



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 08:10 AM EDT

PDB ID : 6Y2J
Title : Crystal structure of M. tuberculosis KasA in complex with 4,4,4-trifluoro-N-(isoquinolin-6-yl)butane-1-sulfonamide
Authors : Chung, C.
Deposited on : 2020-02-16
Resolution : 2.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

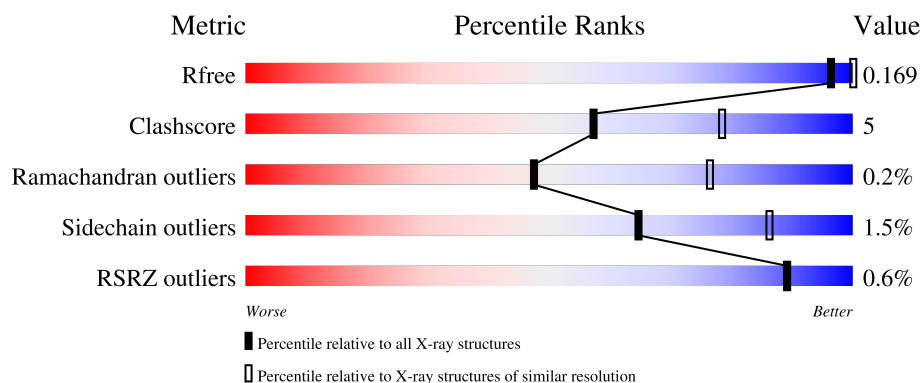
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.89 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}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	AAA	435	
1	BBB	435	
1	CCC	435	
1	DDD	435	
1	EEE	435	

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Mol	Chain	Length	Quality of chain
1	FFF	435	 83% 12% 5%
1	GGG	435	 85% 10% 5%
1	HHH	435	 86% 9% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PG4	DDD	901	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25455 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 3-oxoacyl-[acyl-carrier-protein] synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	415	Total	C	N	O	S	0	1	0
			3039	1895	541	585	18			
1	BBB	415	Total	C	N	O	S	0	1	0
			3039	1895	541	585	18			
1	CCC	415	Total	C	N	O	S	0	1	0
			3039	1895	541	585	18			
1	DDD	414	Total	C	N	O	S	0	1	0
			3023	1887	536	582	18			
1	EEE	415	Total	C	N	O	S	0	0	0
			3029	1889	538	584	18			
1	FFF	415	Total	C	N	O	S	0	0	0
			3029	1889	538	584	18			
1	GGG	415	Total	C	N	O	S	0	0	0
			3029	1889	538	584	18			
1	HHH	415	Total	C	N	O	S	0	2	0
			3050	1901	545	586	18			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-18	MET	-	initiating methionine	UNP P9WQD9
AAA	-17	GLY	-	expression tag	UNP P9WQD9
AAA	-16	SER	-	expression tag	UNP P9WQD9
AAA	-15	SER	-	expression tag	UNP P9WQD9
AAA	-14	HIS	-	expression tag	UNP P9WQD9
AAA	-13	HIS	-	expression tag	UNP P9WQD9
AAA	-12	HIS	-	expression tag	UNP P9WQD9
AAA	-11	HIS	-	expression tag	UNP P9WQD9
AAA	-10	HIS	-	expression tag	UNP P9WQD9
AAA	-9	HIS	-	expression tag	UNP P9WQD9
AAA	-8	SER	-	expression tag	UNP P9WQD9
AAA	-7	SER	-	expression tag	UNP P9WQD9
AAA	-6	GLY	-	expression tag	UNP P9WQD9

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-5	LEU	-	expression tag	UNP P9WQD9
AAA	-4	VAL	-	expression tag	UNP P9WQD9
AAA	-3	PRO	-	expression tag	UNP P9WQD9
AAA	-2	ARG	-	expression tag	UNP P9WQD9
AAA	-1	GLY	-	expression tag	UNP P9WQD9
AAA	0	SER	-	expression tag	UNP P9WQD9
AAA	1	HIS	-	expression tag	UNP P9WQD9
BBB	-18	MET	-	initiating methionine	UNP P9WQD9
BBB	-17	GLY	-	expression tag	UNP P9WQD9
BBB	-16	SER	-	expression tag	UNP P9WQD9
BBB	-15	SER	-	expression tag	UNP P9WQD9
BBB	-14	HIS	-	expression tag	UNP P9WQD9
BBB	-13	HIS	-	expression tag	UNP P9WQD9
BBB	-12	HIS	-	expression tag	UNP P9WQD9
BBB	-11	HIS	-	expression tag	UNP P9WQD9
BBB	-10	HIS	-	expression tag	UNP P9WQD9
BBB	-9	HIS	-	expression tag	UNP P9WQD9
BBB	-8	SER	-	expression tag	UNP P9WQD9
BBB	-7	SER	-	expression tag	UNP P9WQD9
BBB	-6	GLY	-	expression tag	UNP P9WQD9
BBB	-5	LEU	-	expression tag	UNP P9WQD9
BBB	-4	VAL	-	expression tag	UNP P9WQD9
BBB	-3	PRO	-	expression tag	UNP P9WQD9
BBB	-2	ARG	-	expression tag	UNP P9WQD9
BBB	-1	GLY	-	expression tag	UNP P9WQD9
BBB	0	SER	-	expression tag	UNP P9WQD9
BBB	1	HIS	-	expression tag	UNP P9WQD9
CCC	-18	MET	-	initiating methionine	UNP P9WQD9
CCC	-17	GLY	-	expression tag	UNP P9WQD9
CCC	-16	SER	-	expression tag	UNP P9WQD9
CCC	-15	SER	-	expression tag	UNP P9WQD9
CCC	-14	HIS	-	expression tag	UNP P9WQD9
CCC	-13	HIS	-	expression tag	UNP P9WQD9
CCC	-12	HIS	-	expression tag	UNP P9WQD9
CCC	-11	HIS	-	expression tag	UNP P9WQD9
CCC	-10	HIS	-	expression tag	UNP P9WQD9
CCC	-9	HIS	-	expression tag	UNP P9WQD9
CCC	-8	SER	-	expression tag	UNP P9WQD9
CCC	-7	SER	-	expression tag	UNP P9WQD9
CCC	-6	GLY	-	expression tag	UNP P9WQD9
CCC	-5	LEU	-	expression tag	UNP P9WQD9
CCC	-4	VAL	-	expression tag	UNP P9WQD9

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-3	PRO	-	expression tag	UNP P9WQD9
CCC	-2	ARG	-	expression tag	UNP P9WQD9
CCC	-1	GLY	-	expression tag	UNP P9WQD9
CCC	0	SER	-	expression tag	UNP P9WQD9
CCC	1	HIS	-	expression tag	UNP P9WQD9
DDD	-18	MET	-	initiating methionine	UNP P9WQD9
DDD	-17	GLY	-	expression tag	UNP P9WQD9
DDD	-16	SER	-	expression tag	UNP P9WQD9
DDD	-15	SER	-	expression tag	UNP P9WQD9
DDD	-14	HIS	-	expression tag	UNP P9WQD9
DDD	-13	HIS	-	expression tag	UNP P9WQD9
DDD	-12	HIS	-	expression tag	UNP P9WQD9
DDD	-11	HIS	-	expression tag	UNP P9WQD9
DDD	-10	HIS	-	expression tag	UNP P9WQD9
DDD	-9	HIS	-	expression tag	UNP P9WQD9
DDD	-8	SER	-	expression tag	UNP P9WQD9
DDD	-7	SER	-	expression tag	UNP P9WQD9
DDD	-6	GLY	-	expression tag	UNP P9WQD9
DDD	-5	LEU	-	expression tag	UNP P9WQD9
DDD	-4	VAL	-	expression tag	UNP P9WQD9
DDD	-3	PRO	-	expression tag	UNP P9WQD9
DDD	-2	ARG	-	expression tag	UNP P9WQD9
DDD	-1	GLY	-	expression tag	UNP P9WQD9
DDD	0	SER	-	expression tag	UNP P9WQD9
DDD	1	HIS	-	expression tag	UNP P9WQD9
EEE	-18	MET	-	initiating methionine	UNP P9WQD9
EEE	-17	GLY	-	expression tag	UNP P9WQD9
EEE	-16	SER	-	expression tag	UNP P9WQD9
EEE	-15	SER	-	expression tag	UNP P9WQD9
EEE	-14	HIS	-	expression tag	UNP P9WQD9
EEE	-13	HIS	-	expression tag	UNP P9WQD9
EEE	-12	HIS	-	expression tag	UNP P9WQD9
EEE	-11	HIS	-	expression tag	UNP P9WQD9
EEE	-10	HIS	-	expression tag	UNP P9WQD9
EEE	-9	HIS	-	expression tag	UNP P9WQD9
EEE	-8	SER	-	expression tag	UNP P9WQD9
EEE	-7	SER	-	expression tag	UNP P9WQD9
EEE	-6	GLY	-	expression tag	UNP P9WQD9
EEE	-5	LEU	-	expression tag	UNP P9WQD9
EEE	-4	VAL	-	expression tag	UNP P9WQD9
EEE	-3	PRO	-	expression tag	UNP P9WQD9
EEE	-2	ARG	-	expression tag	UNP P9WQD9

