WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 02:54 PM EST

PDB ID : 3SSN
Title : MycE Methyltransferase from the Mycinamycin Biosynthetic Pathway in Complex with Mg, SAH, and Mycinamycin VI
Authors : Akey, D.L.; Smith, J.L.
Deposited on : 2011-07-08
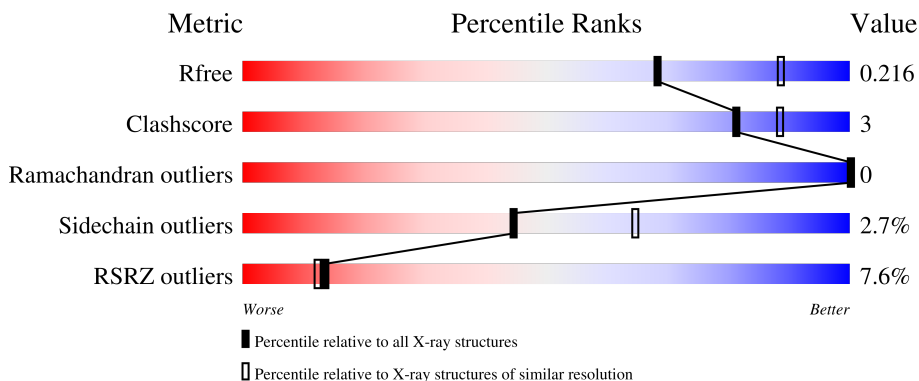Resolution : 2.39 Å(reported)

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 2.39 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		0.216
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		2.7%
RSRZ outliers		7.6%

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	A	419	5% / 81% / 10% · 8%
1	B	419	8% / 78% / 5% 16%
1	C	419	5% / 81% / 5% 13%
1	D	419	9% / 87% / 7% 6%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 12616 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 Methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total 3077	C 1955	N 543	O 571	S 8	0	0	0
1	B	350	Total 2774	C 1748	N 496	O 524	S 6	0	0	0
1	C	366	Total 2924	C 1860	N 518	O 538	S 8	0	0	0
1	D	393	Total 3126	C 1982	N 554	O 582	S 8	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q83WF2
A	-18	GLY	-	expression tag	UNP Q83WF2
A	-17	SER	-	expression tag	UNP Q83WF2
A	-16	SER	-	expression tag	UNP Q83WF2
A	-15	HIS	-	expression tag	UNP Q83WF2
A	-14	HIS	-	expression tag	UNP Q83WF2
A	-13	HIS	-	expression tag	UNP Q83WF2
A	-12	HIS	-	expression tag	UNP Q83WF2
A	-11	HIS	-	expression tag	UNP Q83WF2
A	-10	HIS	-	expression tag	UNP Q83WF2
A	-9	SER	-	expression tag	UNP Q83WF2
A	-8	SER	-	expression tag	UNP Q83WF2
A	-7	GLY	-	expression tag	UNP Q83WF2
A	-6	LEU	-	expression tag	UNP Q83WF2
A	-5	VAL	-	expression tag	UNP Q83WF2
A	-4	PRO	-	expression tag	UNP Q83WF2
A	-3	ARG	-	expression tag	UNP Q83WF2
A	-2	GLY	-	expression tag	UNP Q83WF2
A	-1	SER	-	expression tag	UNP Q83WF2
A	0	HIS	-	expression tag	UNP Q83WF2
B	-19	MET	-	expression tag	UNP Q83WF2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q83WF2
B	-17	SER	-	expression tag	UNP Q83WF2
B	-16	SER	-	expression tag	UNP Q83WF2
B	-15	HIS	-	expression tag	UNP Q83WF2
B	-14	HIS	-	expression tag	UNP Q83WF2
B	-13	HIS	-	expression tag	UNP Q83WF2
B	-12	HIS	-	expression tag	UNP Q83WF2
B	-11	HIS	-	expression tag	UNP Q83WF2
B	-10	HIS	-	expression tag	UNP Q83WF2
B	-9	SER	-	expression tag	UNP Q83WF2
B	-8	SER	-	expression tag	UNP Q83WF2
B	-7	GLY	-	expression tag	UNP Q83WF2
B	-6	LEU	-	expression tag	UNP Q83WF2
B	-5	VAL	-	expression tag	UNP Q83WF2
B	-4	PRO	-	expression tag	UNP Q83WF2
B	-3	ARG	-	expression tag	UNP Q83WF2
B	-2	GLY	-	expression tag	UNP Q83WF2
B	-1	SER	-	expression tag	UNP Q83WF2
B	0	HIS	-	expression tag	UNP Q83WF2
C	-19	MET	-	expression tag	UNP Q83WF2
C	-18	GLY	-	expression tag	UNP Q83WF2
C	-17	SER	-	expression tag	UNP Q83WF2
C	-16	SER	-	expression tag	UNP Q83WF2
C	-15	HIS	-	expression tag	UNP Q83WF2
C	-14	HIS	-	expression tag	UNP Q83WF2
C	-13	HIS	-	expression tag	UNP Q83WF2
C	-12	HIS	-	expression tag	UNP Q83WF2
C	-11	HIS	-	expression tag	UNP Q83WF2
C	-10	HIS	-	expression tag	UNP Q83WF2
C	-9	SER	-	expression tag	UNP Q83WF2
C	-8	SER	-	expression tag	UNP Q83WF2
C	-7	GLY	-	expression tag	UNP Q83WF2
C	-6	LEU	-	expression tag	UNP Q83WF2
C	-5	VAL	-	expression tag	UNP Q83WF2
C	-4	PRO	-	expression tag	UNP Q83WF2
C	-3	ARG	-	expression tag	UNP Q83WF2
C	-2	GLY	-	expression tag	UNP Q83WF2
C	-1	SER	-	expression tag	UNP Q83WF2
C	0	HIS	-	expression tag	UNP Q83WF2
D	-19	MET	-	expression tag	UNP Q83WF2
D	-18	GLY	-	expression tag	UNP Q83WF2
D	-17	SER	-	expression tag	UNP Q83WF2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q83WF2
D	-15	HIS	-	expression tag	UNP Q83WF2
D	-14	HIS	-	expression tag	UNP Q83WF2
D	-13	HIS	-	expression tag	UNP Q83WF2
D	-12	HIS	-	expression tag	UNP Q83WF2
D	-11	HIS	-	expression tag	UNP Q83WF2
D	-10	HIS	-	expression tag	UNP Q83WF2
D	-9	SER	-	expression tag	UNP Q83WF2
D	-8	SER	-	expression tag	UNP Q83WF2
D	-7	GLY	-	expression tag	UNP Q83WF2
D	-6	LEU	-	expression tag	UNP Q83WF2
D	-5	VAL	-	expression tag	UNP Q83WF2
D	-4	PRO	-	expression tag	UNP Q83WF2
D	-3	ARG	-	expression tag	UNP Q83WF2
D	-2	GLY	-	expression tag	UNP Q83WF2
D	-1	SER	-	expression tag	UNP Q83WF2
D	0	HIS	-	expression tag	UNP Q83WF2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

SAH
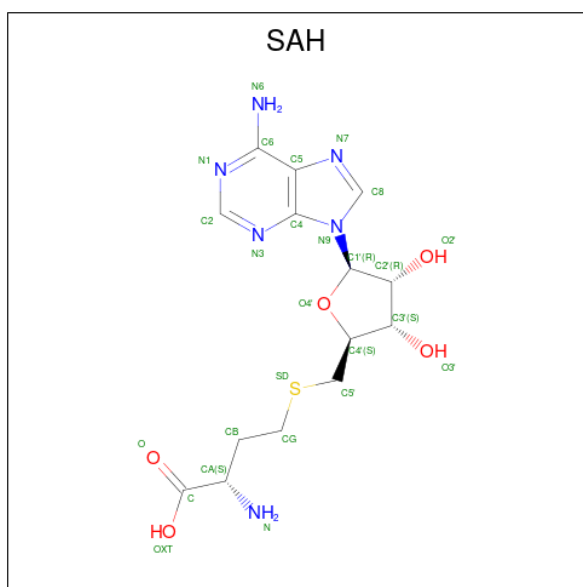
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is Mycinamicin VI (three-letter code: MVI) (formula: $C_{35}H_{57}NO_{11}$).

