



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:29 AM UTC

PDB ID : 8R7B / pdb_00008r7b
Title : SARS-CoV-2 NSP14 in complex with SAH and TDI-015051
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Deposited on : 2023-11-24
Resolution : 2.18 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

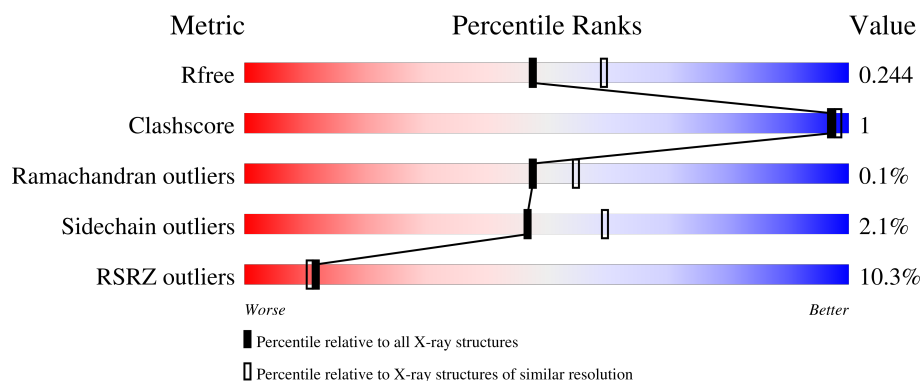
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	528	9% 76% 20%
1	B	528	7% 79% 17%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7252 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 Guanine-N7 methyltransferase nsp14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	17	0	0
			3395	2190	576	598	31			
1	B	436	Total	C	N	O	S	7	0	0
			3504	2257	595	619	33			

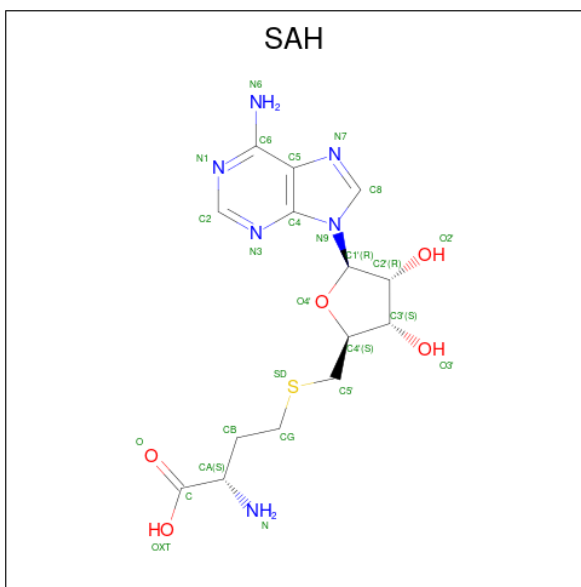
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P0DTD1
A	90	ALA	ASP	conflict	UNP P0DTD1
A	92	ALA	GLU	conflict	UNP P0DTD1
B	0	SER	-	expression tag	UNP P0DTD1
B	90	ALA	ASP	conflict	UNP P0DTD1
B	92	ALA	GLU	conflict	UNP P0DTD1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	4	Total	Zn	0	0
			4	4		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



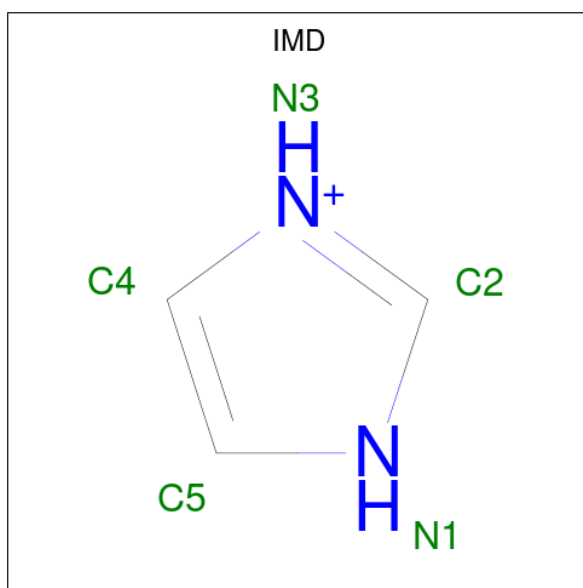
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



