WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2024 – 07:11 pm GMT

PDB ID	:	6T75
Title	:	Bacteroides salyersiae GH164 beta-mannosidase 2-deoxy-2-fluoro-beta-D-mannosyl enzyme intermediate
Authors	:	Armstrong, Z.; Davies, G.
Deposited on	:	2019-10-21
Resolution	:	2.55 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:

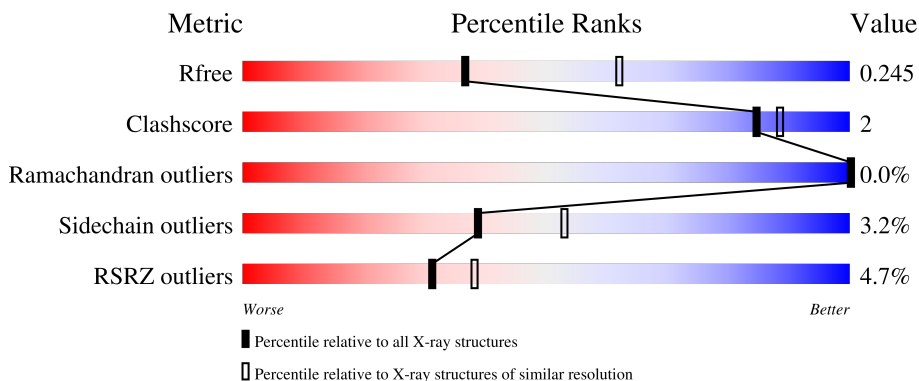|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.55 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.
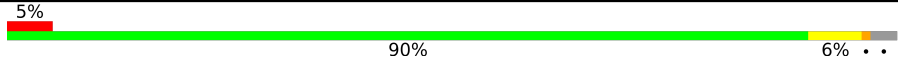
Metric	Percentile Ranks	Value
Rfree		0.245
Clashscore		2
Ramachandran outliers		0.0%
Sidechain outliers		3.2%
RSRZ outliers		4.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	674	2% / 90% / 7% ·
1	BBB	674	3% / 89% / 7% ·
1	CCC	674	5% / 87% / 9% · ·
1	DDD	674	5% / 88% / 8% ·
1	EEE	674	8% / 86% / 9% / 5%

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Mol	Chain	Length	Quality of chain
1	FFF	674	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 62440 atoms, of which 30823 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 Glyco_hydro_42M domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	657	Total	C	H	N	O	S	285	0	0
			10469	3416	5181	874	979	19			
1	DDD	652	Total	C	H	N	O	S	283	0	0
			10391	3392	5146	867	967	19			
1	CCC	649	Total	C	H	N	O	S	282	0	0
			10351	3376	5123	865	968	19			
1	BBB	648	Total	C	H	N	O	S	283	0	0
			10330	3371	5112	861	967	19			
1	FFF	652	Total	C	H	N	O	S	283	0	0
			10382	3386	5138	868	971	19			
1	EEE	642	Total	C	H	N	O	S	278	0	0
			10228	3338	5063	852	956	19			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	10	MET	-	initiating methionine	UNP I9SUA3
AAA	11	GLY	-	expression tag	UNP I9SUA3
AAA	12	SER	-	expression tag	UNP I9SUA3
AAA	13	SER	-	expression tag	UNP I9SUA3
AAA	14	HIS	-	expression tag	UNP I9SUA3
AAA	15	HIS	-	expression tag	UNP I9SUA3
AAA	16	HIS	-	expression tag	UNP I9SUA3
AAA	17	HIS	-	expression tag	UNP I9SUA3
AAA	18	HIS	-	expression tag	UNP I9SUA3
AAA	19	HIS	-	expression tag	UNP I9SUA3
AAA	20	SER	-	expression tag	UNP I9SUA3
AAA	21	SER	-	expression tag	UNP I9SUA3
AAA	22	GLY	-	expression tag	UNP I9SUA3
AAA	23	LEU	-	expression tag	UNP I9SUA3
AAA	24	GLU	-	expression tag	UNP I9SUA3
AAA	25	VAL	-	expression tag	UNP I9SUA3
AAA	26	LEU	-	expression tag	UNP I9SUA3

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	27	PHE	-	expression tag	UNP I9SUA3
AAA	28	GLN	-	expression tag	UNP I9SUA3
AAA	29	GLY	-	expression tag	UNP I9SUA3
AAA	30	PRO	-	expression tag	UNP I9SUA3
AAA	31	ALA	-	expression tag	UNP I9SUA3
DDD	10	MET	-	initiating methionine	UNP I9SUA3
DDD	11	GLY	-	expression tag	UNP I9SUA3
DDD	12	SER	-	expression tag	UNP I9SUA3
DDD	13	SER	-	expression tag	UNP I9SUA3
DDD	14	HIS	-	expression tag	UNP I9SUA3
DDD	15	HIS	-	expression tag	UNP I9SUA3
DDD	16	HIS	-	expression tag	UNP I9SUA3
DDD	17	HIS	-	expression tag	UNP I9SUA3
DDD	18	HIS	-	expression tag	UNP I9SUA3
DDD	19	HIS	-	expression tag	UNP I9SUA3
DDD	20	SER	-	expression tag	UNP I9SUA3
DDD	21	SER	-	expression tag	UNP I9SUA3
DDD	22	GLY	-	expression tag	UNP I9SUA3
DDD	23	LEU	-	expression tag	UNP I9SUA3
DDD	24	GLU	-	expression tag	UNP I9SUA3
DDD	25	VAL	-	expression tag	UNP I9SUA3
DDD	26	LEU	-	expression tag	UNP I9SUA3
DDD	27	PHE	-	expression tag	UNP I9SUA3
DDD	28	GLN	-	expression tag	UNP I9SUA3
DDD	29	GLY	-	expression tag	UNP I9SUA3
DDD	30	PRO	-	expression tag	UNP I9SUA3
DDD	31	ALA	-	expression tag	UNP I9SUA3
CCC	10	MET	-	initiating methionine	UNP I9SUA3
CCC	11	GLY	-	expression tag	UNP I9SUA3
CCC	12	SER	-	expression tag	UNP I9SUA3
CCC	13	SER	-	expression tag	UNP I9SUA3
CCC	14	HIS	-	expression tag	UNP I9SUA3
CCC	15	HIS	-	expression tag	UNP I9SUA3
CCC	16	HIS	-	expression tag	UNP I9SUA3
CCC	17	HIS	-	expression tag	UNP I9SUA3
CCC	18	HIS	-	expression tag	UNP I9SUA3
CCC	19	HIS	-	expression tag	UNP I9SUA3
CCC	20	SER	-	expression tag	UNP I9SUA3
CCC	21	SER	-	expression tag	UNP I9SUA3
CCC	22	GLY	-	expression tag	UNP I9SUA3
CCC	23	LEU	-	expression tag	UNP I9SUA3
CCC	24	GLU	-	expression tag	UNP I9SUA3

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	25	VAL	-	expression tag	UNP I9SUA3
CCC	26	LEU	-	expression tag	UNP I9SUA3
CCC	27	PHE	-	expression tag	UNP I9SUA3
CCC	28	GLN	-	expression tag	UNP I9SUA3
CCC	29	GLY	-	expression tag	UNP I9SUA3
CCC	30	PRO	-	expression tag	UNP I9SUA3
CCC	31	ALA	-	expression tag	UNP I9SUA3
BBB	10	MET	-	initiating methionine	UNP I9SUA3
BBB	11	GLY	-	expression tag	UNP I9SUA3
BBB	12	SER	-	expression tag	UNP I9SUA3
BBB	13	SER	-	expression tag	UNP I9SUA3
BBB	14	HIS	-	expression tag	UNP I9SUA3
BBB	15	HIS	-	expression tag	UNP I9SUA3
BBB	16	HIS	-	expression tag	UNP I9SUA3
BBB	17	HIS	-	expression tag	UNP I9SUA3
BBB	18	HIS	-	expression tag	UNP I9SUA3
BBB	19	HIS	-	expression tag	UNP I9SUA3
BBB	20	SER	-	expression tag	UNP I9SUA3
BBB	21	SER	-	expression tag	UNP I9SUA3
BBB	22	GLY	-	expression tag	UNP I9SUA3
BBB	23	LEU	-	expression tag	UNP I9SUA3
BBB	24	GLU	-	expression tag	UNP I9SUA3
BBB	25	VAL	-	expression tag	UNP I9SUA3
BBB	26	LEU	-	expression tag	UNP I9SUA3
BBB	27	PHE	-	expression tag	UNP I9SUA3
BBB	28	GLN	-	expression tag	UNP I9SUA3
BBB	29	GLY	-	expression tag	UNP I9SUA3
BBB	30	PRO	-	expression tag	UNP I9SUA3
BBB	31	ALA	-	expression tag	UNP I9SUA3
FFF	10	MET	-	initiating methionine	UNP I9SUA3
FFF	11	GLY	-	expression tag	UNP I9SUA3
FFF	12	SER	-	expression tag	UNP I9SUA3
FFF	13	SER	-	expression tag	UNP I9SUA3
FFF	14	HIS	-	expression tag	UNP I9SUA3
FFF	15	HIS	-	expression tag	UNP I9SUA3
FFF	16	HIS	-	expression tag	UNP I9SUA3
FFF	17	HIS	-	expression tag	UNP I9SUA3
FFF	18	HIS	-	expression tag	UNP I9SUA3
FFF	19	HIS	-	expression tag	UNP I9SUA3
FFF	20	SER	-	expression tag	UNP I9SUA3
FFF	21	SER	-	expression tag	UNP I9SUA3
FFF	22	GLY	-	expression tag	UNP I9SUA3