MVI
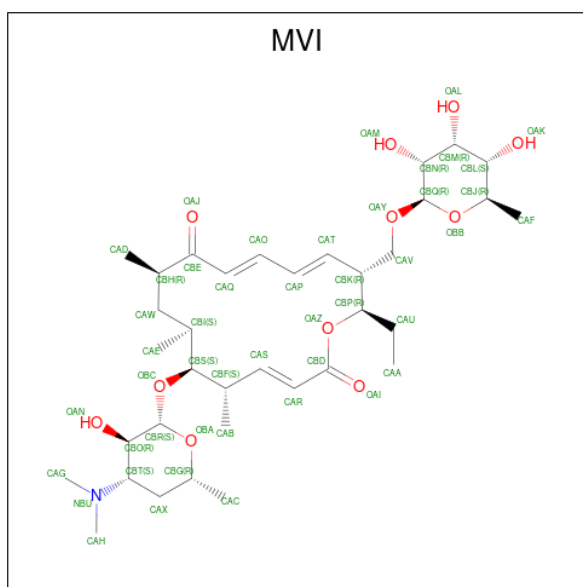
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			47	35	1	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total 47	C 35	N 1	O 11	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).
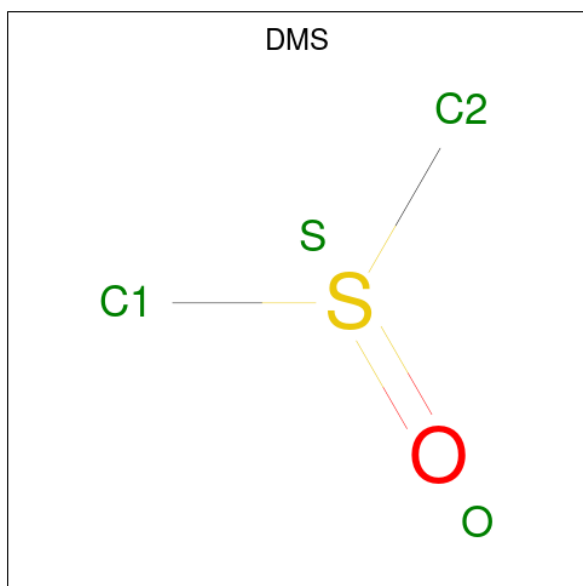
DMS

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	166	Total 166	O 166	0	0
7	B	109	Total 109	O 109	0	0
7	C	130	Total 130	O 130	0	0
7	D	117	Total 117	O 117	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 sh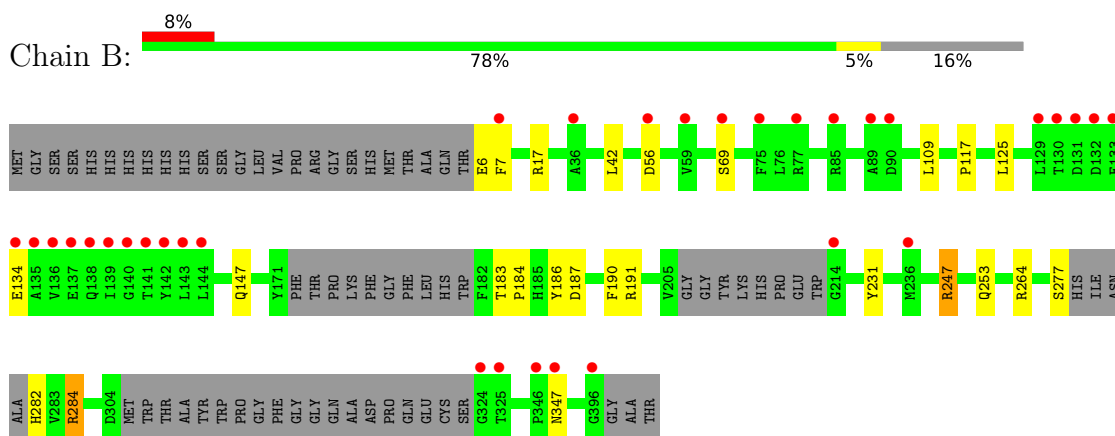ows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit 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: Methyltransferase
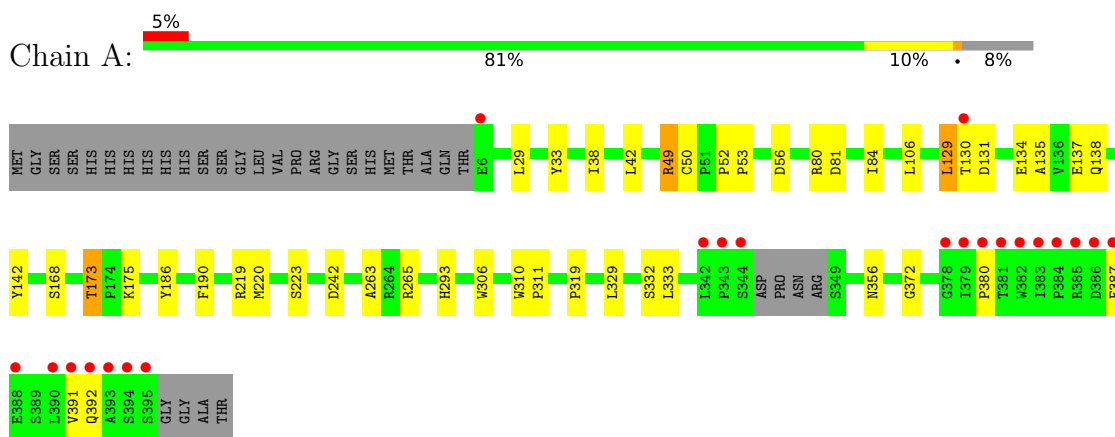
Chain A:

- Molecule 1: Methyltransferase

Chain B:

- Molecule 1: Methyltransferase

Chain C:

Y442 S168 T173 K209 E212 D242 L333 A336 H339 GLN GLU LEU PRO SER ASP PRO ASN ARG SER PRO G351 Y352 V353 D354 I357 H361 F368 V369 R373 N374 D375 G378 I379 P380 T381 W382 ILE PRO ARG ASP PHE GLU SER LEU VAL GLN
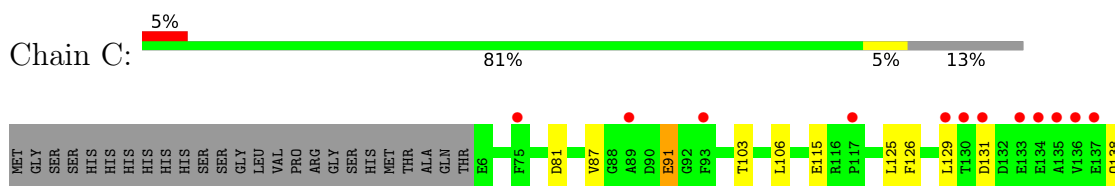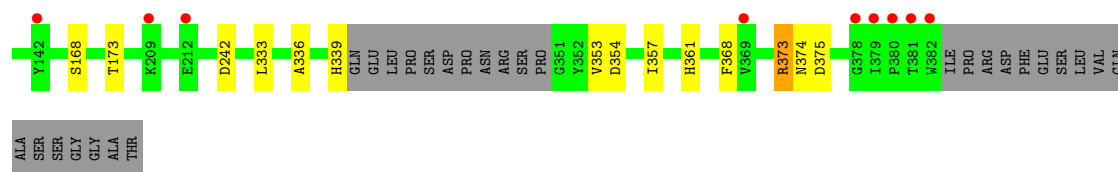
ALA SER SER GLY ALA THR

• Molecule 1: Methyltransferase

Chain D:

9%

87%   7%   6%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET THR ALA GLN T5 E6 Y33 I38 V59 L60 R77 G92 T130 D131 D132 E133 E134 A135 V136 E137 Q138 I139 G140 T141 Y142 L143 L144 Q147 R160 G177 F178

R188 R194 K209 H210 P211 I235 M236 D237 K238 Q253 S286 A308 Y309 W310 P311 G312 F313 G314 G315 Q316 A317 E321 C322 S323 G324 L329 L333 L342 N347 N356 G372 I379 P380 E388 Q392 G397 ALA THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.11Å 142.11Å 83.86Å 90.00° 105.61° 90.00°	Depositor
Resolution (Å)	46.70 – 2.39 46.71 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.70-2.39) 98.7 (46.71-2.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.218 0.164 , 0.216	Depositor DCC
R_{free} test set	3264 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12616	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: GOL, MVI, DMS, SAH, 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	0.45	0/3159	0.56	0/4287
1	B	0.41	0/2833	0.55	0/3835
1	C	0.44	0/3002	0.55	0/4072
1	D	0.43	0/3210	0.55	0/4358
All	All	0.43	0/12204	0.55	0/16552

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts   ⓘ

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	3077	0	2969	27	0
1	B	2774	0	2704	12	0
1	C	2924	0	2822	11	0
1	D	3126	0	3013	17	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	19	0	0
3	C	26	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	26	0	19	0	0
4	A	47	0	56	1	0
4	C	47	0	56	0	0
5	A	8	0	12	1	0
5	C	4	0	6	0	0
6	D	6	0	8	1	0
7	A	166	0	0	2	0
7	B	109	0	0	1	0
7	C	130	0	0	0	0
7	D	117	0	0	2	0
All	All	12616	0	11703	61	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 3.

All (61) 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:A:173:THR:HG21	1:A:220:MET:HE3	1.59	0.84
1:A:319:PRO:HG3	1:D:342:LEU:HD21	1.80	0.64
1:A:219:ARG:HD2	7:A:462:HOH:O	1.97	0.64
1:B:231:TYR:HD2	1:B:247:ARG:HG2	1.65	0.61
1:A:173:THR:HG21	1:A:220:MET:CE	2.31	0.60
1:D:33:TYR:HB2	1:D:38:ILE:HD11	1.84	0.60
1:C:125:LEU:HD11	1:D:380:PRO:HG3	1.84	0.60
1:A:49:ARG:HG2	5:A:401:DMS:S	2.44	0.56
1:A:129:LEU:HD23	1:A:135:ALA:HA	1.87	0.56
1:B:147:GLN:HG3	1:D:177:GLY:HA3	1.88	0.54
1:D:6:GLU:HB2	7:D:481:HOH:O	2.09	0.52
1:A:50:CYS:HB3	1:A:84:ILE:HD12	1.91	0.52
1:D:77:ARG:HD2	6:D:400:GOL:H31	1.93	0.51
1:C:333:LEU:HD22	1:C:357:ILE:HD12	1.93	0.51
1:B:264:ARG:NH2	7:B:459:HOH:O	2.44	0.50
1:C:353:VAL:HG13	1:C:357:ILE:HD11	1.94	0.50
1:A:265:ARG:HD2	7:A:521:HOH:O	2.12	0.50
1:C:361:HIS:HB2	1:C:368:PHE:HB2	1.93	0.50
1:A:33:TYR:HB2	1:A:38:ILE:HD11	1.94	0.49
1:C:103:THR:HA	1:C:106:LEU:HD12	1.95	0.48
1:B:186:TYR:O	1:B:190:PHE:HB2	2.14	0.47
1:A:173:THR:CG2	1:A:220:MET:CE	2.92	0.47
1:A:173:THR:OG1	1:A:175:LYS:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ARG:NH2	1:C:375:ASP:OD1	2.47	0.47
1:B:117:PRO:HG3	1:D:188:ARG:CZ	2.45	0.46
1:A:80:ARG:O	1:A:81:ASP:HB2	2.15	0.46
1:B:183:THR:N	1:B:184:PRO:CD	2.77	0.46
1:D:253:GLN:HG3	1:D:286:SER:OG	2.16	0.46
1:D:236:MET:HB2	1:D:238:LYS:HE2	1.98	0.46
1:C:126:PHE:HB3	1:C:129:LEU:HD22	1.98	0.45
1:D:388:GLU:H	1:D:388:GLU:CD	2.20	0.45
1:C:87:VAL:HB	1:C:91:GLU:HG3	1.98	0.45
1:A:387:PHE:O	1:A:391:VAL:HG23	2.16	0.45
1:A:310:TRP:HA	1:A:311:PRO:HD3	1.86	0.45
1:D:329:LEU:O	1:D:333:LEU:HG	2.16	0.44
1:C:336:ALA:HB1	1:C:354:ASP:HA	1.99	0.44
1:A:134:GLU:O	1:A:137:GLU:HG2	2.18	0.44
1:D:136:VAL:HA	1:D:139:ILE:HD12	2.00	0.44
1:D:60:LEU:HD13	1:D:92:GLY:HA3	2.01	0.43
1:A:29:LEU:C	1:A:29:LEU:HD23	2.40	0.42
1:A:306:TRP:CD2	1:D:379:ILE:HG13	2.55	0.42
1:D:310:TRP:HA	1:D:311:PRO:HD3	1.84	0.42
1:A:80:ARG:NH1	1:C:81:ASP:OD2	2.50	0.42
1:D:194:ARG:HD3	7:D:439:HOH:O	2.19	0.42
1:B:6:GLU:HG3	1:B:7:PHE:CD1	2.55	0.42
1:A:50:CYS:CB	1:A:84:ILE:HD12	2.49	0.41
1:A:138:GLN:HG3	1:A:142:TYR:HD2	1.84	0.41
1:A:186:TYR:O	1:A:190:PHE:HB2	2.20	0.41
4:A:701:MVI:CAP	4:A:701:MVI:CBD	2.99	0.41
1:D:356:ASN:HA	1:D:372:GLY:O	2.20	0.41
1:A:329:LEU:O	1:A:333:LEU:HG	2.21	0.41
1:A:42:LEU:HD21	1:A:106:LEU:HD23	2.02	0.41
1:B:231:TYR:CD2	1:B:247:ARG:HG2	2.50	0.41
1:B:284:ARG:H	1:B:284:ARG:HG2	1.73	0.41
1:A:52:PRO:HA	1:A:53:PRO:HD3	1.77	0.41
1:A:380:PRO:HB3	1:B:125:LEU:HD11	2.03	0.41
1:C:339:HIS:CE1	1:C:374:ASN:ND2	2.89	0.40
1:B:187:ASP:OD1	1:B:191:ARG:HD3	2.21	0.40
1:A:263:ALA:HB1	1:A:293:HIS:CG	2.57	0.40
1:A:356:ASN:HA	1:A:372:GLY:O	2.22	0.40
1:B:42:LEU:HD22	1:B:109:LEU:HD12	2.04	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	A	382/419 (91%)	372 (97%)	10 (3%)	0	100	100
1	B	340/419 (81%)	330 (97%)	10 (3%)	0	100	100
1	C	362/419 (86%)	353 (98%)	9 (2%)	0	100	100
1	D	391/419 (93%)	378 (97%)	13 (3%)	0	100	100
All	All	1475/1676 (88%)	1433 (97%)	42 (3%)	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	327/353 (93%)	316 (97%)	11 (3%)	37	56
1	B	299/353 (85%)	289 (97%)	10 (3%)	38	57
1	C	308/353 (87%)	300 (97%)	8 (3%)	46	66
1	D	332/353 (94%)	327 (98%)	5 (2%)	65	80
All	All	1266/1412 (90%)	1232 (97%)	34 (3%)	44	65

