



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 02:09 PM EDT

PDB ID : 6NT2
Title : type 1 PRMT in complex with the inhibitor GSK3368715
Authors : Concha, N.O.
Deposited on : 2019-01-28
Resolution : 2.48 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

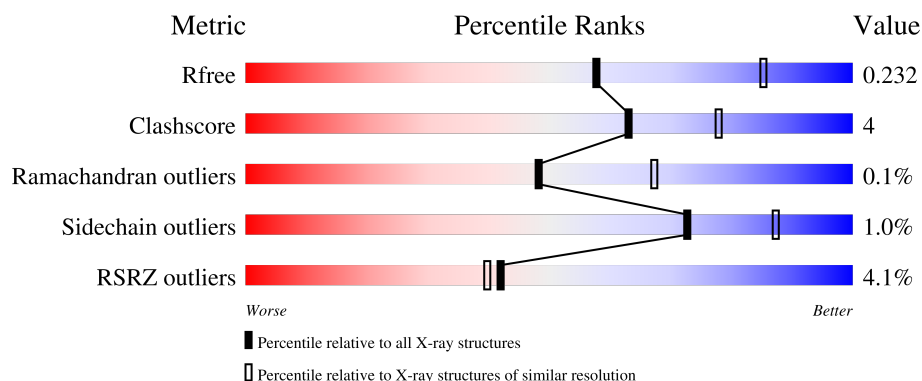
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	164625	7106 (2.50-2.46)
Clashscore	180529	7991 (2.50-2.46)
Ramachandran outliers	177936	7888 (2.50-2.46)
Sidechain outliers	177891	7890 (2.50-2.46)
RSRZ outliers	164620	7106 (2.50-2.46)

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	371	 4% 83% 6% 11%
1	B	371	 2% 84% 5% 11%
1	C	371	 4% 85% • 11%
1	D	371	 4% 85% • 11%

2 Entry composition [i](#)

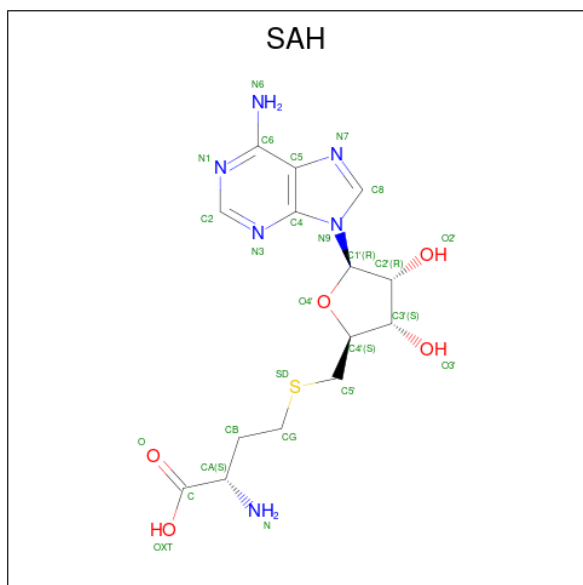
There are 6 unique types of molecules in this entry. The entry contains 12135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein arginine N-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	14	0
			2798	1802	452	523	21			
1	D	330	Total	C	N	O	S	0	10	0
			2771	1786	447	517	21			
1	B	330	Total	C	N	O	S	0	11	0
			2774	1788	448	517	21			
1	C	330	Total	C	N	O	S	8	11	0
			2774	1788	448	517	21			

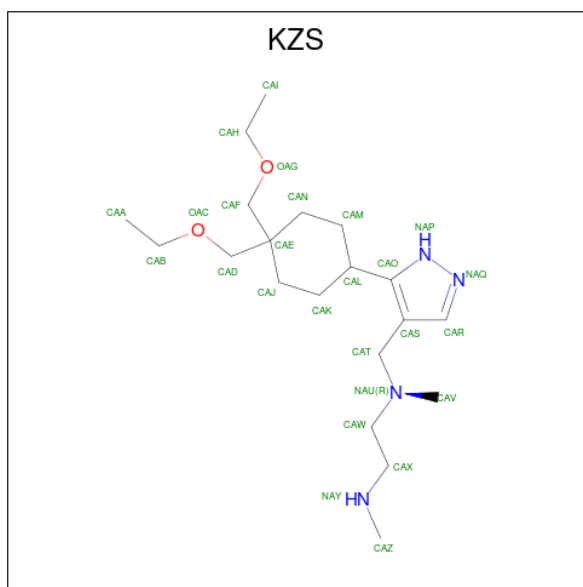
- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 3 is N 1 -({5-[4,4-bis(ethoxymethyl)cyclohexyl]-1H-pyrazol-4-yl}methyl)-N 1 ,N 2 -dimethylethane-1,2-diamine (three-letter code: KZS) (formula: C₂₀H₃₈N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			26	20	4	2			
3	D	1	Total	C	N	O		0	0
			26	20	4	2			
3	B	1	Total	C	N	O		0	0
			26	20	4	2			
3	C	1	Total	C	N	O		0	0
			26	20	4	2			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



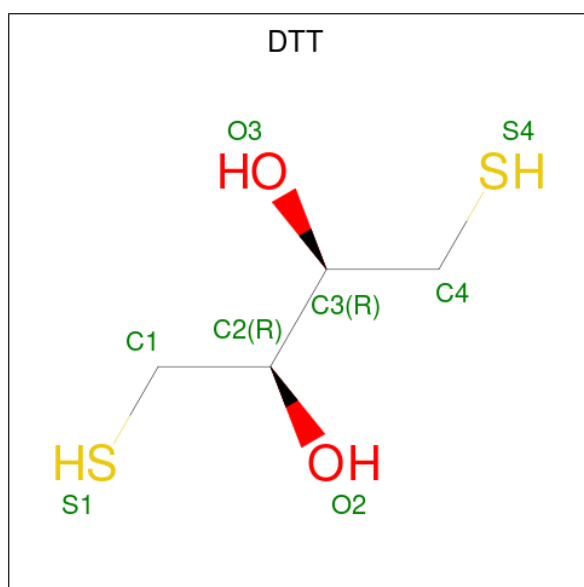
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total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

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

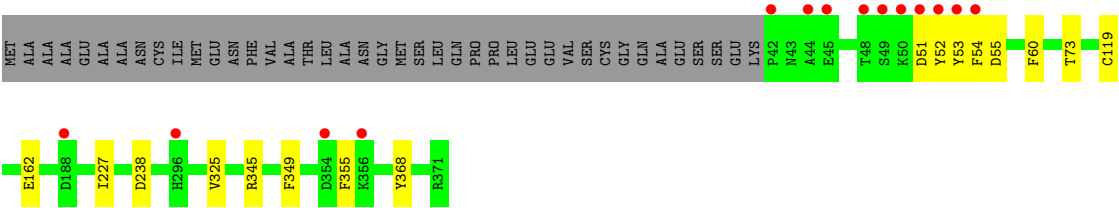
- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	186	Total 186	O 186	0	0
6	D	134	Total 134	O 134	0	0
6	B	180	Total 180	O 180	0	0
6	C	164	Total 164	O 164	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	174.15Å 174.15Å 142.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.94 – 2.48 38.94 – 2.48	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.94-2.48) 99.9 (38.94-2.48)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.190 , 0.222 0.202 , 0.232	Depositor DCC
R_{free} test set	3909 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtrriage
Anisotropy	0.252	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12135	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.00 % 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 3.9407e-04. 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/2879	0.57	0/3895
1	B	0.35	0/2852	0.58	0/3860
1	C	0.36	0/2852	0.58	0/3860
1	D	0.35	0/2845	0.59	0/3849
All	All	0.35	0/11428	0.58	0/15464

