Full wwPDB X-ray Structure Validation Report (i)

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)

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

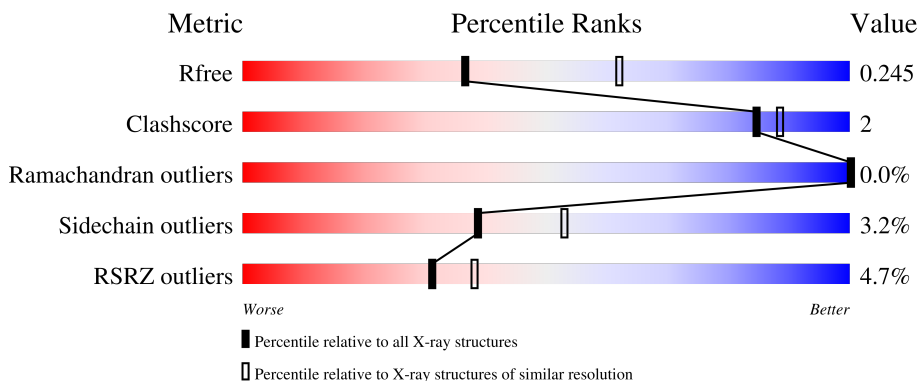|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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.
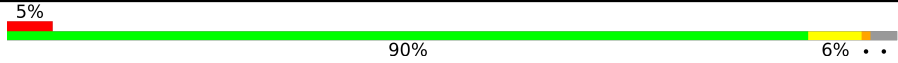
Metric	Percentile Ranks	Value
Rfree		0.245
Clashscore		2
Ramachandran outliers		0.0%
Sidechain outliers		3.2%
RSRZ outliers		4.7%

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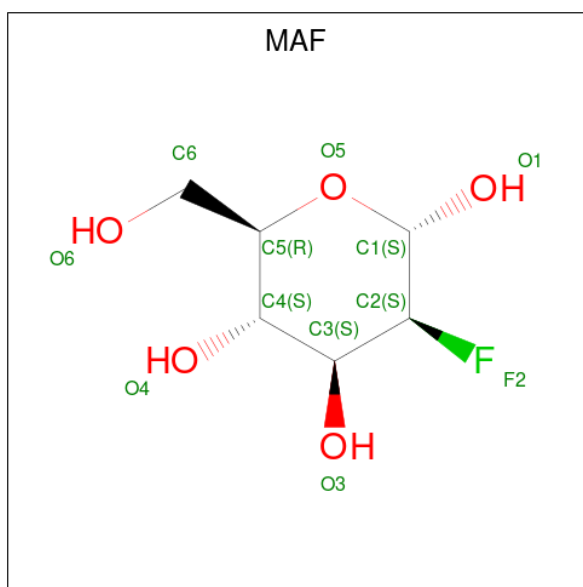
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total 21	C 6	F 1	H 10	O 4	3	0
2	DDD	1	Total 21	C 6	F 1	H 10	O 4	3	0
2	CCC	1	Total 21	C 6	F 1	H 10	O 4	3	0
2	BBB	1	Total 21	C 6	F 1	H 10	O 4	3	0
2	FFF	1	Total 21	C 6	F 1	H 10	O 4	3	0
2	EEE	1	Total 21	C 6	F 1	H 10	O 4	3	0

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

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

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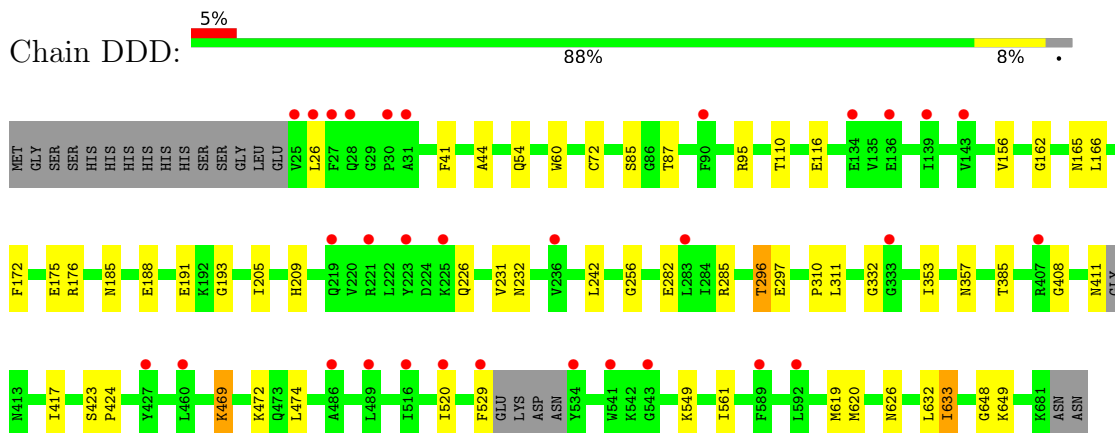ric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues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

• Molecule 1: Glyco_hydro_42M domain-containing protein
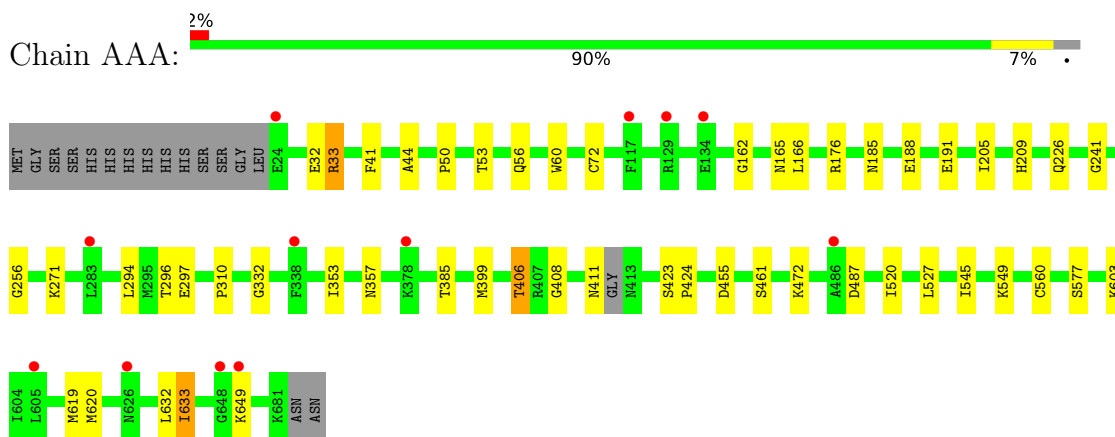
Chain AAA:

• Molecule 1: Glyco_hydro_42M domain-containing protein

Chain DDD:

• Molecule 1: Glyco_hydro_42M domain-containing protein

Chain CCC:

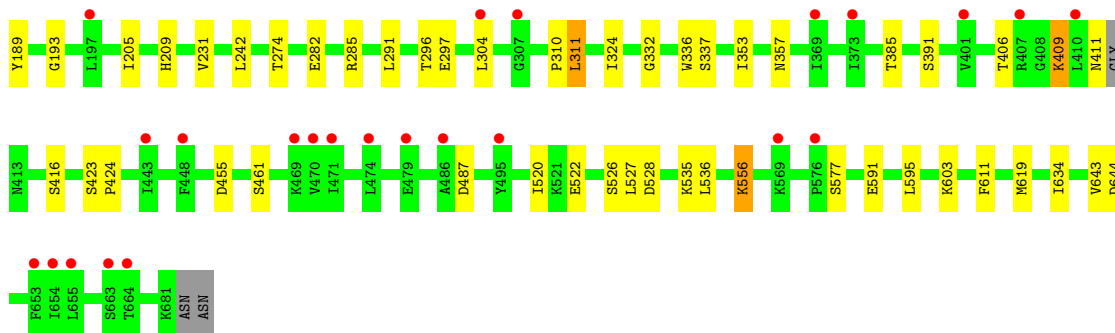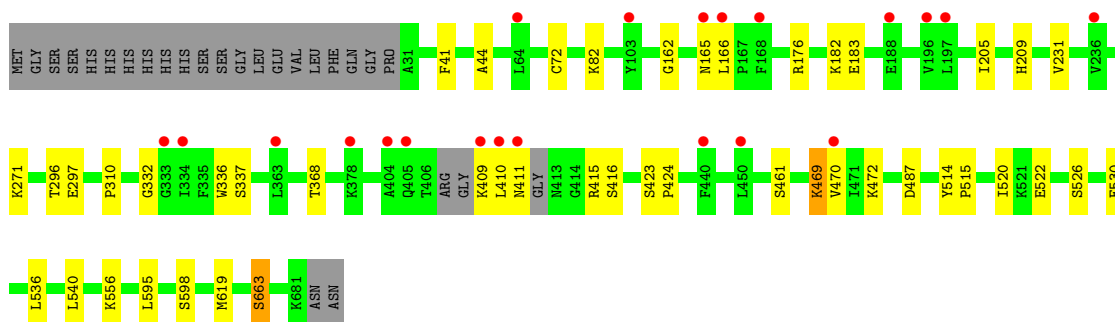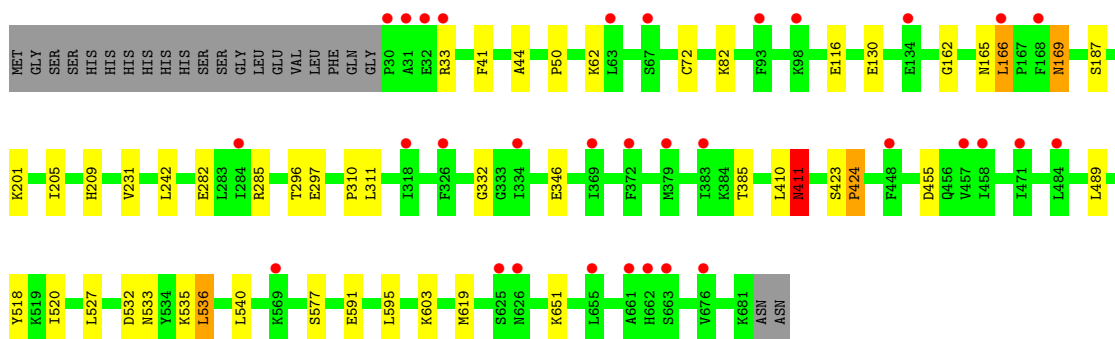• Molecule 1: Glyco_hydro_42M domain-containing protein