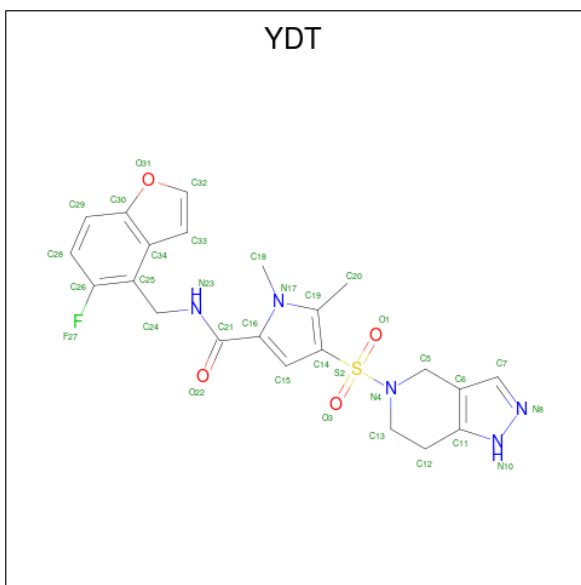
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is N-[(5-fluoranyl-1-benzofuran-4-yl)methyl]-1,5-dimethyl-4-(1,4,6,7-tetrahydropyrazolo[4,3-c]pyridin-5-ylsulfonyl)pyrrole-2-carboxamide (CCD ID: YDT) (formula: $C_{22}H_{22}FN_5O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	S	1	0
			33	22	1	5	4	1		
6	B	1	Total	C	F	N	O	S	0	0
			33	22	1	5	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	4	Total	Cl	0	0
			4	4		

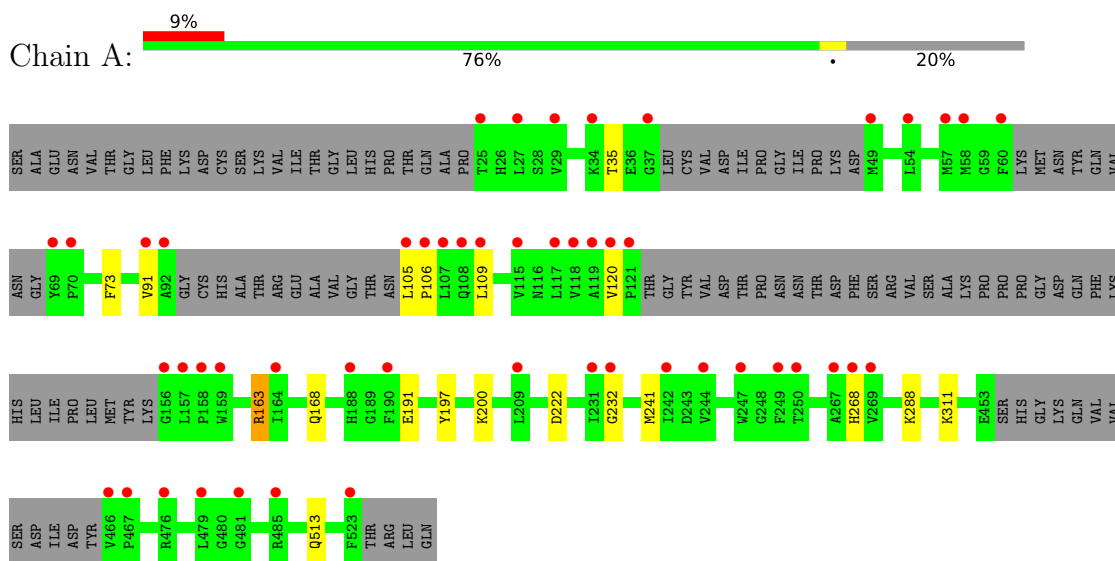
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	88	Total	O	0	0
			88	88		
8	B	103	Total	O	0	0
			103	103		

