[B]	ELO	OAK-CBO-CBY	2.20	110.75	107.12
4	F	501	ELO	OAQ-CCM-CCQ	-2.19	116.25	123.69
4	F	501	ELO	CCG-CBY-CBO	-2.18	107.28	111.11
4	F	501	ELO	CCS-CCR-CCN	2.17	128.36	123.21
4	F	501	ELO	CBQ-CBW-CCA	2.15	117.75	111.34
4	B	501[A]	ELO	CBY-CCI-CCO	-2.13	121.71	126.11
4	E	501[A]	ELO	OAL-CCN-OAR	-2.12	119.94	123.34
4	F	501	ELO	OAN-CCB-CCD	2.10	114.51	110.15
4	E	501[A]	ELO	CBR-OAJ-CCF	-2.10	108.07	113.82
4	E	501[A]	ELO	CBY-CCI-CCO	-2.09	121.79	126.11
4	F	501	ELO	OAC-CBQ-CBW	2.08	112.29	108.28
4	F	501	ELO	OAD-CAX-CAV	-2.08	104.48	107.42
4	C	501[B]	ELO	OAK-CCM-OAQ	2.08	126.66	123.34
4	B	501[A]	ELO	OAK-CCM-OAQ	2.07	126.66	123.34
4	F	501	ELO	OAJ-CCF-CCD	2.07	113.28	109.55
4	C	501[B]	ELO	CBV-CBJ-CBF	-2.05	107.40	111.43
4	B	501[A]	ELO	CCK-CCE-CCC	2.04	116.82	113.08
4	E	501[A]	ELO	OAI-CCE-CCK	2.02	111.21	106.74
4	C	501[B]	ELO	OAK-CCM-CCQ	2.01	115.77	111.39
4	B	501[A]	ELO	OAC-CBQ-OAI	2.00	116.44	109.97

There are no chirality outliers.

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	GOL	C1-C2-C3-O3
3	C	502	GOL	O1-C1-C2-C3
3	E	503	GOL	C1-C2-C3-O3
3	F	505	GOL	O1-C1-C2-C3
3	G	504	GOL	O1-C1-C2-C3
3	G	505	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	G	505	GOL	O1-C1-C2-C3
4	B	501[A]	ELO	CAY-CAS-CBA-CBK
4	B	501[A]	ELO	CAY-CAS-CBA-CBE
4	B	501[A]	ELO	OAA-CAS-CBA-CBK
4	B	501[A]	ELO	OAA-CAS-CBA-CBE
4	B	501[A]	ELO	OAE-CAS-CBA-CBK
4	B	501[A]	ELO	OAE-CAS-CBA-CBE
4	B	501[A]	ELO	CAS-CBA-CBE-OAG
4	B	501[A]	ELO	CBK-CBA-CBE-OAG
4	B	501[A]	ELO	CBK-CBA-CBE-CBI
4	B	501[A]	ELO	CCR-CCN-OAL-CBP
4	B	501[A]	ELO	CCQ-CCM-OAK-CBO
4	B	501[A]	ELO	CBJ-CBP-CBZ-CCH
4	C	501[B]	ELO	CAW-CAU-CBG-CBS
4	C	501[B]	ELO	OAA-CAS-CBA-CBK
4	C	501[B]	ELO	OAE-CAS-CBA-CBK
4	C	501[B]	ELO	OAR-CCN-OAL-CBP
4	C	501[B]	ELO	OAQ-CCM-OAK-CBO
4	C	501[B]	ELO	CBJ-CBP-CBZ-CCH
4	D	501[B]	ELO	CAY-CAS-CBA-CBK
4	D	501[B]	ELO	CAY-CAS-CBA-CBE
4	D	501[B]	ELO	OAA-CAS-CBA-CBK
4	D	501[B]	ELO	OAA-CAS-CBA-CBE
4	D	501[B]	ELO	OAE-CAS-CBA-CBK
4	D	501[B]	ELO	OAE-CAS-CBA-CBE
4	D	501[B]	ELO	CBK-CBA-CBE-OAG
4	D	501[B]	ELO	CCR-CCN-OAL-CBP
4	D	501[B]	ELO	CCQ-CCM-OAK-CBO
4	D	501[B]	ELO	CAZ-CAT-CBB-CBF
4	D	501[B]	ELO	OAF-CAT-CBB-CBF
4	D	501[B]	ELO	OAB-CAT-CBB-CBF
4	D	501[B]	ELO	CAZ-CAT-CBB-CBL
4	D	501[B]	ELO	OAF-CAT-CBB-CBL
4	D	501[B]	ELO	OAB-CAT-CBB-CBL
4	D	501[B]	ELO	CBX-CBR-OAD-CAX
4	E	501[A]	ELO	CAY-CAS-CBA-CBK
4	E	501[A]	ELO	CAY-CAS-CBA-CBE
4	E	501[A]	ELO	OAA-CAS-CBA-CBK
4	E	501[A]	ELO	OAA-CAS-CBA-CBE
4	E	501[A]	ELO	OAE-CAS-CBA-CBK
4	E	501[A]	ELO	OAE-CAS-CBA-CBE
4	E	501[A]	ELO	CAS-CBA-CBE-OAG

