



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2021 – 10:11 AM JST

PDB ID : 7EC0
Title : Crystal structure of juvenile hormone acid methyltransferase JHAMT in complex with S-Adenosyl homocysteine and methyl farnesoate
Authors : Guo, P.C.; Zhang, Y.S.; Zhang, L.; Xu, H.Y.; Xia, Q.Y.
Deposited on : 2021-03-11
Resolution : 2.49 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

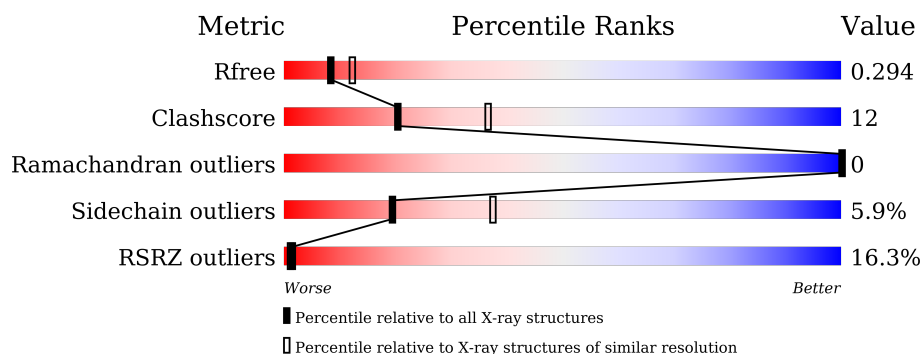
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	288	<div> <div>17%</div> <div>66%</div> <div>21%</div> <div>•</div> <div>11%</div> </div>
1	D	288	<div> <div>9%</div> <div>65%</div> <div>23%</div> <div>•</div> <div>11%</div> </div>
1	G	288	<div> <div>12%</div> <div>65%</div> <div>23%</div> <div>•</div> <div>11%</div> </div>
1	J	288	<div> <div>17%</div> <div>67%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>
1	M	288	<div> <div>16%</div> <div>67%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>
1	P	288	<div> <div>11%</div> <div>50%</div> <div>16%</div> <div>•</div> <div>31%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	J10	A	302	-	-	X	X
3	J10	J	302	-	-	X	X
3	J10	M	302	-	-	-	X

2 Entry composition [i](#)

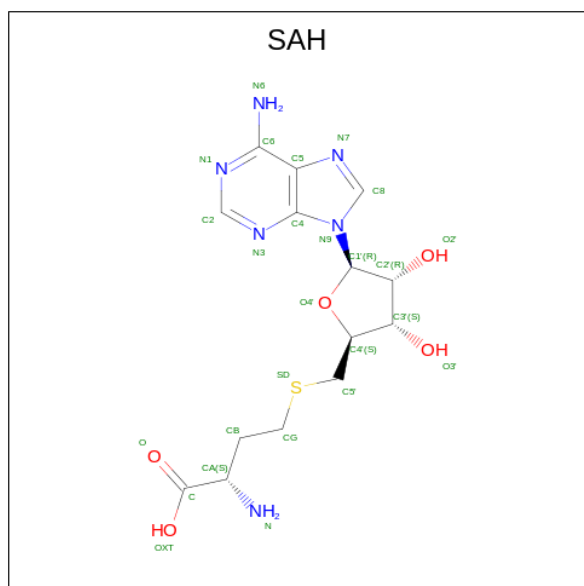
There are 4 unique types of molecules in this entry. The entry contains 24931 atoms, of which 12415 are hydrogens and 0 are deuteriums.

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 Juvenile hormone acid methyltransferase.

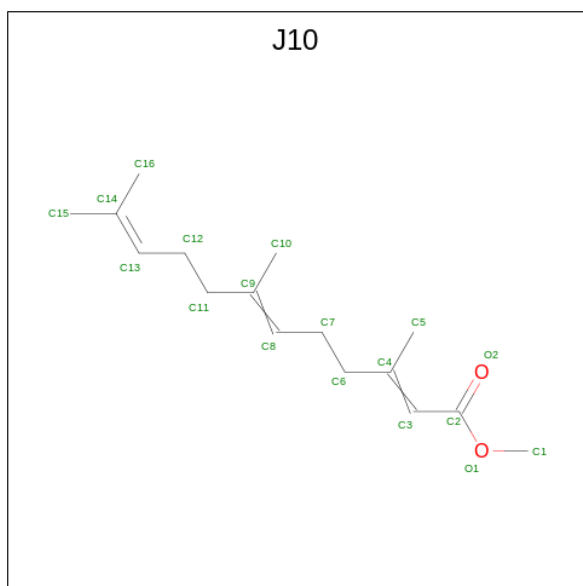
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	255	Total	C	H	N	O	S	93	0	0
			4224	1363	2105	351	391	14			
1	D	256	Total	C	H	N	O	S	94	0	0
			4238	1367	2112	352	393	14			
1	G	256	Total	C	H	N	O	S	94	0	0
			4238	1367	2112	352	393	14			
1	J	256	Total	C	H	N	O	S	94	0	0
			4238	1367	2112	352	393	14			
1	M	256	Total	C	H	N	O	S	94	0	0
			4238	1367	2112	352	393	14			
1	P	198	Total	C	H	N	O	S	66	0	0
			3291	1067	1642	266	306	10			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	
			44	14	18	6	5	1	
2	D	1	Total	C	H	N	O	S	
			44	14	18	6	5	1	
2	G	1	Total	C	H	N	O	S	
			44	14	18	6	5	1	
2	J	1	Total	C	H	N	O	S	
			44	14	18	6	5	1	
2	M	1	Total	C	H	N	O	S	
			44	14	18	6	5	1	

- Molecule 3 is Methyl farnesoate (three-letter code: J10) (formula: $C_{16}H_{26}O_2$) (labeled as "Ligand of Interest" by depositor).



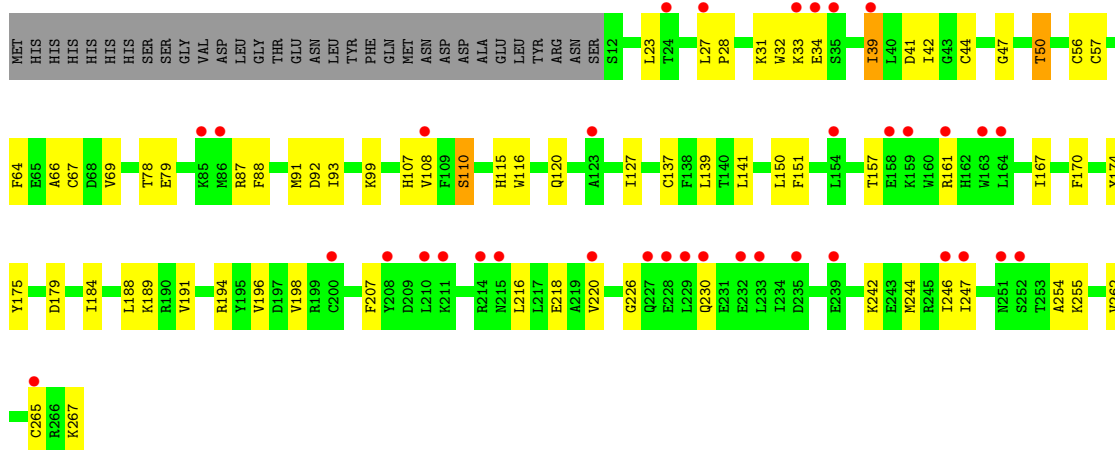
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	H	O	
			44	16	26	2	
3	D	1	Total	C	H	O	
			44	16	26	2	
3	G	1	Total	C	H	O	
			44	16	26	2	
3	J	1	Total	C	H	O	
			44	16	26	2	
3	M	1	Total	C	H	O	
			44	16	26	2	

- Molecule 4 is water.

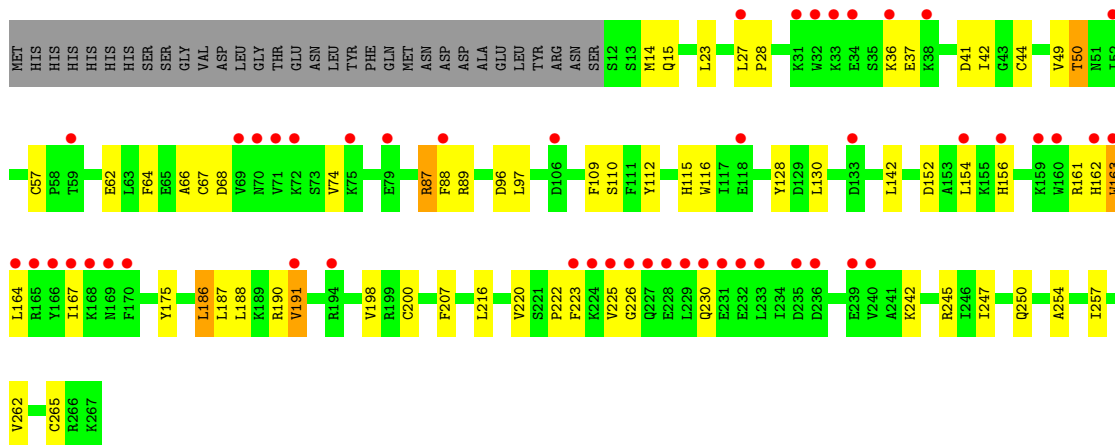
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	O 4	0	0
4	D	6	Total 6	O 6	0	0
4	G	5	Total 5	O 5	0	0
4	J	1	Total 1	O 1	0	0
4	M	4	Total 4	O 4	0	0
4	P	4	Total 4	O 4	0	0

- Molecule 1: Juvenile hormone acid methyltransferase

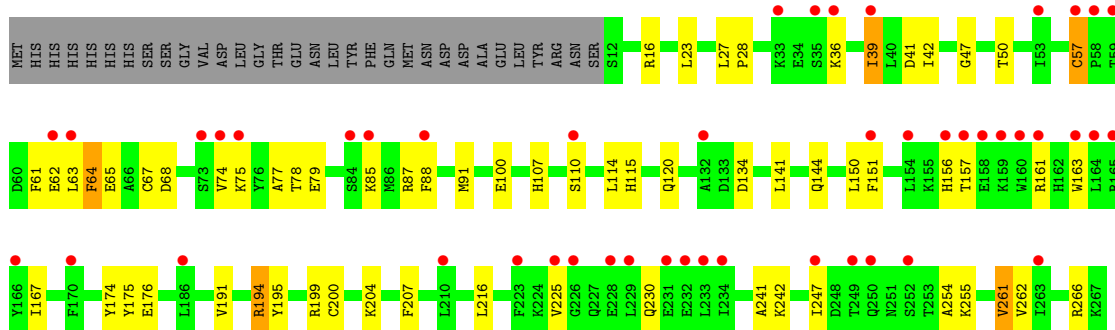




• Molecule 1: Juvenile hormone acid methyltransferase

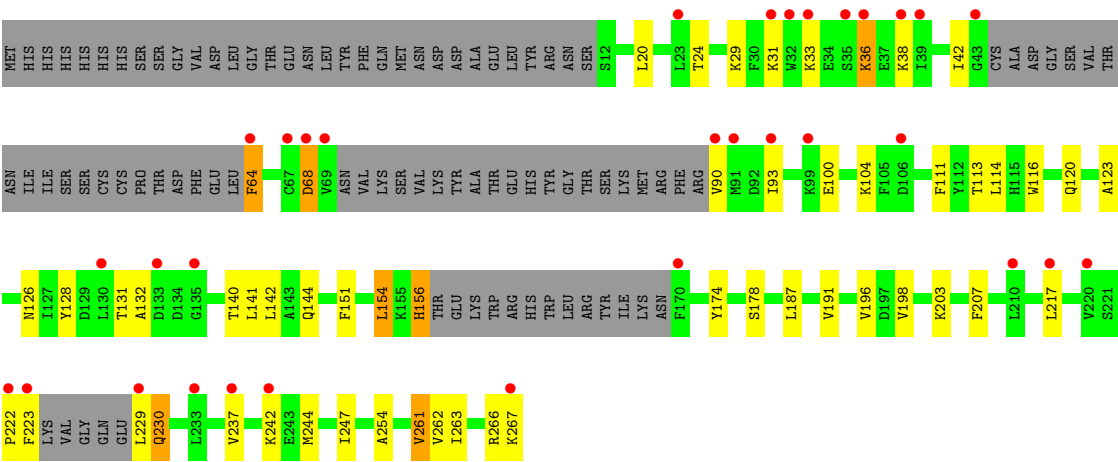


• Molecule 1: Juvenile hormone acid methyltransferase



• Molecule 1: Juvenile hormone acid methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.46Å 101.20Å 103.36Å 90.00° 93.50° 90.00°	Depositor
Resolution (Å)	72.26 – 2.49 55.48 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (72.26-2.49) 99.2 (55.48-2.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.245 , 0.293 0.245 , 0.294	Depositor DCC
R_{free} test set	3103 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24931	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: J10, SAH

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	0.64	0/2166	0.71	0/2917
1	D	0.64	0/2174	0.71	0/2930
1	G	0.64	0/2174	0.70	0/2930
1	J	0.64	0/2174	0.71	0/2930
1	M	0.64	0/2174	0.71	0/2930
1	P	0.65	0/1681	0.72	0/2259
All	All	0.64	0/12543	0.71	0/16896

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2119	2105	2097	61	1
1	D	2126	2112	2105	54	0
1	G	2126	2112	2105	46	1
1	J	2126	2112	2105	60	1
1	M	2126	2112	2105	49	0
1	P	1649	1642	1633	42	0
2	A	26	18	19	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	26	18	19	2	0
2	G	26	18	19	0	0
2	J	26	18	19	6	0
2	M	26	18	19	1	0
3	A	18	26	0	17	0
3	D	18	26	0	3	0
3	G	18	26	0	8	0
3	J	18	26	0	12	0
3	M	18	26	0	3	0
4	A	4	0	0	0	0
4	D	6	0	0	0	0
4	G	5	0	0	0	0
4	J	1	0	0	0	0
4	M	4	0	0	2	0
4	P	4	0	0	0	0
All	All	12516	12415	12245	307	2

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 12.