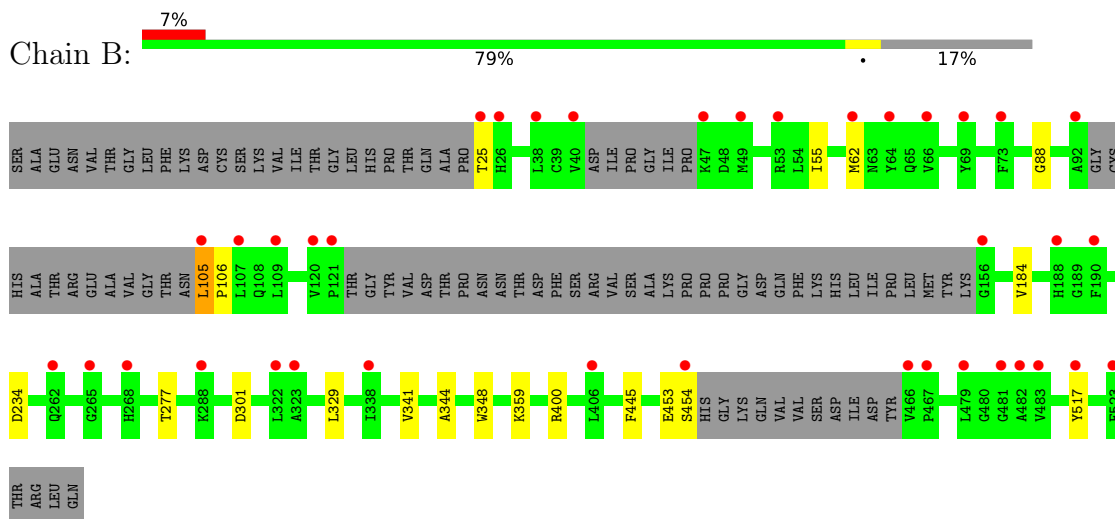
3 Residue-property plots [i](#)

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: Guanine-N7 methyltransferase nsp14



• Molecule 1: Guanine-N7 methyltransferase nsp14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.45Å 101.07Å 90.47Å 90.00° 108.43° 90.00°	Depositor
Resolution (Å)	65.51 – 2.18 65.51 – 2.18	Depositor EDS
% Data completeness (in resolution range)	69.5 (65.51-2.18) 69.4 (65.51-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.190 , 0.244 0.192 , 0.244	Depositor DCC
R_{free} test set	1019 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7252	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, IMD, SAH, YDT, ZN

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	1.01	0/3490	1.40	0/4736
1	B	1.03	0/3601	1.40	2/4886 (0.0%)
All	All	1.02	0/7091	1.40	2/9622 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	88	GLY	CA-C-O	-5.41	116.65	121.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	GLY	Peptide

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	3395	0	3287	5	0
1	B	3504	0	3397	8	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
4	A	8	0	12	0	0
5	A	5	0	5	0	0
5	B	20	0	17	2	0
6	A	33	0	0	0	0
6	B	33	0	0	0	0
7	B	4	0	0	0	0
8	A	88	0	0	1	0
8	B	103	0	0	1	0
All	All	7252	0	6756	13	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 1.

