



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:15 PM UTC

PDB ID : 7EC0 / pdb_00007ec0
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 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

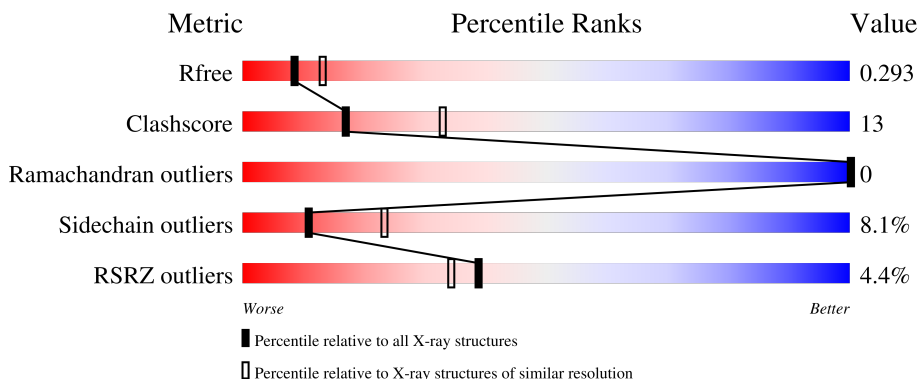
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	 6% 64% 23% 11%
1	D	288	 2% 64% 23% 11%
1	G	288	 3% 64% 23% 11%
1	J	288	 2% 65% 21% 11%
1	M	288	 6% 65% 22% 11%

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Mol	Chain	Length	Quality of chain
1	P	288	

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	-
3	J10	J	302	-	-	X	-

2 Entry composition [i](#)

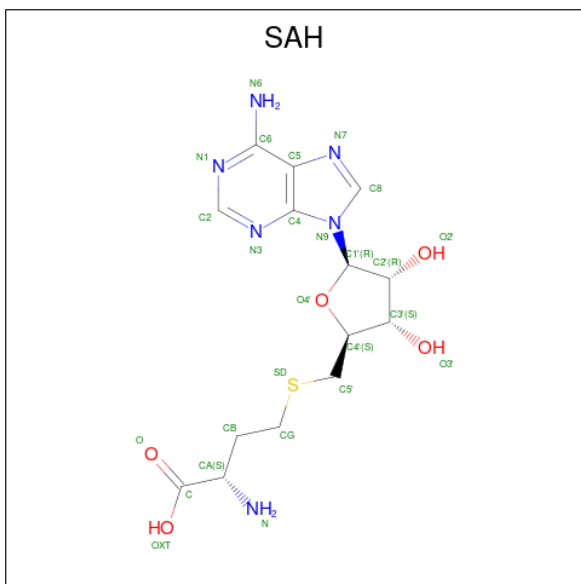
There are 4 unique types of molecules in this entry. The entry contains 24931 atoms, of which 12415 are hydrogens and 0 are deuteriums.

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.

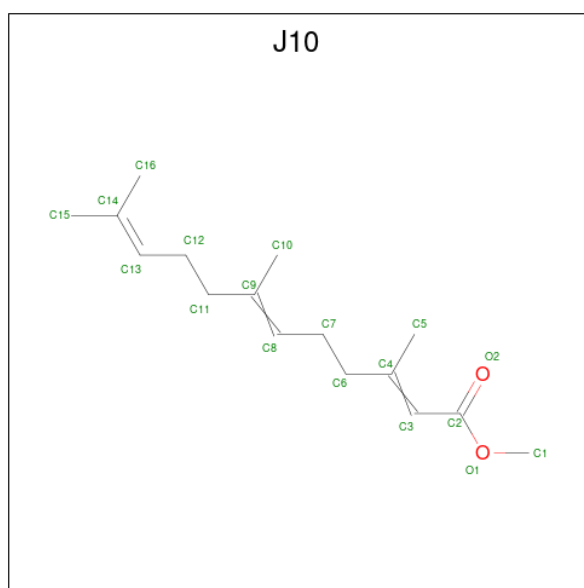
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	255	Total 4224	C 1363	H 2105	N 351	O 391	S 14	93	0	0
1	D	256	Total 4238	C 1367	H 2112	N 352	O 393	S 14	94	0	0
1	G	256	Total 4238	C 1367	H 2112	N 352	O 393	S 14	94	0	0
1	J	256	Total 4238	C 1367	H 2112	N 352	O 393	S 14	94	0	0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

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
2	A	1	44	14	18	6	5	1	4	0
2	D	1	44	14	18	6	5	1	4	0
2	G	1	44	14	18	6	5	1	4	0
2	J	1	44	14	18	6	5	1	4	0
2	M	1	44	14	18	6	5	1	4	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
3	A	1	44	16	26	2	0	0
3	D	1	44	16	26	2	0	0
3	G	1	44	16	26	2	0	0
3	J	1	44	16	26	2	0	0
3	M	1	44	16	26	2	0	0

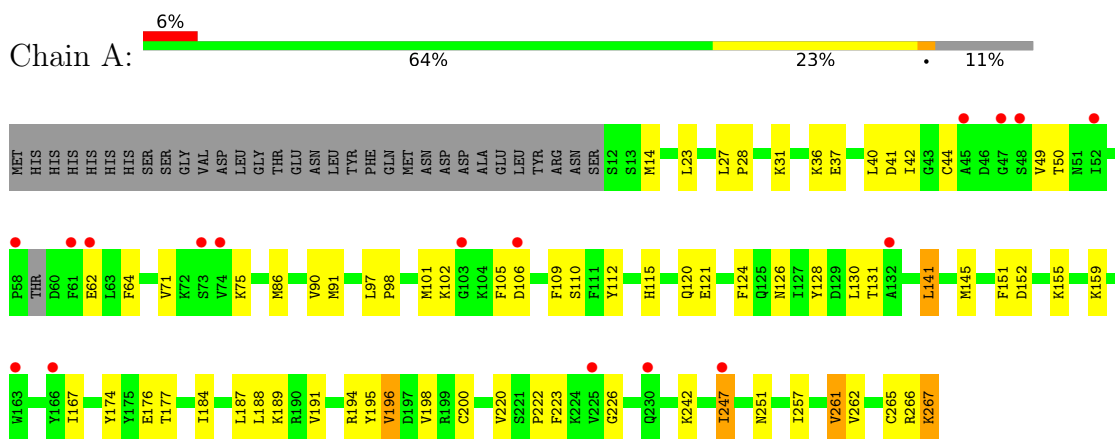
- Molecule 4 is water.

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

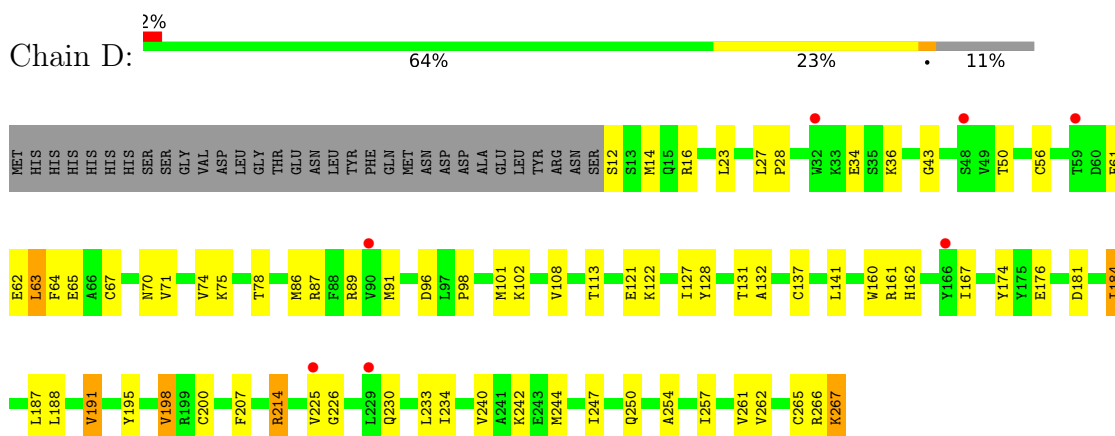
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

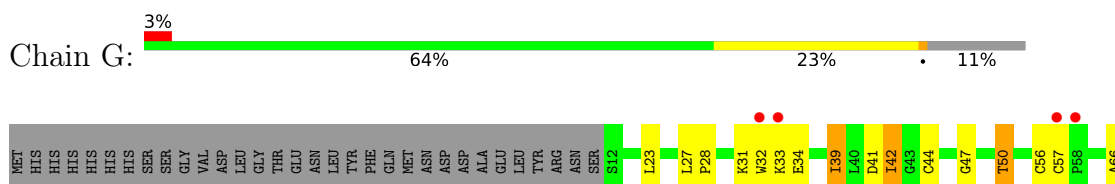
- Molecule 1: Juvenile hormone acid methyltransferase