All (307) 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:G:194:ARG:HG3	1:G:267:LYS:O	1.41	1.18
1:J:49:VAL:HG11	2:J:301:SAH:HA	1.28	1.09
1:P:222:PRO:HD2	1:P:223:PHE:CD2	1.89	1.07
1:J:163:TRP:HD1	1:J:225:VAL:HG12	1.21	1.04
1:M:151:PHE:CD1	3:M:302:J10:C15	2.42	1.03
1:A:220:VAL:HB	3:A:302:J10:C7	1.93	0.97
1:P:31:LYS:HD2	1:P:33:LYS:HE2	1.47	0.96
1:A:115:HIS:CE1	3:A:302:J10:C1	2.48	0.95
1:A:98:PRO:HG2	1:A:101:MET:HG3	1.51	0.91
1:P:222:PRO:HD2	1:P:223:PHE:CE2	2.05	0.91
1:J:163:TRP:CD1	1:J:225:VAL:HG12	2.09	0.85
1:M:36:LYS:HG3	1:M:62:GLU:HB2	1.60	0.83
1:A:115:HIS:NE2	3:A:302:J10:C1	2.42	0.83
1:D:14:MET:HE1	3:D:302:J10:C5	2.09	0.82
1:G:31:LYS:HE2	1:G:33:LYS:HE3	1.62	0.82
1:D:226:GLY:O	1:D:230:GLN:HB2	1.80	0.81
1:M:114:LEU:HB2	1:M:141:LEU:HD13	1.61	0.81
1:G:79:GLU:O	1:M:194:ARG:HG2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD21	1:A:130:LEU:HD21	1.64	0.79
1:A:49:VAL:HG11	2:A:301:SAH:HN2	1.47	0.78
1:M:36:LYS:HE3	1:M:62:GLU:HG2	1.65	0.78
1:A:151:PHE:CD2	3:A:302:J10:C15	2.67	0.78
1:J:49:VAL:HG11	2:J:301:SAH:CA	2.12	0.78
1:M:61:PHE:O	1:M:85:LYS:HE3	1.83	0.77
3:D:302:J10:C3	3:D:302:J10:C8	2.60	0.76
1:D:43:GLY:O	2:D:301:SAH:N	2.17	0.75
1:M:151:PHE:CE1	3:M:302:J10:C15	2.71	0.73
1:A:115:HIS:HE2	3:A:302:J10:C1	2.02	0.72
1:A:97:LEU:CD2	1:A:130:LEU:HD21	2.18	0.72
1:D:50:THR:HG22	1:D:86:MET:CE	2.19	0.72
1:J:49:VAL:CG1	2:J:301:SAH:HA	2.15	0.72
1:J:225:VAL:HG23	1:J:230:GLN:CD	2.09	0.72
1:P:29:LYS:O	1:P:266:ARG:NH2	2.23	0.71
1:P:229:LEU:HG	1:P:229:LEU:O	1.89	0.71
1:D:36:LYS:HG3	1:D:62:GLU:HB2	1.72	0.71
1:D:63:LEU:HD11	1:D:65:GLU:HG3	1.72	0.70
1:M:163:TRP:CD2	1:M:225:VAL:HG12	2.28	0.69
1:A:151:PHE:CG	3:A:302:J10:C15	2.75	0.69
1:M:68:ASP:OD2	2:M:301:SAH:O3'	2.11	0.68
1:A:151:PHE:HB2	3:A:302:J10:C15	2.22	0.68
1:M:115:HIS:N	1:M:141:LEU:HD11	2.08	0.67
1:J:225:VAL:HG23	1:J:230:GLN:NE2	2.09	0.67
1:M:63:LEU:HD21	1:M:65:GLU:HG3	1.76	0.67
1:A:49:VAL:HG11	2:A:301:SAH:N	2.09	0.66
1:P:114:LEU:HB2	1:P:141:LEU:HD21	1.78	0.66
1:P:42:ILE:CG2	1:P:93:ILE:HD11	2.26	0.66
1:A:97:LEU:HD21	1:A:130:LEU:CD2	2.25	0.66
1:D:50:THR:CG2	1:D:86:MET:CE	2.75	0.65
1:J:164:LEU:N	1:J:164:LEU:HD12	2.12	0.64
1:D:50:THR:HG22	1:D:86:MET:HE1	1.78	0.64
1:G:115:HIS:HB3	1:G:141:LEU:HD23	1.80	0.64
1:J:36:LYS:HG3	1:J:62:GLU:HB2	1.80	0.64
1:D:98:PRO:HG2	1:D:101:MET:HG3	1.79	0.64
1:J:116:TRP:HE1	3:J:302:J10:C1	2.09	0.64
1:G:220:VAL:HB	3:G:302:J10:C7	2.27	0.64
1:A:145:MET:HE2	3:A:302:J10:C5	2.29	0.63
1:A:222:PRO:HD2	1:A:223:PHE:CE2	2.33	0.63
1:A:42:ILE:HB	1:A:110:SER:HB2	1.81	0.62
1:M:47:GLY:HA2	1:M:50:THR:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:HD11	1:D:176:GLU:HG2	1.81	0.62
1:P:38:LYS:HD2	1:P:104:LYS:O	1.98	0.62
1:G:194:ARG:CG	1:G:267:LYS:O	2.33	0.62
1:A:41:ASP:OD2	1:A:50:THR:HG22	2.00	0.61
1:J:163:TRP:C	1:J:164:LEU:HD12	2.21	0.61
1:M:151:PHE:CG	3:M:302:J10:C15	2.83	0.61
3:G:302:J10:C15	3:G:302:J10:C11	2.79	0.61
1:J:225:VAL:CG2	1:J:230:GLN:NE2	2.64	0.61
1:P:113:THR:O	1:P:116:TRP:HB2	2.01	0.60
1:P:187:LEU:O	1:P:191:VAL:HG23	2.01	0.60
1:A:145:MET:CE	3:A:302:J10:C5	2.79	0.60
1:J:225:VAL:CG2	1:J:230:GLN:OE1	2.48	0.60
1:D:87:ARG:NH2	1:G:99:LYS:NZ	2.50	0.60
1:J:97:LEU:HD11	1:J:130:LEU:HG	1.83	0.60
1:D:71:VAL:HG21	1:G:69:VAL:HB	1.84	0.60
1:D:87:ARG:HH22	1:G:99:LYS:HZ2	1.49	0.60
1:A:36:LYS:HA	1:A:62:GLU:HB2	1.84	0.60
1:P:128:TYR:CE2	1:P:267:LYS:HE3	2.37	0.59
1:P:120:GLN:HG2	1:P:174:TYR:OH	2.03	0.59
1:M:36:LYS:CG	1:M:62:GLU:HB2	2.31	0.59
1:M:207:PHE:HB2	1:M:254:ALA:HB3	1.85	0.59
1:M:75:LYS:O	1:M:79:GLU:HG3	2.02	0.59
3:A:302:J10:C16	3:A:302:J10:C11	2.81	0.58
1:P:36:LYS:NZ	1:P:36:LYS:HB3	2.17	0.58
1:J:164:LEU:N	1:J:164:LEU:CD1	2.67	0.58
1:D:225:VAL:HG23	1:D:230:GLN:HA	1.85	0.58
1:A:151:PHE:CB	3:A:302:J10:C15	2.82	0.57
1:M:242:LYS:HG3	1:M:247:ILE:HD11	1.86	0.57
1:P:222:PRO:CD	1:P:223:PHE:CE2	2.85	0.57
1:J:163:TRP:HD1	1:J:225:VAL:CG1	2.07	0.57
1:G:244:MET:HA	1:P:244:MET:HA	1.87	0.56
1:D:50:THR:CG2	1:D:86:MET:HE1	2.33	0.56
1:J:257:ILE:HD13	4:M:403:HOH:O	2.05	0.56
1:M:36:LYS:CE	1:M:62:GLU:HG2	2.35	0.56
1:D:50:THR:HG22	1:D:86:MET:HE2	1.88	0.56
1:D:63:LEU:HD13	1:D:63:LEU:C	2.25	0.56
1:A:176:GLU:HG2	1:D:257:ILE:HD11	1.87	0.56
1:G:151:PHE:HB2	3:G:302:J10:C16	2.36	0.56
1:A:194:ARG:HG3	1:A:194:ARG:HH11	1.70	0.56
1:G:242:LYS:HG2	1:G:247:ILE:HD11	1.88	0.55
1:P:132:ALA:O	1:P:267:LYS:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:230:GLN:HE21	1:P:230:GLN:C	2.11	0.55
1:J:225:VAL:HG22	1:J:230:GLN:HE22	1.73	0.54
1:J:36:LYS:CG	1:J:62:GLU:HB2	2.37	0.54
1:P:93:ILE:HG22	1:P:123:ALA:HA	1.89	0.54
1:P:131:THR:HG22	1:P:132:ALA:O	2.08	0.54
1:D:87:ARG:HH22	1:G:99:LYS:NZ	2.04	0.54
1:M:57:CYS:O	1:M:57:CYS:SG	2.66	0.54
1:A:115:HIS:NE2	3:A:302:J10:O2	2.39	0.54
1:D:87:ARG:NH2	1:G:99:LYS:HZ1	2.06	0.54
1:A:124:PHE:CD2	1:A:187:LEU:HD22	2.43	0.54
1:J:225:VAL:CG2	1:J:230:GLN:CD	2.76	0.54
1:P:230:GLN:O	1:P:230:GLN:HG2	2.07	0.54
1:A:40:LEU:HD22	1:A:105:PHE:CE2	2.44	0.53
1:G:115:HIS:NE2	3:G:302:J10:O2	2.41	0.53
1:A:97:LEU:CD2	1:A:130:LEU:CD2	2.84	0.53
1:J:68:ASP:OD2	2:J:301:SAH:O3'	2.25	0.53
1:J:112:TYR:O	3:J:302:J10:C1	2.57	0.53
1:D:14:MET:CE	3:D:302:J10:C5	2.85	0.53
1:J:186:LEU:O	1:J:190:ARG:HG3	2.09	0.53
1:A:131:THR:O	1:A:267:LYS:HE2	2.09	0.52
1:G:137:CYS:SG	1:G:265:CYS:HB2	2.49	0.52
1:J:27:LEU:HB3	1:J:28:PRO:HD3	1.92	0.52
1:J:41:ASP:OD2	1:J:50:THR:HG22	2.09	0.52
1:J:230:GLN:OE1	1:J:230:GLN:HA	2.09	0.52
1:A:242:LYS:HG2	1:A:247:ILE:HD11	1.91	0.52
1:D:36:LYS:HE2	1:D:62:GLU:HG2	1.92	0.52
3:A:302:J10:C7	3:A:302:J10:C12	2.88	0.52
1:D:96:ASP:OD1	1:D:122:LYS:NZ	2.39	0.52
1:D:131:THR:O	1:D:267:LYS:HE2	2.09	0.52
1:D:36:LYS:CG	1:D:62:GLU:HB2	2.37	0.52
1:M:120:GLN:HG2	1:M:174:TYR:OH	2.09	0.52
1:J:242:LYS:HG2	1:J:247:ILE:HD11	1.91	0.52
1:J:257:ILE:HD11	1:M:176:GLU:HG2	1.92	0.52
1:J:188:LEU:HD13	1:J:265:CYS:SG	2.50	0.52
1:D:242:LYS:HG2	1:D:247:ILE:HD11	1.92	0.51
1:D:137:CYS:SG	1:D:265:CYS:HB2	2.49	0.51
1:A:115:HIS:HB3	1:A:141:LEU:HD23	1.93	0.51
3:A:302:J10:C2	3:A:302:J10:C8	2.88	0.51
1:A:222:PRO:HD2	1:A:223:PHE:CD2	2.45	0.51
1:D:225:VAL:CG2	1:D:230:GLN:HA	2.40	0.51
1:A:189:LYS:HE3	1:A:196:VAL:CG1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:O	1:A:86:MET:HA	2.10	0.51
1:D:226:GLY:O	1:D:230:GLN:CB	2.56	0.51
1:G:188:LEU:HD13	1:G:265:CYS:SG	2.50	0.51
1:J:225:VAL:CG2	1:J:230:GLN:HE22	2.24	0.51
1:A:115:HIS:HE1	3:A:302:J10:C1	2.15	0.51
1:G:41:ASP:OD2	1:G:50:THR:HB	2.10	0.50
1:A:141:LEU:HB3	1:A:261:VAL:HG22	1.93	0.50
1:A:128:TYR:CE1	1:A:267:LYS:HD2	2.46	0.50
1:G:170:PHE:O	3:G:302:J10:C10	2.60	0.50
1:G:207:PHE:HB2	1:G:254:ALA:HB3	1.94	0.50
1:J:222:PRO:HD2	1:J:223:PHE:CE2	2.47	0.50
3:J:302:J10:C7	3:J:302:J10:C12	2.89	0.50
1:J:44:CYS:HB2	1:J:50:THR:HG21	1.92	0.50