Chain BBB:

• Molecule 1: Glyco_hydro_42M domain-containing protein

Chain FFF:

• Molecule 1: Glyco_hydro_42M domain-containing protein

Chain EEE:
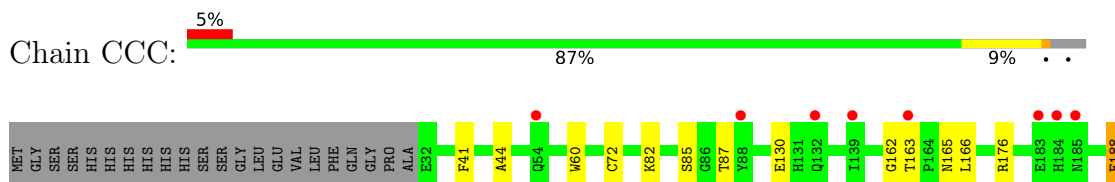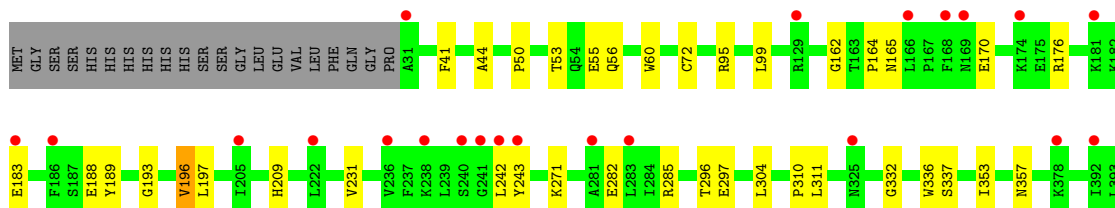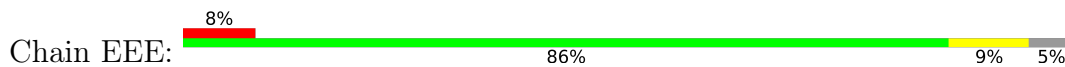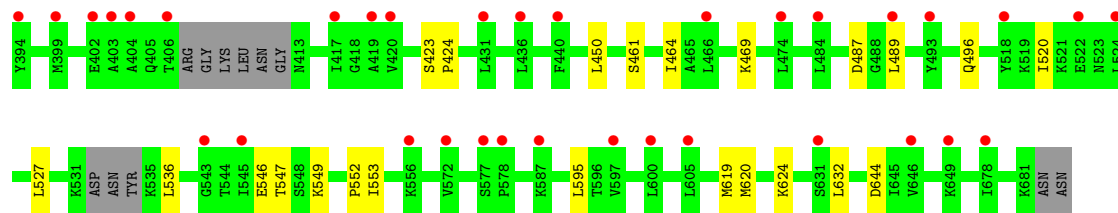
4 Data and refinement statistics ⓘ

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%)

All (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
1	DDD	297	GLU	CD-OE1	14.58	1.41	1.25
1	DDD	175	GLU	CD-OE1	5.68	1.31	1.25
1	DDD	297	GLU	CD-OE2	-5.17	1.20	1.25
1	BBB	530	GLU	CD-OE1	5.13	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 ⓘ