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2798	0	2733	50	0
1	B	2774	0	2706	17	0
1	C	2774	0	2706	20	0
1	D	2771	0	2711	47	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	0	0	0
3	C	26	0	0	0	0
3	D	26	0	0	0	0
4	A	42	0	56	0	0
4	B	36	0	48	0	0
4	C	24	0	32	0	0
4	D	36	0	48	0	0
5	B	8	0	10	0	0
6	A	186	0	0	0	0
6	B	180	0	0	0	0
6	C	164	0	0	1	0
6	D	134	0	0	0	0
All	All	12135	0	11126	89	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 4.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53[A]:TYR:CE2	1:D:53[A]:TYR:HA	1.18	1.63
1:A:53[A]:TYR:CE2	1:D:53[A]:TYR:CD1	1.86	1.63
1:A:53[A]:TYR:CE2	1:D:53[A]:TYR:CA	1.85	1.55
1:A:53[A]:TYR:CZ	1:D:53[A]:TYR:CD1	1.95	1.51
1:A:53[A]:TYR:CD2	1:D:53[A]:TYR:CG	2.03	1.47
1:A:53[A]:TYR:CD2	1:D:53[A]:TYR:CB	2.01	1.41
1:A:53[A]:TYR:CE2	1:D:53[A]:TYR:HD1	1.31	1.31
1:A:53[A]:TYR:HE2	1:D:53[A]:TYR:CA	1.27	1.31
1:A:53[A]:TYR:CZ	1:D:53[A]:TYR:HD1	1.39	1.25
1:D:51[B]:ASP:HB2	1:D:55[B]:ASP:CB	1.68	1.23
1:C:51[B]:ASP:HB2	1:C:55[B]:ASP:CB	1.69	1.23
1:A:53[A]:TYR:CE1	1:D:53[A]:TYR:CE1	2.27	1.21
1:A:53[A]:TYR:CD2	1:D:53[A]:TYR:CA	2.22	1.21
1:B:50[B]:LYS:HE2	1:C:52[B]:TYR:CE2	1.79	1.18
1:A:53[A]:TYR:CD2	1:D:53[A]:TYR:CD1	2.24	1.15
1:A:51[B]:ASP:CB	1:A:55[B]:ASP:HB3	1.78	1.13
1:D:51[B]:ASP:CB	1:D:55[B]:ASP:HB3	1.80	1.12
1:A:51[B]:ASP:HB2	1:A:55[B]:ASP:CB	1.80	1.10
1:A:53[A]:TYR:HD2	1:D:53[A]:TYR:HB3	1.15	1.09
1:A:53[A]:TYR:CE1	1:D:53[A]:TYR:CD1	2.39	1.08
1:C:51[B]:ASP:CB	1:C:55[B]:ASP:HB3	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53[A]:TYR:CE2	1:D:53[A]:TYR:C	2.32	1.02
1:A:53[A]:TYR:CD2	1:D:53[A]:TYR:HB3	1.89	1.02
1:A:53[A]:TYR:CE2	1:D:53[A]:TYR:CG	2.37	1.02
1:A:53[A]:TYR:CZ	1:D:53[A]:TYR:CE1	2.47	1.01
1:A:53[A]:TYR:CG	1:D:53[A]:TYR:CG	2.53	0.97
1:C:51[B]:ASP:HB2	1:C:55[B]:ASP:HB3	0.99	0.97
1:A:53[A]:TYR:CD2	1:D:53[A]:TYR:C	2.38	0.96
1:D:51[B]:ASP:HB2	1:D:55[B]:ASP:HB3	0.96	0.96
1:A:51[B]:ASP:HB2	1:A:55[B]:ASP:HB3	0.93	0.93
1:A:53[A]:TYR:CE2	1:D:53[A]:TYR:O	2.24	0.89
1:B:52[B]:TYR:H	1:B:55[B]:ASP:HB2	1.37	0.89
1:A:53[A]:TYR:HD2	1:D:53[A]:TYR:CB	1.62	0.87
1:B:50[B]:LYS:CE	1:C:52[B]:TYR:CE2	2.57	0.87
1:A:53[A]:TYR:CE2	1:D:53[A]:TYR:CB	2.43	0.84
1:A:53[A]:TYR:CD1	1:D:53[A]:TYR:CE1	2.66	0.84
1:A:53[A]:TYR:CG	1:D:53[A]:TYR:CD1	2.64	0.83
1:A:53[A]:TYR:CD1	1:D:53[A]:TYR:CD1	2.69	0.80
1:C:52[B]:TYR:H	1:C:55[B]:ASP:HB2	1.47	0.80
1:C:54[A]:PHE:CD1	1:C:54[A]:PHE:O	2.38	0.76
1:A:54[B]:PHE:CD1	1:A:119[B]:CYS:HB3	2.23	0.73
1:B:50[B]:LYS:NZ	1:C:52[B]:TYR:CD2	2.56	0.73
1:B:50[B]:LYS:HE2	1:C:52[B]:TYR:HE2	1.52	0.71
1:B:50[B]:LYS:HZ3	1:C:52[B]:TYR:HD2	1.32	0.70
1:B:50[B]:LYS:CE	1:C:52[B]:TYR:CD2	2.74	0.69
1:B:52[B]:TYR:CG	1:B:53[B]:TYR:N	2.60	0.68
1:A:53[A]:TYR:HA	1:D:53[A]:TYR:CE2	2.31	0.66
1:D:303:THR:HG22	1:D:310:THR:HG21	1.78	0.66
1:D:54[B]:PHE:CE1	1:D:119[B]:CYS:HB3	2.33	0.64
1:C:54[A]:PHE:O	1:C:54[A]:PHE:CG	2.51	0.63
1:A:54[B]:PHE:CE1	1:A:119[B]:CYS:HB3	2.33	0.62
1:A:52[B]:TYR:H	1:A:55[B]:ASP:HB2	1.66	0.61
1:C:52[B]:TYR:CG	1:C:53[B]:TYR:N	2.68	0.60
1:A:53[A]:TYR:CD2	1:D:53[A]:TYR:O	2.50	0.59
1:A:53[A]:TYR:HD2	1:D:53[A]:TYR:C	1.98	0.59
1:D:54[B]:PHE:CD1	1:D:119[B]:CYS:HB3	2.38	0.59
1:D:52[B]:TYR:H	1:D:55[B]:ASP:HB2	1.69	0.58
1:D:51[B]:ASP:CB	1:D:55[B]:ASP:CB	2.57	0.58
1:A:53[A]:TYR:O	1:A:54[A]:PHE:CD1	2.59	0.56
1:B:51[B]:ASP:C	1:B:51[B]:ASP:OD1	2.43	0.56
1:D:51[B]:ASP:HB2	1:D:55[B]:ASP:HB2	1.78	0.55
1:B:325:VAL:HG12	1:B:355:PHE:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53[A]:TYR:CG	1:D:53[A]:TYR:CD2	2.95	0.54
1:C:345:ARG:NH2	6:C:501:HOH:O	2.42	0.53
1:A:53[A]:TYR:HE2	1:D:53[A]:TYR:HA	0.53	0.51
1:A:160:ILE:HG22	1:A:192:PHE:HB2	1.93	0.50
1:D:160:ILE:HG22	1:D:192:PHE:HB2	1.94	0.49
1:A:53[A]:TYR:CE1	1:D:53[A]:TYR:HE1	2.17	0.49
1:B:51[B]:ASP:HB2	1:B:55[B]:ASP:HB3	1.94	0.48
1:D:50[B]:LYS:O	1:D:51[B]:ASP:HB3	2.13	0.48
1:A:95:VAL:HG13	1:A:146:VAL:HG21	1.95	0.47
1:B:54[B]:PHE:CD1	1:B:119[B]:CYS:HB3	2.50	0.47
1:A:325:VAL:HG12	1:A:355:PHE:CZ	2.51	0.46
1:A:227:ILE:HG23	1:D:60[B]:PHE:CD1	2.51	0.46
1:A:270:PRO:HB2	1:B:270:PRO:HB2	1.98	0.45
1:C:325:VAL:HG12	1:C:355:PHE:CZ	2.51	0.45
1:C:54[B]:PHE:CD1	1:C:119[B]:CYS:HB3	2.53	0.43
1:B:60[B]:PHE:CD1	1:C:227:ILE:HG23	2.53	0.43
1:B:160:ILE:HG22	1:B:192:PHE:HB2	2.00	0.43
1:B:227:ILE:HG23	1:C:60[B]:PHE:CD1	2.55	0.42
1:A:220:TYR:CE2	1:D:73:THR:HG21	2.54	0.42
1:D:52[B]:TYR:N	1:D:55[B]:ASP:HB2	2.32	0.42
1:A:60[B]:PHE:CD1	1:D:227:ILE:HG23	2.54	0.42
1:C:349:PHE:HB2	1:C:368:TYR:HB2	2.02	0.41
1:A:52[B]:TYR:CG	1:A:53[B]:TYR:N	2.88	0.41
1:B:220:TYR:CE2	1:C:73:THR:HG21	2.55	0.41
1:A:52[B]:TYR:O	1:A:56:SER:OG	2.23	0.41
1:A:315:THR:HG21	1:A:370:MET:HE1	2.03	0.40
1:A:52[B]:TYR:N	1:A:55[B]:ASP:HB2	2.34	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	342/371 (92%)	327 (96%)	15 (4%)	0	100	100
1	B	339/371 (91%)	324 (96%)	15 (4%)	0	100	100
1	C	339/371 (91%)	324 (96%)	15 (4%)	0	100	100
1	D	338/371 (91%)	323 (96%)	13 (4%)	2 (1%)	22	36
All	All	1358/1484 (92%)	1298 (96%)	58 (4%)	2 (0%)	48	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	53[A]	TYR
1	D	53[B]	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/329 (94%)	306 (98%)	5 (2%)	58	79
1	B	307/329 (93%)	304 (99%)	3 (1%)	73	87
1	C	307/329 (93%)	305 (99%)	2 (1%)	81	92
1	D	307/329 (93%)	303 (99%)	4 (1%)	65	83
All	All	1232/1316 (94%)	1218 (99%)	14 (1%)	73	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53[A]	TYR
1	A	53[B]	TYR
1	A	162	GLU
1	A	238	ASP
1	A	313	LYS
1	D	53[A]	TYR
1	D	53[B]	TYR
1	D	162	GLU
1	D	310	THR