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Chain	Residue	Modelled	Actual	Comment	Reference
FFF	23	LEU	-	expression tag	UNP I9SUA3
FFF	24	GLU	-	expression tag	UNP I9SUA3
FFF	25	VAL	-	expression tag	UNP I9SUA3
FFF	26	LEU	-	expression tag	UNP I9SUA3
FFF	27	PHE	-	expression tag	UNP I9SUA3
FFF	28	GLN	-	expression tag	UNP I9SUA3
FFF	29	GLY	-	expression tag	UNP I9SUA3
FFF	30	PRO	-	expression tag	UNP I9SUA3
FFF	31	ALA	-	expression tag	UNP I9SUA3
EEE	10	MET	-	initiating methionine	UNP I9SUA3
EEE	11	GLY	-	expression tag	UNP I9SUA3
EEE	12	SER	-	expression tag	UNP I9SUA3
EEE	13	SER	-	expression tag	UNP I9SUA3
EEE	14	HIS	-	expression tag	UNP I9SUA3
EEE	15	HIS	-	expression tag	UNP I9SUA3
EEE	16	HIS	-	expression tag	UNP I9SUA3
EEE	17	HIS	-	expression tag	UNP I9SUA3
EEE	18	HIS	-	expression tag	UNP I9SUA3
EEE	19	HIS	-	expression tag	UNP I9SUA3
EEE	20	SER	-	expression tag	UNP I9SUA3
EEE	21	SER	-	expression tag	UNP I9SUA3
EEE	22	GLY	-	expression tag	UNP I9SUA3
EEE	23	LEU	-	expression tag	UNP I9SUA3
EEE	24	GLU	-	expression tag	UNP I9SUA3
EEE	25	VAL	-	expression tag	UNP I9SUA3
EEE	26	LEU	-	expression tag	UNP I9SUA3
EEE	27	PHE	-	expression tag	UNP I9SUA3
EEE	28	GLN	-	expression tag	UNP I9SUA3
EEE	29	GLY	-	expression tag	UNP I9SUA3
EEE	30	PRO	-	expression tag	UNP I9SUA3
EEE	31	ALA	-	expression tag	UNP I9SUA3

- Molecule 2 is 2-deoxy-2-fluoro-alpha-D-mannopyranose (three-letter code: MAF) (formula: $C_6H_{11}FO_5$) (labeled as "Ligand of Interest" by depositor).

MAF
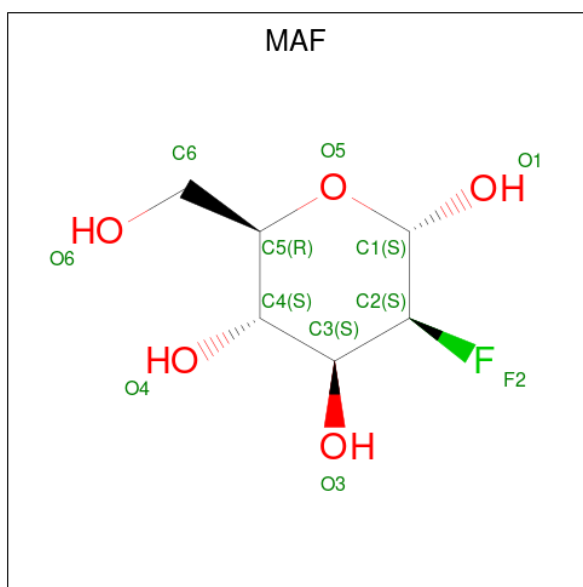
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	F	H	O	3	0
			21	6	1	10	4		
2	DDD	1	Total	C	F	H	O	3	0
			21	6	1	10	4		
2	CCC	1	Total	C	F	H	O	3	0
			21	6	1	10	4		
2	BBB	1	Total	C	F	H	O	3	0
			21	6	1	10	4		
2	FFF	1	Total	C	F	H	O	3	0
			21	6	1	10	4		
2	EEE	1	Total	C	F	H	O	3	0
			21	6	1	10	4		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	31	Total 31	O 31	0	0
4	DDD	13	Total 13	O 13	0	0
4	CCC	25	Total 25	O 25	0	0
4	BBB	37	Total 37	O 37	0	0
4	FFF	27	Total 27	O 27	0	0
4	EEE	24	Total 24	O 24	0	0

3   Residue-property plots ⓘ

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: Glyco_hydro_42M domain-containing protein
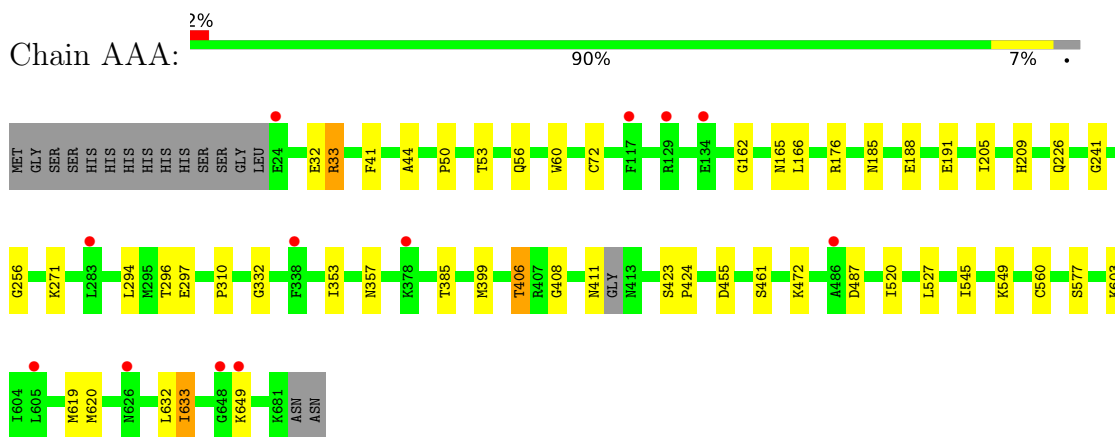
Chain AAA:

- Molecule 1: Glyco_hydro_42M domain-containing protein

Chain DDD:

- Molecule 1: Glyco_hydro_42M domain-containing protein

Chain CCC:
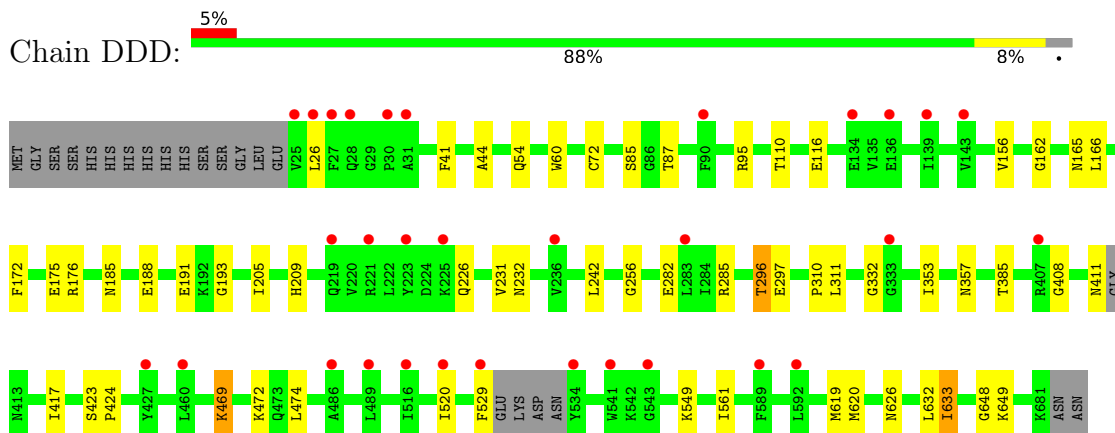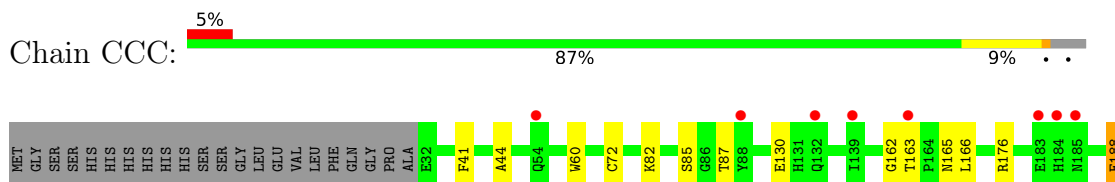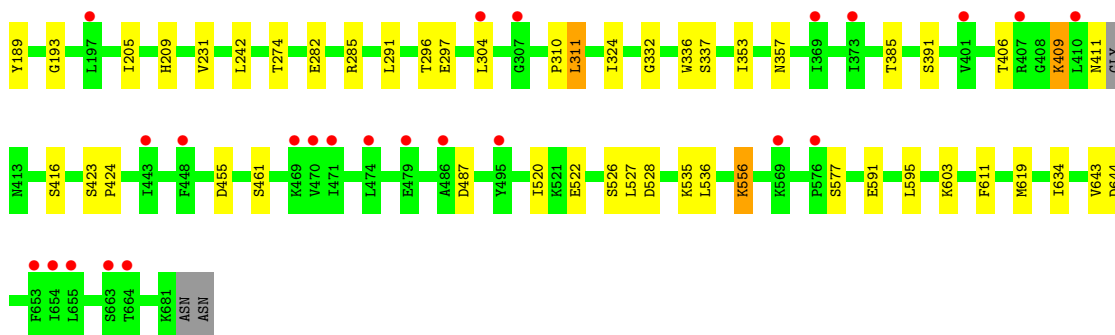
• Molecule 1: Glyco_hydro_42M domain-containing protein
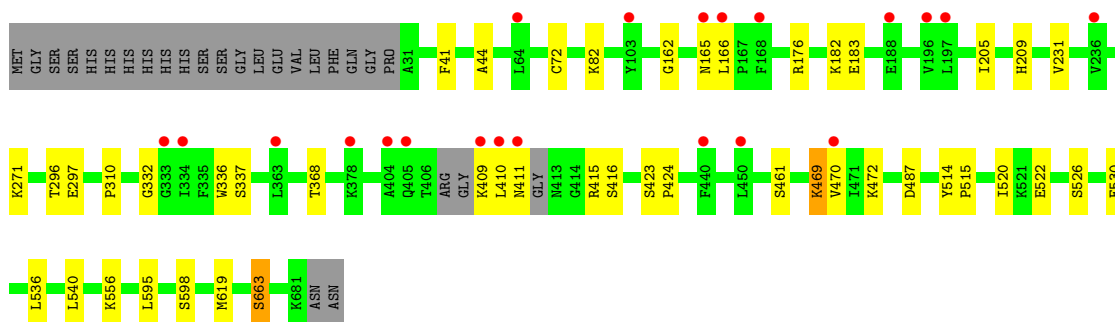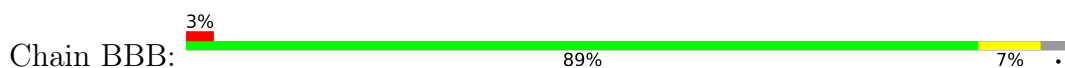
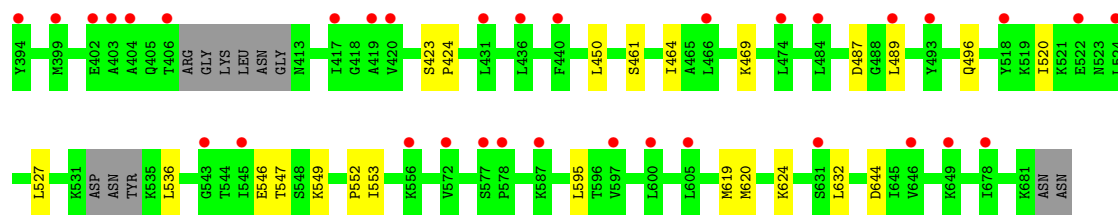• Molecule 1: Glyco_hydro_42M domain-containing protein
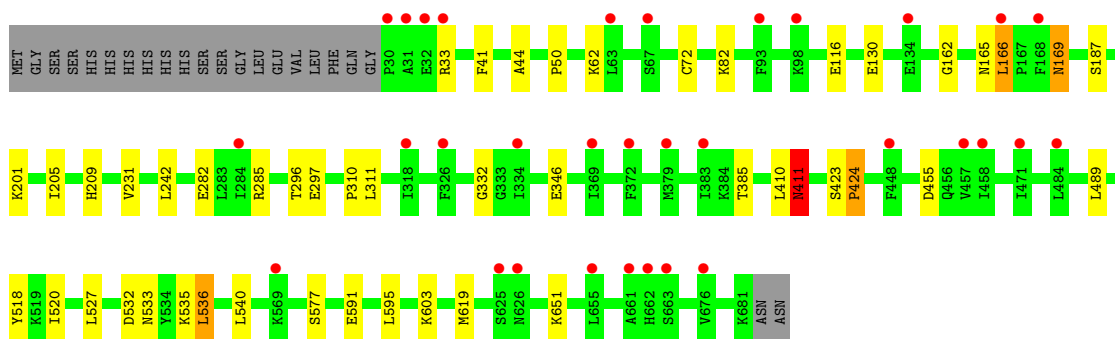
• Molecule 1: Glyco_hydro_42M domain-containing protein
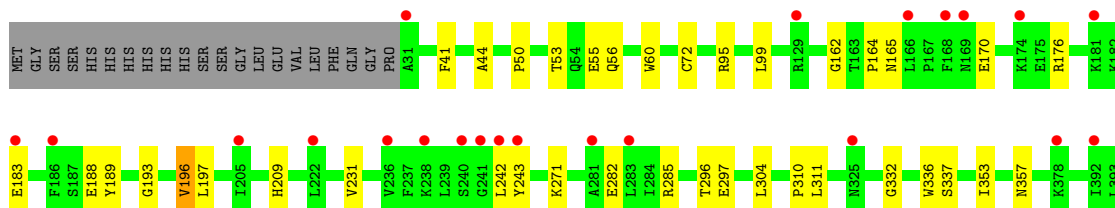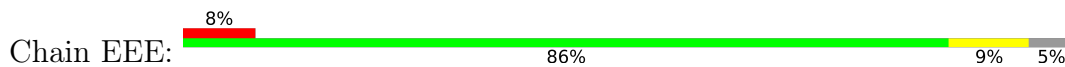
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.16Å 104.87Å 171.63Å 91.98° 97.73° 107.16°	Depositor
Resolution (Å)	89.34 – 2.55 89.18 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.6 (89.34-2.55) 98.7 (89.18-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.214 , 0.245 0.215 , 0.245	Depositor DCC
R_{free} test set	7529 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 14.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	62440	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.76	1/5433 (0.0%)	0.83	0/7354
1	BBB	0.79	2/5360 (0.0%)	0.84	1/7254 (0.0%)
1	CCC	0.76	1/5371 (0.0%)	0.83	1/7269 (0.0%)
1	DDD	0.75	3/5389 (0.1%)	0.82	1/7294 (0.0%)
1	EEE	0.76	1/5306 (0.0%)	0.83	1/7181 (0.0%)
1	FFF	0.76	1/5389 (0.0%)	0.83	0/7295
All	All	0.76	9/32248 (0.0%)	0.83	4/43647 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	297	GLU	CD-OE1	19.36	1.47	1.25
1	FFF	297	GLU	CD-OE1	18.57	1.46	1.25
1	EEE	297	GLU	CD-OE1	18.45	1.46	1.25
1	AAA	297	GLU	CD-OE1	17.39	1.44	1.25
1	CCC	297	GLU	CD-OE1	16.32	1.43	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	188	GLU	CB-CG-CD	5.84	129.98	114.20
1	BBB	176	ARG	CG-CD-NE	5.35	123.03	111.80
1	EEE	170	GLU	CB-CA-C	5.16	120.73	110.40
1	DDD	626	ASN	CB-CA-C	5.13	120.67	110.40

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	5288	5181	5161	27	0
1	BBB	5218	5112	5091	20	0
1	CCC	5228	5123	5103	30	0
1	DDD	5245	5146	5125	27	0
1	EEE	5165	5063	5042	31	0
1	FFF	5244	5138	5120	22	0
2	AAA	11	10	9	0	0
2	BBB	11	10	9	0	0
2	CCC	11	10	9	0	0
2	DDD	11	10	9	0	0
2	EEE	11	10	9	0	0
2	FFF	11	10	9	1	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
4	AAA	31	0	0	3	0
4	BBB	37	0	0	1	0
4	CCC	25	0	0	0	0
4	DDD	13	0	0	0	0
4	EEE	24	0	0	1	0
4	FFF	27	0	0	0	0
All	All	31617	30823	30696	145	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 2.