1:M:41:ASP:OD2	1:M:50:THR:HB	2.11	0.50
1:A:120:GLN:HG2	1:A:174:TYR:OH	2.13	0.49
1:D:67:CYS:HB2	1:D:91:MET:HB3	1.94	0.49
3:J:302:J10:C2	3:J:302:J10:C8	2.90	0.49
1:D:113:THR:HG23	2:D:301:SAH:O4'	2.12	0.49
1:J:115:HIS:CE1	3:J:302:J10:O2	2.66	0.49
1:M:39:ILE:HG22	1:M:107:HIS:HB2	1.93	0.49
1:A:220:VAL:HB	3:A:302:J10:C6	2.42	0.49
1:P:114:LEU:HB2	1:P:141:LEU:CD2	2.42	0.49
1:J:207:PHE:HB2	1:J:254:ALA:HB3	1.95	0.48
1:M:114:LEU:HB2	1:M:141:LEU:CD1	2.37	0.48
1:M:114:LEU:C	1:M:141:LEU:HD11	2.33	0.48
1:G:116:TRP:HE1	3:G:302:J10:C1	2.26	0.48
3:J:302:J10:C8	3:J:302:J10:C13	2.90	0.48
1:J:66:ALA:O	1:J:88:PHE:HA	2.14	0.48
1:A:152:ASP:O	1:A:155:LYS:HG2	2.12	0.48
1:J:162:HIS:HB3	1:J:163:TRP:CE3	2.48	0.48
1:P:156:HIS:ND1	1:P:156:HIS:N	2.61	0.48
1:G:42:ILE:HD12	1:G:93:ILE:HD13	1.96	0.48
1:G:110:SER:O	1:G:139:LEU:HA	2.14	0.48
1:G:47:GLY:HA2	1:G:50:THR:HG23	1.95	0.47
1:G:108:VAL:HG21	1:G:127:ILE:HG23	1.96	0.47
1:J:156:HIS:HB2	4:M:401:HOH:O	2.13	0.47
1:J:115:HIS:NE2	3:J:302:J10:O2	2.48	0.47
1:A:194:ARG:HG3	1:A:194:ARG:NH1	2.29	0.47
1:A:44:CYS:HB2	1:A:50:THR:HG21	1.96	0.47
3:J:302:J10:C7	3:J:302:J10:C13	2.93	0.47
1:M:36:LYS:HG3	1:M:62:GLU:CB	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:128:TYR:CZ	1:P:267:LYS:HE3	2.49	0.47
1:D:23:LEU:O	1:D:27:LEU:HB2	2.15	0.47
1:P:198:VAL:HG22	1:P:263:ILE:HG12	1.96	0.47
1:A:112:TYR:O	2:A:301:SAH:H5'2	2.15	0.47
1:D:214:ARG:HD3	1:D:234:ILE:HG21	1.97	0.47
1:A:200:CYS:HB3	1:D:200:CYS:O	2.13	0.47
1:J:247:ILE:HA	1:J:254:ALA:HA	1.96	0.46
1:D:75:LYS:HE3	1:G:92:ASP:OD2	2.16	0.46
1:G:66:ALA:O	1:G:88:PHE:HA	2.16	0.46
1:G:79:GLU:O	1:M:194:ARG:CG	2.56	0.46
1:J:142:LEU:HD12	3:J:302:J10:O2	2.15	0.46
1:J:222:PRO:HD2	1:J:223:PHE:CD2	2.50	0.46
1:P:207:PHE:HB2	1:P:254:ALA:HB3	1.97	0.46
1:A:71:VAL:HG12	1:A:75:LYS:NZ	2.31	0.46
1:A:189:LYS:HG3	1:A:196:VAL:HG11	1.98	0.46
1:A:124:PHE:CD2	1:A:187:LEU:CD2	2.99	0.46
1:P:68:ASP:O	1:P:90:VAL:HA	2.16	0.46
1:G:150:LEU:HD21	1:G:246:ILE:HD12	1.98	0.45
1:J:128:TYR:HB2	1:J:191:VAL:CG1	2.45	0.45
1:J:200:CYS:HB3	1:M:200:CYS:O	2.17	0.45
1:M:247:ILE:HA	1:M:254:ALA:HA	1.97	0.45
1:G:31:LYS:CE	1:G:33:LYS:HE3	2.41	0.45
3:G:302:J10:C7	3:G:302:J10:C12	2.94	0.45
1:M:23:LEU:O	1:M:27:LEU:HB2	2.16	0.45
1:G:23:LEU:O	1:G:27:LEU:HB2	2.17	0.45
1:P:142:LEU:HD23	1:P:142:LEU:HA	1.85	0.45
1:P:247:ILE:HA	1:P:254:ALA:HA	1.99	0.45
1:P:196:VAL:HG13	1:P:196:VAL:O	2.17	0.45
1:J:23:LEU:O	1:J:27:LEU:HB2	2.17	0.45
1:J:44:CYS:CB	1:J:50:THR:HG21	2.47	0.44
1:M:195:TYR:HB3	1:M:266:ARG:HB2	1.99	0.44
1:P:114:LEU:CB	1:P:141:LEU:HD21	2.45	0.44
1:J:14:MET:CE	3:J:302:J10:C5	2.95	0.44
1:P:100:GLU:H	1:P:100:GLU:HG3	1.52	0.44
1:A:31:LYS:HE2	1:A:31:LYS:HB3	1.80	0.44
1:D:27:LEU:HB3	1:D:28:PRO:HD3	1.98	0.44
1:P:93:ILE:O	1:P:126:ASN:ND2	2.50	0.44
1:M:199:ARG:O	1:M:261:VAL:HA	2.18	0.44
1:A:41:ASP:HA	1:A:109:PHE:O	2.17	0.44
1:D:160:TRP:CZ2	1:D:233:LEU:HA	2.52	0.44
1:G:32:TRP:CH2	1:G:57:CYS:HB2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:ILE:HG22	1:G:107:HIS:HB2	1.99	0.44
1:P:64:PHE:CD1	1:P:64:PHE:C	2.91	0.44
1:D:174:TYR:CE2	1:D:184:ILE:HD11	2.53	0.44
1:A:27:LEU:HB3	1:A:28:PRO:HD3	2.00	0.44
1:P:217:LEU:HD13	1:P:237:VAL:HG11	1.99	0.44
1:A:188:LEU:HD13	1:A:265:CYS:SG	2.58	0.44
1:A:189:LYS:HE3	1:A:196:VAL:HG13	2.00	0.43
1:D:70:ASN:O	1:D:74:VAL:HG23	2.18	0.43
1:G:226:GLY:O	1:G:230:GLN:N	2.50	0.43
1:J:14:MET:HE1	3:J:302:J10:C5	2.48	0.43
1:J:41:ASP:HA	1:J:109:PHE:O	2.18	0.43
1:D:61:PHE:CD1	1:D:64:PHE:HB2	2.53	0.43
1:A:126:ASN:O	1:A:130:LEU:HG	2.18	0.43
1:P:242:LYS:CG	1:P:247:ILE:HD11	2.49	0.43
1:G:31:LYS:HB3	1:G:33:LYS:HD2	2.01	0.43
1:P:111:PHE:CD1	1:P:140:THR:HG23	2.53	0.43
1:G:67:CYS:HB2	1:G:91:MET:HB3	2.01	0.43
1:J:207:PHE:CZ	1:J:216:LEU:HD22	2.54	0.43
1:D:242:LYS:HE3	1:D:247:ILE:HD11	2.01	0.43
1:M:77:ALA:HB1	1:M:88:PHE:CE2	2.54	0.43
1:P:154:LEU:HD13	1:P:237:VAL:HG22	1.99	0.43
1:A:174:TYR:HA	1:A:177:THR:OG1	2.18	0.43
1:D:181:ASP:O	1:D:198:VAL:HG21	2.18	0.43
3:G:302:J10:C7	3:G:302:J10:C2	2.96	0.43
1:D:188:LEU:HD13	1:D:265:CYS:SG	2.59	0.42
1:J:162:HIS:HB3	1:J:163:TRP:HE3	1.83	0.42
1:P:20:LEU:O	1:P:24:THR:OG1	2.30	0.42
1:J:74:VAL:HG13	1:J:88:PHE:HB3	2.00	0.42
1:M:64:PHE:C	1:M:64:PHE:HD1	2.23	0.42
1:G:66:ALA:HB3	1:G:88:PHE:CD1	2.54	0.42
1:G:207:PHE:CZ	1:G:216:LEU:HD22	2.54	0.42
1:A:49:VAL:HG11	2:A:301:SAH:CA	2.48	0.42
1:G:242:LYS:HE3	1:G:247:ILE:HD11	2.02	0.42
1:M:64:PHE:C	1:M:64:PHE:CD1	2.93	0.42
1:D:108:VAL:HG21	1:D:127:ILE:HG23	2.01	0.42
1:M:115:HIS:N	1:M:141:LEU:CD1	2.79	0.42
1:D:207:PHE:HB2	1:D:254:ALA:HB3	2.02	0.42
1:P:141:LEU:N	1:P:261:VAL:O	2.47	0.42
1:M:67:CYS:HB2	1:M:91:MET:HB3	2.01	0.42
1:J:15:GLN:NE2	2:J:301:SAH:OXT	2.26	0.41
1:A:242:LYS:HE3	1:A:247:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:HIS:HB3	1:G:141:LEU:CD2	2.48	0.41
1:G:157:THR:O	1:G:161:ARG:N	2.53	0.41
1:J:161:ARG:O	1:J:161:ARG:HG3	2.19	0.41
1:A:37:GLU:HG3	1:A:106:ASP:HB2	2.03	0.41
1:J:67:CYS:HA	1:J:89:ARG:O	2.20	0.41
1:P:151:PHE:HA	1:P:154:LEU:HD22	2.01	0.41
1:D:128:TYR:HB2	1:D:191:VAL:CG1	2.50	0.41
1:J:97:LEU:CD1	1:J:130:LEU:HG	2.49	0.41
1:D:75:LYS:HA	1:D:78:THR:HG22	2.02	0.41
1:D:132:ALA:O	1:D:267:LYS:HG3	2.20	0.41
1:M:39:ILE:HD11	1:M:64:PHE:CD2	2.55	0.41
1:M:207:PHE:CZ	1:M:216:LEU:HD22	2.56	0.41
1:P:64:PHE:C	1:P:64:PHE:HD1	2.24	0.41
1:A:40:LEU:HB2	1:A:105:PHE:CD1	2.55	0.41
1:D:131:THR:O	1:D:267:LYS:CE	2.69	0.41
1:J:200:CYS:O	1:M:200:CYS:HB3	2.20	0.41
1:A:112:TYR:O	3:A:302:J10:C1	2.68	0.41
1:D:161:ARG:NH2	1:D:162:HIS:NE2	2.68	0.41
1:G:120:GLN:HG2	1:G:174:TYR:OH	2.21	0.41
1:J:42:ILE:HB	1:J:110:SER:HB3	2.02	0.41
1:M:225:VAL:HG23	1:M:230:GLN:HA	2.02	0.41
1:D:128:TYR:HB2	1:D:191:VAL:HG11	2.01	0.41
1:J:68:ASP:OD1	2:J:301:SAH:O2'	2.34	0.41
1:M:63:LEU:CD2	1:M:65:GLU:HG3	2.48	0.41
1:M:150:LEU:HD21	1:M:241:ALA:HA	2.03	0.41
1:A:195:TYR:HB3	1:A:266:ARG:HB2	2.03	0.40
1:G:179:ASP:OD1	1:P:203:LYS:HE2	2.21	0.40
1:M:204:LYS:HD2	1:M:255:LYS:HE3	2.04	0.40
1:D:195:TYR:HB3	1:D:266:ARG:HB2	2.03	0.40
1:G:27:LEU:N	1:G:28:PRO:CD	2.84	0.40
1:J:220:VAL:O	3:J:302:J10:C12	2.70	0.40
1:A:23:LEU:O	1:A:27:LEU:HB2	2.21	0.40
1:J:226:GLY:O	1:J:230:GLN:HB2	2.21	0.40
1:M:157:THR:O	1:M:161:ARG:N	2.55	0.40
1:M:207:PHE:HZ	1:M:216:LEU:HD22	1.86	0.40
1:D:91:MET:HB2	1:D:91:MET:HE2	1.82	0.40
1:M:27:LEU:N	1:M:28:PRO:CD	2.84	0.40
1:M:36:LYS:CG	1:M:62:GLU:CB	2.97	0.40
1:M:42:ILE:HB	1:M:110:SER:HB3	2.03	0.40
1:A:71:VAL:HG12	1:A:75:LYS:HZ2	1.86	0.40
1:D:12:SER:O	1:D:16:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:CYS:HB2	1:G:50:THR:HG21	2.03	0.40
1:G:189:LYS:HE3	1:G:196:VAL:CG1	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:ARG:HD2	1:J:87:ARG:HH12[1_455]	1.20	0.40
1:A:62:GLU:OE2	1:A:159:LYS:HD2[2_656]	1.53	0.07