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Mol	Chain	Res	Type
1	B	162	GLU
1	B	319	MET
1	B	354	ASP
1	C	162	GLU
1	C	238	ASP

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

Mol	Chain	Res	Type
1	D	244	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 [i](#)

32 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	$\# Z > 2$
4	GOL	C	406	-	5,5,5	0.38	0	5,5,5	0.27	0
4	GOL	A	405	-	5,5,5	0.29	0	5,5,5	0.23	0
4	GOL	A	403	-	5,5,5	0.24	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	409	-	5,5,5	0.32	0	5,5,5	0.20	0
4	GOL	D	404	-	5,5,5	0.35	0	5,5,5	0.56	0
3	KZS	B	402	-	27,27,27	1.91	3 (11%)	24,35,35	1.22	3 (12%)
4	GOL	D	406	-	5,5,5	0.31	0	5,5,5	0.19	0
4	GOL	D	408	-	5,5,5	0.28	0	5,5,5	0.21	0
4	GOL	A	407	-	5,5,5	0.40	0	5,5,5	0.39	0
4	GOL	A	408	-	5,5,5	0.28	0	5,5,5	0.16	0
4	GOL	B	407	-	5,5,5	0.40	0	5,5,5	0.19	0
4	GOL	D	405	-	5,5,5	0.24	0	5,5,5	0.21	0
2	SAH	D	401	-	23,28,28	1.00	2 (8%)	22,40,40	1.42	3 (13%)
4	GOL	D	407	-	5,5,5	0.32	0	5,5,5	0.34	0
4	GOL	C	403	-	5,5,5	0.24	0	5,5,5	0.31	0
5	DTT	B	409	-	7,7,7	0.54	0	4,8,8	0.46	0
2	SAH	C	401	-	23,28,28	1.01	2 (8%)	22,40,40	1.45	3 (13%)
4	GOL	A	404	-	5,5,5	0.29	0	5,5,5	0.25	0
4	GOL	A	406	-	5,5,5	0.33	0	5,5,5	0.18	0
2	SAH	A	401	-	23,28,28	1.01	2 (8%)	22,40,40	1.46	3 (13%)
4	GOL	B	408	-	5,5,5	0.30	0	5,5,5	0.16	0
4	GOL	B	405	-	5,5,5	0.27	0	5,5,5	0.21	0
4	GOL	B	404	-	5,5,5	0.26	0	5,5,5	0.21	0
4	GOL	B	403	-	5,5,5	0.29	0	5,5,5	0.27	0
4	GOL	C	405	-	5,5,5	0.27	0	5,5,5	0.25	0
3	KZS	D	402	-	27,27,27	1.86	3 (11%)	24,35,35	1.23	3 (12%)
4	GOL	B	406	-	5,5,5	0.29	0	5,5,5	0.20	0
3	KZS	C	402	-	27,27,27	1.97	3 (11%)	24,35,35	1.12	3 (12%)
3	KZS	A	402	-	27,27,27	1.77	3 (11%)	24,35,35	1.23	2 (8%)
4	GOL	D	403	-	5,5,5	0.29	0	5,5,5	0.27	0
2	SAH	B	401	-	23,28,28	0.99	2 (8%)	22,40,40	1.45	3 (13%)
4	GOL	C	404	-	5,5,5	0.29	0	5,5,5	0.18	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
4	GOL	C	406	-	-	2/4/4/4	-
4	GOL	A	405	-	-	2/4/4/4	-
4	GOL	A	403	-	-	0/4/4/4	-
4	GOL	A	409	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	404	-	-	2/4/4/4	-
3	KZS	B	402	-	-	3/17/34/34	0/2/2/2
4	GOL	D	406	-	-	2/4/4/4	-
4	GOL	D	408	-	-	0/4/4/4	-
4	GOL	A	407	-	-	1/4/4/4	-
4	GOL	A	408	-	-	0/4/4/4	-
4	GOL	B	407	-	-	4/4/4/4	-
4	GOL	D	405	-	-	2/4/4/4	-
2	SAH	D	401	-	-	2/11/31/31	0/3/3/3
4	GOL	D	407	-	-	0/4/4/4	-
4	GOL	C	403	-	-	0/4/4/4	-
5	DTT	B	409	-	-	6/8/8/8	-
2	SAH	C	401	-	-	1/11/31/31	0/3/3/3
4	GOL	A	404	-	-	0/4/4/4	-
4	GOL	A	406	-	-	0/4/4/4	-
2	SAH	A	401	-	-	0/11/31/31	0/3/3/3
4	GOL	B	408	-	-	2/4/4/4	-
4	GOL	B	405	-	-	2/4/4/4	-
4	GOL	B	404	-	-	0/4/4/4	-
4	GOL	B	403	-	-	2/4/4/4	-
4	GOL	C	405	-	-	4/4/4/4	-
3	KZS	D	402	-	-	6/17/34/34	0/2/2/2
4	GOL	B	406	-	-	0/4/4/4	-
3	KZS	C	402	-	-	3/17/34/34	0/2/2/2
3	KZS	A	402	-	-	3/17/34/34	0/2/2/2
4	GOL	D	403	-	-	0/4/4/4	-
2	SAH	B	401	-	-	1/11/31/31	0/3/3/3
4	GOL	C	404	-	-	0/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	KZS	NAQ-NAP	-6.60	1.23	1.37
3	B	402	KZS	CAS-CAO	-6.22	1.33	1.41
3	A	402	KZS	CAS-CAO	-6.19	1.33	1.41
3	C	402	KZS	CAS-CAO	-6.14	1.33	1.41
3	D	402	KZS	CAS-CAO	-6.12	1.33	1.41
3	B	402	KZS	NAQ-NAP	-5.67	1.25	1.37
3	D	402	KZS	NAQ-NAP	-5.42	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	KZS	NAQ-NAP	-4.87	1.27	1.37
3	B	402	KZS	CAO-CAL	3.75	1.56	1.50
3	A	402	KZS	CAO-CAL	3.39	1.55	1.50
3	D	402	KZS	CAO-CAL	3.39	1.55	1.50
3	C	402	KZS	CAO-CAL	3.13	1.55	1.50
2	D	401	SAH	OXT-C	-2.23	1.23	1.30
2	B	401	SAH	C2-N3	2.17	1.35	1.32
2	D	401	SAH	C2-N3	2.16	1.35	1.32
2	C	401	SAH	OXT-C	-2.16	1.23	1.30
2	B	401	SAH	OXT-C	-2.15	1.23	1.30
2	A	401	SAH	OXT-C	-2.13	1.23	1.30
2	C	401	SAH	C2-N3	2.12	1.35	1.32
2	A	401	SAH	C2-N3	2.10	1.35	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SAH	N3-C2-N1	-4.36	122.75	128.67
2	A	401	SAH	N3-C2-N1	-4.28	122.87	128.67
2	C	401	SAH	N3-C2-N1	-4.25	122.90	128.67
2	D	401	SAH	N3-C2-N1	-4.14	123.05	128.67
3	A	402	KZS	CAR-CAS-CAO	3.84	108.21	104.56
3	D	402	KZS	CAR-CAS-CAO	3.52	107.91	104.56
3	B	402	KZS	CAR-CAS-CAO	3.35	107.75	104.56
3	C	402	KZS	CAR-CAS-CAO	2.89	107.31	104.56
2	A	401	SAH	OXT-C-O	-2.82	117.69	124.08
2	C	401	SAH	OXT-C-O	-2.75	117.85	124.08
2	D	401	SAH	OXT-C-O	-2.73	117.89	124.08
2	B	401	SAH	OXT-C-O	-2.69	117.98	124.08
2	D	401	SAH	C4-C5-N7	-2.67	106.51	109.34
2	C	401	SAH	C4-C5-N7	-2.60	106.59	109.34
3	B	402	KZS	CAK-CAL-CAO	-2.55	107.76	111.43
2	A	401	SAH	C4-C5-N7	-2.48	106.72	109.34
3	A	402	KZS	CAV-NAU-CAT	2.32	114.13	110.53
3	C	402	KZS	CAV-NAU-CAT	2.23	113.99	110.53
2	B	401	SAH	C4-C5-N7	-2.19	107.03	109.34
3	B	402	KZS	CAV-NAU-CAT	2.16	113.89	110.53
3	D	402	KZS	CAV-NAU-CAT	2.13	113.84	110.53
3	D	402	KZS	CAK-CAL-CAO	-2.04	108.51	111.43
3	C	402	KZS	CAK-CAL-CAO	-2.02	108.53	111.43