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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:CCC:611:PHE:CD1	1:CCC:643:VAL:HG11	2.26	0.71
1:DDD:310:PRO:HB2	1:FFF:520:ILE:HD13	1.74	0.68
1:DDD:172:PHE:O	1:DDD:176:ARG:HG2	1.95	0.66
1:CCC:611:PHE:CE1	1:CCC:643:VAL:HG11	2.31	0.65
1:EEE:547:THR:HG21	1:EEE:552:PRO:HD3	1.80	0.63
1:CCC:619:MET:HE3	1:CCC:634:ILE:HD12	1.80	0.63
1:DDD:529:PHE:CE2	1:DDD:561:ILE:HD11	2.35	0.62
1:EEE:282:GLU:OE1	1:EEE:285:ARG:NH1	2.34	0.61
1:AAA:310:PRO:HB2	1:CCC:520:ILE:HD13	1.83	0.60
1:FFF:535:LYS:O	1:FFF:591:GLU:HG2	2.02	0.60
1:FFF:282:GLU:OE1	1:FFF:285:ARG:NH1	2.35	0.60
1:CCC:353:ILE:HD12	1:CCC:357:ASN:HD22	1.67	0.59
1:DDD:87:THR:HG21	1:BBB:368:THR:HG21	1.84	0.59
1:CCC:282:GLU:OE1	1:CCC:285:ARG:NH1	2.36	0.59
1:CCC:310:PRO:HB2	1:BBB:520:ILE:HD13	1.83	0.58
1:DDD:520:ILE:HD13	1:EEE:310:PRO:HB2	1.85	0.58
1:DDD:529:PHE:CZ	1:DDD:561:ILE:HD11	2.39	0.58
1:CCC:619:MET:CE	1:CCC:634:ILE:HD12	2.33	0.58
1:AAA:406:THR:HG23	1:AAA:408:GLY:H	1.68	0.57
1:DDD:282:GLU:OE1	1:DDD:285:ARG:NH1	2.37	0.57
1:BBB:409:LYS:HE2	1:BBB:415:ARG:O	2.04	0.57
1:AAA:33:ARG:NH1	1:AAA:226:GLN:O	2.38	0.56
1:CCC:188:GLU:HG2	1:CCC:189:TYR:CD2	2.41	0.56
1:BBB:469:LYS:HE2	1:BBB:470:VAL:HG13	1.87	0.56
1:DDD:54:GLN:HG2	1:DDD:95:ARG:HD2	1.88	0.55
1:DDD:648:GLY:O	1:DDD:649:LYS:HD2	2.06	0.55
1:BBB:663:SER:O	1:FFF:187:SER:HB2	2.08	0.54
1:AAA:353:ILE:HD12	1:AAA:357:ASN:HD22	1.71	0.54
1:DDD:620:MET:SD	1:DDD:633:ILE:HD11	2.48	0.54
1:EEE:188:GLU:HG3	1:EEE:189:TYR:CD2	2.43	0.53
1:AAA:620:MET:SD	1:AAA:633:ILE:HD11	2.48	0.53
1:FFF:242:LEU:HD12	1:FFF:242:LEU:N	2.22	0.53
1:BBB:409:LYS:C	1:BBB:410:LEU:HD12	2.29	0.53
1:EEE:95:ARG:O	1:EEE:99:LEU:HD13	2.08	0.53
1:FFF:50:PRO:HB2	1:EEE:193:GLY:O	2.08	0.53
1:CCC:611:PHE:CD1	1:CCC:643:VAL:CG1	2.92	0.53
1:CCC:535:LYS:O	1:CCC:591:GLU:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:182:LYS:HE2	1:BBB:182:LYS:HA	1.91	0.52
1:DDD:353:ILE:HD12	1:DDD:357:ASN:HD22	1.74	0.52
1:EEE:353:ILE:HD12	1:EEE:357:ASN:HD22	1.74	0.52
1:AAA:176:ARG:HG2	4:AAA:831:HOH:O	2.10	0.51
1:FFF:410:LEU:O	1:FFF:411:ASN:HB2	2.10	0.51
1:FFF:242:LEU:N	1:FFF:242:LEU:CD1	2.74	0.51
1:CCC:188:GLU:HG2	1:CCC:189:TYR:CE2	2.45	0.51
1:DDD:193:GLY:O	1:EEE:50:PRO:HB2	2.09	0.51
1:DDD:54:GLN:HE21	1:DDD:95:ARG:HG3	1.77	0.50
1:CCC:406:THR:O	1:CCC:409:LYS:HD2	2.12	0.49
1:BBB:536:LEU:HD11	1:BBB:595:LEU:HD22	1.95	0.49
1:CCC:274:THR:HB	1:CCC:619:MET:CE	2.44	0.48
1:DDD:166:LEU:HD22	1:DDD:205:ILE:HG12	1.96	0.47
1:BBB:423:SER:HB3	1:BBB:424:PRO:HD3	1.95	0.47
1:EEE:162:GLY:HA2	1:EEE:209:HIS:NE2	2.30	0.47
1:AAA:32:GLU:CA	4:AAA:804:HOH:O	2.62	0.46
1:EEE:196:VAL:HG22	1:EEE:496:GLN:HB2	1.96	0.46
1:CCC:162:GLY:HA2	1:CCC:209:HIS:NE2	2.30	0.46
1:AAA:423:SER:HB3	1:AAA:424:PRO:HD3	1.97	0.46
1:AAA:44:ALA:O	1:AAA:72:CYS:HA	2.16	0.46
1:FFF:166:LEU:HD22	1:FFF:205:ILE:HG12	1.97	0.46
1:DDD:408:GLY:HA2	1:DDD:417:ILE:HD11	1.97	0.46
1:FFF:532:ASP:O	1:FFF:533:ASN:OD1	2.34	0.46
1:EEE:196:VAL:HG13	1:EEE:197:LEU:O	2.15	0.46
1:BBB:162:GLY:HA2	1:BBB:209:HIS:NE2	2.30	0.45
1:EEE:423:SER:HB3	1:EEE:424:PRO:HD3	1.99	0.45
1:AAA:455:ASP:OD2	1:AAA:603:LYS:HD3	2.16	0.45
1:FFF:346:GLU:OE1	2:FFF:701:MAF:H6C1	2.17	0.45
1:FFF:169:ASN:H	1:FFF:169:ASN:HD22	1.63	0.45
1:CCC:423:SER:HB3	1:CCC:424:PRO:HD3	1.98	0.45
1:FFF:527:LEU:HD11	1:FFF:577:SER:HB2	1.98	0.45
1:AAA:166:LEU:HD22	1:AAA:205:ILE:HG12	1.98	0.45
1:DDD:232:ASN:HB3	1:DDD:296:THR:HG21	1.99	0.45
1:DDD:162:GLY:HA2	1:DDD:209:HIS:NE2	2.32	0.44
1:AAA:545:ILE:O	1:AAA:560:CYS:HB3	2.17	0.44
1:DDD:205:ILE:HG21	1:DDD:242:LEU:HD22	2.00	0.44
1:BBB:183:GLU:HG2	4:BBB:826:HOH:O	2.17	0.44
1:AAA:53:THR:H	1:AAA:56:GLN:NE2	2.04	0.44
1:DDD:232:ASN:HB3	1:DDD:296:THR:CG2	2.46	0.44
1:FFF:44:ALA:O	1:FFF:72:CYS:HA	2.18	0.44
1:FFF:423:SER:HB3	1:FFF:424:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:455:ASP:OD2	1:FFF:603:LYS:HD3	2.17	0.44
1:DDD:44:ALA:O	1:DDD:72:CYS:HA	2.17	0.44
1:FFF:540:LEU:HD23	1:FFF:540:LEU:HA	1.82	0.44
1:AAA:162:GLY:HA2	1:AAA:209:HIS:NE2	2.33	0.44
1:AAA:41:PHE:O	1:AAA:332:GLY:HA2	2.18	0.44
1:CCC:527:LEU:HD11	1:CCC:577:SER:HB2	1.99	0.44
1:CCC:528:ASP:HB2	1:CCC:556:LYS:HG3	2.01	0.43
1:DDD:423:SER:HB3	1:DDD:424:PRO:HD3	2.00	0.43
1:CCC:274:THR:HB	1:CCC:619:MET:HE1	2.00	0.43
1:CCC:311:LEU:HA	1:BBB:520:ILE:CG2	2.48	0.43
1:EEE:44:ALA:O	1:EEE:72:CYS:HA	2.18	0.43
1:CCC:44:ALA:O	1:CCC:72:CYS:HA	2.18	0.43
1:BBB:336:TRP:HA	1:BBB:337:SER:HA	1.83	0.43
1:AAA:527:LEU:HD11	1:AAA:577:SER:HB2	2.00	0.43
1:AAA:520:ILE:HD13	1:BBB:310:PRO:HB2	2.00	0.43
1:CCC:41:PHE:O	1:CCC:332:GLY:HA2	2.18	0.43
1:BBB:44:ALA:O	1:BBB:72:CYS:HA	2.19	0.43
1:FFF:162:GLY:HA2	1:FFF:209:HIS:NE2	2.34	0.43
1:CCC:536:LEU:HD11	1:CCC:595:LEU:HD22	2.00	0.43
1:BBB:166:LEU:HD22	1:BBB:205:ILE:HG12	2.00	0.43
1:AAA:241:GLY:H	1:AAA:399:MET:HE1	1.84	0.43
1:CCC:60:TRP:HE1	1:CCC:357:ASN:ND2	2.17	0.43
1:AAA:60:TRP:HE1	1:AAA:357:ASN:ND2	2.16	0.42
1:CCC:166:LEU:HD22	1:CCC:205:ILE:HG12	2.01	0.42
1:EEE:336:TRP:HA	1:EEE:337:SER:HA	1.84	0.42
1:AAA:53:THR:OG1	1:AAA:56:GLN:HG3	2.19	0.42
1:DDD:469:LYS:HA	1:DDD:469:LYS:HD2	1.79	0.42
1:CCC:324:ILE:HD11	1:CCC:619:MET:HE1	2.00	0.42
1:CCC:455:ASP:OD2	1:CCC:603:LYS:HD3	2.17	0.42
1:CCC:336:TRP:HA	1:CCC:337:SER:HA	1.82	0.42
1:DDD:620:MET:HA	1:DDD:632:LEU:O	2.19	0.42
1:FFF:489:LEU:HD22	1:FFF:518:TYR:CE2	2.55	0.42
1:FFF:536:LEU:HD11	1:FFF:595:LEU:HD22	2.01	0.42
1:EEE:304:LEU:HD12	1:EEE:304:LEU:HA	1.92	0.42
1:EEE:464:ILE:HG22	1:EEE:489:LEU:HB2	2.02	0.42
1:EEE:547:THR:HG21	1:EEE:552:PRO:CD	2.48	0.42
1:EEE:60:TRP:HE1	1:EEE:357:ASN:ND2	2.18	0.42
1:EEE:41:PHE:O	1:EEE:332:GLY:HA2	2.20	0.42
1:EEE:461:SER:HA	1:EEE:487:ASP:OD1	2.20	0.42
1:BBB:461:SER:HA	1:BBB:487:ASP:OD1	2.18	0.42
1:AAA:32:GLU:N	4:AAA:804:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:620:MET:HA	1:AAA:632:LEU:O	2.20	0.41
1:CCC:461:SER:HA	1:CCC:487:ASP:OD1	2.20	0.41
1:FFF:41:PHE:O	1:FFF:332:GLY:HA2	2.20	0.41
1:FFF:310:PRO:HB2	1:EEE:520:ILE:HD13	2.01	0.41
1:EEE:620:MET:HA	1:EEE:632:LEU:O	2.20	0.41
1:DDD:41:PHE:O	1:DDD:332:GLY:HA2	2.21	0.41
1:BBB:41:PHE:O	1:BBB:332:GLY:HA2	2.21	0.41
1:AAA:461:SER:HA	1:AAA:487:ASP:OD1	2.21	0.41
1:DDD:60:TRP:HE1	1:DDD:357:ASN:ND2	2.18	0.41
1:EEE:53:THR:OG1	1:EEE:56:GLN:HG3	2.21	0.41
1:EEE:242:LEU:HD12	1:EEE:243:TYR:CD1	2.56	0.41
1:AAA:33:ARG:HA	1:AAA:33:ARG:HE	1.86	0.40
1:AAA:256:GLY:HA2	1:AAA:294:LEU:O	2.21	0.40
1:DDD:110:THR:HA	1:DDD:156:VAL:HB	2.03	0.40
1:DDD:256:GLY:HA3	1:DDD:296:THR:CG2	2.51	0.40
1:AAA:50:PRO:HB2	1:CCC:193:GLY:O	2.21	0.40
1:BBB:423:SER:HB3	1:BBB:424:PRO:CD	2.51	0.40
1:EEE:196:VAL:CG2	1:EEE:496:GLN:HB3	2.43	0.40
1:EEE:536:LEU:HD11	1:EEE:595:LEU:HD22	2.04	0.40
1:BBB:514:TYR:CD1	1:BBB:515:PRO:HD2	2.57	0.40
1:EEE:196:VAL:HG11	1:EEE:496:GLN:NE2	2.37	0.40

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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	33	ARG
1	AAA	165	ASN
1	AAA	185	ASN
1	AAA	188	GLU
1	AAA	191	GLU
1	AAA	271	LYS
1	AAA	296	THR
1	AAA	385	THR
1	AAA	406	THR

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Mol	Chain	Res	Type
1	AAA	411	ASN
1	AAA	472	LYS
1	AAA	549	LYS
1	AAA	619	MET
1	AAA	633	ILE
1	AAA	649	LYS
1	DDD	26	LEU
1	DDD	85	SER
1	DDD	116	GLU
1	DDD	165	ASN
1	DDD	185	ASN
1	DDD	188	GLU
1	DDD	191	GLU
1	DDD	226	GLN
1	DDD	231	VAL
1	DDD	296	THR
1	DDD	311	LEU
1	DDD	385	THR
1	DDD	411	ASN
1	DDD	469	LYS
1	DDD	472	LYS
1	DDD	474	LEU
1	DDD	549	LYS
1	DDD	619	MET
1	DDD	633	ILE
1	CCC	82	LYS
1	CCC	85	SER
1	CCC	87	THR
1	CCC	130	GLU
1	CCC	163	THR
1	CCC	165	ASN
1	CCC	176	ARG
1	CCC	231	VAL
1	CCC	242	LEU
1	CCC	291	LEU
1	CCC	296	THR
1	CCC	304	LEU
1	CCC	311	LEU
1	CCC	385	THR
1	CCC	391	SER
1	CCC	409	LYS
1	CCC	411	ASN

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Mol	Chain	Res	Type
1	CCC	416	SER
1	CCC	522	GLU
1	CCC	526	SER
1	CCC	556	LYS
1	CCC	644	ASP
1	BBB	82	LYS
1	BBB	165	ASN
1	BBB	231	VAL
1	BBB	271	LYS
1	BBB	296	THR
1	BBB	411	ASN
1	BBB	416	SER
1	BBB	469	LYS
1	BBB	472	LYS
1	BBB	522	GLU
1	BBB	526	SER
1	BBB	540	LEU
1	BBB	556	LYS
1	BBB	598	SER
1	BBB	619	MET
1	BBB	663	SER
1	FFF	33	ARG
1	FFF	62	LYS
1	FFF	82	LYS
1	FFF	116	GLU
1	FFF	130	GLU
1	FFF	165	ASN
1	FFF	166	LEU
1	FFF	169	ASN
1	FFF	201	LYS
1	FFF	231	VAL
1	FFF	296	THR
1	FFF	311	LEU
1	FFF	385	THR
1	FFF	411	ASN
1	FFF	424	PRO
1	FFF	536	LEU
1	FFF	619	MET
1	FFF	651	LYS
1	EEE	55	GLU
1	EEE	164	PRO
1	EEE	165	ASN