The worst 5 of 145 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:AAA:53:THR:H	1:AAA:56:GLN:HE21	1.25	0.82
1:EEE:196:VAL:HG22	1:EEE:496:GLN:HB3	1.64	0.80
1:EEE:176:ARG:HG2	4:EEE:824:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:196:VAL:HG22	1:EEE:496:GLN:CB	2.19	0.72
1:EEE:188:GLU:HG3	1:EEE:189:TYR:CE2	2.24	0.72

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	AAA	653/674 (97%)	634 (97%)	19 (3%)	0	100	100
1	BBB	642/674 (95%)	617 (96%)	25 (4%)	0	100	100
1	CCC	645/674 (96%)	621 (96%)	24 (4%)	0	100	100
1	DDD	646/674 (96%)	621 (96%)	25 (4%)	0	100	100
1	EEE	636/674 (94%)	616 (97%)	20 (3%)	0	100	100
1	FFF	650/674 (96%)	625 (96%)	24 (4%)	1 (0%)	47	60
All	All	3872/4044 (96%)	3734 (96%)	137 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	FFF	411	ASN

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	AAA	568/582 (98%)	553 (97%)	15 (3%)	46	61
1	BBB	561/582 (96%)	545 (97%)	16 (3%)	42	57
1	CCC	562/582 (97%)	540 (96%)	22 (4%)	32	44
1	DDD	563/582 (97%)	544 (97%)	19 (3%)	37	50
1	EEE	555/582 (95%)	537 (97%)	18 (3%)	39	53
1	FFF	563/582 (97%)	545 (97%)	18 (3%)	39	53
All	All	3372/3492 (97%)	3264 (97%)	108 (3%)	39	53

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	165	ASN
1	BBB	663	SER
1	EEE	450	LEU
1	BBB	271	LYS
1	BBB	522	GLU

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	MAF	CCC	701	1	11,11,12	1.29	1 (9%)	10,15,17	2.25	2 (20%)
2	MAF	AAA	701	1	11,11,12	1.28	1 (9%)	10,15,17	1.50	1 (10%)
2	MAF	EEE	701	1	11,11,12	1.04	0	10,15,17	2.39	4 (40%)
2	MAF	FFF	701	1	11,11,12	1.64	1 (9%)	10,15,17	2.47	4 (40%)
2	MAF	DDD	701	1	11,11,12	0.91	0	10,15,17	1.79	3 (30%)
2	MAF	BBB	701	1	11,11,12	1.48	1 (9%)	10,15,17	1.72	3 (30%)

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	MAF	CCC	701	1	-	2/2/19/22	0/1/1/1
2	MAF	AAA	701	1	-	0/2/19/22	0/1/1/1
2	MAF	EEE	701	1	-	0/2/19/22	0/1/1/1
2	MAF	FFF	701	1	-	0/2/19/22	0/1/1/1
2	MAF	DDD	701	1	-	1/2/19/22	0/1/1/1
2	MAF	BBB	701	1	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	FFF	701	MAF	C1-C2	4.68	1.58	1.52
2	BBB	701	MAF	C1-C2	4.31	1.58	1.52
2	AAA	701	MAF	C1-C2	2.84	1.56	1.52
2	CCC	701	MAF	C1-C2	2.38	1.55	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	FFF	701	MAF	C1-O5-C5	6.25	120.65	112.19
2	CCC	701	MAF	C1-O5-C5	5.69	119.91	112.19
2	EEE	701	MAF	C1-O5-C5	4.90	118.83	112.19
2	DDD	701	MAF	O5-C5-C4	-3.51	102.28	110.83
2	BBB	701	MAF	C1-O5-C5	3.31	116.68	112.19

There are no chirality outliers.
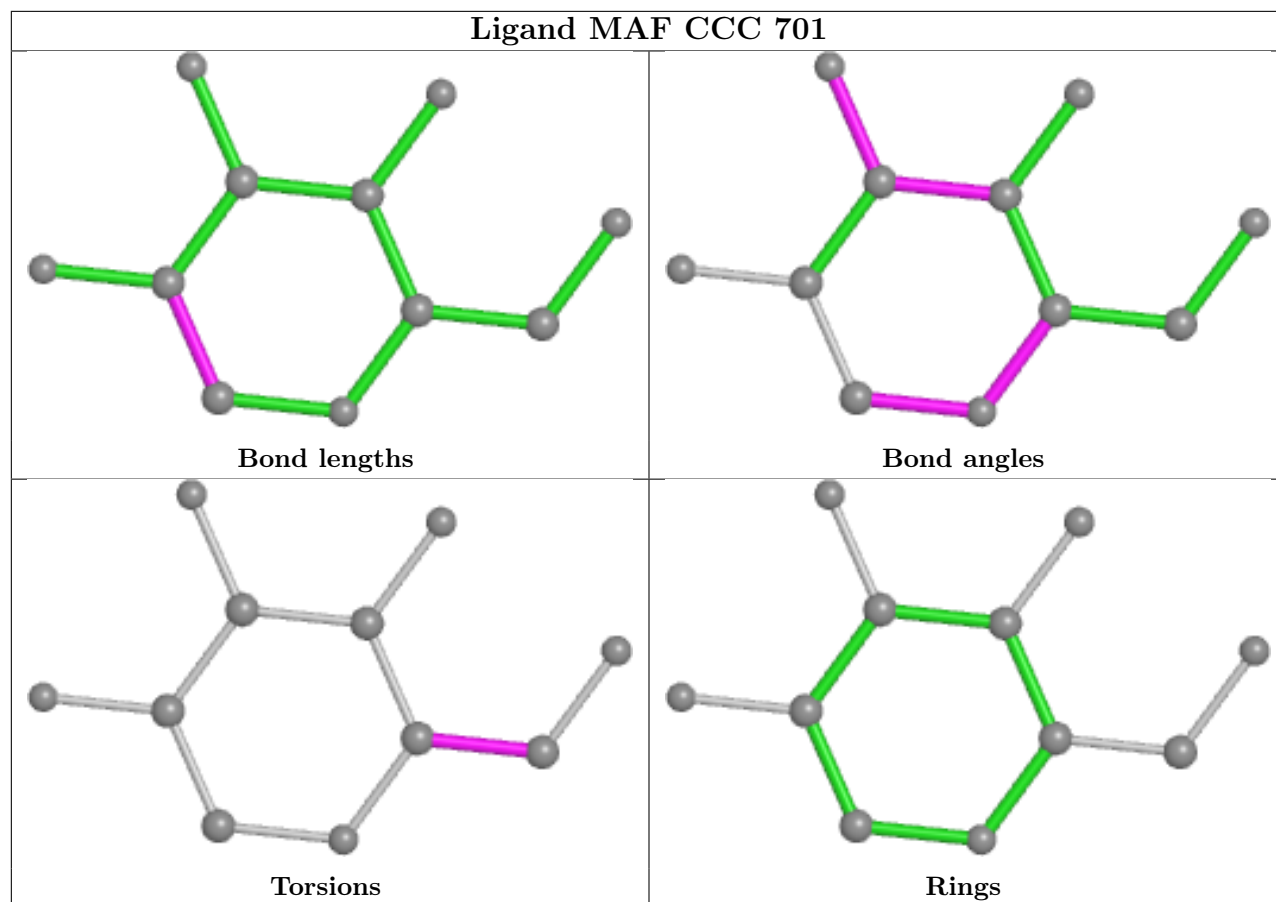
All (3) torsion outliers are listed below:

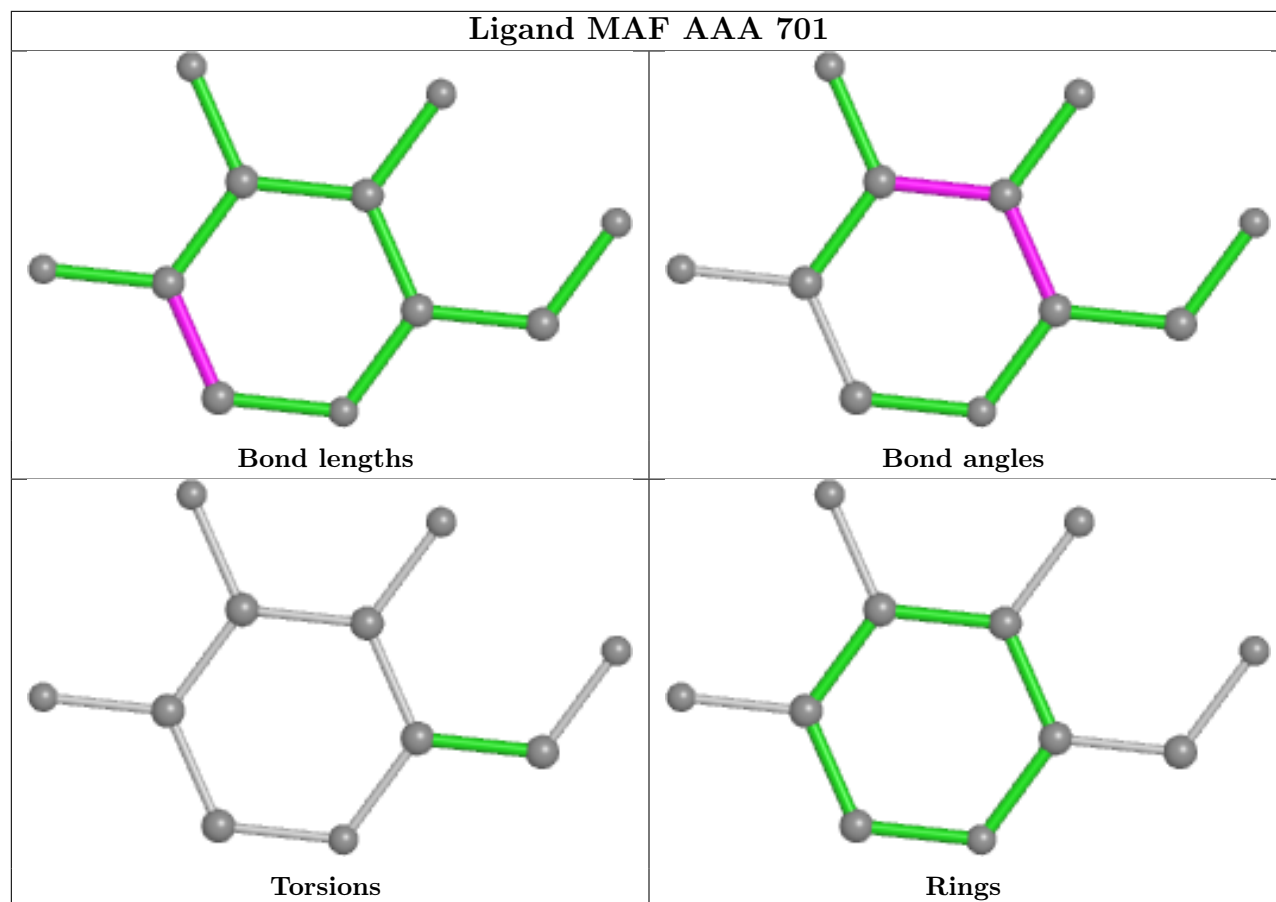| Mol	Chain	Res	Type	Atoms
2	DDD	701	MAF	C4-C5-C6-O6
2	CCC	701	MAF	C4-C5-C6-O6
2	CCC	701	MAF	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	FFF	701	MAF	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 then 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 MAF CCC 701