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	402	KZS	CAW-CAX-NAY-CAZ
4	A	405	GOL	C1-C2-C3-O3
4	D	406	GOL	O1-C1-C2-O2
4	D	406	GOL	O1-C1-C2-C3
4	B	405	GOL	O1-C1-C2-C3
4	B	408	GOL	O1-C1-C2-C3
5	B	409	DTT	S1-C1-C2-O2
5	B	409	DTT	S1-C1-C2-C3
5	B	409	DTT	C1-C2-C3-O3
5	B	409	DTT	C1-C2-C3-C4
5	B	409	DTT	O2-C2-C3-O3
5	B	409	DTT	O2-C2-C3-C4
4	A	409	GOL	O1-C1-C2-C3
4	D	404	GOL	O1-C1-C2-C3
4	D	405	GOL	C1-C2-C3-O3
4	B	403	GOL	C1-C2-C3-O3
4	B	407	GOL	O1-C1-C2-C3
4	B	407	GOL	C1-C2-C3-O3
4	C	405	GOL	O1-C1-C2-C3
4	C	405	GOL	C1-C2-C3-O3
4	C	406	GOL	C1-C2-C3-O3
4	A	405	GOL	O2-C2-C3-O3
4	D	404	GOL	O1-C1-C2-O2
4	B	403	GOL	O2-C2-C3-O3
4	B	405	GOL	O1-C1-C2-O2
4	B	407	GOL	O1-C1-C2-O2
4	B	407	GOL	O2-C2-C3-O3
4	B	408	GOL	O1-C1-C2-O2
3	D	402	KZS	CAN-CAE-CAF-OAG
4	D	405	GOL	O2-C2-C3-O3
4	C	405	GOL	O1-C1-C2-O2
3	A	402	KZS	CAE-CAF-OAG-CAH
3	D	402	KZS	CAA-CAB-OAC-CAD
3	B	402	KZS	CAA-CAB-OAC-CAD
3	D	402	KZS	CAJ-CAE-CAF-OAG
4	A	407	GOL	O2-C2-C3-O3
3	D	402	KZS	CAE-CAF-OAG-CAH
3	A	402	KZS	CAA-CAB-OAC-CAD
3	C	402	KZS	CAA-CAB-OAC-CAD
4	C	405	GOL	O2-C2-C3-O3
3	B	402	KZS	CAE-CAF-OAG-CAH
3	C	402	KZS	CAE-CAF-OAG-CAH

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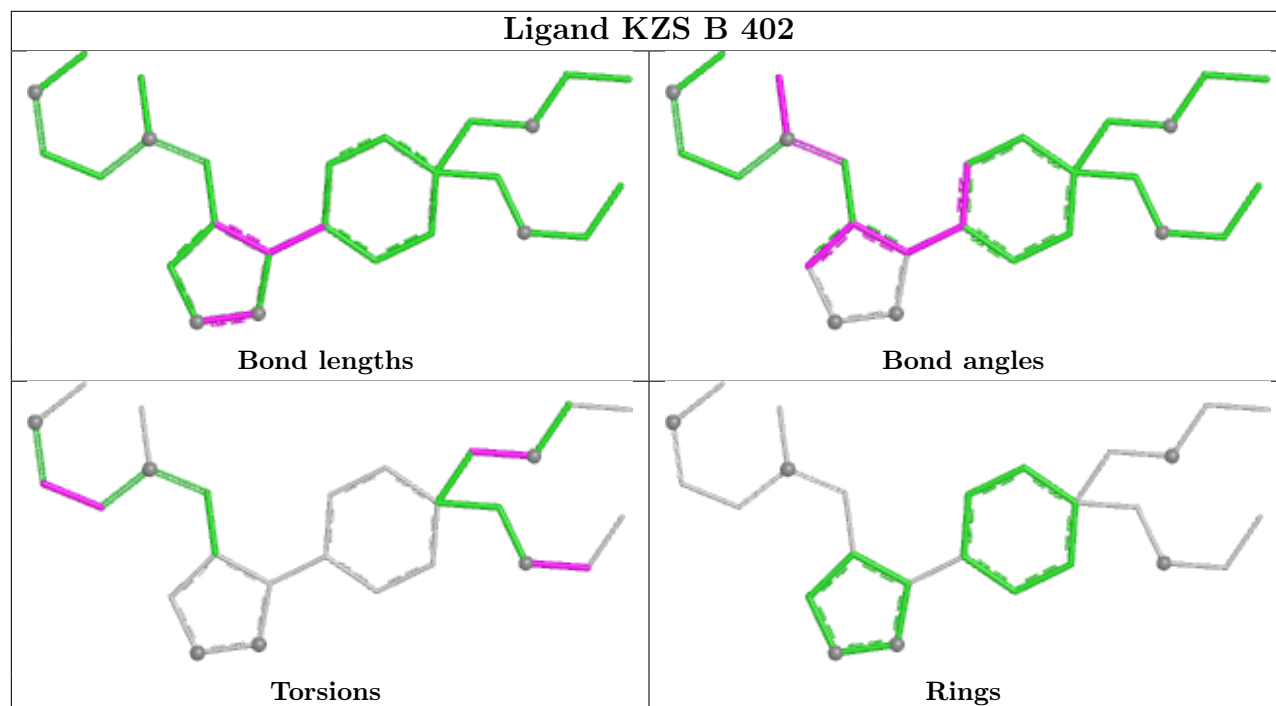
Mol	Chain	Res	Type	Atoms
3	A	402	KZS	CAW-CAX-NAY-CAZ
4	A	409	GOL	O1-C1-C2-O2
3	D	402	KZS	CAD-CAE-CAF-OAG
2	D	401	SAH	C-CA-CB-CG
4	C	406	GOL	O2-C2-C3-O3
2	D	401	SAH	CB-CG-SD-C5'
2	C	401	SAH	CB-CG-SD-C5'
3	C	402	KZS	NAU-CAW-CAX-NAY
3	B	402	KZS	NAU-CAW-CAX-NAY
2	B	401	SAH	CB-CG-SD-C5'

There are no ring outliers.

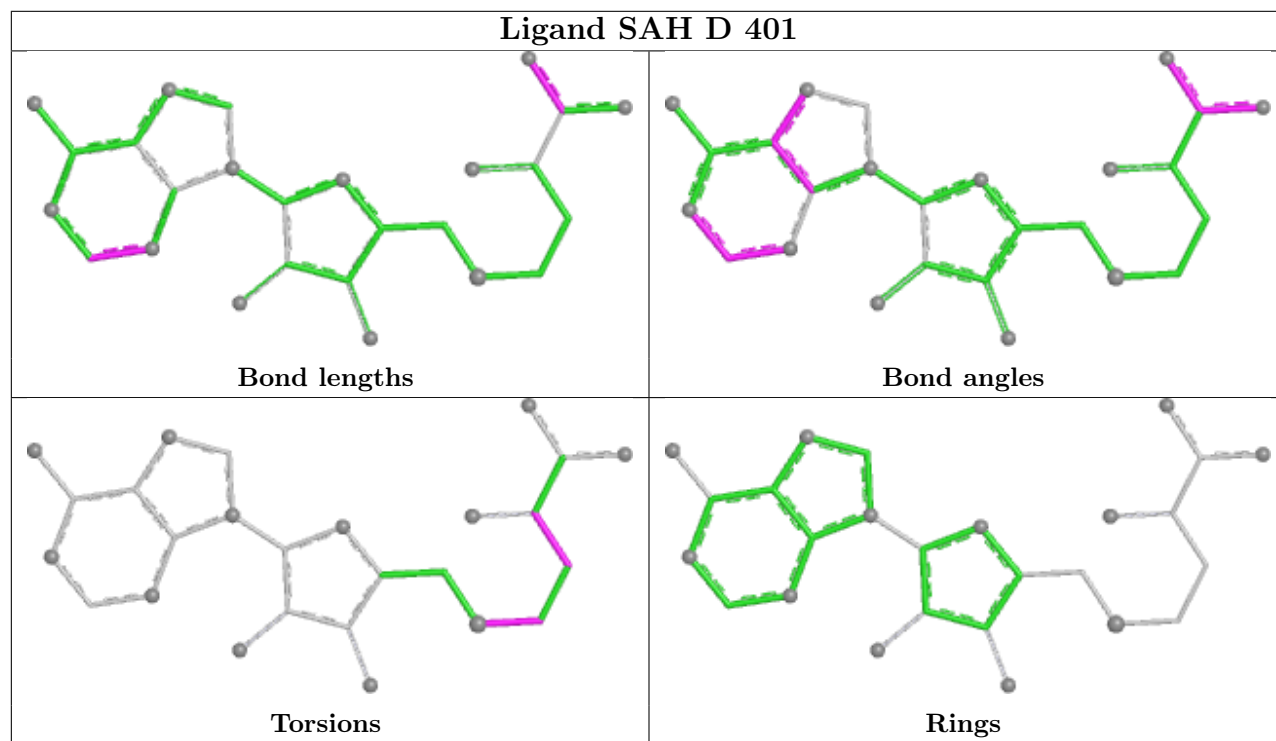
No monomer is involved in short contacts.