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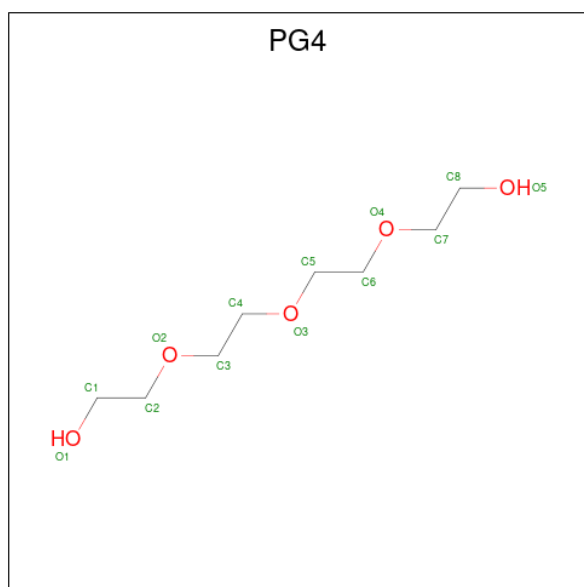
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	-1	GLY	-	expression tag	UNP P9WQD9
EEE	0	SER	-	expression tag	UNP P9WQD9
EEE	1	HIS	-	expression tag	UNP P9WQD9
FFF	-18	MET	-	initiating methionine	UNP P9WQD9
FFF	-17	GLY	-	expression tag	UNP P9WQD9
FFF	-16	SER	-	expression tag	UNP P9WQD9
FFF	-15	SER	-	expression tag	UNP P9WQD9
FFF	-14	HIS	-	expression tag	UNP P9WQD9
FFF	-13	HIS	-	expression tag	UNP P9WQD9
FFF	-12	HIS	-	expression tag	UNP P9WQD9
FFF	-11	HIS	-	expression tag	UNP P9WQD9
FFF	-10	HIS	-	expression tag	UNP P9WQD9
FFF	-9	HIS	-	expression tag	UNP P9WQD9
FFF	-8	SER	-	expression tag	UNP P9WQD9
FFF	-7	SER	-	expression tag	UNP P9WQD9
FFF	-6	GLY	-	expression tag	UNP P9WQD9
FFF	-5	LEU	-	expression tag	UNP P9WQD9
FFF	-4	VAL	-	expression tag	UNP P9WQD9
FFF	-3	PRO	-	expression tag	UNP P9WQD9
FFF	-2	ARG	-	expression tag	UNP P9WQD9
FFF	-1	GLY	-	expression tag	UNP P9WQD9
FFF	0	SER	-	expression tag	UNP P9WQD9
FFF	1	HIS	-	expression tag	UNP P9WQD9
GGG	-18	MET	-	initiating methionine	UNP P9WQD9
GGG	-17	GLY	-	expression tag	UNP P9WQD9
GGG	-16	SER	-	expression tag	UNP P9WQD9
GGG	-15	SER	-	expression tag	UNP P9WQD9
GGG	-14	HIS	-	expression tag	UNP P9WQD9
GGG	-13	HIS	-	expression tag	UNP P9WQD9
GGG	-12	HIS	-	expression tag	UNP P9WQD9
GGG	-11	HIS	-	expression tag	UNP P9WQD9
GGG	-10	HIS	-	expression tag	UNP P9WQD9
GGG	-9	HIS	-	expression tag	UNP P9WQD9
GGG	-8	SER	-	expression tag	UNP P9WQD9
GGG	-7	SER	-	expression tag	UNP P9WQD9
GGG	-6	GLY	-	expression tag	UNP P9WQD9
GGG	-5	LEU	-	expression tag	UNP P9WQD9
GGG	-4	VAL	-	expression tag	UNP P9WQD9
GGG	-3	PRO	-	expression tag	UNP P9WQD9
GGG	-2	ARG	-	expression tag	UNP P9WQD9
GGG	-1	GLY	-	expression tag	UNP P9WQD9
GGG	0	SER	-	expression tag	UNP P9WQD9

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Chain	Residue	Modelled	Actual	Comment	Reference
GGG	1	HIS	-	expression tag	UNP P9WQD9
HHH	-18	MET	-	initiating methionine	UNP P9WQD9
HHH	-17	GLY	-	expression tag	UNP P9WQD9
HHH	-16	SER	-	expression tag	UNP P9WQD9
HHH	-15	SER	-	expression tag	UNP P9WQD9
HHH	-14	HIS	-	expression tag	UNP P9WQD9
HHH	-13	HIS	-	expression tag	UNP P9WQD9
HHH	-12	HIS	-	expression tag	UNP P9WQD9
HHH	-11	HIS	-	expression tag	UNP P9WQD9
HHH	-10	HIS	-	expression tag	UNP P9WQD9
HHH	-9	HIS	-	expression tag	UNP P9WQD9
HHH	-8	SER	-	expression tag	UNP P9WQD9
HHH	-7	SER	-	expression tag	UNP P9WQD9
HHH	-6	GLY	-	expression tag	UNP P9WQD9
HHH	-5	LEU	-	expression tag	UNP P9WQD9
HHH	-4	VAL	-	expression tag	UNP P9WQD9
HHH	-3	PRO	-	expression tag	UNP P9WQD9
HHH	-2	ARG	-	expression tag	UNP P9WQD9
HHH	-1	GLY	-	expression tag	UNP P9WQD9
HHH	0	SER	-	expression tag	UNP P9WQD9
HHH	1	HIS	-	expression tag	UNP P9WQD9

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			13	8	5		

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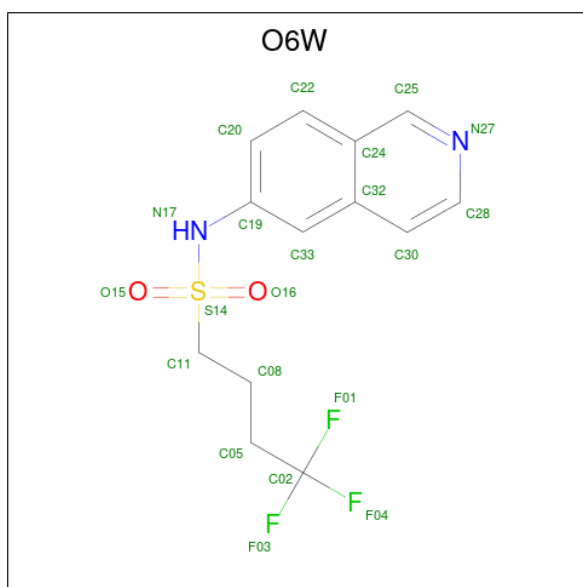
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	BBB	1	Total	C	O	0	0
			13	8	5		
2	CCC	1	Total	C	O	0	0
			13	8	5		
2	DDD	1	Total	C	O	0	0
			13	8	5		
2	EEE	1	Total	C	O	0	0
			13	8	5		
2	FFF	1	Total	C	O	0	0
			13	8	5		
2	GGG	1	Total	C	O	0	0
			13	8	5		
2	HHH	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Na	0	0
			1	1		
3	BBB	1	Total	Na	0	0
			1	1		
3	CCC	1	Total	Na	0	0
			1	1		
3	DDD	1	Total	Na	0	0
			1	1		
3	EEE	1	Total	Na	0	0
			1	1		
3	FFF	1	Total	Na	0	0
			1	1		
3	GGG	1	Total	Na	0	0
			1	1		
3	HHH	1	Total	Na	0	0
			1	1		

- Molecule 4 is 4,4,4-tris(fluoranyl)- {N}-isoquinolin-6-yl-butane-1-sulfonamide (three-letter code: O6W) (formula: C₁₃H₁₃F₃N₂O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	AAA	1	Total 21	C 13	F 3	N 2	O 2	S 1	0	0
4	BBB	1	Total 21	C 13	F 3	N 2	O 2	S 1	0	0
4	CCC	1	Total 21	C 13	F 3	N 2	O 2	S 1	0	0
4	DDD	1	Total 21	C 13	F 3	N 2	O 2	S 1	0	0
4	EEE	1	Total 21	C 13	F 3	N 2	O 2	S 1	0	0
4	FFF	1	Total 21	C 13	F 3	N 2	O 2	S 1	0	0
4	GGG	1	Total 21	C 13	F 3	N 2	O 2	S 1	0	0
4	HHH	1	Total 21	C 13	F 3	N 2	O 2	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	139	Total	O	0	0
			139	139		
5	BBB	160	Total	O	0	0
			160	160		
5	CCC	110	Total	O	0	0
			110	110		
5	DDD	115	Total	O	0	0
			115	115		

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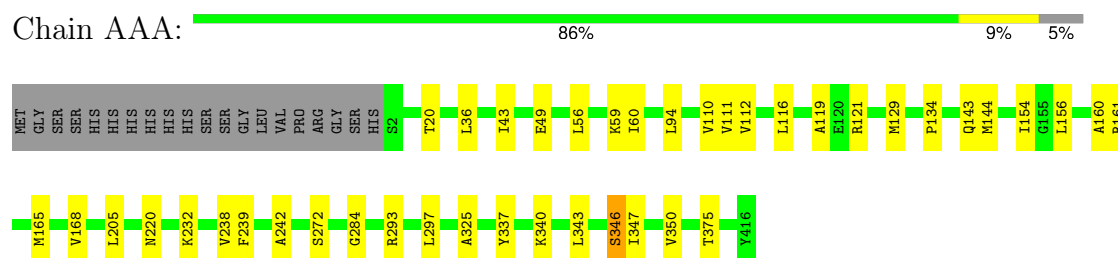
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	EEE	76	Total 76	O 76	0	0
5	FFF	109	Total 109	O 109	0	0
5	GGG	85	Total 85	O 85	0	0
5	HHH	104	Total 104	O 104	0	0

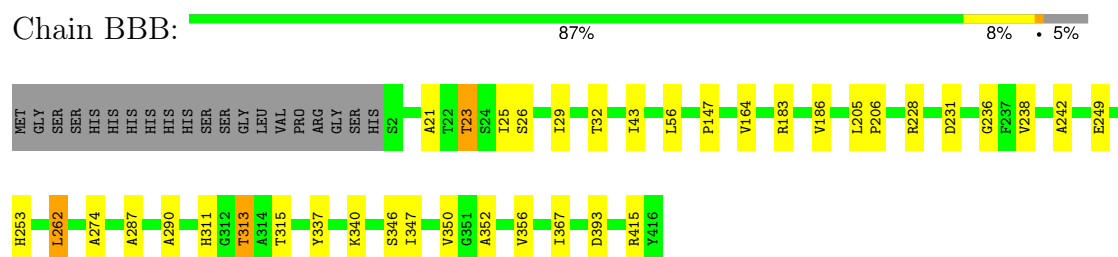
3 Residue-property plots [i](#)

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 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.

