



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:48 AM UTC

PDB ID : 2Y1X / pdb_00002y1x
Title : CRYSTAL STRUCTURE OF COACTIVATOR ASSOCIATED ARGININE METHYLTRANSFERASE 1 (CARM1) IN COMPLEX WITH SINEFUNGIN AND INDOLE INHIBITOR
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Deposited on : 2010-12-10
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

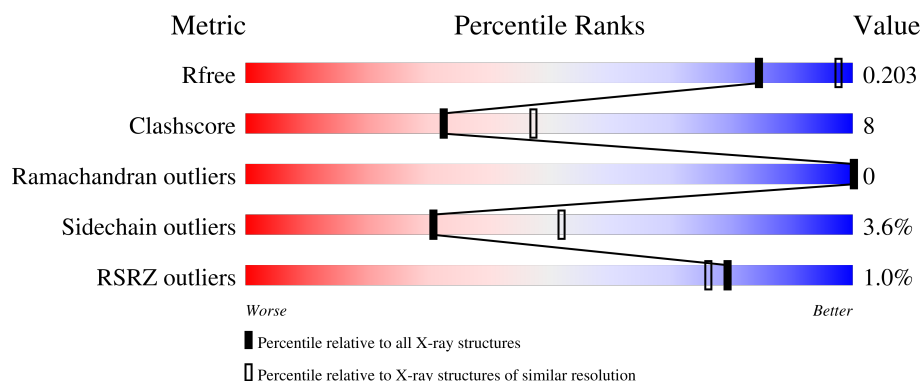
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	348	
1	B	348	
1	C	348	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	348	% 83% 14% ..

2 Entry composition [i](#)

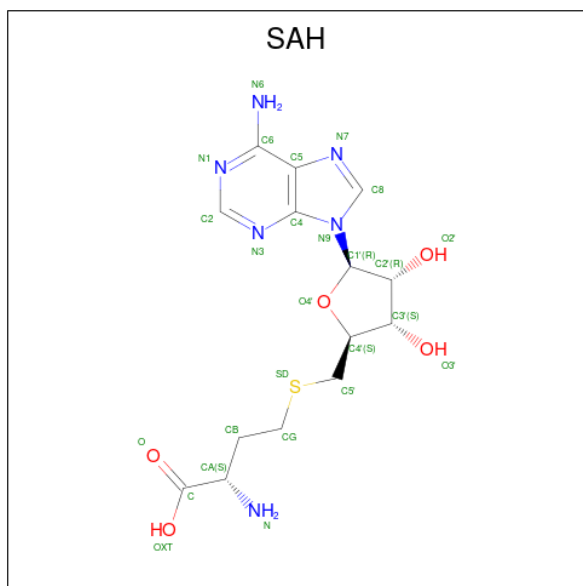
There are 5 unique types of molecules in this entry. The entry contains 11692 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called HISTONE-ARGININE METHYLTRANSFERASE CARM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	1
			2745	1772	454	505	14			
1	B	343	Total	C	N	O	S	0	0	1
			2745	1772	454	505	14			
1	C	343	Total	C	N	O	S	0	0	1
			2745	1772	454	505	14			
1	D	343	Total	C	N	O	S	0	0	1
			2745	1772	454	505	14			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



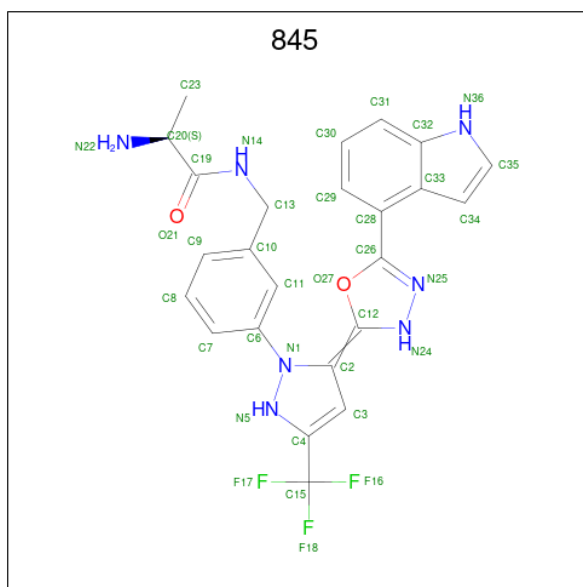
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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

- Molecule 3 is N-(3-{5-[5-(1H-INDOL-4-YL)-1,3,4-OXADIAZOL-2-YL]-3-(TRIFLUOROMETHYL)-1H-PYRAZOL-1-YL}BENZYL)-L-ALANINAMIDE (CCD ID: 845) (formula: $C_{24}H_{22}F_3N_7O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			36	24	3	7	2		
3	B	1	Total	C	F	N	O	0	0
			36	24	3	7	2		
3	C	1	Total	C	F	N	O	0	0
			36	24	3	7	2		
3	D	1	Total	C	F	N	O	0	0
			36	24	3	7	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total 1 Cl	0	0
4	B	1	Total 1 Cl	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0

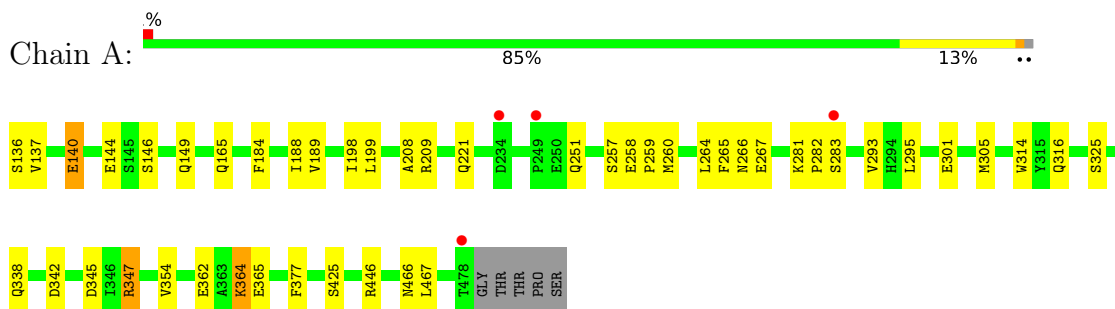
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total 124	O 124	0	0
5	B	86	Total 86	O 86	0	0
5	C	137	Total 137	O 137	0	0
5	D	113	Total 113	O 113	0	0

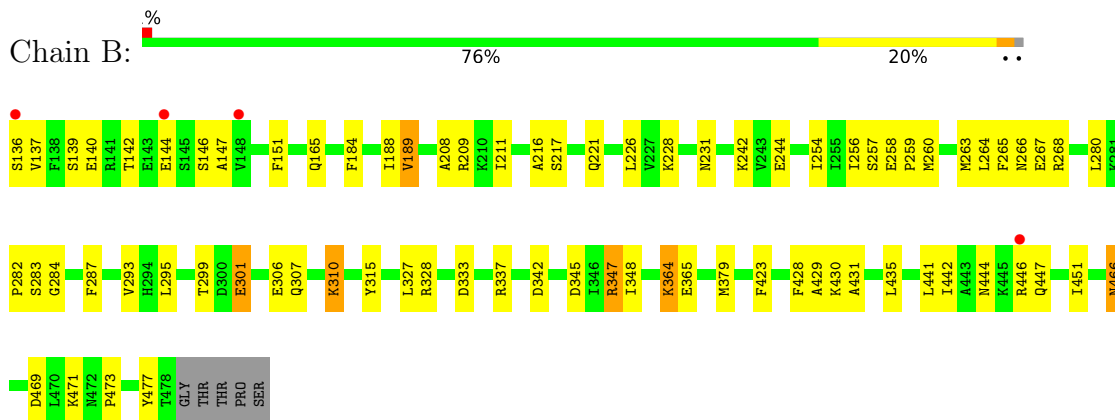
3 Residue-property plots [i](#)

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.

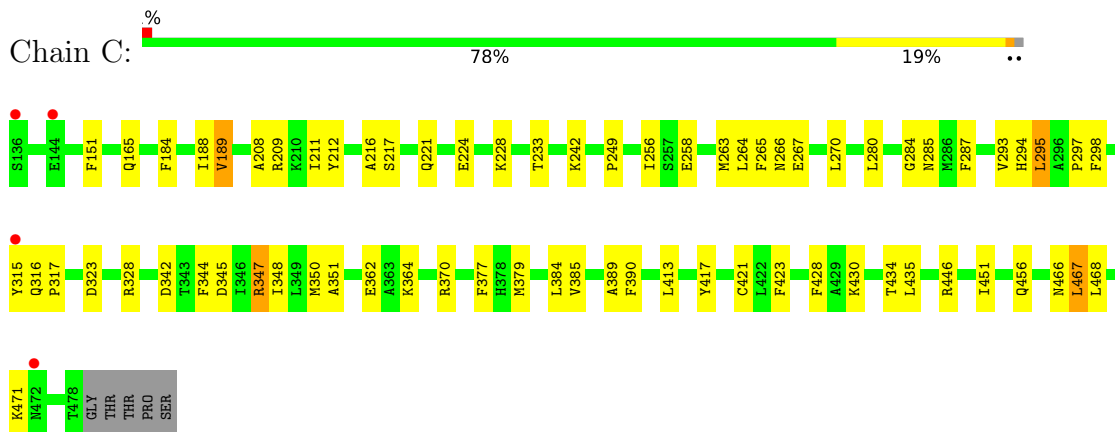
• Molecule 1: HISTONE-ARGININE METHYLTRANSFERASE CARM1



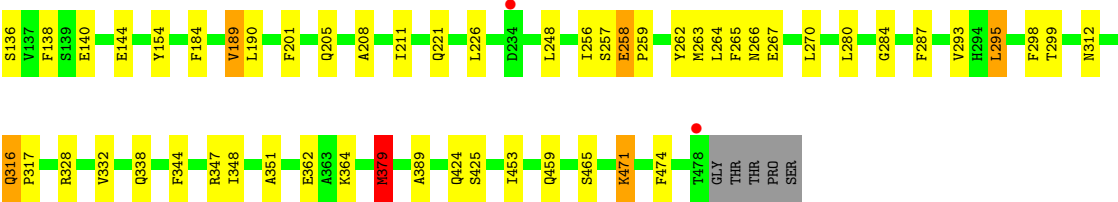
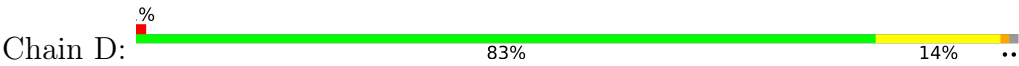
• Molecule 1: HISTONE-ARGININE METHYLTRANSFERASE CARM1