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Mol	Chain	Res	Type
1	EEE	183	GLU
1	EEE	196	VAL
1	EEE	231	VAL
1	EEE	271	LYS
1	EEE	296	THR
1	EEE	311	LEU
1	EEE	450	LEU
1	EEE	469	LYS
1	EEE	527	LEU
1	EEE	546	GLU
1	EEE	549	LYS
1	EEE	553	ILE
1	EEE	619	MET
1	EEE	624	LYS
1	EEE	644	ASP

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

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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 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

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	EEE	701	MAF	C3-C4-C5	3.19	115.94	110.24
2	DDD	701	MAF	C1-O5-C5	3.06	116.34	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	701	MAF	O3-C3-C4	-2.87	103.71	110.35
2	EEE	701	MAF	O5-C5-C6	-2.81	102.81	107.20
2	BBB	701	MAF	C3-C4-C5	2.79	115.22	110.24
2	FFF	701	MAF	O3-C3-C2	-2.67	104.50	109.58
2	AAA	701	MAF	C3-C4-C5	-2.60	105.61	110.24
2	FFF	701	MAF	C3-C4-C5	-2.28	106.18	110.24
2	BBB	701	MAF	O3-C3-C2	-2.24	105.32	109.58
2	EEE	701	MAF	O4-C4-C3	-2.23	105.19	110.35
2	CCC	701	MAF	O3-C3-C4	-2.11	105.47	110.35
2	FFF	701	MAF	O4-C4-C5	2.08	114.46	109.30

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:

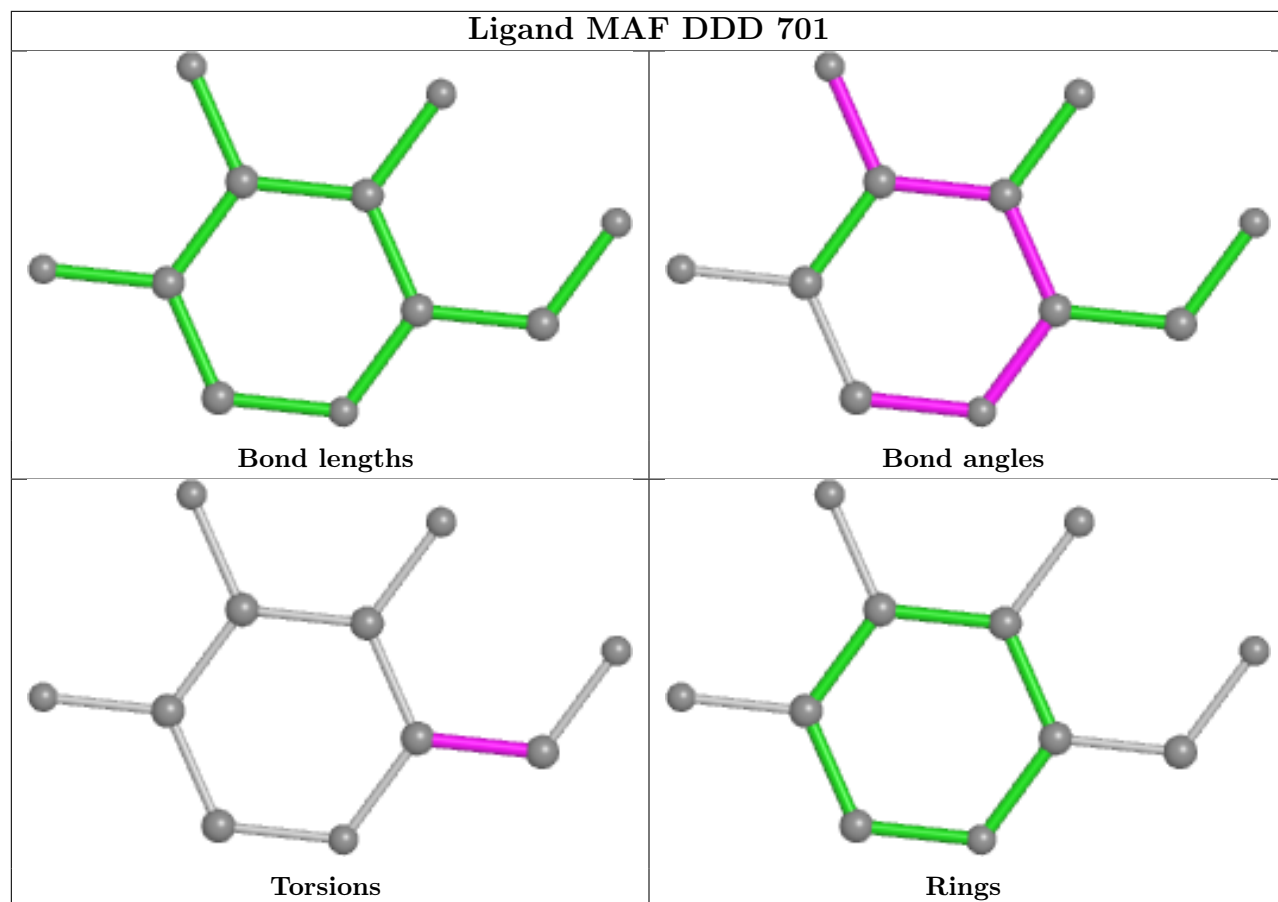| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	FFF	701	MAF	1	0

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.
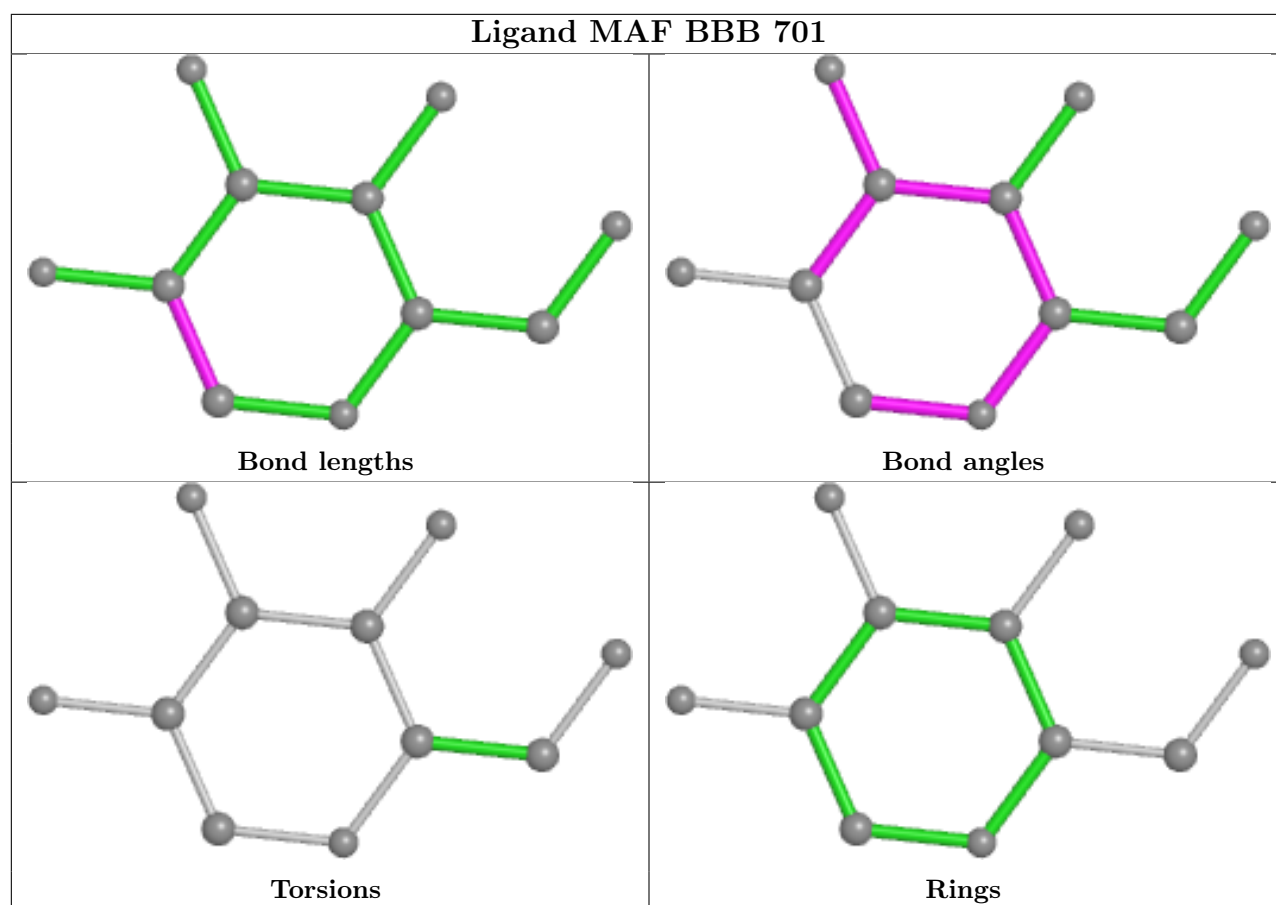
Ligand MAF CCC 701

