



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:33 PM UTC

PDB ID : 8P4H / pdb_00008p4h
Title : Crystal structure of human methionine adenosyltransferase 2A (MAT2A) in complex with SAM and allosteric compound IDEAYA cmpd A
Authors : Thomsen, M.; Thieulin-Pardo, G.; Neumann, L.
Deposited on : 2023-05-21
Resolution : 1.71 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

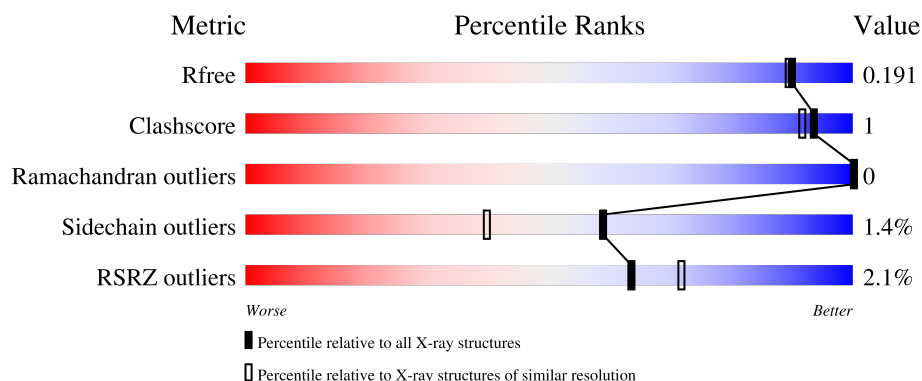
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	412	0% 89% 5% 6%
1	B	412	2% 84% 6% 10%
1	C	412	3% 87% • 9%
1	D	412	2% 88% • 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13205 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called S-adenosylmethionine synthase isoform type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	25	7	0
			3073	1943	536	582	12			
1	B	371	Total	C	N	O	S	29	4	0
			2913	1843	506	552	12			
1	C	376	Total	C	N	O	S	22	8	0
			2979	1881	517	568	13			
1	D	376	Total	C	N	O	S	39	4	0
			2961	1871	514	564	12			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP P31153
A	-15	ALA	-	expression tag	UNP P31153
A	-14	HIS	-	expression tag	UNP P31153
A	-13	HIS	-	expression tag	UNP P31153
A	-12	HIS	-	expression tag	UNP P31153
A	-11	HIS	-	expression tag	UNP P31153
A	-10	HIS	-	expression tag	UNP P31153
A	-9	HIS	-	expression tag	UNP P31153
A	-8	SER	-	expression tag	UNP P31153
A	-7	SER	-	expression tag	UNP P31153
A	-6	GLY	-	expression tag	UNP P31153
A	-5	GLU	-	expression tag	UNP P31153
A	-4	ASN	-	expression tag	UNP P31153
A	-3	LEU	-	expression tag	UNP P31153
A	-2	TYR	-	expression tag	UNP P31153
A	-1	PHE	-	expression tag	UNP P31153
A	0	GLN	-	expression tag	UNP P31153
A	1	GLY	-	expression tag	UNP P31153
B	-16	MET	-	initiating methionine	UNP P31153
B	-15	ALA	-	expression tag	UNP P31153
B	-14	HIS	-	expression tag	UNP P31153

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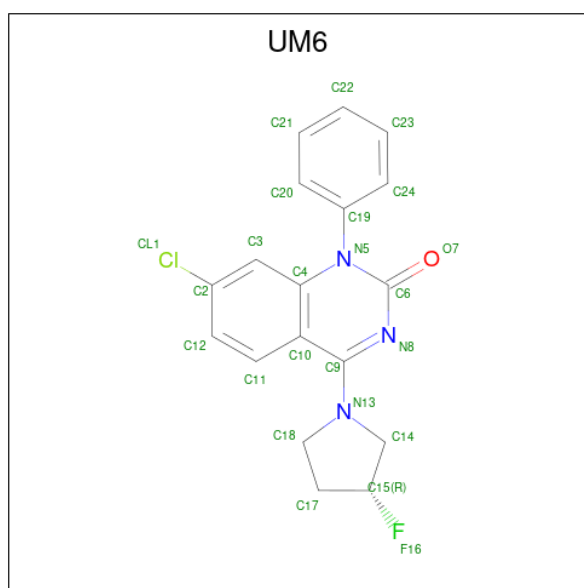
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP P31153
B	-12	HIS	-	expression tag	UNP P31153
B	-11	HIS	-	expression tag	UNP P31153
B	-10	HIS	-	expression tag	UNP P31153
B	-9	HIS	-	expression tag	UNP P31153
B	-8	SER	-	expression tag	UNP P31153
B	-7	SER	-	expression tag	UNP P31153
B	-6	GLY	-	expression tag	UNP P31153
B	-5	GLU	-	expression tag	UNP P31153
B	-4	ASN	-	expression tag	UNP P31153
B	-3	LEU	-	expression tag	UNP P31153
B	-2	TYR	-	expression tag	UNP P31153
B	-1	PHE	-	expression tag	UNP P31153
B	0	GLN	-	expression tag	UNP P31153
B	1	GLY	-	expression tag	UNP P31153
C	-16	MET	-	initiating methionine	UNP P31153
C	-15	ALA	-	expression tag	UNP P31153
C	-14	HIS	-	expression tag	UNP P31153
C	-13	HIS	-	expression tag	UNP P31153
C	-12	HIS	-	expression tag	UNP P31153
C	-11	HIS	-	expression tag	UNP P31153
C	-10	HIS	-	expression tag	UNP P31153
C	-9	HIS	-	expression tag	UNP P31153
C	-8	SER	-	expression tag	UNP P31153
C	-7	SER	-	expression tag	UNP P31153
C	-6	GLY	-	expression tag	UNP P31153
C	-5	GLU	-	expression tag	UNP P31153
C	-4	ASN	-	expression tag	UNP P31153
C	-3	LEU	-	expression tag	UNP P31153
C	-2	TYR	-	expression tag	UNP P31153
C	-1	PHE	-	expression tag	UNP P31153
C	0	GLN	-	expression tag	UNP P31153
C	1	GLY	-	expression tag	UNP P31153
D	-16	MET	-	initiating methionine	UNP P31153
D	-15	ALA	-	expression tag	UNP P31153
D	-14	HIS	-	expression tag	UNP P31153
D	-13	HIS	-	expression tag	UNP P31153
D	-12	HIS	-	expression tag	UNP P31153
D	-11	HIS	-	expression tag	UNP P31153
D	-10	HIS	-	expression tag	UNP P31153
D	-9	HIS	-	expression tag	UNP P31153
D	-8	SER	-	expression tag	UNP P31153

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	SER	-	expression tag	UNP P31153
D	-6	GLY	-	expression tag	UNP P31153
D	-5	GLU	-	expression tag	UNP P31153
D	-4	ASN	-	expression tag	UNP P31153
D	-3	LEU	-	expression tag	UNP P31153
D	-2	TYR	-	expression tag	UNP P31153
D	-1	PHE	-	expression tag	UNP P31153
D	0	GLN	-	expression tag	UNP P31153
D	1	GLY	-	expression tag	UNP P31153

- Molecule 2 is 7-chloranyl-4-[(3R)-3-fluoranylpyrrolidin-1-yl]-1-phenyl-quinazolin-2-one (CCD ID: UM6) (formula: C₁₈H₁₅ClFN₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 29	C 22	Cl 1	F 2	N 3	O 1	0	1
2	B	1	Total 24	C 18	Cl 1	F 1	N 3	O 1	0	0
2	C	1	Total 24	C 18	Cl 1	F 1	N 3	O 1	0	0
2	D	1	Total 24	C 18	Cl 1	F 1	N 3	O 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

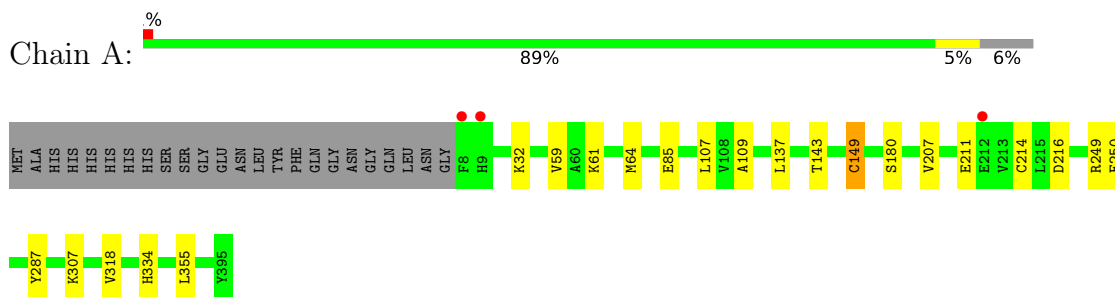
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).