• Molecule 1: HISTONE-ARGININE METHYLTRANSFERASE CARM1



● Molecule 1: HISTONE-ARGININE METHYLTRANSFERASE CARM1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	75.56Å 98.76Å 207.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.40 29.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.96-2.40) 99.3 (29.96-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.39Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.207 , 0.264 0.207 , 0.203	Depositor DCC
R_{free} test set	3108 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.4	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	11692	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5598e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 845, CL, 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	0.61	0/2815	0.86	2/3815 (0.1%)
1	B	0.60	1/2815 (0.0%)	0.84	0/3815
1	C	0.62	0/2815	0.84	2/3815 (0.1%)
1	D	0.61	1/2815 (0.0%)	0.81	4/3815 (0.1%)
All	All	0.61	2/11260 (0.0%)	0.84	8/15260 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	379	MET	SD-CE	-6.50	1.63	1.79
1	B	477	TYR	C-N	-5.10	1.26	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316	GLN	CA-C-N	8.73	128.46	119.64
1	C	316	GLN	C-N-CA	8.73	128.46	119.64
1	A	338	GLN	CA-C-N	-5.60	114.16	119.76
1	A	338	GLN	C-N-CA	-5.60	114.16	119.76
1	D	316	GLN	CA-C-N	5.59	125.29	119.64
1	D	316	GLN	C-N-CA	5.59	125.29	119.64
1	D	258	GLU	CA-C-N	5.21	127.34	121.04
1	D	258	GLU	C-N-CA	5.21	127.34	121.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2745	0	2692	27	0
1	B	2745	0	2692	60	0
1	C	2745	0	2692	49	0
1	D	2745	0	2692	41	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
2	C	26	0	19	1	0
2	D	26	0	19	0	0
3	A	36	0	22	1	0
3	B	36	0	22	2	0
3	C	36	0	22	0	0
3	D	36	0	22	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	124	0	0	2	0
5	B	86	0	0	7	0
5	C	137	0	0	5	0
5	D	113	0	0	4	0
All	All	11692	0	10932	176	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (176) 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:D:338:GLN:HE21	1:D:474:PHE:HB2	1.30	0.95
1:C:315:TYR:HB2	1:C:328:ARG:HD3	1.55	0.88
1:B:345:ASP:OD2	1:B:347:ARG:HB2	1.82	0.80
1:D:338:GLN:NE2	1:D:474:PHE:HB2	1.96	0.79
1:C:379:MET:HA	1:C:379:MET:HE2	1.64	0.78
1:C:328:ARG:HG2	1:C:328:ARG:HH11	1.47	0.77
1:B:333:ASP:O	1:B:337:ARG:HG3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ASN:HB2	5:C:2073:HOH:O	1.86	0.76
1:B:140:GLU:HA	1:B:140:GLU:OE1	1.92	0.70
1:A:342:ASP:HB2	5:A:2071:HOH:O	1.91	0.69
1:C:342:ASP:HB2	5:C:2088:HOH:O	1.94	0.68
1:D:144:GLU:HA	1:D:144:GLU:OE1	1.93	0.68
1:D:312:ASN:HD21	1:D:328:ARG:HH21	1.41	0.67
1:B:342:ASP:HB2	5:B:2054:HOH:O	1.96	0.65
1:D:379:MET:HA	1:D:379:MET:HE3	1.77	0.65
1:D:379:MET:HA	1:D:379:MET:CE	2.27	0.65
1:C:421:CYS:SG	1:C:468:LEU:HD22	2.37	0.65
1:C:297:PRO:HG3	1:C:379:MET:HE1	1.78	0.65
1:A:301:GLU:HG3	1:A:305:MET:HE2	1.78	0.64
1:D:189:VAL:HG22	1:D:211:ILE:HG23	1.82	0.62
1:C:270:LEU:HB2	5:C:2066:HOH:O	1.99	0.62
1:D:266:ASN:O	1:D:267:GLU:HB2	1.99	0.62
1:B:315:TYR:HB2	1:B:328:ARG:HG3	1.82	0.61
1:B:442:ILE:HD12	5:B:2080:HOH:O	2.00	0.60
1:D:351:ALA:HB2	1:D:379:MET:HE3	1.83	0.59
1:C:328:ARG:HG2	1:C:328:ARG:NH1	2.17	0.59
1:B:280:LEU:HD11	1:B:284:GLY:HA3	1.85	0.59
1:D:312:ASN:ND2	1:D:328:ARG:HE	2.01	0.59
1:D:265:PHE:CE2	1:D:293:VAL:HG21	2.40	0.57
1:B:228:LYS:HE3	5:B:2022:HOH:O	2.05	0.56
1:A:265:PHE:CE2	1:A:293:VAL:HG21	2.40	0.56
1:C:189:VAL:HG22	1:C:211:ILE:HG23	1.87	0.56
1:C:428:PHE:CE1	1:C:430:LYS:HE2	2.41	0.56
1:C:351:ALA:HB2	1:C:379:MET:HE2	1.86	0.56
1:A:266:ASN:O	1:A:267:GLU:HB2	2.06	0.55
1:B:379:MET:HE3	1:B:435:LEU:HB3	1.87	0.55
1:A:466:ASN:ND2	1:A:467:LEU:H	2.05	0.55
1:A:354:VAL:HG23	1:A:377:PHE:CE1	2.42	0.54
1:C:435:LEU:HD12	1:C:456:GLN:O	2.06	0.54
1:B:268:ARG:NH1	1:B:444:ASN:O	2.37	0.54
1:C:265:PHE:CE2	1:C:293:VAL:HG21	2.42	0.54
1:C:317:PRO:O	1:C:323:ASP:HA	2.09	0.53
1:B:184:PHE:O	1:B:208:ALA:HA	2.08	0.53
1:C:377:PHE:O	1:C:434:THR:HA	2.09	0.53
1:C:224:GLU:OE2	1:C:228:LYS:HE2	2.09	0.53
1:C:233:THR:HG22	5:C:2040:HOH:O	2.09	0.53
1:A:184:PHE:O	1:A:208:ALA:HA	2.09	0.52
1:B:136:SER:OG	1:B:137:VAL:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:PRO:HD2	5:D:2061:HOH:O	2.08	0.52
1:C:451:ILE:HB	1:C:468:LEU:HB2	1.91	0.52
1:B:146:SER:HB2	1:B:446:ARG:NH1	2.25	0.52
1:D:136:SER:O	1:D:140:GLU:HG2	2.10	0.52
1:B:379:MET:HE3	1:B:435:LEU:CB	2.40	0.52
1:C:266:ASN:O	1:C:267:GLU:HB2	2.09	0.52
1:C:151:PHE:CE1	1:C:216:ALA:HB3	2.45	0.51
1:D:459:GLN:N	1:D:459:GLN:OE1	2.42	0.51
1:A:188:ILE:HD11	1:A:209:ARG:HH21	1.76	0.51
1:B:471:LYS:C	1:B:473:PRO:HD3	2.36	0.51
1:D:295:LEU:HA	1:D:389:ALA:O	2.11	0.50
1:A:314:TRP:O	1:A:325:SER:HA	2.12	0.50
1:D:184:PHE:O	1:D:208:ALA:HA	2.11	0.50
1:B:428:PHE:HD1	1:B:429:ALA:N	2.10	0.50
1:A:144:GLU:HA	1:A:144:GLU:OE1	2.12	0.50
1:B:469:ASP:OD2	1:B:471:LYS:HG2	2.11	0.50
1:C:265:PHE:HE2	1:C:293:VAL:HG21	1.77	0.50
1:D:138:PHE:CD1	1:D:138:PHE:C	2.90	0.49
1:B:267:GLU:CD	3:B:1002:845:H35	2.37	0.49
1:B:189:VAL:HG22	1:B:211:ILE:HG23	1.95	0.49
1:C:295:LEU:N	1:C:295:LEU:HD23	2.28	0.49
1:B:282:PRO:O	1:B:283:SER:HB2	2.12	0.49
1:C:423:PHE:CD1	1:C:466:ASN:ND2	2.82	0.48
1:A:267:GLU:OE2	3:A:1002:845:H35	2.14	0.48
1:A:466:ASN:HD22	1:A:467:LEU:H	1.61	0.48
1:D:265:PHE:HE2	1:D:293:VAL:HG21	1.75	0.47
1:B:301:GLU:O	1:B:301:GLU:HG2	2.14	0.47
1:B:364:LYS:O	1:B:365:GLU:C	2.58	0.47
1:B:142:THR:HG21	1:B:147:ALA:HB2	1.95	0.47
1:D:299:THR:HG23	1:D:299:THR:O	2.14	0.47
1:A:264:LEU:HD23	1:A:293:VAL:CG2	2.45	0.47
1:B:267:GLU:OE2	3:B:1002:845:H35	2.15	0.47
1:A:345:ASP:OD1	1:A:347:ARG:HG2	2.14	0.47
1:D:190:LEU:HD13	1:D:248:LEU:HD11	1.97	0.47
1:B:266:ASN:O	1:B:267:GLU:HB2	2.15	0.47
1:C:344:PHE:CD1	1:C:348:ILE:HD11	2.49	0.47
1:D:453:ILE:O	1:D:465:SER:HA	2.15	0.47
1:A:264:LEU:HD23	1:A:293:VAL:HG22	1.95	0.46
1:B:231:ASN:HA	5:B:2023:HOH:O	2.16	0.46
1:A:282:PRO:O	1:A:283:SER:HB2	2.15	0.46
1:C:428:PHE:HE1	1:C:430:LYS:CE	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:LEU:HD11	1:C:417:TYR:CD2	2.49	0.46
1:B:188:ILE:HD11	1:B:209:ARG:HH21	1.79	0.46
1:B:263:MET:O	1:B:264:LEU:HB3	2.14	0.46
1:B:268:ARG:HD3	1:B:447:GLN:HA	1.98	0.46
1:D:328:ARG:O	1:D:332:VAL:HG23	2.16	0.46
1:B:265:PHE:CE2	1:B:293:VAL:HG21	2.51	0.46
1:A:136:SER:O	1:A:140:GLU:HB2	2.16	0.46
1:C:264:LEU:HD23	1:C:293:VAL:CG2	2.45	0.46
1:B:147:ALA:O	1:B:151:PHE:HD2	2.00	0.45
1:C:295:LEU:HA	1:C:389:ALA:O	2.16	0.45
1:A:257:SER:C	1:A:259:PRO:HD3	2.41	0.45
1:C:347:ARG:HE	1:C:347:ARG:HB3	1.33	0.45
1:B:264:LEU:HD23	1:B:293:VAL:CG2	2.46	0.45
1:D:266:ASN:O	1:D:267:GLU:CB	2.63	0.45
1:A:137:VAL:HG23	5:A:2001:HOH:O	2.16	0.45
1:B:469:ASP:CG	1:B:471:LYS:HG2	2.42	0.45
1:B:469:ASP:OD1	1:B:471:LYS:HE2	2.16	0.45
1:C:263:MET:O	1:C:264:LEU:HB3	2.17	0.45
1:D:316:GLN:HB2	5:D:2061:HOH:O	2.17	0.45
1:B:144:GLU:C	1:B:146:SER:H	2.25	0.44
1:C:184:PHE:O	1:C:208:ALA:HA	2.17	0.44
1:B:307:GLN:OE1	1:B:310:LYS:HE2	2.17	0.44
1:C:379:MET:HE2	1:C:379:MET:CA	2.43	0.44
1:B:256:ILE:HA	1:B:287:PHE:O	2.17	0.44
1:D:201:PHE:O	1:D:205:GLN:HG3	2.18	0.44
1:B:327:LEU:HD11	1:D:226:LEU:HG	2.00	0.44
1:C:151:PHE:O	1:C:217:SER:HB2	2.18	0.44
1:B:430:LYS:O	1:B:431:ALA:C	2.60	0.43
1:B:244:GLU:C	5:B:2028:HOH:O	2.61	0.43
1:B:299:THR:O	1:B:348:ILE:HB	2.18	0.43
1:B:257:SER:C	1:B:259:PRO:HD3	2.43	0.43
1:D:256:ILE:HA	1:D:287:PHE:O	2.18	0.43
1:D:270:LEU:HB2	5:D:2043:HOH:O	2.19	0.43
1:B:428:PHE:CD1	1:B:429:ALA:N	2.87	0.43
1:C:350:MET:SD	1:C:385:VAL:HG22	2.59	0.43
1:A:259:PRO:HD2	1:A:260:MET:SD	2.59	0.43
1:A:364:LYS:O	1:A:365:GLU:C	2.62	0.43
1:C:294:HIS:O	1:C:390:PHE:HA	2.18	0.43
1:C:377:PHE:HB3	1:C:379:MET:HE3	2.01	0.43
1:B:144:GLU:C	1:B:146:SER:N	2.73	0.43
1:C:256:ILE:HA	1:C:287:PHE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LYS:HA	2:B:1001:SAH:N1	2.34	0.43
1:C:328:ARG:NH1	1:C:328:ARG:CG	2.82	0.42
1:B:423:PHE:HA	1:B:466:ASN:OD1	2.19	0.42
1:D:344:PHE:CD1	1:D:344:PHE:C	2.97	0.42
1:D:312:ASN:HD21	1:D:328:ARG:NH2	2.10	0.42
1:D:471:LYS:HE2	5:D:2108:HOH:O	2.19	0.42
1:A:345:ASP:OD1	1:A:347:ARG:CG	2.68	0.42
1:B:144:GLU:O	1:B:146:SER:N	2.53	0.42
1:B:259:PRO:HD2	1:B:260:MET:SD	2.60	0.42
1:C:242:LYS:HA	2:C:1001:SAH:N1	2.35	0.42
1:D:257:SER:C	1:D:259:PRO:HD3	2.45	0.42
1:B:142:THR:CG2	1:B:147:ALA:HB2	2.50	0.42
1:C:370:ARG:NE	5:C:2100:HOH:O	2.45	0.42
1:C:446:ARG:HB3	1:C:471:LYS:HE2	2.02	0.42
1:D:263:MET:O	1:D:264:LEU:HB3	2.20	0.42
1:B:189:VAL:HB	1:B:254:ILE:HG23	2.02	0.42
1:C:212:TYR:OH	1:C:249:PRO:HG2	2.20	0.42
1:D:262:TYR:O	1:D:263:MET:HB2	2.20	0.42
1:A:198:ILE:HG23	1:A:199:LEU:N	2.35	0.41
1:A:251:GLN:HB3	1:A:281:LYS:HG3	2.03	0.41
1:B:428:PHE:CD1	1:B:428:PHE:C	2.97	0.41
1:B:471:LYS:O	1:B:473:PRO:HD3	2.20	0.41
1:B:226:LEU:HD23	1:B:226:LEU:HA	1.80	0.41
1:C:188:ILE:HD11	1:C:209:ARG:HH21	1.86	0.41
1:C:345:ASP:O	1:C:348:ILE:HG12	2.21	0.41
1:D:298:PHE:HA	1:D:348:ILE:O	2.20	0.41
1:B:217:SER:HB2	5:B:2002:HOH:O	2.19	0.41
1:B:441:LEU:CD2	1:B:451:ILE:HG12	2.51	0.41
1:D:154:TYR:OH	3:D:1002:845:H232	2.21	0.41
1:A:265:PHE:HE2	1:A:293:VAL:HG21	1.81	0.41
1:B:306:GLU:HB2	5:B:2039:HOH:O	2.20	0.41
1:C:467:LEU:C	1:C:468:LEU:HD12	2.46	0.41
1:C:298:PHE:CD1	1:C:298:PHE:C	2.99	0.41
1:B:147:ALA:O	1:B:151:PHE:CD2	2.74	0.41
1:D:295:LEU:HD23	1:D:295:LEU:N	2.36	0.41
1:B:151:PHE:CE1	1:B:216:ALA:HB3	2.56	0.41
1:D:267:GLU:CD	3:D:1002:845:H35	2.45	0.41
1:D:280:LEU:HD11	1:D:284:GLY:HA3	2.03	0.41
1:A:345:ASP:CG	1:A:347:ARG:CG	2.94	0.40
1:D:264:LEU:HD23	1:D:293:VAL:CG2	2.50	0.40
1:D:347:ARG:HE	1:D:347:ARG:HB2	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:HB2	1:A:446:ARG:NH1	2.36	0.40
1:C:212:TYR:CZ	1:C:249:PRO:HG2	2.56	0.40
1:C:280:LEU:HD11	1:C:284:GLY:HA3	2.04	0.40
1:B:151:PHE:CE2	1:B:242:LYS:HE3	2.57	0.40
1:B:151:PHE:O	1:B:217:SER:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/348 (98%)	327 (96%)	14 (4%)	0	100	100
1	B	341/348 (98%)	324 (95%)	17 (5%)	0	100	100
1	C	341/348 (98%)	327 (96%)	14 (4%)	0	100	100
1	D	341/348 (98%)	327 (96%)	14 (4%)	0	100	100
All	All	1364/1392 (98%)	1305 (96%)	59 (4%)	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	298/303 (98%)	286 (96%)	12 (4%)	28	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	298/303 (98%)	287 (96%)	11 (4%)	30	51
1	C	298/303 (98%)	288 (97%)	10 (3%)	32	54
1	D	298/303 (98%)	288 (97%)	10 (3%)	32	54
All	All	1192/1212 (98%)	1149 (96%)	43 (4%)	31	52