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	A	251/288 (87%)	242 (96%)	9 (4%)	0	100	100
1	D	254/288 (88%)	240 (94%)	14 (6%)	0	100	100
1	G	254/288 (88%)	242 (95%)	12 (5%)	0	100	100
1	J	254/288 (88%)	246 (97%)	8 (3%)	0	100	100
1	M	254/288 (88%)	240 (94%)	14 (6%)	0	100	100
1	P	188/288 (65%)	178 (95%)	10 (5%)	0	100	100
All	All	1455/1728 (84%)	1388 (95%)	67 (5%)	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	A	237/267 (89%)	228 (96%)	9 (4%)	33	58
1	D	238/267 (89%)	227 (95%)	11 (5%)	27	50
1	G	238/267 (89%)	222 (93%)	16 (7%)	16	31
1	J	238/267 (89%)	220 (92%)	18 (8%)	13	25
1	M	238/267 (89%)	221 (93%)	17 (7%)	14	28
1	P	185/267 (69%)	175 (95%)	10 (5%)	22	42
All	All	1374/1602 (86%)	1293 (94%)	81 (6%)	19	37

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	PHE
1	A	141	LEU
1	A	167	ILE
1	A	175	TYR
1	A	184	ILE
1	A	198	VAL
1	A	251	ASN
1	A	262	VAL
1	A	267	LYS
1	D	56	CYS
1	D	64	PHE
1	D	89	ARG
1	D	141	LEU
1	D	167	ILE
1	D	175	TYR
1	D	187	LEU
1	D	191	VAL
1	D	214	ARG
1	D	250	GLN
1	D	262	VAL
1	G	34	GLU
1	G	39	ILE
1	G	50	THR
1	G	56	CYS
1	G	64	PHE
1	G	78	THR
1	G	87	ARG

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Mol	Chain	Res	Type
1	G	110	SER
1	G	167	ILE
1	G	175	TYR
1	G	184	ILE
1	G	191	VAL
1	G	198	VAL
1	G	218	GLU
1	G	255	LYS
1	G	262	VAL
1	J	37	GLU
1	J	50	THR
1	J	57	CYS
1	J	64	PHE
1	J	87	ARG
1	J	96	ASP
1	J	152	ASP
1	J	154	LEU
1	J	163	TRP
1	J	167	ILE
1	J	175	TYR
1	J	186	LEU
1	J	187	LEU
1	J	191	VAL
1	J	198	VAL
1	J	245	ARG
1	J	250	GLN
1	J	262	VAL
1	M	16	ARG
1	M	39	ILE
1	M	57	CYS
1	M	64	PHE
1	M	74	VAL
1	M	78	THR
1	M	87	ARG
1	M	100	GLU
1	M	134	ASP
1	M	144	GLN
1	M	156	HIS
1	M	167	ILE
1	M	175	TYR
1	M	191	VAL
1	M	194	ARG

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Mol	Chain	Res	Type
1	M	261	VAL
1	M	262	VAL
1	P	36	LYS
1	P	64	PHE
1	P	68	ASP
1	P	144	GLN
1	P	154	LEU
1	P	156	HIS
1	P	178	SER
1	P	230	GLN
1	P	261	VAL
1	P	262	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	230	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands 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	$\# Z > 2$
3	J10	G	302	-	17,17,17	0.32	0	20,20,20	0.44	0
2	SAH	A	301	-	21,28,28	0.67	1 (4%)	20,40,40	0.82	1 (5%)
3	J10	J	302	-	17,17,17	0.42	0	20,20,20	0.49	0
2	SAH	G	301	-	21,28,28	0.84	1 (4%)	20,40,40	1.02	2 (10%)
3	J10	A	302	-	17,17,17	0.36	0	20,20,20	0.52	0
3	J10	M	302	-	17,17,17	0.47	0	20,20,20	0.54	0
3	J10	D	302	-	17,17,17	0.49	0	20,20,20	0.57	0
2	SAH	D	301	-	21,28,28	0.78	1 (4%)	20,40,40	0.90	2 (10%)
2	SAH	J	301	-	21,28,28	0.78	1 (4%)	20,40,40	1.04	2 (10%)
2	SAH	M	301	-	21,28,28	0.73	1 (4%)	20,40,40	0.93	2 (10%)

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	J10	G	302	-	-	9/18/18/18	-
2	SAH	A	301	-	-	2/7/31/31	0/3/3/3
3	J10	J	302	-	-	10/18/18/18	-
2	SAH	G	301	-	-	1/7/31/31	0/3/3/3
3	J10	A	302	-	-	11/18/18/18	-
3	J10	M	302	-	-	10/18/18/18	-
3	J10	D	302	-	-	10/18/18/18	-
2	SAH	D	301	-	-	1/7/31/31	0/3/3/3
2	SAH	J	301	-	-	4/7/31/31	0/3/3/3
2	SAH	M	301	-	-	1/7/31/31	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	SAH	C8-N7	-2.29	1.30	1.34
2	D	301	SAH	C8-N7	-2.28	1.30	1.34
2	J	301	SAH	C8-N7	-2.17	1.30	1.34
2	M	301	SAH	C8-N7	-2.10	1.31	1.34
2	A	301	SAH	C8-N7	-2.00	1.31	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	SAH	O4'-C1'-C2'	-2.69	102.99	106.93
2	G	301	SAH	C5-C6-N6	2.58	124.28	120.35
2	J	301	SAH	C5-C6-N6	2.49	124.14	120.35
2	J	301	SAH	O3'-C3'-C2'	-2.46	103.86	111.82
2	M	301	SAH	C5-C6-N6	2.38	123.97	120.35
2	A	301	SAH	C5-C6-N6	2.37	123.95	120.35
2	D	301	SAH	C5-C6-N6	2.29	123.83	120.35
2	M	301	SAH	O4'-C1'-C2'	-2.26	103.62	106.93
2	D	301	SAH	O4'-C1'-C2'	-2.16	103.77	106.93

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	SAH	N-CA-CB-CG
2	A	301	SAH	C-CA-CB-CG
2	G	301	SAH	C-CA-CB-CG
2	J	301	SAH	C-CA-CB-CG
3	A	302	J10	C2-C3-C4-C5
3	A	302	J10	C2-C3-C4-C6
3	A	302	J10	C11-C12-C13-C14
3	D	302	J10	C3-C2-O1-C1
3	D	302	J10	C2-C3-C4-C5
3	D	302	J10	C2-C3-C4-C6
3	D	302	J10	C7-C8-C9-C10
3	D	302	J10	C7-C8-C9-C11
3	D	302	J10	C11-C12-C13-C14
3	G	302	J10	C2-C3-C4-C5
3	G	302	J10	C2-C3-C4-C6
3	G	302	J10	C4-C6-C7-C8
3	G	302	J10	C11-C12-C13-C14
3	J	302	J10	C2-C3-C4-C5
3	J	302	J10	C2-C3-C4-C6
3	M	302	J10	C3-C2-O1-C1
3	M	302	J10	C2-C3-C4-C5
3	M	302	J10	C2-C3-C4-C6
3	J	302	J10	C12-C13-C14-C15
3	J	302	J10	C12-C13-C14-C16
3	M	302	J10	C7-C8-C9-C10
3	M	302	J10	O2-C2-O1-C1
3	M	302	J10	C7-C8-C9-C11

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Mol	Chain	Res	Type	Atoms
3	D	302	J10	O2-C2-O1-C1
3	D	302	J10	C12-C13-C14-C15
3	D	302	J10	C9-C11-C12-C13
3	A	302	J10	C7-C8-C9-C11
3	D	302	J10	C12-C13-C14-C16
3	A	302	J10	C7-C8-C9-C10
3	J	302	J10	C4-C6-C7-C8
3	A	302	J10	C5-C4-C6-C7
3	G	302	J10	C5-C4-C6-C7
3	J	302	J10	C5-C4-C6-C7
3	A	302	J10	C6-C7-C8-C9
3	A	302	J10	C3-C4-C6-C7
3	G	302	J10	C3-C4-C6-C7
3	G	302	J10	C6-C7-C8-C9
3	J	302	J10	C3-C4-C6-C7
3	A	302	J10	C12-C11-C9-C10
3	G	302	J10	C12-C11-C9-C10
3	G	302	J10	C12-C11-C9-C8
3	J	302	J10	C12-C11-C9-C8
3	J	302	J10	C12-C11-C9-C10
3	A	302	J10	C12-C11-C9-C8
3	J	302	J10	C9-C11-C12-C13
2	J	301	SAH	N-CA-CB-CG
2	J	301	SAH	C3'-C4'-C5'-SD
3	M	302	J10	O1-C2-C3-C4
2	J	301	SAH	O4'-C4'-C5'-SD
2	M	301	SAH	CB-CG-SD-C5'
3	M	302	J10	C12-C11-C9-C10
3	M	302	J10	C12-C11-C9-C8
3	M	302	J10	O2-C2-C3-C4
3	A	302	J10	C4-C6-C7-C8
2	D	301	SAH	CB-CG-SD-C5'

There are no ring outliers.

9 monomers are involved in 56 short contacts:

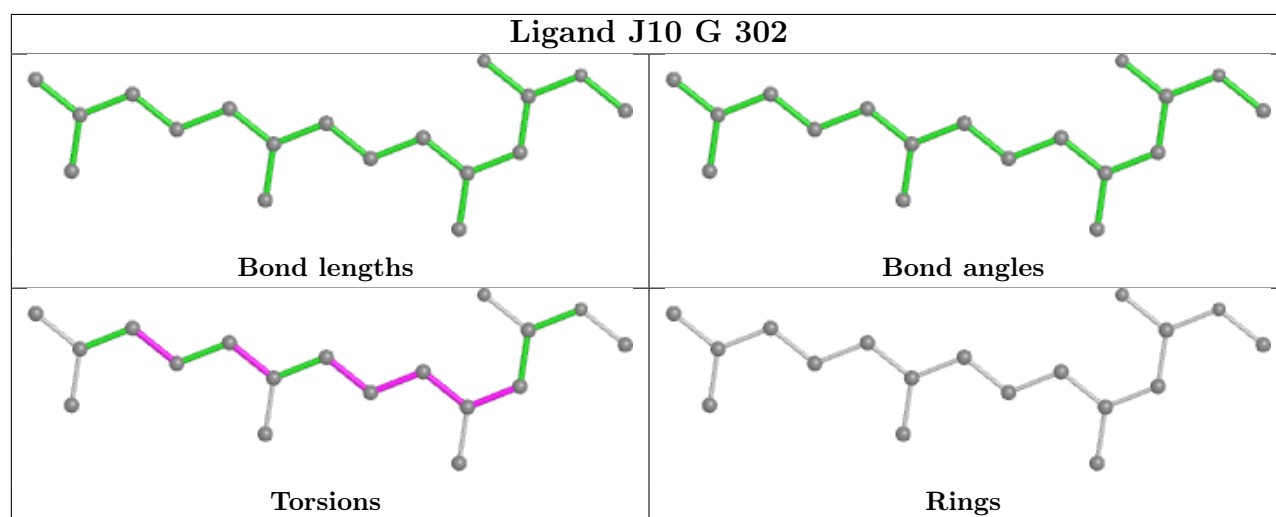
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	302	J10	8	0
2	A	301	SAH	4	0
3	J	302	J10	12	0
3	A	302	J10	17	0
3	M	302	J10	3	0