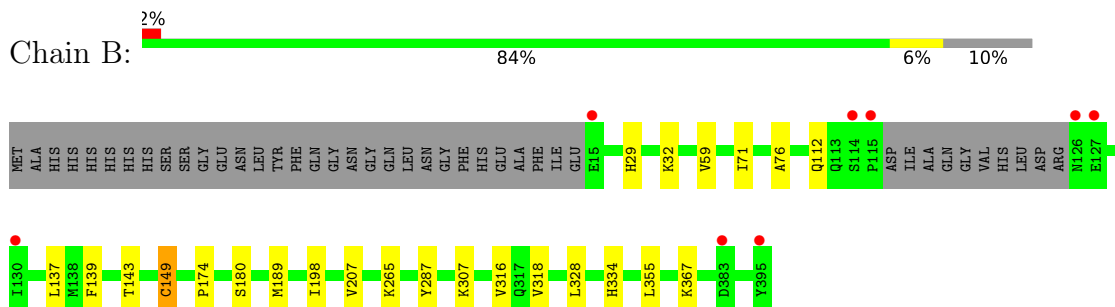
3 Residue-property plots [i](#)

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.

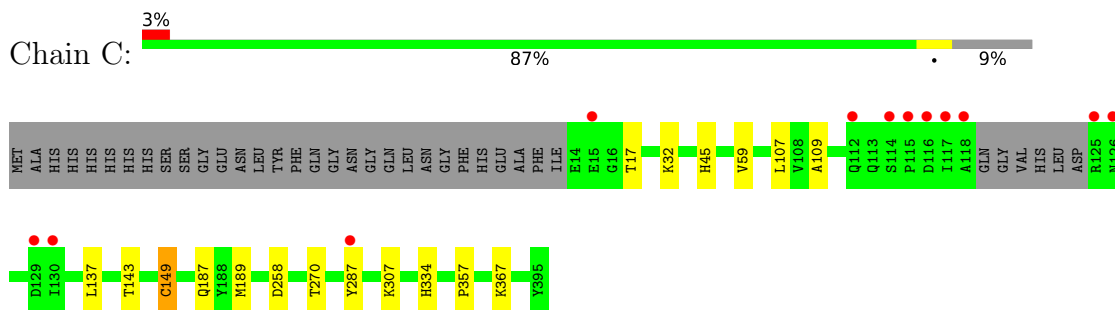
- Molecule 1: S-adenosylmethionine synthase isoform type-2



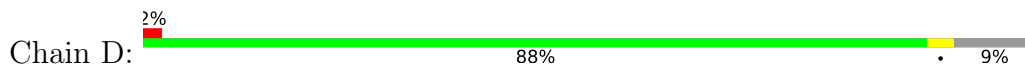
- Molecule 1: S-adenosylmethionine synthase isoform type-2

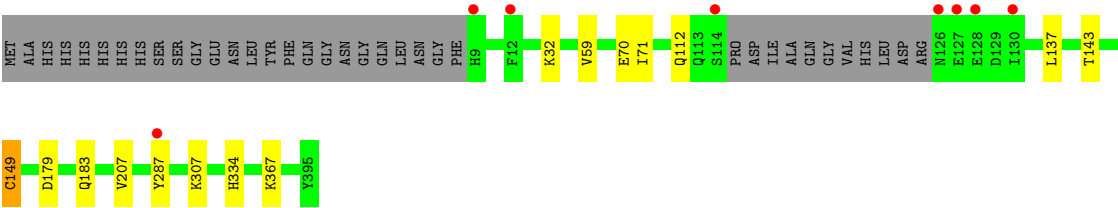


- Molecule 1: S-adenosylmethionine synthase isoform type-2



- Molecule 1: S-adenosylmethionine synthase isoform type-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.90Å 106.74Å 115.00Å 90.00° 93.18° 90.00°	Depositor
Resolution (Å)	78.30 – 1.71 78.30 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.9 (78.30-1.71) 99.9 (78.30-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.153 , 0.184 0.164 , 0.191	Depositor DCC
R_{free} test set	8747 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13205	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, CL, UM6, GOL, SAM, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.10	0/3130	1.21	2/4233 (0.0%)
1	B	1.08	0/2965	1.17	0/4008
1	C	1.09	2/3031 (0.1%)	1.19	3/4096 (0.1%)
1	D	1.05	2/3011 (0.1%)	1.21	1/4069 (0.0%)
All	All	1.08	4/12137 (0.0%)	1.20	6/16406 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	207	VAL	C-O	6.40	1.30	1.24
1	C	45	HIS	CE1-NE2	5.95	1.38	1.32
1	D	183	GLN	C-O	5.67	1.30	1.23
1	C	357	PRO	C-O	-5.01	1.17	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	258	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	250	PHE	CA-CB-CG	6.11	119.91	113.80
1	D	179	ASP	CA-CB-CG	5.66	118.26	112.60
1	C	187	GLN	CB-CG-CD	-5.23	103.71	112.60
1	A	216	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	270	THR	O-C-N	5.04	124.56	120.83

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	A	3073	0	3051	11	0
1	B	2913	0	2910	12	0
1	C	2979	0	2963	8	0
1	D	2961	0	2939	7	0
2	A	29	0	0	0	0
2	B	24	0	0	0	0
2	C	24	0	0	0	0
2	D	24	0	0	0	0
3	A	24	0	32	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	27	0	22	0	0
5	D	27	0	22	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	306	0	0	1	0
7	B	259	0	0	2	0
7	C	272	0	0	0	0
7	D	241	0	0	2	0
All	All	13205	0	11963	34	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 1.

All (34) 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:B:149:CYS:SG	1:B:307:LYS:NZ	2.51	0.83
1:B:76:ALA:HB3	7:B:639:HOH:O	1.89	0.72
1:D:70:GLU:OE1	7:D:501:HOH:O	2.08	0.71
1:D:149:CYS:SG	1:D:307:LYS:NZ	2.57	0.65
1:C:149:CYS:SG	1:C:307:LYS:NZ	2.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:CYS:SG	1:A:307:LYS:NZ	2.64	0.63
1:A:85:GLU:HG2	7:A:751:HOH:O	2.01	0.61
1:C:59:VAL:HG21	1:D:59:VAL:HG21	1.82	0.61
1:D:71:ILE:O	1:D:112:GLN:HA	2.02	0.59
1:C:17:THR:HG22	1:C:189[B]:MET:HG2	1.86	0.58
1:A:211:GLU:OE2	1:A:249:ARG:NH2	2.37	0.54
1:B:71:ILE:O	1:B:112:GLN:HA	2.10	0.52
1:A:59:VAL:HG21	1:B:59:VAL:HG21	1.91	0.52
1:B:318[A]:VAL:HG11	1:B:355:LEU:HD13	1.94	0.49
1:D:143:THR:O	1:D:149:CYS:HA	2.14	0.48
1:A:143:THR:O	1:A:149:CYS:HA	2.14	0.47
1:C:143:THR:O	1:C:149:CYS:HA	2.14	0.47
1:B:143:THR:O	1:B:149:CYS:HA	2.14	0.47
1:C:287:TYR:CZ	1:C:367:LYS:HG2	2.50	0.46
1:A:107:LEU:HD23	1:C:109:ALA:HB2	1.98	0.46
1:B:174:PRO:HA	7:B:670:HOH:O	2.16	0.44
1:C:17:THR:HG22	1:C:189[B]:MET:CG	2.47	0.44
1:B:287:TYR:CZ	1:B:367:LYS:HG2	2.52	0.44
1:A:318[A]:VAL:HG21	1:A:355:LEU:HD13	1.99	0.44
1:A:109:ALA:HB2	1:C:107:LEU:HD23	2.01	0.43
1:A:180:SER:HB3	1:A:207:VAL:HG23	2.00	0.43
1:D:287:TYR:CZ	1:D:367:LYS:HG2	2.54	0.43
1:D:112:GLN:HB2	7:D:516:HOH:O	2.19	0.43
1:A:61:LYS:HG2	1:A:64:MET:HE2	2.01	0.42
1:B:29:HIS:CE1	1:B:265:LYS:HE2	2.54	0.42
1:B:139:PHE:HA	1:B:316:VAL:O	2.20	0.42
1:B:180:SER:HB3	1:B:207:VAL:HG23	2.03	0.41
1:A:287:TYR:CD1	1:A:287:TYR:C	2.99	0.41
1:B:189:MET:HB2	1:B:198:ILE:HD11	2.03	0.41