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	GLU
1	A	149	GLN
1	A	165	GLN
1	A	189	VAL
1	A	221	GLN
1	A	258	GLU
1	A	295	LEU
1	A	316	GLN
1	A	347	ARG
1	A	362	GLU
1	A	364	LYS
1	A	425	SER
1	B	139	SER
1	B	165	GLN
1	B	189	VAL
1	B	221	GLN
1	B	258	GLU
1	B	295	LEU
1	B	301	GLU
1	B	310	LYS
1	B	347	ARG
1	B	364	LYS
1	B	466	ASN
1	C	165	GLN
1	C	189	VAL
1	C	221	GLN
1	C	258	GLU
1	C	295	LEU
1	C	347	ARG
1	C	362	GLU
1	C	364	LYS
1	C	384	LEU
1	C	467	LEU

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Mol	Chain	Res	Type
1	D	189	VAL
1	D	221	GLN
1	D	258	GLU
1	D	295	LEU
1	D	362	GLU
1	D	364	LYS
1	D	379	MET
1	D	424	GLN
1	D	425	SER
1	D	471	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	160	GLN
1	A	161	GLN
1	A	174	GLN
1	A	466	ASN
1	A	472	ASN
1	B	160	GLN
1	B	161	GLN
1	B	174	GLN
1	B	221	GLN
1	B	472	ASN
1	C	160	GLN
1	C	161	GLN
1	C	174	GLN
1	C	316	GLN
1	C	369	HIS
1	C	447	GLN
1	C	456	GLN
1	D	161	GLN
1	D	174	GLN
1	D	179	GLN
1	D	312	ASN
1	D	338	GLN
1	D	369	HIS
1	D	381	HIS
1	D	424	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SAH	D	1001	-	27,28,28	1.17	1 (3%)	36,40,40	1.82	7 (19%)
2	SAH	C	1001	-	27,28,28	1.24	2 (7%)	36,40,40	1.86	7 (19%)
2	SAH	B	1001	-	27,28,28	1.21	2 (7%)	36,40,40	1.85	7 (19%)
3	845	C	1002	-	36,40,40	2.76	14 (38%)	49,59,59	2.99	12 (24%)
2	SAH	A	1001	-	27,28,28	1.17	3 (11%)	36,40,40	1.88	7 (19%)
3	845	D	1002	-	36,40,40	2.87	13 (36%)	49,59,59	2.85	10 (20%)
3	845	B	1002	-	36,40,40	2.76	13 (36%)	49,59,59	2.90	11 (22%)
3	845	A	1002	-	36,40,40	2.84	16 (44%)	49,59,59	2.77	7 (14%)

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	D	1001	-	-	0/15/31/31	0/3/3/3
2	SAH	C	1001	-	-	0/15/31/31	0/3/3/3
2	SAH	B	1001	-	-	0/15/31/31	0/3/3/3
3	845	C	1002	-	-	5/23/27/27	0/5/5/5
2	SAH	A	1001	-	-	0/15/31/31	0/3/3/3
3	845	D	1002	-	-	4/23/27/27	0/5/5/5
3	845	B	1002	-	-	5/23/27/27	0/5/5/5
3	845	A	1002	-	-	5/23/27/27	0/5/5/5

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1002	845	C6-N1	-11.77	1.27	1.42
3	A	1002	845	C6-N1	-10.67	1.28	1.42
3	C	1002	845	C6-N1	-9.87	1.29	1.42
3	B	1002	845	C6-N1	-9.74	1.29	1.42
3	C	1002	845	C26-N25	6.63	1.39	1.29
3	B	1002	845	C26-N25	6.48	1.39	1.29
3	D	1002	845	C26-N25	5.71	1.38	1.29
3	A	1002	845	C26-N25	5.64	1.38	1.29
3	C	1002	845	C28-C33	5.11	1.47	1.41
3	B	1002	845	C28-C33	5.04	1.47	1.41
3	D	1002	845	C28-C33	4.20	1.46	1.41
3	A	1002	845	C28-C33	3.99	1.46	1.41
3	D	1002	845	C28-C26	-3.93	1.40	1.47
2	C	1001	SAH	C2-N3	3.85	1.40	1.33
3	A	1002	845	C33-C32	3.85	1.45	1.41
3	A	1002	845	C29-C28	3.84	1.45	1.39
3	C	1002	845	C33-C32	3.62	1.45	1.41
3	C	1002	845	C29-C28	3.44	1.45	1.39
3	B	1002	845	C28-C26	-3.42	1.41	1.47
3	A	1002	845	C28-C26	-3.36	1.41	1.47
2	D	1001	SAH	C2-N3	3.35	1.39	1.33
3	A	1002	845	C31-C32	3.30	1.45	1.39
2	B	1001	SAH	C2-N3	3.26	1.39	1.33
3	D	1002	845	C31-C32	3.24	1.45	1.39
3	D	1002	845	C29-C28	3.23	1.44	1.39
3	A	1002	845	C11-C6	3.19	1.45	1.39
2	A	1001	SAH	C5-N7	-3.12	1.33	1.39
3	D	1002	845	N5-N1	-3.06	1.34	1.39
3	B	1002	845	C30-C29	2.99	1.44	1.38
3	B	1002	845	C4-N5	2.94	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	845	C33-C32	2.89	1.44	1.41
3	A	1002	845	C30-C29	2.88	1.43	1.38
3	A	1002	845	C9-C10	2.84	1.44	1.38
3	B	1002	845	C29-C28	2.78	1.44	1.39
3	C	1002	845	C9-C10	2.76	1.44	1.38
2	A	1001	SAH	C2-N3	2.71	1.38	1.33
3	C	1002	845	C28-C26	-2.65	1.42	1.47
3	B	1002	845	C11-C10	2.65	1.43	1.39
2	C	1001	SAH	C5-N7	-2.58	1.34	1.39
3	C	1002	845	C7-C6	2.55	1.44	1.39
3	C	1002	845	C35-C34	2.53	1.40	1.36
3	D	1002	845	C33-C32	2.52	1.44	1.41
3	C	1002	845	C31-C32	2.49	1.43	1.39
3	C	1002	845	C11-C6	2.48	1.43	1.39
3	A	1002	845	C35-C34	2.44	1.40	1.36
3	D	1002	845	C9-C10	2.43	1.43	1.38
3	A	1002	845	N5-N1	-2.42	1.35	1.39
3	B	1002	845	N5-N1	-2.39	1.35	1.39
3	A	1002	845	C13-N14	2.38	1.50	1.46
3	C	1002	845	C11-C10	2.38	1.43	1.39
3	A	1002	845	C7-C6	2.36	1.43	1.39
3	D	1002	845	C4-N5	2.34	1.38	1.35
3	B	1002	845	C13-C10	2.34	1.56	1.51
3	D	1002	845	C7-C6	2.33	1.43	1.39
3	B	1002	845	C31-C32	2.28	1.43	1.39
3	D	1002	845	C30-C29	2.26	1.42	1.38
3	A	1002	845	C35-N36	2.17	1.42	1.38
2	B	1001	SAH	C5-N7	-2.15	1.35	1.39
2	A	1001	SAH	OXT-C	-2.14	1.23	1.30
3	C	1002	845	C35-N36	2.14	1.41	1.38
3	C	1002	845	C30-C29	2.13	1.42	1.38
3	B	1002	845	C11-C6	2.10	1.43	1.39
3	A	1002	845	C13-C10	2.04	1.56	1.51
3	D	1002	845	C35-C34	2.02	1.39	1.36