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	56	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	129	LEU
1	A	130	THR
1	A	131	ASP
1	A	168	SER
1	A	173	THR
1	A	223	SER
1	A	242	ASP
1	A	332	SER
1	A	392	GLN
1	B	17	ARG
1	B	56	ASP
1	B	69	SER
1	B	134	GLU
1	B	247	ARG
1	B	253	GLN
1	B	277	SER
1	B	282	HIS
1	B	284	ARG
1	B	347	ASN
1	C	91	GLU
1	C	115	GLU
1	C	131	ASP
1	C	138	GLN
1	C	168	SER
1	C	173	THR
1	C	242	ASP
1	C	373	ARG
1	D	59	VAL
1	D	134	GLU
1	D	147	GLN
1	D	188	ARG
1	D	347	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	282	HIS
1	C	339	HIS
1	D	74	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	#$|Z| > 2$
5	DMS	A	400	-	3,3,3	2.66	1 (33%)	3,3,3	0.45	0
4	MVI	A	701	2	49,49,49	1.33	5 (10%)	60,69,69	1.32	9 (15%)
5	DMS	C	400	-	3,3,3	2.64	1 (33%)	3,3,3	0.56	0
4	MVI	C	701	2	49,49,49	1.36	5 (10%)	60,69,69	1.33	9 (15%)
6	GOL	D	400	-	5,5,5	0.40	0	5,5,5	0.20	0
3	SAH	C	601	-	24,28,28	1.05	1 (4%)	25,40,40	1.39	4 (16%)
5	DMS	A	401	-	3,3,3	2.67	1 (33%)	3,3,3	0.64	0
3	SAH	D	601	-	24,28,28	1.08	1 (4%)	25,40,40	1.42	5 (20%)
3	SAH	A	601	-	24,28,28	1.03	3 (12%)	25,40,40	1.47	5 (20%)

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
4	MVI	A	701	2	-	3/51/87/87	0/2/3/3
4	MVI	C	701	2	-	4/51/87/87	0/2/3/3
6	GOL	D	400	-	-	0/4/4/4	-
3	SAH	C	601	-	-	0/11/31/31	0/3/3/3
3	SAH	D	601	-	-	2/11/31/31	0/3/3/3
3	SAH	A	601	-	-	0/11/31/31	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	DMS	O-S	4.48	1.80	1.50
5	A	400	DMS	O-S	4.47	1.80	1.50
5	C	400	DMS	O-S	4.42	1.80	1.50
4	A	701	MVI	CAR-CBD	-3.43	1.40	1.48
4	C	701	MVI	CAR-CBD	-3.42	1.40	1.48
4	C	701	MVI	CAR-CAS	3.36	1.40	1.32
4	A	701	MVI	CAR-CAS	3.12	1.39	1.32
3	D	601	SAH	C5-C4	2.81	1.48	1.40
4	C	701	MVI	OAY-CBQ	2.55	1.44	1.40
3	C	601	SAH	C5-C4	2.55	1.47	1.40
3	A	601	SAH	C5-C4	2.32	1.47	1.40
4	A	701	MVI	CAX-CBG	2.13	1.55	1.51
4	C	701	MVI	CBH-CBE	2.12	1.54	1.51
4	C	701	MVI	CAP-CAO	-2.07	1.38	1.44
3	A	601	SAH	C2-N3	2.06	1.35	1.32
4	A	701	MVI	CBH-CBE	2.03	1.54	1.51
3	A	601	SAH	OXT-C	-2.00	1.24	1.30
4	A	701	MVI	OBB-CBQ	2.00	1.46	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	MVI	OBB-CBJ-CAF	3.98	115.28	106.70
4	C	701	MVI	OBB-CBJ-CBL	3.70	116.17	109.52
3	A	601	SAH	N3-C2-N1	-3.62	123.01	128.68
4	A	701	MVI	CAP-CAO-CAQ	-3.39	116.19	124.67
3	D	601	SAH	N3-C2-N1	-3.35	123.44	128.68
4	C	701	MVI	OBB-CBJ-CAF	3.27	113.76	106.70
4	A	701	MVI	OAZ-CBD-CAR	3.15	118.53	111.38
3	C	601	SAH	N3-C2-N1	-3.05	123.91	128.68
4	C	701	MVI	CAP-CAO-CAQ	-3.00	117.18	124.67
4	C	701	MVI	CBQ-OBB-CBJ	2.98	118.79	113.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	SAH	C4-C5-N7	-2.93	106.35	109.40
3	C	601	SAH	C4-C5-N7	-2.86	106.42	109.40
3	C	601	SAH	OXT-C-O	-2.81	117.70	124.09
4	C	701	MVI	OAZ-CBP-CBK	2.74	113.42	107.42
4	C	701	MVI	OAZ-CBD-CAR	2.68	117.45	111.38
4	C	701	MVI	CBF-CAS-CAR	-2.67	119.14	126.44
4	A	701	MVI	OAZ-CBP-CBK	2.65	113.24	107.42
4	C	701	MVI	CBM-CBL-CBJ	2.63	113.87	109.77
3	D	601	SAH	C4-C5-N7	-2.51	106.78	109.40
3	A	601	SAH	OXT-C-O	-2.47	118.47	124.09
3	D	601	SAH	OXT-C-O	-2.47	118.47	124.09
4	C	701	MVI	CBK-CAT-CAP	-2.41	119.36	125.45
3	A	601	SAH	OXT-C-CA	2.32	121.27	113.38
3	A	601	SAH	CB-CG-SD	-2.29	108.18	113.31
4	A	701	MVI	CBQ-OBB-CBJ	2.26	117.55	113.67
3	D	601	SAH	OXT-C-CA	2.22	120.95	113.38
3	D	601	SAH	C3'-C2'-C1'	2.22	104.32	100.98
3	C	601	SAH	OXT-C-CA	2.20	120.89	113.38
4	A	701	MVI	CBF-CAS-CAR	-2.19	120.45	126.44
4	A	701	MVI	OAY-CBQ-CBN	-2.09	105.04	108.30
4	A	701	MVI	OBA-CBG-CAC	2.06	111.25	106.88
4	A	701	MVI	CBM-CBL-CBJ	2.05	112.97	109.77

