wwPDB X-ray Structure Validation Summary Report (i)

Mar 6, 2026 – 05:23 PM UTC

PDB ID	:	6T7G / pdb_00006t7g
Title	:	Bacteroides salyersiae GH164 beta-mannosidase in complex with mannoimidazole
Authors	:	Armstrong, Z.; Davies, G.
Deposited on	:	2019-10-21
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

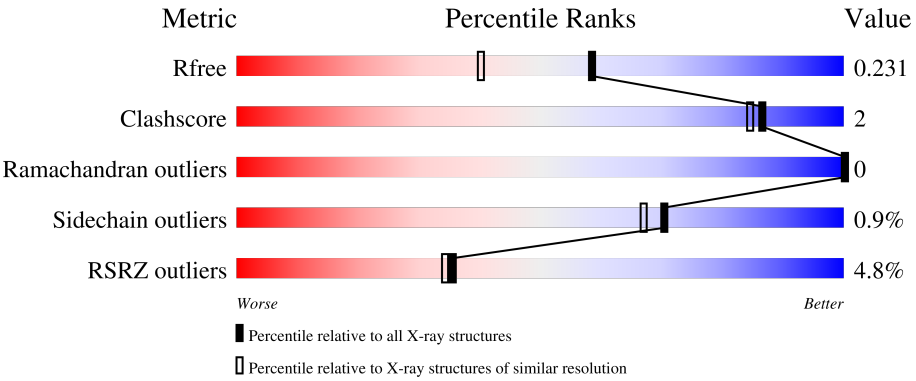
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	9% 92% 5% ·
1	BBB	674	4% 90% 6% ·
1	CCC	674	3% 91% 6% ·
1	DDD	674	5% 91% 6% ·
1	EEE	674	4% 90% 6% ·

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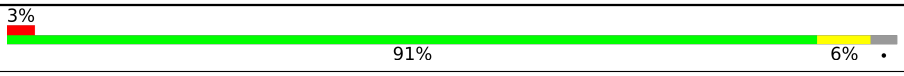
Mol	Chain	Length	Quality of chain
1	FFF	674	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 64543 atoms, of which 31126 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	661	Total	C	H	N	O	S	289	1	0
			10531	3434	5211	880	987	19			
1	DDD	658	Total	C	H	N	O	S	285	0	0
			10465	3415	5179	874	978	19			
1	CCC	654	Total	C	H	N	O	S	286	1	0
			10432	3399	5164	876	974	19			
1	BBB	652	Total	C	H	N	O	S	285	0	0
			10390	3388	5142	869	972	19			
1	FFF	654	Total	C	H	N	O	S	286	1	0
			10417	3396	5154	872	976	19			
1	EEE	648	Total	C	H	N	O	S	281	0	0
			10320	3367	5108	862	964	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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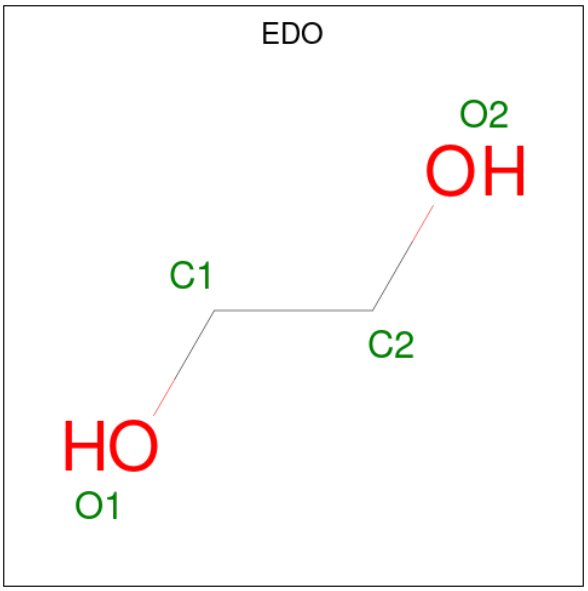
Chain	Residue	Modelled	Actual	Comment	Reference
FFF	23	LEU	-	expression tag	UNP I9SUA3
FFF	24	GLU	-	expression tag	UNP I9SUA3
FFF	25	VAL	-	expression tag	UNP I9SUA3
FFF	26	LEU	-	expression tag	UNP I9SUA3
FFF	27	PHE	-	expression tag	UNP I9SUA3
FFF	28	GLN	-	expression tag	UNP I9SUA3
FFF	29	GLY	-	expression 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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
2	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	FFF	1	Total	C	H	O	1	0
			10	2	6	2		
2	FFF	1	Total	C	H	O	1	0
			10	2	6	2		
2	FFF	1	Total	C	H	O	1	0
			10	2	6	2		

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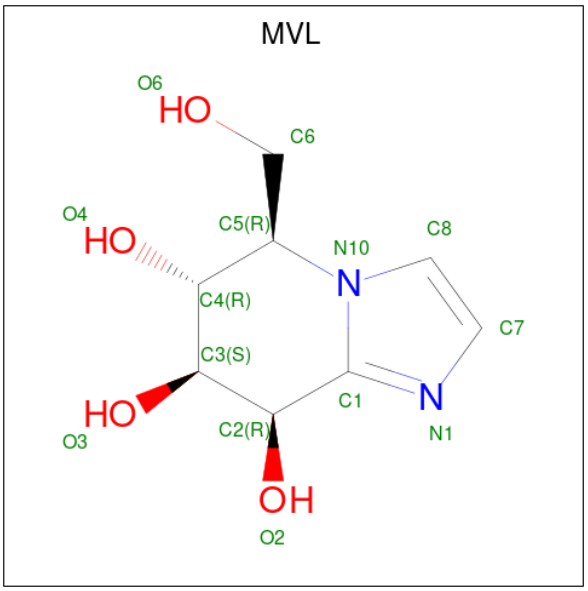
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	EEE	1	Total C H O 10 2 6 2	1	0
2	EEE	1	Total C H O 10 2 6 2	1	0

- Molecule 3 is (5R,6R,7S,8R)-5-(HYDROXYMETHYL)-5,6,7,8-TETRAHYDROIMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (CCD ID: MVL) (formula: $C_8H_{12}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C H N O 26 8 12 2 4	3	0
3	DDD	1	Total C H N O 26 8 12 2 4	3	0
3	CCC	1	Total C H N O 26 8 12 2 4	3	0
3	BBB	1	Total C H N O 26 8 12 2 4	3	0
3	FFF	1	Total C H N O 26 8 12 2 4	3	0
3	EEE	1	Total C H N O 26 8 12 2 4	3	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is water.

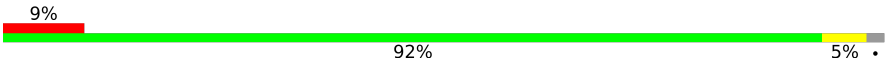
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	251	Total O 251 251	0	0
5	DDD	255	Total O 255 255	0	0
5	CCC	296	Total O 296 296	0	0
5	BBB	347	Total O 347 347	0	0
5	FFF	275	Total O 275 275	0	0
5	EEE	242	Total O 242 242	0	0

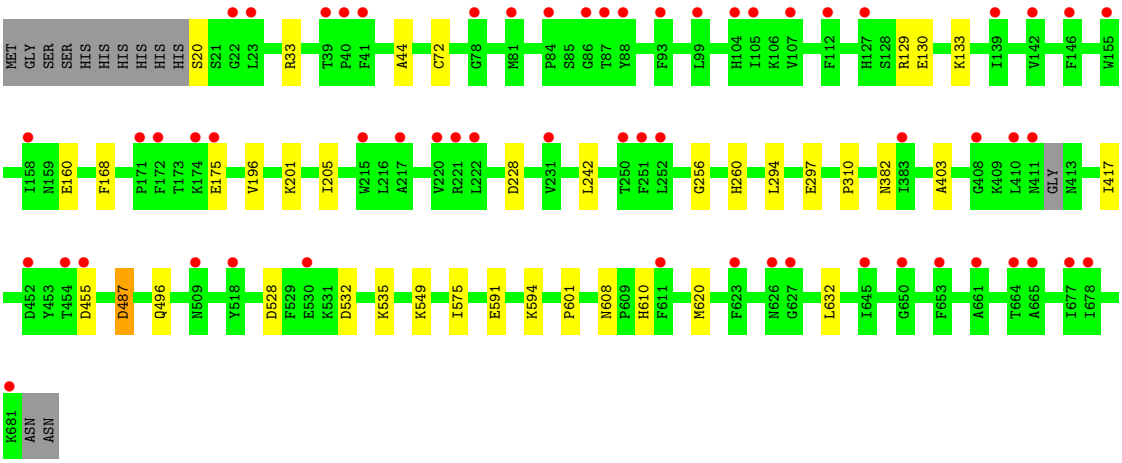
3 Residue-property plots (i)

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: Glyco_hydro_42M domain-containing protein

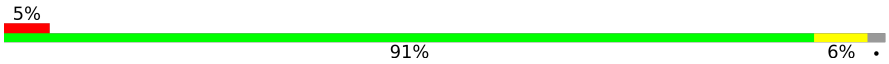
Chain AAA:

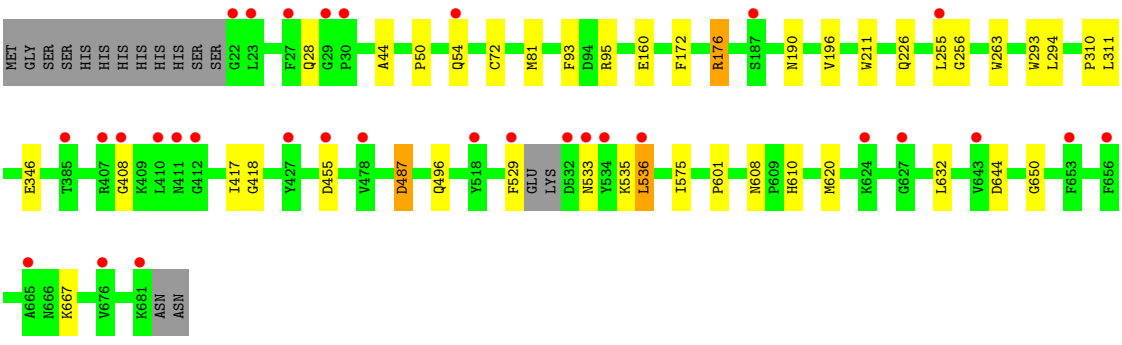




• Molecule 1: Glyco_hydro_42M domain-containing protein

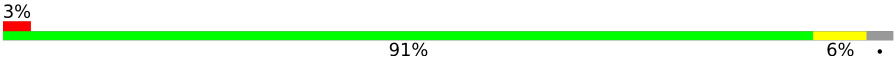
Chain DDD:

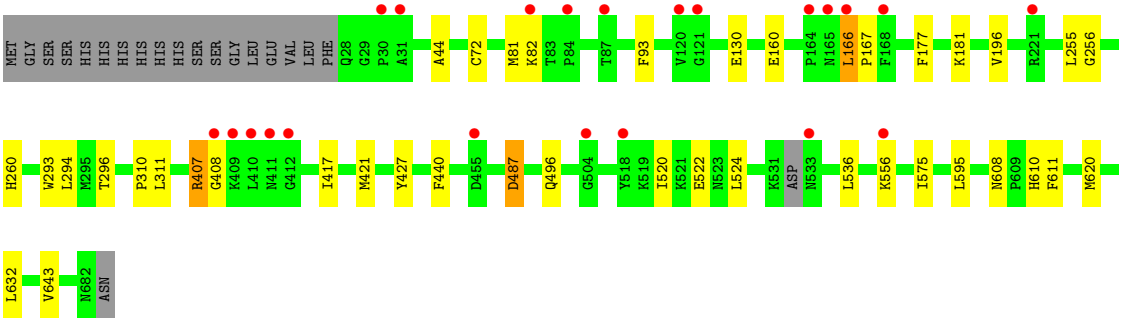




• Molecule 1: Glyco_hydro_42M domain-containing protein

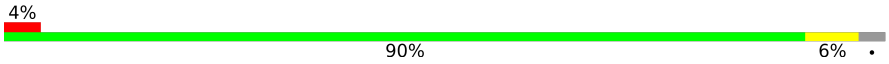
Chain CCC:

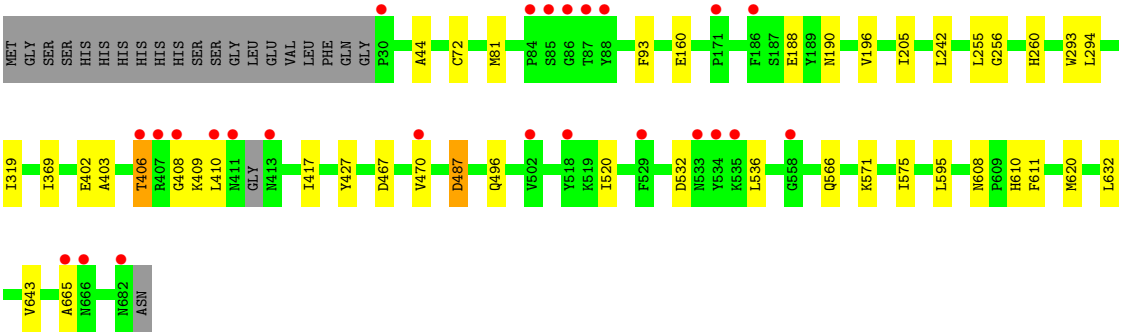




• Molecule 1: Glyco_hydro_42M domain-containing protein

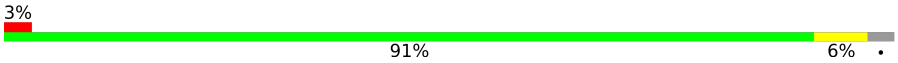
Chain BBB:

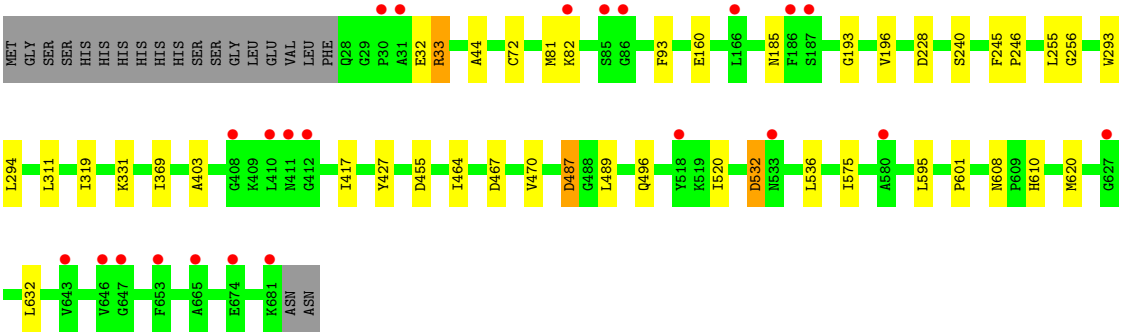




• Molecule 1: Glyco_hydro_42M domain-containing protein

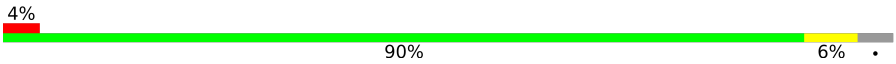
Chain FFF:

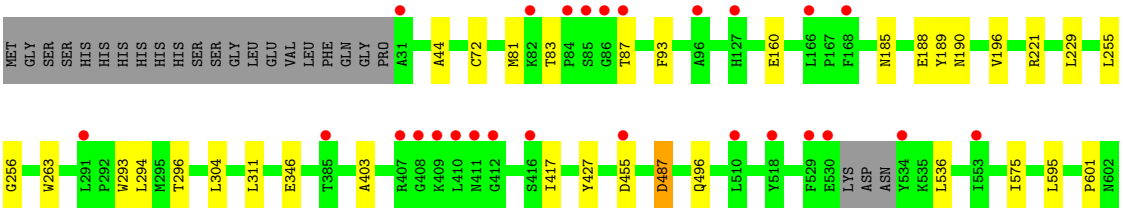


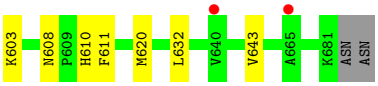


• Molecule 1: Glyco_hydro_42M domain-containing protein

Chain EEE:






K603
N608
P609
H610
F611
M620
L632
V640
V643
A665
K681
ASN
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.71Å 104.74Å 170.57Å 92.29° 97.27° 106.30°	Depositor
Resolution (Å)	168.66 – 1.80 168.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (168.66-1.80) 100.0 (168.66-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.206 , 0.231 0.206 , 0.231	Depositor DCC
R_{free} test set	21073 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	64543	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, MVL, EDO

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	1.00	0/5465	1.23	0/7397
1	BBB	1.02	0/5392	1.22	1/7298 (0.0%)
1	CCC	1.00	0/5412	1.22	0/7324
1	DDD	0.98	0/5431	1.22	3/7352 (0.0%)
1	EEE	0.99	1/5355 (0.0%)	1.21	0/7248
1	FFF	1.00	0/5408	1.22	2/7321 (0.0%)
All	All	1.00	1/32463 (0.0%)	1.22	6/43940 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	304	LEU	C-O	-6.63	1.18	1.23

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	406	THR	CA-CB-OG1	-8.67	96.59	109.60
1	DDD	176	ARG	CB-CG-CD	5.78	124.60	111.30
1	DDD	650	GLY	CA-C-O	-5.48	118.37	122.37
1	DDD	28	GLN	CB-CA-C	5.33	118.25	110.26
1	FFF	532	ASP	CA-C-N	5.14	129.43	122.07