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Mol	Chain	Res	Type	Atoms
4	E	501[A]	ELO	CBK-CBA-CBE-OAG
4	E	501[A]	ELO	CBK-CBA-CBE-CBI
4	E	501[A]	ELO	CCR-CCN-OAL-CBP
4	E	501[A]	ELO	CAX-CAV-CBH-CBT
4	E	501[A]	ELO	CAZ-CAX-OAD-CBR
4	E	501[A]	ELO	OAJ-CBR-OAD-CAX
4	F	501	ELO	CAW-CAU-CBG-CBS
4	F	501	ELO	CAY-CAS-CBA-CBK
4	F	501	ELO	CAY-CAS-CBA-CBE
4	F	501	ELO	OAA-CAS-CBA-CBK
4	F	501	ELO	OAA-CAS-CBA-CBE
4	F	501	ELO	OAE-CAS-CBA-CBK
4	F	501	ELO	OAE-CAS-CBA-CBE
4	F	501	ELO	CBK-CBA-CBE-OAG
4	F	501	ELO	CBK-CBA-CBE-CBI
4	F	501	ELO	OAQ-CCM-OAK-CBO
4	F	501	ELO	CBD-CAV-CBH-CBT
4	F	501	ELO	CAX-CAV-CBH-CBT
4	D	501[B]	ELO	OAG-CBE-CBI-CBO
4	B	501[A]	ELO	OAR-CCN-OAL-CBP
4	B	501[A]	ELO	OAQ-CCM-OAK-CBO
4	D	501[B]	ELO	OAR-CCN-OAL-CBP
4	D	501[B]	ELO	OAQ-CCM-OAK-CBO
4	E	501[A]	ELO	OAR-CCN-OAL-CBP
4	F	501	ELO	OAR-CCN-OAL-CBP
4	F	501	ELO	CCR-CCN-OAL-CBP
4	E	501[A]	ELO	CBX-CBR-OAD-CAX
3	G	504	GOL	O2-C2-C3-O3
4	F	501	ELO	OAG-CBE-CBI-CBO
4	D	501[B]	ELO	CBA-CBE-CBI-CBU
4	D	501[B]	ELO	CAZ-CAX-OAD-CBR
4	C	501[B]	ELO	CCR-CCN-OAL-CBP
4	C	501[B]	ELO	CCQ-CCM-OAK-CBO
4	F	501	ELO	CCQ-CCM-OAK-CBO
4	E	501[A]	ELO	CBU-CBI-CBO-CBY
4	D	501[B]	ELO	OAG-CBE-CBI-CBU
4	E	501[A]	ELO	CCG-CBY-CCI-CCO
4	B	501[A]	ELO	OAG-CBE-CBI-CBO
4	B	501[A]	ELO	CBA-CBE-CBI-CBU
4	E	501[A]	ELO	OAQ-CCM-OAK-CBO
3	A	504	GOL	C1-C2-C3-O3
3	B	505	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	505	GOL	C1-C2-C3-O3
3	F	505	GOL	C1-C2-C3-O3
3	F	507	GOL	O1-C1-C2-C3
3	G	504	GOL	C1-C2-C3-O3
4	D	501[B]	ELO	CBK-CBA-CBE-CBI
4	B	501[A]	ELO	OAG-CBE-CBI-CBU
4	F	501	ELO	OAG-CBE-CBI-CBU
4	F	501	ELO	CCG-CBY-CCI-CCO
3	A	505	GOL	O2-C2-C3-O3
3	E	503	GOL	O2-C2-C3-O3
3	F	505	GOL	O1-C1-C2-O2
3	F	505	GOL	O2-C2-C3-O3
4	D	501[B]	ELO	CBA-CBE-CBI-CBO
4	E	501[A]	ELO	CCQ-CCM-OAK-CBO
4	E	501[A]	ELO	CBU-CBI-CBO-OAK
4	F	501	ELO	CBA-CBE-CBI-CBU
4	D	501[B]	ELO	OAJ-CBR-OAD-CAX
3	F	507	GOL	O1-C1-C2-O2
4	D	501[B]	ELO	OAH-CBF-CBJ-CBP
4	B	501[A]	ELO	CBL-CBB-CBF-CBJ
4	B	501[A]	ELO	CBA-CBE-CBI-CBO
4	C	501[B]	ELO	CBC-CAU-CBG-CBS
4	F	501	ELO	CBA-CBE-CBI-CBO
3	A	504	GOL	O2-C2-C3-O3
3	B	505	GOL	O2-C2-C3-O3
3	C	502	GOL	O1-C1-C2-O2
3	G	504	GOL	O1-C1-C2-O2
4	B	501[A]	ELO	CCG-CBY-CCI-CCO
4	D	501[B]	ELO	CBB-CBF-CBJ-CBP
4	B	501[A]	ELO	CBL-CBB-CBF-OAH
4	C	501[B]	ELO	CBZ-CBP-OAL-CCN
4	D	501[B]	ELO	CBB-CBF-CBJ-CBV
4	D	501[B]	ELO	CCG-CBY-CCI-CCO
3	B	505	GOL	O1-C1-C2-O2
3	F	507	GOL	O2-C2-C3-O3
4	B	501[A]	ELO	CBY-CBO-OAK-CCM
4	B	501[A]	ELO	CBZ-CBP-OAL-CCN
4	D	501[B]	ELO	CBY-CBO-OAK-CCM
4	D	501[B]	ELO	CBZ-CBP-OAL-CCN
4	F	501	ELO	CBY-CBO-OAK-CCM
4	D	501[B]	ELO	CBO-CBY-CCI-CCO
4	F	501	ELO	CBO-CBY-CCI-CCO

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Mol	Chain	Res	Type	Atoms
4	E	501[A]	ELO	OAG-CBE-CBI-CBO
4	C	501[B]	ELO	CCG-CBY-CCI-CCO
4	C	501[B]	ELO	CBJ-CBP-OAL-CCN
4	E	501[A]	ELO	CBY-CBO-OAK-CCM
4	F	501	ELO	CBZ-CBP-OAL-CCN
4	D	501[B]	ELO	CBI-CBO-OAK-CCM
4	D	501[B]	ELO	CBJ-CBP-CBZ-CCH
4	E	501[A]	ELO	CBJ-CBP-CBZ-CCH
4	D	501[B]	ELO	OAH-CBF-CBJ-CBV
4	B	501[A]	ELO	CBJ-CBP-OAL-CCN
4	C	501[B]	ELO	CBW-CBQ-OAC-CAW
4	E	501[A]	ELO	CBA-CBE-CBI-CBO
4	E	501[A]	ELO	CBO-CBY-CCI-CCO
4	E	501[A]	ELO	CBZ-CBP-OAL-CCN
4	C	501[B]	ELO	OAE-CAS-CBA-CBE
4	D	501[B]	ELO	CBJ-CBP-OAL-CCN
3	A	505	GOL	O1-C1-C2-O2
4	B	501[A]	ELO	CBI-CBO-OAK-CCM
3	A	505	GOL	O1-C1-C2-C3
4	F	501	ELO	CBL-CBB-CBF-CBJ
4	F	501	ELO	CBJ-CBP-OAL-CCN
4	B	501[A]	ELO	CBO-CBY-CCI-CCO
4	F	501	ELO	CBC-CAU-CBG-CBS
4	F	501	ELO	CBI-CBO-OAK-CCM
4	E	501[A]	ELO	OAG-CBE-CBI-CBU
4	F	501	ELO	CBU-CBI-CBO-CBY
4	B	501[A]	ELO	CBW-CBQ-OAC-CAW
4	B	501[A]	ELO	OAL-CBP-CBZ-CCH
4	F	501	ELO	CAS-CBA-CBE-OAG
4	E	501[A]	ELO	CBE-CBI-CBO-CBY

There are no ring outliers.