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

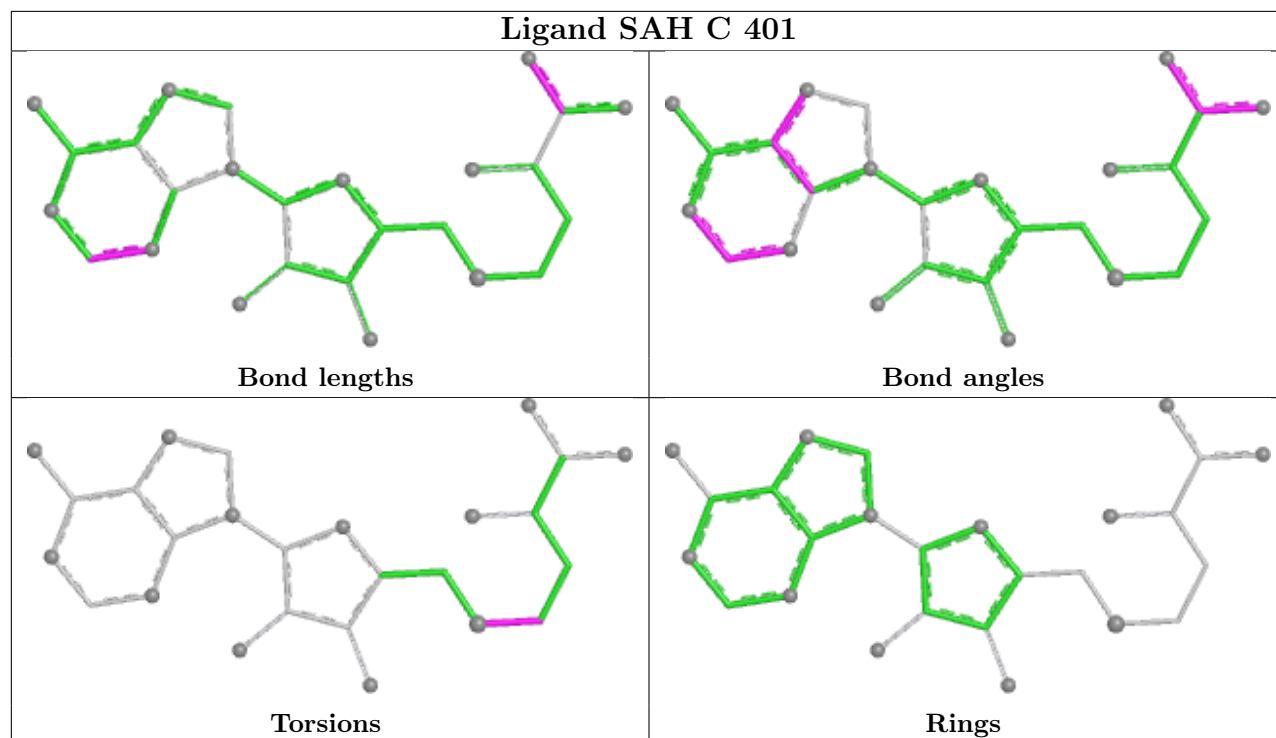
Ligand KZS B 402



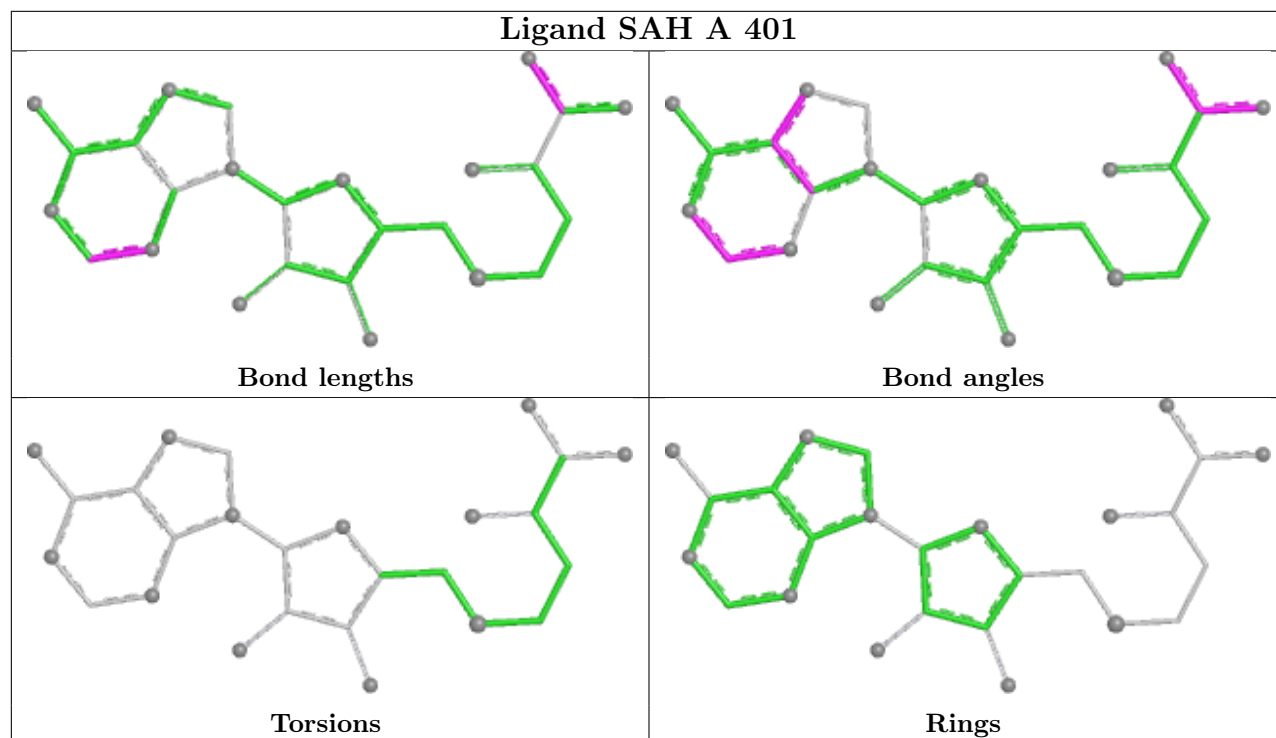
Ligand SAH D 401



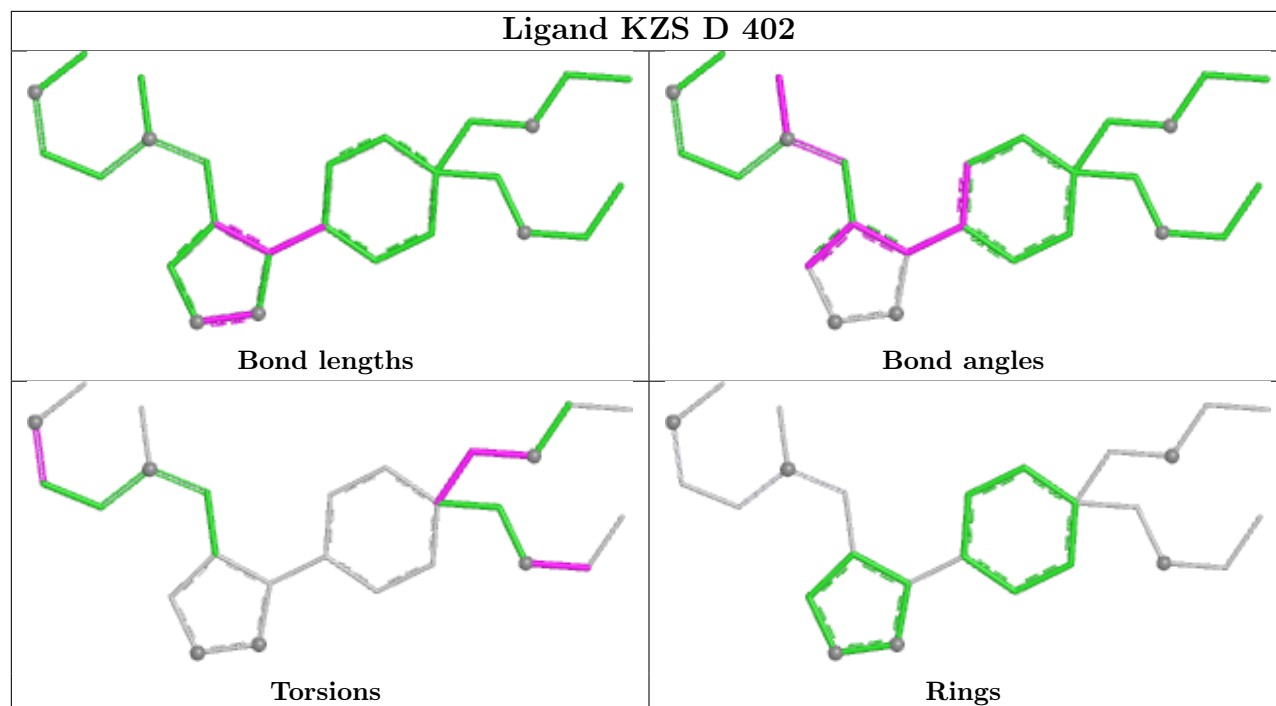
Ligand SAH C 401



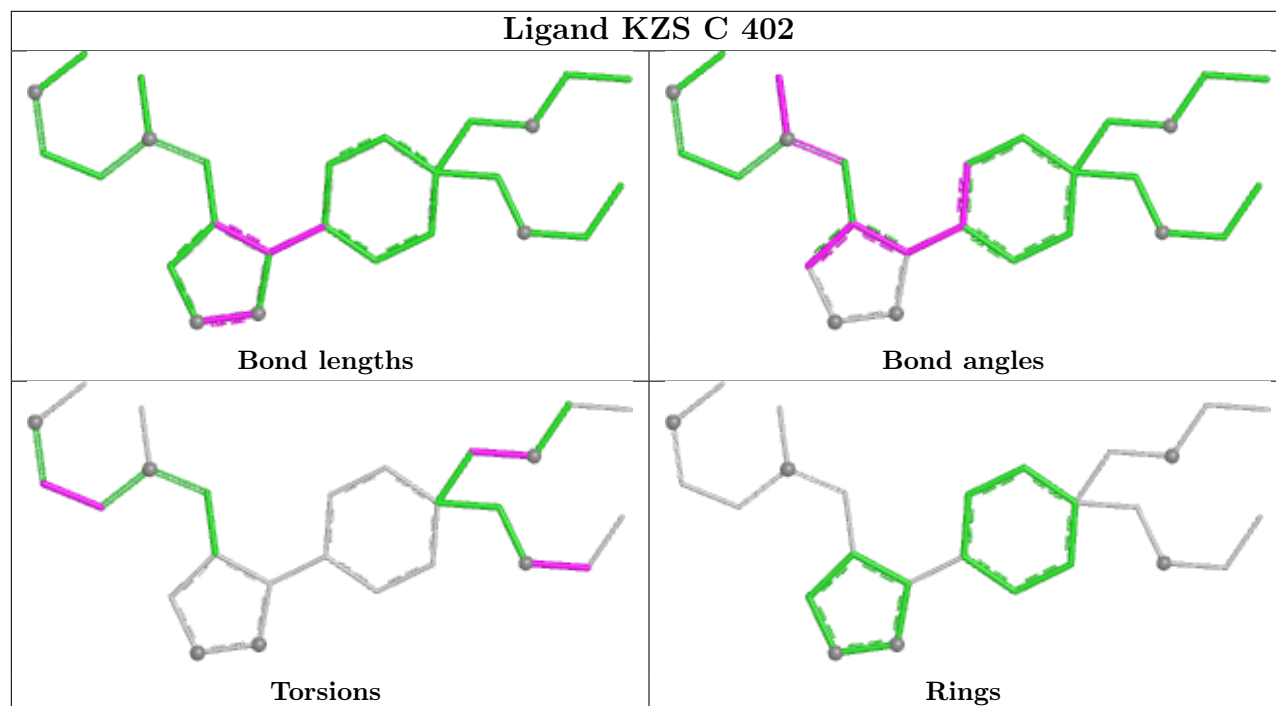
Ligand SAH A 401

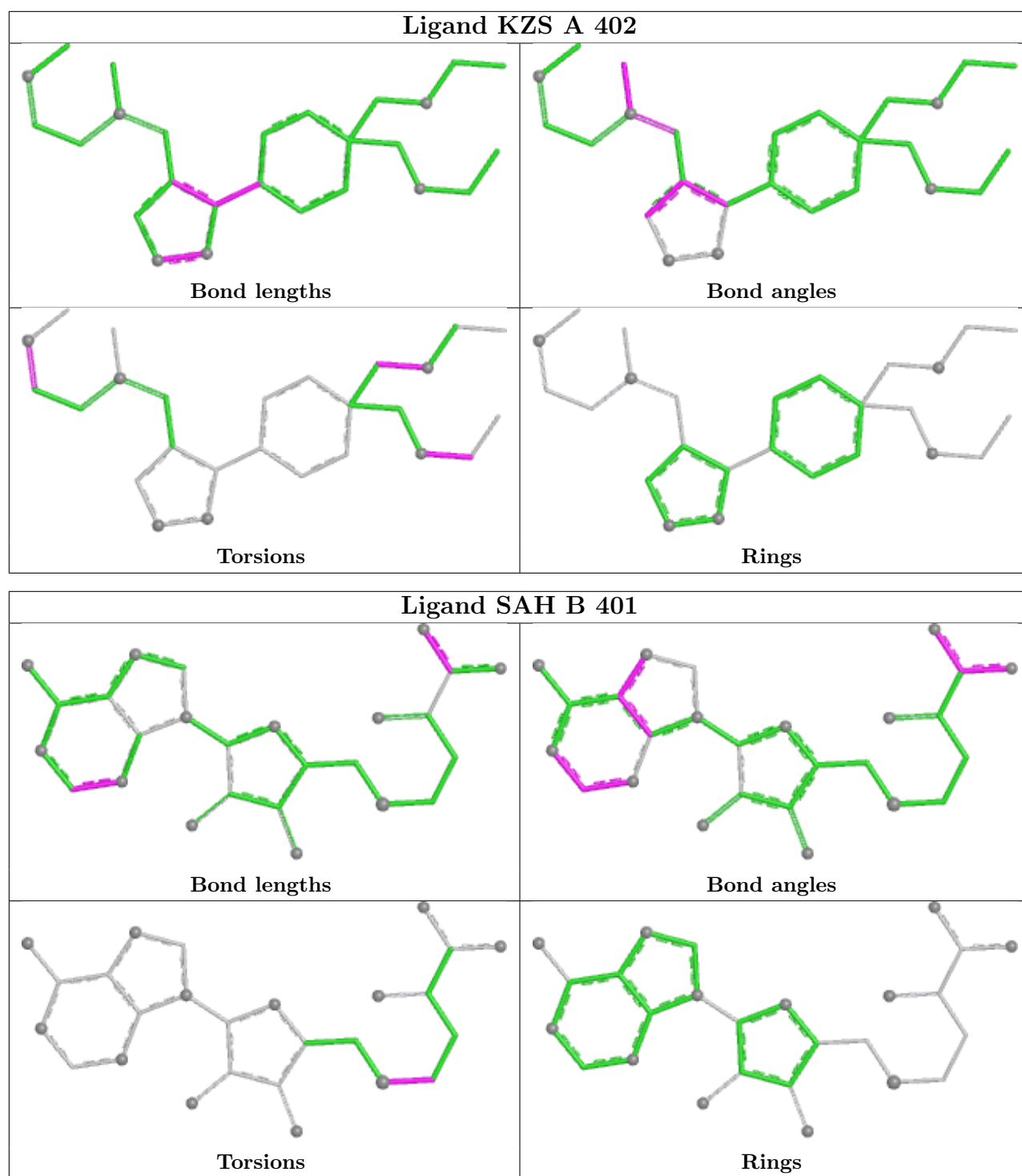


Ligand KZS D 402



Ligand KZS C 402





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/371 (88%)	-0.10	15 (4%) 39 36	8, 19, 31, 61	14 (4%)
1	B	330/371 (88%)	-0.13	9 (2%) 56 54	8, 18, 29, 59	11 (3%)
1	C	330/371 (88%)	-0.14	14 (4%) 41 39	9, 18, 30, 72	11 (3%)
1	D	330/371 (88%)	-0.06	16 (4%) 36 34	8, 19, 31, 69	10 (3%)
All	All	1320/1484 (88%)	-0.11	54 (4%) 42 40	8, 19, 30, 72	46 (3%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	54[A]	PHE	9.5
1	C	54[A]	PHE	8.8
1	D	52[A]	TYR	7.1
1	A	53[A]	TYR	6.6
1	B	54[A]	PHE	6.5
1	D	53[A]	TYR	6.4
1	A	54[A]	PHE	6.3
1	A	52[A]	TYR	6.1
1	C	52[A]	TYR	5.9
1	B	52[A]	TYR	5.6
1	A	50[A]	LYS	5.6
1	D	50[A]	LYS	5.6
1	D	51[A]	ASP	5.2
1	D	42	PRO	4.7
1	D	45	GLU	4.6
1	C	51[A]	ASP	4.4
1	B	42	PRO	4.3
1	A	51[A]	ASP	4.2
1	B	51[A]	ASP	4.2
1	B	50[A]	LYS	4.1