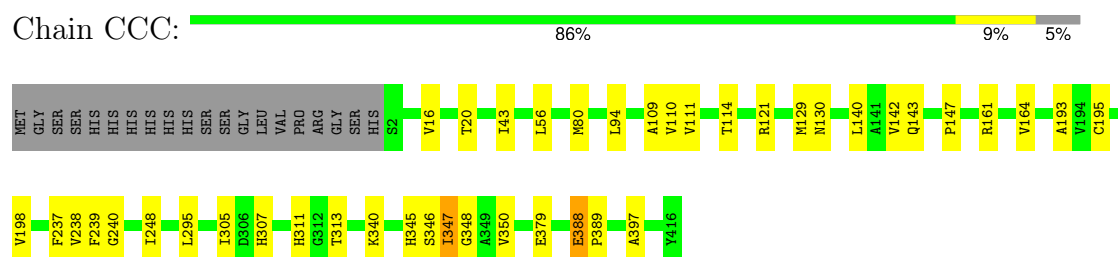
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 1



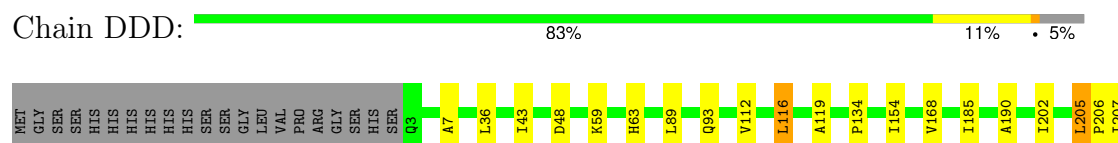
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 1

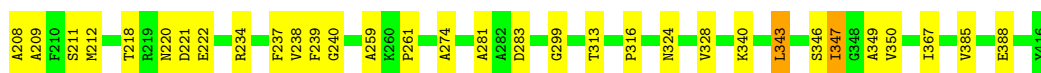


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 1

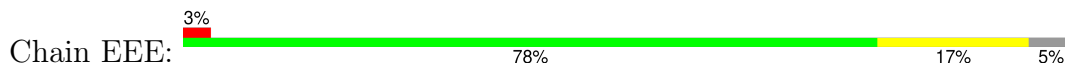


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 1

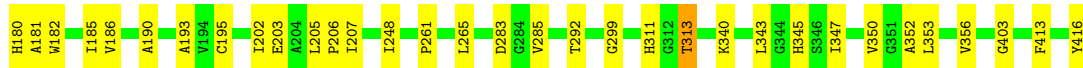
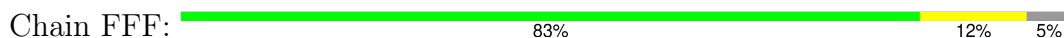




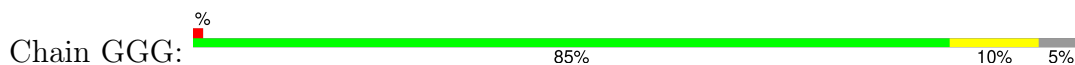
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 1



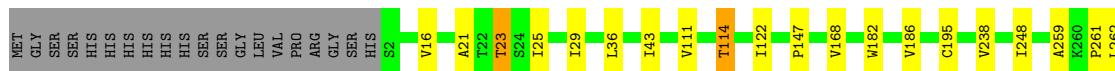
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 1



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 1



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	151.24Å 151.24Å 147.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	130.98 – 2.89 130.98 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.3 (130.98-2.89) 99.7 (130.98-2.89)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.116 , 0.166 0.126 , 0.169	Depositor DCC
R_{free} test set	4375 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l 0.025 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
Reported twinning fraction	0.612 for H, K, L 0.389 for K, H, -L	Depositor
Outliers	0 of 84863 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25455	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, O6W, PG4

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	AAA	0.64	0/3100	0.71	0/4212
1	BBB	0.63	0/3100	0.69	0/4212
1	CCC	0.64	0/3100	0.70	0/4212
1	DDD	0.64	0/3084	0.70	0/4192
1	EEE	0.66	0/3089	0.71	0/4197
1	FFF	0.65	0/3089	0.71	0/4197
1	GGG	0.65	0/3089	0.70	0/4197
1	HHH	0.64	0/3111	0.70	0/4226
All	All	0.64	0/24762	0.70	0/33645

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3039	0	2988	30	0
1	BBB	3039	0	2988	26	0
1	CCC	3039	0	2988	29	0
1	DDD	3023	0	2966	35	0
1	EEE	3029	0	2982	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FFF	3029	0	2982	32	0
1	GGG	3029	0	2982	28	0
1	HHH	3050	0	3000	27	0
2	AAA	13	0	18	2	0
2	BBB	13	0	18	0	0
2	CCC	13	0	18	0	0
2	DDD	13	0	18	2	0
2	EEE	13	0	18	0	0
2	FFF	13	0	18	0	0
2	GGG	13	0	18	0	0
2	HHH	13	0	18	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	1	0	0	0	0
3	EEE	1	0	0	0	0
3	FFF	1	0	0	0	0
3	GGG	1	0	0	0	0
3	HHH	1	0	0	0	0
4	AAA	21	0	0	0	0
4	BBB	21	0	0	0	0
4	CCC	21	0	0	0	0
4	DDD	21	0	0	0	0
4	EEE	21	0	0	1	0
4	FFF	21	0	0	0	0
4	GGG	21	0	0	1	0
4	HHH	21	0	0	0	0
5	AAA	139	0	0	1	0
5	BBB	160	0	0	0	0
5	CCC	110	0	0	2	0
5	DDD	115	0	0	0	0
5	EEE	76	0	0	2	0
5	FFF	109	0	0	0	0
5	GGG	85	0	0	5	0
5	HHH	104	0	0	1	0
All	All	25455	0	24020	238	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 5.

The worst 5 of 238 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:23:THR:HG22	1:FFF:26:SER:H	1.37	0.87
1:BBB:23:THR:HG22	1:BBB:26:SER:H	1.43	0.82
1:EEE:86:MET:HE3	1:EEE:243:GLY:HA3	1.60	0.82
1:EEE:86:MET:HE3	1:EEE:243:GLY:CA	2.12	0.79
1:CCC:20:THR:HG22	1:CCC:94:LEU:HD13	1.62	0.79

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	AAA	414/435 (95%)	400 (97%)	13 (3%)	1 (0%)	47	76
1	BBB	414/435 (95%)	401 (97%)	12 (3%)	1 (0%)	47	76
1	CCC	414/435 (95%)	397 (96%)	16 (4%)	1 (0%)	47	76
1	DDD	413/435 (95%)	397 (96%)	15 (4%)	1 (0%)	47	76
1	EEE	413/435 (95%)	394 (95%)	18 (4%)	1 (0%)	47	76
1	FFF	413/435 (95%)	396 (96%)	16 (4%)	1 (0%)	47	76
1	GGG	413/435 (95%)	397 (96%)	15 (4%)	1 (0%)	47	76
1	HHH	415/435 (95%)	404 (97%)	10 (2%)	1 (0%)	47	76
All	All	3309/3480 (95%)	3186 (96%)	115 (4%)	8 (0%)	47	76

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	EEE	347	ILE
1	HHH	347	ILE
1	DDD	347	ILE
1	AAA	347	ILE
1	BBB	347	ILE

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	AAA	308/324 (95%)	304 (99%)	4 (1%)	69	88
1	BBB	308/324 (95%)	305 (99%)	3 (1%)	76	91
1	CCC	308/324 (95%)	304 (99%)	4 (1%)	69	88
1	DDD	305/324 (94%)	300 (98%)	5 (2%)	62	85
1	EEE	307/324 (95%)	301 (98%)	6 (2%)	55	81
1	FFF	307/324 (95%)	301 (98%)	6 (2%)	55	81
1	GGG	307/324 (95%)	301 (98%)	6 (2%)	55	81
1	HHH	309/324 (95%)	305 (99%)	4 (1%)	69	88
All	All	2459/2592 (95%)	2421 (98%)	38 (2%)	65	86

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	GGG	48	ASP
1	HHH	114	THR
1	GGG	120	GLU
1	GGG	315	THR
1	HHH	346	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PG4	EEE	901	-	12,12,12	0.28	0	11,11,11	0.18	0
2	PG4	CCC	901	-	12,12,12	0.28	0	11,11,11	0.13	0
2	PG4	GGG	901	-	12,12,12	0.28	0	11,11,11	0.15	0
2	PG4	DDD	901	-	12,12,12	0.25	0	11,11,11	0.12	0
4	O6W	AAA	903	-	22,22,22	0.32	0	31,32,32	0.90	1 (3%)
4	O6W	BBB	903	-	22,22,22	0.35	0	31,32,32	0.51	0
4	O6W	HHH	903	-	22,22,22	0.37	0	31,32,32	0.73	1 (3%)
2	PG4	HHH	901	-	12,12,12	0.37	0	11,11,11	0.23	0
2	PG4	BBB	901	-	12,12,12	0.35	0	11,11,11	0.19	0
4	O6W	FFF	903	-	22,22,22	0.45	0	31,32,32	0.47	0
2	PG4	AAA	901	-	12,12,12	0.27	0	11,11,11	0.16	0
2	PG4	FFF	901	-	12,12,12	0.27	0	11,11,11	0.12	0
4	O6W	DDD	903	-	22,22,22	0.34	0	31,32,32	0.56	1 (3%)
4	O6W	CCC	903	-	22,22,22	0.35	0	31,32,32	0.68	1 (3%)
4	O6W	EEE	903	-	22,22,22	0.35	0	31,32,32	0.44	0
4	O6W	GGG	903	-	22,22,22	0.33	0	31,32,32	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	EEE	901	-	-	4/10/10/10	-
2	PG4	CCC	901	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	GGG	901	-	-	5/10/10/10	-
2	PG4	DDD	901	-	-	6/10/10/10	-
4	O6W	AAA	903	-	-	5/13/13/13	0/2/2/2
4	O6W	BBB	903	-	-	3/13/13/13	0/2/2/2
4	O6W	HHH	903	-	-	0/13/13/13	0/2/2/2
2	PG4	HHH	901	-	-	5/10/10/10	-
2	PG4	BBB	901	-	-	6/10/10/10	-
4	O6W	FFF	903	-	-	8/13/13/13	0/2/2/2
2	PG4	AAA	901	-	-	6/10/10/10	-
2	PG4	FFF	901	-	-	6/10/10/10	-
4	O6W	DDD	903	-	-	3/13/13/13	0/2/2/2
4	O6W	CCC	903	-	-	5/13/13/13	0/2/2/2
4	O6W	EEE	903	-	-	7/13/13/13	0/2/2/2
4	O6W	GGG	903	-	-	9/13/13/13	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	903	O6W	C11-S14-N17	4.22	112.71	106.72
4	HHH	903	O6W	C11-S14-N17	3.31	111.42	106.72
4	CCC	903	O6W	C11-S14-N17	2.97	110.93	106.72
4	DDD	903	O6W	C08-C11-S14	-2.19	108.39	113.74