All (13) 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:163:ARG:NH1	1:A:197:TYR:O	2.30	0.64
1:A:106:PRO:HB3	1:A:120:VAL:HG12	1.82	0.61
1:A:513:GLN:NE2	8:A:701:HOH:O	2.33	0.60
1:B:341:VAL:HG12	1:B:344:ALA:HB2	1.90	0.53
1:B:445:PHE:CD2	5:B:613:IMD:H2	2.44	0.52
1:A:91:VAL:HG22	1:A:109:LEU:HD23	1.92	0.52
1:B:445:PHE:CE2	5:B:613:IMD:H2	2.46	0.50
1:B:55:ILE:HG21	1:B:62:MET:HG2	1.99	0.44
1:B:400:ARG:NE	8:B:701:HOH:O	2.33	0.43
1:B:105:LEU:HG	1:B:106:PRO:HD2	2.01	0.43
1:B:329:LEU:HD22	1:B:348:TRP:CE2	2.54	0.43
1:B:184:VAL:HG12	1:B:277:THR:HG22	2.01	0.41
1:A:73:PHE:HA	1:A:241:MET:O	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/528 (78%)	398 (97%)	11 (3%)	1 (0%)	43	49
1	B	426/528 (81%)	411 (96%)	15 (4%)	0	100	100
All	All	836/1056 (79%)	809 (97%)	26 (3%)	1 (0%)	48	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	HIS

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	369/461 (80%)	360 (98%)	9 (2%)	43	55
1	B	382/461 (83%)	375 (98%)	7 (2%)	51	65
All	All	751/922 (82%)	735 (98%)	16 (2%)	47	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	105	LEU
1	A	163	ARG
1	A	168	GLN
1	A	191	GLU

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Mol	Chain	Res	Type
1	A	200	LYS
1	A	222	ASP
1	A	288	LYS
1	A	311	LYS
1	B	25	THR
1	B	105	LEU
1	B	301	ASP
1	B	359	LYS
1	B	453	GLU
1	B	454	SER
1	B	517	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	GLN
1	B	256	ASN

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](#)