9 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	505	GOL	1	0
4	B	501[A]	ELO	7	0
3	F	506	GOL	1	0
3	A	505	GOL	1	0
4	E	501[A]	ELO	13	0
2	F	504	ACT	1	0
4	C	501[B]	ELO	9	0

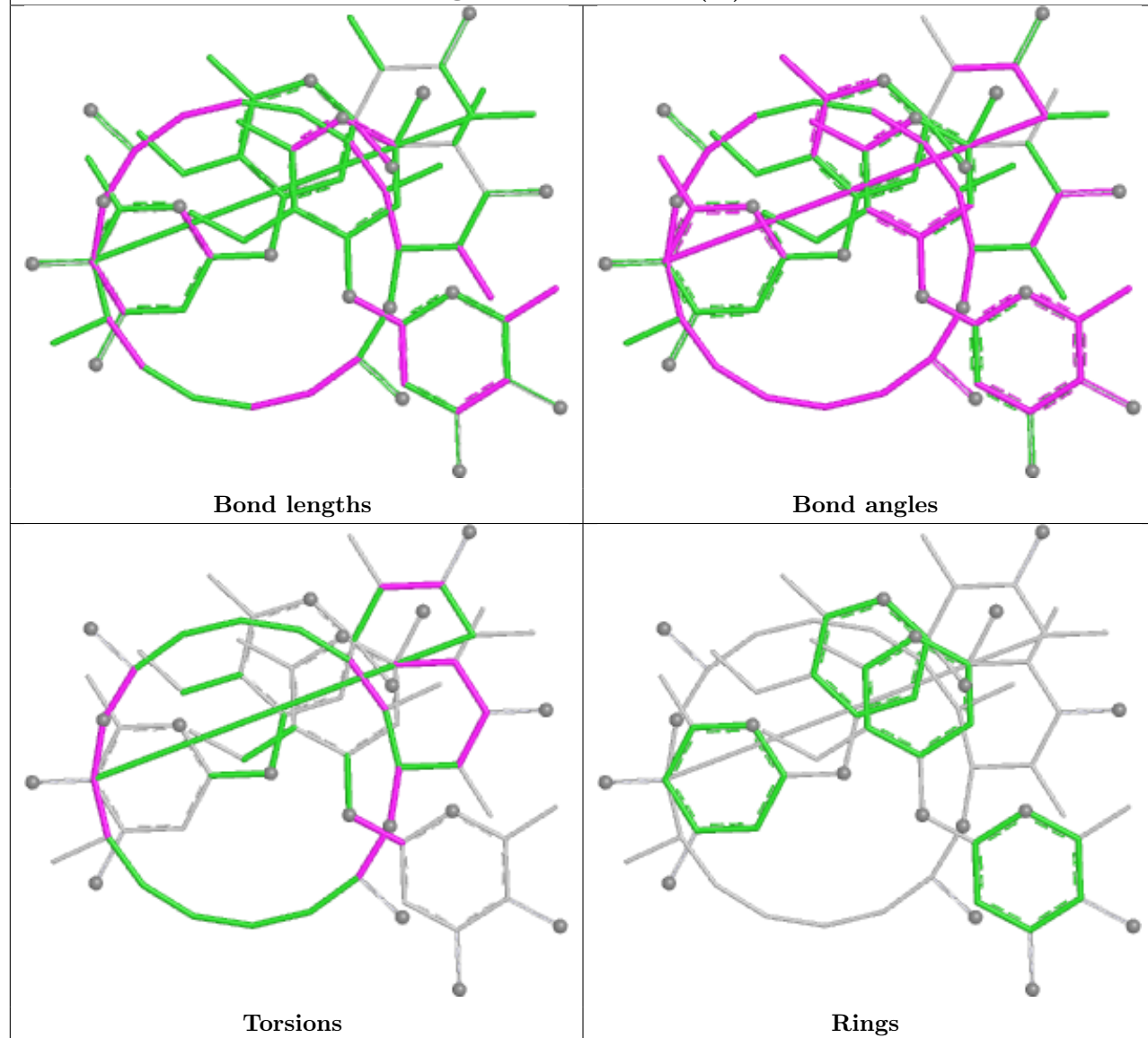
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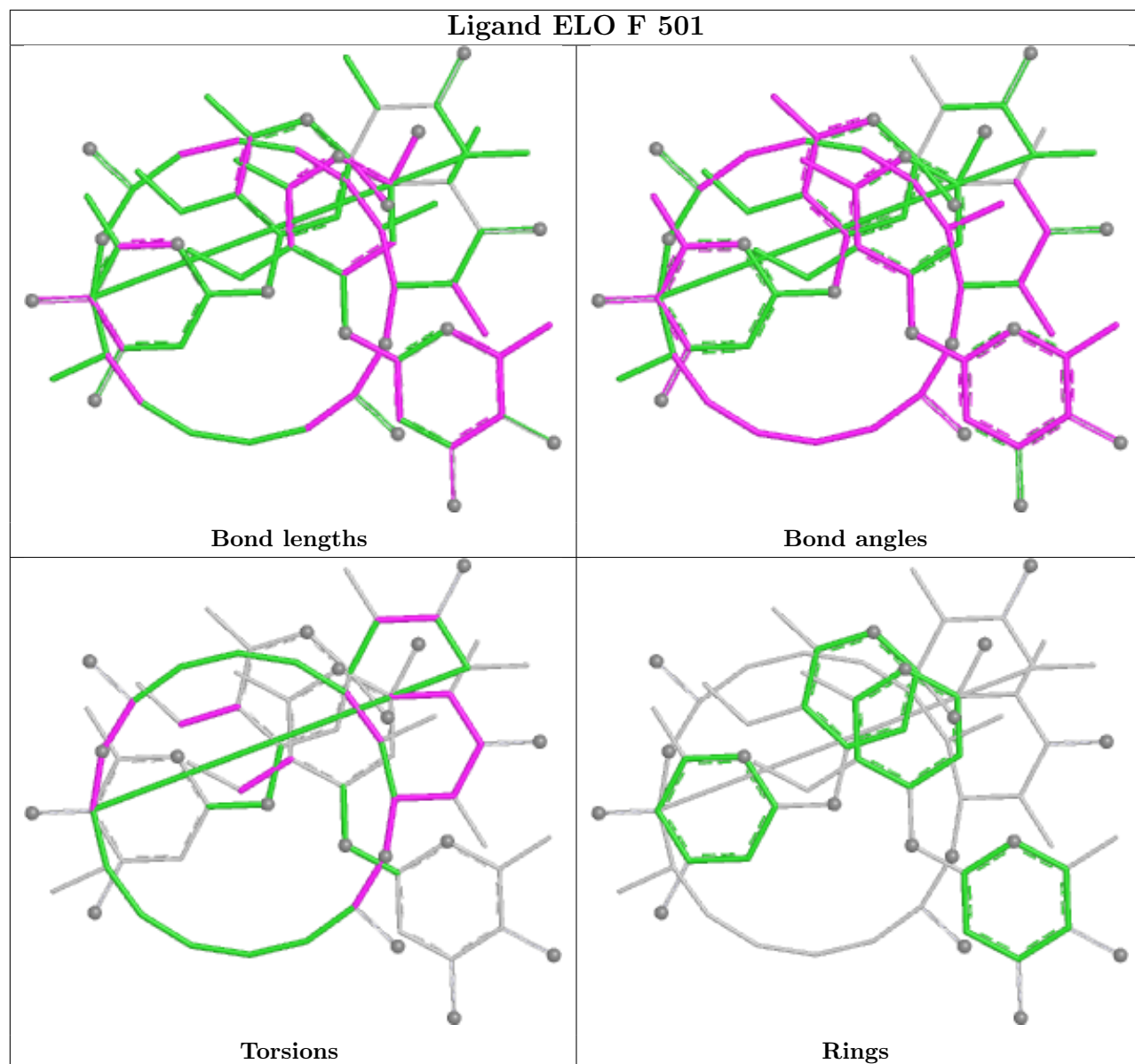
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501[B]	ELO	11	0
2	G	502	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