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	5320	5211	5190	20	0
1	BBB	5248	5142	5122	25	0
1	CCC	5268	5164	5143	23	0
1	DDD	5286	5179	5159	25	0
1	EEE	5212	5108	5088	21	0
1	FFF	5263	5154	5134	21	0
2	AAA	8	12	12	1	0
2	BBB	16	24	24	0	0
2	CCC	12	18	18	0	0
2	DDD	8	12	12	0	0
2	EEE	8	12	12	0	0
2	FFF	12	18	18	0	0
3	AAA	14	12	12	2	0
3	BBB	14	12	12	2	0
3	CCC	14	12	12	2	0
3	DDD	14	12	12	3	0
3	EEE	14	12	12	3	0
3	FFF	14	12	12	1	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
4	DDD	1	0	0	0	0
4	EEE	1	0	0	0	0
4	FFF	1	0	0	0	0
5	AAA	251	0	0	2	0
5	BBB	347	0	0	1	0
5	CCC	296	0	0	1	0
5	DDD	255	0	0	1	0
5	EEE	242	0	0	0	0
5	FFF	275	0	0	1	0
All	All	33417	31126	31004	131	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 131 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:536:LEU:HD11	1:FFF:595:LEU:HD22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:408:GLY:O	1:BBB:410:LEU:CD1	2.41	0.68
1:FFF:33:ARG:HD3	1:FFF:228:ASP:OD1	1.93	0.68
1:BBB:408:GLY:O	1:BBB:410:LEU:HD13	1.94	0.67
1:CCC:536:LEU:HD11	1:CCC:595:LEU:HD22	1.75	0.67

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	658/674 (98%)	640 (97%)	18 (3%)	0	100	100
1	BBB	648/674 (96%)	629 (97%)	19 (3%)	0	100	100
1	CCC	651/674 (97%)	631 (97%)	20 (3%)	0	100	100
1	DDD	654/674 (97%)	635 (97%)	19 (3%)	0	100	100
1	EEE	644/674 (96%)	625 (97%)	19 (3%)	0	100	100
1	FFF	653/674 (97%)	632 (97%)	21 (3%)	0	100	100
All	All	3908/4044 (97%)	3792 (97%)	116 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	572/582 (98%)	568 (99%)	4 (1%)	76	73
1	BBB	564/582 (97%)	561 (100%)	3 (0%)	81	80
1	CCC	565/582 (97%)	557 (99%)	8 (1%)	59	52
1	DDD	567/582 (97%)	564 (100%)	3 (0%)	81	80
1	EEE	559/582 (96%)	555 (99%)	4 (1%)	76	73
1	FFF	565/582 (97%)	556 (98%)	9 (2%)	55	47
All	All	3392/3492 (97%)	3361 (99%)	31 (1%)	70	67

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	556	LYS
1	EEE	296	THR
1	BBB	532	ASP
1	EEE	427	TYR
1	FFF	427	TYR

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MVL	FFF	704	-	14,15,15	1.03	1 (7%)	14,22,22	0.98	0
3	MVL	EEE	703	-	14,15,15	0.50	0	14,22,22	0.90	1 (7%)
3	MVL	AAA	702	-	14,15,15	1.04	1 (7%)	14,22,22	1.05	1 (7%)
2	EDO	FFF	702	-	3,3,3	0.11	0	2,2,2	0.18	0
2	EDO	FFF	701	-	3,3,3	0.22	0	2,2,2	0.12	0
2	EDO	BBB	702	-	3,3,3	0.17	0	2,2,2	0.11	0
2	EDO	AAA	703	-	3,3,3	0.12	0	2,2,2	0.17	0
3	MVL	CCC	704	-	14,15,15	0.77	1 (7%)	14,22,22	0.90	0
2	EDO	BBB	703	-	3,3,3	0.19	0	2,2,2	0.54	0
2	EDO	BBB	705	-	3,3,3	0.07	0	2,2,2	0.09	0
3	MVL	DDD	702	-	14,15,15	1.13	2 (14%)	14,22,22	1.03	1 (7%)
3	MVL	BBB	704	-	14,15,15	0.80	0	14,22,22	0.92	1 (7%)
2	EDO	EEE	701	-	3,3,3	0.34	0	2,2,2	0.19	0
2	EDO	BBB	701	-	3,3,3	0.34	0	2,2,2	0.48	0
2	EDO	DDD	703	-	3,3,3	0.32	0	2,2,2	0.42	0
2	EDO	FFF	703	-	3,3,3	0.25	0	2,2,2	0.43	0
2	EDO	CCC	702	-	3,3,3	0.22	0	2,2,2	0.15	0
2	EDO	DDD	701	-	3,3,3	0.13	0	2,2,2	0.23	0
2	EDO	EEE	702	-	3,3,3	0.23	0	2,2,2	0.16	0
2	EDO	CCC	703	-	3,3,3	0.03	0	2,2,2	0.12	0
2	EDO	CCC	701	-	3,3,3	0.32	0	2,2,2	0.05	0
2	EDO	AAA	701	-	3,3,3	0.19	0	2,2,2	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MVL	FFF	704	-	-	0/2/22/22	0/2/2/2
3	MVL	EEE	703	-	-	0/2/22/22	0/2/2/2
3	MVL	AAA	702	-	-	0/2/22/22	0/2/2/2
2	EDO	FFF	702	-	-	0/1/1/1	-
2	EDO	FFF	701	-	-	1/1/1/1	-
2	EDO	BBB	702	-	-	0/1/1/1	-
2	EDO	AAA	703	-	-	1/1/1/1	-
3	MVL	CCC	704	-	-	0/2/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	BBB	703	-	-	1/1/1/1	-
2	EDO	BBB	705	-	-	0/1/1/1	-
3	MVL	DDD	702	-	-	0/2/22/22	0/2/2/2
3	MVL	BBB	704	-	-	0/2/22/22	0/2/2/2
2	EDO	EEE	701	-	-	1/1/1/1	-
2	EDO	BBB	701	-	-	0/1/1/1	-
2	EDO	DDD	703	-	-	1/1/1/1	-
2	EDO	FFF	703	-	-	1/1/1/1	-
2	EDO	CCC	702	-	-	0/1/1/1	-
2	EDO	DDD	701	-	-	0/1/1/1	-
2	EDO	EEE	702	-	-	0/1/1/1	-
2	EDO	CCC	703	-	-	0/1/1/1	-
2	EDO	CCC	701	-	-	0/1/1/1	-
2	EDO	AAA	701	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	702	MVL	C1-N10	-3.18	1.32	1.36
3	FFF	704	MVL	C1-N1	3.09	1.36	1.32
3	DDD	702	MVL	C1-N1	2.90	1.36	1.32
3	DDD	702	MVL	C1-N10	-2.62	1.33	1.36
3	CCC	704	MVL	C1-N1	2.33	1.35	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	EEE	703	MVL	C4-C3-C2	2.58	114.30	110.22
3	BBB	704	MVL	C6-C5-C4	2.38	116.53	112.93
3	AAA	702	MVL	O6-C6-C5	-2.33	106.39	111.55
3	DDD	702	MVL	C6-C5-C4	2.19	116.23	112.93

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	FFF	701	EDO	O1-C1-C2-O2
2	BBB	703	EDO	O1-C1-C2-O2
2	FFF	703	EDO	O1-C1-C2-O2
2	DDD	703	EDO	O1-C1-C2-O2
2	AAA	703	EDO	O1-C1-C2-O2

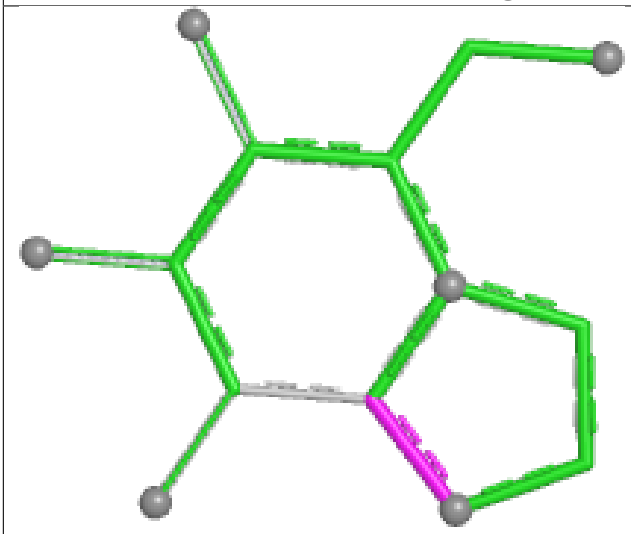
There are no ring outliers.

7 monomers are involved in 13 short contacts:

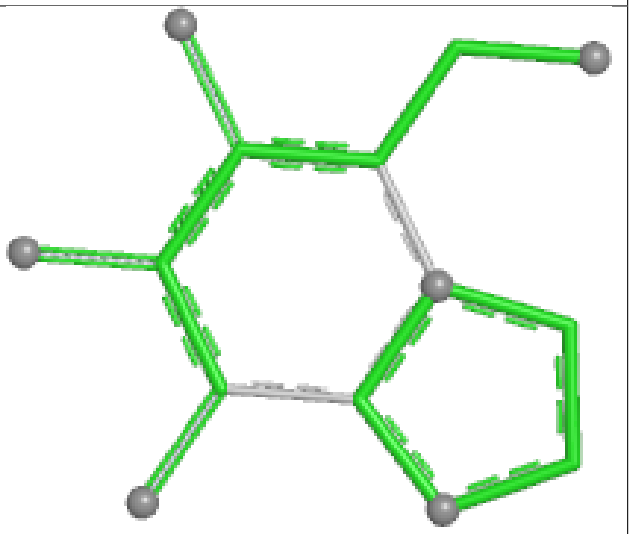
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	FFF	704	MVL	1	0
3	EEE	703	MVL	3	0
3	AAA	702	MVL	2	0
2	AAA	703	EDO	1	0
3	CCC	704	MVL	2	0
3	DDD	702	MVL	3	0
3	BBB	704	MVL	2	0

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.