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

Full wwPDB X-ray Structure Validation Report

Ligand MAF BBB 701

Bond lengths

Bond angles

Torsions

Rings
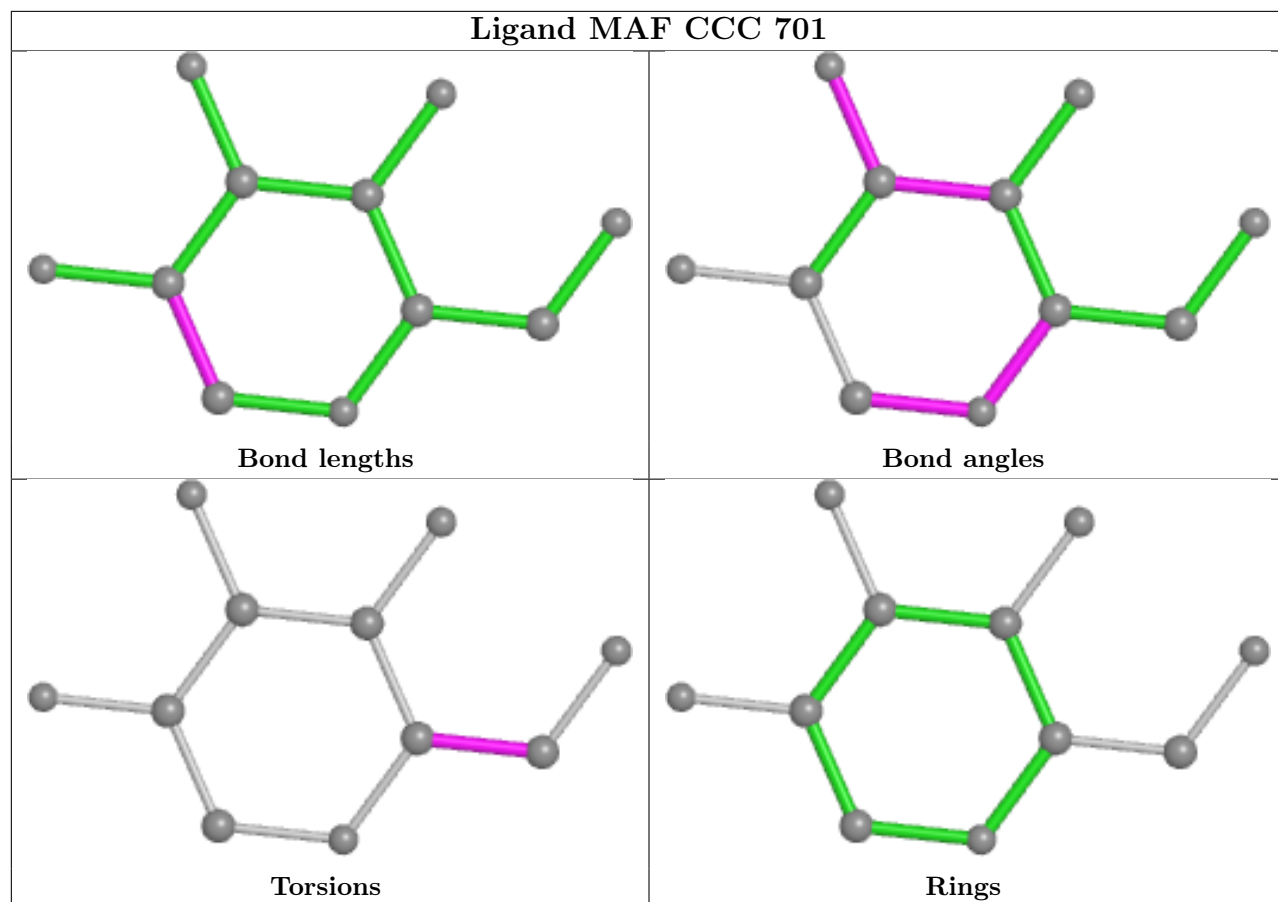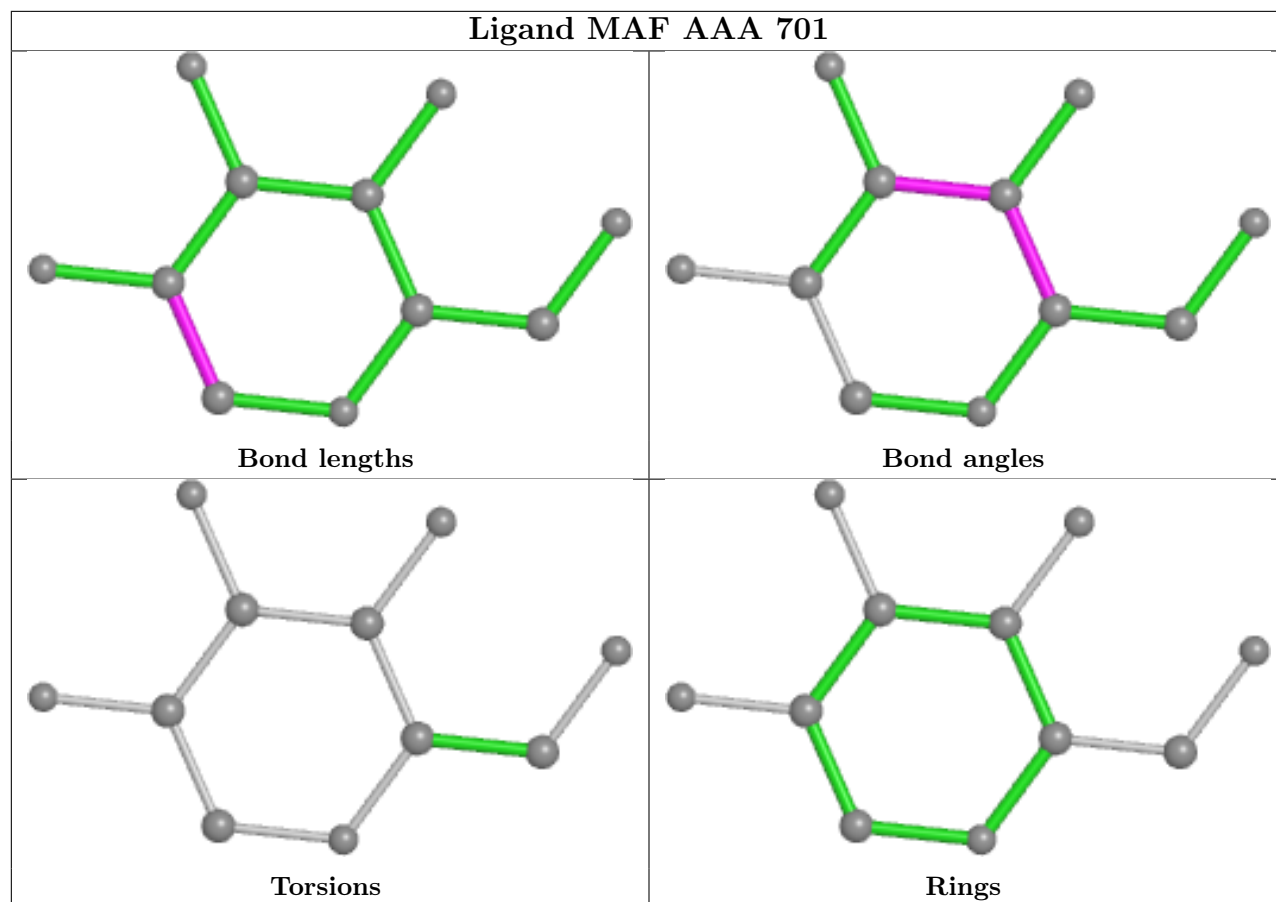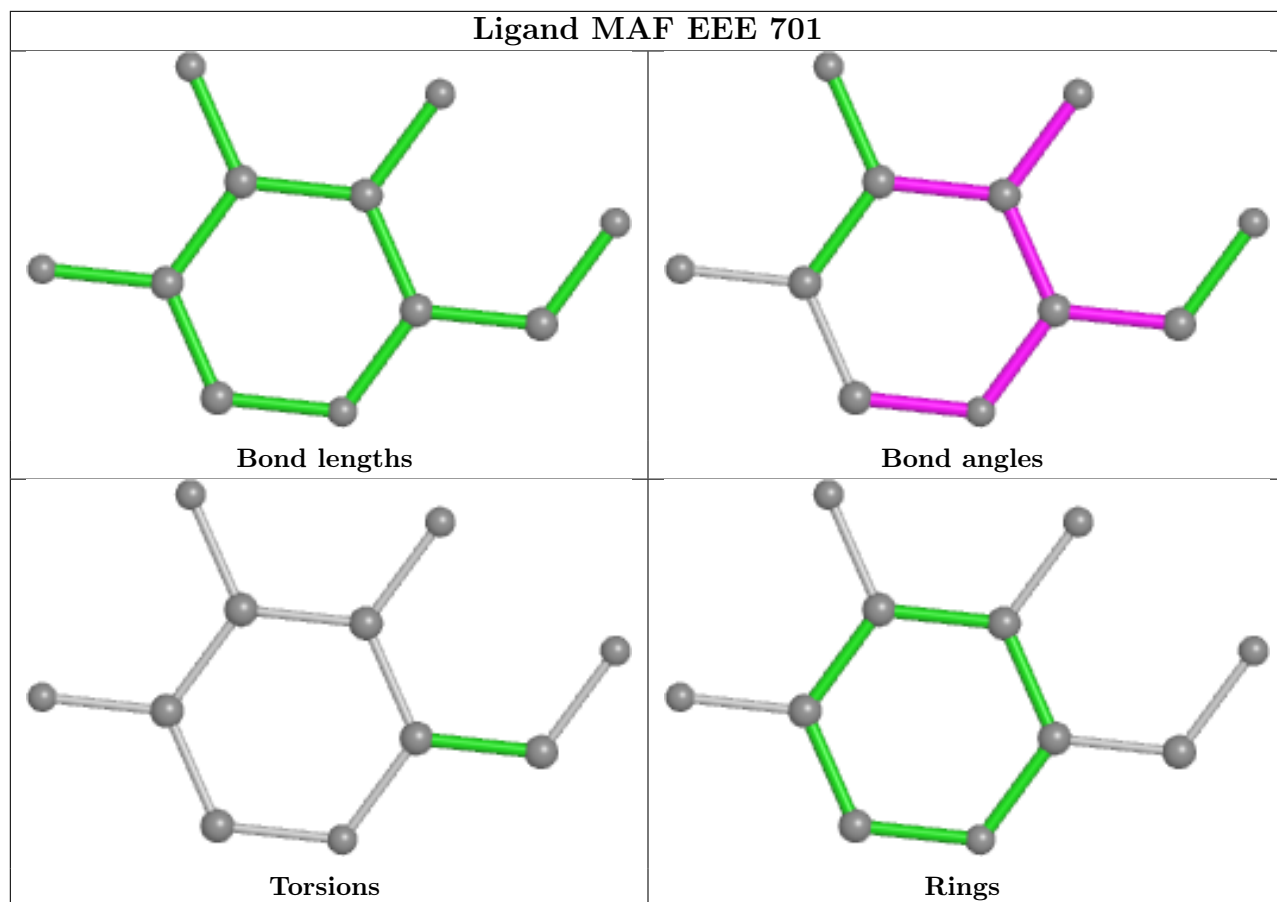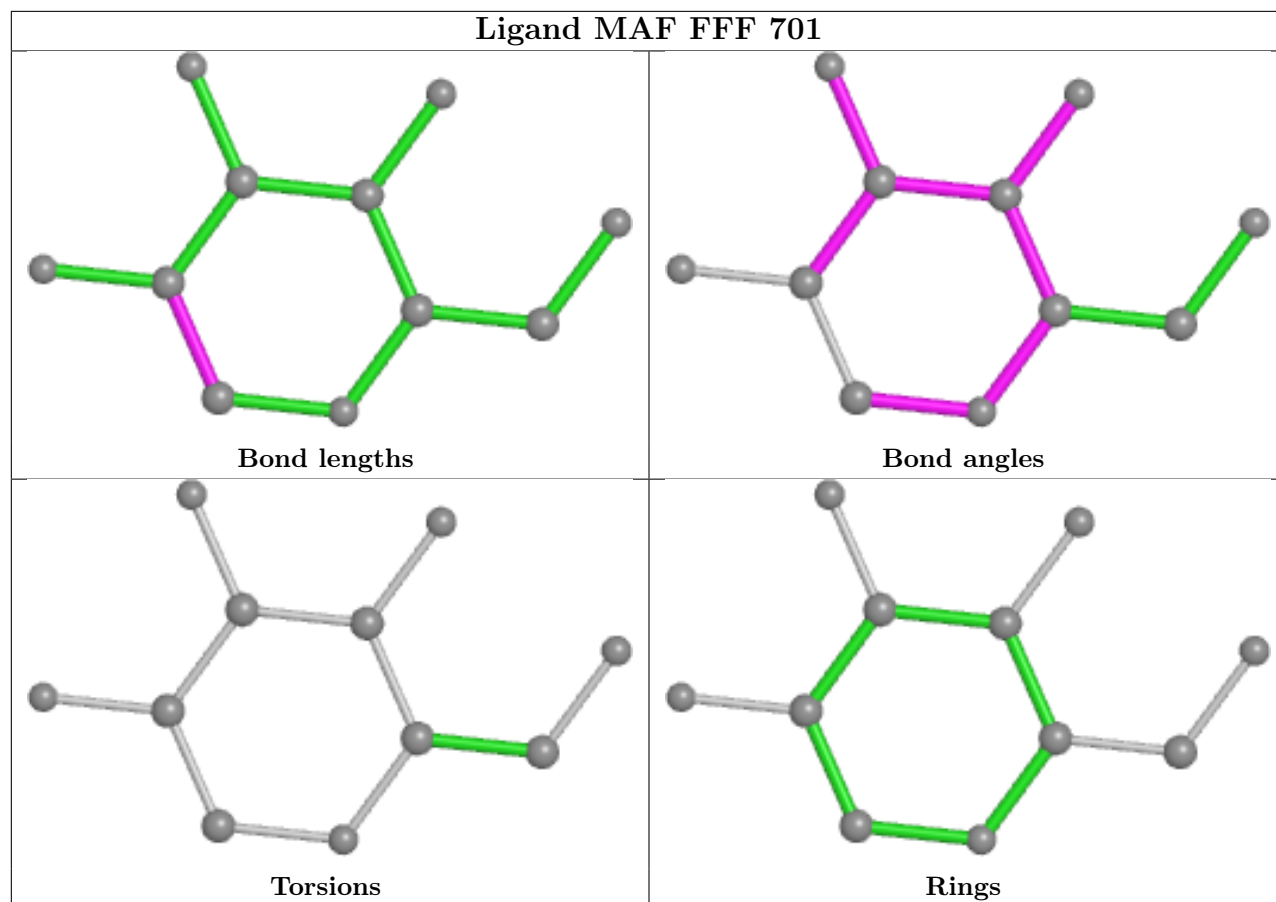
5.7 Other polymers ⓘ