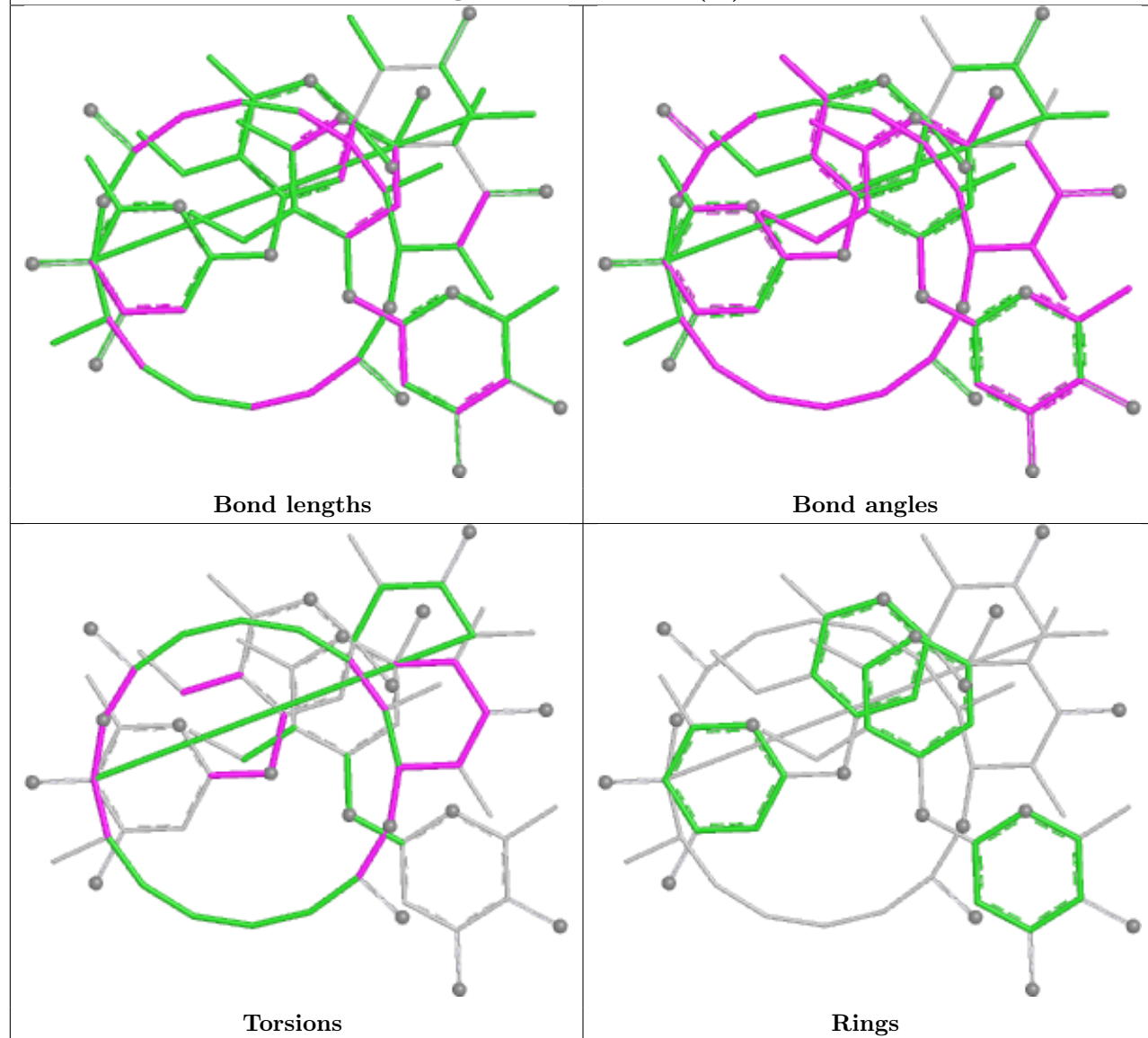
Ligand ELO B 501 (A)