Of 22 ligands modelled in this entry, 11 are monoatomic - leaving 11 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	$\# Z > 2$
4	EDO	A	606	-	3,3,3	0.14	0	2,2,2	0.22	0
5	IMD	B	605	2	5,5,5	0.24	0	5,5,5	0.55	0
6	YDT	B	614	-	34,37,37	1.87	8 (23%)	44,56,56	2.83	16 (36%)
3	SAH	A	604	-	27,28,28	0.43	0	36,40,40	0.53	0
5	IMD	A	607	-	5,5,5	0.21	0	5,5,5	0.57	0
6	YDT	A	608	-	34,37,37	2.21	9 (26%)	44,56,56	2.76	19 (43%)
5	IMD	B	604	2	5,5,5	0.14	0	5,5,5	0.47	0
3	SAH	B	607	-	27,28,28	0.53	1 (3%)	36,40,40	0.74	1 (2%)
5	IMD	B	606	2	5,5,5	0.22	0	5,5,5	0.52	0
4	EDO	A	605	-	3,3,3	0.26	0	2,2,2	0.32	0
5	IMD	B	613	-	5,5,5	0.30	0	5,5,5	0.48	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	EDO	A	606	-	-	1/1/1/1	-
5	IMD	B	605	2	-	-	0/1/1/1
6	YDT	B	614	-	-	2/19/30/30	0/5/5/5
3	SAH	A	604	-	-	4/15/31/31	0/3/3/3
5	IMD	A	607	-	-	-	0/1/1/1
6	YDT	A	608	-	-	3/19/30/30	0/5/5/5
5	IMD	B	604	2	-	-	0/1/1/1
3	SAH	B	607	-	-	2/15/31/31	0/3/3/3
5	IMD	B	606	2	-	-	0/1/1/1
4	EDO	A	605	-	-	1/1/1/1	-
5	IMD	B	613	-	-	-	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	608	YDT	C13-N4	-6.38	1.41	1.47
6	A	608	YDT	C7-C6	-5.97	1.33	1.40
6	B	614	YDT	C11-N10	-5.62	1.29	1.35
6	B	614	YDT	C7-C6	-5.27	1.34	1.40
6	A	608	YDT	C11-N10	-5.13	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	614	YDT	N10-N8	2.93	1.42	1.36
6	A	608	YDT	C5-N4	-2.85	1.44	1.47
6	A	608	YDT	O1-S2	-2.56	1.40	1.43
6	B	614	YDT	O31-C30	-2.36	1.34	1.37
6	A	608	YDT	N10-N8	2.30	1.41	1.36
3	B	607	SAH	OXT-C	-2.26	1.23	1.30
6	A	608	YDT	O31-C32	-2.25	1.35	1.38
6	B	614	YDT	C21-N23	2.25	1.37	1.33
6	A	608	YDT	O31-C30	-2.21	1.34	1.37
6	B	614	YDT	C34-C30	2.12	1.42	1.39
6	A	608	YDT	C7-N8	2.12	1.37	1.33
6	B	614	YDT	O31-C32	-2.07	1.35	1.38
6	B	614	YDT	C11-C6	2.04	1.40	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	614	YDT	C12-C13-N4	7.46	116.20	109.21
6	A	608	YDT	O31-C30-C34	-7.21	106.01	110.29
6	A	608	YDT	C12-C11-C6	-6.27	120.83	125.65
6	A	608	YDT	C30-O31-C32	6.05	111.28	105.19
6	B	614	YDT	C30-O31-C32	6.01	111.24	105.19
6	B	614	YDT	O31-C30-C34	-6.01	106.72	110.29
6	B	614	YDT	C6-C7-N8	-5.58	106.56	111.45
6	A	608	YDT	C12-C13-N4	5.23	114.11	109.21
6	B	614	YDT	C29-C30-C34	-5.05	119.69	124.10
6	B	614	YDT	O31-C30-C29	4.57	133.59	125.99
6	A	608	YDT	O31-C30-C29	4.50	133.47	125.99
6	B	614	YDT	C5-N4-C13	4.48	119.94	113.34
6	B	614	YDT	C20-C19-C14	-4.23	126.23	132.34
6	A	608	YDT	O3-S2-N4	4.12	114.44	107.26
6	A	608	YDT	C29-C30-C34	-4.10	120.52	124.10
6	B	614	YDT	C11-N10-N8	-4.03	105.47	111.02
6	B	614	YDT	C21-C16-N17	4.02	127.94	122.81
6	A	608	YDT	C11-N10-N8	-3.88	105.67	111.02
6	B	614	YDT	C12-C11-C6	-3.73	122.79	125.65
6	A	608	YDT	C5-N4-C13	3.72	118.82	113.34
6	B	614	YDT	C20-C19-N17	3.54	125.47	122.18
6	A	608	YDT	C6-C7-N8	-3.52	108.37	111.45
3	B	607	SAH	OXT-C-O	-3.52	116.10	124.08
6	A	608	YDT	C25-C24-N23	-3.13	104.84	111.26
6	B	614	YDT	C7-N8-N10	2.77	109.34	105.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	608	YDT	C5-N4-S2	2.76	122.69	117.08
6	A	608	YDT	C16-C21-N23	2.62	122.12	117.20
6	B	614	YDT	O31-C32-C33	-2.58	110.37	112.49
6	A	608	YDT	O3-S2-C14	-2.48	103.45	107.98
6	A	608	YDT	C20-C19-C14	-2.45	128.80	132.34
6	B	614	YDT	O3-S2-N4	2.39	111.43	107.26
6	B	614	YDT	O1-S2-C14	-2.39	103.61	107.98
6	A	608	YDT	C34-C33-C32	-2.25	104.80	106.36
6	A	608	YDT	C30-C34-C33	2.25	107.07	105.41
6	A	608	YDT	O3-S2-O1	-2.11	116.66	119.69
6	A	608	YDT	O1-S2-N4	2.06	110.86	107.26