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	845	C26-N25-N24	12.23	109.17	103.64
3	D	1002	845	C26-N25-N24	12.22	109.17	103.64
3	A	1002	845	C26-N25-N24	11.42	108.80	103.64
3	B	1002	845	C26-N25-N24	11.40	108.80	103.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	845	O27-C26-N25	-10.95	106.10	112.99
3	B	1002	845	O27-C26-N25	-10.64	106.30	112.99
3	A	1002	845	O27-C26-N25	-10.60	106.32	112.99
3	D	1002	845	O27-C26-N25	-10.41	106.44	112.99
3	C	1002	845	C32-N36-C35	-6.45	104.21	108.91
3	A	1002	845	C32-N36-C35	-6.41	104.24	108.91
3	C	1002	845	C33-C32-N36	6.38	110.73	107.09
3	B	1002	845	C32-N36-C35	-6.36	104.27	108.91
2	A	1001	SAH	C4-N9-C8	-6.20	99.22	105.74
2	B	1001	SAH	C4-N9-C8	-6.00	99.43	105.74
3	D	1002	845	C32-N36-C35	-5.99	104.54	108.91
3	B	1002	845	C33-C32-N36	5.95	110.48	107.09
2	C	1001	SAH	C4-N9-C8	-5.91	99.54	105.74
2	D	1001	SAH	C4-N9-C8	-5.79	99.66	105.74
3	D	1002	845	C33-C32-N36	5.71	110.35	107.09
3	A	1002	845	C33-C32-N36	5.58	110.27	107.09
2	C	1001	SAH	C5-C4-N9	5.23	111.51	105.81
2	B	1001	SAH	C5-C4-N9	4.98	111.24	105.81
2	A	1001	SAH	C5-C4-N9	4.89	111.14	105.81
2	D	1001	SAH	C5-C4-N9	4.84	111.09	105.81
3	B	1002	845	O27-C12-N24	4.11	108.18	104.91
3	C	1002	845	O27-C12-N24	3.92	108.03	104.91
3	B	1002	845	C6-N1-N5	3.88	124.74	120.54
2	A	1001	SAH	N3-C4-N9	-3.74	120.81	127.17
2	C	1001	SAH	N3-C4-N9	-3.70	120.88	127.17
2	B	1001	SAH	N3-C4-N9	-3.58	121.07	127.17
2	D	1001	SAH	N3-C4-N9	-3.58	121.08	127.17
3	D	1002	845	O27-C26-C28	3.47	125.87	118.68
3	A	1002	845	O27-C12-N24	3.16	107.42	104.91
3	D	1002	845	O27-C12-N24	3.09	107.37	104.91
3	C	1002	845	C15-C4-N5	2.95	125.23	121.13
2	A	1001	SAH	N3-C2-N1	-2.93	124.15	128.58
2	B	1001	SAH	N3-C2-N1	-2.92	124.16	128.58
3	C	1002	845	O27-C26-C28	2.90	124.69	118.68
3	D	1002	845	C6-N1-N5	2.88	123.66	120.54
3	A	1002	845	O27-C26-C28	2.85	124.58	118.68
3	B	1002	845	C15-C4-N5	2.85	125.09	121.13
2	D	1001	SAH	N3-C2-N1	-2.84	124.28	128.58
2	D	1001	SAH	O2'-C2'-C3'	2.84	120.92	111.82
2	C	1001	SAH	OXT-C-O	2.81	130.45	124.08
2	C	1001	SAH	N3-C2-N1	-2.73	124.46	128.58
3	B	1002	845	O27-C26-C28	2.71	124.29	118.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	845	C33-C28-C26	2.66	125.75	122.33
3	C	1002	845	C15-C4-C3	-2.57	126.07	130.12
2	A	1001	SAH	O2'-C2'-C3'	2.49	119.80	111.82
3	D	1002	845	C15-C4-N5	2.45	124.54	121.13
2	D	1001	SAH	OXT-C-O	2.43	129.60	124.08
2	C	1001	SAH	C4-C5-N7	-2.41	107.82	110.58
2	A	1001	SAH	OXT-C-O	2.38	129.48	124.08
2	B	1001	SAH	OXT-C-O	2.30	129.30	124.08
2	C	1001	SAH	O2'-C2'-C3'	2.29	119.14	111.82
3	D	1002	845	C33-C28-C26	2.27	125.25	122.33
3	C	1002	845	C13-N14-C19	2.26	125.40	122.29
3	B	1002	845	C15-C4-C3	-2.22	126.62	130.12
3	B	1002	845	C3-C2-N1	2.20	107.38	105.57
3	A	1002	845	C15-C4-N5	2.18	124.16	121.13
2	A	1001	SAH	C2-N1-C6	2.17	122.30	118.73
3	C	1002	845	C31-C32-C33	-2.15	120.95	122.66
3	C	1002	845	C29-C28-C33	-2.14	116.08	119.55
2	B	1001	SAH	O2'-C2'-C3'	2.13	118.64	111.82
2	B	1001	SAH	C4-C5-N7	-2.08	108.20	110.58
3	B	1002	845	C29-C28-C33	-2.07	116.19	119.55
3	D	1002	845	C31-C32-C33	-2.07	121.02	122.66
2	D	1001	SAH	C4-C5-N7	-2.05	108.24	110.58

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	845	C7-C6-N1-N5
3	A	1002	845	C11-C6-N1-N5
3	A	1002	845	O21-C19-C20-C23
3	B	1002	845	C7-C6-N1-N5
3	B	1002	845	C11-C6-N1-N5
3	C	1002	845	C7-C6-N1-N5
3	C	1002	845	C11-C6-N1-N5
3	D	1002	845	C7-C6-N1-N5
3	D	1002	845	C11-C6-N1-N5
3	A	1002	845	C7-C6-N1-C2
3	C	1002	845	C7-C6-N1-C2
3	A	1002	845	C11-C6-N1-C2
3	B	1002	845	C7-C6-N1-C2
3	B	1002	845	C11-C6-N1-C2
3	C	1002	845	C11-C6-N1-C2

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Mol	Chain	Res	Type	Atoms
3	D	1002	845	C7-C6-N1-C2
3	D	1002	845	C11-C6-N1-C2
3	C	1002	845	C10-C13-N14-C19
3	B	1002	845	N25-C26-C28-C29

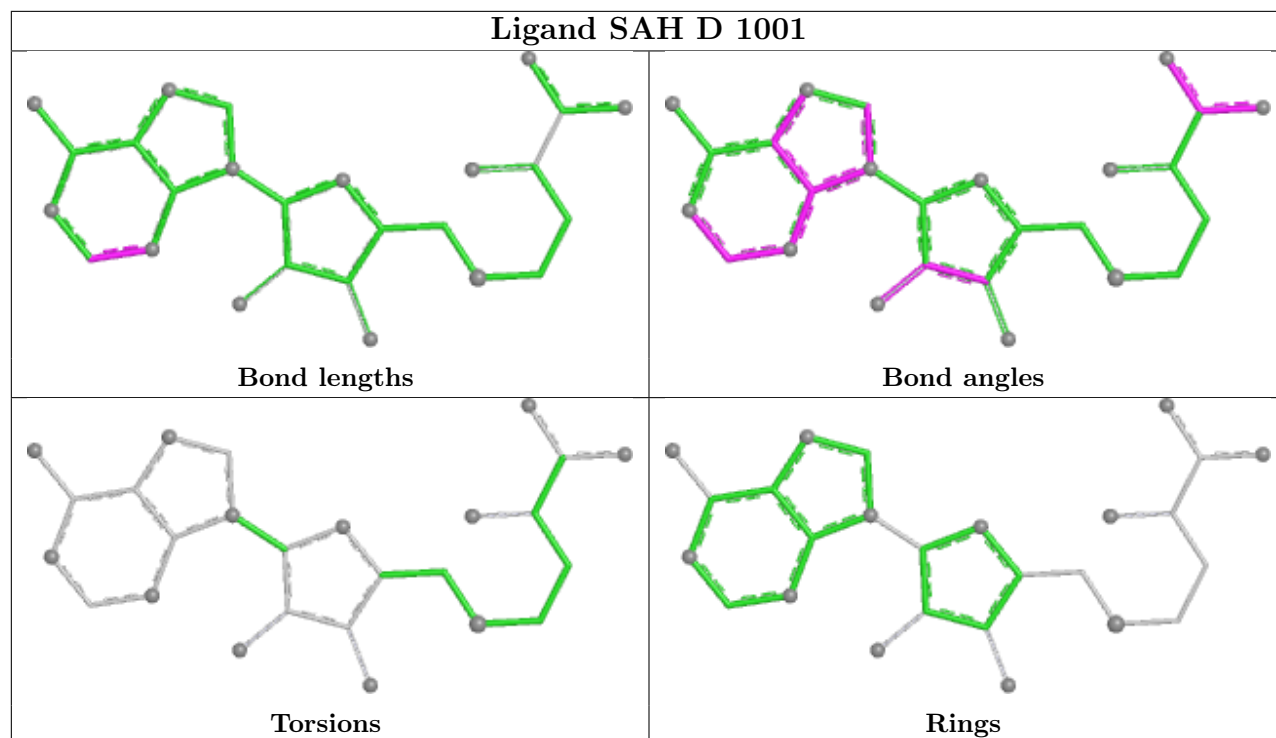
There are no ring outliers.