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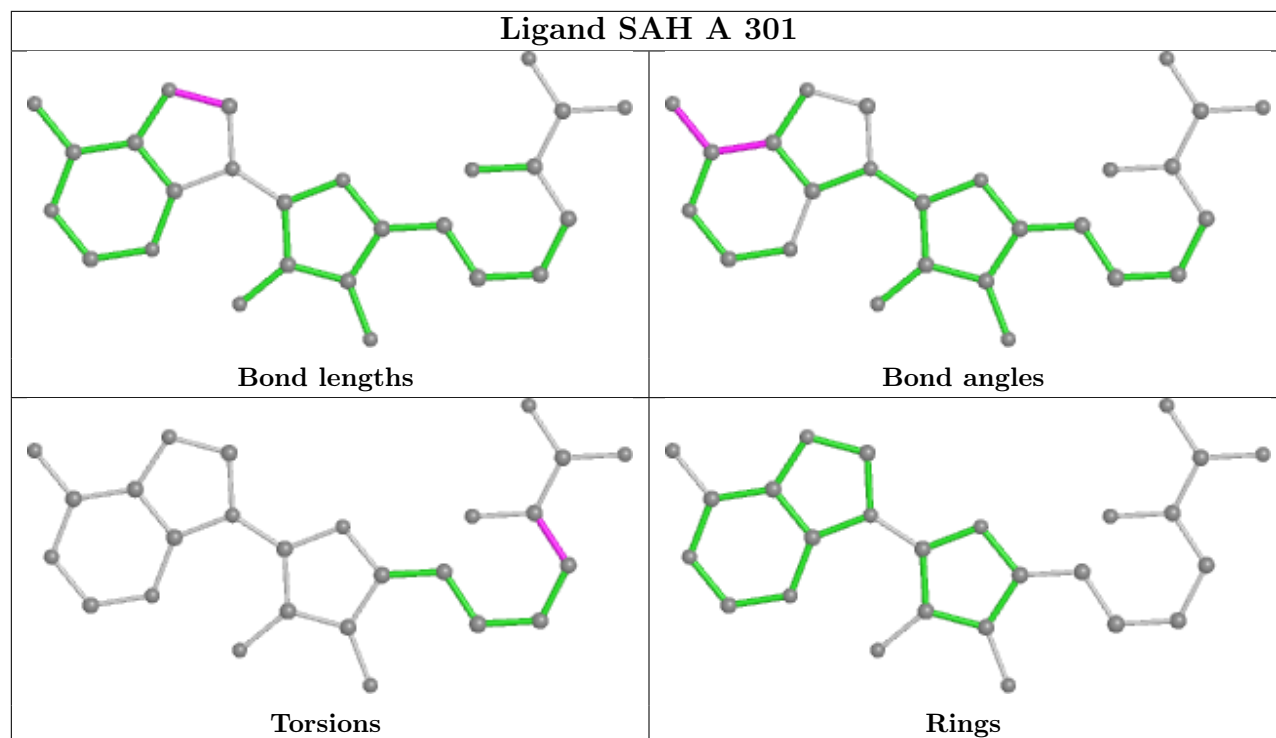
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	J10	3	0
2	D	301	SAH	2	0
2	J	301	SAH	6	0
2	M	301	SAH	1	0

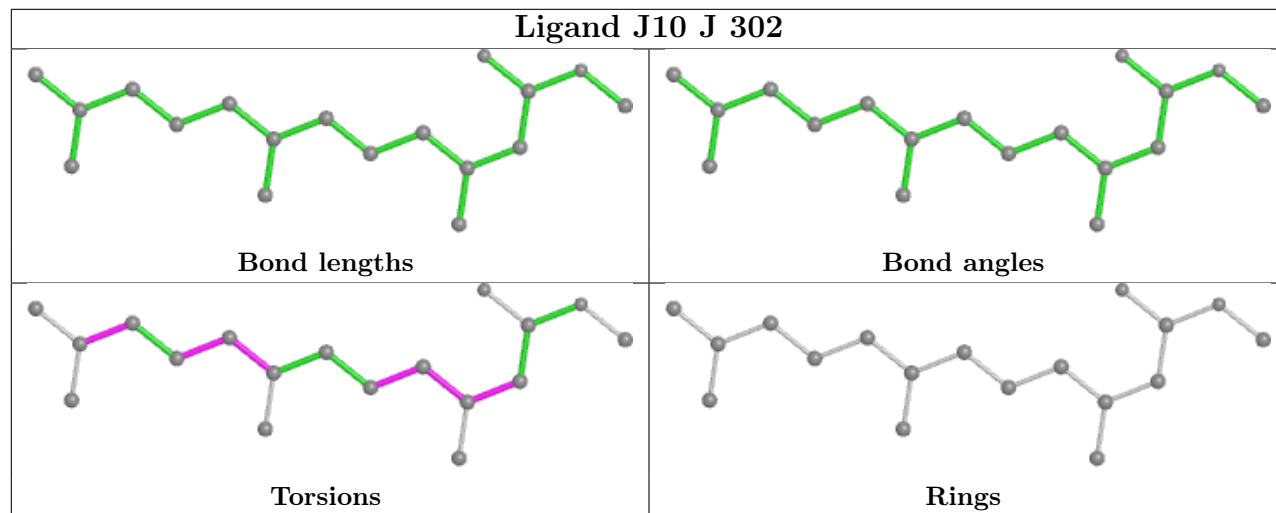
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

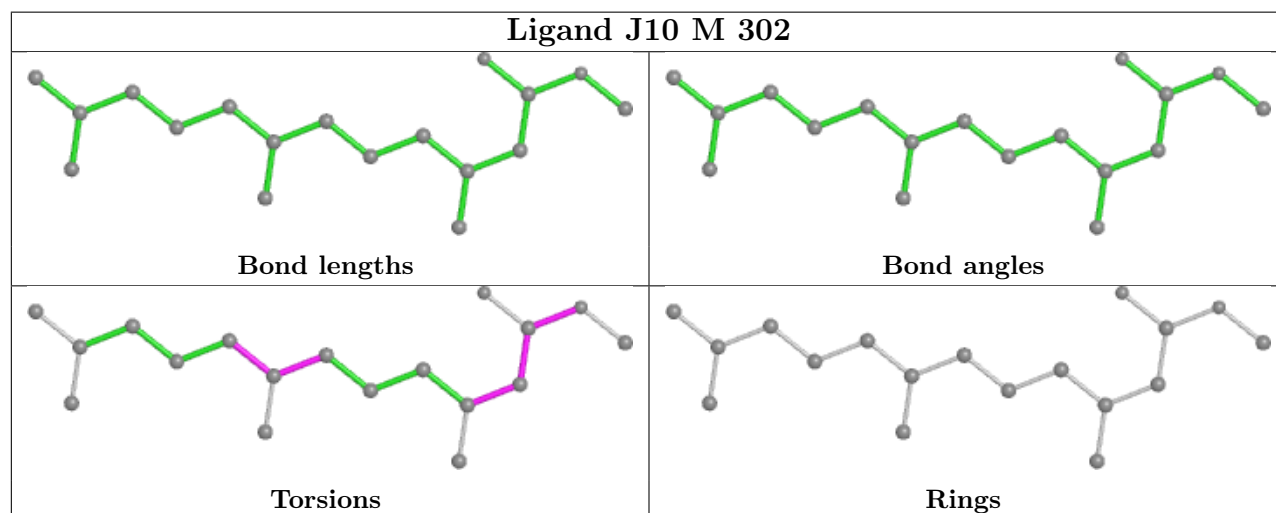
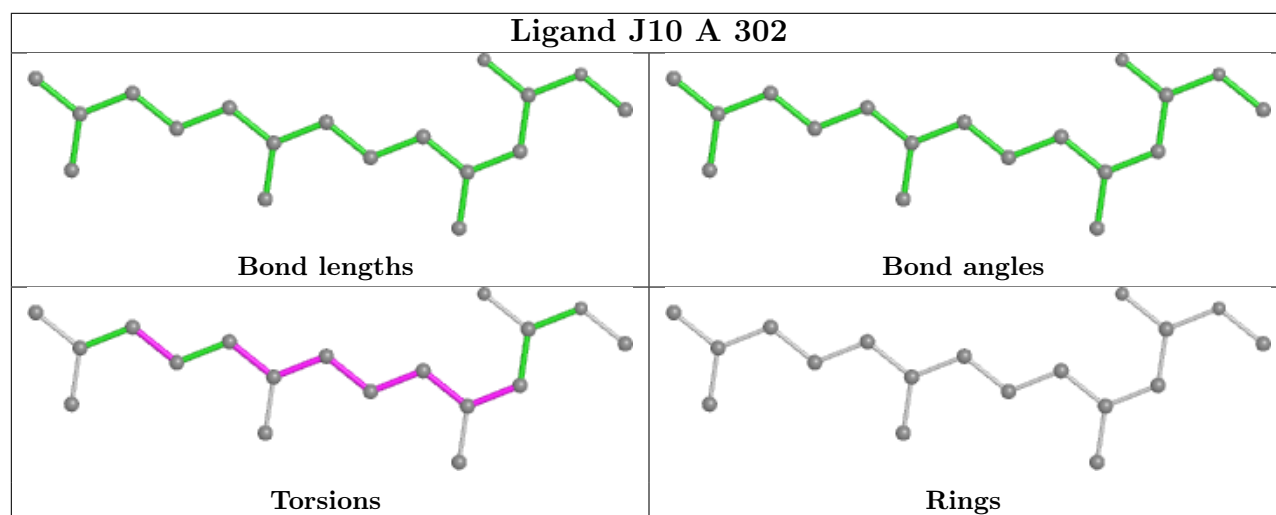
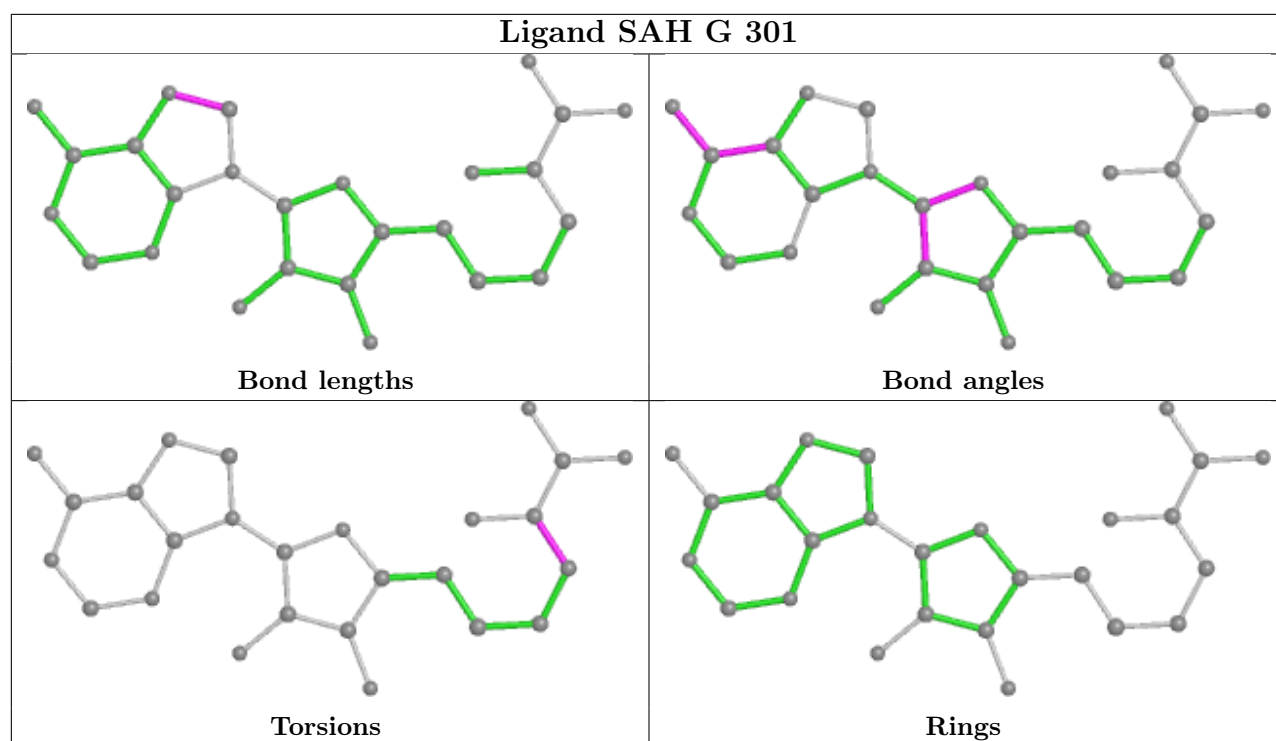