1	B	45	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	42	PRO	4.0
1	C	42	PRO	4.0
1	C	296	HIS	4.0
1	C	45	GLU	3.9
1	A	44	ALA	3.9
1	C	48	THR	3.7
1	A	45	GLU	3.7
1	C	50[A]	LYS	3.6
1	D	44	ALA	3.6
1	B	44	ALA	3.1
1	D	43	ASN	3.1
1	A	296	HIS	3.1
1	D	356	LYS	3.0
1	A	85	HIS	3.0
1	D	46	ASP	3.0
1	D	137	HIS	2.9
1	B	53[A]	TYR	2.8
1	A	49	SER	2.8
1	C	53[A]	TYR	2.8
1	A	46	ASP	2.7
1	C	44	ALA	2.6
1	D	296	HIS	2.6
1	D	49	SER	2.6
1	B	296[A]	HIS	2.4
1	D	48	THR	2.4
1	C	49	SER	2.3
1	A	43	ASN	2.2
1	A	48	THR	2.2
1	C	188	ASP	2.2
1	D	338	ARG	2.2
1	A	188	ASP	2.2
1	C	356	LYS	2.1
1	C	354	ASP	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

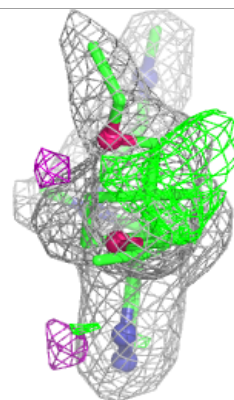
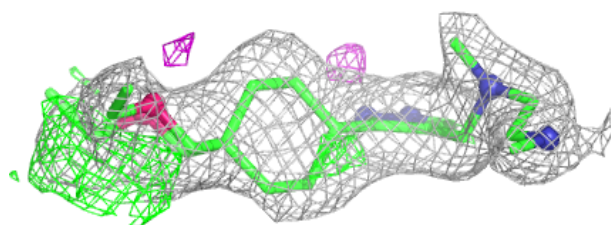
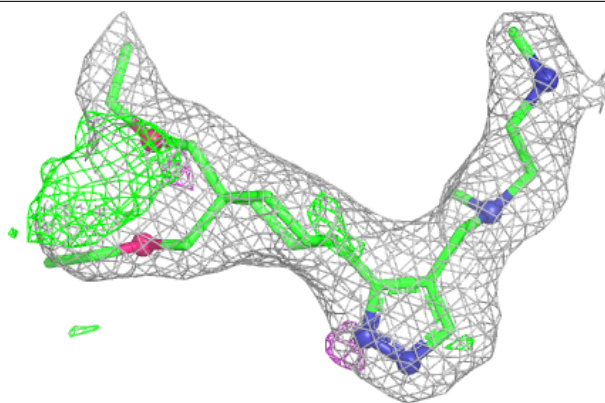
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	D	408	6/6	0.67	0.29	63,65,66,67	0
4	GOL	A	407	6/6	0.69	0.24	43,45,46,47	0
4	GOL	D	407	6/6	0.70	0.25	55,56,57,57	0
4	GOL	B	407	6/6	0.72	0.24	41,43,43,43	0
4	GOL	D	406	6/6	0.77	0.31	64,66,66,67	0
4	GOL	A	409	6/6	0.77	0.25	67,67,67,68	0
4	GOL	C	405	6/6	0.78	0.19	48,49,49,49	0
4	GOL	B	403	6/6	0.80	0.19	39,40,41,42	0
5	DTT	B	409	8/8	0.81	0.21	49,53,56,58	0