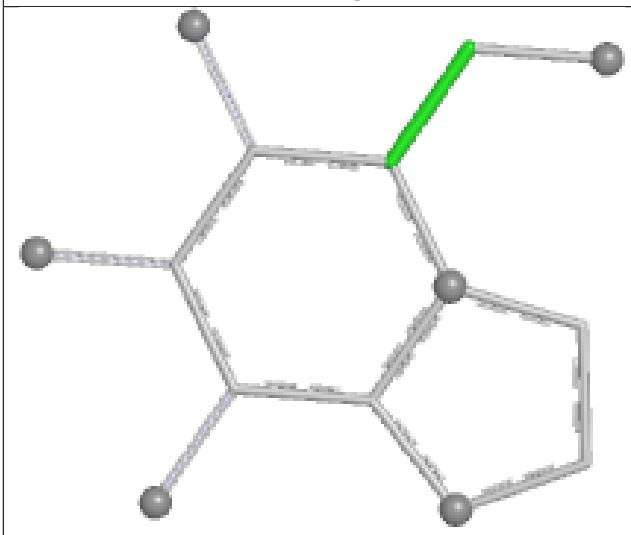
Ligand MVL FFF 704



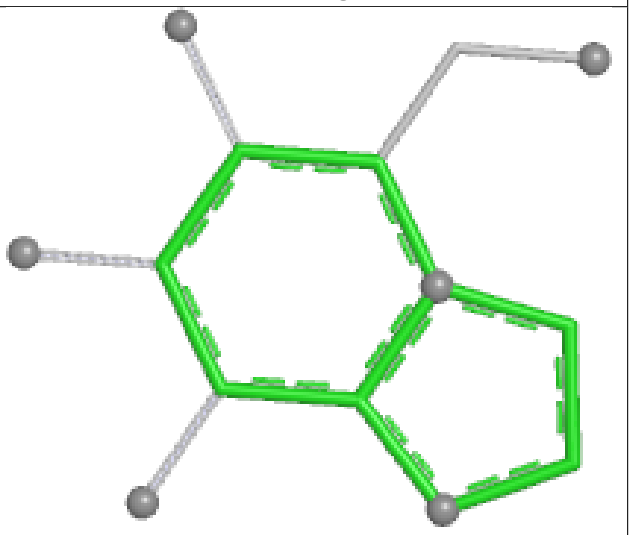
Bond lengths



Bond angles

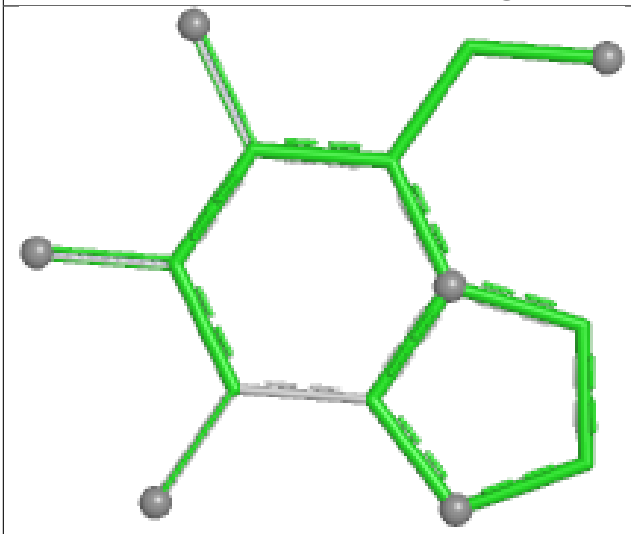


Torsions



Rings

Ligand MVL EEE 703



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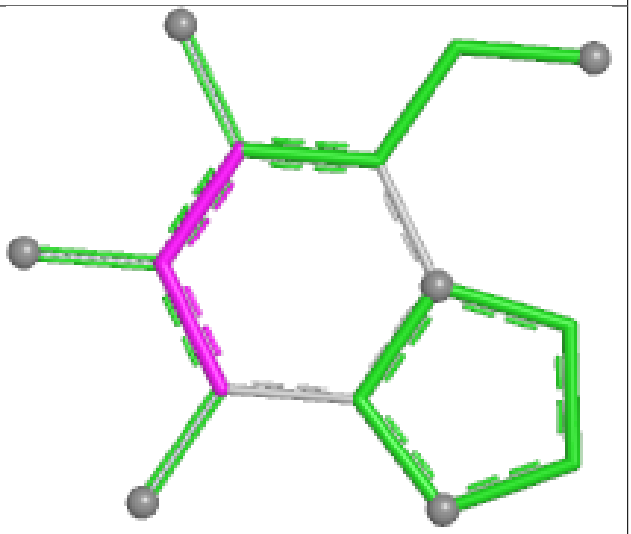

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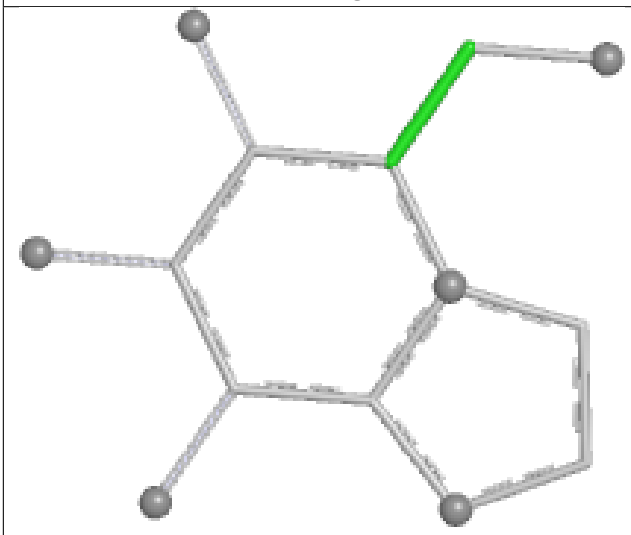
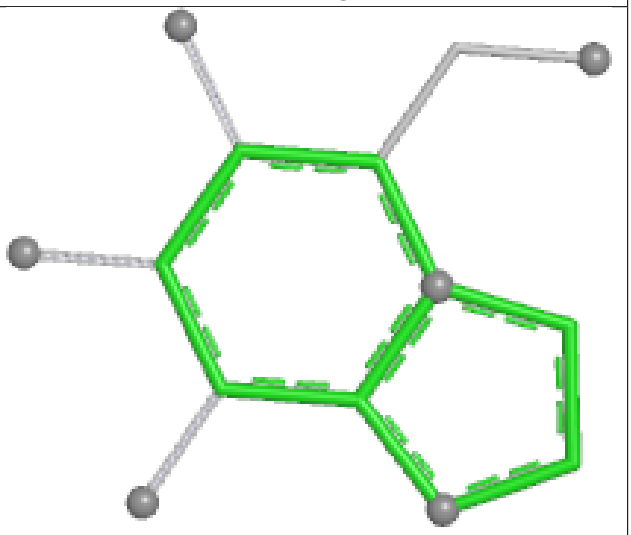
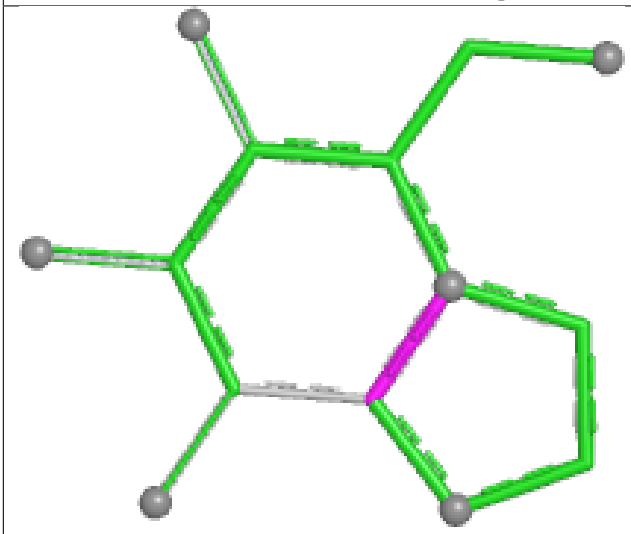


Torsions



Rings

Ligand MVL AAA 702



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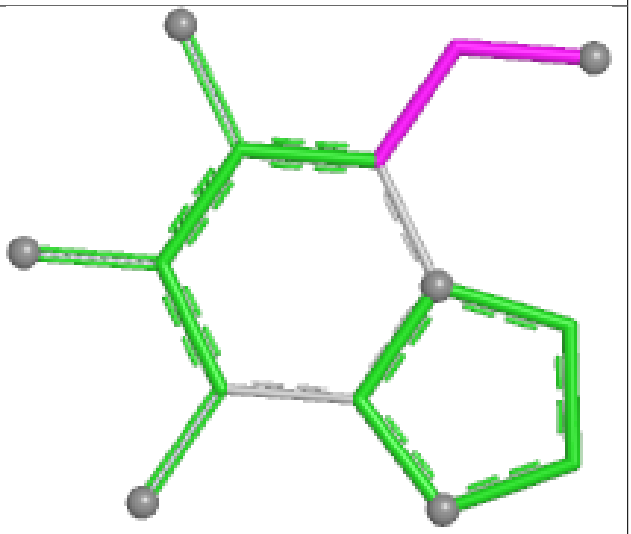