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	A	391/412 (95%)	384 (98%)	7 (2%)	0	100	100
1	B	370/412 (90%)	363 (98%)	7 (2%)	0	100	100
1	C	378/412 (92%)	371 (98%)	7 (2%)	0	100	100
1	D	375/412 (91%)	370 (99%)	5 (1%)	0	100	100
All	All	1514/1648 (92%)	1488 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	327/340 (96%)	323 (99%)	4 (1%)	63	46
1	B	311/340 (92%)	306 (98%)	5 (2%)	55	34
1	C	318/340 (94%)	314 (99%)	4 (1%)	61	43
1	D	315/340 (93%)	311 (99%)	4 (1%)	61	43
All	All	1271/1360 (94%)	1254 (99%)	17 (1%)	59	43

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	137	LEU
1	A	149	CYS
1	A	334	HIS
1	B	32	LYS
1	B	137	LEU
1	B	149	CYS
1	B	328	LEU
1	B	334	HIS
1	C	32	LYS
1	C	137	LEU
1	C	149	CYS
1	C	334	HIS

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Mol	Chain	Res	Type
1	D	32	LYS
1	D	137	LEU
1	D	149	CYS
1	D	334	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	339	GLN
1	B	372	GLN
1	C	113	GLN
1	C	208	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSO	D	214	1	3,6,7	0.54	0	1,6,8	0.37	0
1	CSO	B	214	1	3,6,7	1.08	0	1,6,8	0.02	0
1	CSO	C	214	1	3,6,7	1.03	0	1,6,8	0.10	0
1	CSO	A	214	1	3,6,7	1.52	1 (33%)	1,6,8	0.39	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
1	CSO	D	214	1	-	0/1/5/7	-
1	CSO	B	214	1	-	0/1/5/7	-
1	CSO	C	214	1	-	0/1/5/7	-
1	CSO	A	214	1	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	CSO	O-C	2.07	1.27	1.20

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	UM6	A	401[B]	-	27,27,27	1.51	4 (14%)	32,39,39	2.06	11 (34%)
2	UM6	A	401[A]	-	27,27,27	1.54	5 (18%)	32,39,39	1.94	9 (28%)
3	GOL	A	402	-	5,5,5	0.13	0	5,5,5	0.40	0
5	SAM	B	502	-	27,29,29	0.47	0	34,42,42	1.01	2 (5%)
3	GOL	C	402	-	5,5,5	0.11	0	5,5,5	0.25	0
2	UM6	D	403	-	27,27,27	1.39	3 (11%)	32,39,39	1.98	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UM6	C	401	-	27,27,27	1.51	4 (14%)	32,39,39	1.92	7 (21%)
3	GOL	A	403	-	5,5,5	0.09	0	5,5,5	0.23	0
3	GOL	B	505	-	5,5,5	0.11	0	5,5,5	0.25	0
2	UM6	B	503	-	27,27,27	1.13	2 (7%)	32,39,39	2.01	11 (34%)
3	GOL	A	405	-	5,5,5	0.12	0	5,5,5	0.34	0
5	SAM	D	401[A]	-	27,29,29	0.52	1 (3%)	34,42,42	0.82	1 (2%)
3	GOL	A	404	-	5,5,5	0.10	0	5,5,5	0.28	0
3	GOL	D	404	-	5,5,5	0.08	0	5,5,5	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UM6	A	401[B]	-	-	0/8/17/17	0/4/4/4
2	UM6	A	401[A]	-	-	0/8/17/17	0/4/4/4
3	GOL	A	402	-	-	0/4/4/4	-
5	SAM	B	502	-	-	5/17/33/33	0/3/3/3
3	GOL	C	402	-	-	0/4/4/4	-
2	UM6	D	403	-	-	0/8/17/17	0/4/4/4
2	UM6	C	401	-	-	0/8/17/17	0/4/4/4
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	B	505	-	-	0/4/4/4	-
2	UM6	B	503	-	-	0/8/17/17	0/4/4/4
3	GOL	A	405	-	-	0/4/4/4	-
5	SAM	D	401[A]	-	-	5/17/33/33	0/3/3/3
3	GOL	A	404	-	-	0/4/4/4	-
3	GOL	D	404	-	-	0/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	403	UM6	C6-N5	-4.84	1.34	1.42
2	C	401	UM6	C6-N5	-4.29	1.35	1.42
2	A	401[A]	UM6	C6-N5	-4.20	1.35	1.42
2	A	401[B]	UM6	C6-N5	-4.20	1.35	1.42
2	C	401	UM6	C17-C18	3.79	1.59	1.52
2	B	503	UM6	C6-N5	-3.21	1.36	1.42
2	A	401[A]	UM6	C19-N5	-2.98	1.40	1.44
2	A	401[B]	UM6	C19-N5	-2.98	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	UM6	C17-C18	2.84	1.58	1.52
2	C	401	UM6	C19-N5	-2.66	1.40	1.44
2	A	401[A]	UM6	C17-C18	2.61	1.57	1.52
2	A	401[A]	UM6	C11-C10	2.46	1.43	1.39
2	A	401[B]	UM6	C11-C10	2.46	1.43	1.39
2	D	403	UM6	C10-C4	2.39	1.44	1.41
2	A	401[A]	UM6	C12-C11	-2.33	1.35	1.38
2	A	401[B]	UM6	C12-C11	-2.33	1.35	1.38
2	C	401	UM6	C10-C4	2.33	1.44	1.41
2	D	403	UM6	C17-C18	2.27	1.57	1.52
5	D	401[A]	SAM	OXT-C	-2.07	1.24	1.30