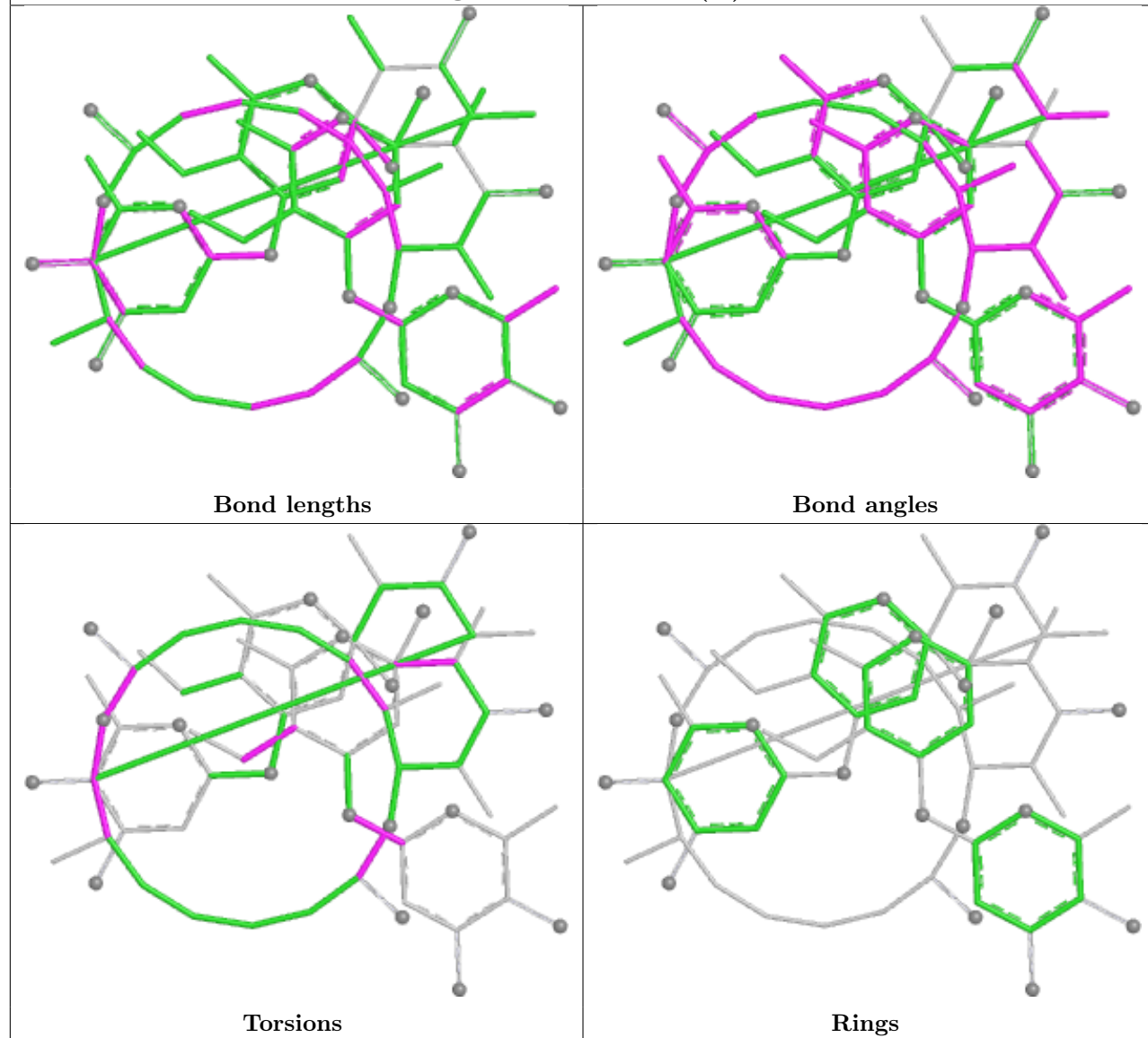
Ligand ELO F 501

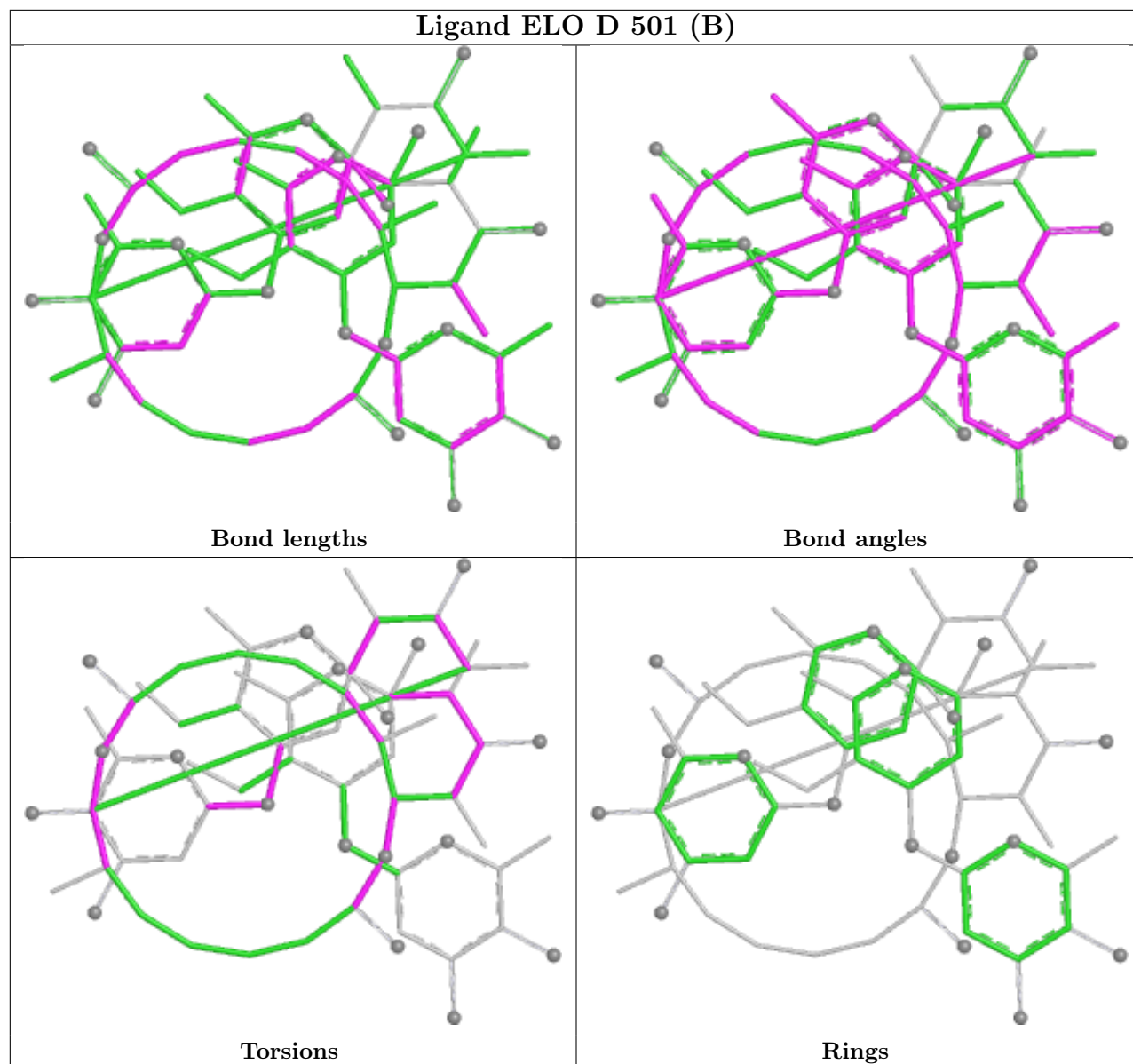


Ligand ELO E 501 (A)



Ligand ELO C 501 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	409/437 (93%)	0.07	14 (3%)	48	50	30, 42, 75, 129	0
1	B	408/437 (93%)	0.33	44 (10%)	11	11	21, 41, 110, 150	3 (0%)
1	C	408/437 (93%)	0.61	40 (9%)	13	13	32, 56, 120, 168	1 (0%)
1	D	408/437 (93%)	0.57	28 (6%)	23	24	39, 57, 104, 146	0
1	E	408/437 (93%)	0.78	43 (10%)	11	12	38, 60, 116, 158	0
1	F	419/437 (95%)	0.05	27 (6%)	25	27	27, 39, 105, 145	1 (0%)
1	G	408/437 (93%)	0.56	32 (7%)	19	20	30, 55, 106, 169	0
All	All	2868/3059 (93%)	0.42	228 (7%)	18	20	21, 50, 109, 169	5 (0%)