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	SAH	N-CA-CB-CG
3	A	604	SAH	C-CA-CB-CG
3	B	607	SAH	N-CA-CB-CG
3	B	607	SAH	C-CA-CB-CG
6	A	608	YDT	C13-N4-S2-O3
4	A	605	EDO	O1-C1-C2-O2
4	A	606	EDO	O1-C1-C2-O2
6	A	608	YDT	C13-N4-S2-O1
6	B	614	YDT	C13-N4-S2-O3
3	A	604	SAH	O-C-CA-CB
3	A	604	SAH	OXT-C-CA-CB
6	A	608	YDT	C13-N4-S2-C14
6	B	614	YDT	C13-N4-S2-C14

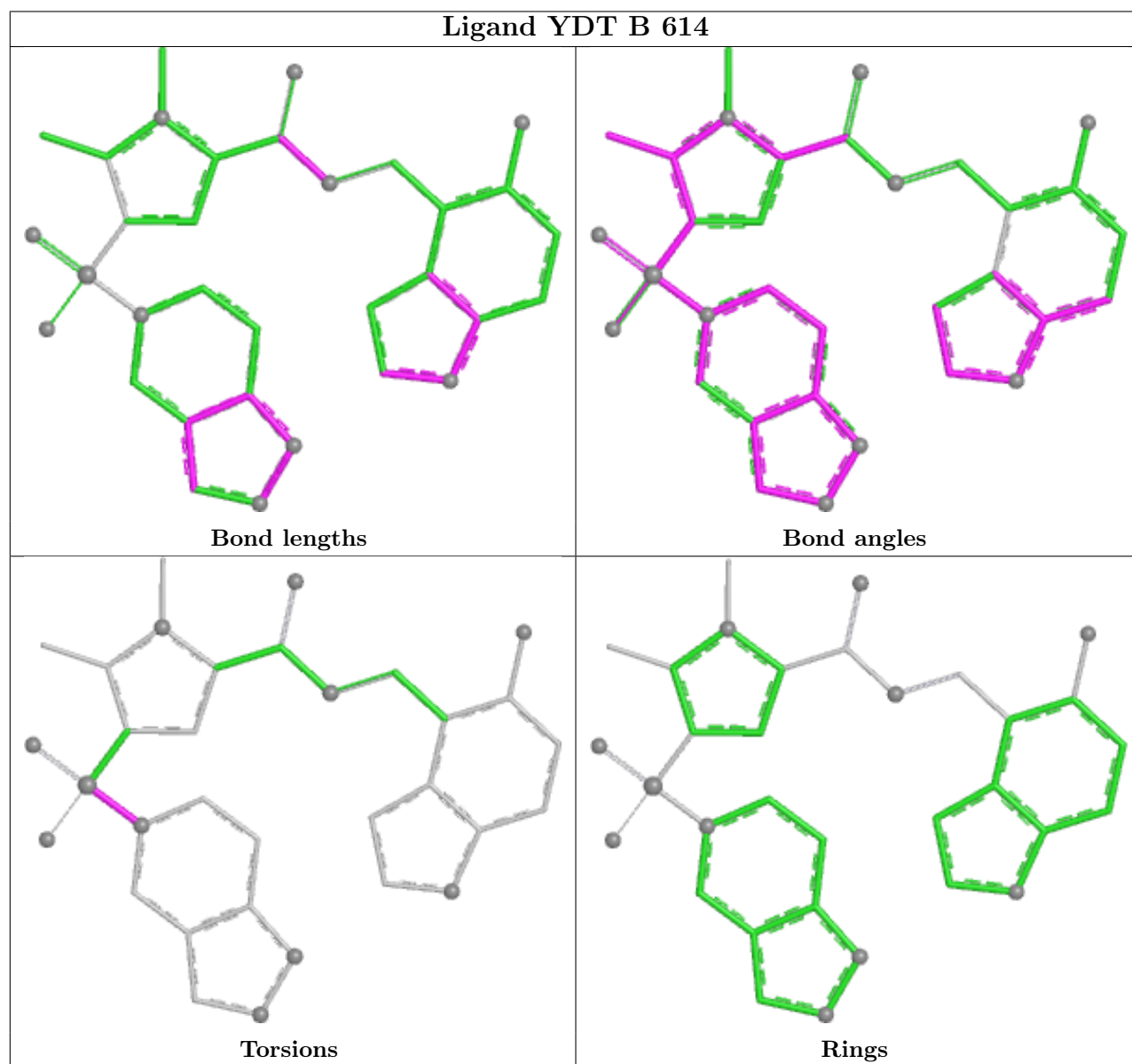
There are no ring outliers.