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	UM6	C24-C19-N5	5.08	125.56	119.72
2	D	403	UM6	C24-C19-N5	4.92	125.37	119.72
2	A	401[A]	UM6	C20-C19-N5	-4.90	114.11	119.72
2	A	401[B]	UM6	C20-C19-N5	-4.90	114.11	119.72
2	C	401	UM6	C20-C19-N5	-4.82	114.20	119.72
5	B	502	SAM	CG-SD-C5'	-4.59	92.21	103.43
2	B	503	UM6	C20-C19-N5	-4.34	114.75	119.72
2	A	401[B]	UM6	C18-N13-C14	-4.26	107.41	112.38
2	D	403	UM6	C20-C19-N5	-4.13	114.99	119.72
2	A	401[A]	UM6	C24-C19-N5	4.08	124.41	119.72
2	A	401[B]	UM6	C24-C19-N5	4.08	124.41	119.72
2	C	401	UM6	C24-C19-N5	3.89	124.19	119.72
2	B	503	UM6	C18-N13-C14	-3.64	108.13	112.38
2	C	401	UM6	C18-N13-C14	-3.50	108.30	112.38
2	D	403	UM6	F16-C15-C14	-3.49	103.39	108.41
5	D	401[A]	SAM	CG-SD-C5'	-3.43	95.04	103.43
2	A	401[A]	UM6	C18-N13-C14	-3.33	108.49	112.38
2	A	401[A]	UM6	O7-C6-N5	3.09	121.58	118.51
2	A	401[B]	UM6	O7-C6-N5	3.09	121.58	118.51
2	A	401[B]	UM6	C17-C18-N13	2.99	106.78	102.93
2	B	503	UM6	C22-C23-C24	2.80	123.70	120.24
2	B	503	UM6	C22-C21-C20	-2.79	116.80	120.24
2	A	401[A]	UM6	C23-C24-C19	-2.75	116.41	119.68
2	A	401[B]	UM6	C23-C24-C19	-2.75	116.41	119.68
2	B	503	UM6	C9-N8-C6	2.71	123.05	119.05
2	A	401[A]	UM6	C22-C21-C20	-2.66	116.95	120.24
2	A	401[B]	UM6	C22-C21-C20	-2.66	116.95	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	SAM	OXT-C-O	-2.55	118.28	124.08
2	A	401[B]	UM6	C17-C15-C14	-2.53	101.89	104.84
2	B	503	UM6	C21-C20-C19	2.52	122.67	119.68
2	D	403	UM6	C18-N13-C14	-2.52	109.44	112.38
2	B	503	UM6	C23-C24-C19	-2.50	116.71	119.68
2	A	401[A]	UM6	C11-C10-C9	2.49	127.17	121.61
2	A	401[B]	UM6	C11-C10-C9	2.49	127.17	121.61
2	D	403	UM6	C21-C20-C19	2.48	122.63	119.68
2	C	401	UM6	O7-C6-N8	-2.47	118.43	122.33
2	C	401	UM6	C4-C3-C2	2.42	122.38	117.95
2	B	503	UM6	O7-C6-N5	2.39	120.88	118.51
2	B	503	UM6	C18-N13-C9	2.38	130.47	123.73
2	A	401[A]	UM6	C17-C15-C14	-2.32	102.13	104.84
2	C	401	UM6	C23-C24-C19	-2.30	116.96	119.68
2	A	401[B]	UM6	C14-N13-C9	2.18	129.93	123.73
2	D	403	UM6	N5-C6-N8	2.18	121.22	118.51
2	D	403	UM6	C4-C3-C2	2.17	121.93	117.95
2	C	401	UM6	C18-N13-C9	2.17	129.88	123.73
2	D	403	UM6	C3-C2-CL1	2.08	121.77	119.17
2	A	401[A]	UM6	C9-N8-C6	2.07	122.10	119.05
2	A	401[B]	UM6	C9-N8-C6	2.07	122.10	119.05
2	D	403	UM6	C15-C14-N13	2.06	106.12	103.19
2	B	503	UM6	C15-C14-N13	2.04	106.09	103.19
2	D	403	UM6	C11-C10-C9	2.00	126.09	121.61

There are no chirality outliers.

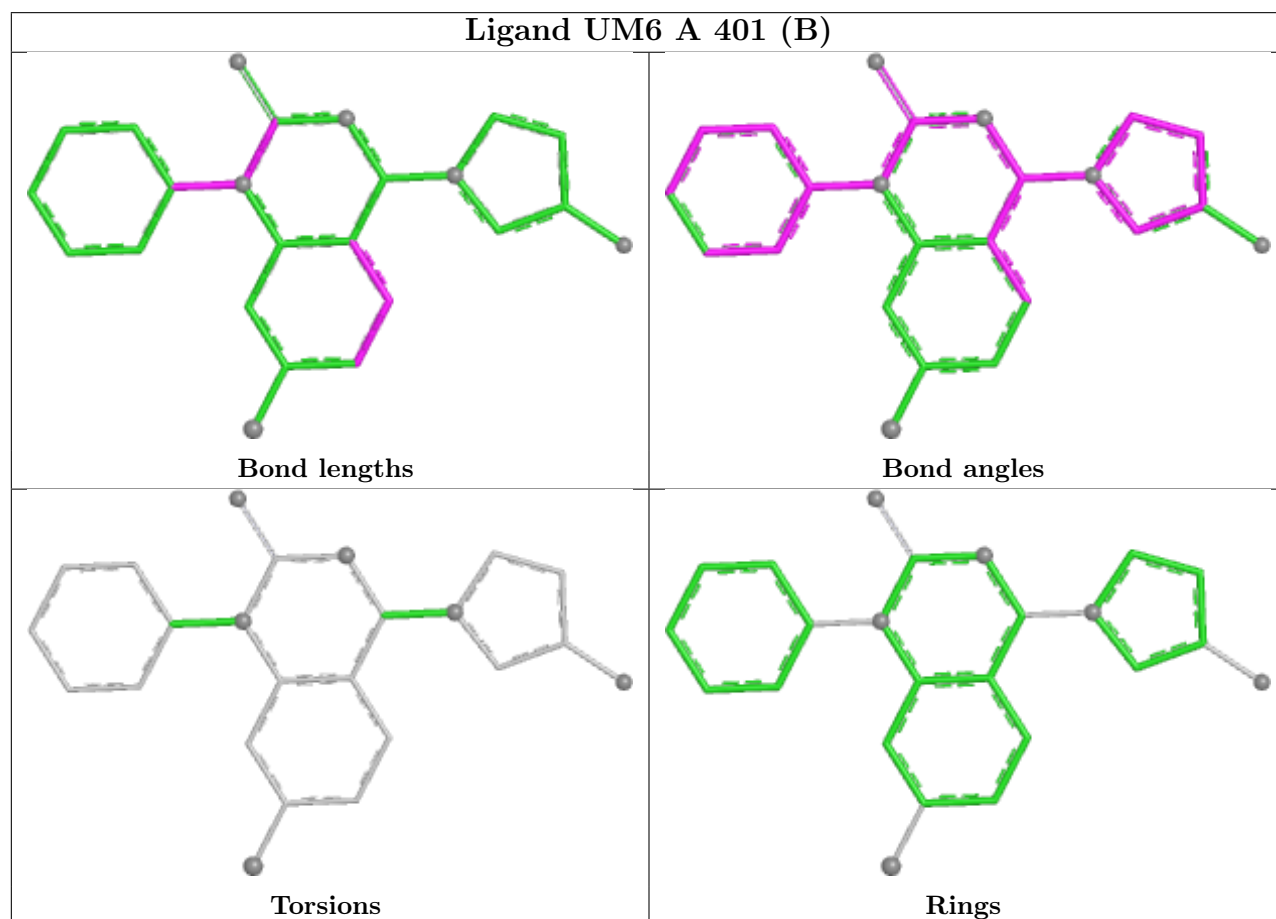
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	401[A]	SAM	O-C-CA-CB
5	D	401[A]	SAM	OXT-C-CA-CB
5	B	502	SAM	C2'-C1'-N9-C8
5	D	401[A]	SAM	C2'-C1'-N9-C8
3	A	403	GOL	C1-C2-C3-O3
5	B	502	SAM	O-C-CA-CB
5	B	502	SAM	O4'-C1'-N9-C8
5	B	502	SAM	OXT-C-CA-CB
5	D	401[A]	SAM	O4'-C1'-N9-C8
5	D	401[A]	SAM	OXT-C-CA-N
3	A	403	GOL	O2-C2-C3-O3
5	B	502	SAM	OXT-C-CA-N