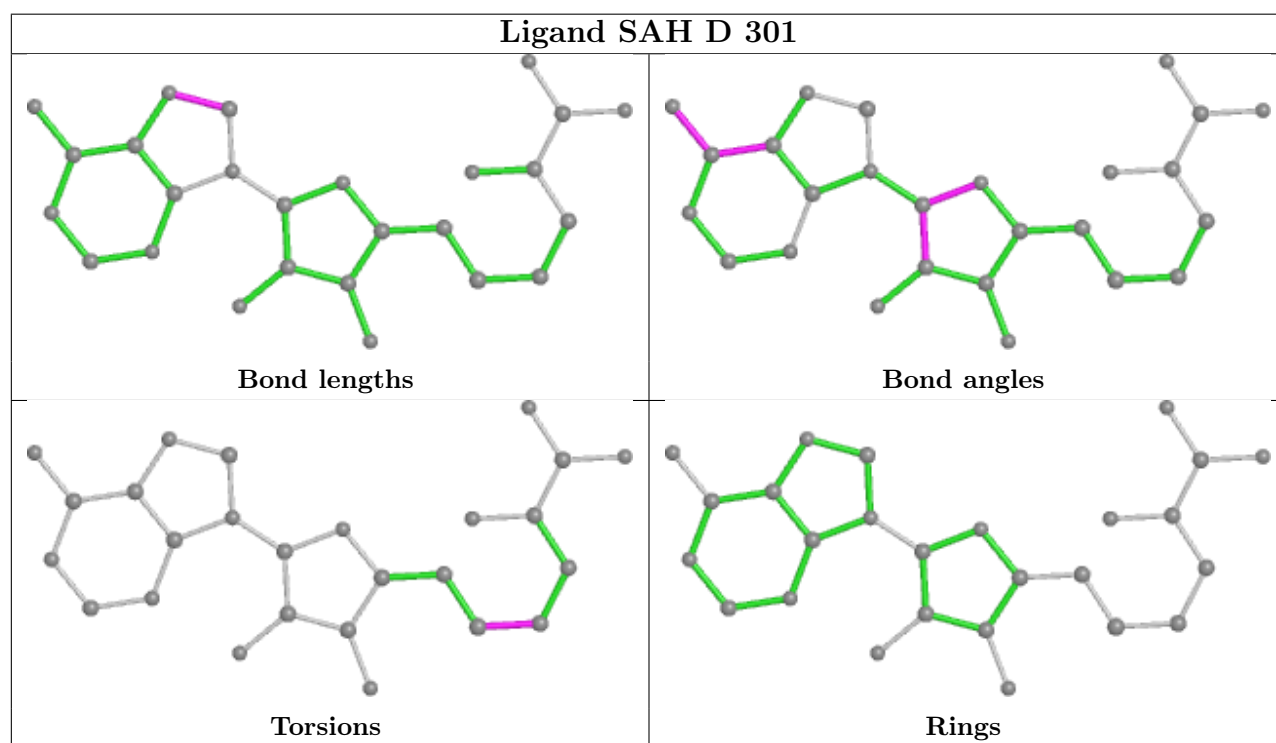
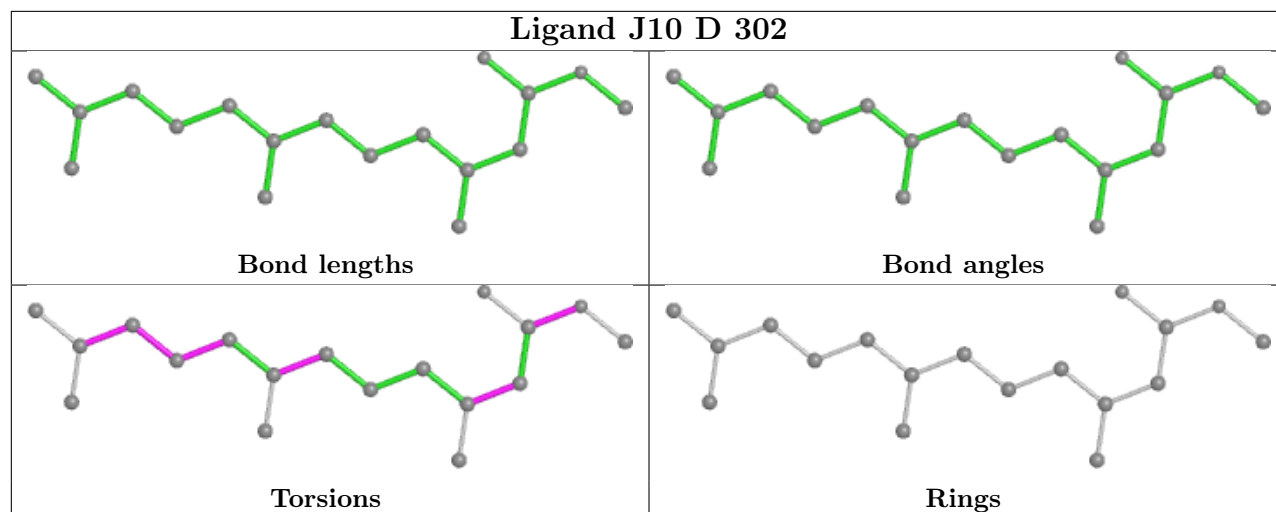
Ligand SAH A 301

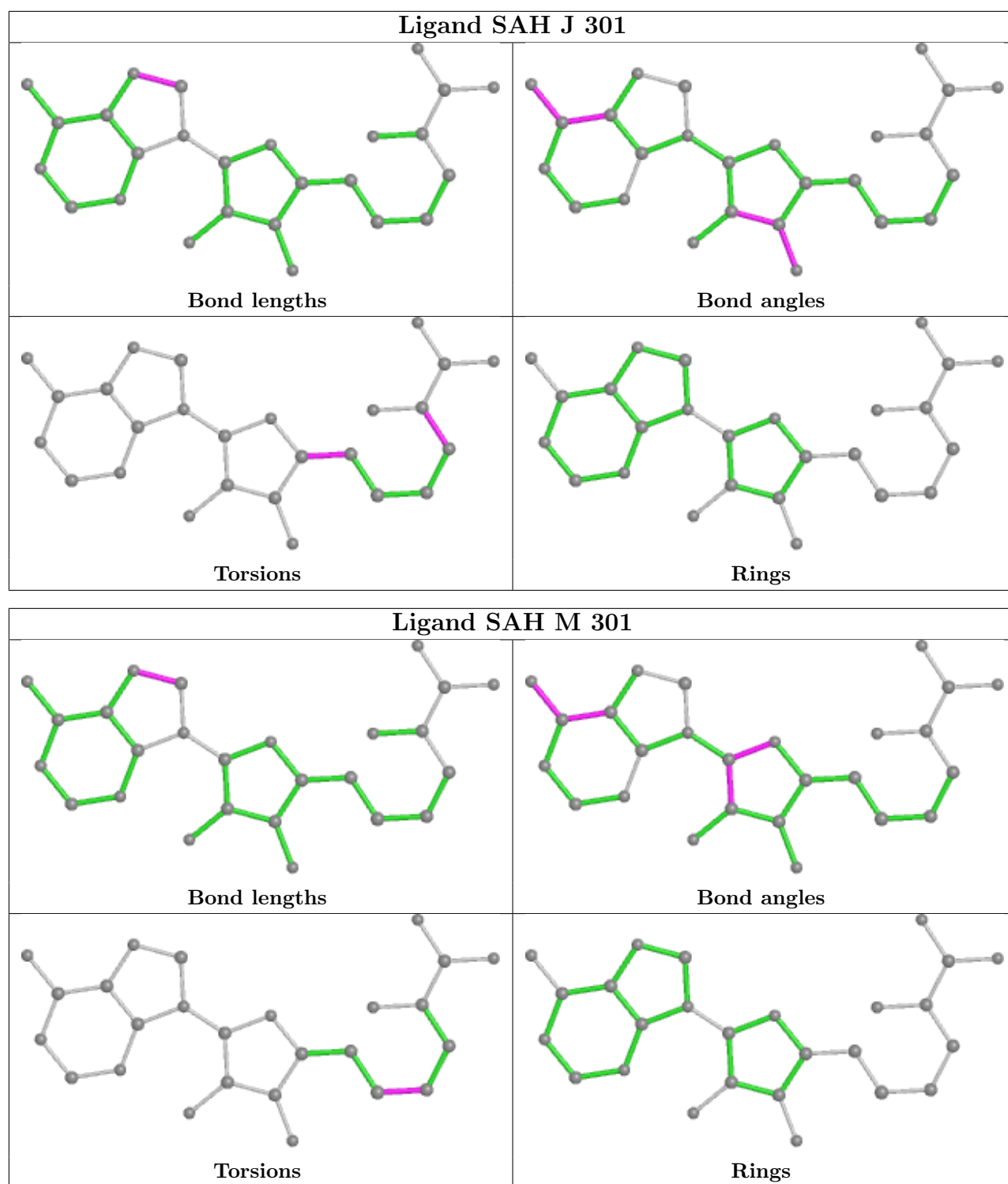


Ligand J10 J 302









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	255/288 (88%)	1.43	50 (19%) 1 1	46, 74, 110, 118	0
1	D	256/288 (88%)	0.96	27 (10%) 6 6	44, 65, 90, 102	0
1	G	256/288 (88%)	1.12	36 (14%) 2 2	47, 65, 94, 105	0
1	J	256/288 (88%)	1.25	49 (19%) 1 1	50, 76, 112, 129	0
1	M	256/288 (88%)	1.37	47 (18%) 1 1	44, 75, 112, 133	0
1	P	198/288 (68%)	1.24	32 (16%) 1 1	35, 77, 107, 118	0
All	All	1477/1728 (85%)	1.23	241 (16%) 1 1	35, 71, 107, 133	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	229	LEU	9.1
1	G	33	LYS	7.2
1	M	160	TRP	7.1
1	A	80	HIS	6.8
1	M	58	PRO	6.8
1	J	166	TYR	6.7
1	J	163	TRP	6.3
1	A	87	ARG	6.2
1	M	229	LEU	6.2
1	J	165	ARG	6.1
1	A	163	TRP	6.1
1	P	69	VAL	6.1
1	A	74	VAL	6.0
1	J	162	HIS	5.8
1	A	158	GLU	5.7
1	P	90	VAL	5.7
1	A	71	VAL	5.6
1	J	232	GLU	5.6
1	J	225	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	J	59	THR	5.5
1	P	33	LYS	5.5
1	P	64	PHE	5.5
1	A	45	ALA	5.4
1	M	163	TRP	5.4
1	A	229	LEU	5.3
1	M	228	GLU	5.2
1	J	227	GLN	5.1
1	J	223	PHE	5.0
1	D	48	SER	5.0
1	M	33	LYS	5.0
1	P	233	LEU	5.0
1	A	228	GLU	5.0
1	A	79	GLU	5.0
1	P	223	PHE	5.0
1	A	230	GLN	4.9
1	A	62	GLU	4.8
1	M	36	LYS	4.8
1	D	59	THR	4.8
1	J	230	GLN	4.7
1	J	33	LYS	4.7
1	A	227	GLN	4.7
1	P	170	PHE	4.7
1	P	91	MET	4.6
1	M	35	SER	4.6
1	J	164	LEU	4.5
1	J	72	LYS	4.5
1	P	36	LYS	4.4
1	A	48	SER	4.3
1	G	233	LEU	4.3
1	J	159	LYS	4.3
1	A	77	ALA	4.3
1	J	31	LYS	4.3
1	A	86	MET	4.2
1	G	210	LEU	4.2
1	G	34	GLU	4.2
1	M	164	LEU	4.2
1	G	229	LEU	4.2
1	M	233	LEU	4.1
1	A	81	TYR	4.1
1	P	43	GLY	4.1
1	D	229	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	M	170	PHE	4.0
1	J	228	GLU	4.0
1	M	74	VAL	4.0
1	P	35	SER	4.0
1	P	32	TRP	3.9
1	D	34	GLU	3.9
1	G	158	GLU	3.9
1	G	247	ILE	3.9
1	M	159	LYS	3.9
1	M	88	PHE	3.9
1	M	250	GLN	3.8
1	J	156	HIS	3.8
1	A	70	ASN	3.7
1	D	32	TRP	3.7
1	P	133	ASP	3.7
1	P	237	VAL	3.7
1	A	78	THR	3.7
1	D	35	SER	3.7
1	M	57	CYS	3.7
1	M	247	ILE	3.7
1	A	73	SER	3.7
1	M	226	GLY	3.7
1	J	231	GLU	3.7
1	M	161	ARG	3.7
1	M	156	HIS	3.6
1	J	168	LYS	3.5
1	G	252	SER	3.5
1	M	59	THR	3.5
1	A	106	ASP	3.5
1	M	154	LEU	3.5
1	G	227	GLN	3.4
1	J	233	LEU	3.4
1	M	85	LYS	3.3
1	A	225	VAL	3.3
1	P	222	PRO	3.3
1	G	228	GLU	3.3
1	M	234	ILE	3.2
1	D	33	LYS	3.2
1	G	159	LYS	3.2
1	P	267	LYS	3.2
1	A	161	ARG	3.2
1	A	75	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	225	VAL	3.2
1	J	79	GLU	3.1
1	A	82	GLY	3.1
1	G	220	VAL	3.1
1	M	232	GLU	3.1
1	P	93	ILE	3.1
1	D	232	GLU	3.1
1	M	225	VAL	3.0
1	J	133	ASP	3.0
1	A	83	THR	3.0
1	G	230	GLN	3.0
1	J	160	TRP	3.0
1	M	73	SER	3.0
1	D	156	HIS	3.0
1	A	76	TYR	3.0
1	A	84	SER	3.0
1	A	164	LEU	3.0
1	J	32	TRP	3.0
1	P	31	LYS	3.0
1	A	47	GLY	3.0
1	J	194	ARG	3.0
1	A	85	LYS	2.9
1	M	62	GLU	2.9
1	M	158	GLU	2.9
1	J	154	LEU	2.9
1	A	63	LEU	2.9
1	P	217	LEU	2.9
1	J	34	GLU	2.8
1	D	233	LEU	2.8
1	D	228	GLU	2.8
1	M	166	TYR	2.8
1	J	36	LYS	2.8
1	A	90	VAL	2.8
1	G	200	CYS	2.8
1	G	265	CYS	2.8
1	G	235	ASP	2.8
1	J	169	ASN	2.8
1	P	210	LEU	2.8
1	G	164	LEU	2.8
1	D	166	TYR	2.7
1	J	167	ILE	2.7
1	A	116	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	251	ASN	2.7
1	D	31	LYS	2.7
1	D	36	LYS	2.7
1	D	247	ILE	2.7
1	M	223	PHE	2.7
1	A	49	VAL	2.6
1	P	135	GLY	2.6
1	A	52	ILE	2.6
1	A	224	LYS	2.6
1	P	130	LEU	2.6
1	A	265	CYS	2.5
1	A	210	LEU	2.5
1	G	208	TYR	2.5
1	G	211	LYS	2.5
1	P	67	CYS	2.5
1	D	58	PRO	2.5
1	M	210	LEU	2.5
1	D	163	TRP	2.5
1	M	165	ARG	2.5
1	G	215	ASN	2.5
1	G	163	TRP	2.4
1	J	70	ASN	2.4
1	J	118	GLU	2.4
1	P	39	ILE	2.4
1	J	224	LYS	2.4
1	G	39	ILE	2.4
1	J	52	ILE	2.4
1	M	252	SER	2.4
1	D	167	ILE	2.4
1	A	88	PHE	2.4
1	M	84	SER	2.4
1	A	60	ASP	2.4
1	G	24	THR	2.4
1	M	186	LEU	2.4
1	P	220	VAL	2.3
1	J	236	ASP	2.3
1	G	154	LEU	2.3
1	D	50	THR	2.3
1	A	154	LEU	2.3
1	P	23	LEU	2.3
1	P	106	ASP	2.3
1	D	90	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	210	LEU	2.3
1	G	108	VAL	2.3
1	A	159	LYS	2.3
1	J	75	LYS	2.3
1	A	130	LEU	2.3
1	G	27	LEU	2.3
1	J	88	PHE	2.2
1	M	249	THR	2.2
1	G	161	ARG	2.2
1	G	232	GLU	2.2
1	D	61	PHE	2.2
1	G	85	LYS	2.2
1	J	170	PHE	2.2
1	M	75	LYS	2.2
1	G	239	GLU	2.2
1	M	231	GLU	2.2
1	A	27	LEU	2.2
1	A	141	LEU	2.2
1	D	62	GLU	2.2
1	J	235	ASP	2.2
1	P	68	ASP	2.2
1	A	69	VAL	2.1
1	D	198	VAL	2.1
1	J	191	VAL	2.1
1	P	229	LEU	2.1
1	G	86	MET	2.1
1	A	247	ILE	2.1
1	G	246	ILE	2.1
1	A	61	PHE	2.1
1	M	110	SER	2.1
1	G	214	ARG	2.1
1	J	239	GLU	2.1
1	J	240	VAL	2.1
1	D	79	GLU	2.1
1	J	69	VAL	2.1
1	M	157	THR	2.1
1	M	39	ILE	2.1
1	P	38	LYS	2.1
1	A	56	CYS	2.1
1	J	71	VAL	2.1
1	M	53	ILE	2.1
1	D	64	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	35	SER	2.1
1	P	99	LYS	2.1
1	J	106	ASP	2.0
1	M	151	PHE	2.0
1	J	38	LYS	2.0
1	M	132	ALA	2.0
1	M	263	ILE	2.0
1	P	242	LYS	2.0
1	J	27	LEU	2.0
1	J	226	GLY	2.0
1	M	63	LEU	2.0
1	G	123	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