5 monomers are involved in 7 short contacts:

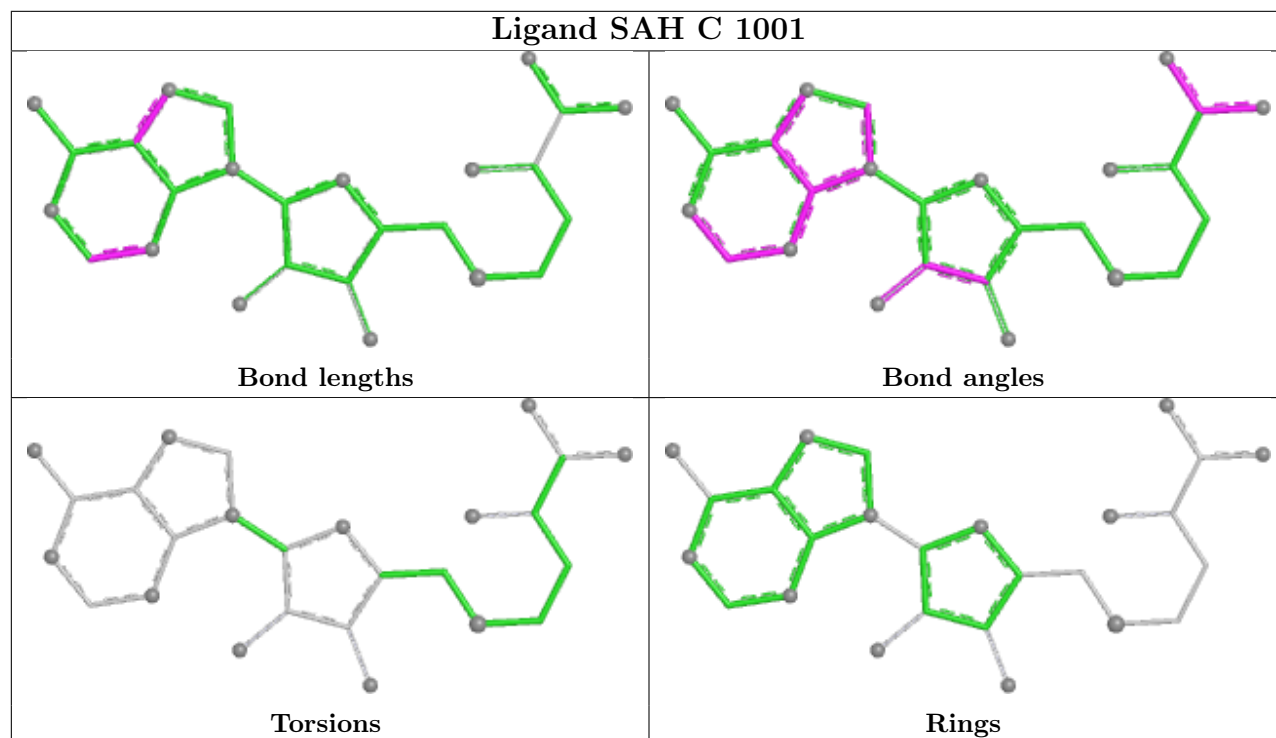
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	SAH	1	0
2	B	1001	SAH	1	0
3	D	1002	845	2	0
3	B	1002	845	2	0
3	A	1002	845	1	0

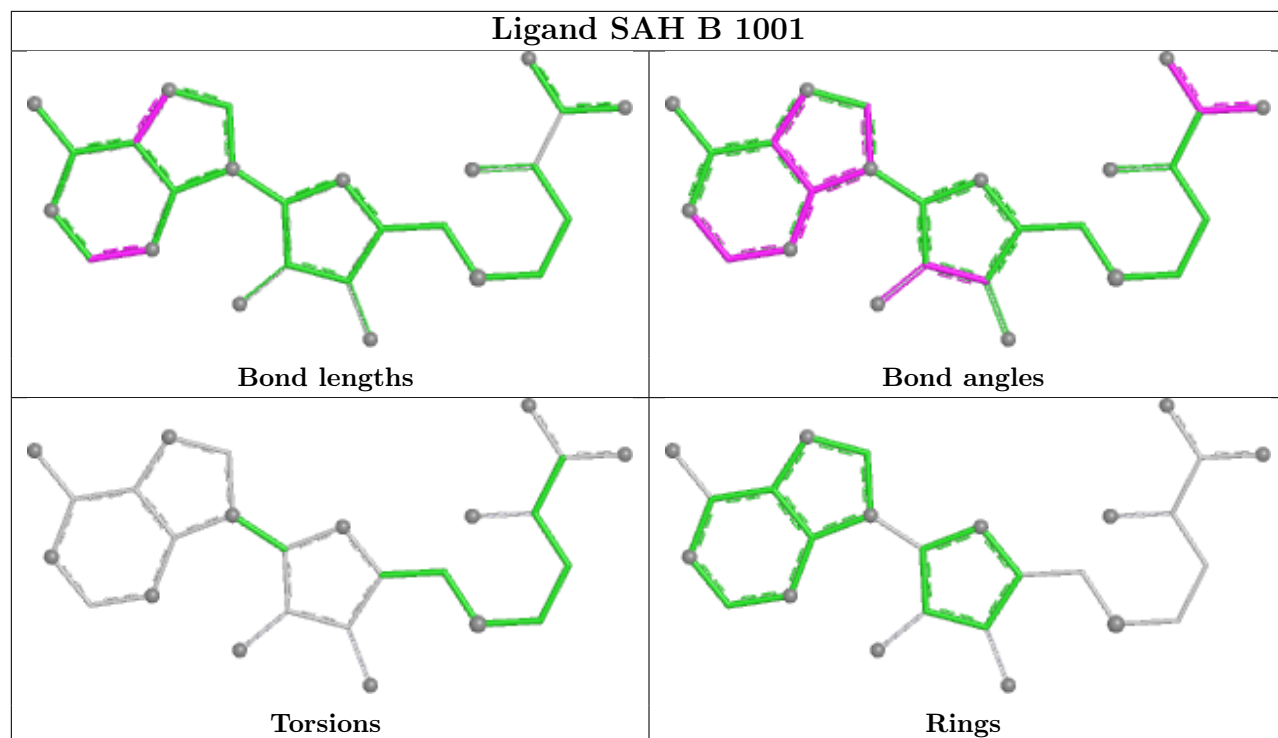
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 D 1001