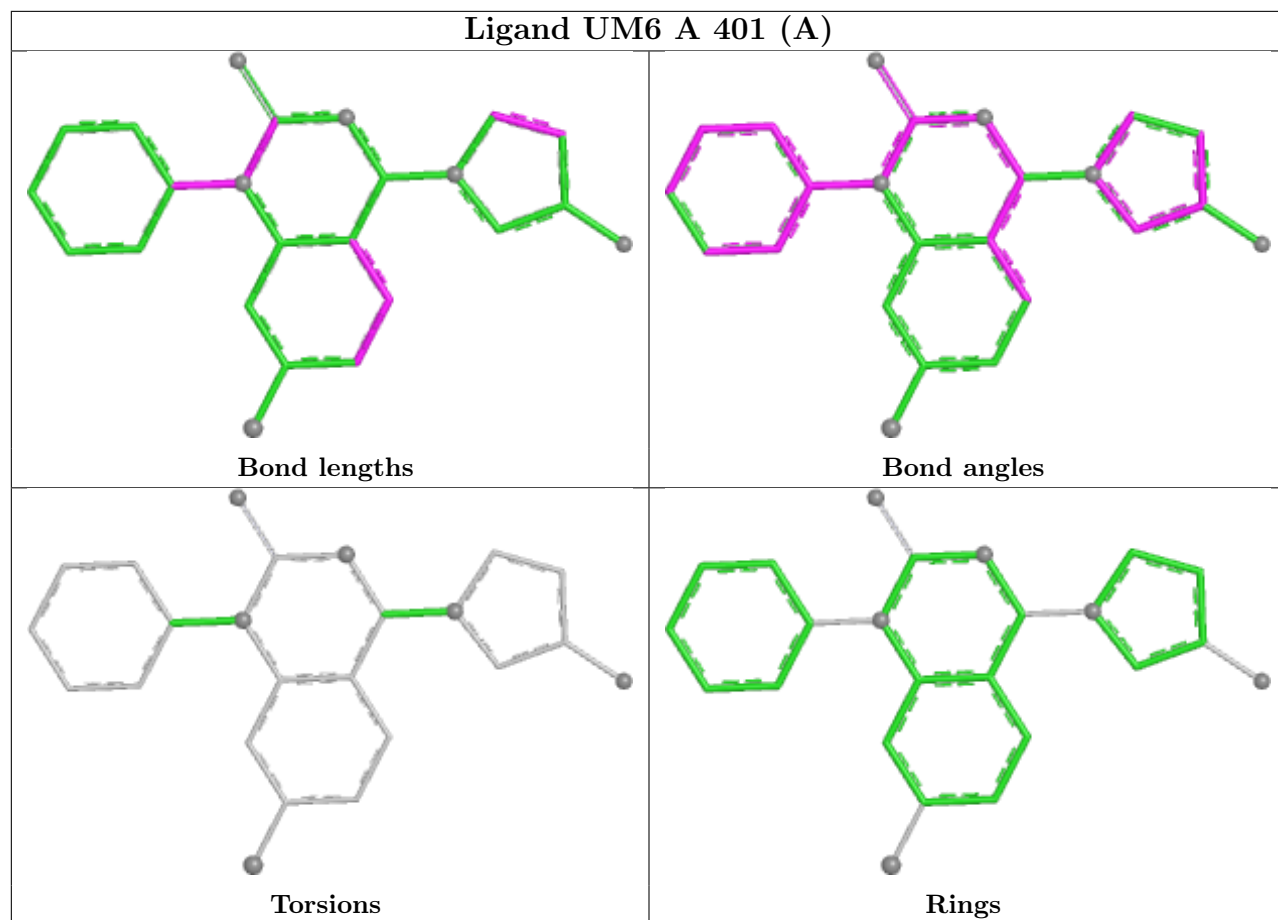
There are no ring outliers.

No monomer is involved in short contacts.

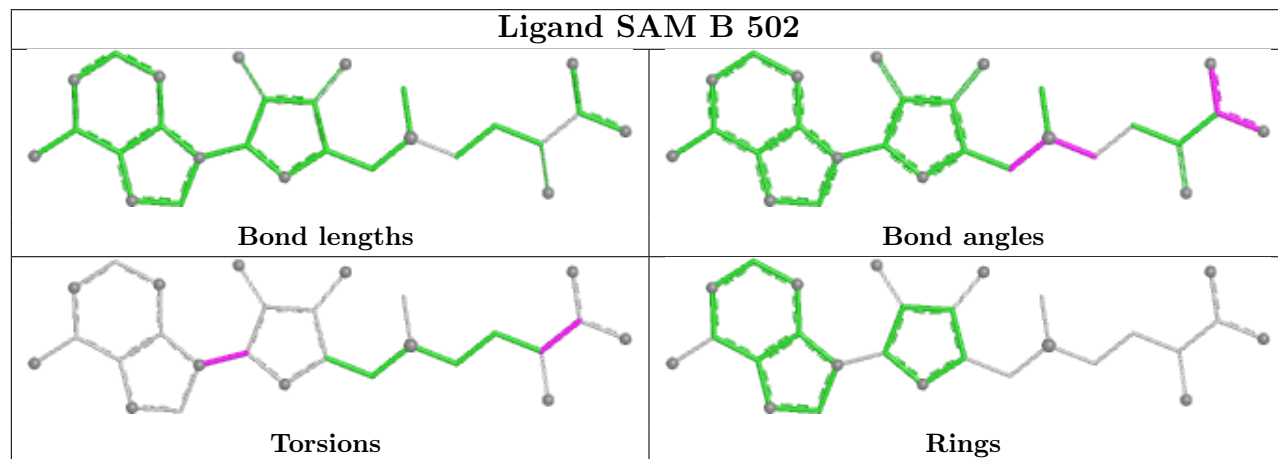
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