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

All (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
1	EEE	436	LEU	5.4
1	FFF	626	ASN	5.3
1	EEE	578	PRO	5.2
1	EEE	417	ILE	5.2
1	EEE	605	LEU	5.1
1	EEE	420	VAL	5.1
1	CCC	569	LYS	5.0
1	BBB	409	LYS	5.0
1	CCC	410	LEU	4.9
1	CCC	654	ILE	4.8
1	AAA	378	LYS	4.7
1	EEE	283	LEU	4.7
1	FFF	318	ILE	4.6
1	DDD	486	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	EEE	403	ALA	4.5
1	FFF	383	ILE	4.4
1	EEE	572	VAL	4.4
1	CCC	470	VAL	4.2
1	CCC	88	TYR	4.2
1	EEE	392	ILE	4.1
1	DDD	529	PHE	4.1
1	DDD	221	ARG	4.1
1	BBB	197	LEU	4.1
1	CCC	663	SER	4.0
1	EEE	646	VAL	4.0
1	BBB	64	LEU	4.0
1	DDD	139	ILE	4.0
1	CCC	369	ILE	4.0
1	CCC	407	ARG	3.9
1	EEE	600	LEU	3.9
1	EEE	597	VAL	3.9
1	EEE	406	THR	3.8
1	FFF	32	GLU	3.8
1	DDD	541	TRP	3.8
1	BBB	196	VAL	3.8
1	DDD	333	GLY	3.7
1	EEE	404	ALA	3.6
1	EEE	399	MET	3.6
1	BBB	411	ASN	3.6
1	DDD	223	TYR	3.5
1	CCC	373	ILE	3.5
1	FFF	448	PHE	3.5
1	CCC	486	ALA	3.4
1	AAA	648	GLY	3.4
1	FFF	458	ILE	3.4
1	EEE	431	LEU	3.4
1	EEE	240	SER	3.3
1	EEE	631	SER	3.3
1	DDD	26	LEU	3.2
1	EEE	678	ILE	3.2
1	BBB	166	LEU	3.2
1	DDD	27	PHE	3.2
1	FFF	655	LEU	3.1
1	FFF	625	SER	3.1
1	EEE	168	PHE	3.1
1	FFF	33	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	CCC	401	VAL	3.1
1	CCC	471	ILE	3.1
1	CCC	495	TYR	3.1
1	EEE	183	GLU	3.1
1	DDD	543	GLY	3.0
1	EEE	241	GLY	3.0
1	CCC	443	ILE	3.0
1	EEE	545	ILE	3.0
1	DDD	90	PHE	3.0
1	EEE	169	ASN	3.0
1	EEE	394	TYR	3.0
1	FFF	369	ILE	3.0
1	DDD	143	VAL	2.9
1	DDD	516	ILE	2.9
1	FFF	457	VAL	2.9
1	AAA	649	LYS	2.9
1	FFF	284	ILE	2.9
1	CCC	197	LEU	2.9
1	BBB	404	ALA	2.9
1	EEE	484	LEU	2.9
1	EEE	524	LEU	2.9
1	EEE	543	GLY	2.8
1	BBB	405	GLN	2.8
1	EEE	649	LYS	2.8
1	BBB	165	ASN	2.8
1	FFF	372	PHE	2.8
1	EEE	466	LEU	2.8
1	EEE	577	SER	2.8
1	DDD	31	ALA	2.8
1	DDD	134	GLU	2.8
1	CCC	653	PHE	2.8
1	DDD	460	LEU	2.7
1	EEE	518	TYR	2.7
1	EEE	129	ARG	2.7
1	EEE	419	ALA	2.7
1	AAA	283	LEU	2.7
1	DDD	407	ARG	2.7
1	CCC	185	ASN	2.6
1	BBB	333	GLY	2.6
1	DDD	427	TYR	2.6
1	AAA	626	ASN	2.6
1	CCC	54	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	FFF	661	ALA	2.6
1	BBB	378	LYS	2.6
1	DDD	30	PRO	2.6
1	DDD	520	ILE	2.6
1	EEE	238	LYS	2.5
1	BBB	440	PHE	2.5
1	CCC	448	PHE	2.5
1	EEE	522	GLU	2.5
1	FFF	484	LEU	2.5
1	EEE	489	LEU	2.5
1	AAA	24	GLU	2.5
1	EEE	236	VAL	2.5
1	DDD	28	GLN	2.5
1	CCC	655	LEU	2.5
1	EEE	556	LYS	2.5
1	CCC	304	LEU	2.4
1	FFF	662	HIS	2.4
1	EEE	402	GLU	2.4
1	BBB	334	ILE	2.4
1	FFF	67	SER	2.4
1	DDD	25	VAL	2.4
1	EEE	181	LYS	2.4
1	AAA	605	LEU	2.4
1	CCC	163	THR	2.4
1	AAA	134	GLU	2.4
1	FFF	569	LYS	2.3
1	CCC	576	PRO	2.3
1	EEE	186	PHE	2.3
1	EEE	243	TYR	2.3
1	BBB	188	GLU	2.3
1	AAA	117	PHE	2.3
1	CCC	184	HIS	2.3
1	CCC	469	LYS	2.3
1	DDD	136	GLU	2.3
1	CCC	132	GLN	2.3
1	BBB	470	VAL	2.3
1	EEE	378	LYS	2.3
1	DDD	489	LEU	2.3
1	BBB	363	LEU	2.3
1	CCC	307	GLY	2.2
1	FFF	93	PHE	2.2
1	EEE	242	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	FFF	326	PHE	2.2
1	FFF	166	LEU	2.2
1	AAA	129	ARG	2.2
1	CCC	664	THR	2.2
1	DDD	592	LEU	2.2
1	BBB	236	VAL	2.2
1	FFF	379	MET	2.2
1	FFF	334	ILE	2.2
1	EEE	281	ALA	2.2
1	CCC	479	GLU	2.2
1	DDD	283	LEU	2.2
1	FFF	168	PHE	2.2
1	BBB	450	LEU	2.2
1	EEE	174	LYS	2.1
1	DDD	534	TYR	2.1
1	BBB	168	PHE	2.1
1	EEE	31	ALA	2.1
1	DDD	225	LYS	2.1
1	FFF	471	ILE	2.1
1	CCC	474	LEU	2.1
1	BBB	103	TYR	2.1
1	FFF	676	VAL	2.1
1	DDD	219	GLN	2.1
1	CCC	183	GLU	2.1
1	EEE	493	TYR	2.1
1	EEE	587	LYS	2.1
1	FFF	63	LEU	2.1
1	FFF	663	SER	2.1
1	AAA	486	ALA	2.1
1	FFF	98	LYS	2.1
1	EEE	205	ILE	2.1
1	DDD	589	PHE	2.1
1	AAA	338	PHE	2.0
1	FFF	134	GLU	2.0
1	EEE	222	LEU	2.0
1	EEE	325	ASN	2.0
1	DDD	236	VAL	2.0
1	CCC	139	ILE	2.0
1	EEE	474	LEU	2.0