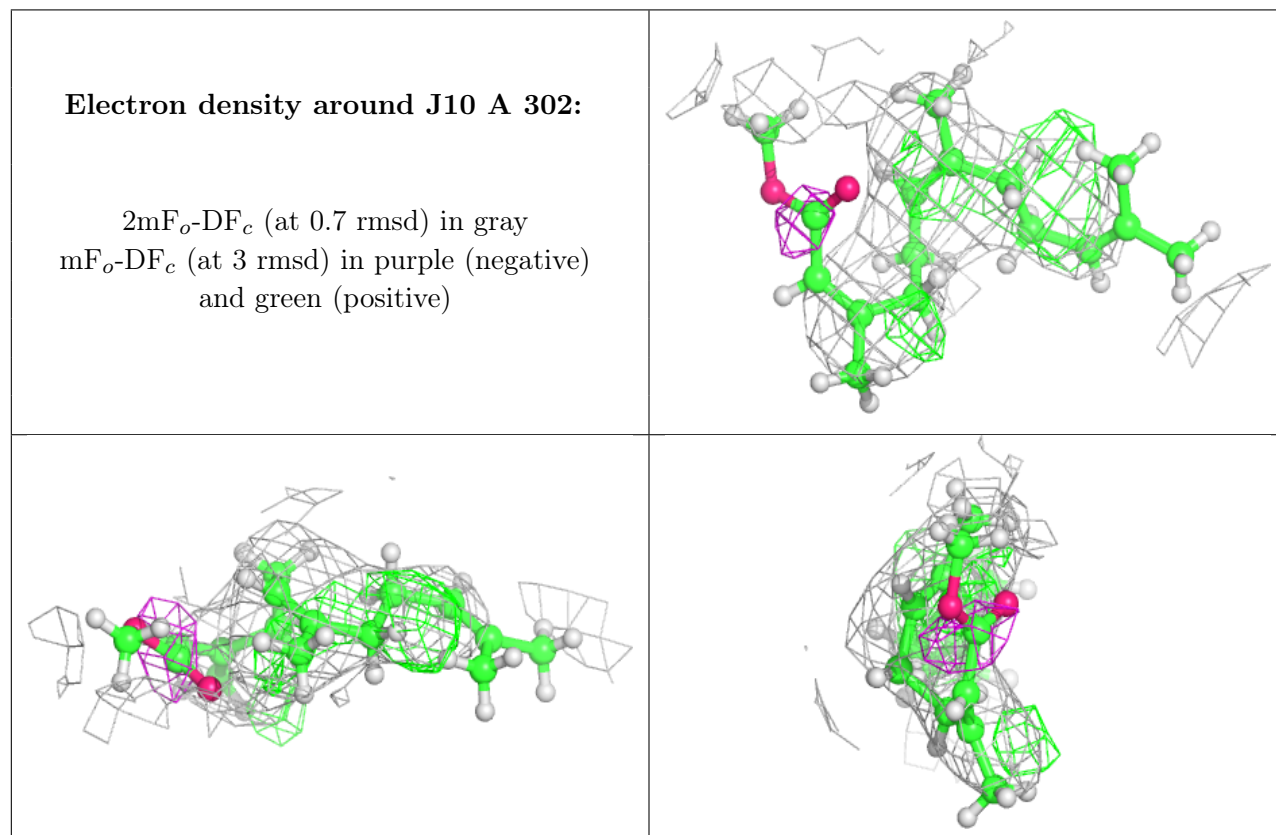
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

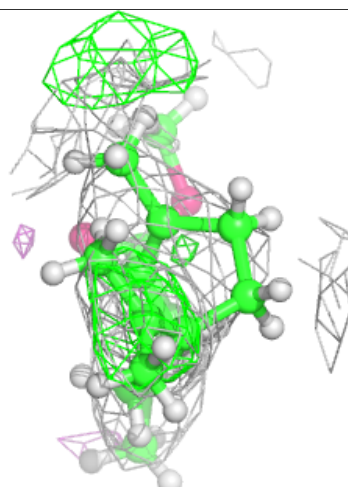
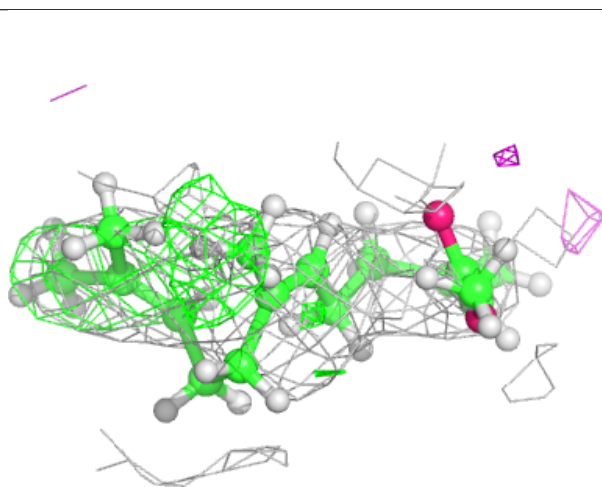
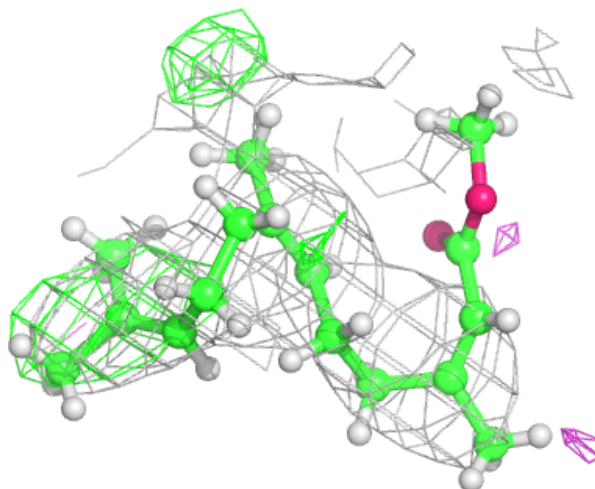
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	J10	A	302	18/18	0.74	0.50	62,65,69,72	24
3	J10	J	302	18/18	0.77	0.40	58,63,67,67	24
3	J10	M	302	18/18	0.78	0.41	64,67,71,72	24
3	J10	G	302	18/18	0.81	0.41	54,57,61,61	24
2	SAH	A	301	26/26	0.82	0.34	56,60,60,62	44
3	J10	D	302	18/18	0.88	0.38	57,60,65,68	7
2	SAH	M	301	26/26	0.93	0.15	63,67,74,76	4
2	SAH	G	301	26/26	0.95	0.18	52,53,63,71	4
2	SAH	J	301	26/26	0.95	0.22	66,70,73,74	4
2	SAH	D	301	26/26	0.96	0.16	59,61,66,69	4

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.



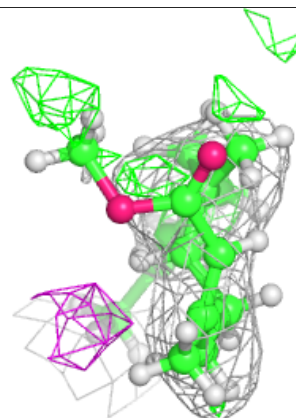
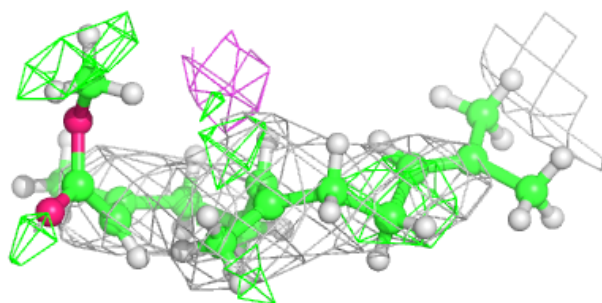
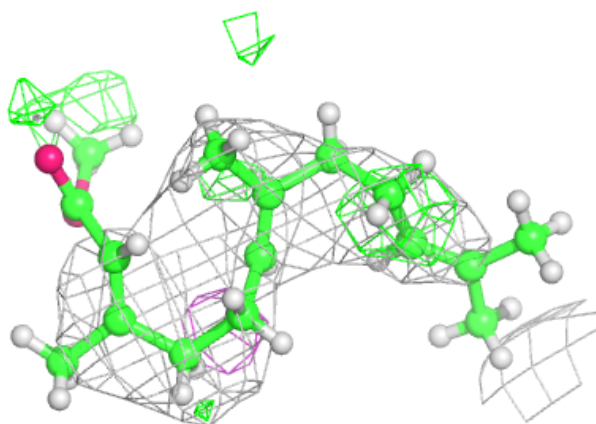
Electron density around J10 J 302:

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

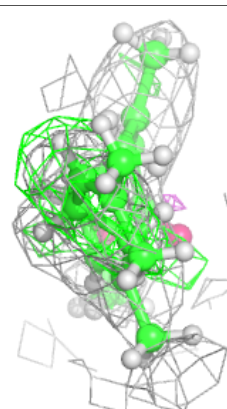
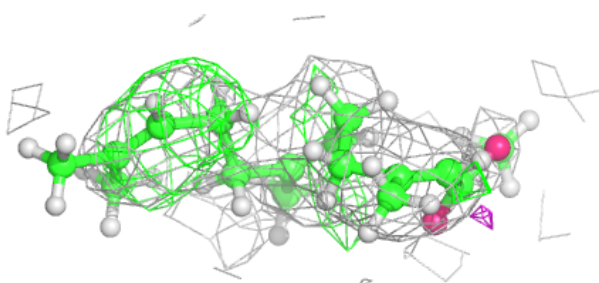
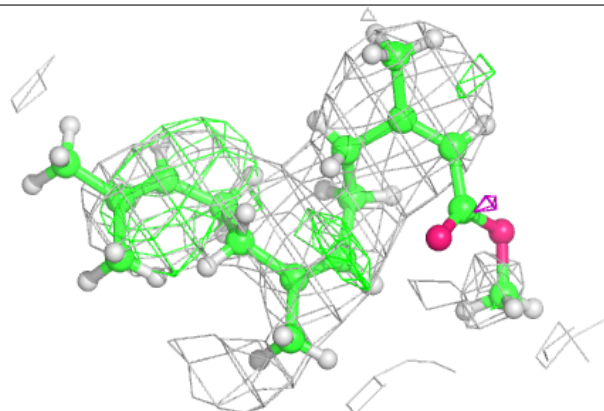


Electron density around J10 M 302:

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

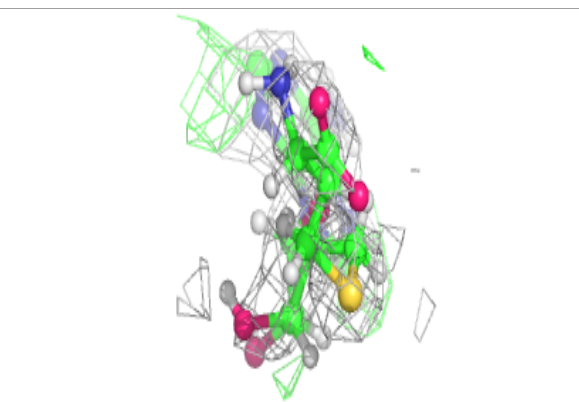
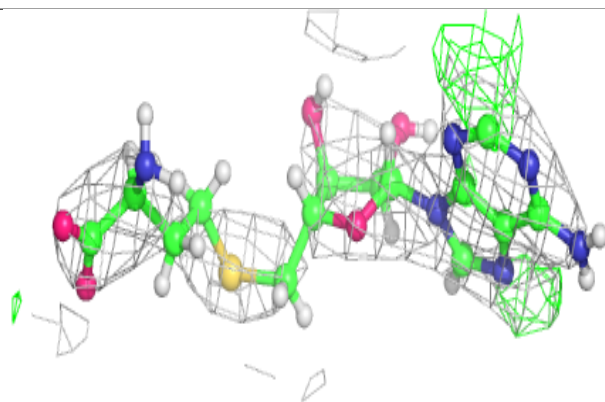
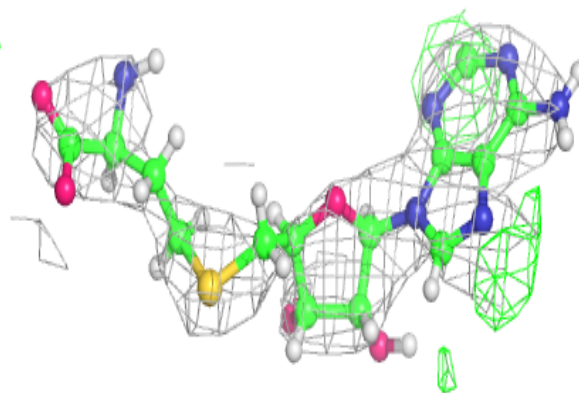
**Electron density around J10 G 302:**

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

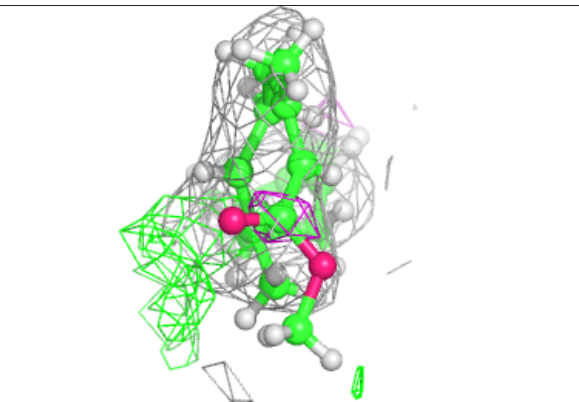
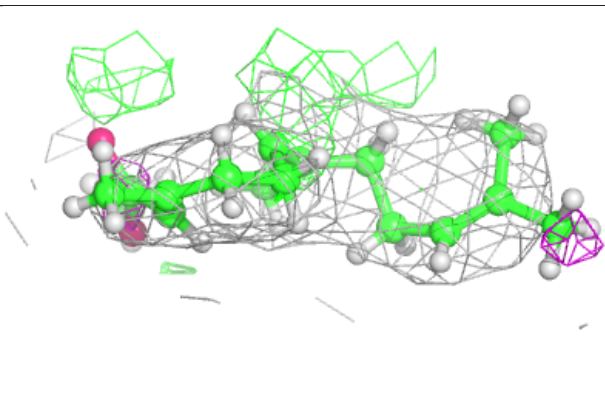
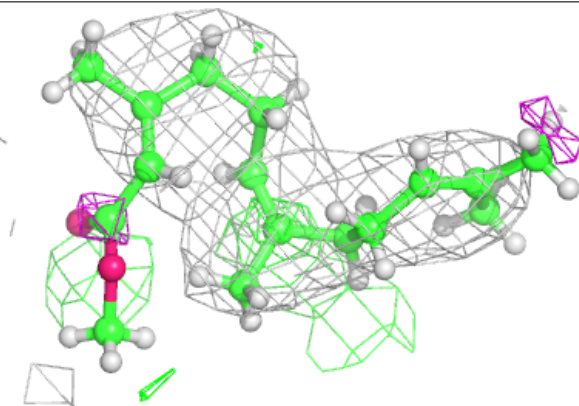


Electron density around SAH A 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

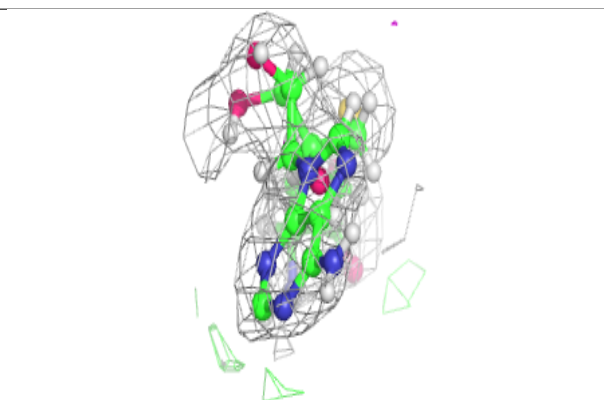
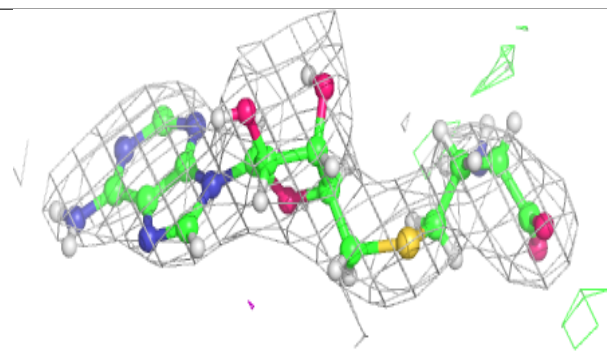
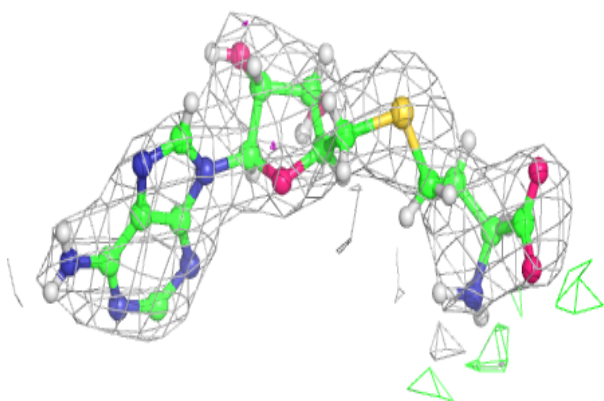
**Electron density around J10 D 302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

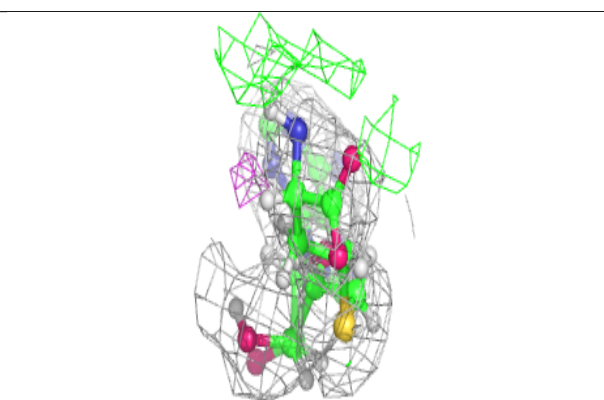
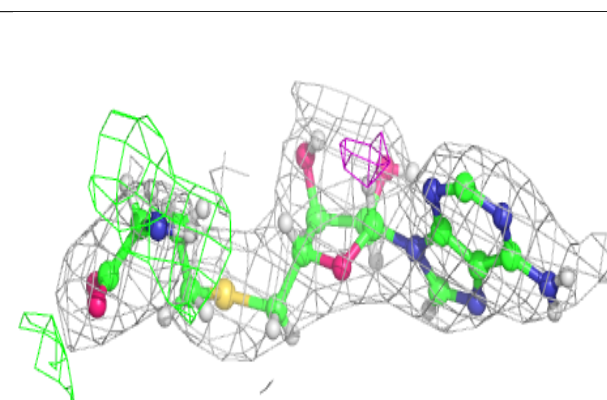
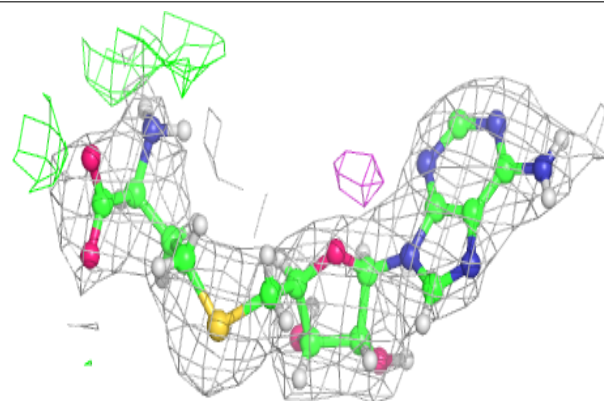


Electron density around SAH M 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

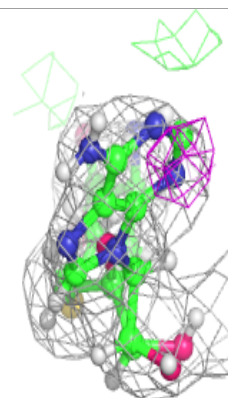
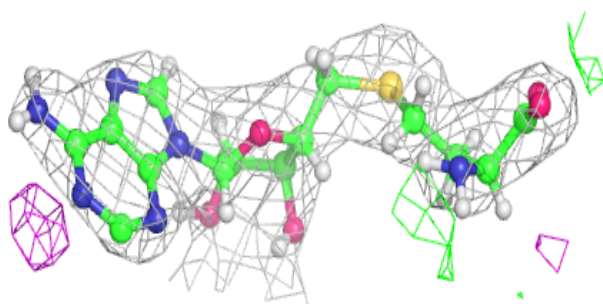
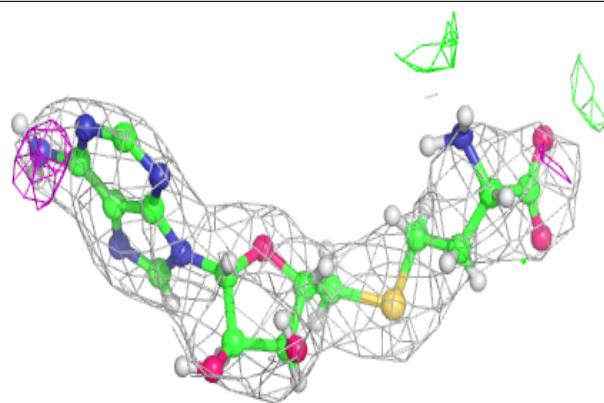
**Electron density around SAH G 301:**

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

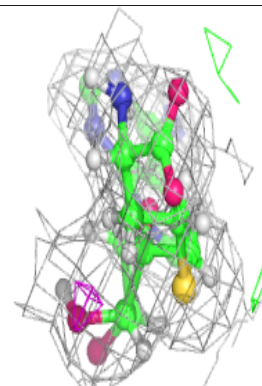
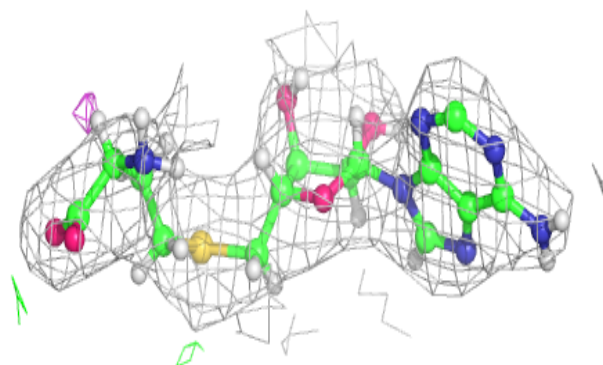
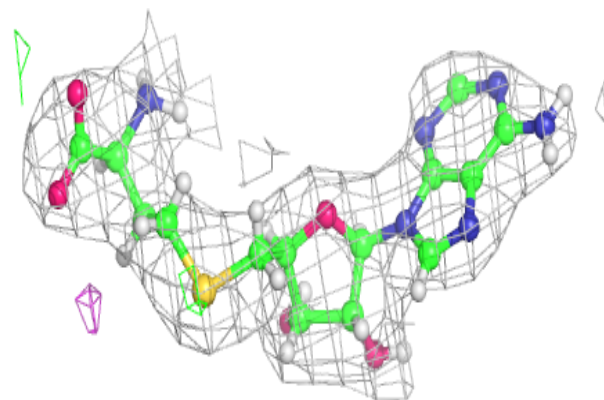


Electron density around SAH J 301:

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

**Electron density around SAH D 301:**

$2mF_o-DF_c$ (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.