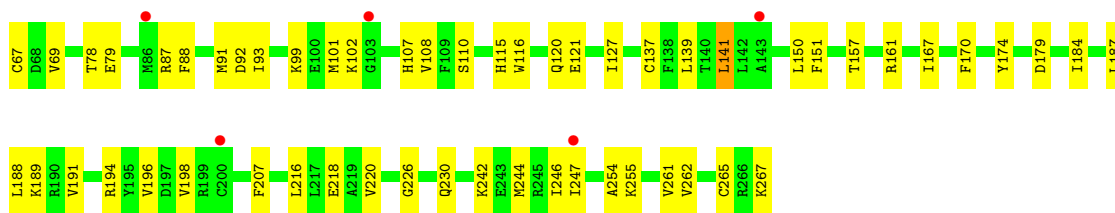


- Molecule 1: Juvenile hormone acid methyltransferase

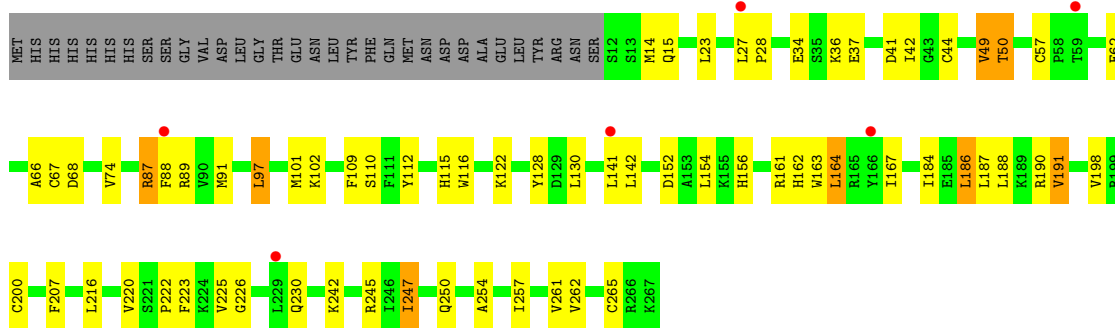


- Molecule 1: Juvenile hormone acid methyltransferase

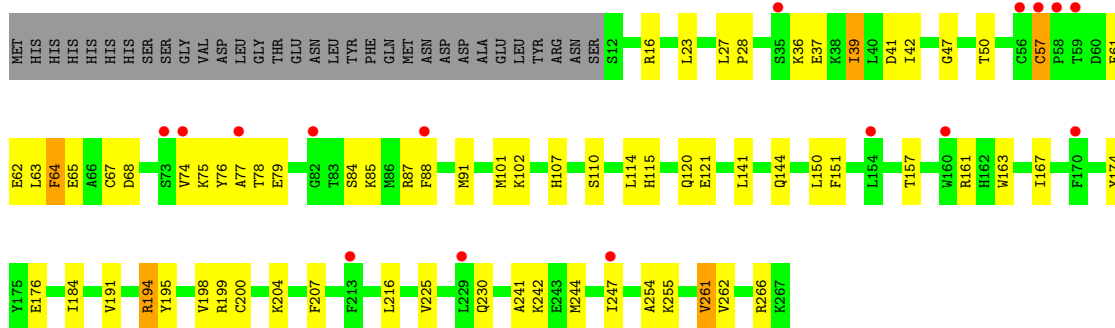




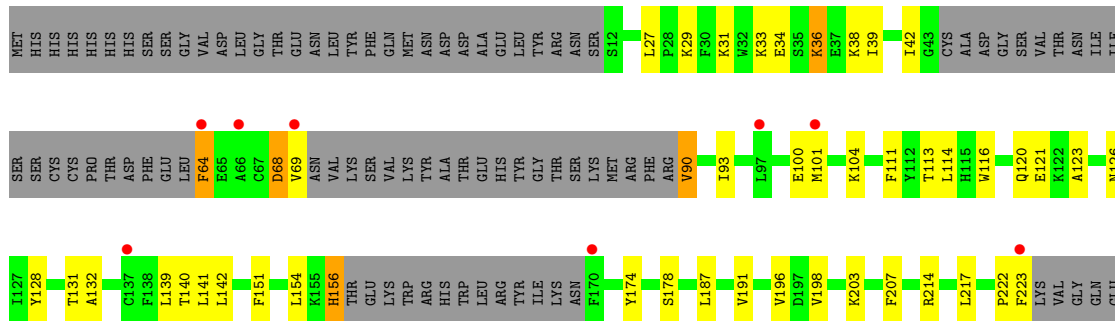
● Molecule 1: Juvenile hormone acid methyltransferase



● 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 72.26 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (72.26-2.49) 99.2 (72.26-2.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.245 , 0.293 0.245 , 0.293	Depositor DCC
R_{free} test set	3103 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.97	0/2166	1.39	2/2917 (0.1%)
1	D	0.97	0/2174	1.37	0/2930
1	G	0.97	0/2174	1.36	0/2930
1	J	0.98	0/2174	1.39	0/2930
1	M	0.98	0/2174	1.39	0/2930
1	P	0.98	0/1681	1.38	1/2259 (0.0%)
All	All	0.97	0/12543	1.38	3/16896 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	230	GLN	N-CA-C	-5.75	106.31	113.15
1	A	226	GLY	CA-C-N	5.47	127.88	120.38
1	A	226	GLY	C-N-CA	5.47	127.88	120.38

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	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2126	2112	2105	49	1
1	J	2126	2112	2105	61	1
1	M	2126	2112	2105	52	0
1	P	1649	1642	1633	44	0
2	A	26	18	19	4	0
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	16	0
3	D	18	26	0	4	0
3	G	18	26	0	7	0
3	J	18	26	0	11	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	313	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 13.

All (313) 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:D:50:THR:HG22	1:D:86:MET:HE1	1.53	0.89
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:HIS:NE2	3:A:302:J10:C1	2.42	0.83
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
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
1:J:225:VAL:HG23	1:J:230:GLN:CD	2.09	0.76
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:A:145:MET:HE2	3:A:302:J10:C5	2.18	0.74
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:J:14:MET:HE1	3:J:302:J10:C5	2.19	0.72
1:J:49:VAL:CG1	2:J:301:SAH:HA	2.15	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:50:THR:HG22	1:D:86:MET:CE	2.19	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:D:50:THR:CG2	1:D:86:MET:HE1	2.21	0.68
1:M:115:HIS:N	1:M:141:LEU:HD11	2.08	0.67
1:D:91:MET:HE1	1:D:101:MET:SD	2.34	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:J:163:TRP:C	1:J:164:LEU:HD12	2.21	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:HD12	1:J:164:LEU:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:MET:HE2	1:P:245:ARG:HG2	1.77	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: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
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:M:151:PHE:CG	3:M:302:J10:C15	2.83	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:D:63:LEU:HD13	1:D:63:LEU:C	2.25	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:P:230:GLN:HE21	1:P:230:GLN:C	2.11	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
1:P:36:LYS:NZ	1:P:36:LYS:HB3	2.17	0.58
1:J:225:VAL:CG2	1:J:230:GLN:CD	2.76	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:J:257:ILE:HD13	4:M:403:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:36:LYS:CE	1:M:62:GLU:HG2	2.35	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:M:91:MET:HE1	1:M:101:MET:SD	2.46	0.56
1:D:14:MET:CE	3:D:302:J10:C5	2.85	0.55
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
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:P:230:GLN:O	1:P:230:GLN:HG2	2.07	0.54
1:M:114:LEU:C	1:M:141:LEU:HD11	2.33	0.53
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:89:ARG:HD2	1:D:91:MET:HE3	1.92	0.50
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:245:ARG:HG2	1:M:244:MET:HE2	1.94	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:P:64:PHE:CD1	1:P:64:PHE:C	2.91	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:D:14:MET:HE1	3:D:302:J10:C5	2.43	0.48
1:M:114:LEU:HB2	1:M:141:LEU:CD1	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:64:PHE:C	1:M:64:PHE:HD1	2.23	0.47
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:M:64:PHE:C	1:M:64:PHE:CD1	2.93	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:P:64:PHE:C	1:P:64:PHE:HD1	2.24	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:A:14:MET:HE1	1:A:145:MET:HE1	1.98	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:D:240:VAL:CG1	1:D:244:MET:HE3	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:LEU:O	1:J:27:LEU:HB2	2.17	0.45
1:P:214:ARG:HA	1:P:238:MET:HE2	1.99	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: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
1:G:39:ILE:HG22	1:G:107:HIS:HB2	1.99	0.44
1:D:174:TYR:CE2	1:D:184:ILE:HD11	2.53	0.44
1:M:76:TYR:CD1	1:M:76:TYR:C	2.96	0.44
1:P:196:VAL:HG13	1:P:196:VAL:O	2.17	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:G:244:MET:HE2	1:P:245:ARG:CG	2.45	0.43
1:J:91:MET:HE1	1:J:101:MET:SD	2.58	0.43
1:D:14:MET:HE2	3:D:302:J10:C5	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:HIS:HB3	1:J:163:TRP:HE3	1.83	0.42
1:J:74:VAL:HG13	1:J:88:PHE:HB3	2.00	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: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:G:91:MET:HE1	1:G:101:MET:SD	2.60	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:12:SER:O	1:D:16:ARG:HD2	2.22	0.40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	222 (94%)	15 (6%)	16	34
1	D	238/267 (89%)	222 (93%)	16 (7%)	15	31
1	G	238/267 (89%)	219 (92%)	19 (8%)	11	24
1	J	238/267 (89%)	215 (90%)	23 (10%)	8	17
1	M	238/267 (89%)	219 (92%)	19 (8%)	11	24
1	P	185/267 (69%)	166 (90%)	19 (10%)	7	14
All	All	1374/1602 (86%)	1263 (92%)	111 (8%)	11	23