There are no chirality outliers.
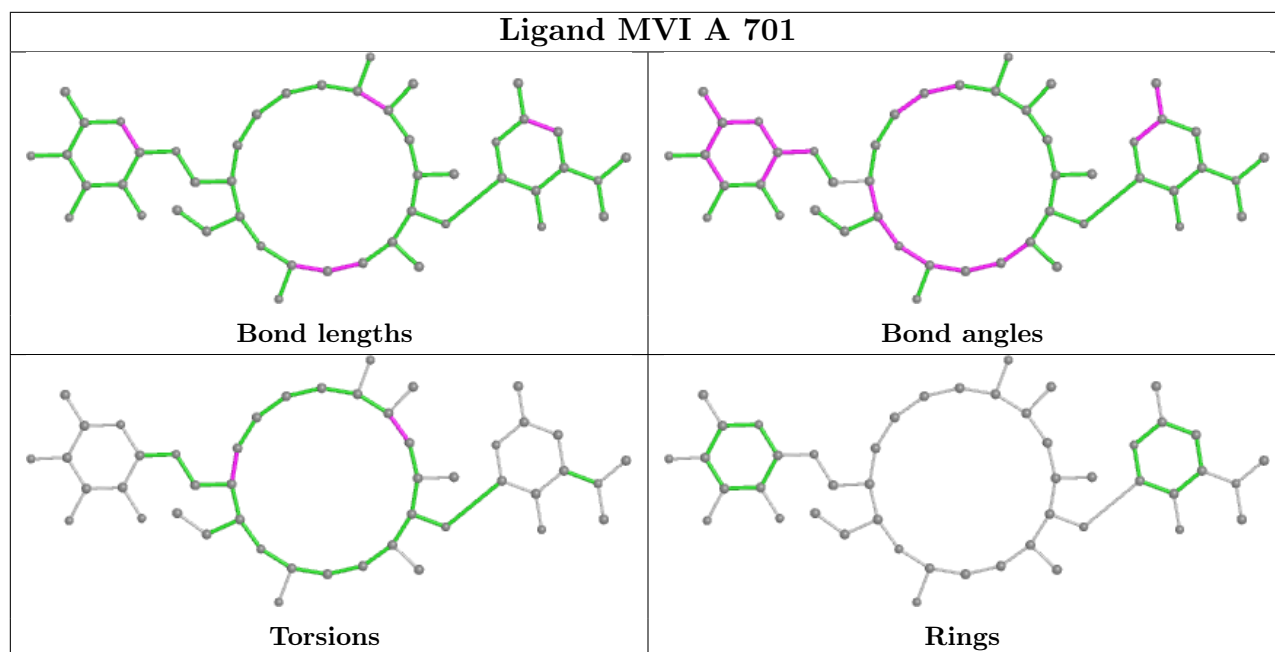
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	701	MVI	CAA-CAU-CBP-OAZ
3	D	601	SAH	O4'-C4'-C5'-SD
4	A	701	MVI	CBI-CAW-CBH-CBE
4	C	701	MVI	CBI-CAW-CBH-CBE
4	C	701	MVI	CAP-CAT-CBK-CAV
4	C	701	MVI	CAP-CAT-CBK-CBP
3	D	601	SAH	CA-CB-CG-SD
4	A	701	MVI	CAP-CAT-CBK-CAV
4	A	701	MVI	CAP-CAT-CBK-CBP

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	MVI	1	0
6	D	400	GOL	1	0
5	A	401	DMS	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 MVI A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand MVI C 701

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH D 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH A 601