Bond lengths

Bond angles

Torsions

Rings

Ligand MAF AAA 701

Bond lengths

Bond angles

Torsions

Rings

Ligand MAF EEE 701

Bond lengths

Bond angles

Torsions

Rings

Ligand MAF FFF 701

Bond lengths

Bond angles

Torsions

Rings

Ligand MAF DDD 701

Bond lengths

Bond angles

Torsions

Rings

Ligand MAF BBB 701

Bond lengths

Bond angles

Torsions

Rings
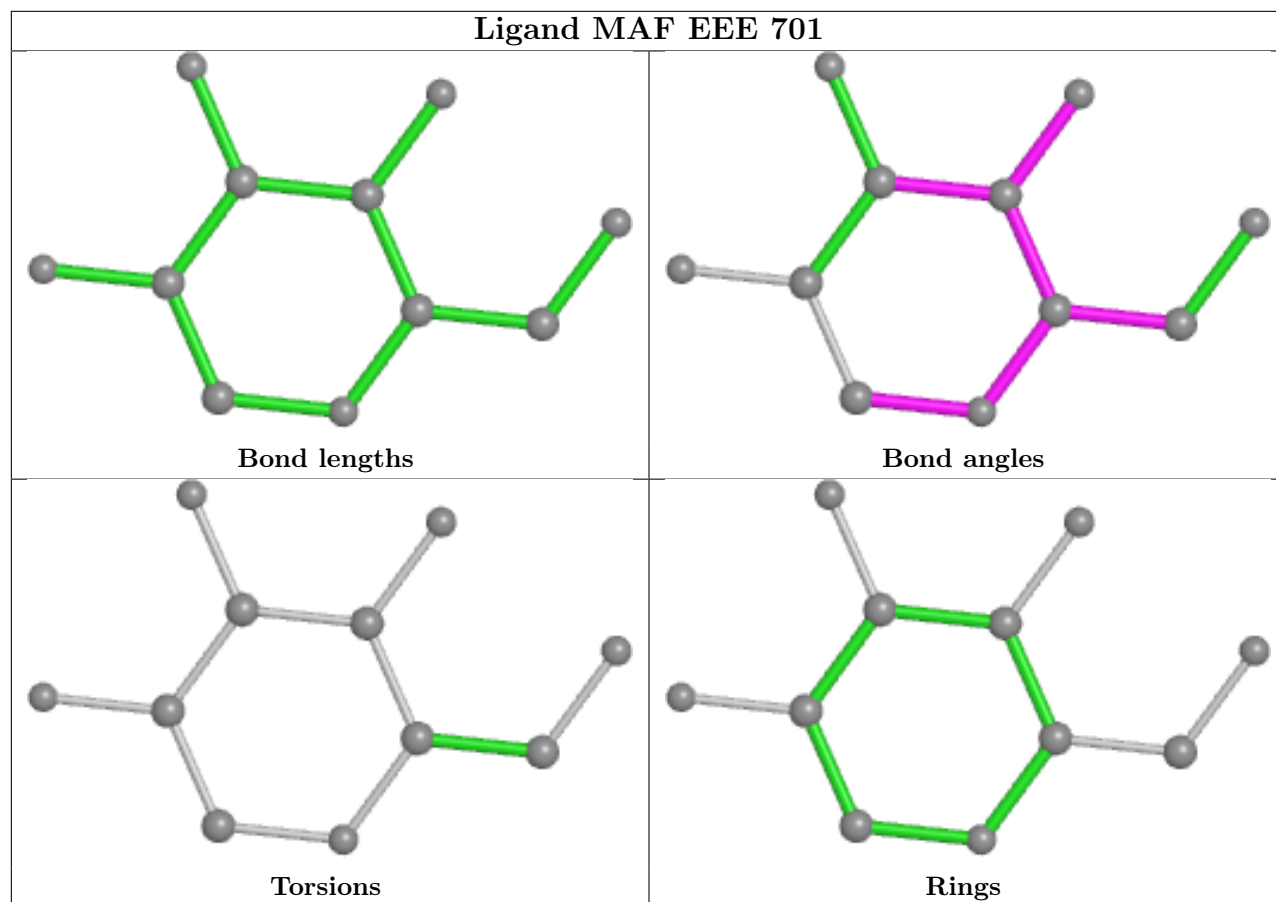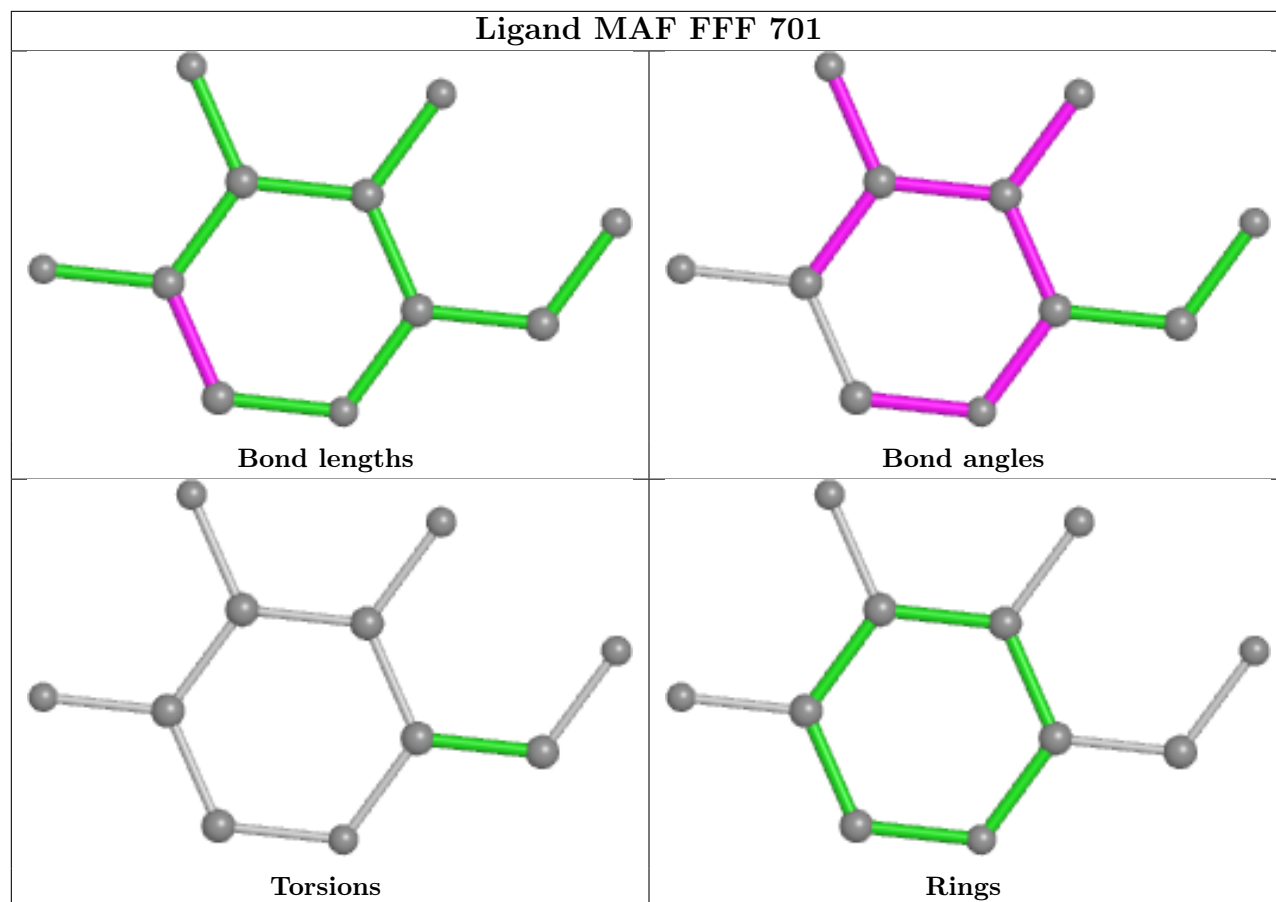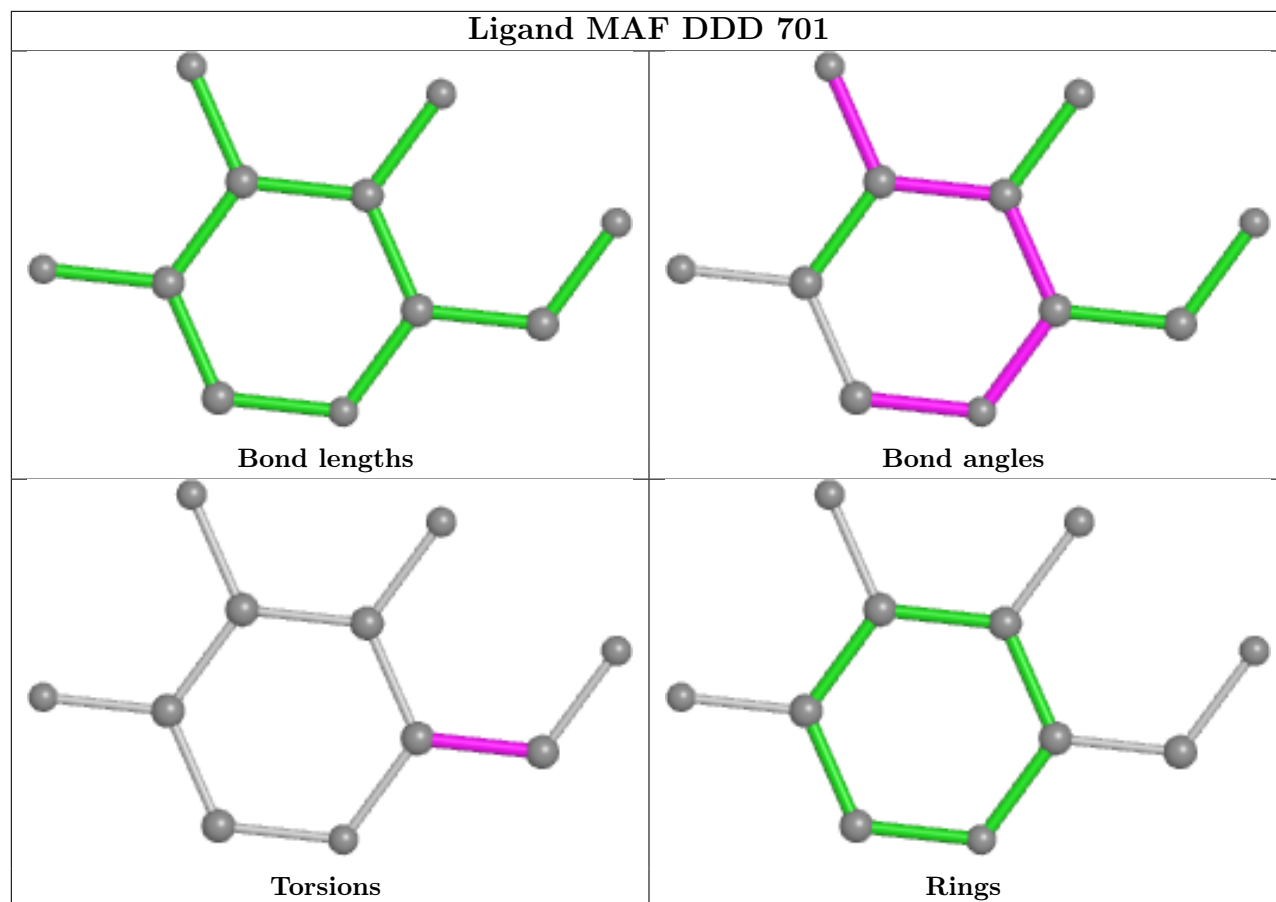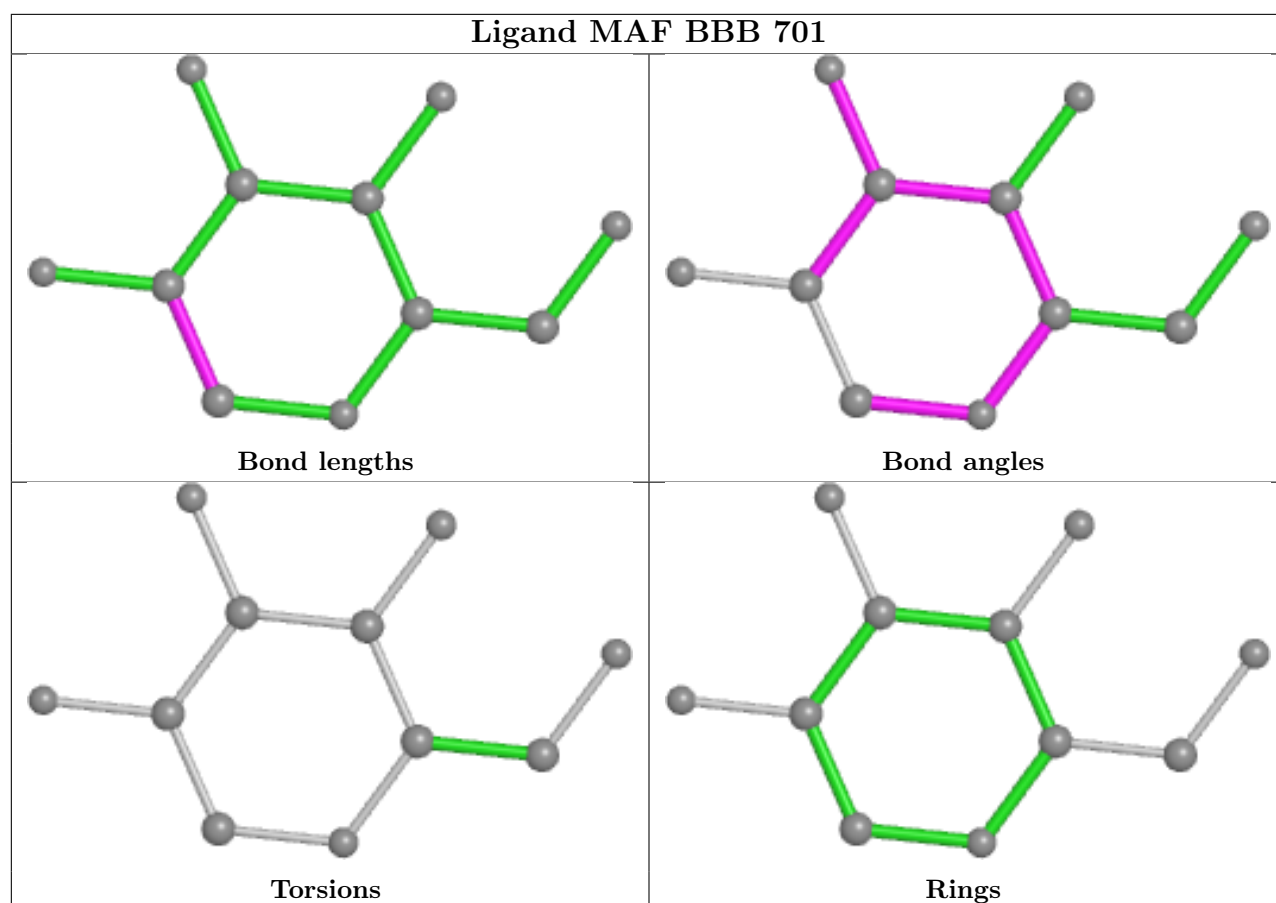
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	AAA	657/674 (97%)	0.12	12 (1%)	68	74	34, 50, 79, 105	0
1	BBB	648/674 (96%)	0.27	21 (3%)	47	55	32, 45, 72, 108	0
1	CCC	649/674 (96%)	0.24	32 (4%)	29	35	32, 48, 75, 102	0
1	DDD	652/674 (96%)	0.24	31 (4%)	30	37	40, 56, 82, 135	0
1	EEE	642/674 (95%)	0.39	56 (8%)	10	12	38, 56, 81, 121	0
1	FFF	652/674 (96%)	0.32	32 (4%)	29	35	35, 51, 83, 112	0
All	All	3900/4044 (96%)	0.26	184 (4%)	31	38	32, 51, 80, 135	0