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 ⓘ

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.
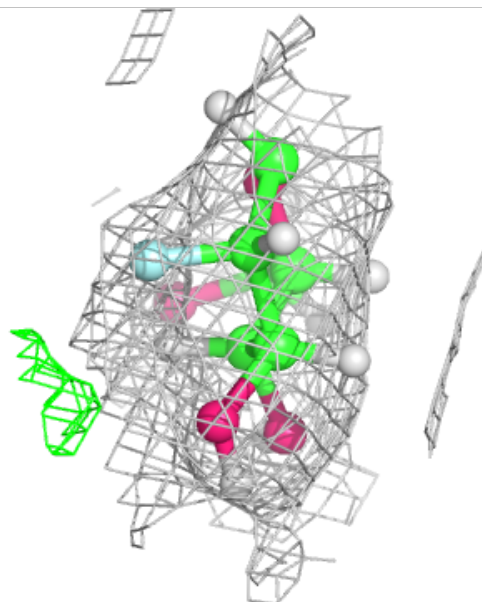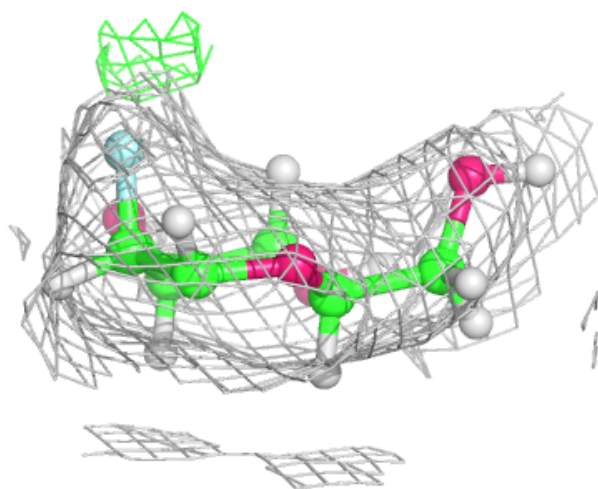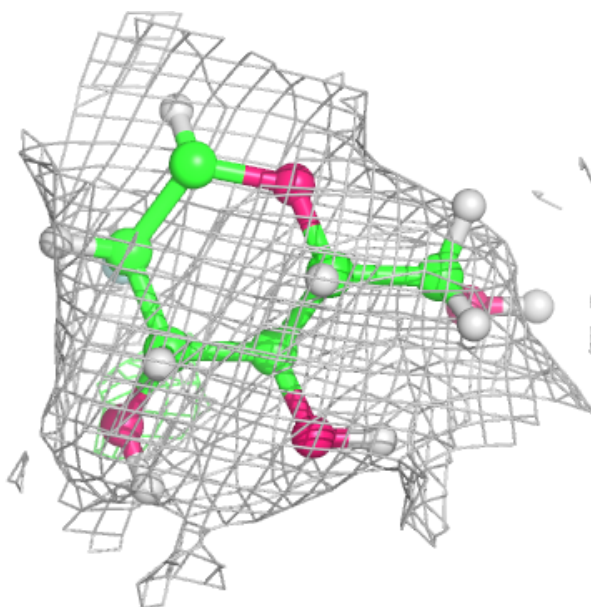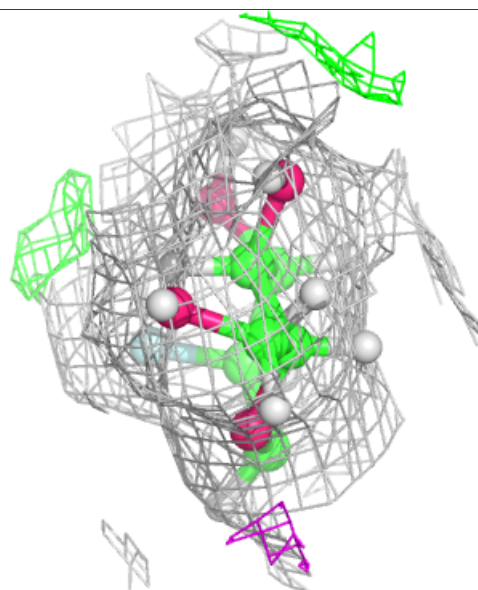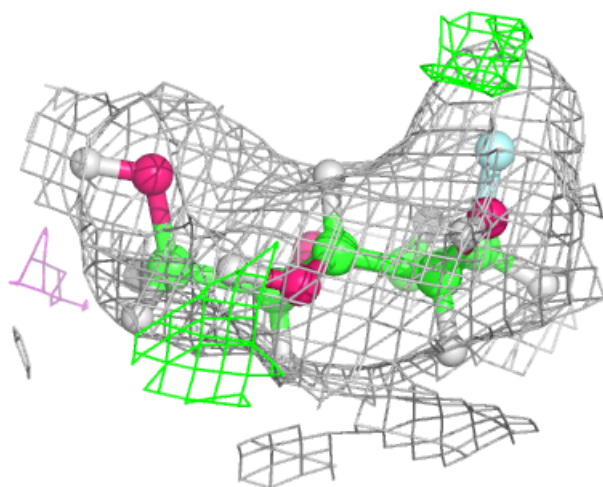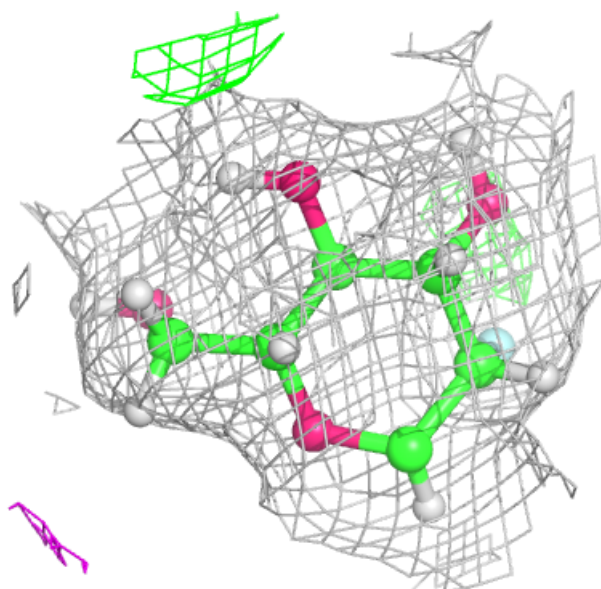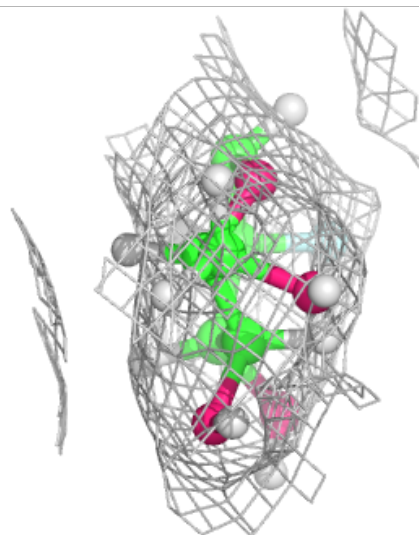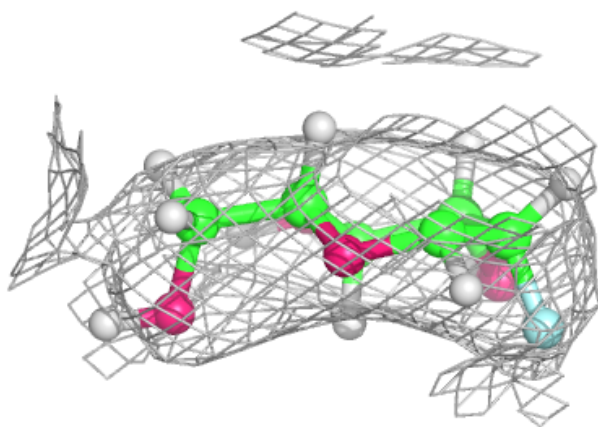
Electron density around MAF EEE 701:

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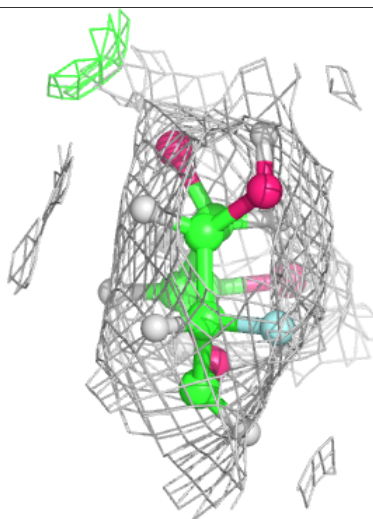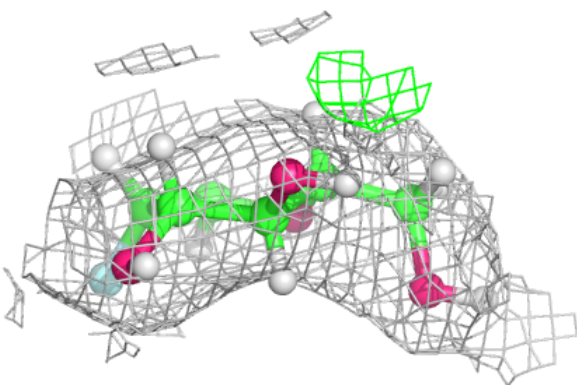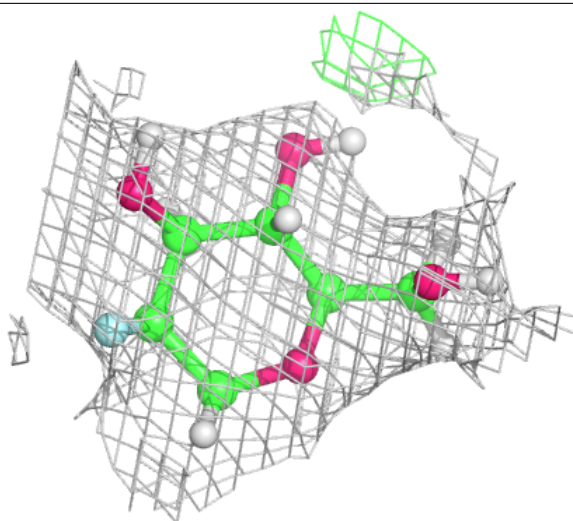
Electron density around MAF FFF 701:

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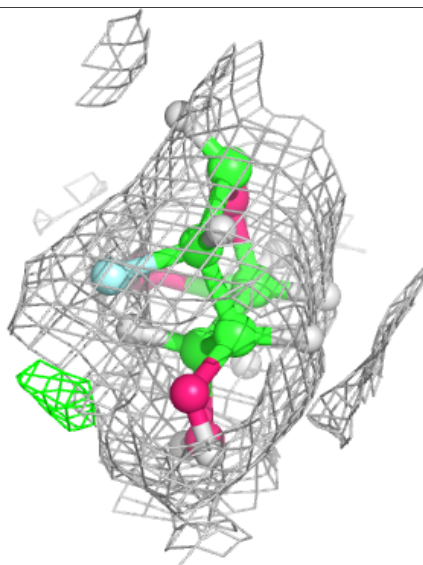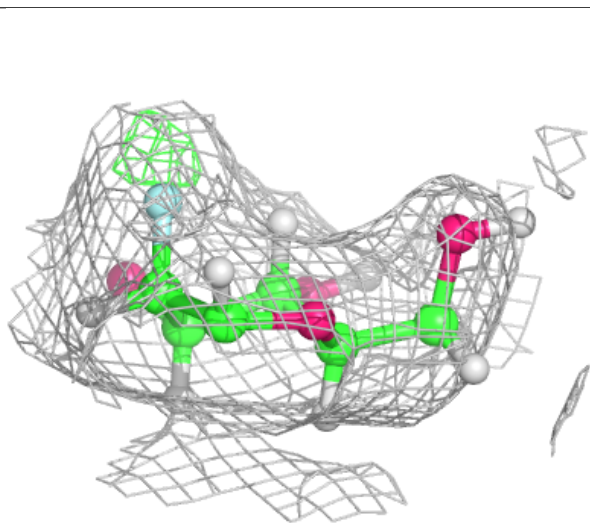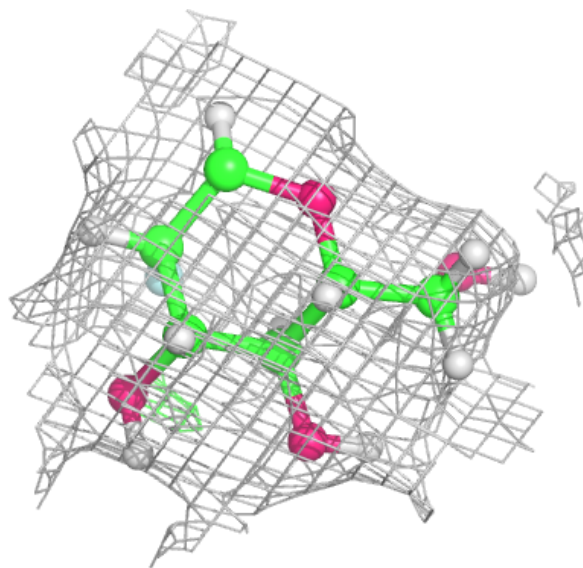
Electron density around MAF CCC 701:

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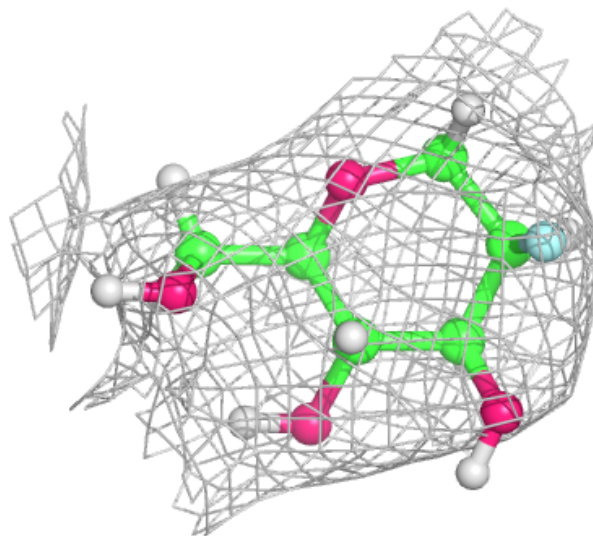and green (positive)
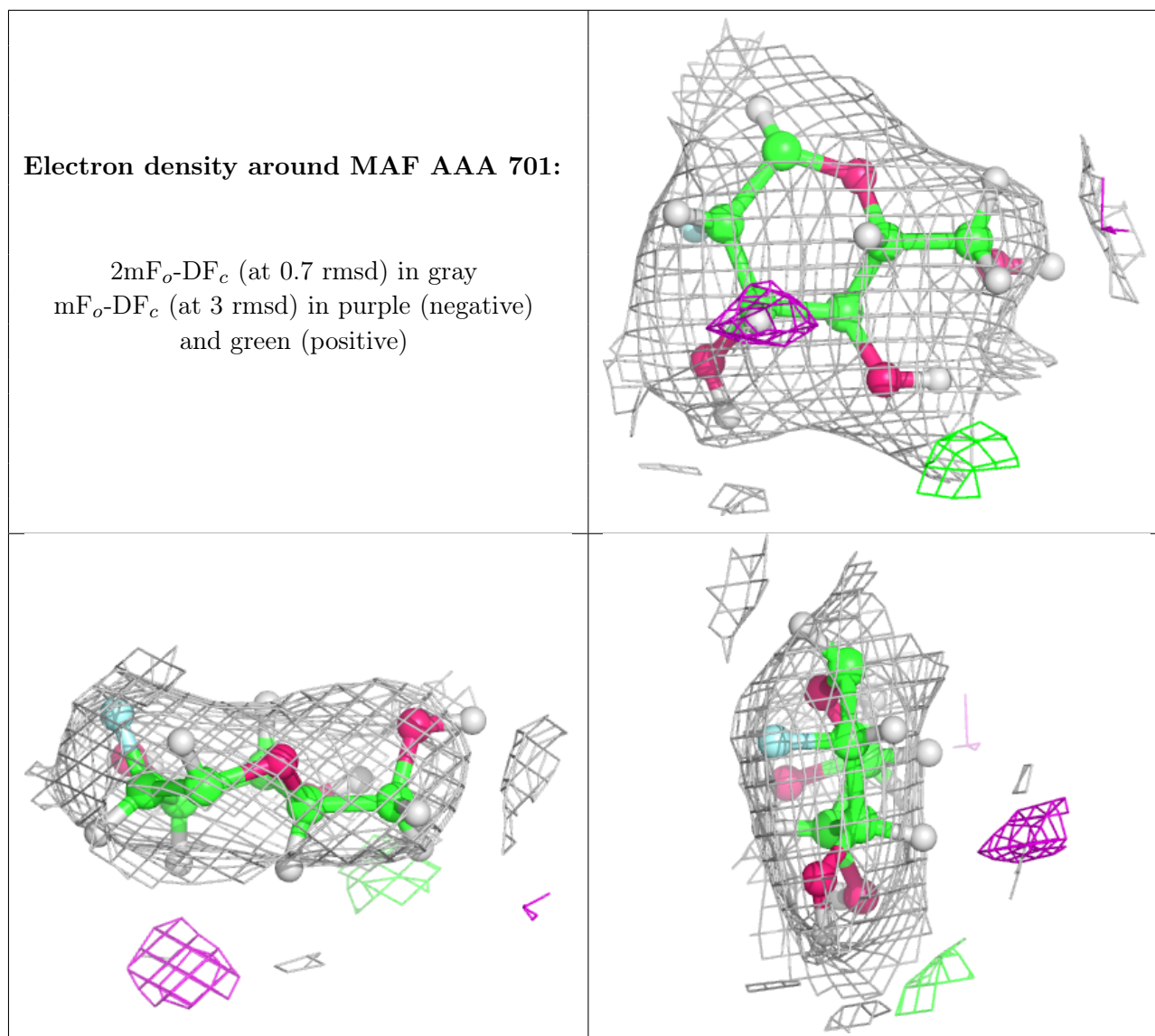
Electron density around MAF BBB 701:

$2mF_o$-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 DDD 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 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.