Bond lengths

Bond angles

Torsions

Rings
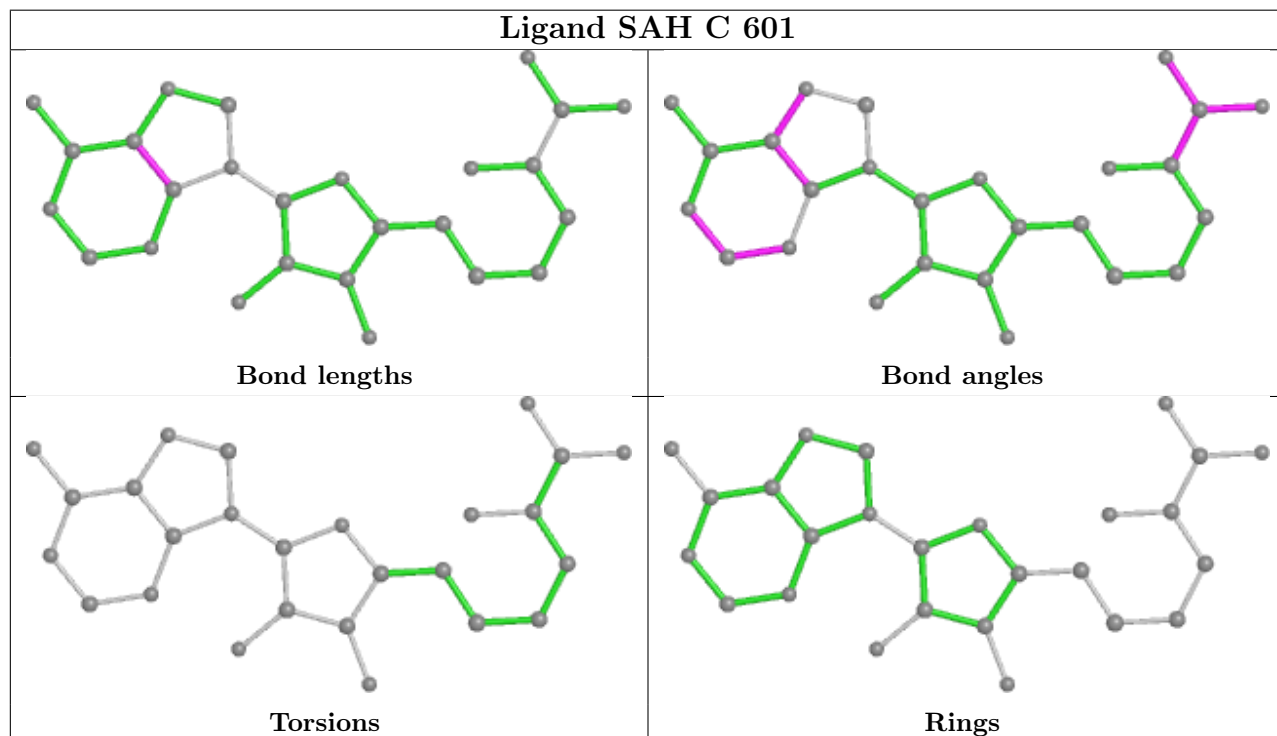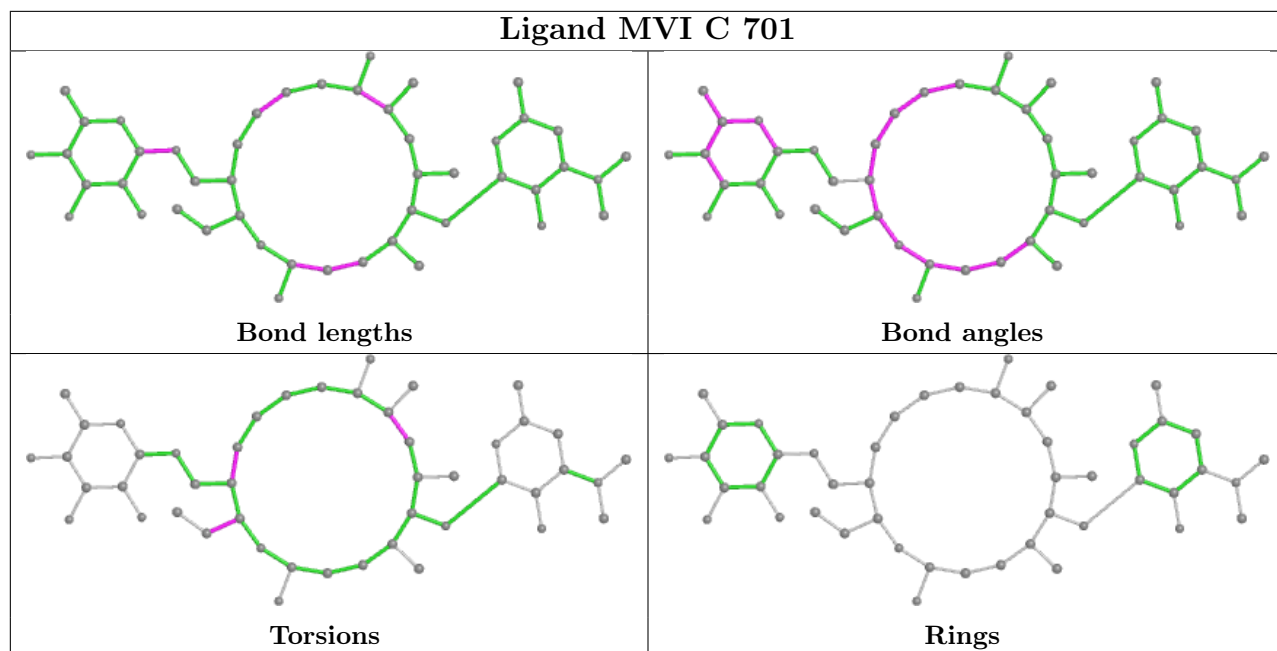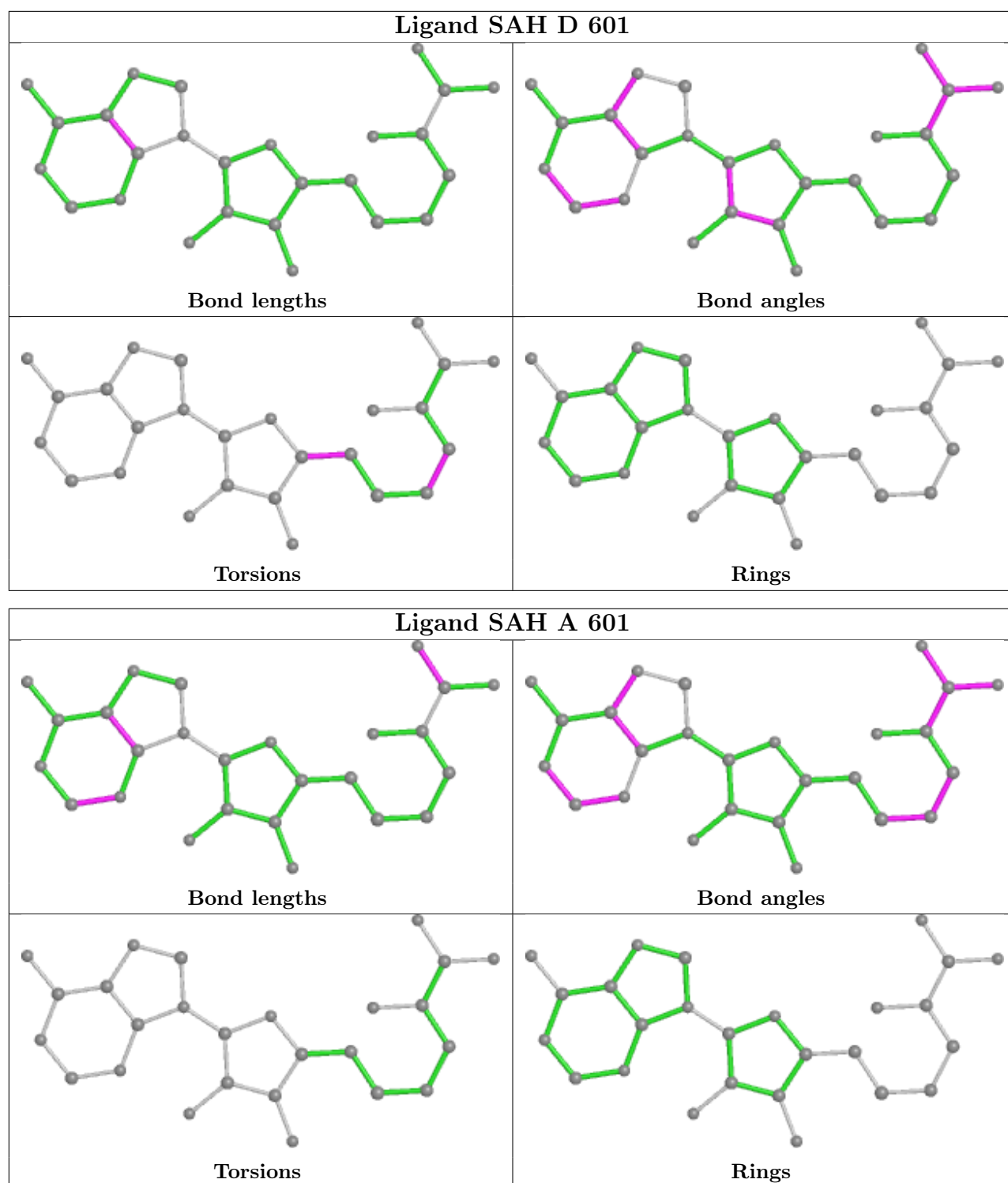
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	386/419 (92%)	0.28	22 (5%)	23	22	25, 41, 86, 123	0
1	B	350/419 (83%)	0.46	33 (9%)	8	7	24, 50, 100, 176	0
1	C	366/419 (87%)	0.35	21 (5%)	23	22	26, 45, 79, 141	0
1	D	393/419 (93%)	0.43	37 (9%)	8	7	27, 48, 98, 119	0
All	All	1495/1676 (89%)	0.38	113 (7%)	13	12	24, 45, 93, 176	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	381	THR	8.2
1	B	130	THR	7.2
1	C	380	PRO	6.2
1	D	311	PRO	6.1
1	C	382	TRP	5.9
1	D	317	ALA	5.8
1	A	344	SER	5.7
1	C	379	ILE	5.6
1	B	133	GLU	5.5
1	B	137	GLU	5.4
1	A	382	TRP	5.2
1	A	392	GLN	5.1
1	B	134	GLU	5.0
1	B	346	PRO	4.8
1	D	136	VAL	4.7
1	A	381	THR	4.6
1	B	139	ILE	4.6
1	B	324	GLY	4.5
1	C	130	THR	4.5
1	B	347	ASN	4.4
1	B	138	GLN	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	143	LEU	4.2
1	A	343	PRO	4.0
1	A	387	PHE	4.0
1	A	385	ARG	4.0
1	D	316	GLN	4.0
1	D	310	TRP	3.9
1	D	178	PHE	3.9
1	A	380	PRO	3.9
1	B	136	VAL	3.9
1	A	394	SER	3.8
1	B	140	GLY	3.8
1	D	139	ILE	3.7
1	D	322	CYS	3.7
1	D	131	ASP	3.6
1	A	391	VAL	3.5
1	D	211	PRO	3.5
1	A	388	GLU	3.5
1	C	212	GLU	3.5
1	D	134	GLU	3.5
1	C	209	LYS	3.4
1	B	325	THR	3.3
1	D	324	GLY	3.3
1	C	129	LEU	3.2
1	A	130	THR	3.2
1	A	384	PRO	3.1
1	B	131	ASP	3.1
1	A	383	ILE	3.0
1	C	133	GLU	3.0
1	A	386	ASP	3.0
1	B	56	ASP	3.0
1	D	5	THR	3.0
1	D	312	GLY	3.0
1	B	132	ASP	3.0
1	B	141	THR	3.0
1	D	133	GLU	2.9
1	D	132	ASP	2.9
1	B	129	LEU	2.9
1	D	143	LEU	2.9
1	B	142	TYR	2.9
1	D	313	PHE	2.8
1	C	134	GLU	2.8
1	B	214	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	209	LYS	2.8