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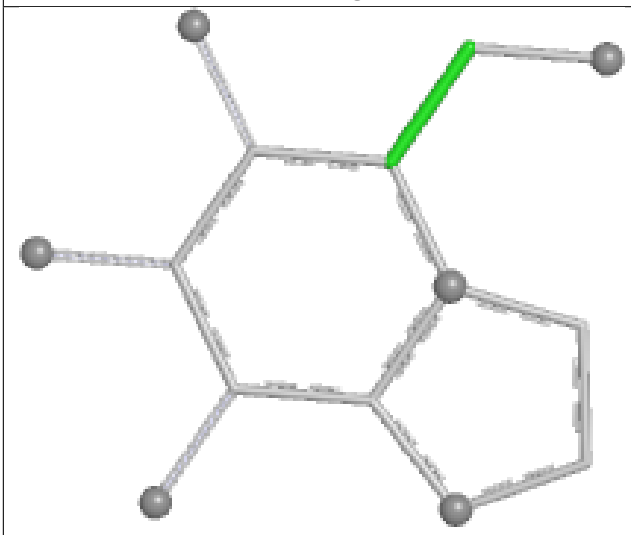
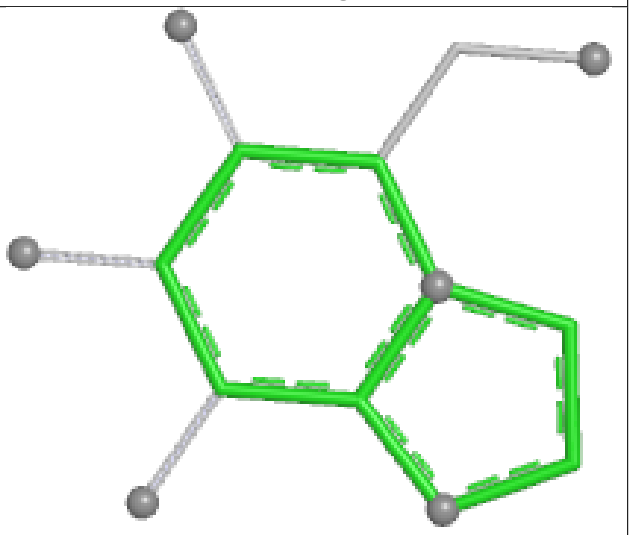
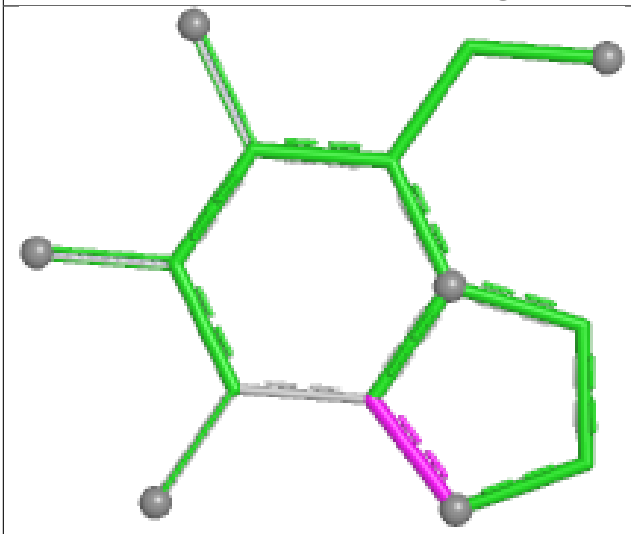