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	91	MET
1	A	102	LYS
1	A	121	GLU
1	A	141	LEU
1	A	167	ILE
1	A	184	ILE
1	A	191	VAL
1	A	196	VAL
1	A	198	VAL
1	A	247	ILE
1	A	251	ASN
1	A	261	VAL

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Mol	Chain	Res	Type
1	A	262	VAL
1	A	267	LYS
1	D	34	GLU
1	D	56	CYS
1	D	63	LEU
1	D	102	LYS
1	D	121	GLU
1	D	141	LEU
1	D	167	ILE
1	D	184	ILE
1	D	187	LEU
1	D	191	VAL
1	D	198	VAL
1	D	214	ARG
1	D	250	GLN
1	D	261	VAL
1	D	262	VAL
1	D	267	LYS
1	G	34	GLU
1	G	39	ILE
1	G	42	ILE
1	G	50	THR
1	G	56	CYS
1	G	78	THR
1	G	87	ARG
1	G	102	LYS
1	G	121	GLU
1	G	141	LEU
1	G	167	ILE
1	G	184	ILE
1	G	187	LEU
1	G	191	VAL
1	G	198	VAL
1	G	218	GLU
1	G	255	LYS
1	G	261	VAL
1	G	262	VAL
1	J	34	GLU
1	J	37	GLU
1	J	49	VAL
1	J	50	THR
1	J	57	CYS

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Mol	Chain	Res	Type
1	J	87	ARG
1	J	97	LEU
1	J	102	LYS
1	J	122	LYS
1	J	141	LEU
1	J	152	ASP
1	J	154	LEU
1	J	164	LEU
1	J	167	ILE
1	J	184	ILE
1	J	186	LEU
1	J	187	LEU
1	J	191	VAL
1	J	198	VAL
1	J	247	ILE
1	J	250	GLN
1	J	261	VAL
1	J	262	VAL
1	M	16	ARG
1	M	37	GLU
1	M	39	ILE
1	M	57	CYS
1	M	64	PHE
1	M	74	VAL
1	M	78	THR
1	M	84	SER
1	M	87	ARG
1	M	102	LYS
1	M	121	GLU
1	M	144	GLN
1	M	167	ILE
1	M	184	ILE
1	M	191	VAL
1	M	194	ARG
1	M	198	VAL
1	M	261	VAL
1	M	262	VAL
1	P	27	LEU
1	P	34	GLU
1	P	36	LYS
1	P	39	ILE
1	P	64	PHE

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Mol	Chain	Res	Type
1	P	68	ASP
1	P	69	VAL
1	P	90	VAL
1	P	101	MET
1	P	121	GLU
1	P	139	LEU
1	P	156	HIS
1	P	178	SER
1	P	229	LEU
1	P	230	GLN
1	P	239	GLU
1	P	247	ILE
1	P	261	VAL
1	P	262	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	215	ASN
1	D	21	ASN
1	G	149	ASN
1	G	227	GLN
1	J	125	GLN
1	J	250	GLN
1	P	144	GLN
1	P	230	GLN
1	P	250	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 oligosaccharides in this entry.

5.6 Ligand geometry

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
2	SAH	M	301	-	27,28,28	0.57	1 (3%)	36,40,40	0.52	0
3	J10	J	302	-	17,17,17	0.44	0	20,20,20	0.45	0
2	SAH	J	301	-	27,28,28	0.63	1 (3%)	36,40,40	0.61	1 (2%)
3	J10	G	302	-	17,17,17	0.34	0	20,20,20	0.43	0
3	J10	M	302	-	17,17,17	0.50	0	20,20,20	0.49	0
2	SAH	G	301	-	27,28,28	0.67	1 (3%)	36,40,40	0.58	0
2	SAH	A	301	-	27,28,28	0.50	0	36,40,40	0.42	0
2	SAH	D	301	-	27,28,28	0.64	1 (3%)	36,40,40	0.47	0
3	J10	A	302	-	17,17,17	0.38	0	20,20,20	0.45	0
3	J10	D	302	-	17,17,17	0.51	0	20,20,20	0.57	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	SAH	M	301	-	-	2/15/31/31	0/3/3/3
3	J10	J	302	-	-	10/18/18/18	-
2	SAH	J	301	-	-	6/15/31/31	0/3/3/3
3	J10	G	302	-	-	9/18/18/18	-
3	J10	M	302	-	-	10/18/18/18	-
2	SAH	G	301	-	-	2/15/31/31	0/3/3/3
2	SAH	A	301	-	-	6/15/31/31	0/3/3/3
2	SAH	D	301	-	-	3/15/31/31	0/3/3/3
3	J10	A	302	-	-	11/18/18/18	-
3	J10	D	302	-	-	10/18/18/18	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	SAH	OXT-C	-2.60	1.22	1.30
2	G	301	SAH	OXT-C	-2.56	1.22	1.30
2	J	301	SAH	OXT-C	-2.48	1.22	1.30
2	M	301	SAH	OXT-C	-2.30	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	301	SAH	O3'-C3'-C2'	-2.48	103.86	111.82

There are no chirality outliers.

All (69) 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
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	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
3	D	302	J10	O2-C2-O1-C1
3	D	302	J10	C9-C11-C12-C13

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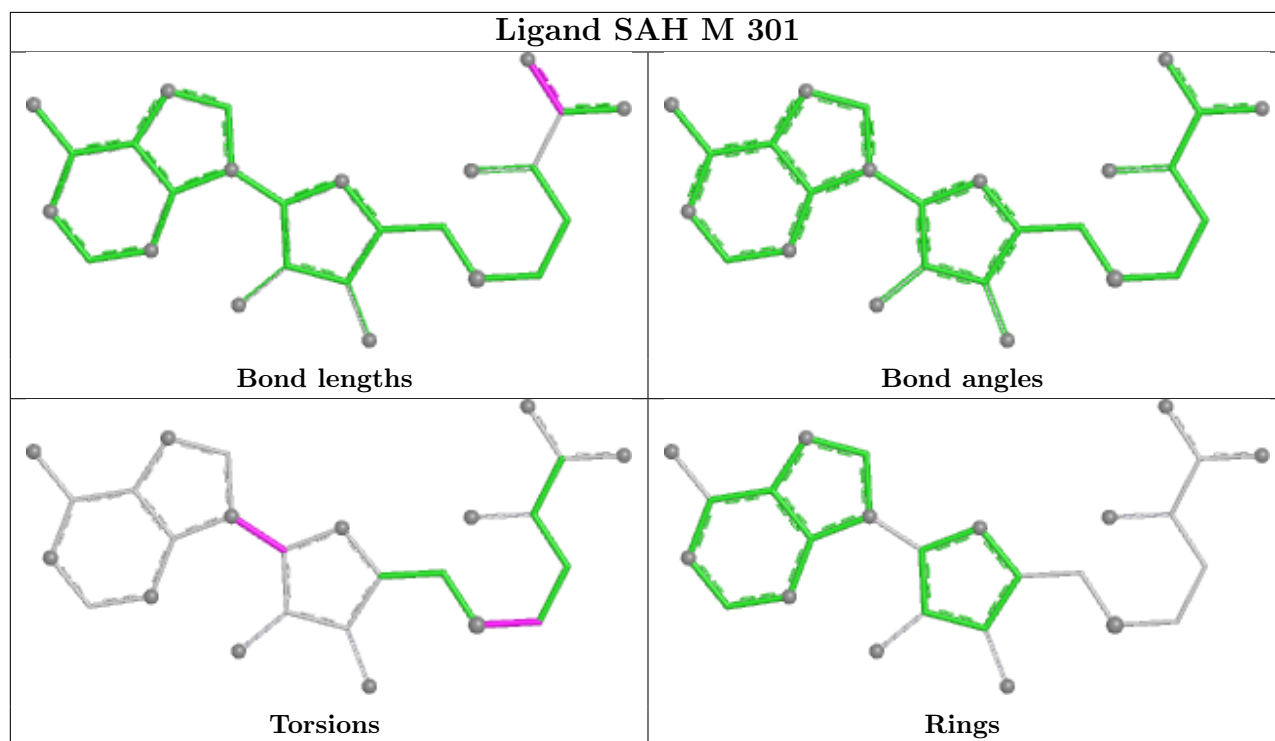
Mol	Chain	Res	Type	Atoms
3	G	302	J10	C4-C6-C7-C8
3	A	302	J10	C7-C8-C9-C11
3	D	302	J10	C12-C13-C14-C15
3	D	302	J10	C12-C13-C14-C16
3	A	302	J10	C7-C8-C9-C10
3	J	302	J10	C4-C6-C7-C8
3	A	302	J10	C6-C7-C8-C9
3	G	302	J10	C6-C7-C8-C9
3	A	302	J10	C5-C4-C6-C7
3	J	302	J10	C5-C4-C6-C7
3	G	302	J10	C5-C4-C6-C7
3	A	302	J10	C3-C4-C6-C7
3	G	302	J10	C3-C4-C6-C7
3	J	302	J10	C3-C4-C6-C7
3	G	302	J10	C12-C11-C9-C10
3	J	302	J10	C12-C11-C9-C10
3	J	302	J10	C9-C11-C12-C13
3	J	302	J10	C12-C11-C9-C8
3	G	302	J10	C12-C11-C9-C8
2	J	301	SAH	C-CA-CB-CG
3	A	302	J10	C12-C11-C9-C10
2	A	301	SAH	C2'-C1'-N9-C8
2	D	301	SAH	C2'-C1'-N9-C8
2	M	301	SAH	C2'-C1'-N9-C8
2	J	301	SAH	N-CA-CB-CG
2	J	301	SAH	C3'-C4'-C5'-SD
3	M	302	J10	O1-C2-C3-C4
3	M	302	J10	C12-C11-C9-C10
2	M	301	SAH	CB-CG-SD-C5'
3	M	302	J10	C12-C11-C9-C8
2	J	301	SAH	O4'-C4'-C5'-SD
2	J	301	SAH	O-C-CA-CB
2	J	301	SAH	OXT-C-CA-CB
3	M	302	J10	O2-C2-C3-C4
3	A	302	J10	C12-C11-C9-C8
3	A	302	J10	C4-C6-C7-C8
2	A	301	SAH	OXT-C-CA-CB
2	D	301	SAH	CB-CG-SD-C5'
2	G	301	SAH	C2'-C1'-N9-C8
2	A	301	SAH	O4'-C1'-N9-C8
2	D	301	SAH	O4'-C1'-N9-C8
2	A	301	SAH	O-C-CA-CB