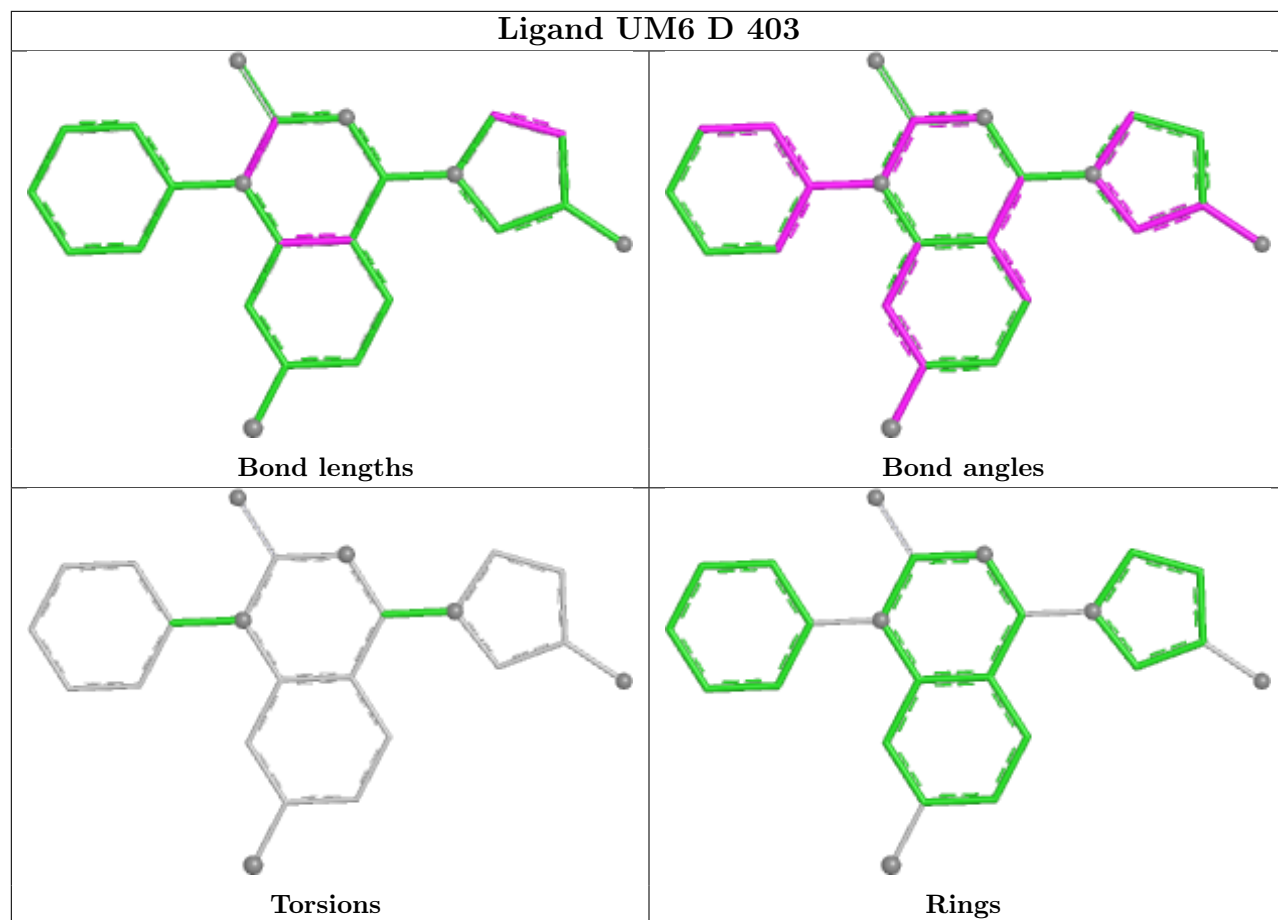


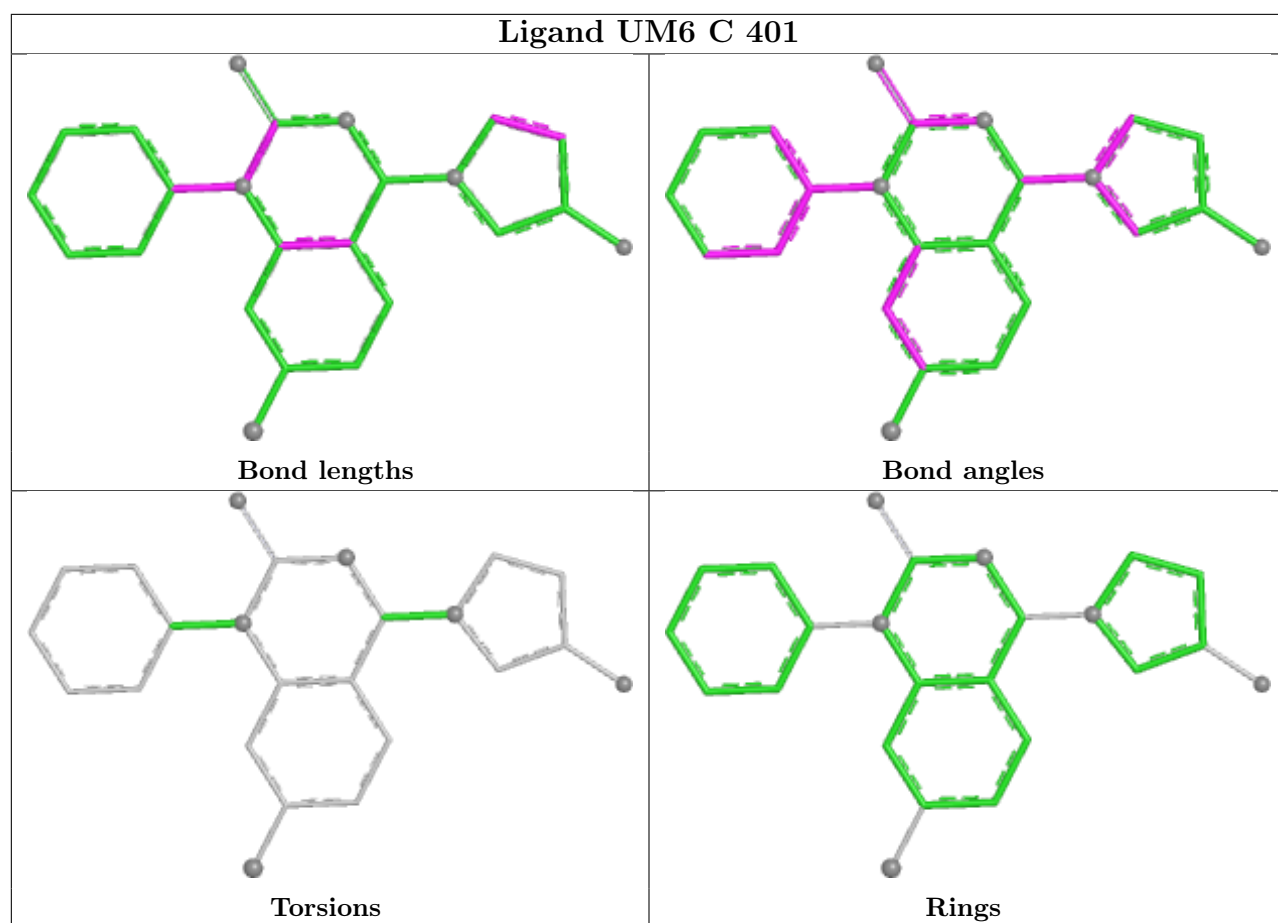
Ligand UM6 A 401 (A)

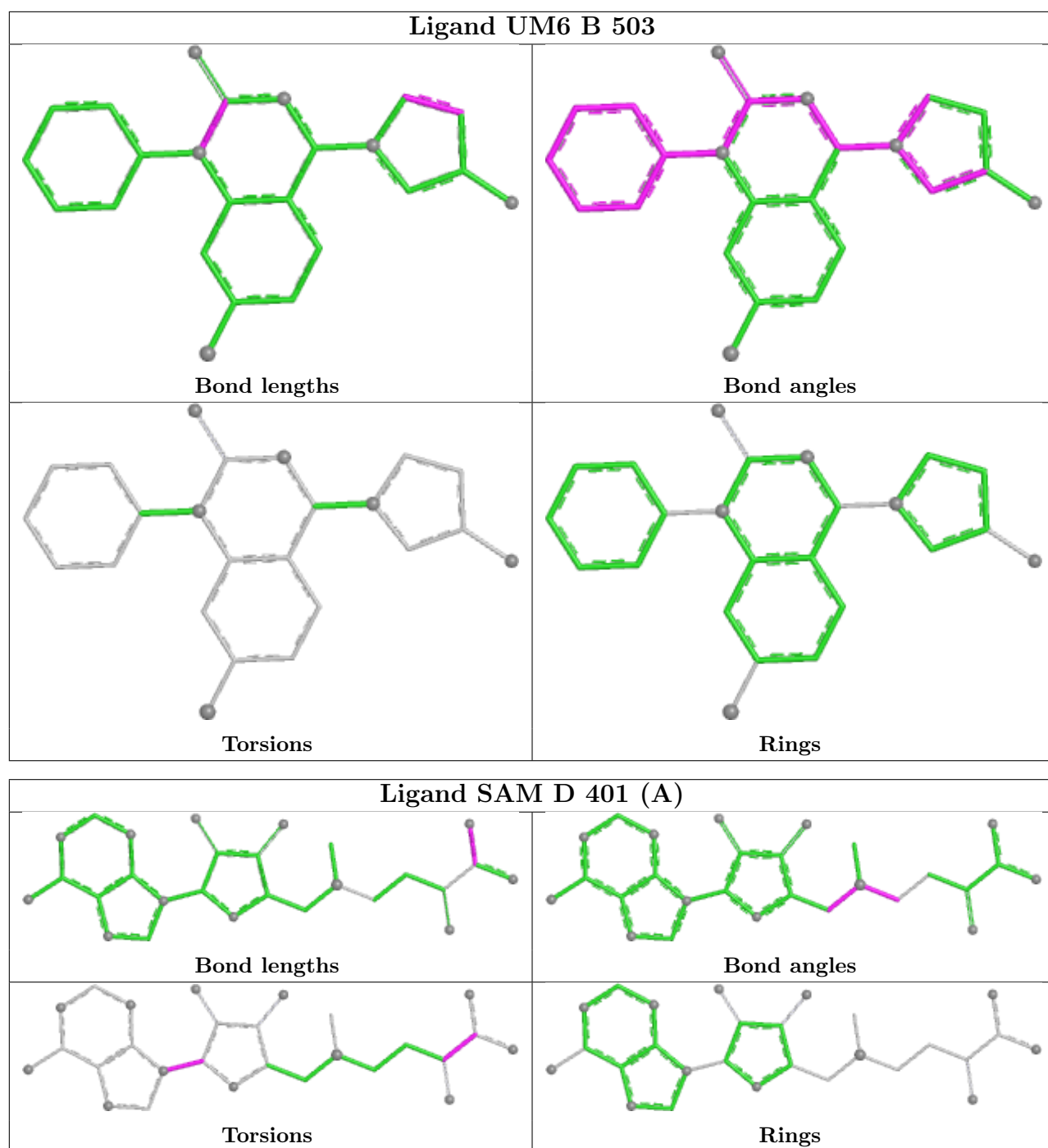


Ligand SAM B 502









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/412 (93%)	-0.29	3 (0%) 82 87	13, 27, 43, 60	16 (4%)
1	B	370/412 (89%)	-0.10	8 (2%) 62 70	15, 31, 49, 104	20 (5%)
1	C	375/412 (91%)	-0.09	12 (3%) 50 59	16, 30, 49, 92	20 (5%)
1	D	375/412 (91%)	-0.08	8 (2%) 63 72	13, 31, 52, 123	22 (5%)
All	All	1507/1648 (91%)	-0.14	31 (2%) 63 72	13, 29, 49, 123	78 (5%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	ALA	10.5
1	C	117	ILE	6.9
1	A	8	PHE	5.0
1	B	126	ASN	4.4
1	B	15	GLU	4.1
1	B	115	PRO	3.8
1	C	115	PRO	3.7
1	D	126	ASN	3.6
1	D	9	HIS	3.4
1	A	9	HIS	3.0
1	C	116	ASP	3.0
1	D	114	SER	3.0
1	C	130	ILE	3.0
1	C	112[A]	GLN	2.8
1	B	130[A]	ILE	2.8
1	B	114	SER	2.8
1	C	287	TYR	2.7
1	C	114	SER	2.7
1	B	127	GLU	2.6
1	D	127	GLU	2.5
1	B	395	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	128	GLU	2.4
1	C	125	ARG	2.4
1	C	126	ASN	2.4
1	C	129	ASP	2.3
1	D	287	TYR	2.3
1	A	212	GLU	2.3
1	D	130	ILE	2.2
1	B	383	ASP	2.1
1	D	12	PHE	2.1
1	C	15	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	B	214	7/8	0.88	0.10	40,43,53,62	0
1	CSO	C	214	7/8	0.89	0.12	30,34,54,59	0
1	CSO	D	214	7/8	0.90	0.11	29,35,51,58	0
1	CSO	A	214	7/8	0.95	0.08	26,34,40,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	405	6/6	0.76	0.14	44,64,78,81	0
3	GOL	B	505	6/6	0.83	0.13	59,62,63,70	0
5	SAM	D	401[A]	27/27	0.83	0.19	22,36,45,51	27
3	GOL	A	403	6/6	0.84	0.14	56,62,65,74	0