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	PHE	6.3
1	C	100	PHE	6.0
1	E	100	PHE	6.0
1	B	70	LEU	6.0
1	E	262	PHE	5.6
1	D	262	PHE	5.4
1	F	288	VAL	5.2
1	E	288	VAL	4.9
1	B	288	VAL	4.8
1	B	262	PHE	4.6
1	F	291	LEU	4.6
1	C	262	PHE	4.5
1	F	100	PHE	4.5
1	C	288	VAL	4.5
1	G	100	PHE	4.4
1	F	303	PHE	4.4
1	B	240	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	100	PHE	4.2
1	G	70	LEU	4.2
1	D	288	VAL	4.2
1	F	240	ALA	4.0
1	A	288	VAL	4.0
1	G	262	PHE	4.0
1	G	288	VAL	4.0
1	C	70	LEU	4.0
1	F	241	PRO	4.0
1	B	242	GLY	4.0
1	C	304	VAL	3.9
1	B	69	SER	3.9
1	B	237	LEU	3.9
1	G	303	PHE	3.9
1	B	100	PHE	3.8
1	F	255	ARG	3.8
1	C	307	HIS	3.7
1	C	241	PRO	3.6
1	B	296	ALA	3.6
1	G	296	ALA	3.6
1	C	250	SER	3.5
1	B	304	VAL	3.5
1	F	285	PRO	3.4
1	G	240	ALA	3.4
1	D	291	LEU	3.4
1	B	250	SER	3.4
1	B	241	PRO	3.3
1	G	304	VAL	3.3
1	B	290	ALA	3.3
1	C	69	SER	3.3
1	F	-1	SER	3.3
1	B	291	LEU	3.2
1	B	303	PHE	3.2
1	B	66	ASN	3.2
1	E	269	ILE	3.2
1	G	366	LEU	3.2
1	A	291	LEU	3.1
1	F	69	SER	3.1
1	E	241	PRO	3.1
1	G	342	TYR	3.1
1	A	99	MET	3.1
1	F	284	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	258	LEU	3.0
1	D	241	PRO	3.0
1	B	275	MET	3.0
1	C	290	ALA	3.0
1	B	285	PRO	3.0
1	D	240	ALA	3.0
1	A	262	PHE	3.0
1	B	238	ARG	2.9
1	A	261	THR	2.9
1	G	241	PRO	2.9
1	D	303	PHE	2.9
1	E	250	SER	2.9
1	A	285	PRO	2.9
1	B	342	TYR	2.9
1	F	262	PHE	2.9
1	C	291	LEU	2.9
1	E	370	VAL	2.9
1	E	303	PHE	2.8
1	E	242	GLY	2.8
1	D	70	LEU	2.8
1	E	272	LEU	2.8
1	E	300	ILE	2.8
1	D	99	MET	2.8
1	F	70	LEU	2.8
1	E	264	PRO	2.8
1	B	307	HIS	2.8
1	C	240	ALA	2.8
1	F	290	ALA	2.8
1	G	290	ALA	2.8
1	E	378	LEU	2.8
1	G	291	LEU	2.8
1	C	308	ALA	2.7
1	E	240	ALA	2.7
1	F	252	VAL	2.7
1	C	269	ILE	2.7
1	E	70	LEU	2.7
1	E	291	LEU	2.7
1	C	285	PRO	2.7
1	D	265	VAL	2.7
1	G	173	ARG	2.7
1	B	368	ALA	2.7
1	D	250	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	280	VAL	2.7
1	B	249	THR	2.6
1	B	272	LEU	2.6
1	C	277	ILE	2.6
1	A	70	LEU	2.6
1	D	283	LEU	2.6
1	B	277	ILE	2.6
1	G	294	VAL	2.6
1	E	296	ALA	2.6
1	C	303	PHE	2.6
1	F	305	PRO	2.6
1	G	282	ALA	2.5
1	A	303	PHE	2.5
1	E	304	VAL	2.5
1	C	319	HIS	2.5
1	C	342	TYR	2.5
1	C	92	MET	2.5
1	F	68	ASP	2.5
1	G	308	ALA	2.5
1	B	243	ARG	2.5
1	A	58	ASN	2.5
1	F	260	GLY	2.4
1	G	312	GLY	2.4
1	F	66	ASN	2.4
1	C	375	VAL	2.4
1	E	265	VAL	2.4
1	E	279	VAL	2.4
1	D	285	PRO	2.4
1	E	285	PRO	2.4
1	D	372	ARG	2.4
1	E	363	ALA	2.4
1	F	67	ARG	2.4
1	G	283	LEU	2.4
1	B	379	VAL	2.4
1	E	277	ILE	2.4
1	E	-1	SER	2.4
1	E	99	MET	2.4
1	D	245	ARG	2.4
1	F	293	LYS	2.4
1	B	305	PRO	2.4
1	G	305	PRO	2.4