Torsions

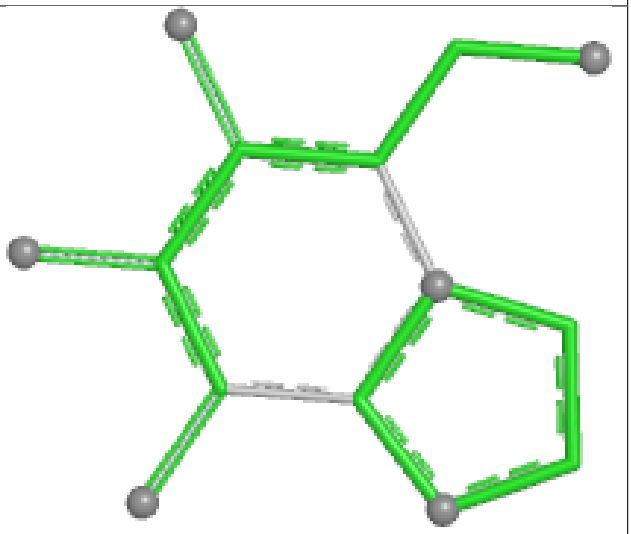


Rings

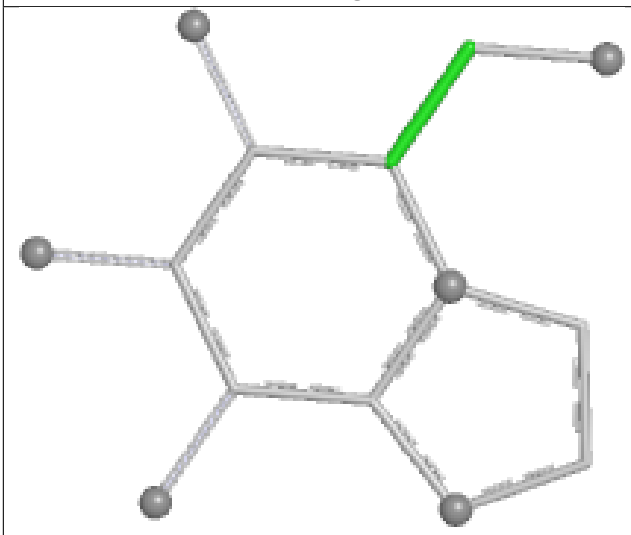
Ligand MVL CCC 704



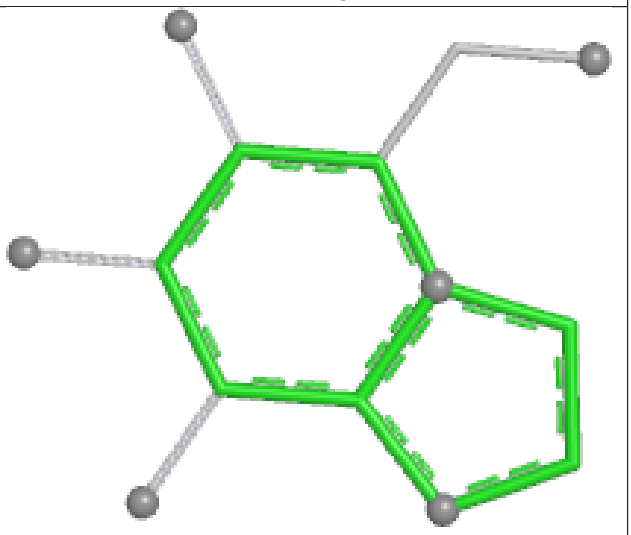
Bond lengths



Bond angles

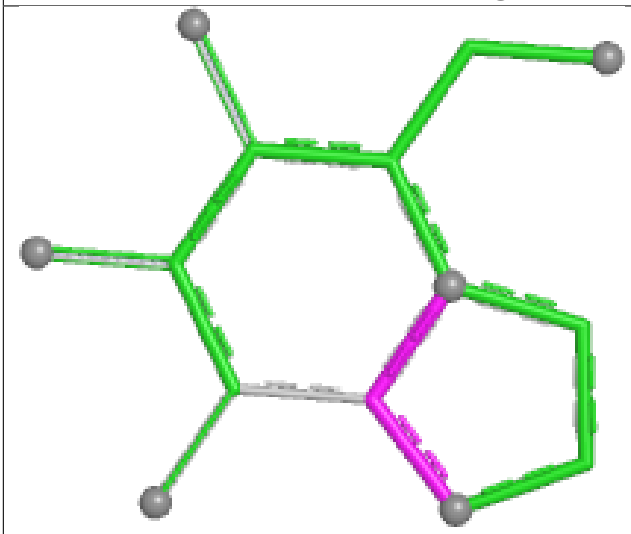


Torsions

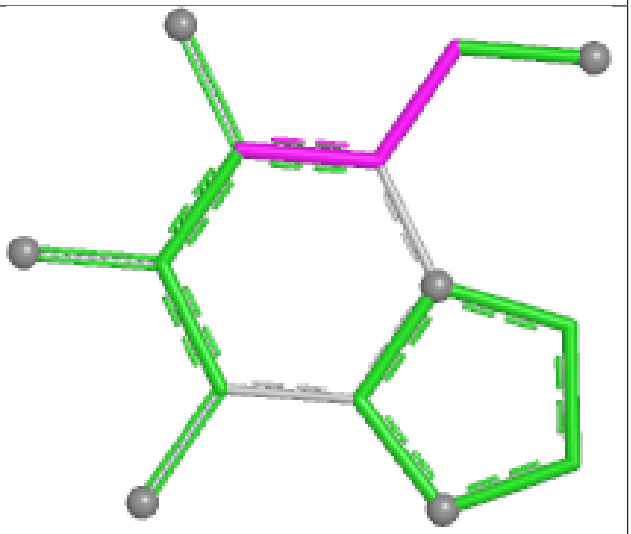


Rings

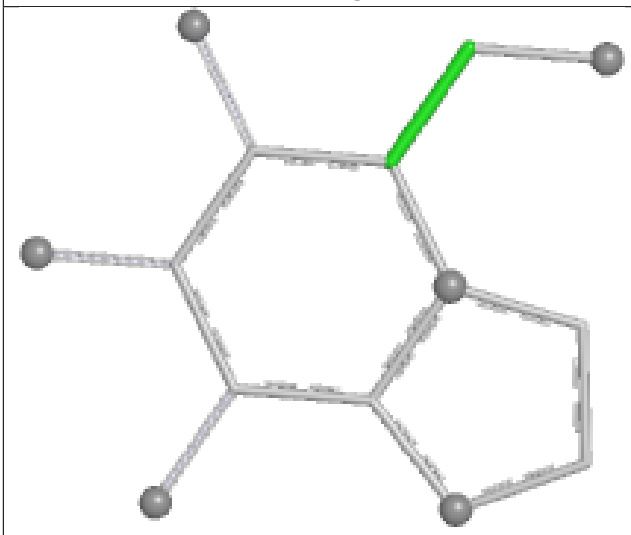
Ligand MVL DDD 702



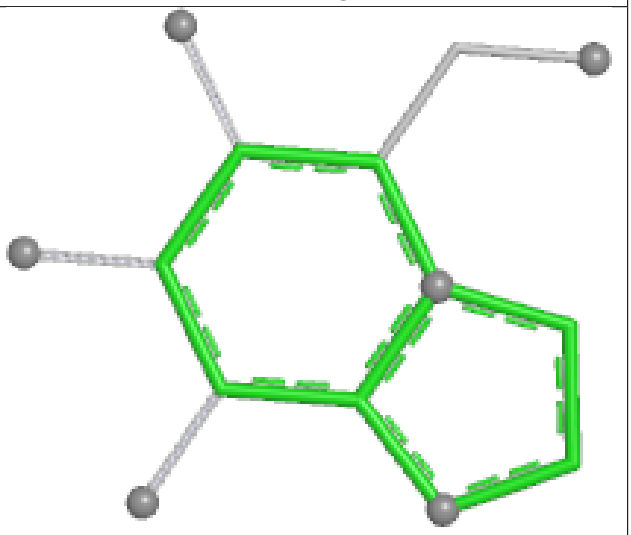
Bond lengths



Bond angles

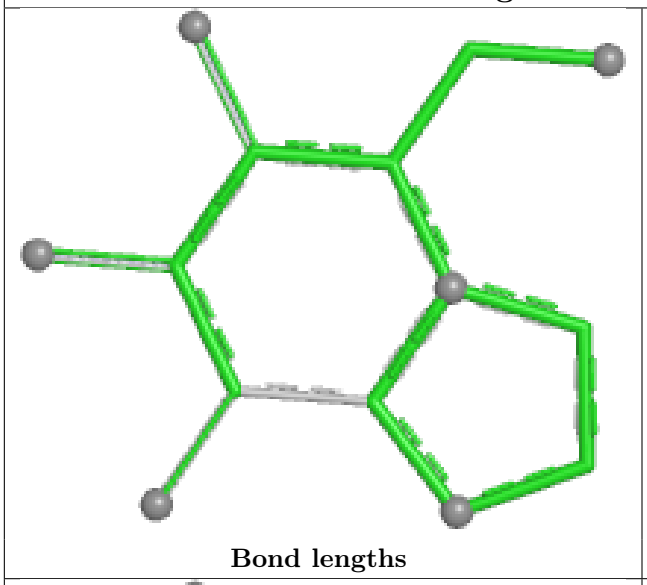


Torsions

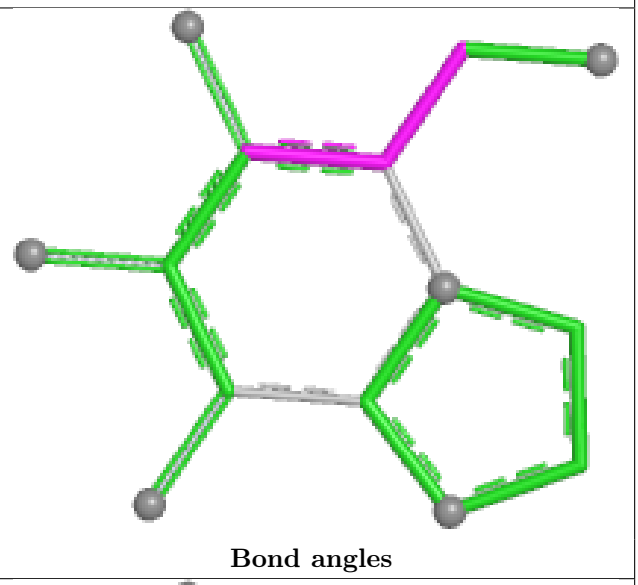


Rings

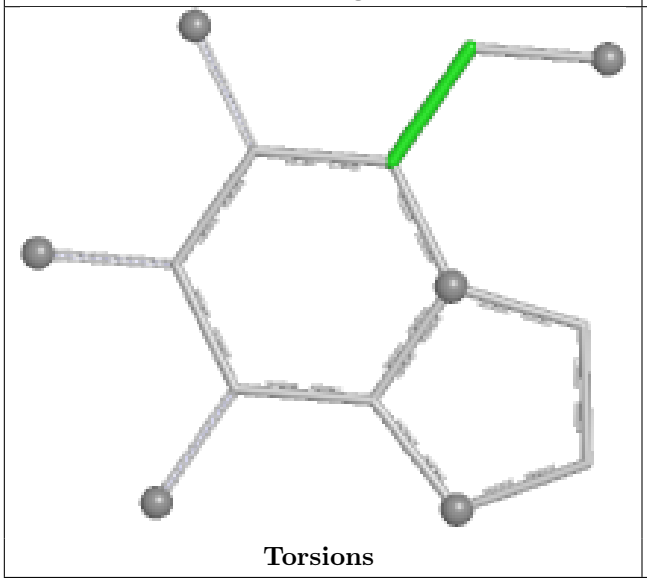
Ligand MVL BBB 704



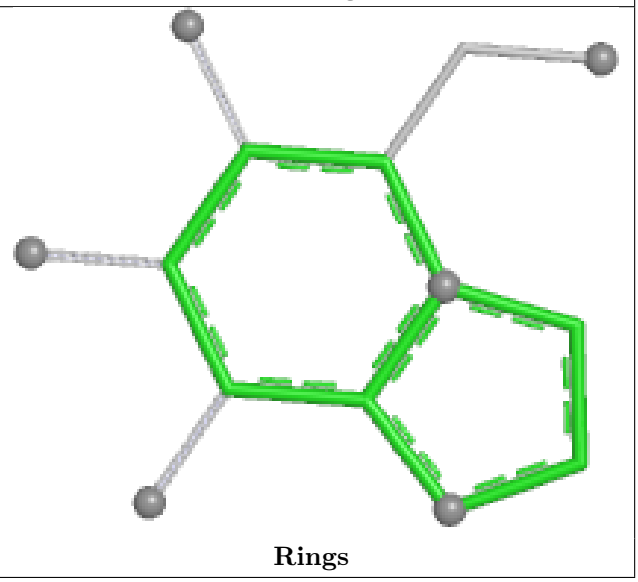
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	661/674 (98%)	0.83	59 (8%)	15	13	16, 41, 66, 105	1 (0%)
1	BBB	652/674 (96%)	0.31	25 (3%)	44	44	23, 34, 56, 89	0
1	CCC	654/674 (97%)	0.46	22 (3%)	48	48	20, 36, 62, 90	1 (0%)
1	DDD	658/674 (97%)	0.60	31 (4%)	36	35	28, 41, 66, 101	0
1	EEE	648/674 (96%)	0.57	28 (4%)	40	39	25, 41, 66, 102	0
1	FFF	654/674 (97%)	0.55	23 (3%)	47	47	14, 38, 61, 95	1 (0%)
All	All	3927/4044 (97%)	0.55	188 (4%)	35	34	14, 39, 64, 105	3 (0%)

The worst 5 of 188 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	412	GLY	6.8
1	DDD	529	PHE	5.7
1	FFF	412	GLY	5.0
1	AAA	78	GLY	5.0
1	AAA	665	ALA	4.9

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 oligosaccharides in this entry.