The worst 5 of 184 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	410	LEU	9.7
1	FFF	30	PRO	6.8
1	FFF	31	ALA	6.6
1	EEE	440	PHE	6.0
1	EEE	166	LEU	6.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
2	MAF	EEE	701	11/12	0.94	0.12	51,55,60,69	3
2	MAF	FFF	701	11/12	0.95	0.13	45,50,55,55	3
2	MAF	CCC	701	11/12	0.96	0.15	41,44,48,51	3
2	MAF	BBB	701	11/12	0.97	0.13	39,43,47,56	3
2	MAF	DDD	701	11/12	0.97	0.15	45,48,53,58	3
2	MAF	AAA	701	11/12	0.97	0.12	38,40,43,49	3
3	CL	CCC	702	1/1	0.98	0.09	39,39,39,39	0
3	CL	BBB	702	1/1	0.98	0.10	50,50,50,50	0
3	CL	AAA	702	1/1	0.99	0.13	46,46,46,46	0
3	CL	DDD	702	1/1	0.99	0.16	48,48,48,48	0
3	CL	FFF	702	1/1	0.99	0.08	41,41,41,41	0
3	CL	EEE	702	1/1	0.99	0.09	51,51,51,51	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 MAF EEE 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
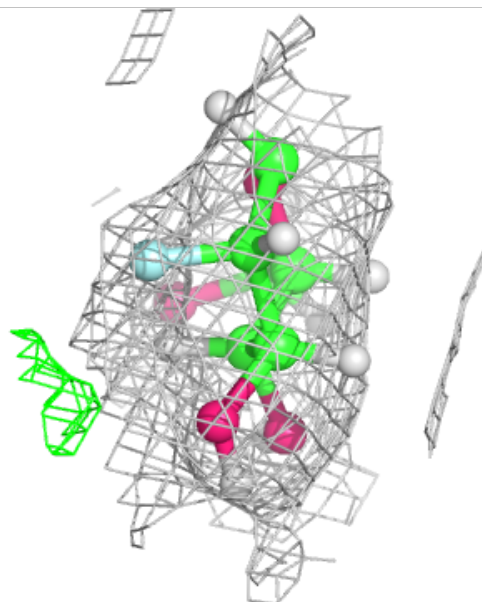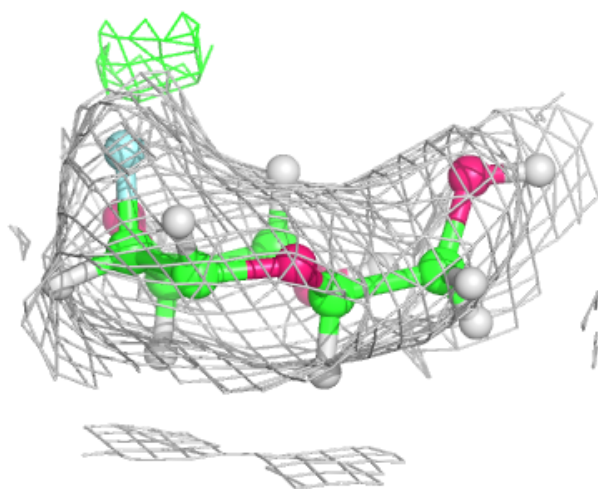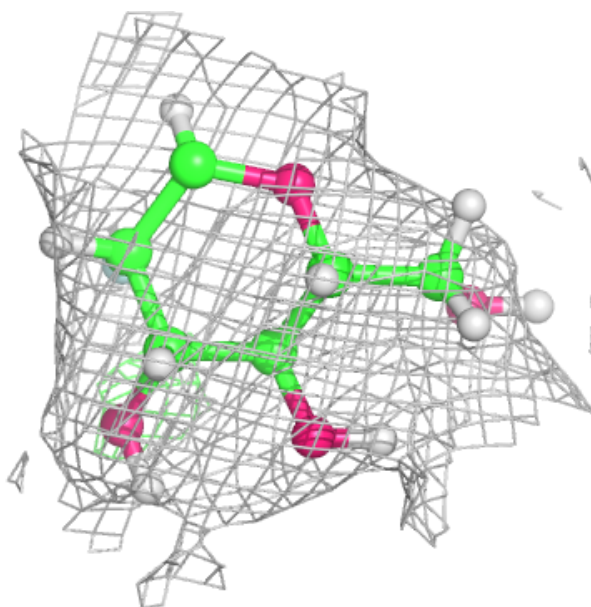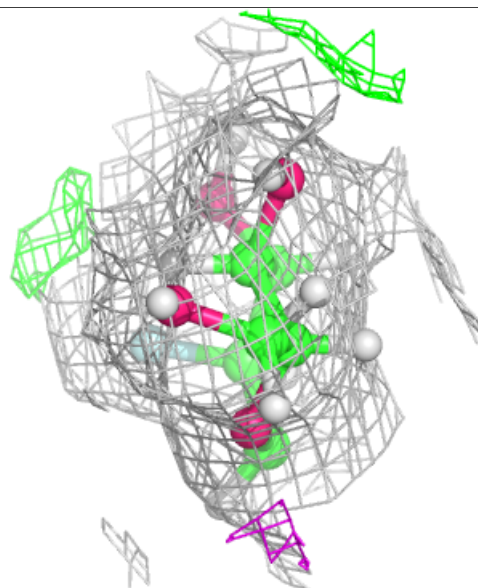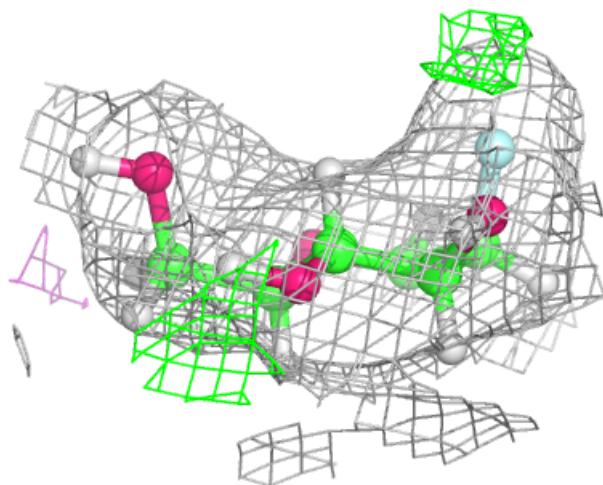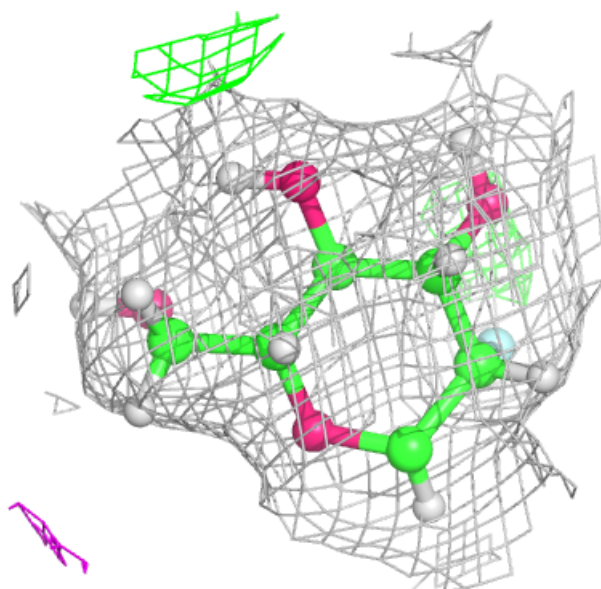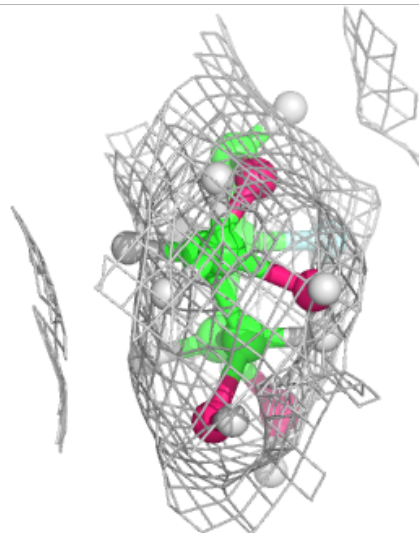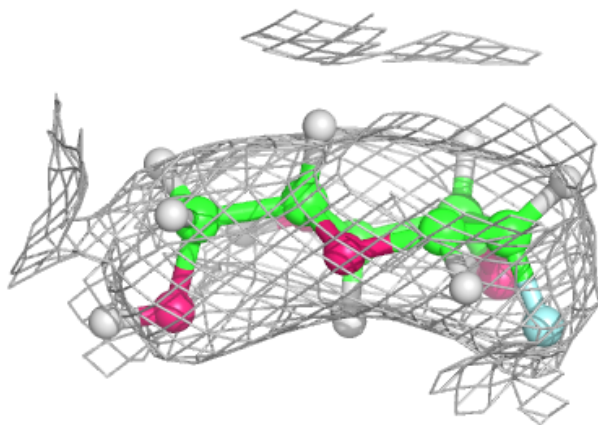mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
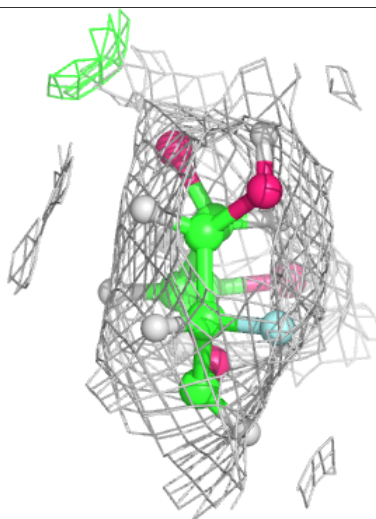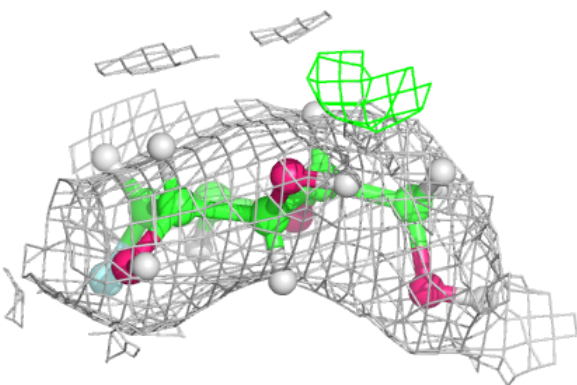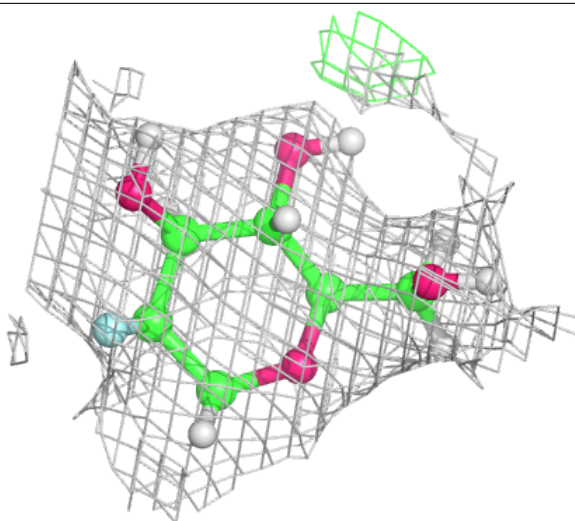
Electron density around MAF FFF 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
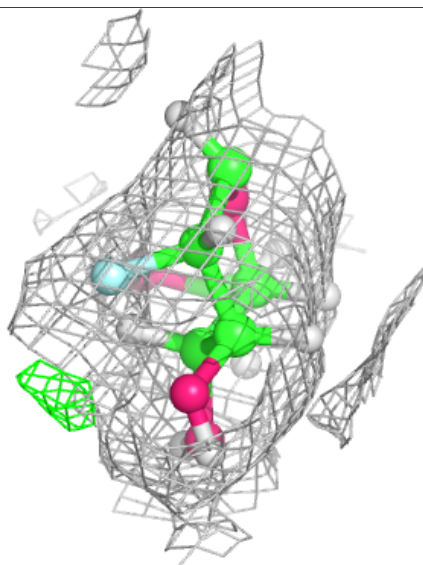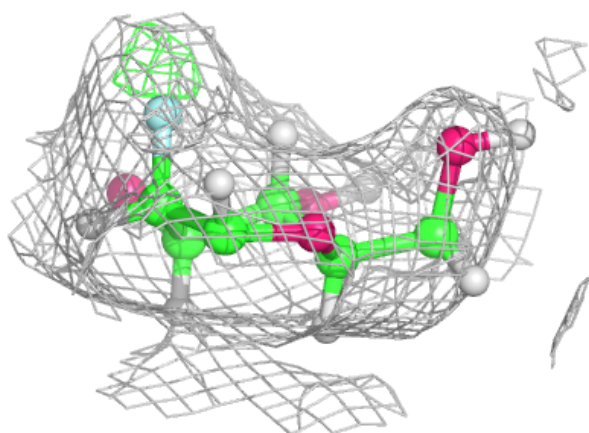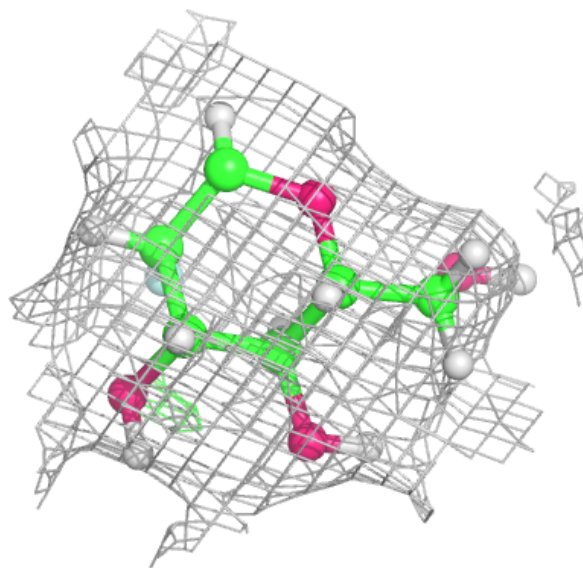
Electron density around MAF CCC 701:

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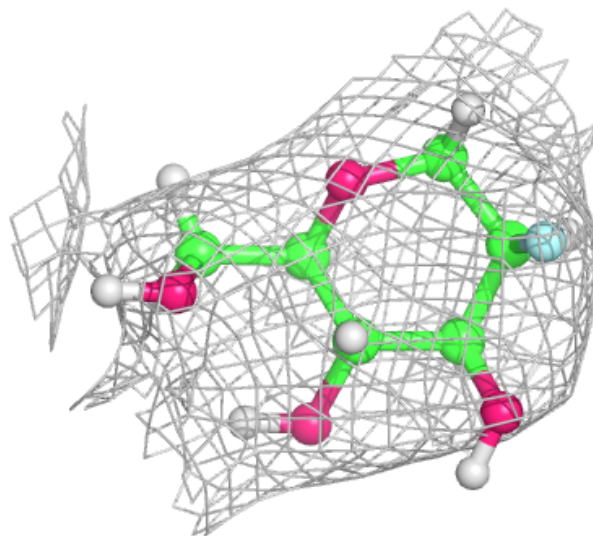mF_o-DF_c (at 3 rmsd) in purple (negative)
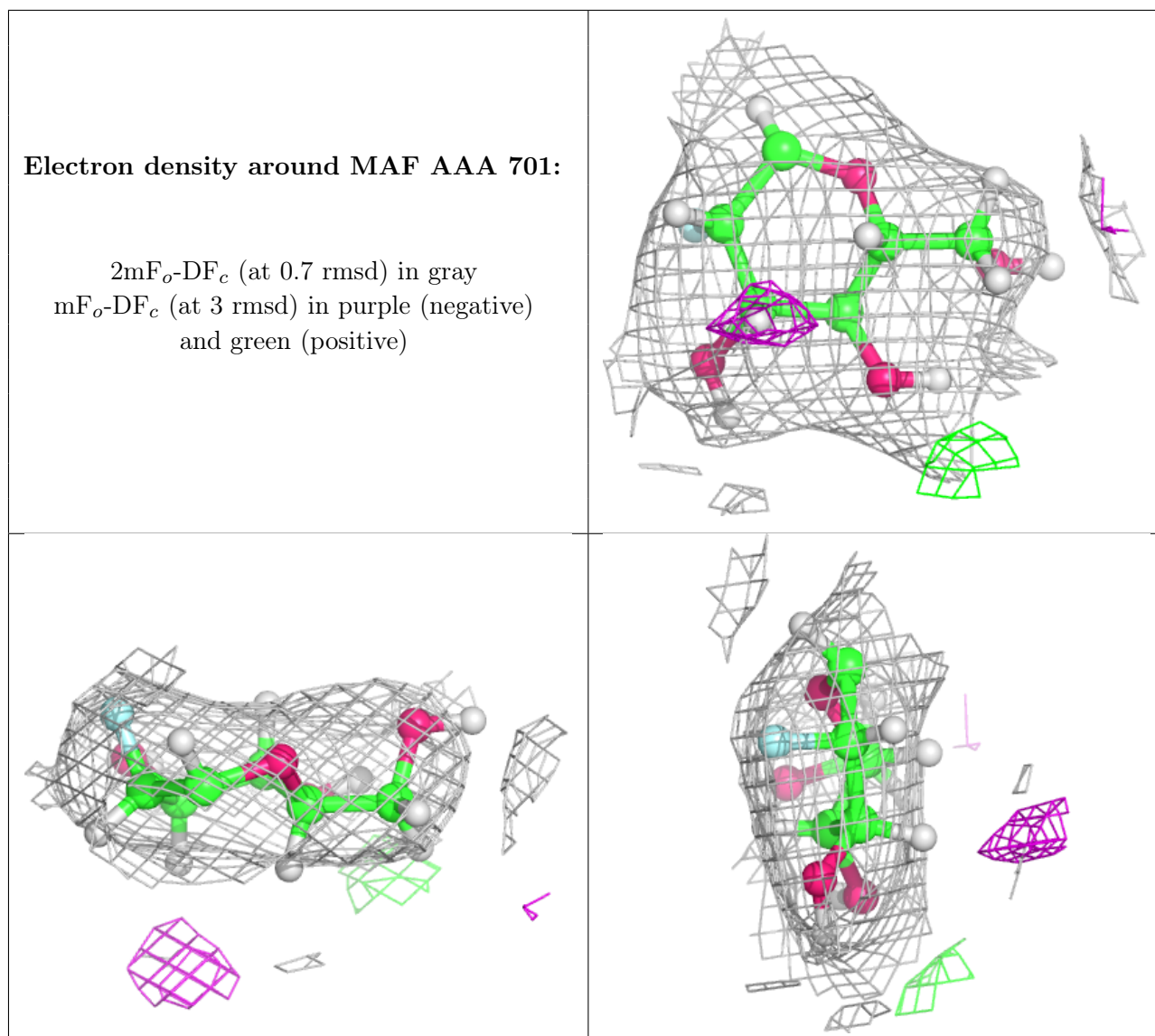and green (positive)

Electron density around MAF BBB 701:

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

Electron density around MAF DDD 701:

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

Electron density around MAF AAA 701:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.