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

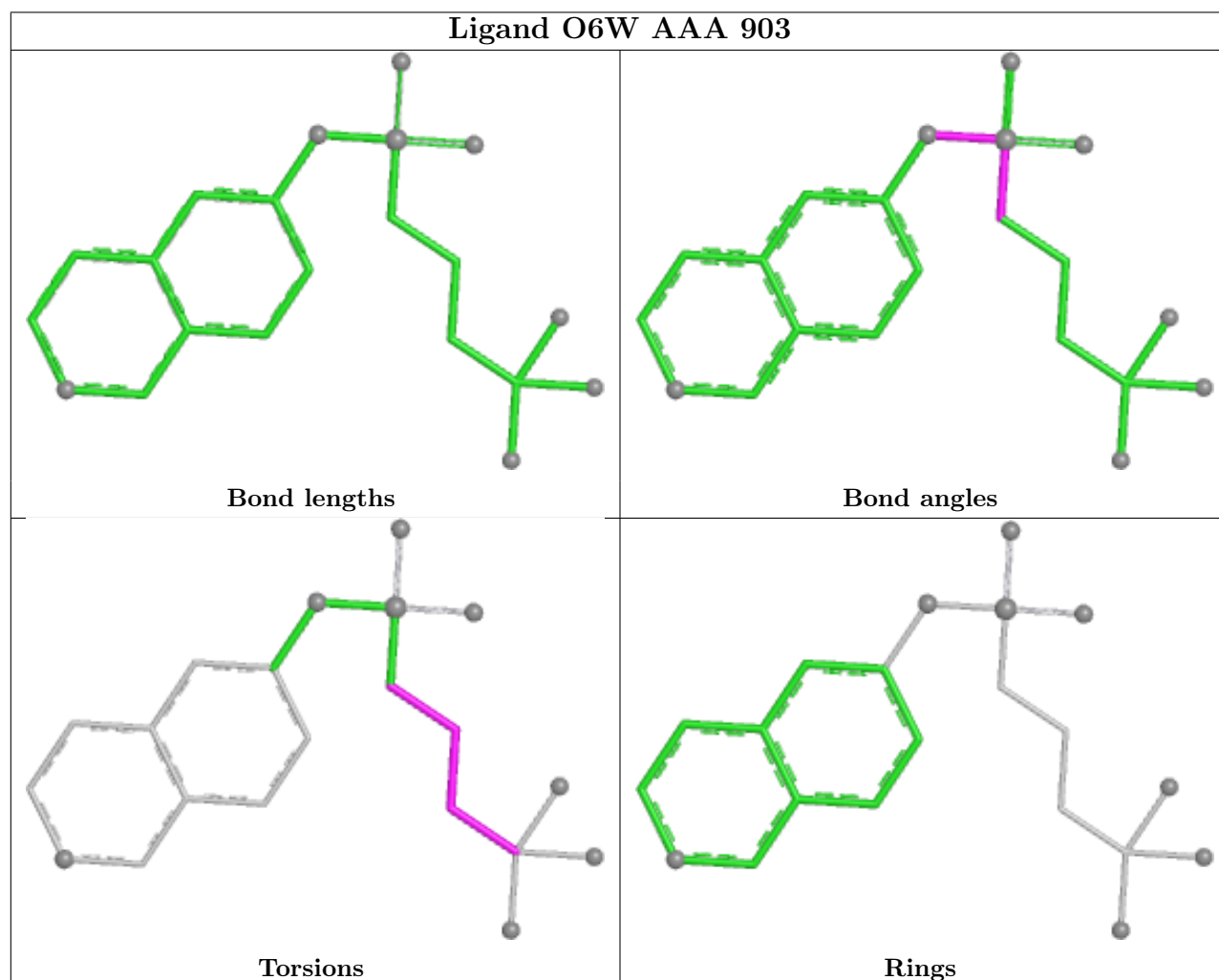
Mol	Chain	Res	Type	Atoms
4	CCC	903	O6W	C05-C08-C11-S14
4	DDD	903	O6W	C02-C05-C08-C11
4	DDD	903	O6W	C08-C11-S14-O15
4	DDD	903	O6W	C08-C11-S14-N17
4	EEE	903	O6W	C08-C11-S14-O15

There are no ring outliers.

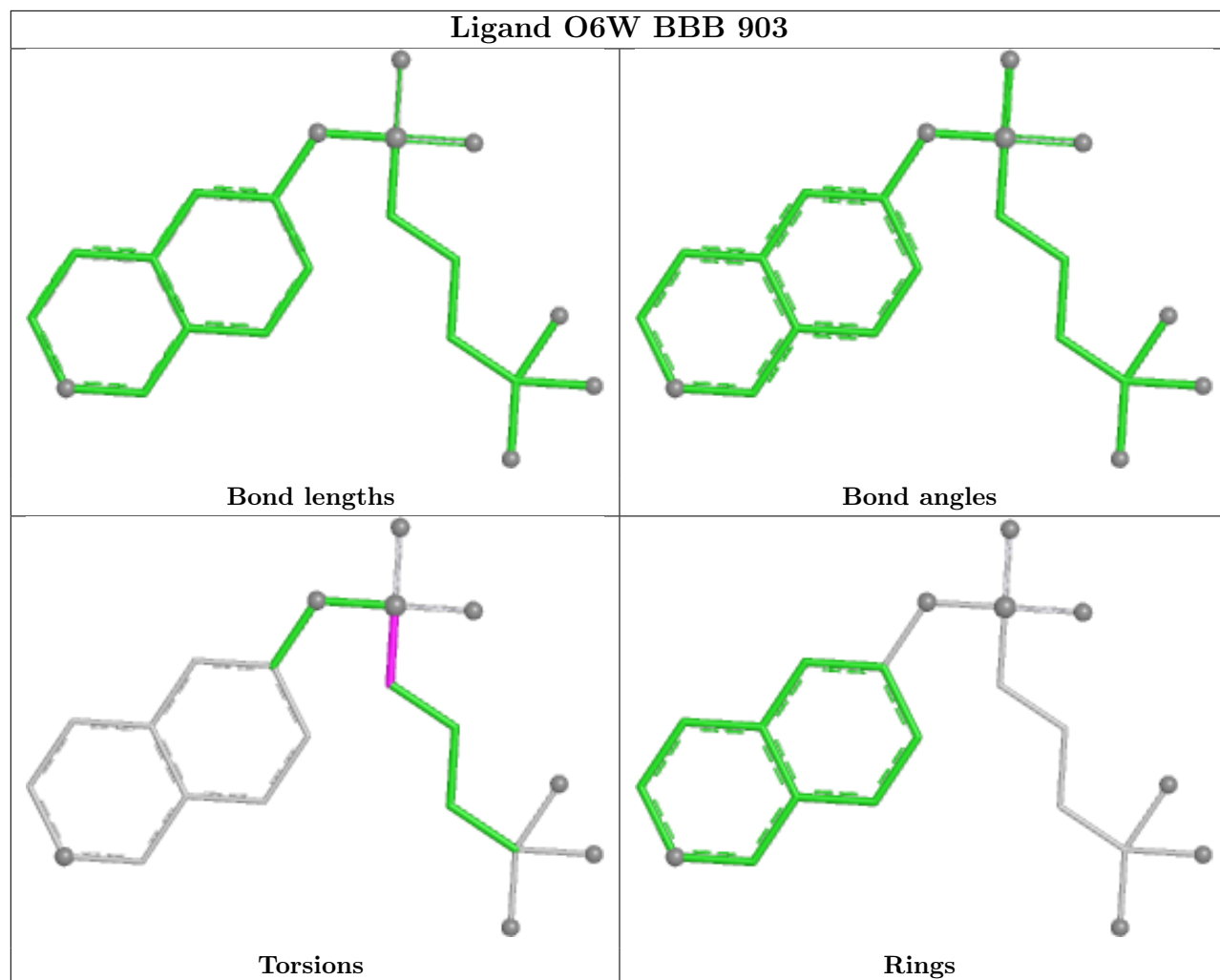
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DDD	901	PG4	2	0
2	AAA	901	PG4	2	0
4	EEE	903	O6W	1	0
4	GGG	903	O6W	1	0