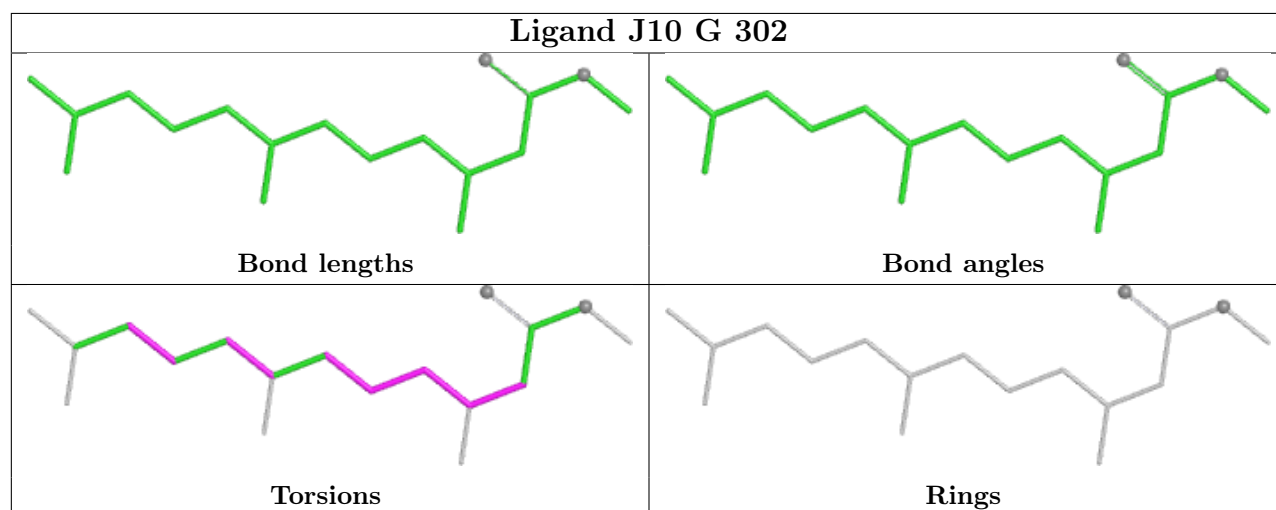
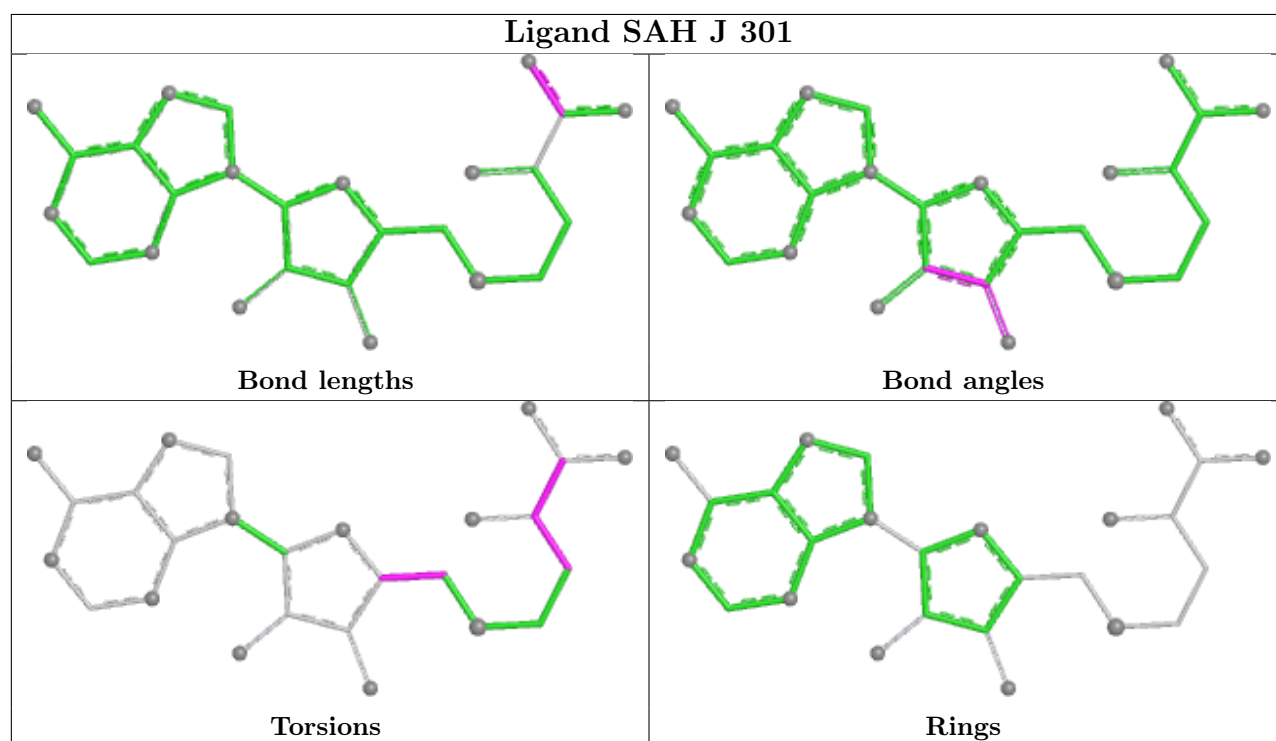
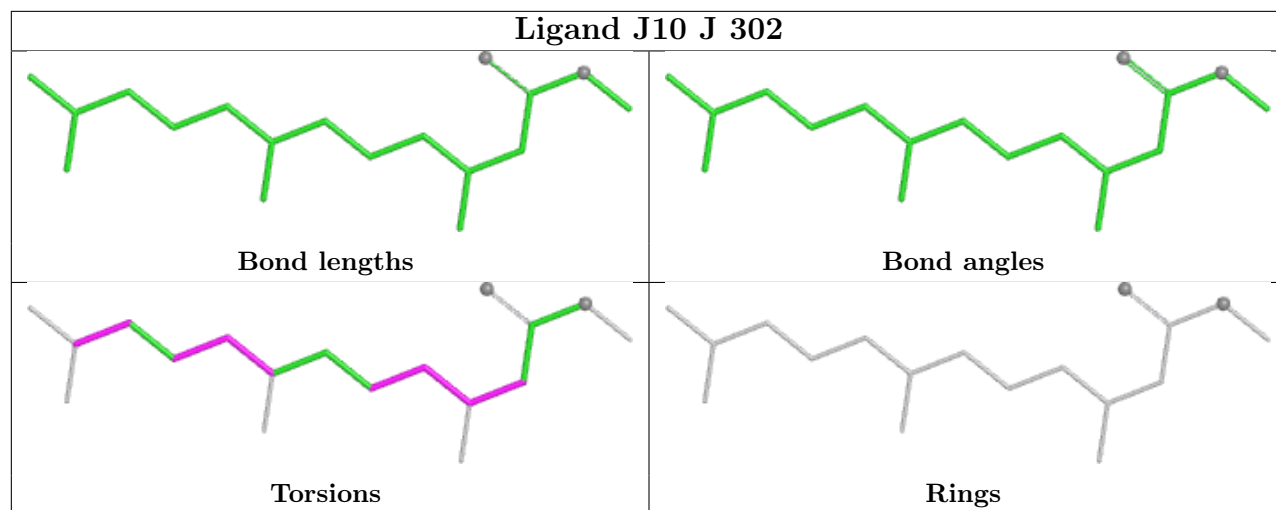
There are no ring outliers.