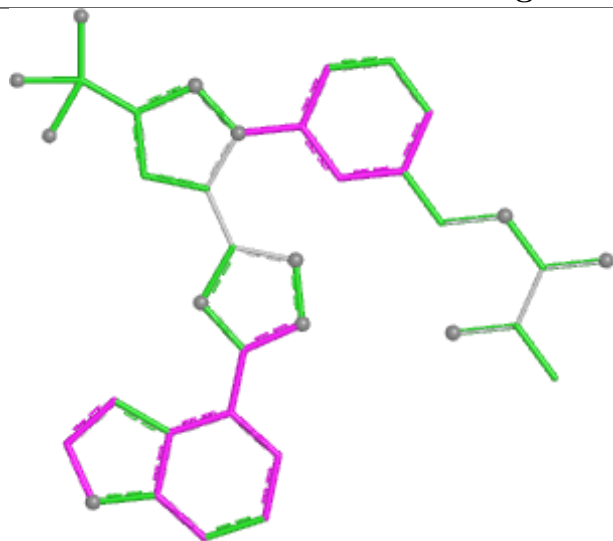


Ligand SAH C 1001

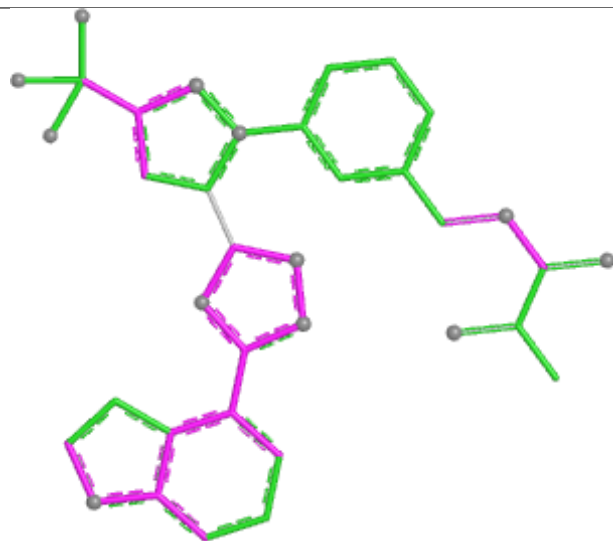




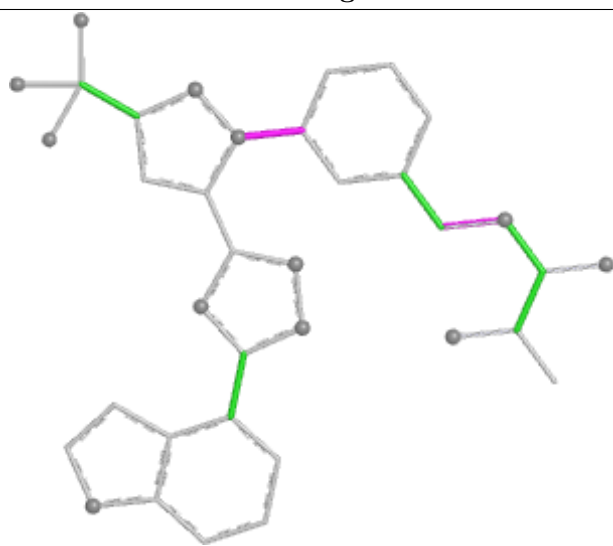
Ligand 845 C 1002



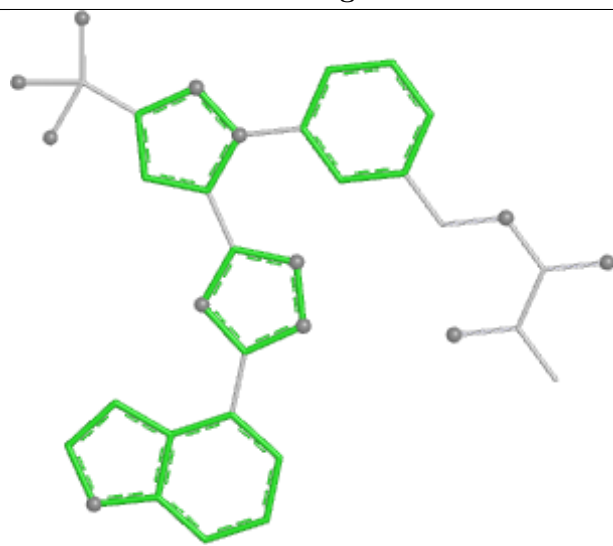
Bond lengths



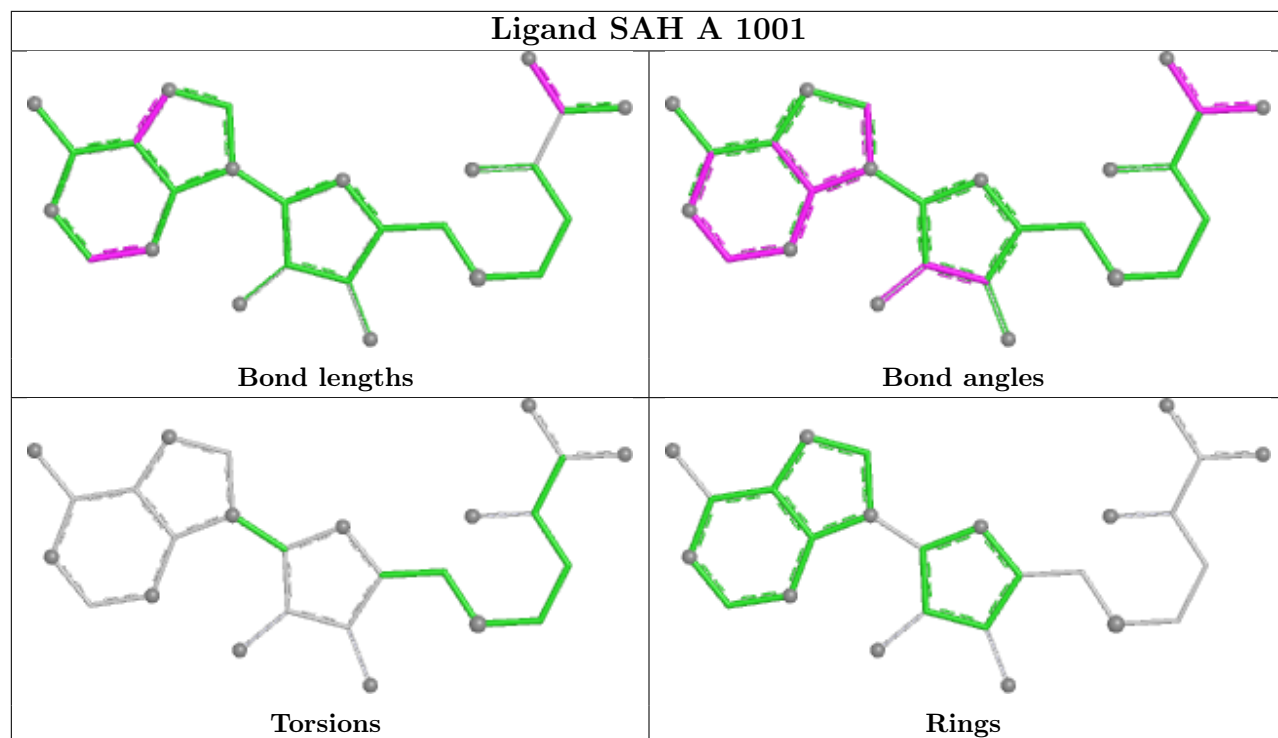
Bond angles



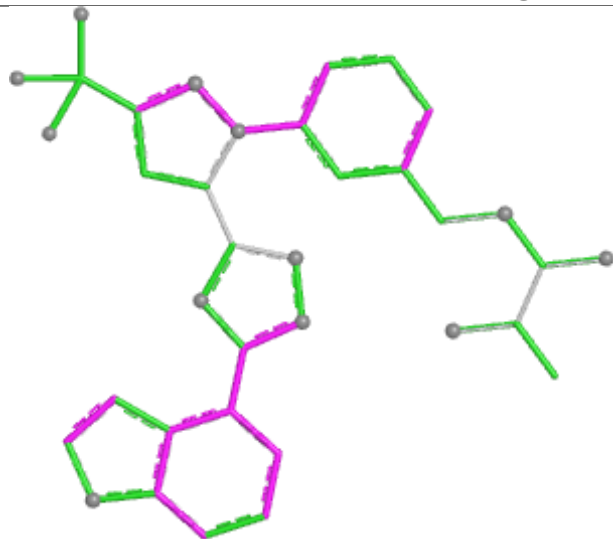
Torsions



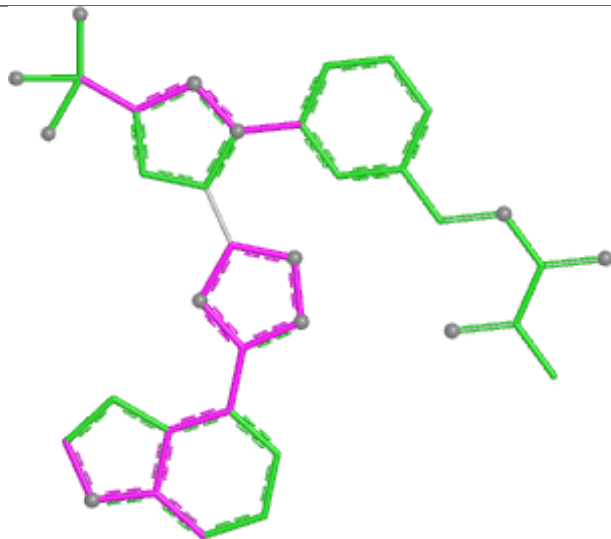
Rings



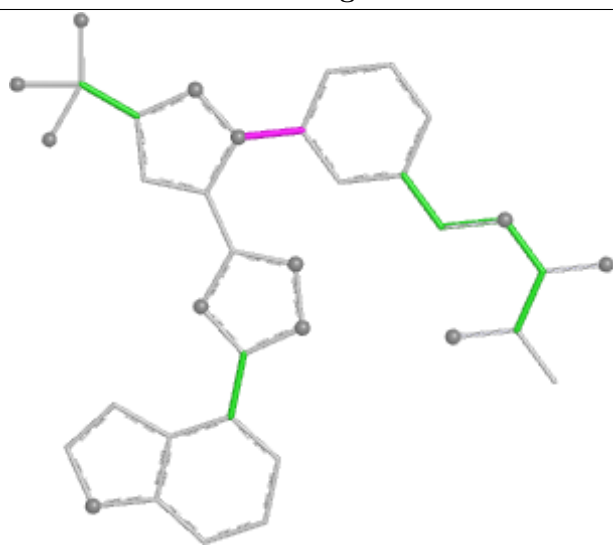
Ligand 845 D 1002



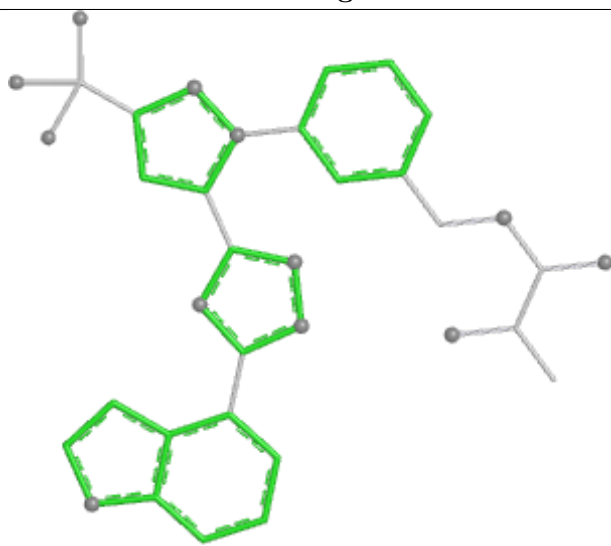
Bond lengths



Bond angles

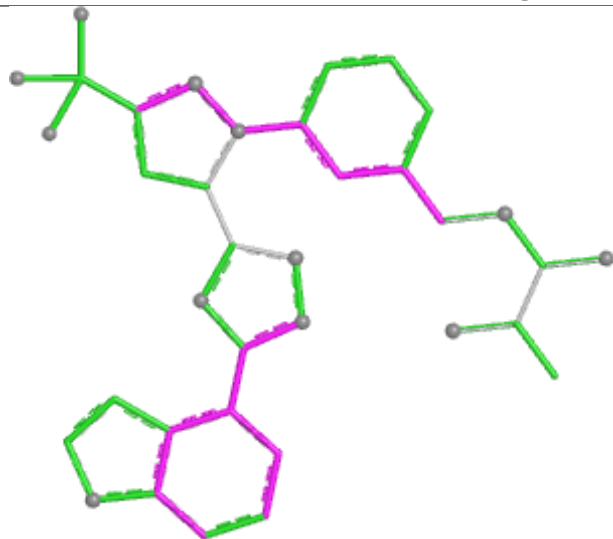


Torsions

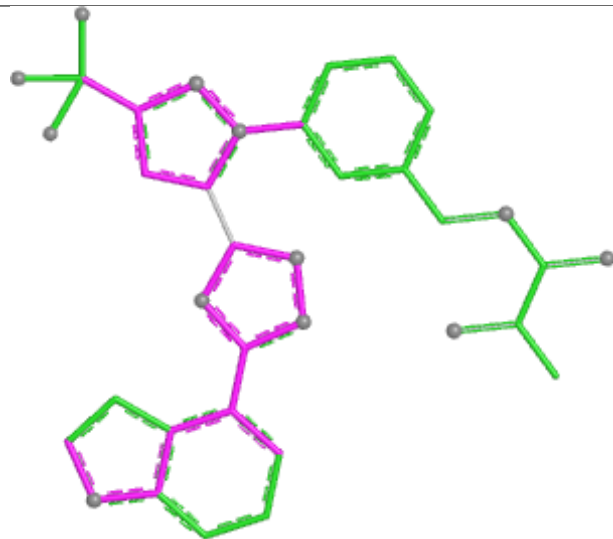


Rings

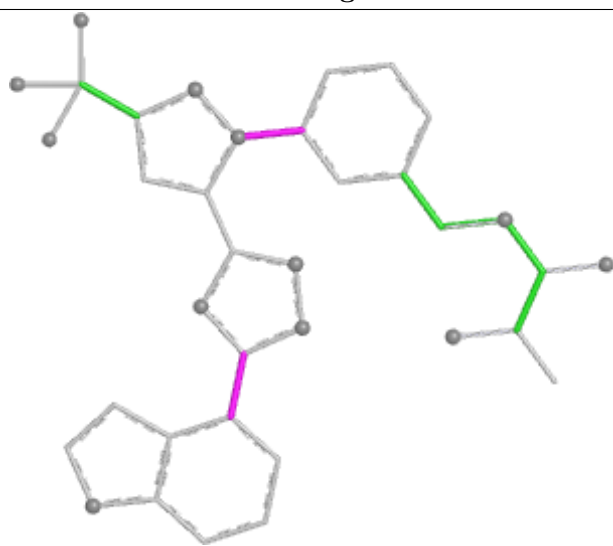
Ligand 845 B 1002



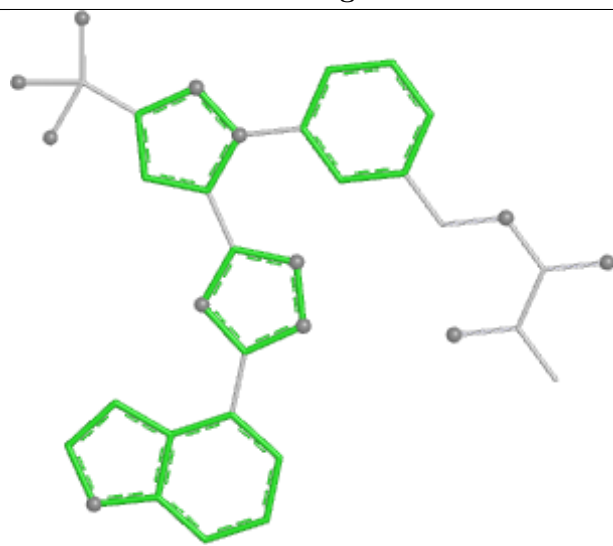
Bond lengths



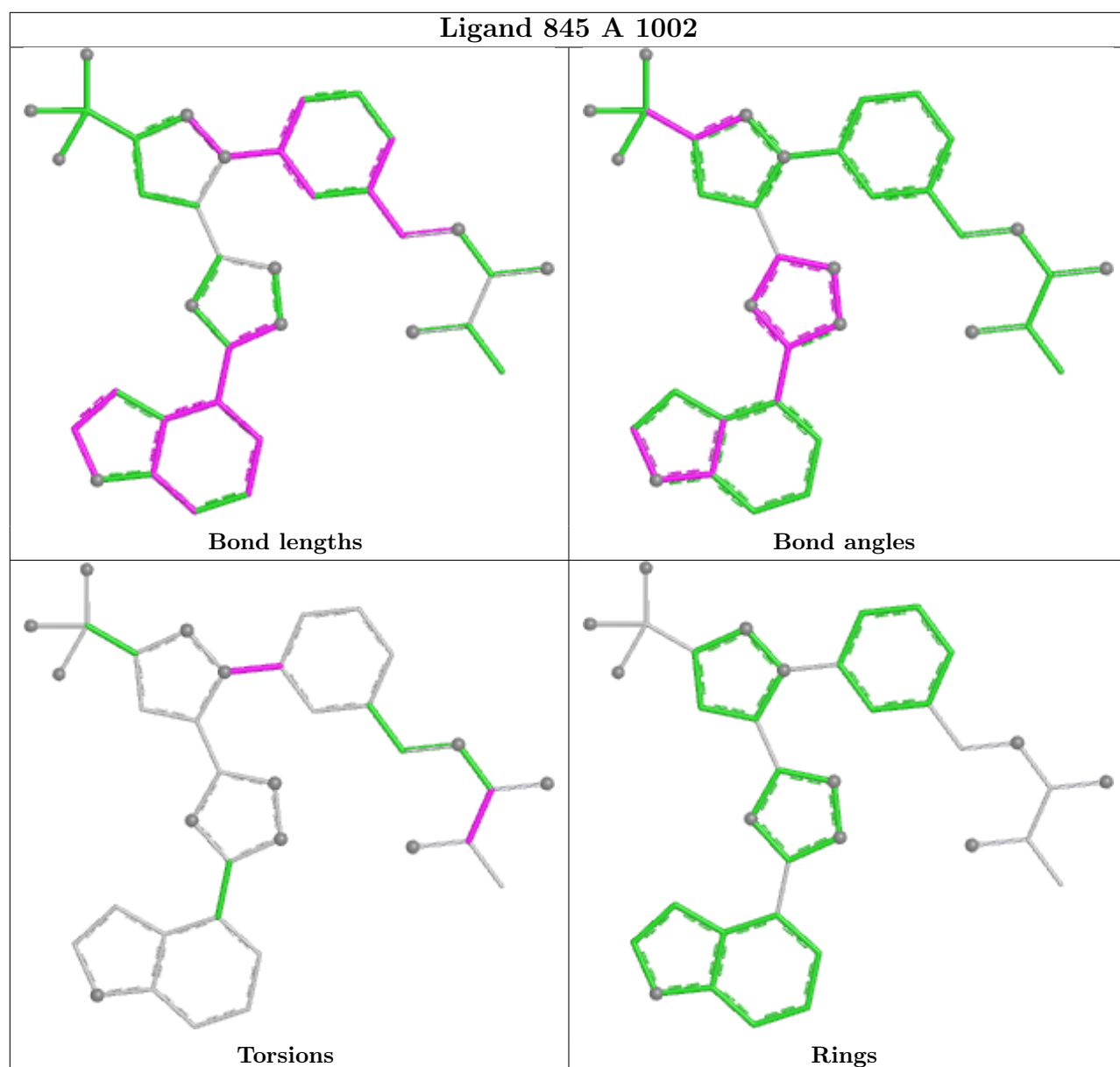
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	343/348 (98%)	-0.23	4 (1%) 76 73	10, 25, 40, 49	0
1	B	343/348 (98%)	-0.20	4 (1%) 76 73	17, 28, 42, 60	0
1	C	343/348 (98%)	-0.30	4 (1%) 76 73	14, 26, 38, 47	0
1	D	343/348 (98%)	-0.36	2 (0%) 85 83	13, 26, 38, 46	0
All	All	1372/1392 (98%)	-0.27	14 (1%) 79 76	10, 26, 40, 60	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	478	THR	3.9
1	B	144	GLU	3.1
1	A	478	THR	3.1
1	C	144	GLU	2.9
1	A	249	PRO	2.8
1	B	148	VAL	2.5
1	C	472	ASN	2.3