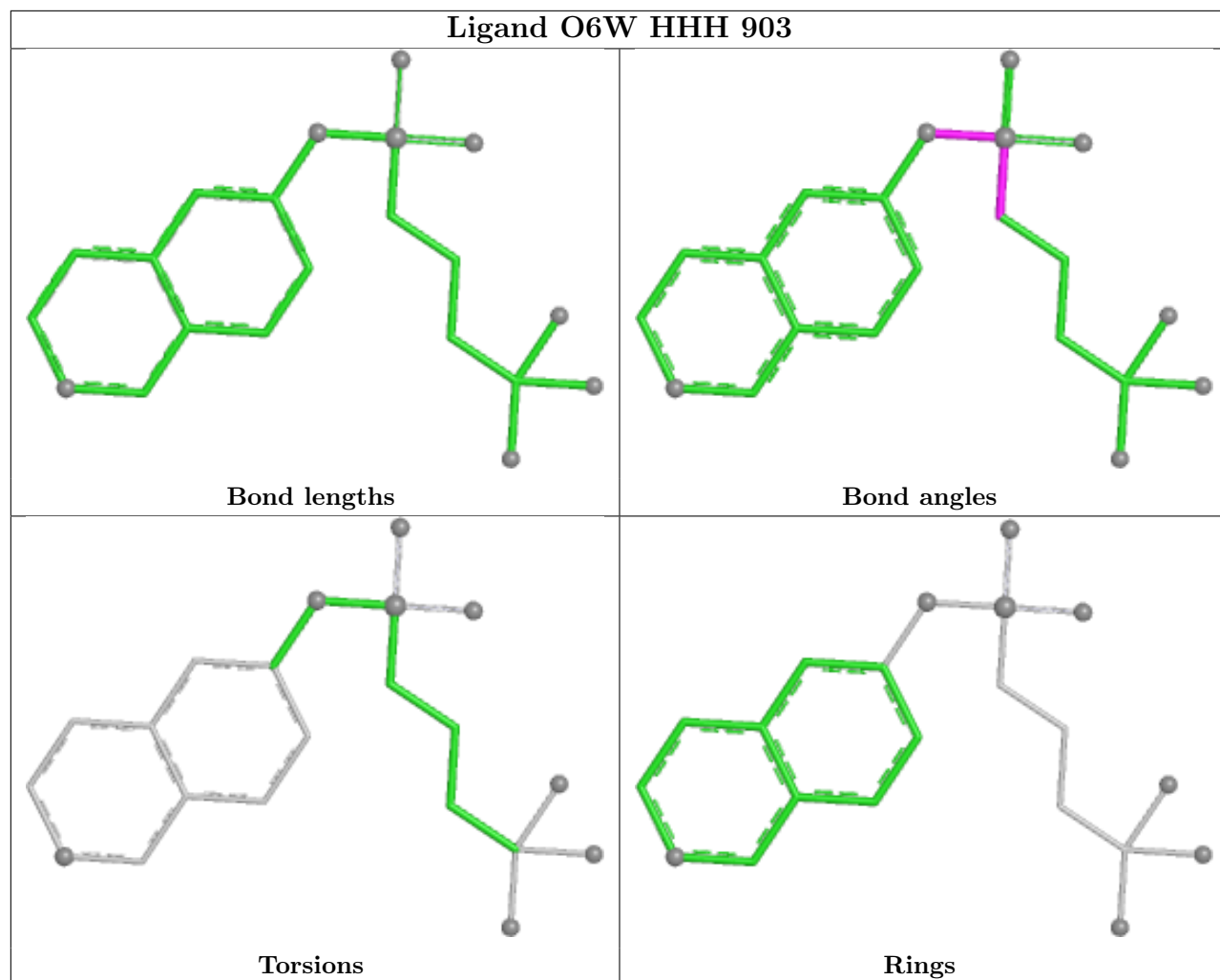
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