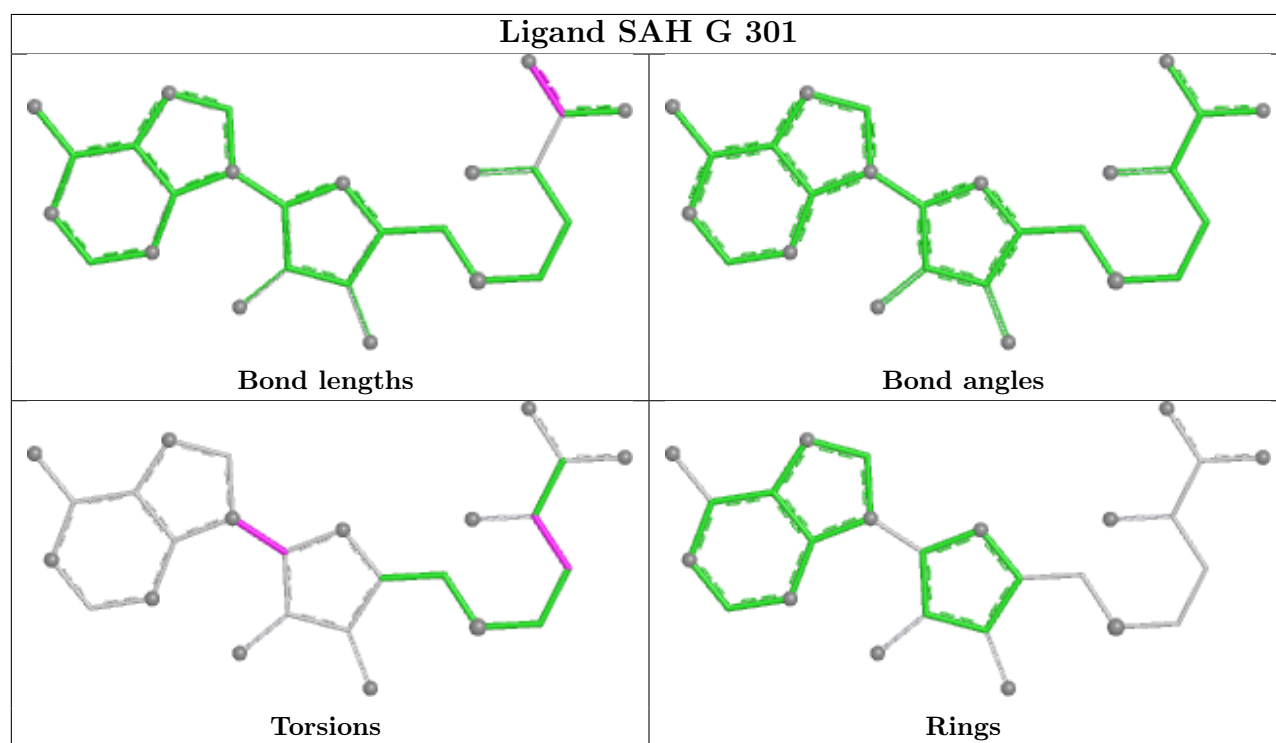
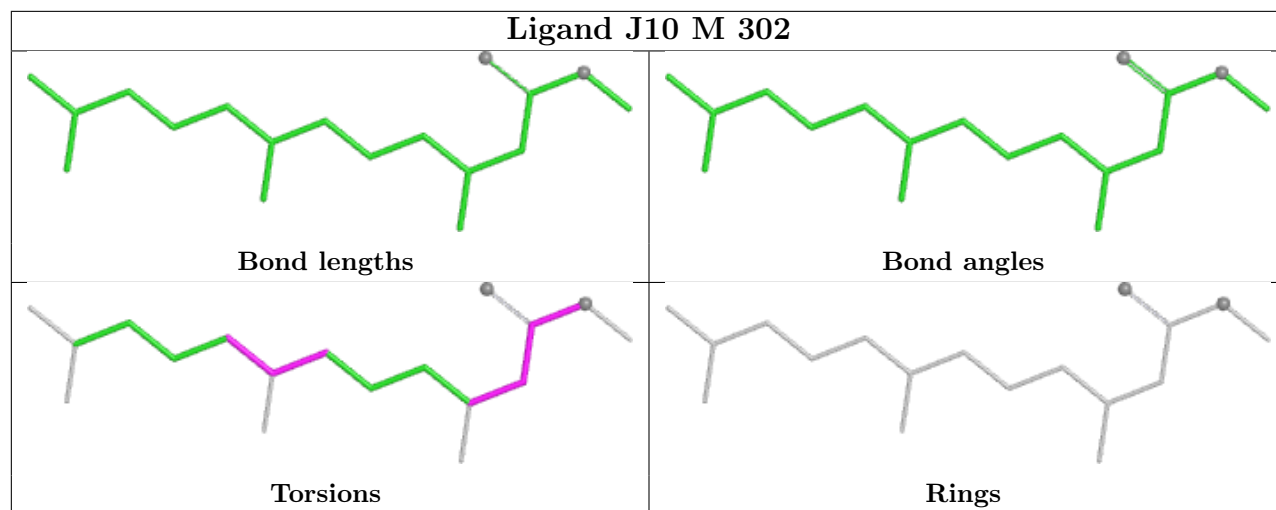
9 monomers are involved in 54 short contacts:

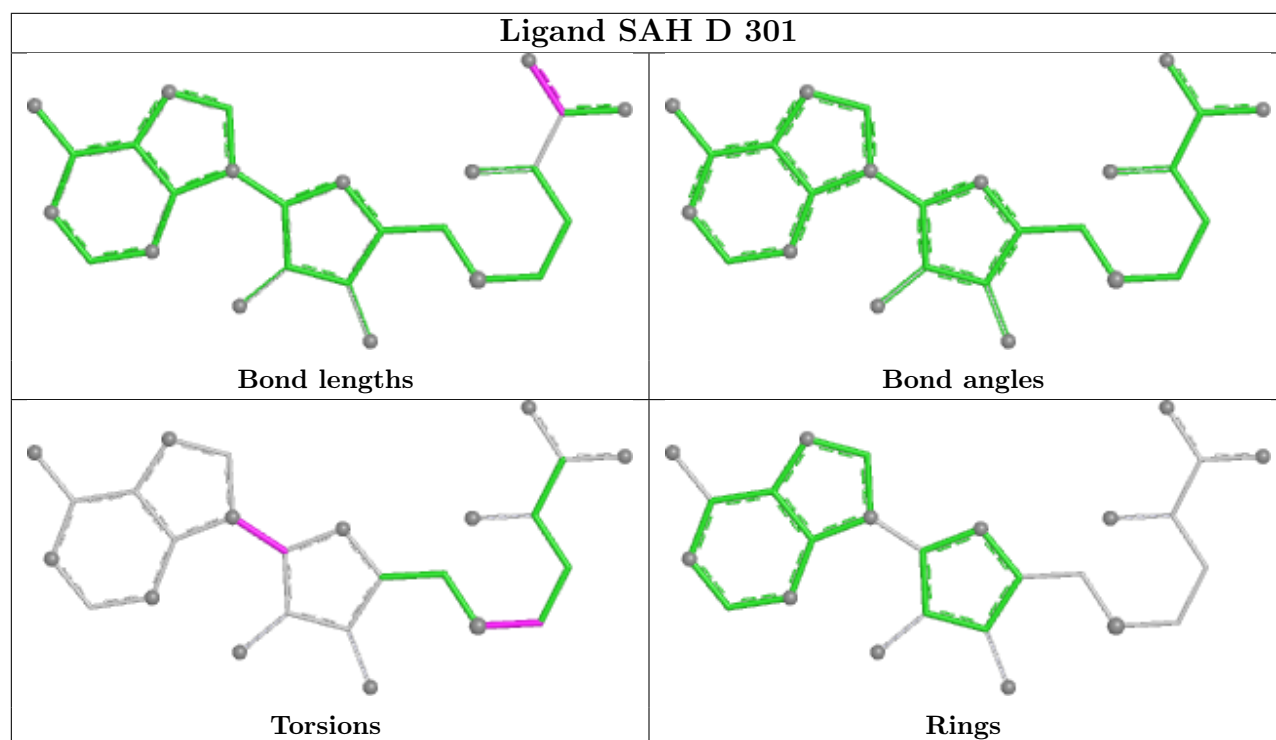
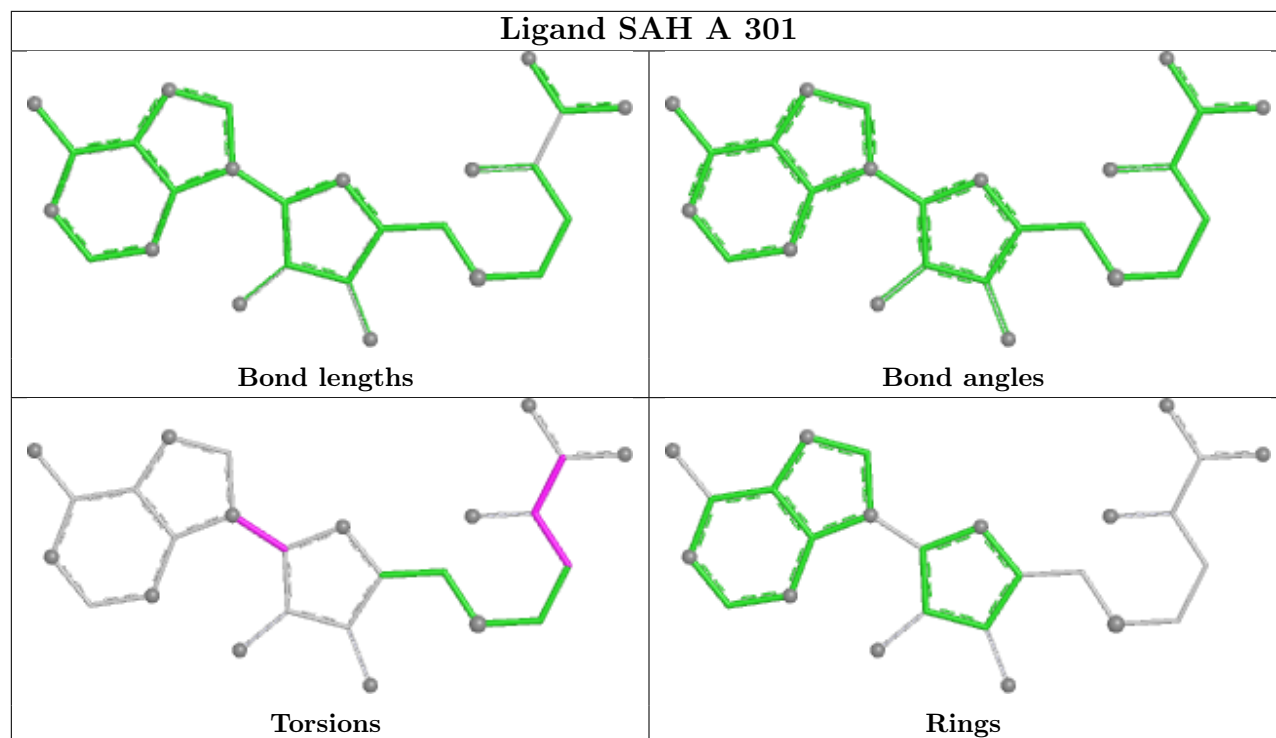
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	301	SAH	1	0
3	J	302	J10	11	0
2	J	301	SAH	6	0
3	G	302	J10	7	0
3	M	302	J10	3	0
2	A	301	SAH	4	0
2	D	301	SAH	2	0
3	A	302	J10	16	0
3	D	302	J10	4	0

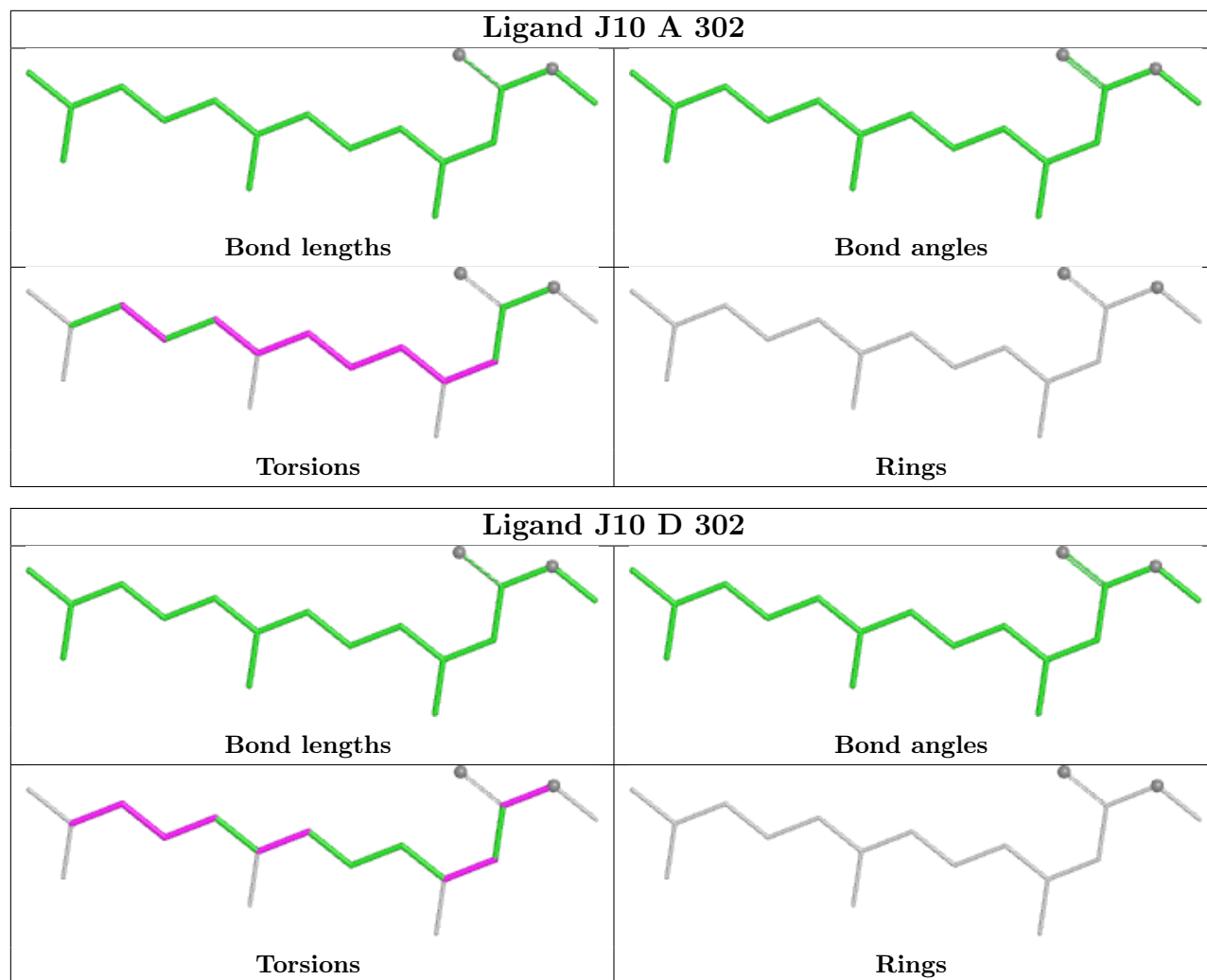
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	255/288 (88%)	0.67	17 (6%) 24 21	41, 72, 108, 118	0
1	D	256/288 (88%)	0.38	7 (2%) 56 51	40, 63, 89, 102	0
1	G	256/288 (88%)	0.45	9 (3%) 47 42	42, 64, 91, 105	0
1	J	256/288 (88%)	0.61	6 (2%) 61 57	44, 74, 109, 129	0
1	M	256/288 (88%)	0.72	16 (6%) 26 23	41, 73, 108, 133	0
1	P	198/288 (68%)	0.71	10 (5%) 33 29	32, 75, 107, 119	0
All	All	1477/1728 (85%)	0.58	65 (4%) 39 34	32, 70, 104, 133	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	48	SER	4.9
1	A	58	PRO	4.4
1	M	88	PHE	3.8
1	P	69	VAL	3.7
1	G	33	LYS	3.5
1	J	59	THR	3.5
1	A	61	PHE	3.3
1	A	74	VAL	3.3
1	M	74	VAL	3.3
1	D	59	THR	3.3
1	A	45	ALA	3.1
1	P	233	LEU	3.1
1	G	200	CYS	3.0
1	D	225	VAL	2.9
1	M	35	SER	2.8
1	M	58	PRO	2.8
1	A	103	GLY	2.8
1	M	229	LEU	2.7
1	P	101	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	229	LEU	2.6
1	M	160	TRP	2.6
1	A	106	ASP	2.6
1	A	48	SER	2.6
1	M	77	ALA	2.6
1	A	47	GLY	2.5
1	M	154	LEU	2.5
1	D	229	LEU	2.5
1	M	57	CYS	2.5
1	P	229	LEU	2.5
1	J	27	LEU	2.4
1	G	143	ALA	2.4
1	A	62	GLU	2.4
1	A	230	GLN	2.4
1	P	170	PHE	2.4
1	J	141	LEU	2.3
1	M	247	ILE	2.3
1	G	57	CYS	2.3
1	G	103	GLY	2.3
1	P	66	ALA	2.3
1	M	73	SER	2.3
1	G	86	MET	2.3
1	A	247	ILE	2.2
1	A	73	SER	2.2
1	D	32	TRP	2.2
1	P	223	PHE	2.2
1	J	166	TYR	2.2
1	M	59	THR	2.2
1	G	32	TRP	2.2
1	P	64	PHE	2.2
1	A	225	VAL	2.1
1	D	90	VAL	2.1
1	D	166	TYR	2.1
1	G	58	PRO	2.1
1	A	163	TRP	2.1
1	G	247	ILE	2.1
1	M	56	CYS	2.1
1	P	137	CYS	2.1
1	J	88	PHE	2.1
1	M	170	PHE	2.1
1	M	213	PHE	2.1
1	A	166	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	82	GLY	2.0
1	A	52	ILE	2.0
1	A	132	ALA	2.0
1	P	97	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