1	D	323	SER	2.7
1	B	144	LEU	2.7
1	B	396	GLY	2.7
1	D	137	GLU	2.7
1	B	77	ARG	2.7
1	A	379	ILE	2.6
1	D	6	GLU	2.6
1	D	392	GLN	2.6
1	D	308	ALA	2.6
1	B	236	MET	2.6
1	C	137	GLU	2.6
1	B	7	PHE	2.6
1	C	93	PHE	2.6
1	D	397	GLY	2.5
1	B	135	ALA	2.5
1	C	131	ASP	2.5
1	A	390	LEU	2.5
1	A	342	LEU	2.5
1	D	309	TYR	2.4
1	B	75	PHE	2.4
1	B	36	ALA	2.4
1	D	144	LEU	2.3
1	C	135	ALA	2.3
1	D	142	TYR	2.3
1	C	89	ALA	2.3
1	C	142	TYR	2.3
1	D	321	GLU	2.3
1	A	378	GLY	2.2
1	C	378	GLY	2.2
1	C	136	VAL	2.2
1	D	235	ILE	2.2
1	B	69	SER	2.2
1	A	393	ALA	2.2
1	B	90	ASP	2.2
1	A	6	GLU	2.2
1	B	59	VAL	2.2
1	D	315	GLY	2.2
1	B	89	ALA	2.1
1	D	138	GLN	2.1
1	D	210	HIS	2.1
1	C	369	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	75	PHE	2.1
1	D	160	ARG	2.0
1	A	395	SER	2.0
1	D	314	GLY	2.0
1	B	85	ARG	2.0
1	D	130	THR	2.0
1	C	117	PRO	2.0
1	D	140	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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
4	MVI	C	701	47/47	0.89	0.20	63,66,68,69	0
6	GOL	D	400	6/6	0.90	0.26	78,78,78,80	0
2	MG	D	501	1/1	0.92	0.26	84,84,84,84	0
3	SAH	D	601	26/26	0.92	0.21	65,67,70,71	0
4	MVI	A	701	47/47	0.94	0.21	54,63,65,66	0
2	MG	C	501	1/1	0.96	0.06	60,60,60,60	0
5	DMS	A	400	4/4	0.96	0.36	74,74,74,75	0
5	DMS	C	400	4/4	0.96	0.18	71,72,72,73	0
3	SAH	C	601	26/26	0.96	0.13	48,50,52,53	0
3	SAH	A	601	26/26	0.97	0.11	36,37,42,43	0
5	DMS	A	401	4/4	0.97	0.13	66,66,67,67	0
2	MG	A	501	1/1	0.99	0.10	47,47,47,47	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.
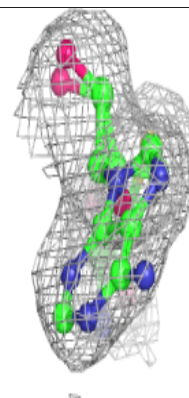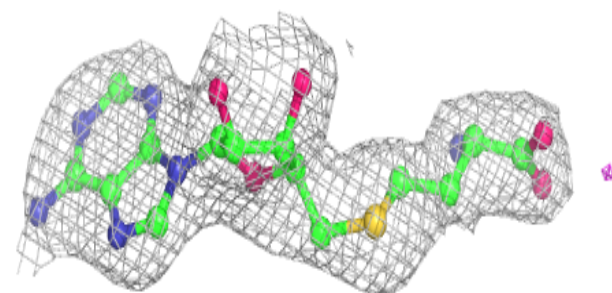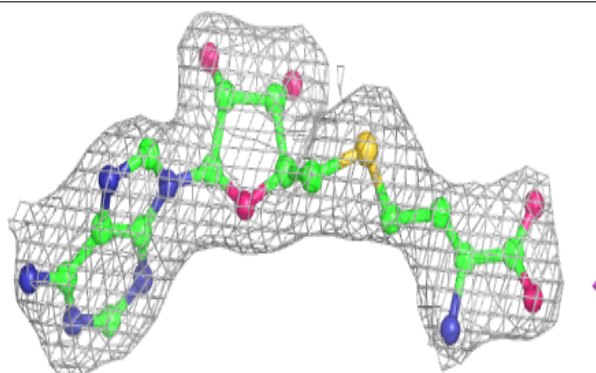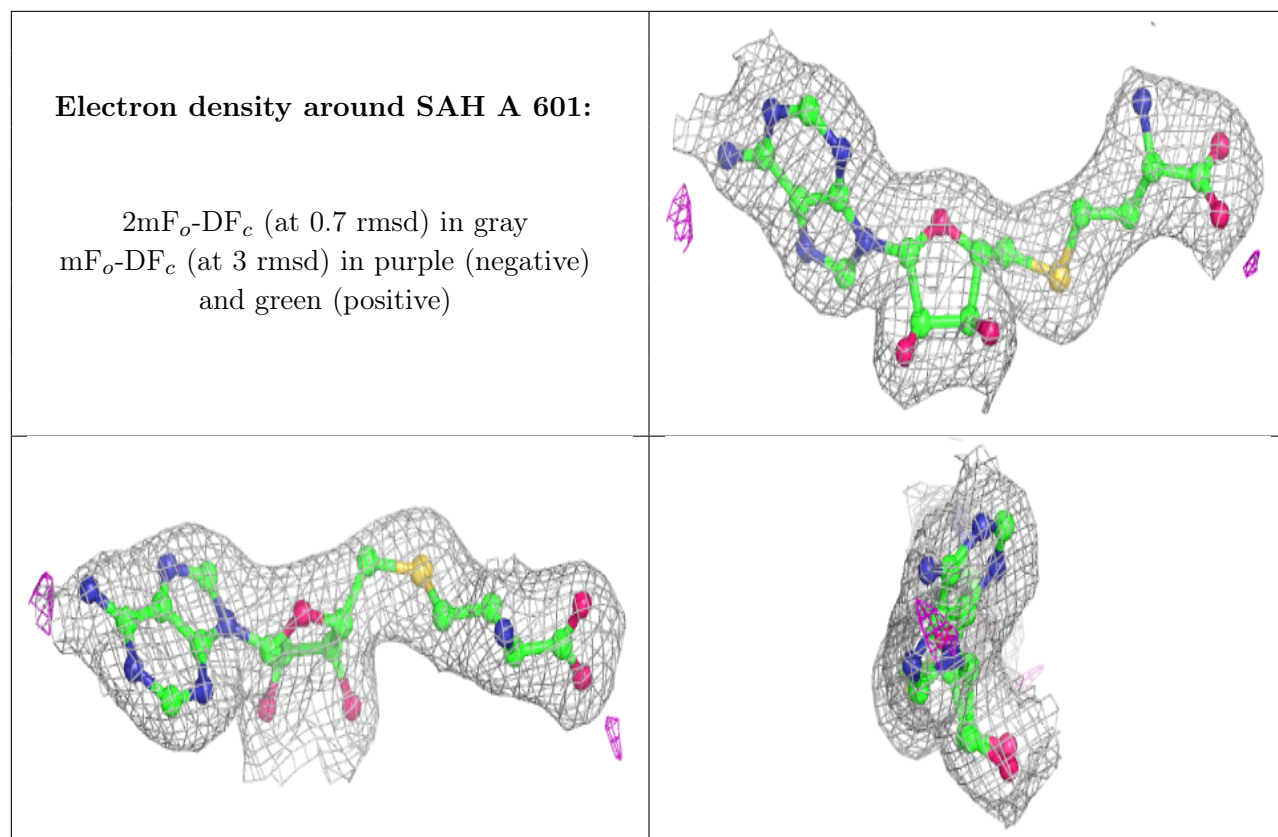
Electron density around MVI C 701:

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

Electron density around SAH D 601:

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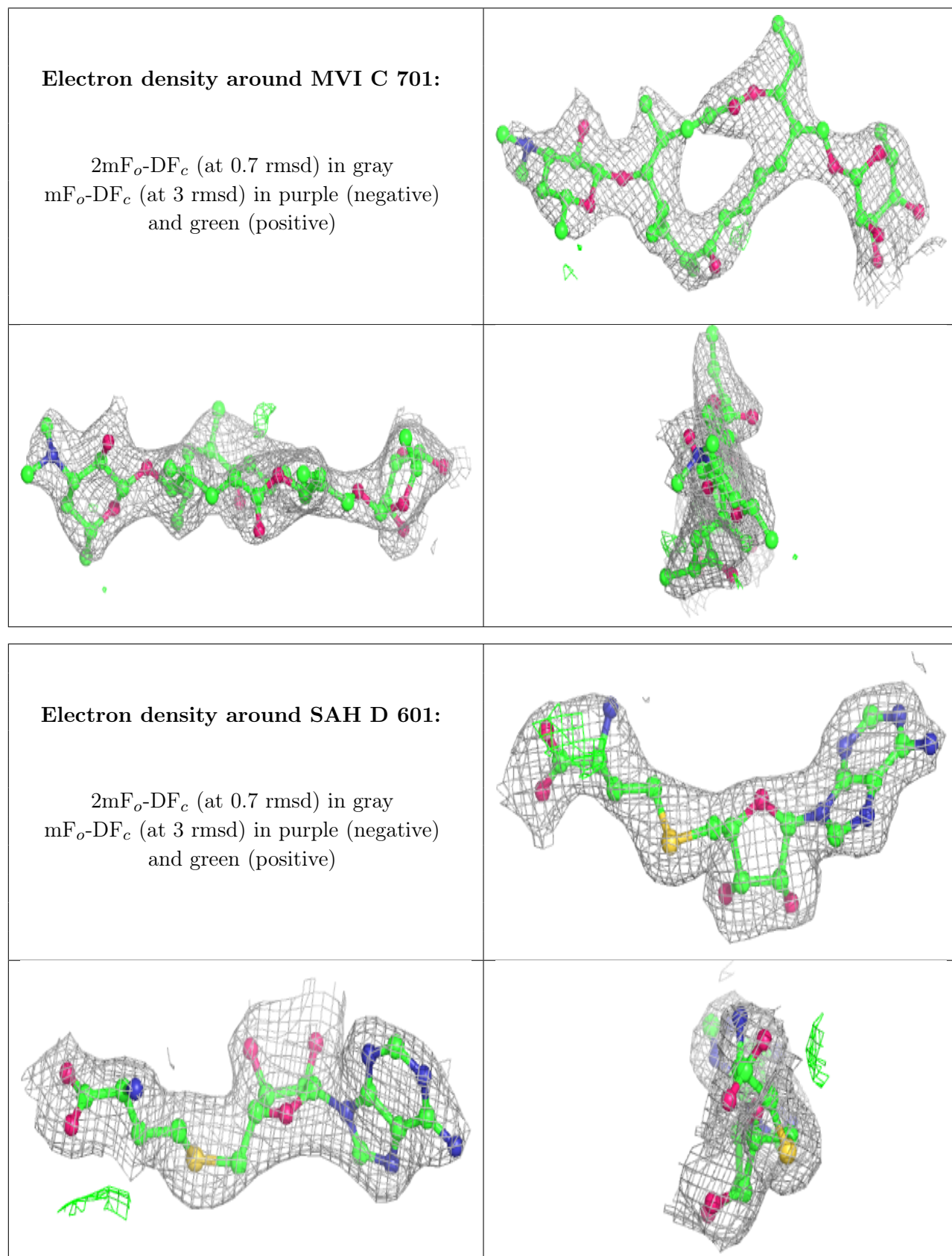
Electron density around MVI A 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
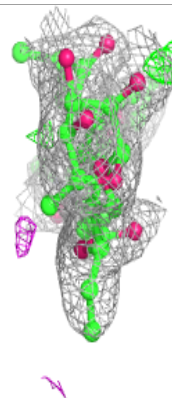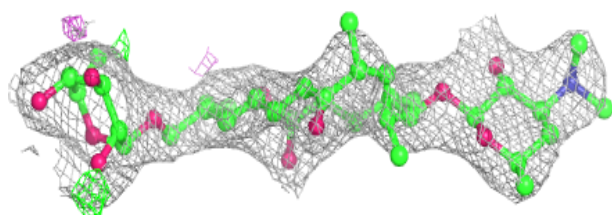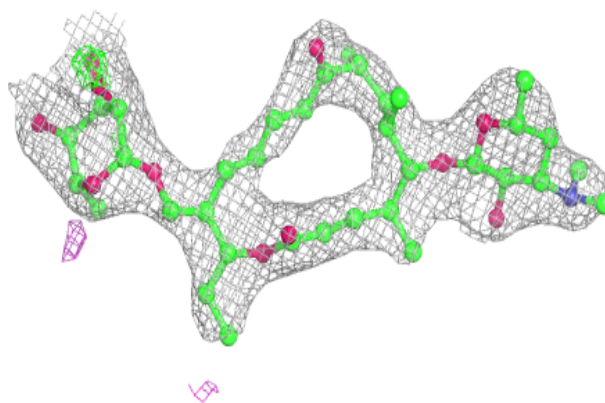
Electron density around SAH C 601:

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 SAH A 601:

$2mF_o\text{-}DF_c$ (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.