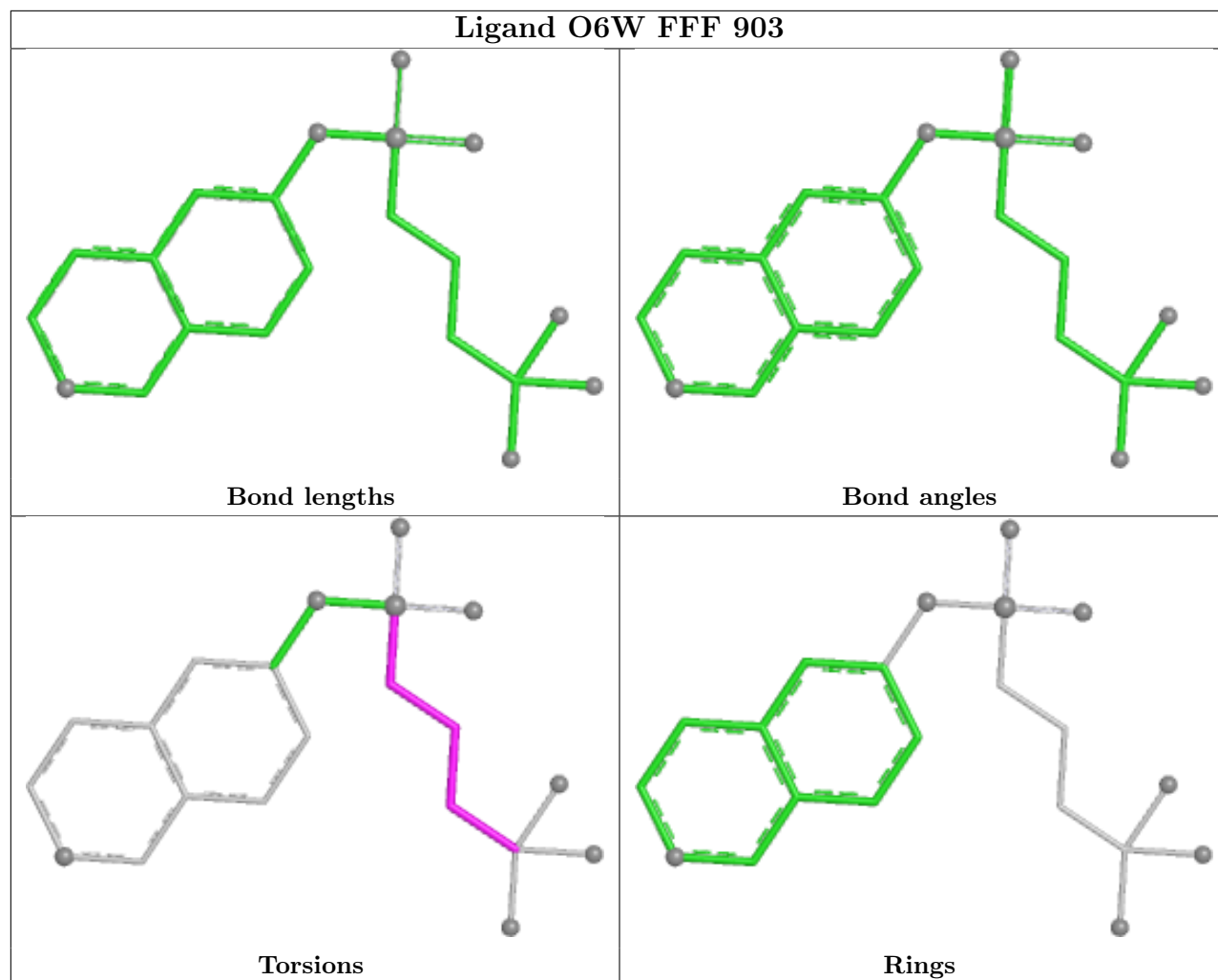
Ligand O6W BBB 903



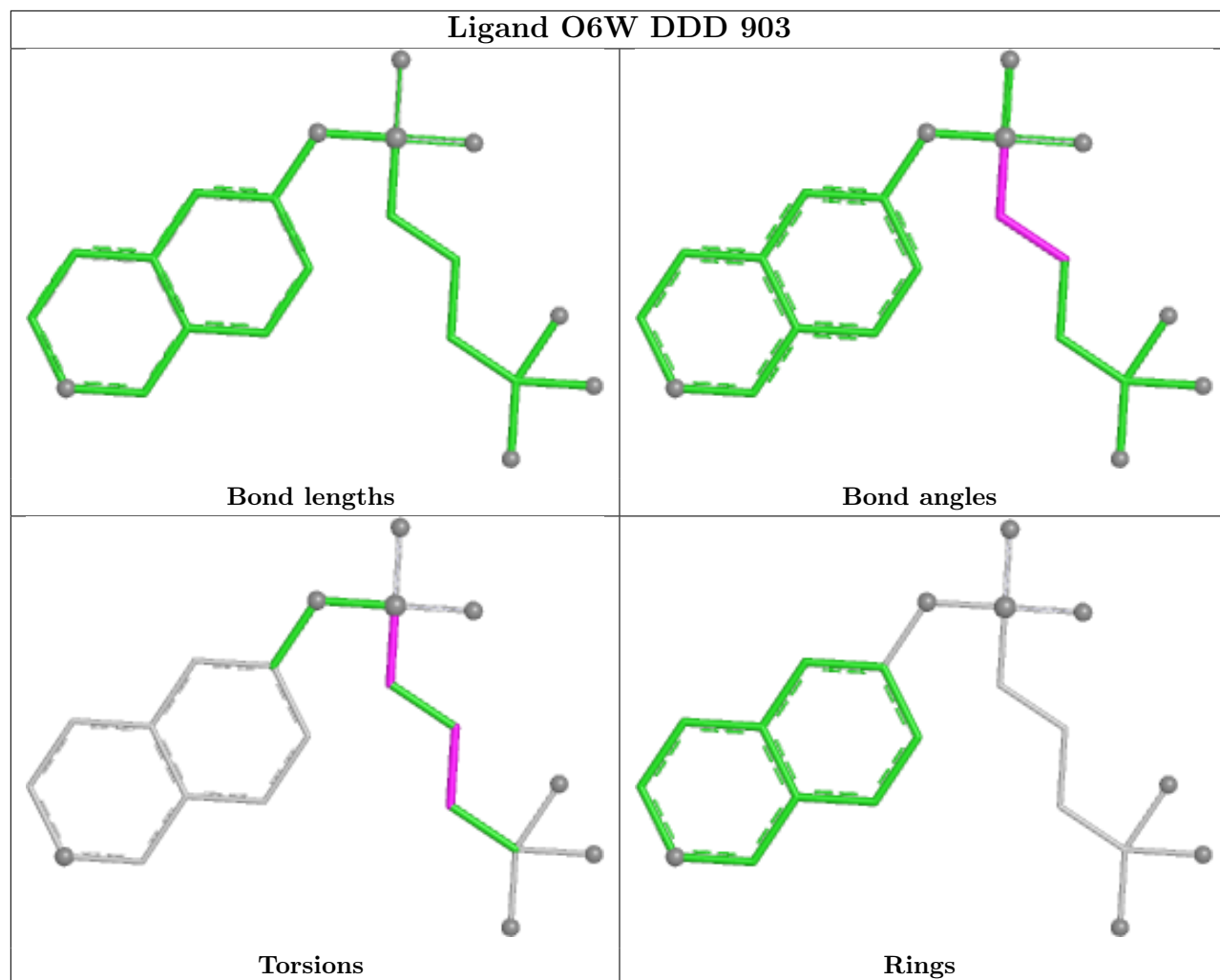
Ligand O6W HHH 903



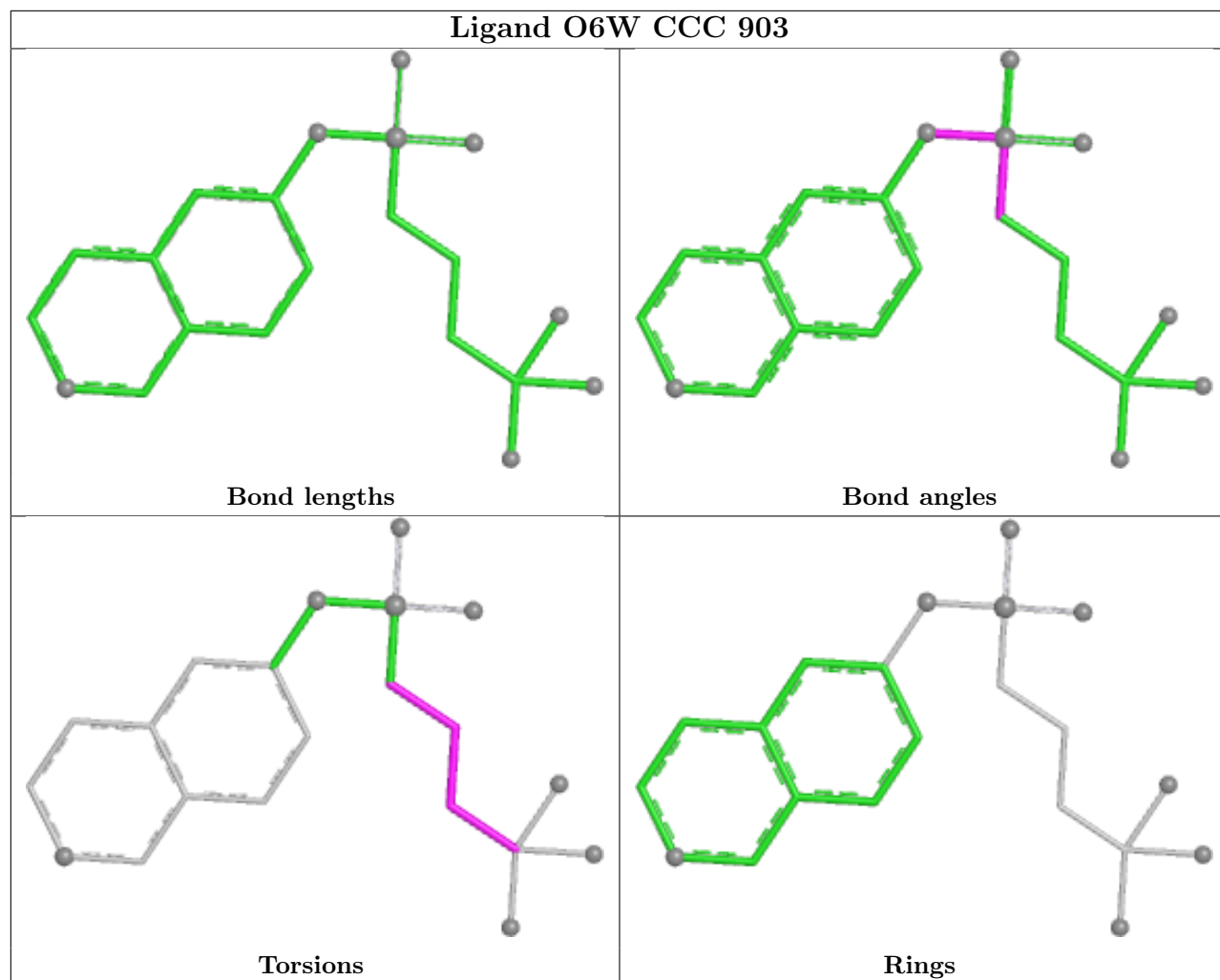
Ligand O6W FFF 903



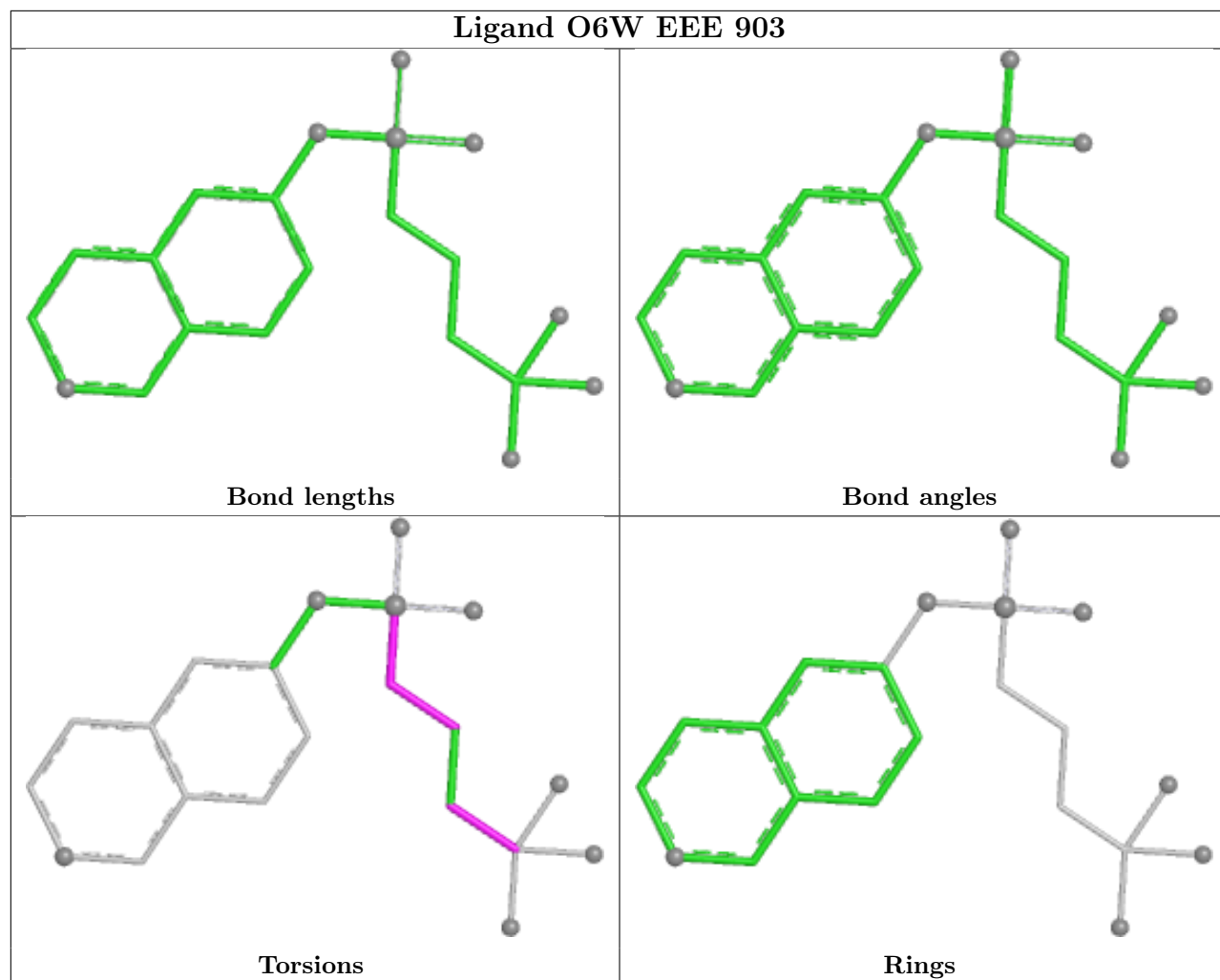
Ligand O6W DDD 903

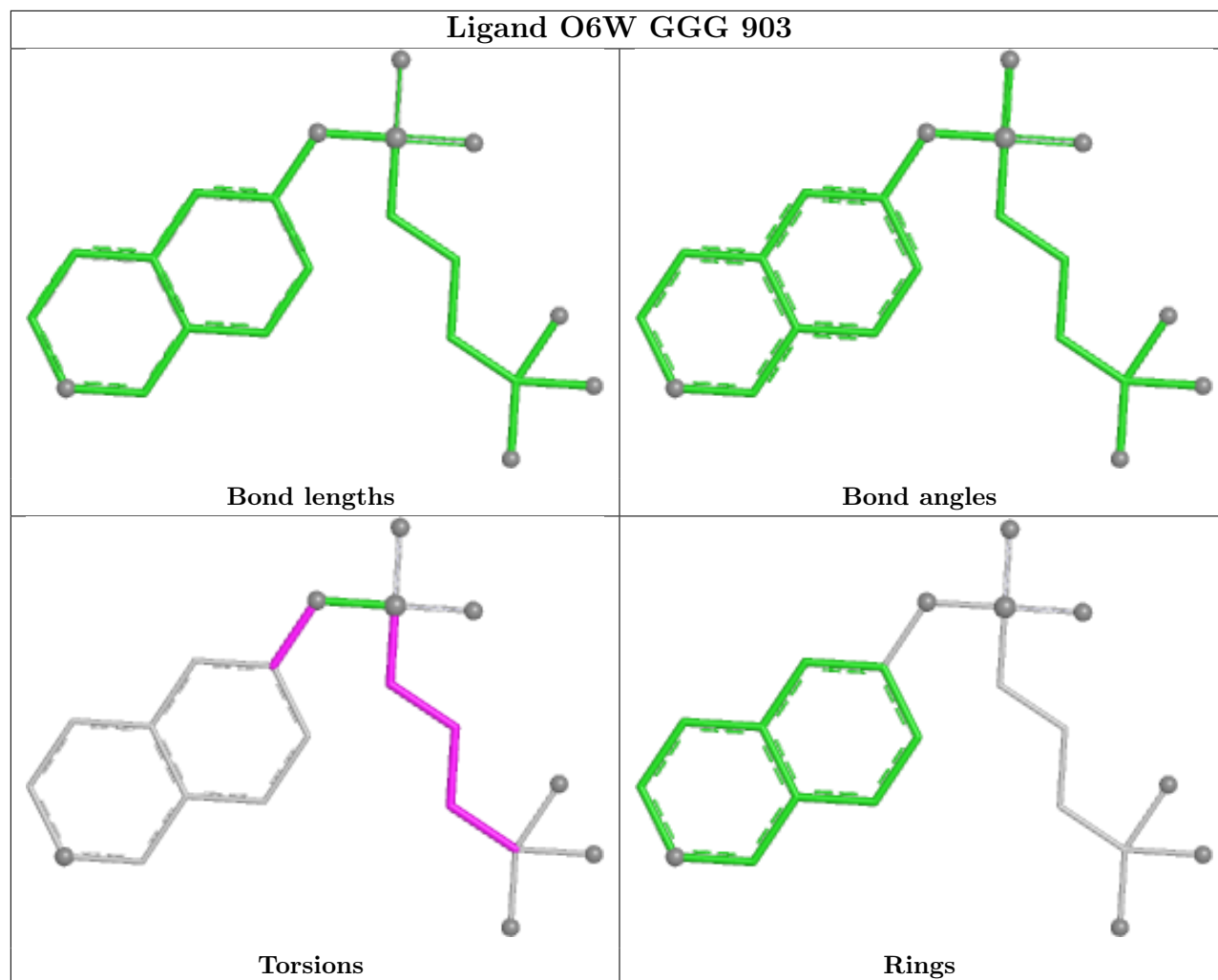


Ligand O6W CCC 903



Ligand O6W EEE 903





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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	AAA	415/435 (95%)	-0.12	0 100 100	32, 46, 68, 116	0
1	BBB	415/435 (95%)	-0.18	0 100 100	27, 40, 60, 93	0
1	CCC	415/435 (95%)	-0.12	0 100 100	36, 50, 80, 115	0
1	DDD	414/435 (95%)	-0.06	0 100 100	35, 52, 87, 118	0
1	EEE	415/435 (95%)	0.21	13 (3%) 49 45	49, 69, 92, 121	0
1	FFF	415/435 (95%)	-0.08	1 (0%) 95 95	35, 54, 79, 116	0
1	GGG	415/435 (95%)	0.06	5 (1%) 79 78	42, 63, 83, 116	0
1	HHH	415/435 (95%)	-0.08	0 100 100	35, 53, 69, 102	0
All	All	3319/3480 (95%)	-0.05	19 (0%) 89 89	27, 53, 82, 121	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	2	SER	3.9
1	EEE	397	ALA	3.1
1	GGG	230	PHE	2.8
1	EEE	366	VAL	2.8
1	EEE	367	ILE	2.8

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 monosaccharides in this entry.

6.4 Ligands ⓘ

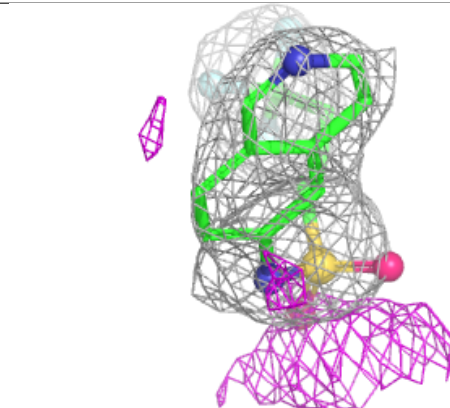
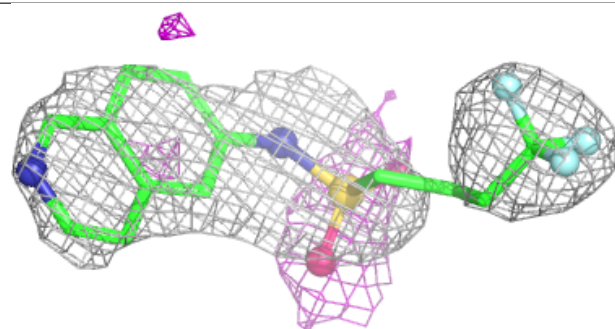
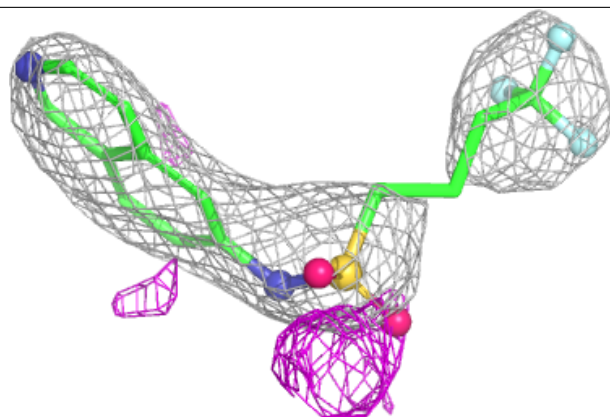