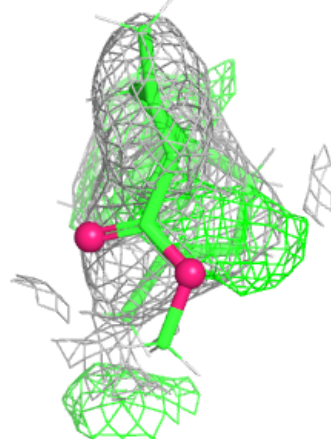
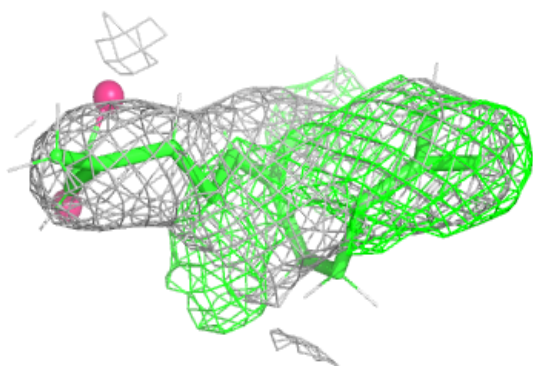
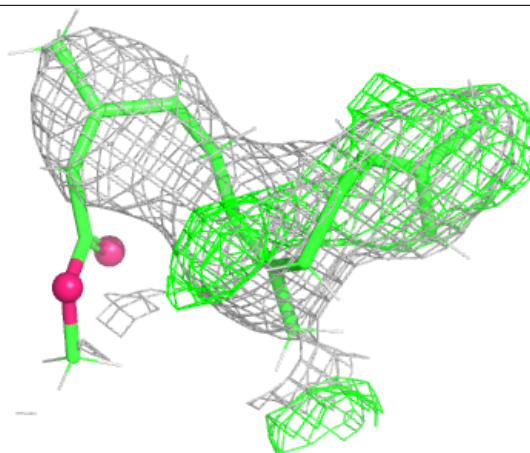
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	J10	J	302	18/18	0.79	0.34	58,63,67,67	24
3	J10	A	302	18/18	0.80	0.31	62,65,69,72	24
3	J10	M	302	18/18	0.83	0.31	64,67,71,72	24
3	J10	D	302	18/18	0.84	0.23	57,60,65,68	7
3	J10	G	302	18/18	0.85	0.32	54,57,61,61	24
2	SAH	M	301	26/26	0.90	0.09	63,67,74,76	4
2	SAH	A	301	26/26	0.90	0.20	56,60,60,62	44
2	SAH	J	301	26/26	0.91	0.08	66,70,73,74	4
2	SAH	G	301	26/26	0.92	0.09	52,53,63,71	4
2	SAH	D	301	26/26	0.95	0.07	59,61,66,69	4

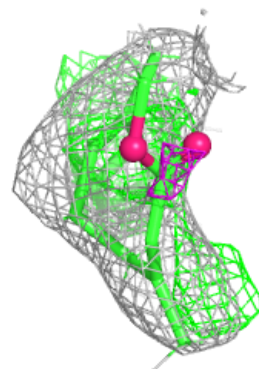
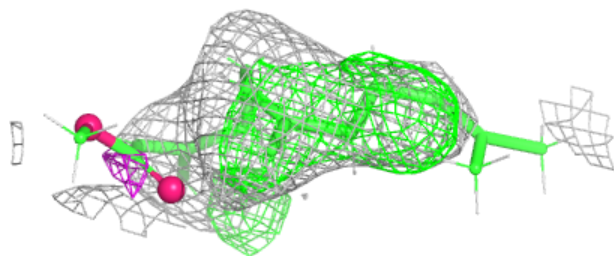
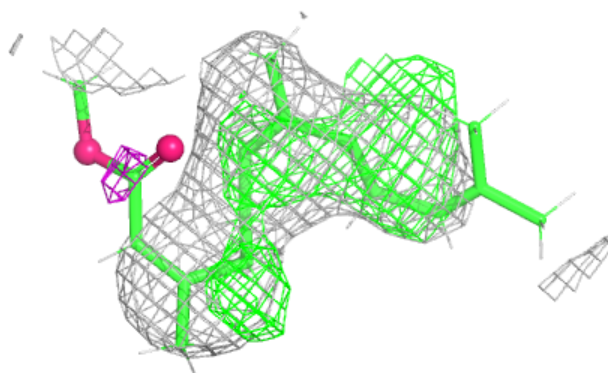
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

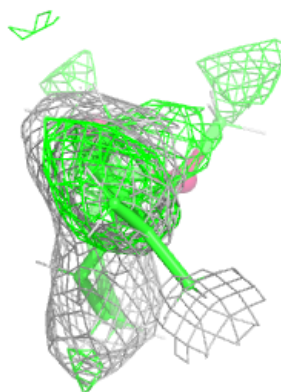
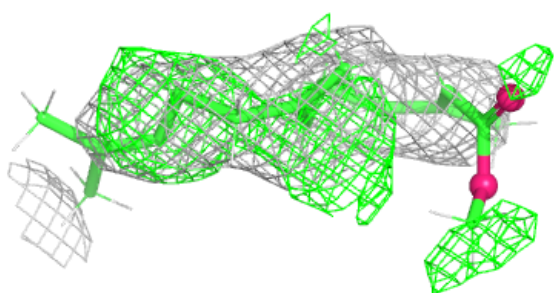
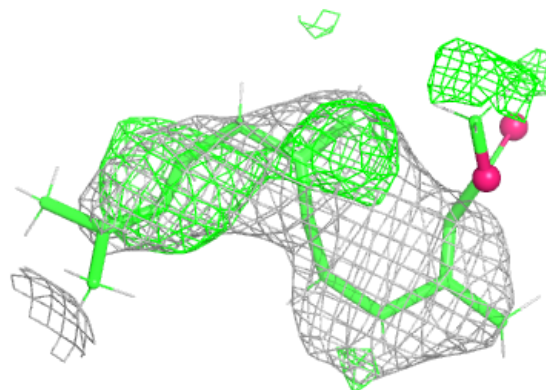
**Electron density around J10 A 302:**

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

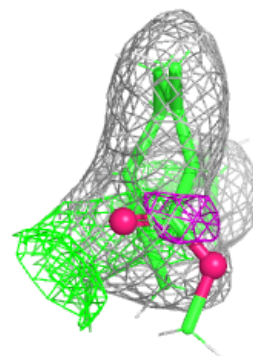
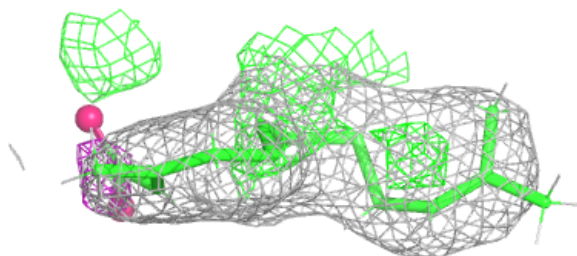
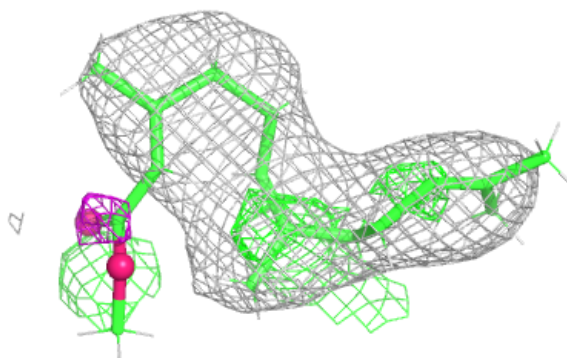


Electron density around J10 M 302:

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

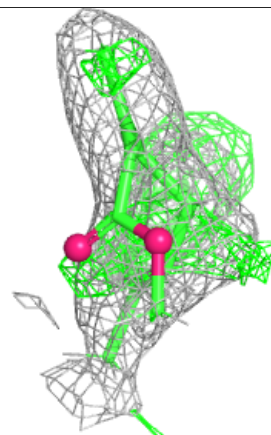
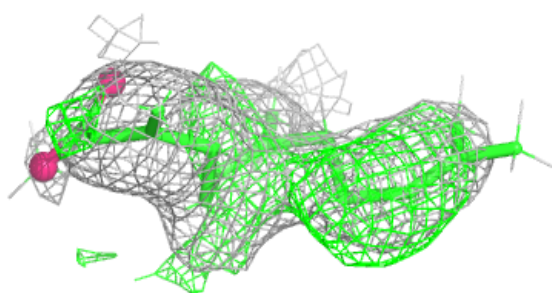
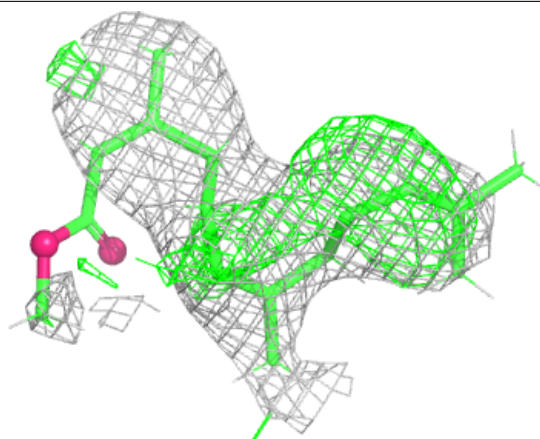
**Electron density around J10 D 302:**

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

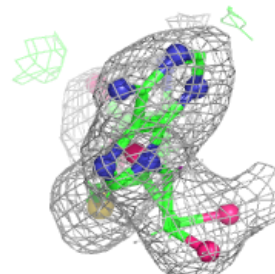
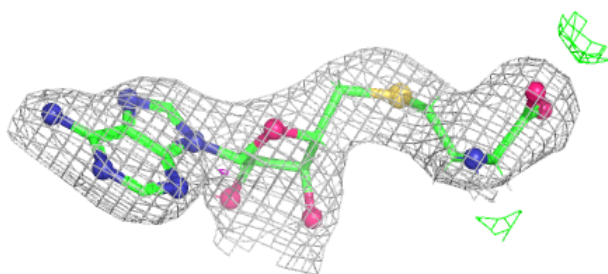
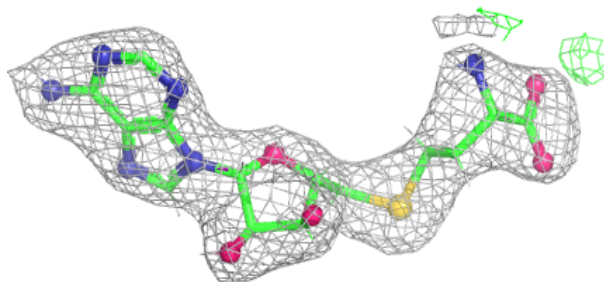


Electron density around J10 G 302:

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

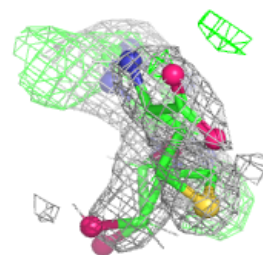
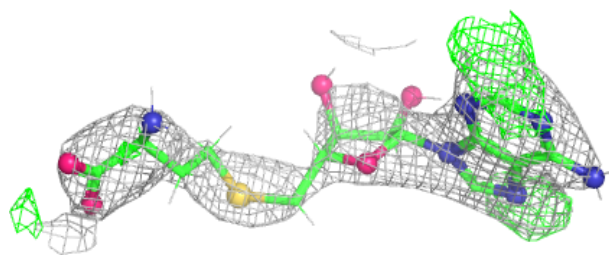
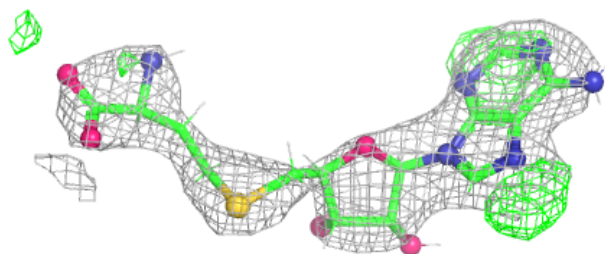
**Electron density around SAH M 301:**

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

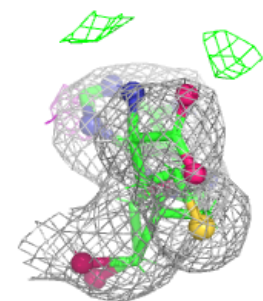
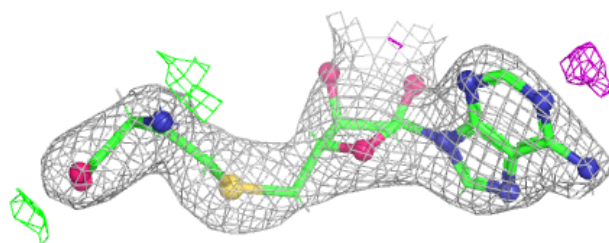
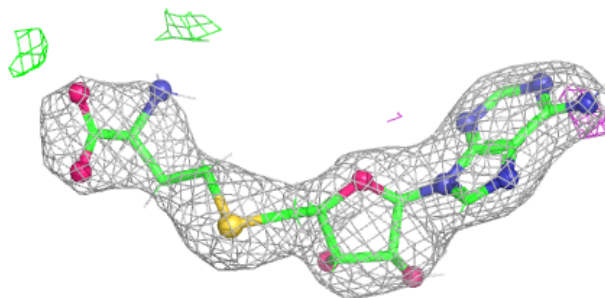


Electron density around SAH A 301:

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

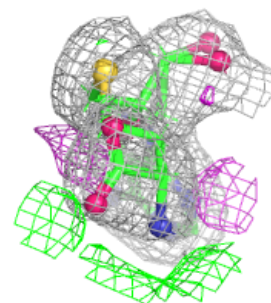
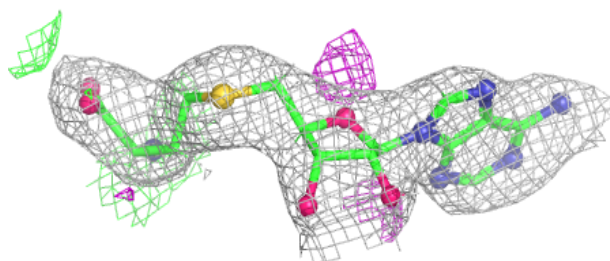
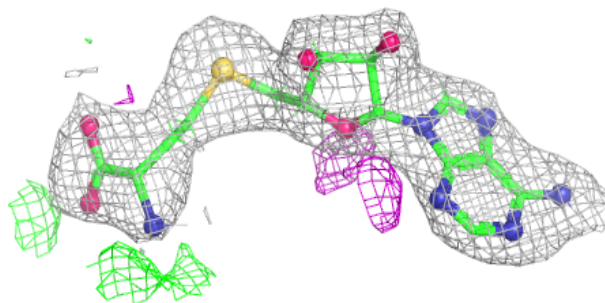
**Electron density around SAH J 301:**

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

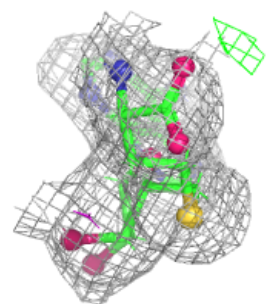
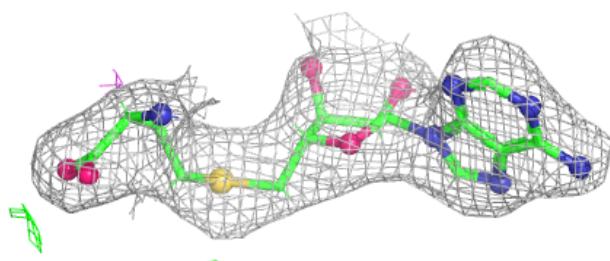
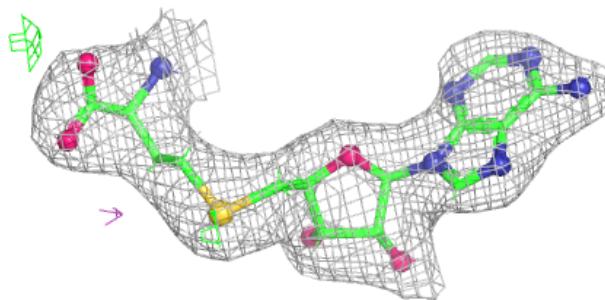


Electron density around SAH G 301:

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

**Electron density around SAH 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.