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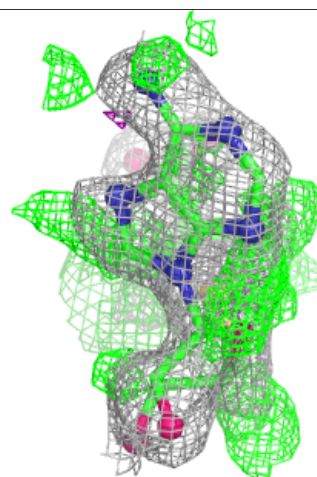
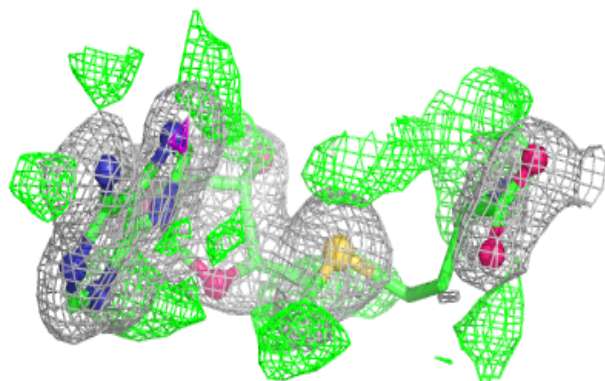
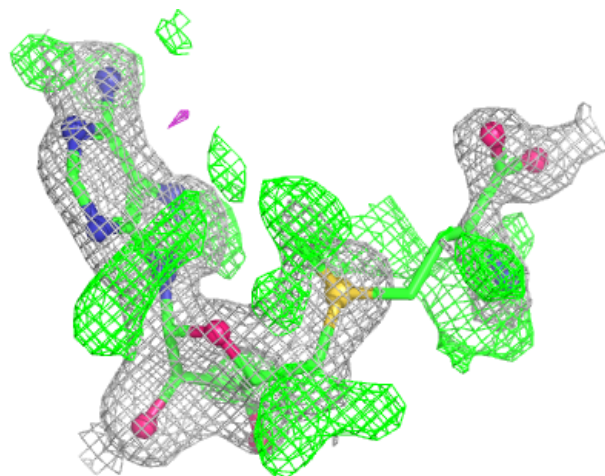
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	404	6/6	0.85	0.15	50,71,86,102	0
3	GOL	C	402	6/6	0.87	0.16	63,64,70,77	0
3	GOL	A	404	6/6	0.89	0.13	36,47,50,62	0
3	GOL	A	402	6/6	0.90	0.11	32,37,40,46	0
4	MG	D	402	1/1	0.95	0.11	40,40,40,40	0
6	CL	D	405	1/1	0.95	0.10	60,60,60,60	0
5	SAM	B	502	27/27	0.96	0.07	24,29,41,47	0
2	UM6	D	403	24/24	0.97	0.06	19,25,29,36	0
2	UM6	C	401	24/24	0.97	0.06	22,25,29,34	0
2	UM6	A	401[A]	24/24	0.98	0.05	19,22,26,29	5
2	UM6	A	401[B]	24/24	0.98	0.05	21,23,29,31	5
2	UM6	B	503	24/24	0.98	0.05	19,24,27,33	0
4	MG	B	501	1/1	0.98	0.06	39,39,39,39	0
6	CL	B	504	1/1	0.99	0.05	35,35,35,35	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.

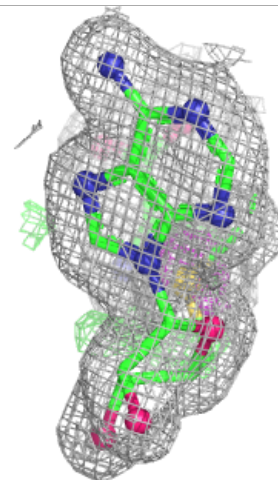
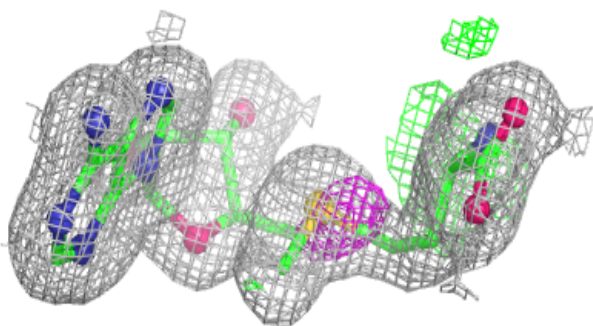
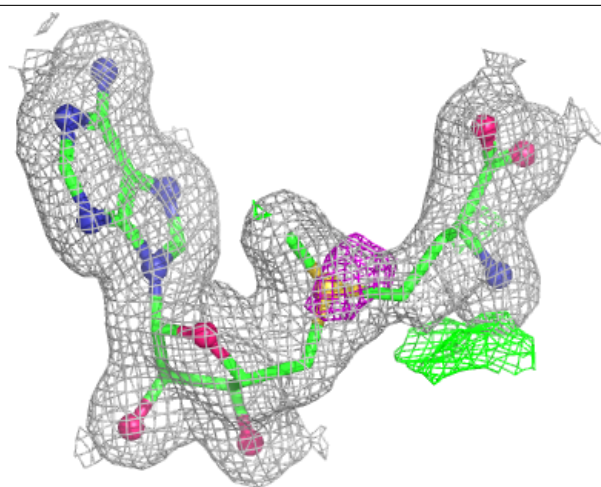
Electron density around SAM D 401 (A):

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



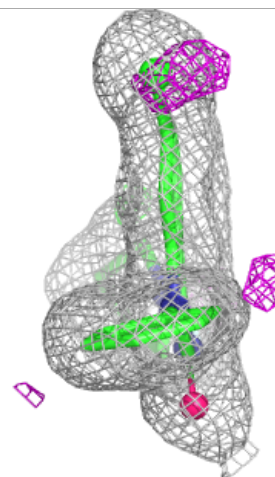
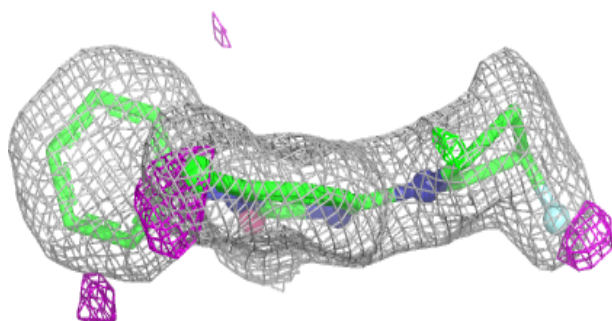
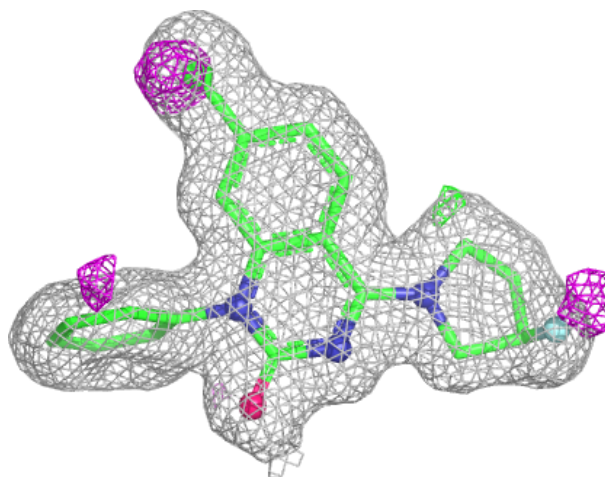
Electron density around SAM B 502:

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



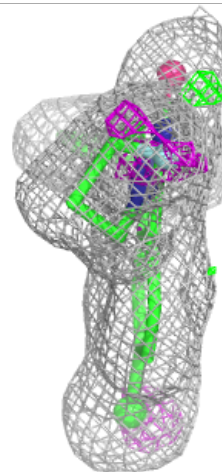
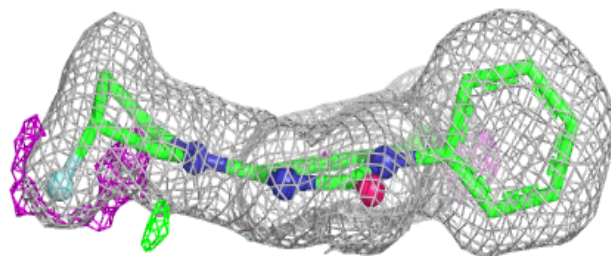
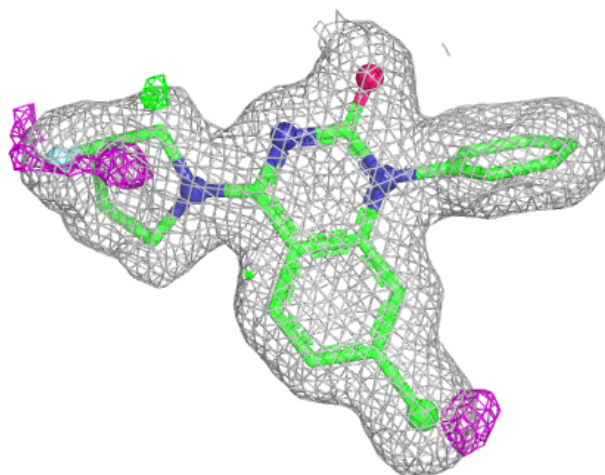
Electron density around UM6 D 403:

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



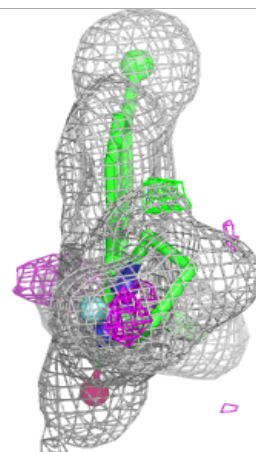
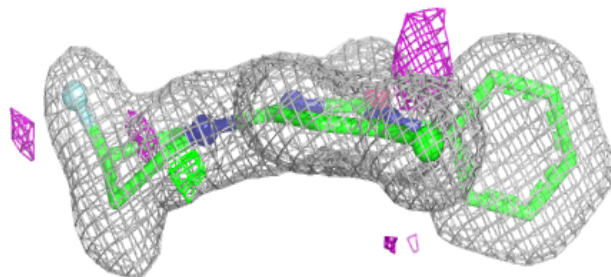
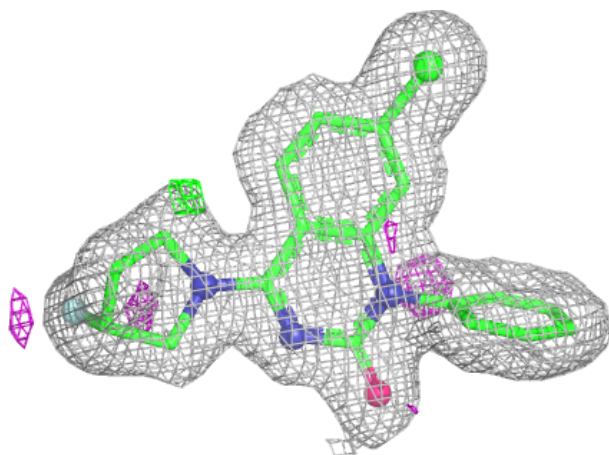
Electron density around UM6 C 401:

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



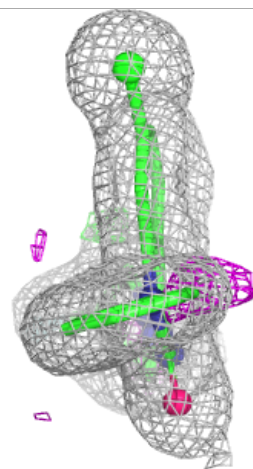
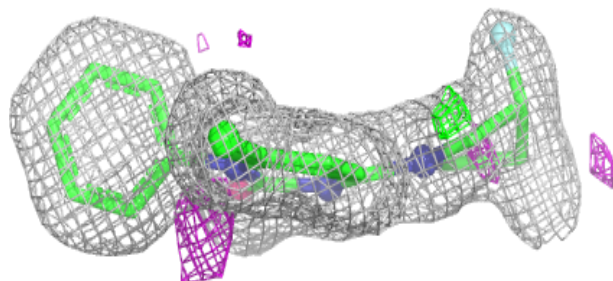
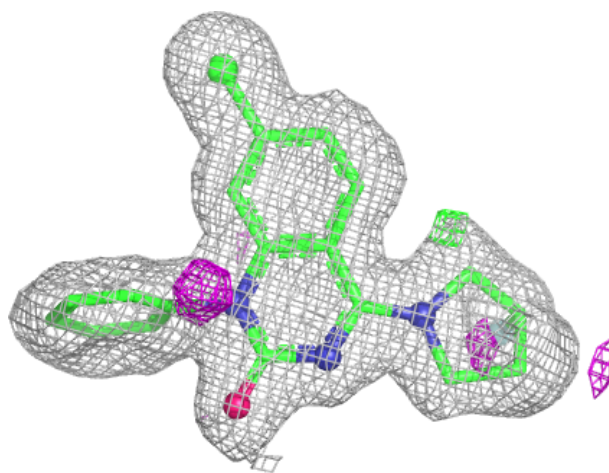
Electron density around UM6 A 401 (A):

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



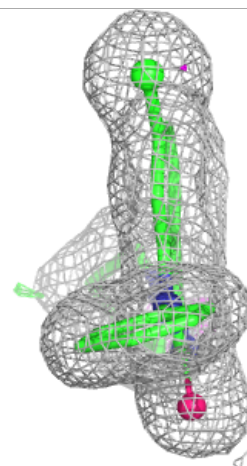
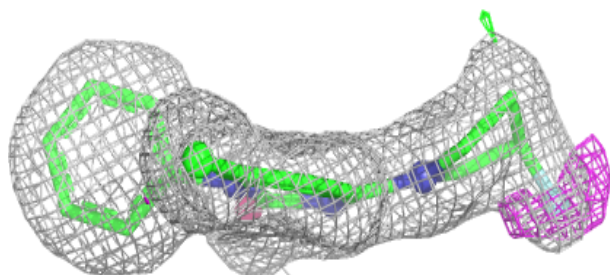
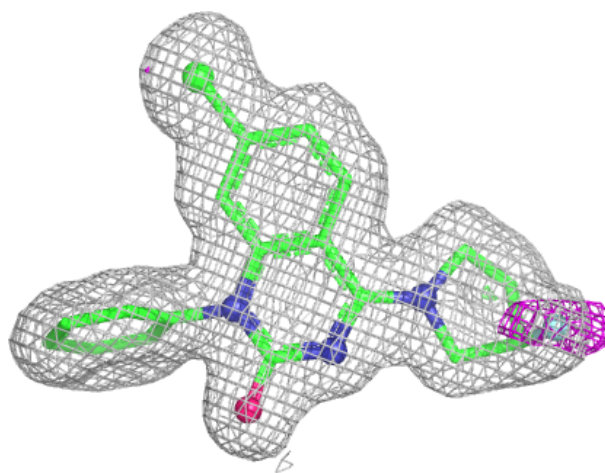
Electron density around UM6 A 401 (B):

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



Electron density around UM6 B 503:

$2mF_o-DF_c$ (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.