1	E	307	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	368	ALA	2.4
1	F	259	GLY	2.4
1	A	92	MET	2.4
1	B	-1	SER	2.4
1	A	290	ALA	2.3
1	C	272	LEU	2.3
1	C	371	LEU	2.3
1	E	248	LEU	2.3
1	E	366	LEU	2.3
1	G	371	LEU	2.3
1	G	242	GLY	2.3
1	B	246	VAL	2.3
1	C	-1	SER	2.3
1	C	274	SER	2.3
1	C	294	VAL	2.3
1	G	250	SER	2.3
1	G	274	SER	2.3
1	C	305	PRO	2.3
1	G	285	PRO	2.3
1	C	384	TYR	2.3
1	B	273	GLY	2.3
1	B	294	VAL	2.3
1	D	249	THR	2.3
1	C	236	TRP	2.3
1	E	263	MET	2.3
1	B	274	SER	2.3
1	A	96	VAL	2.3
1	B	265	VAL	2.3
1	E	246	VAL	2.3
1	E	244	PRO	2.3
1	B	372	ARG	2.3
1	C	173	ARG	2.3
1	D	308	ALA	2.3
1	E	290	ALA	2.3
1	B	283	LEU	2.3
1	D	272	LEU	2.3
1	G	245	ARG	2.2
1	B	276	ASP	2.2
1	E	368	ALA	2.2
1	F	254	ALA	2.2
1	F	283	LEU	2.2
1	E	116	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	245	ARG	2.2
1	E	298	THR	2.2
1	D	379	VAL	2.2
1	C	62	MET	2.2
1	C	242	GLY	2.2
1	E	266	ALA	2.2
1	E	308	ALA	2.2
1	A	250	SER	2.2
1	D	300	ILE	2.2
1	D	304	VAL	2.2
1	E	332	GLY	2.2
1	E	119	HIS	2.2
1	G	237	LEU	2.2
1	F	256	ALA	2.1
1	D	293	LYS	2.1
1	C	244	PRO	2.1
1	C	264	PRO	2.1
1	C	300	ILE	2.1
1	B	270	ASN	2.1
1	G	268	MET	2.1
1	B	295	PRO	2.1
1	D	312	GLY	2.1
1	E	233	ILE	2.1
1	E	236	TRP	2.1
1	C	265	VAL	2.1
1	E	282	ALA	2.1
1	G	309	LEU	2.1
1	D	284	PRO	2.1
1	F	188	ARG	2.1
1	B	300	ILE	2.1
1	B	280	VAL	2.1
1	B	301	VAL	2.1
1	C	370	VAL	2.1
1	D	96	VAL	2.1
1	G	368	ALA	2.1
1	B	306	LEU	2.0
1	G	248	LEU	2.0
1	D	384	TYR	2.0
1	C	279	VAL	2.0
1	D	280	VAL	2.0
1	G	375	VAL	2.0
1	C	266	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	413	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	F	507	6/6	0.76	0.18	70,83,92,93	0
2	ACT	A	503	4/4	0.79	0.15	63,66,70,72	0
4	ELO	B	501[A]	72/72	0.79	0.26	32,56,87,96	72
4	ELO	E	501[A]	72/72	0.79	0.29	44,66,159,169	72
3	GOL	F	506	6/6	0.80	0.14	70,73,77,81	0
4	ELO	D	501[B]	72/72	0.80	0.28	39,73,139,145	72
2	ACT	D	503	4/4	0.80	0.18	59,63,64,71	0
2	ACT	B	502	4/4	0.81	0.18	72,72,75,83	0
4	ELO	C	501[B]	72/72	0.81	0.24	36,53,66,68	72
3	GOL	A	505	6/6	0.83	0.18	67,83,85,87	0
3	GOL	G	504	6/6	0.83	0.20	53,69,70,72	0
4	ELO	F	501	72/72	0.83	0.21	29,44,52,63	72
2	ACT	B	503	4/4	0.84	0.20	76,80,81,87	0
2	ACT	A	501	4/4	0.85	0.14	49,55,60,64	0
3	GOL	A	504	6/6	0.86	0.14	40,58,63,70	0
3	GOL	F	505	6/6	0.86	0.20	48,71,75,83	0
2	ACT	F	504	4/4	0.87	0.14	48,59,62,63	0
3	GOL	B	505	6/6	0.89	0.14	40,53,64,66	0
2	ACT	G	503	4/4	0.89	0.16	61,62,64,66	0
3	GOL	E	503	6/6	0.90	0.13	58,62,69,70	0
2	ACT	F	503	4/4	0.90	0.16	50,50,55,62	0
3	GOL	B	504	6/6	0.90	0.12	43,54,55,60	0