4	GOL	D	405	6/6	0.82	0.21	58,60,60,61	0
4	GOL	B	408	6/6	0.82	0.17	52,53,54,54	0
4	GOL	A	405	6/6	0.83	0.20	68,70,70,71	0
4	GOL	A	408	6/6	0.84	0.26	82,82,83,84	0
4	GOL	C	406	6/6	0.85	0.16	35,35,36,36	0
4	GOL	B	405	6/6	0.86	0.21	63,64,64,64	0
4	GOL	A	403	6/6	0.86	0.16	33,33,34,35	0
3	KZS	A	402	26/26	0.86	0.18	32,37,43,44	0
4	GOL	C	403	6/6	0.87	0.15	38,38,39,39	0
3	KZS	B	402	26/26	0.87	0.17	30,34,40,41	0
4	GOL	A	406	6/6	0.88	0.20	54,55,56,57	0
3	KZS	D	402	26/26	0.88	0.16	29,34,39,39	0
4	GOL	D	403	6/6	0.88	0.16	38,39,39,39	0
4	GOL	D	404	6/6	0.90	0.14	30,30,30,30	0
4	GOL	B	406	6/6	0.90	0.17	47,48,49,49	0
3	KZS	C	402	26/26	0.90	0.15	27,33,39,39	0
4	GOL	A	404	6/6	0.90	0.12	28,28,29,29	0
4	GOL	B	404	6/6	0.93	0.12	30,30,30,30	0
4	GOL	C	404	6/6	0.95	0.09	29,30,30,30	0
2	SAH	D	401	26/26	0.96	0.08	20,20,21,21	0
2	SAH	B	401	26/26	0.97	0.07	19,20,20,20	0
2	SAH	C	401	26/26	0.97	0.07	20,20,21,21	0
2	SAH	A	401	26/26	0.97	0.07	18,18,19,19	0

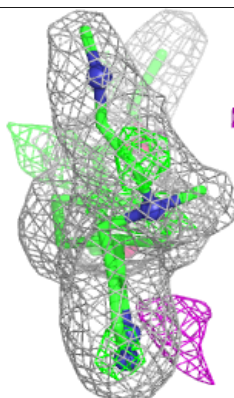
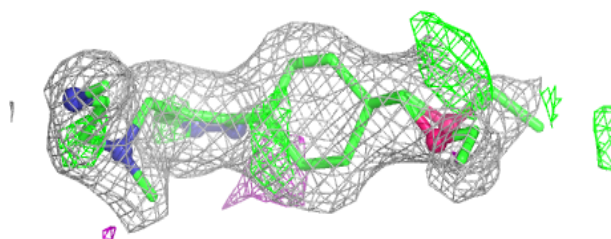
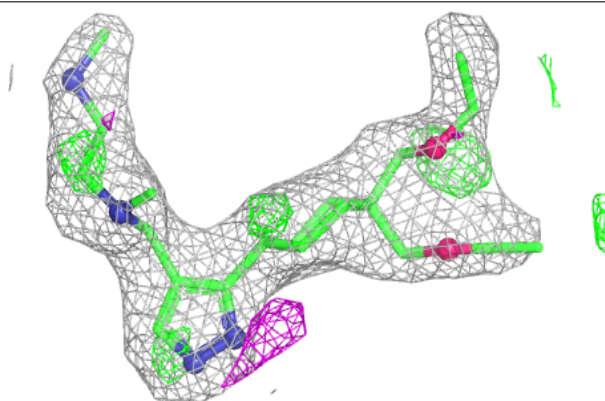
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KZS A 402:

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

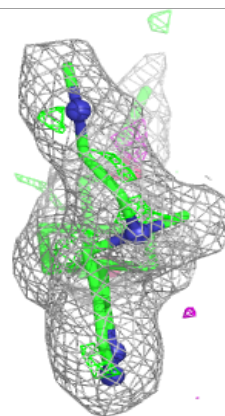
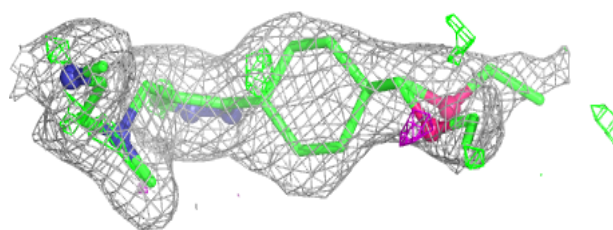
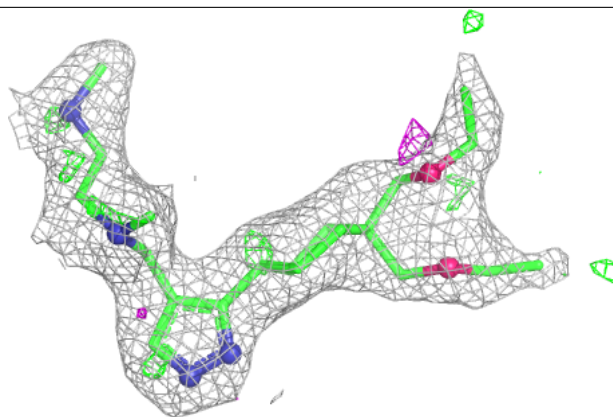
**Electron density around KZS B 402:**

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

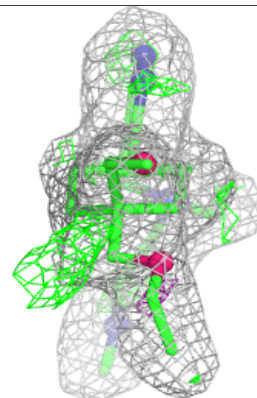
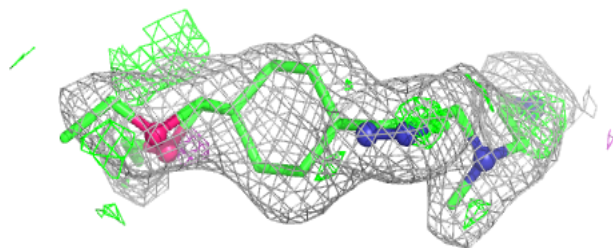
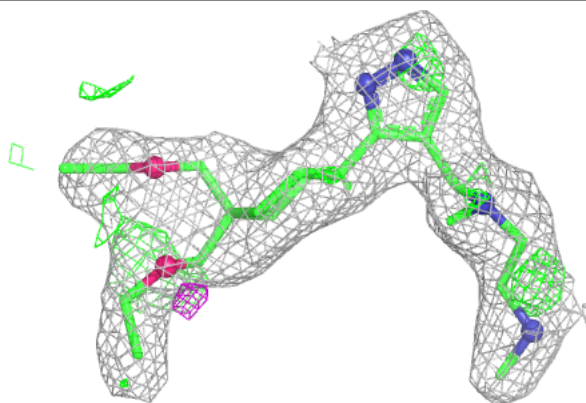


Electron density around KZS D 402:

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

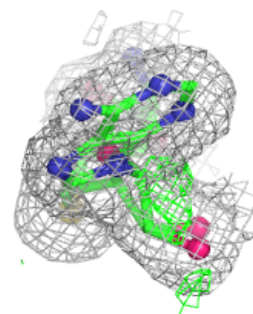
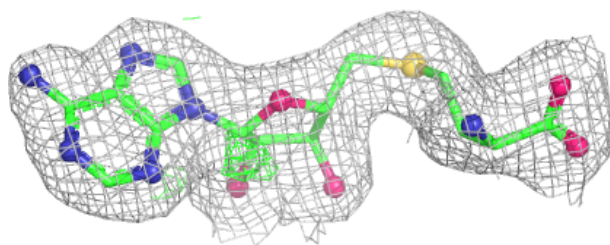
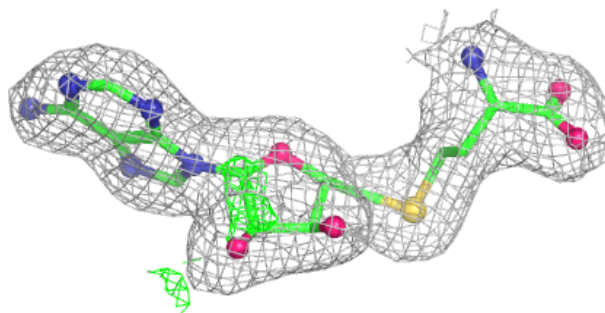
**Electron density around KZS C 402:**

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

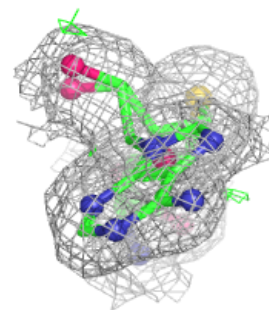
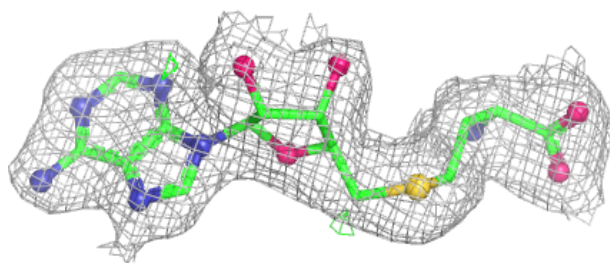
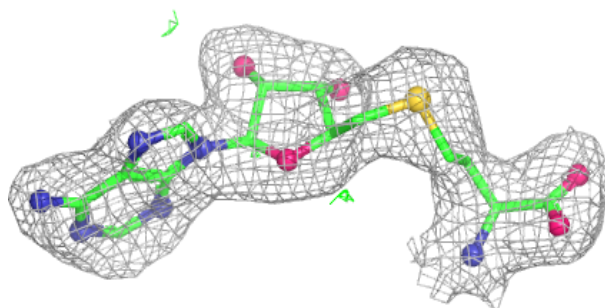


Electron density around SAH D 401:

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

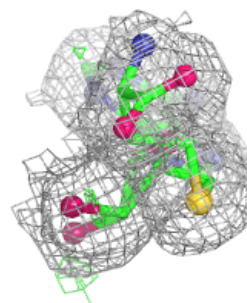
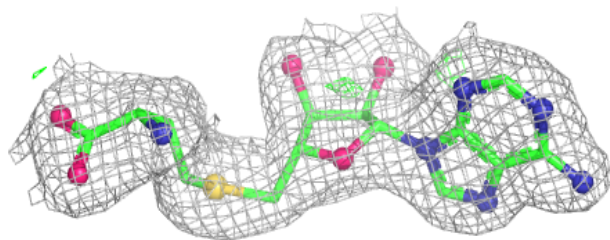
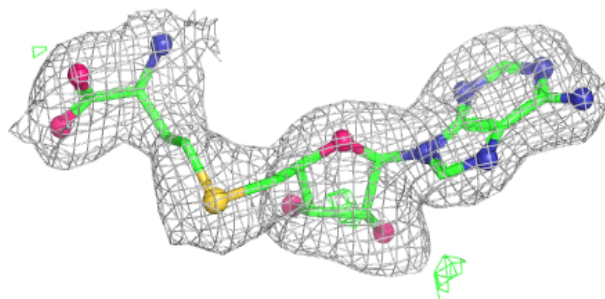
**Electron density around SAH B 401:**

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

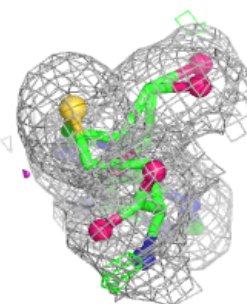
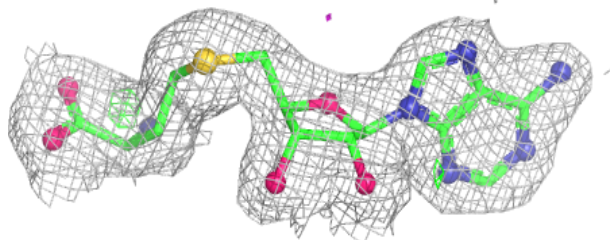
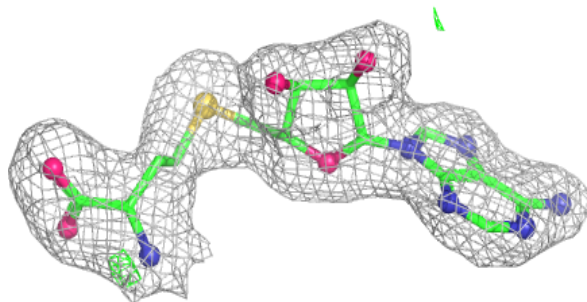


Electron density around SAH C 401:

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

**Electron density around SAH A 401:**

$2mF_o-DF_c$ (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.