1	A	234	ASP	2.3
1	C	315	TYR	2.2
1	A	283	SER	2.1
1	B	446	ARG	2.1
1	B	136	SER	2.1
1	C	136	SER	2.1
1	D	234	ASP	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](#)

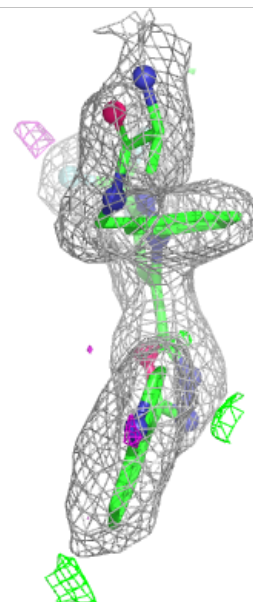
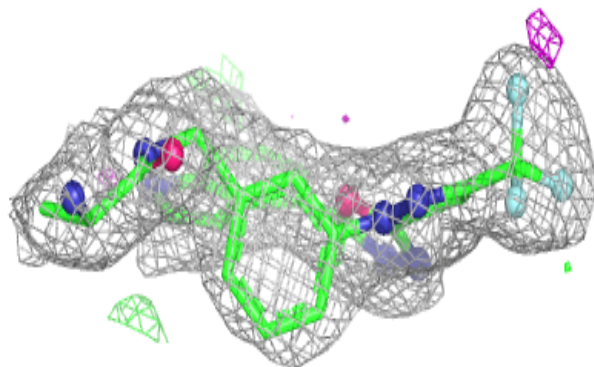
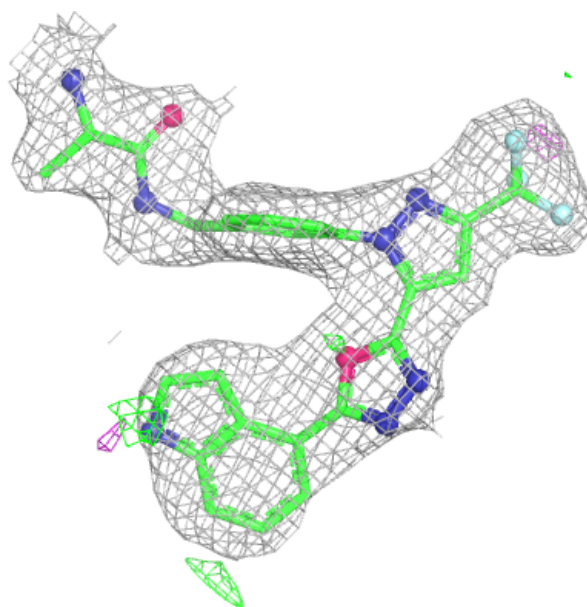
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	D	1003	1/1	0.91	0.14	44,44,44,44	0
4	CL	B	1003	1/1	0.92	0.12	53,53,53,53	0
4	CL	A	1003	1/1	0.92	0.12	47,47,47,47	0
4	CL	C	1003	1/1	0.93	0.12	47,47,47,47	0
3	845	B	1002	36/36	0.93	0.09	11,27,44,45	0
3	845	A	1002	36/36	0.94	0.08	17,26,40,41	0
2	SAH	A	1001	26/26	0.94	0.08	21,26,33,34	0
3	845	C	1002	36/36	0.94	0.09	13,27,39,40	0
3	845	D	1002	36/36	0.94	0.09	18,32,47,47	0
2	SAH	B	1001	26/26	0.96	0.07	13,26,30,32	0
2	SAH	C	1001	26/26	0.97	0.06	14,19,21,23	0
2	SAH	D	1001	26/26	0.97	0.06	16,19,21,22	0

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

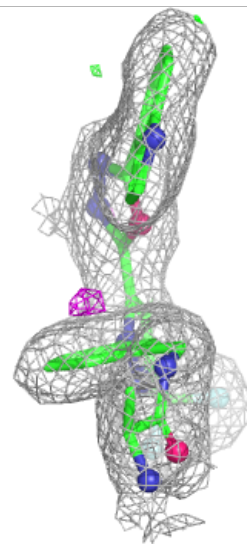
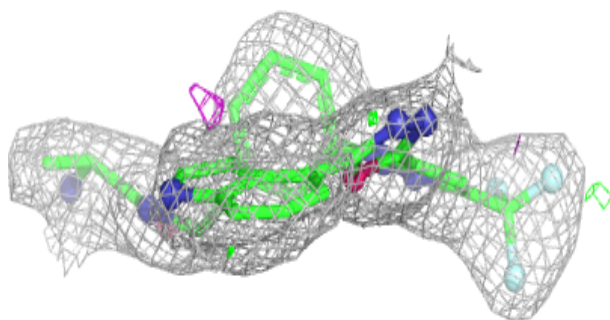
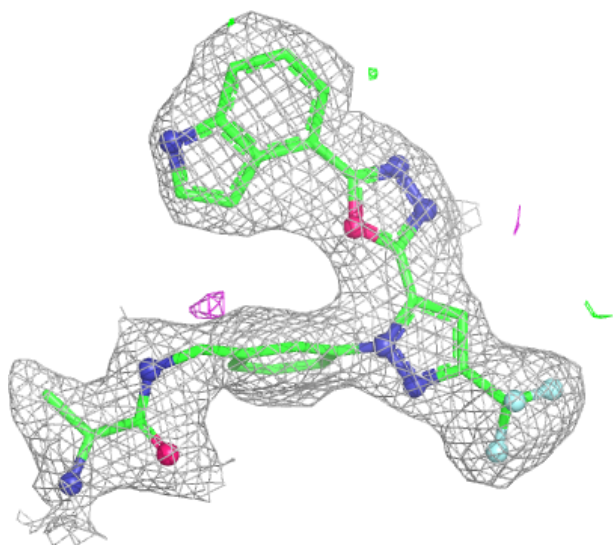
Electron density around 845 B 1002:

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



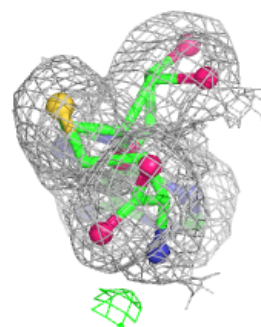
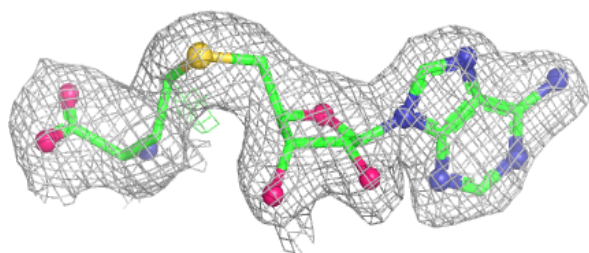
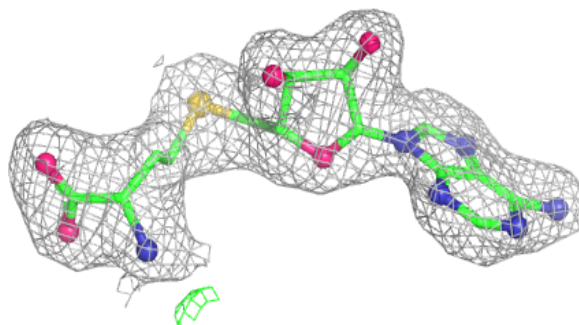
Electron density around 845 A 1002:

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



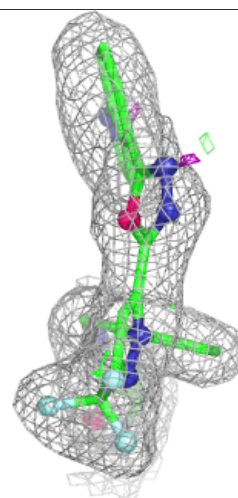
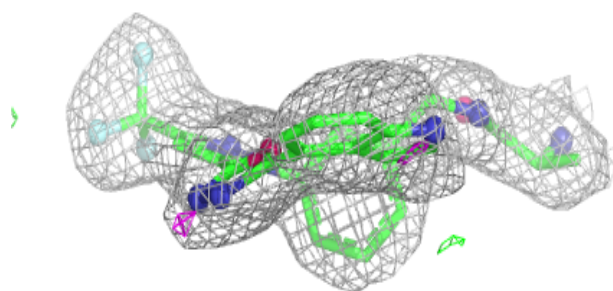
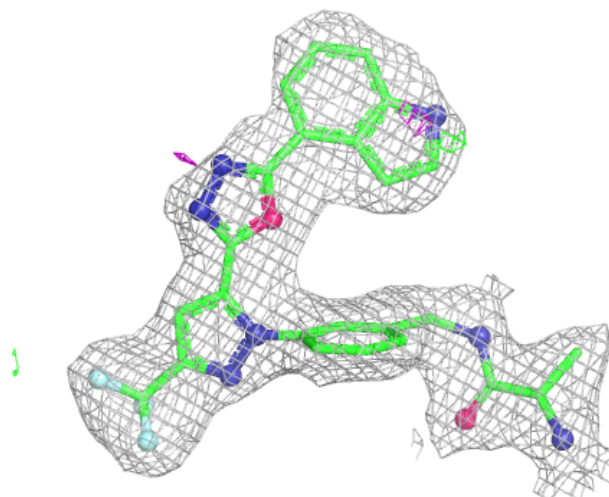
Electron density around SAH A 1001:

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



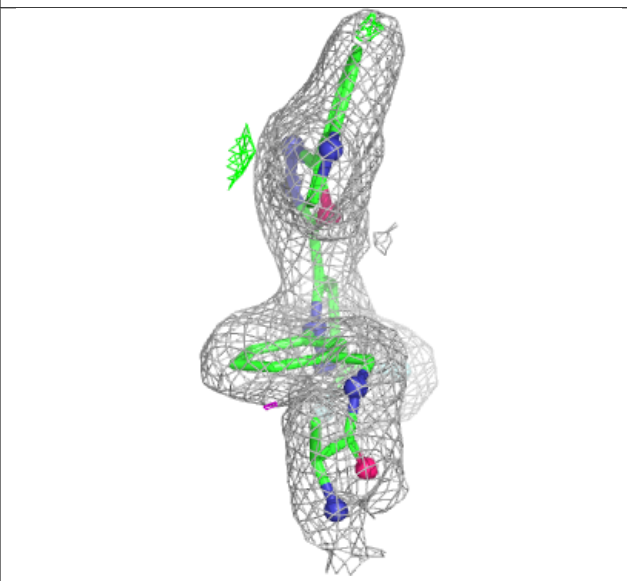
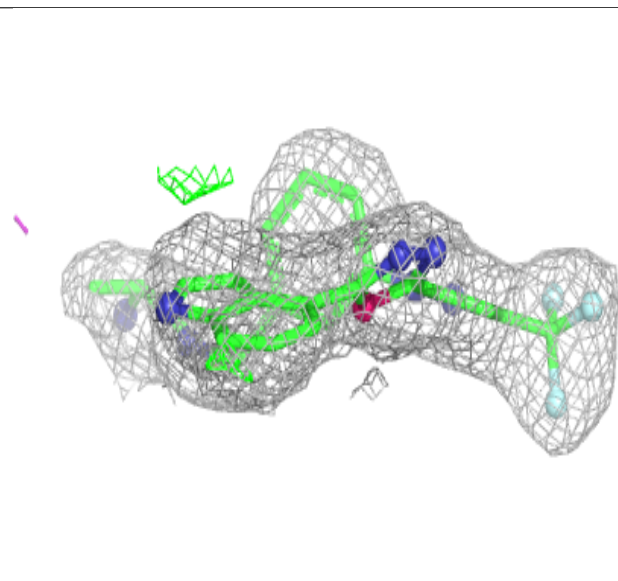
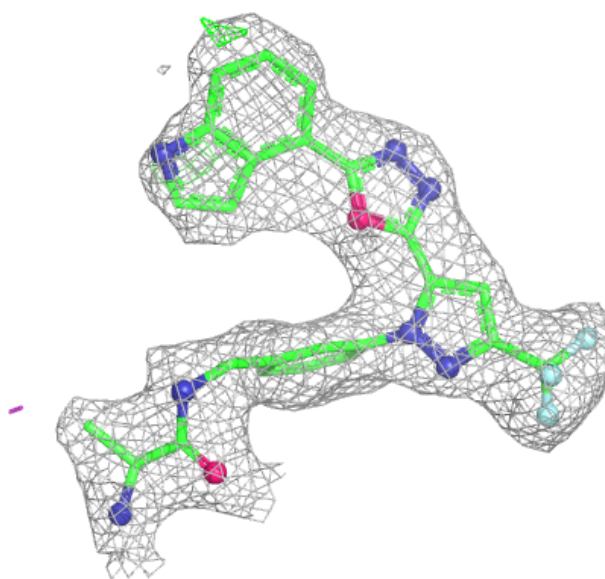
Electron density around 845 C 1002:

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



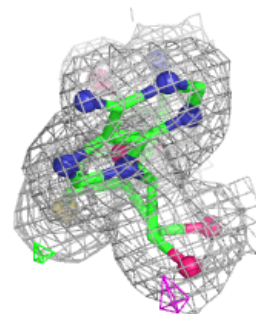
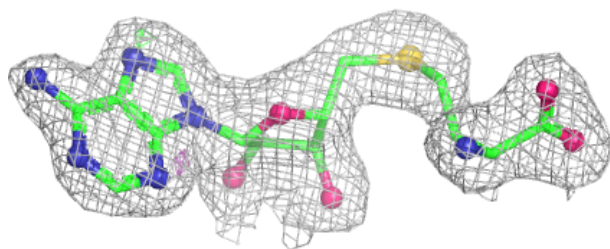
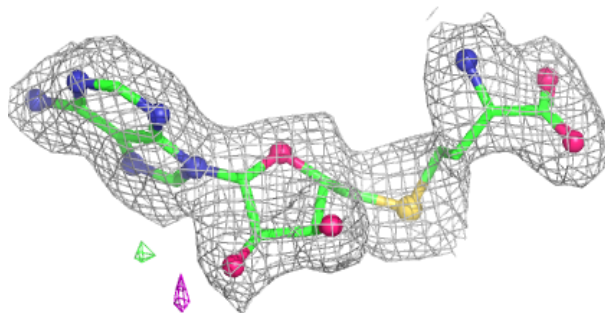
Electron density around 845 D 1002:

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

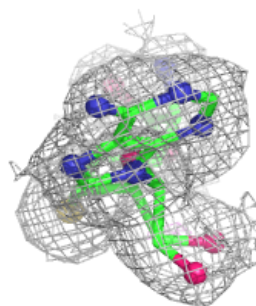
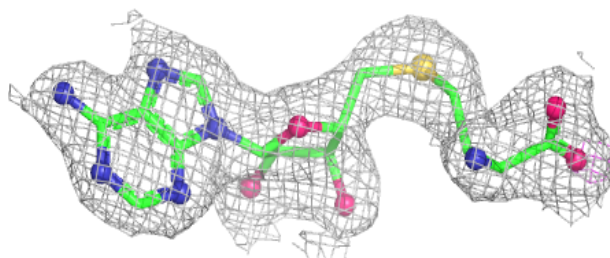
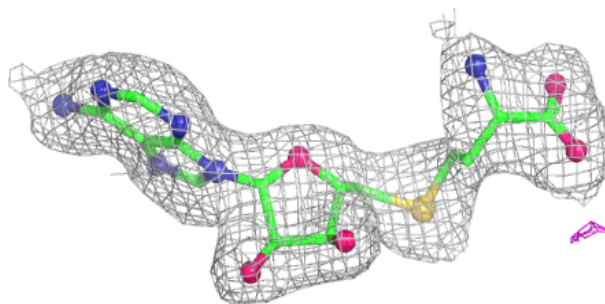


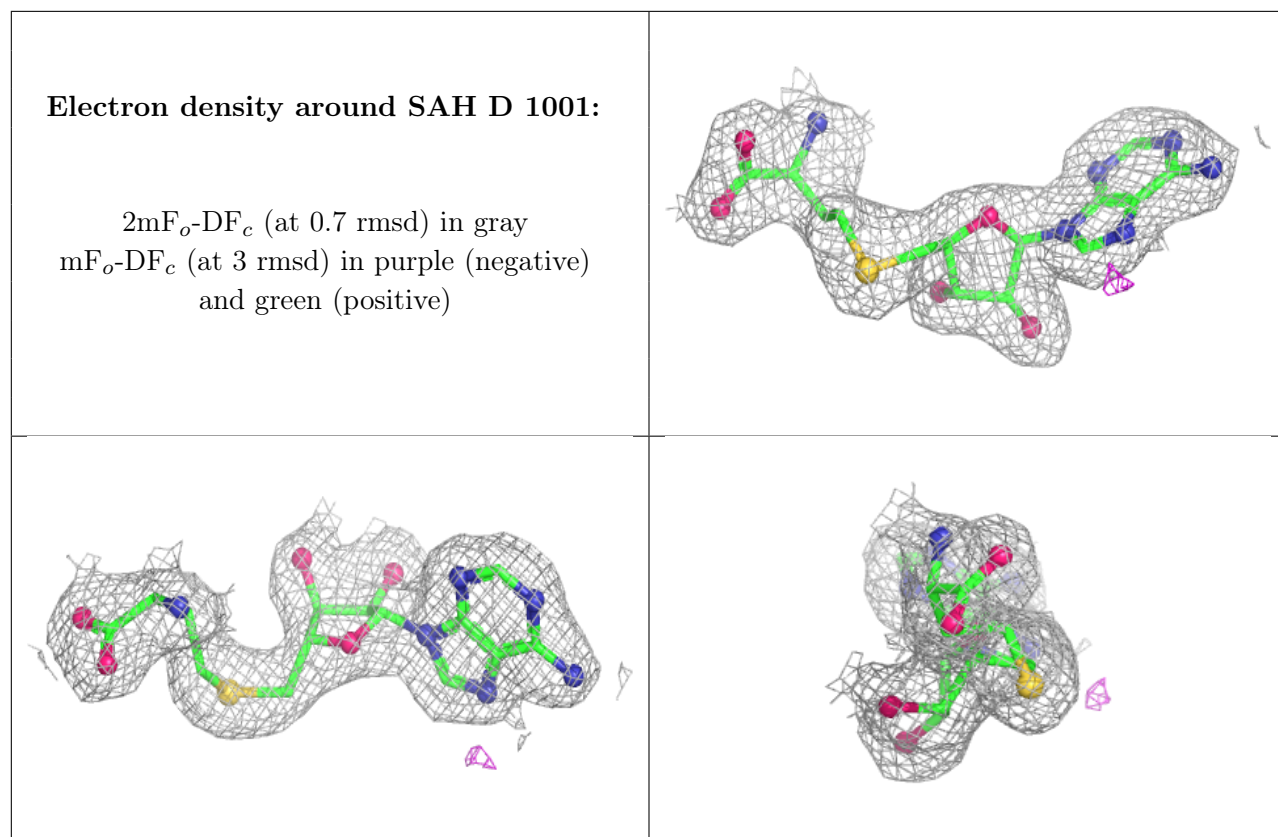
Electron density around SAH B 1001:

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

**Electron density around SAH C 1001:**

$2mF_o-DF_c$ (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.