6.4 Ligands (i)

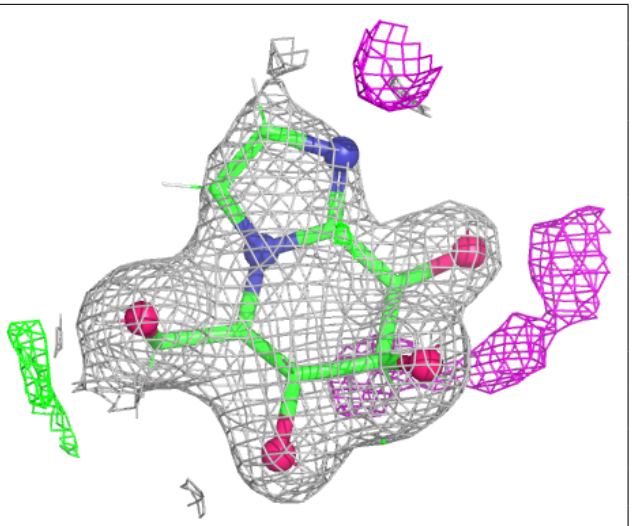
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

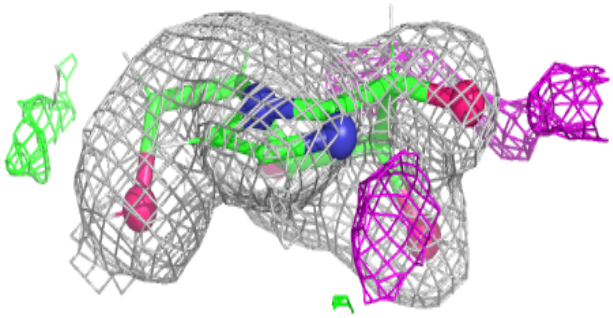
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	DDD	703	4/4	0.82	0.20	51,57,64,64	1
2	EDO	BBB	705	4/4	0.85	0.15	46,53,60,60	1
3	MVL	AAA	702	14/14	0.86	0.12	37,47,57,57	3
2	EDO	EEE	702	4/4	0.87	0.12	53,57,60,60	1
2	EDO	FFF	703	4/4	0.87	0.12	43,44,47,47	1
3	MVL	CCC	704	14/14	0.87	0.13	31,42,56,59	3
3	MVL	FFF	704	14/14	0.88	0.12	35,42,60,61	3
2	EDO	BBB	703	4/4	0.89	0.14	57,62,63,63	1
2	EDO	DDD	701	4/4	0.90	0.16	58,62,69,69	1
3	MVL	DDD	702	14/14	0.90	0.10	38,43,53,54	3
2	EDO	AAA	703	4/4	0.91	0.13	54,56,62,62	1
3	MVL	EEE	703	14/14	0.91	0.10	36,41,52,55	3
2	EDO	CCC	702	4/4	0.92	0.12	44,46,53,53	1
2	EDO	CCC	703	4/4	0.92	0.12	53,55,66,66	1
2	EDO	FFF	701	4/4	0.92	0.12	55,59,62,62	1
3	MVL	BBB	704	14/14	0.92	0.10	32,36,49,49	3
2	EDO	BBB	701	4/4	0.92	0.12	39,44,44,44	1
2	EDO	BBB	702	4/4	0.92	0.13	49,50,53,53	1
2	EDO	AAA	701	4/4	0.93	0.12	46,48,54,54	1
2	EDO	CCC	701	4/4	0.94	0.11	44,48,50,50	1
2	EDO	EEE	701	4/4	0.94	0.09	46,47,52,52	1
2	EDO	FFF	702	4/4	0.94	0.10	48,50,53,53	1
4	CL	AAA	704	1/1	0.98	0.11	41,41,41,41	0
4	CL	CCC	705	1/1	0.98	0.05	32,32,32,32	0
4	CL	BBB	706	1/1	0.98	0.10	33,33,33,33	0
4	CL	FFF	705	1/1	0.98	0.04	31,31,31,31	0
4	CL	DDD	704	1/1	0.99	0.04	34,34,34,34	0
4	CL	EEE	704	1/1	0.99	0.04	37,37,37,37	0

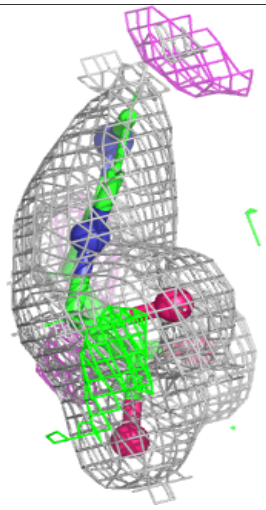
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MVL AAA 702:

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

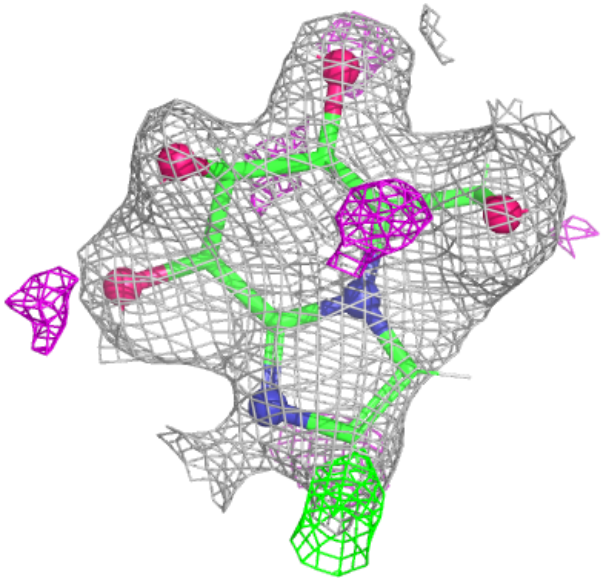


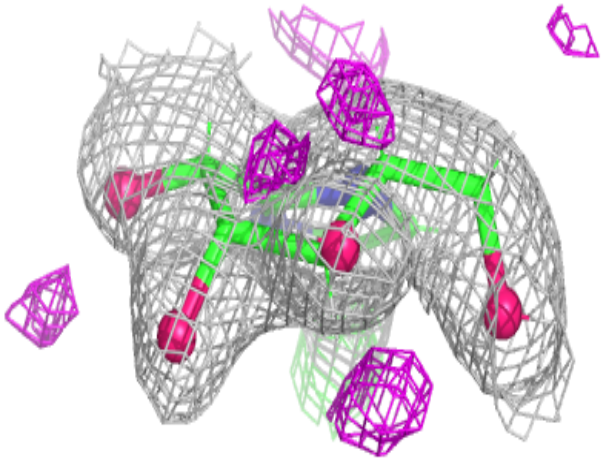


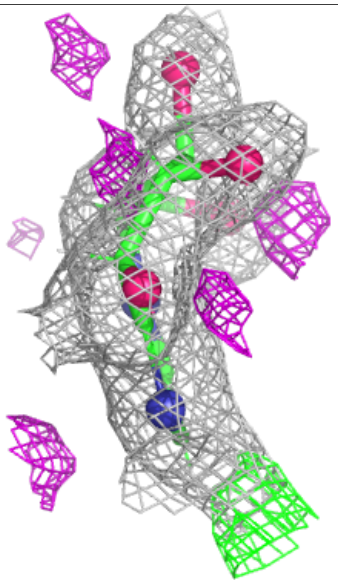


Electron density around MVL CCC 704:

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

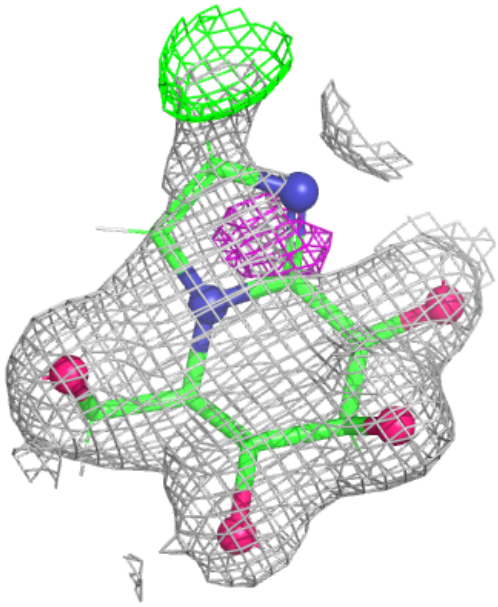


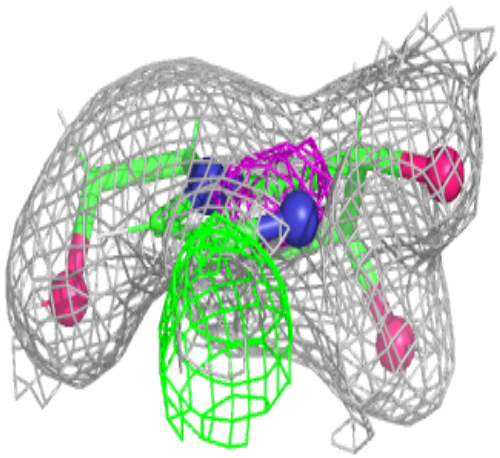


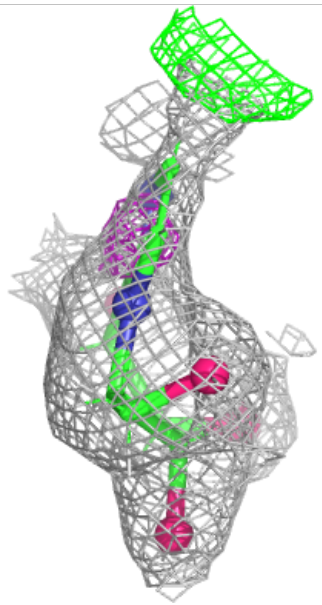


Electron density around MVL FFF 704:

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

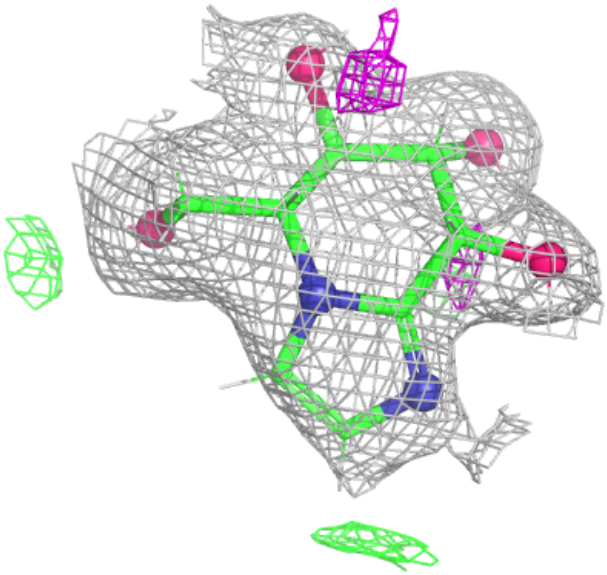


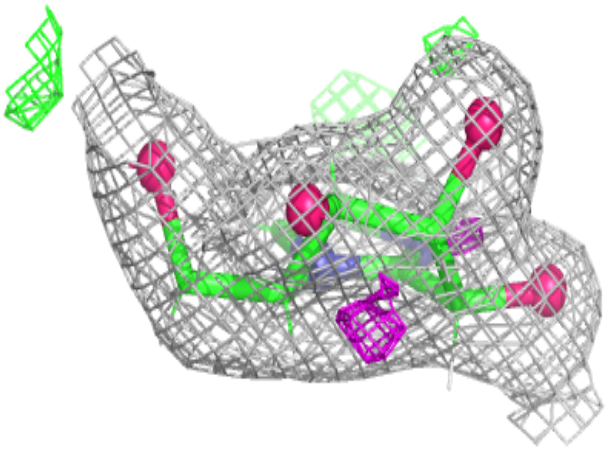


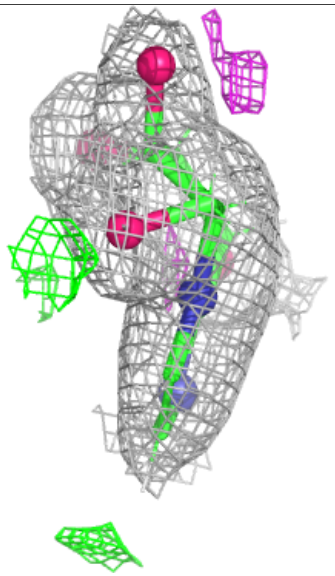


Electron density around MVL DDD 702:

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

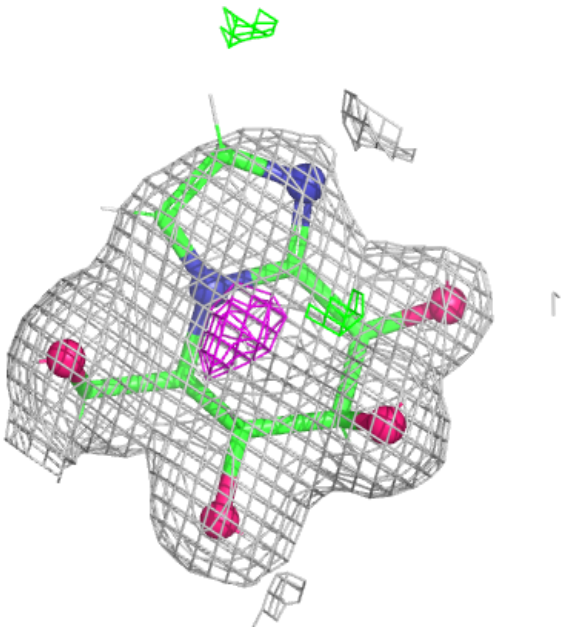


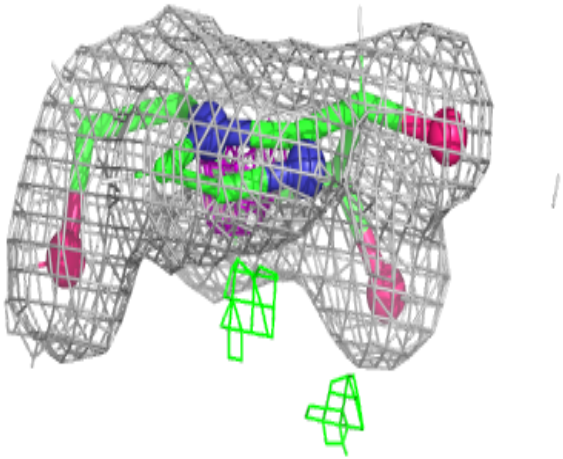


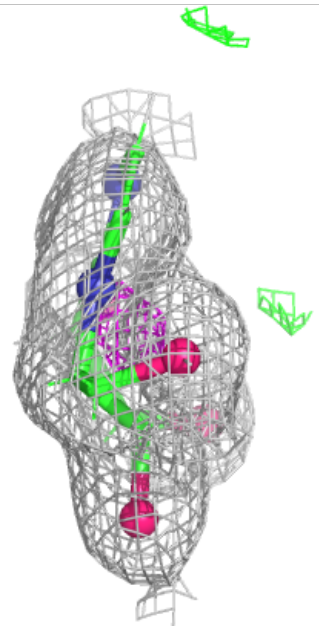


Electron density around MVL EEE 703:

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

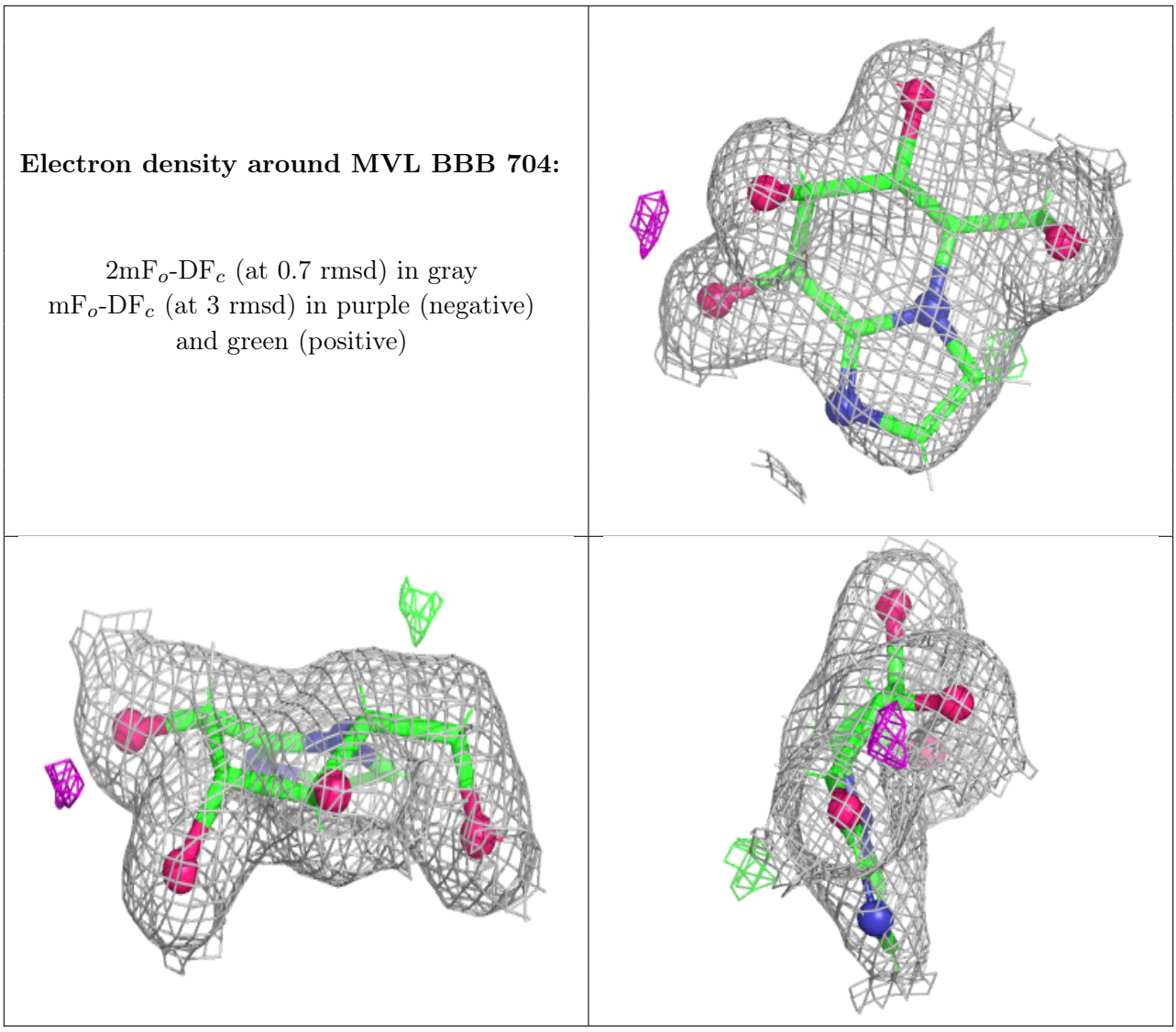






Electron density around MVL BBB 704:

$2mF_o$-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.