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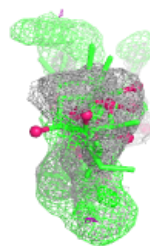
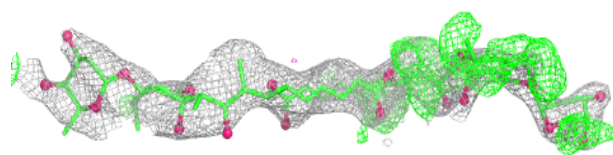
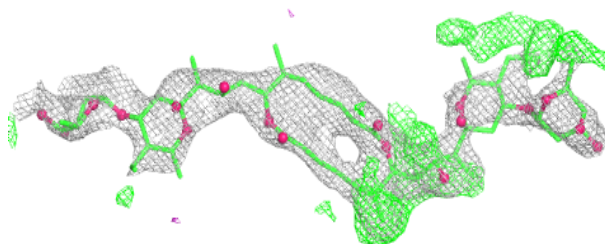
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	G	501	4/4	0.90	0.16	45,57,57,62	0
3	GOL	C	502	6/6	0.90	0.16	67,79,85,94	0
2	ACT	D	502	4/4	0.91	0.12	66,67,69,69	0
2	ACT	A	502	4/4	0.93	0.14	53,58,61,63	0
2	ACT	G	502	4/4	0.93	0.11	54,56,58,59	0
2	ACT	E	502	4/4	0.94	0.10	59,65,71,73	0
3	GOL	G	505	6/6	0.95	0.09	57,63,68,72	0
2	ACT	F	502	4/4	0.95	0.09	43,44,49,49	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

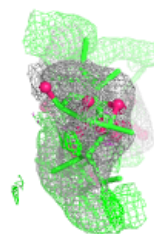
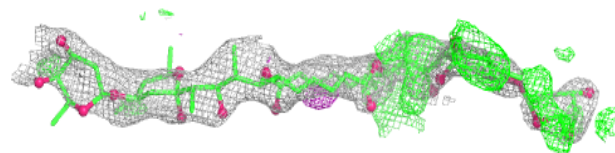
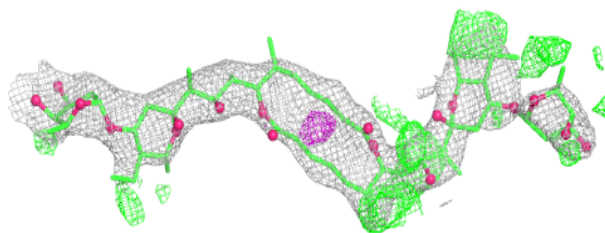
Electron density around ELO B 501 (A):

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

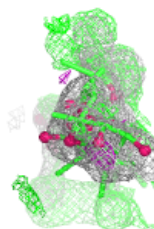
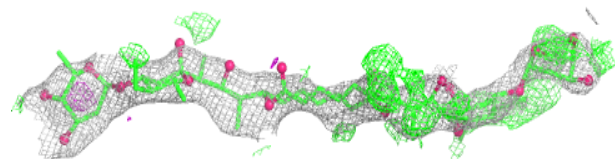
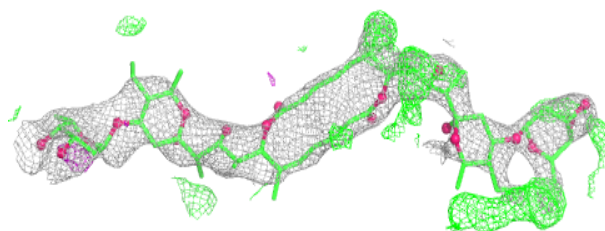


Electron density around ELO E 501 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

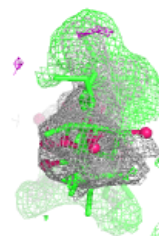
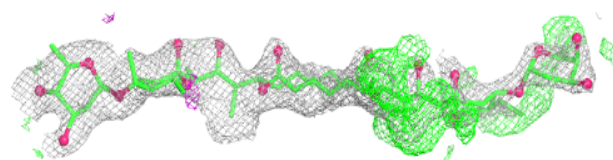
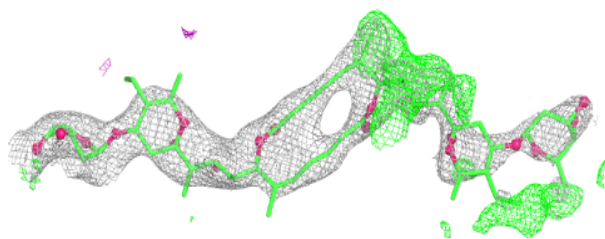
**Electron density around ELO D 501 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

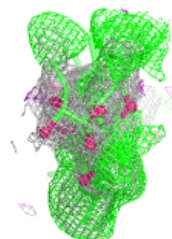
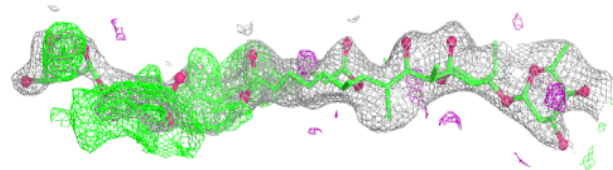
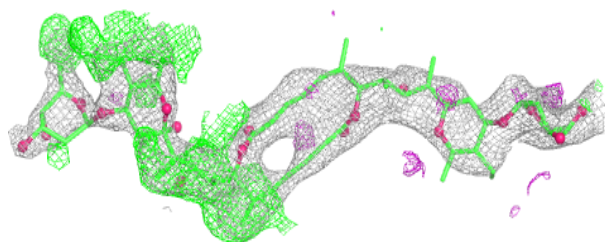


Electron density around ELO C 501 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ELO F 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.