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PG4	DDD	901	13/13	0.80	0.94	94,116,130,134	0
3	NA	GGG	902	1/1	0.86	0.12	73,73,73,73	0
2	PG4	CCC	901	13/13	0.91	0.43	55,70,88,89	0
2	PG4	EEE	901	13/13	0.94	0.39	61,63,68,70	0
2	PG4	FFF	901	13/13	0.96	0.35	56,72,82,82	0
2	PG4	HHH	901	13/13	0.97	0.29	50,53,62,62	0
3	NA	AAA	902	1/1	0.97	0.07	37,37,37,37	0
3	NA	DDD	902	1/1	0.97	0.08	35,35,35,35	0
2	PG4	AAA	901	13/13	0.97	0.28	50,52,64,64	0
4	O6W	DDD	903	21/21	0.97	0.42	74,87,118,125	0
2	PG4	BBB	901	13/13	0.98	0.31	45,53,60,62	0
3	NA	EEE	902	1/1	0.98	0.23	54,54,54,54	0
3	NA	FFF	902	1/1	0.98	0.14	48,48,48,48	0
2	PG4	GGG	901	13/13	0.98	0.45	60,72,81,82	0
4	O6W	AAA	903	21/21	0.98	0.21	48,51,56,63	0
4	O6W	BBB	903	21/21	0.98	0.26	49,53,58,69	0
4	O6W	CCC	903	21/21	0.98	0.28	65,74,89,90	0
3	NA	BBB	902	1/1	0.98	0.06	30,30,30,30	0
4	O6W	EEE	903	21/21	0.98	0.24	55,62,79,82	0
4	O6W	FFF	903	21/21	0.98	0.24	67,70,77,78	0
4	O6W	GGG	903	21/21	0.98	0.21	62,68,86,90	0
4	O6W	HHH	903	21/21	0.98	0.27	54,57,70,79	0
3	NA	CCC	902	1/1	0.99	0.08	35,35,35,35	0
3	NA	HHH	902	1/1	0.99	0.07	43,43,43,43	0

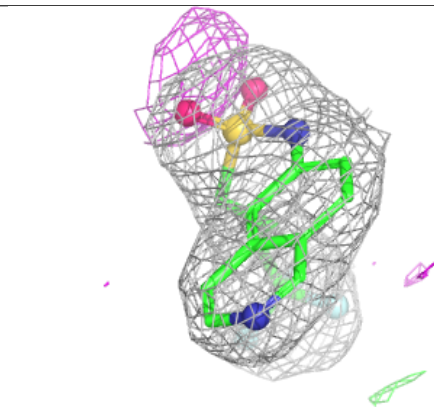
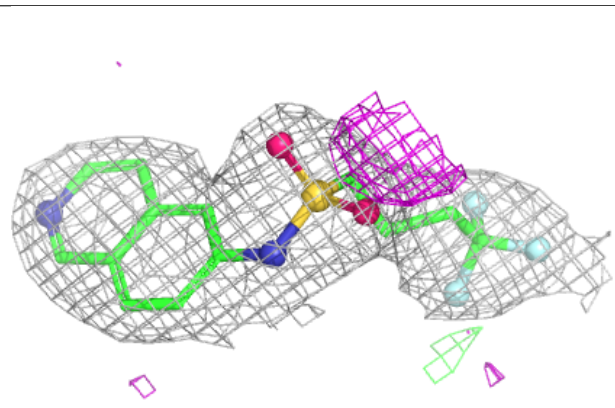
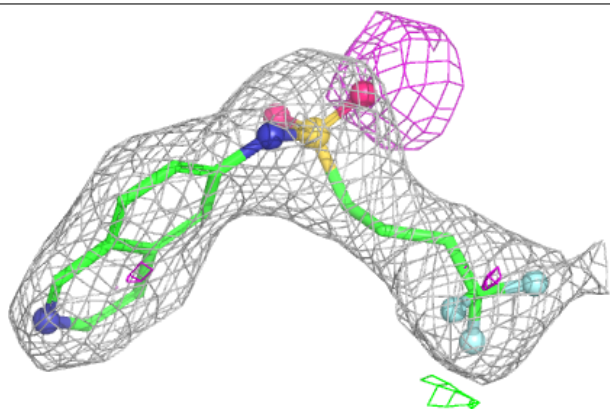
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around O6W DDD 903:

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

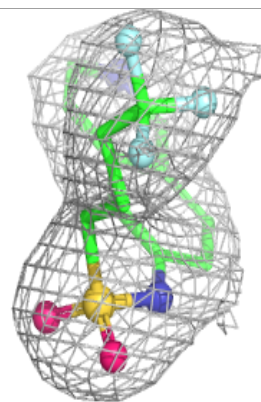
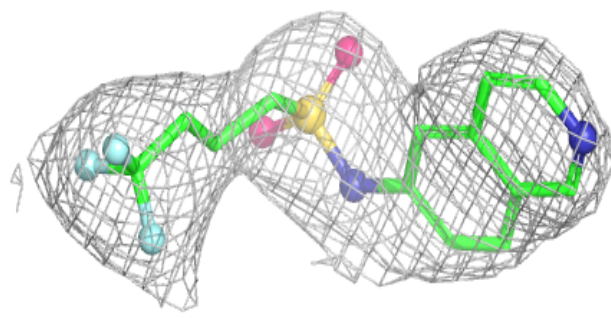
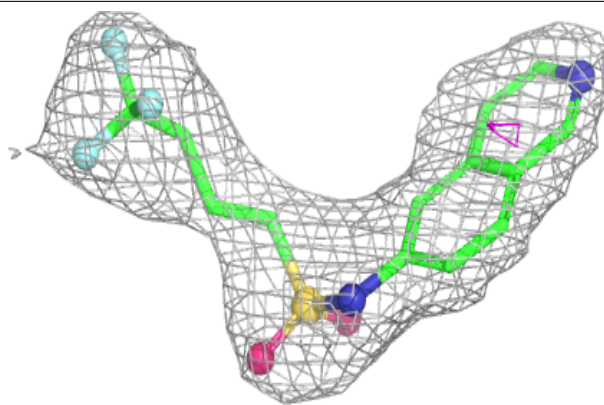
**Electron density around O6W AAA 903:**

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

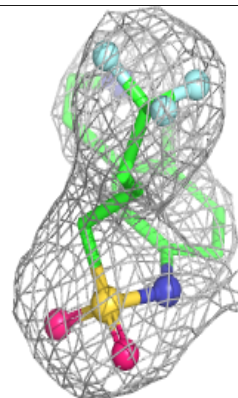
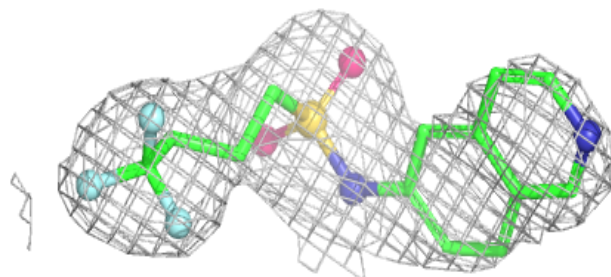
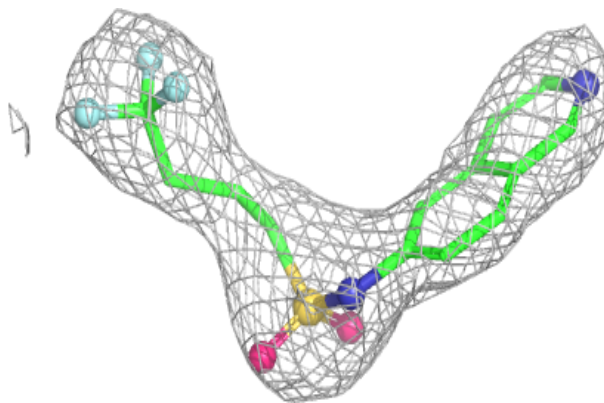


Electron density around O6W BBB 903:

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

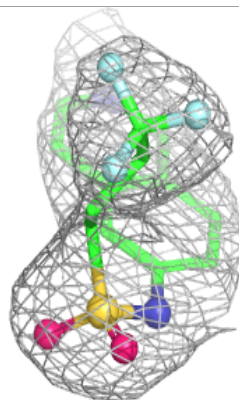
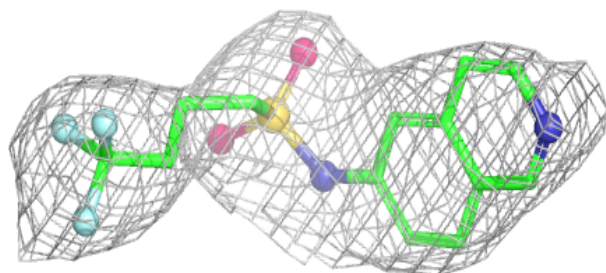
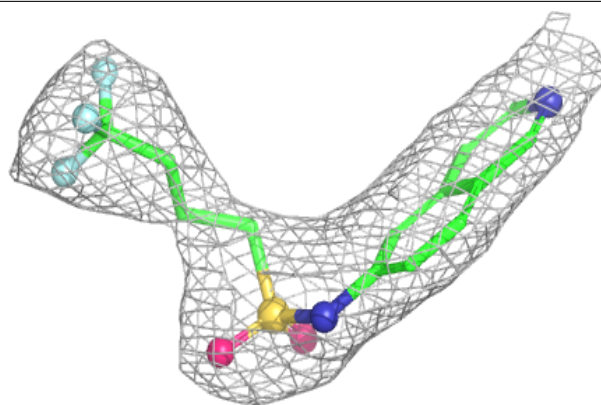
**Electron density around O6W CCC 903:**

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

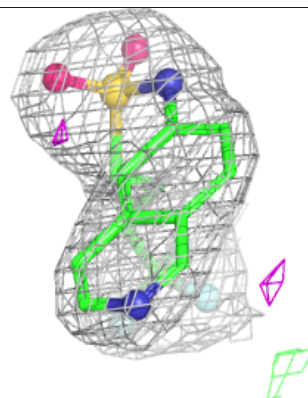
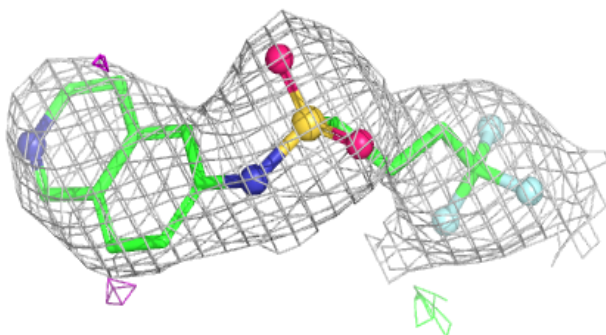
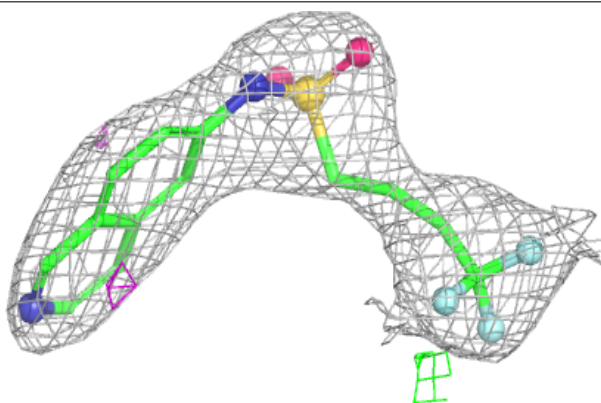


Electron density around O6W EEE 903:

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

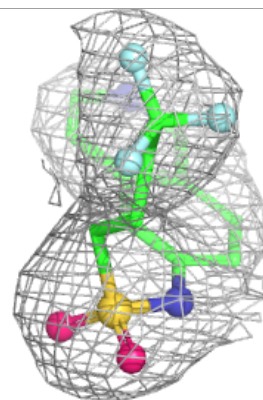
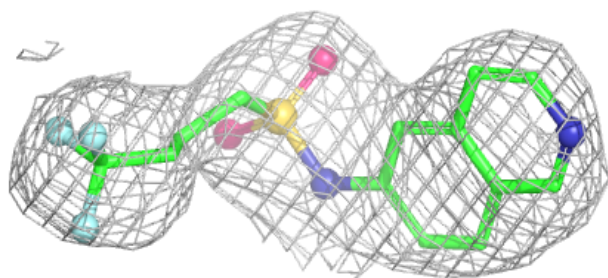
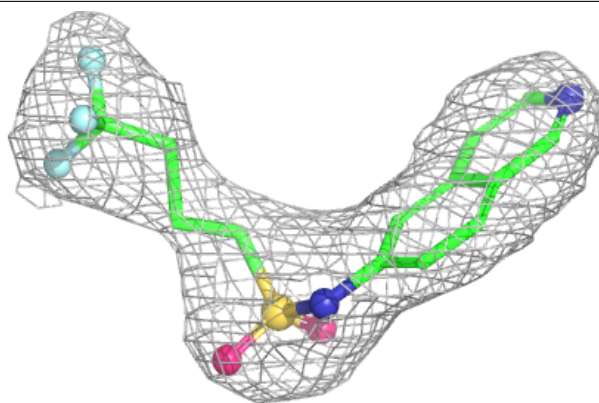
**Electron density around O6W FFF 903:**

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

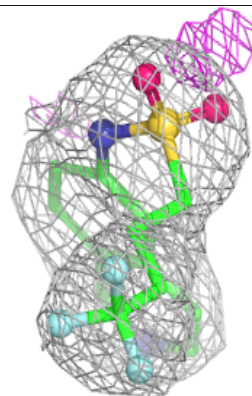
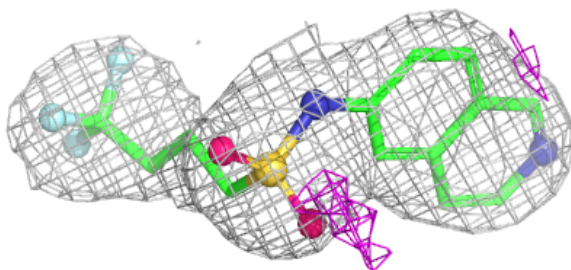
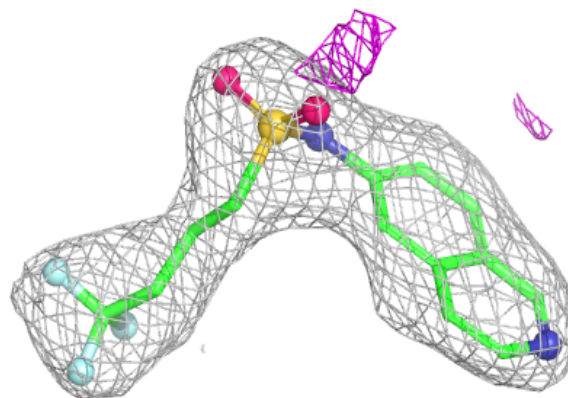


Electron density around O6W GGG 903:

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

**Electron density around O6W HHH 903:**

$2mF_o-DF_c$ (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.