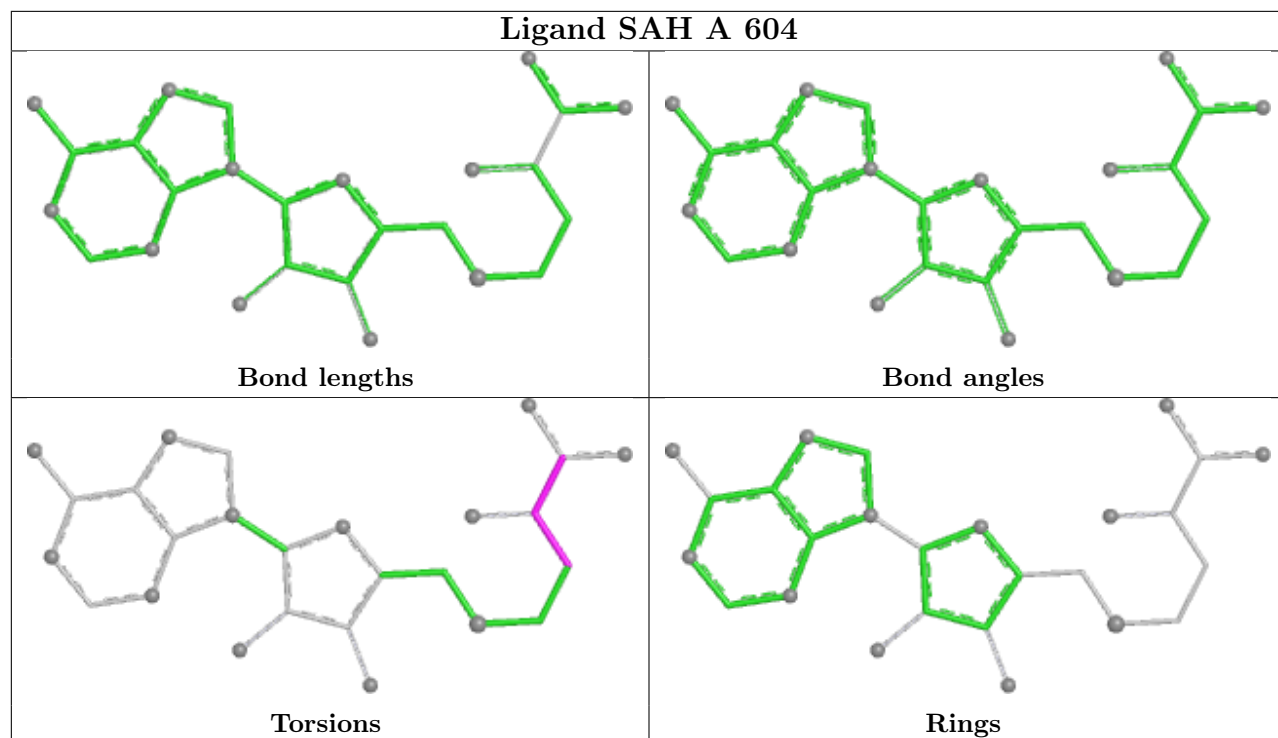
1 monomer is involved in 2 short contacts:

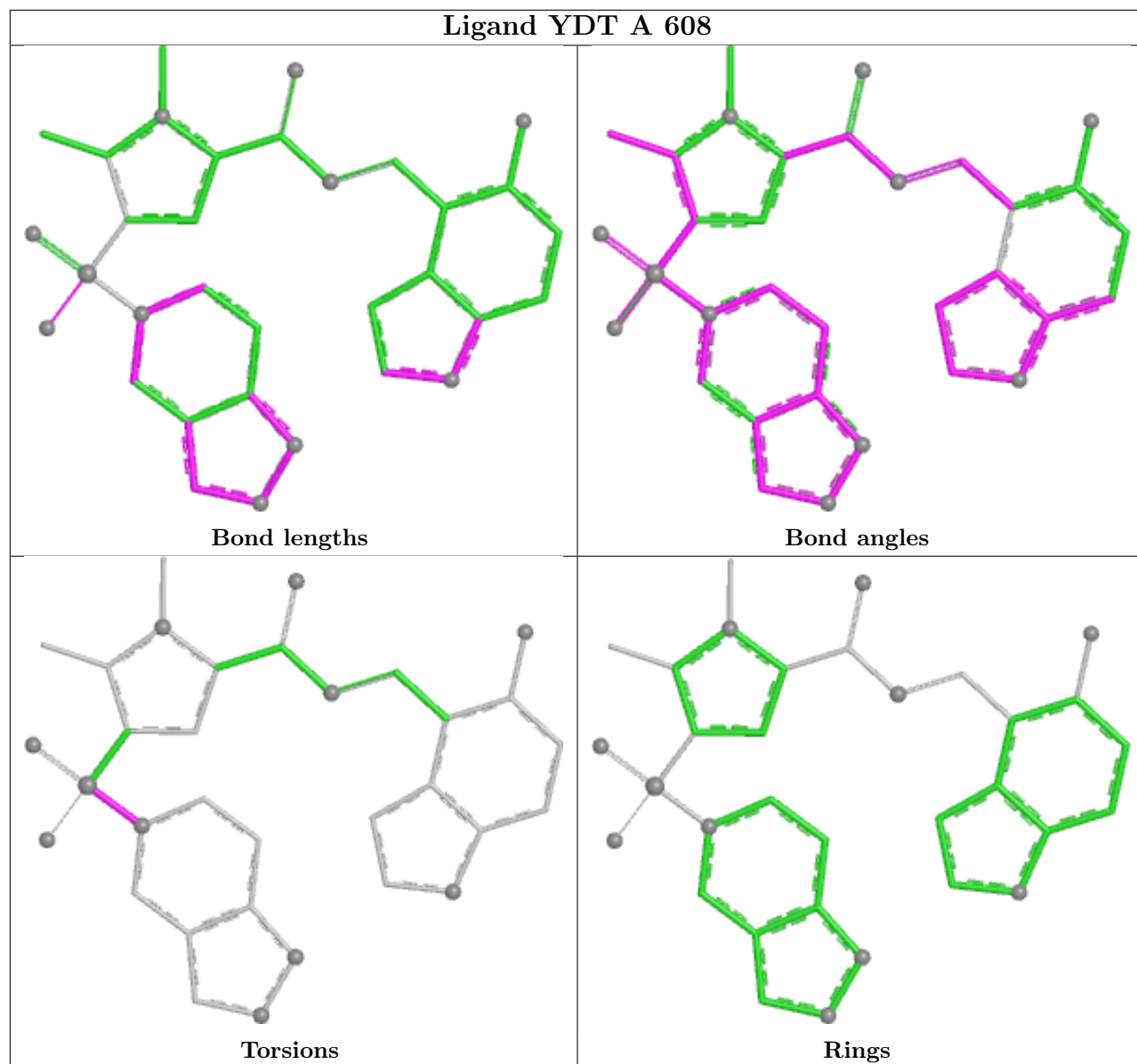
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	613	IMD	2	0

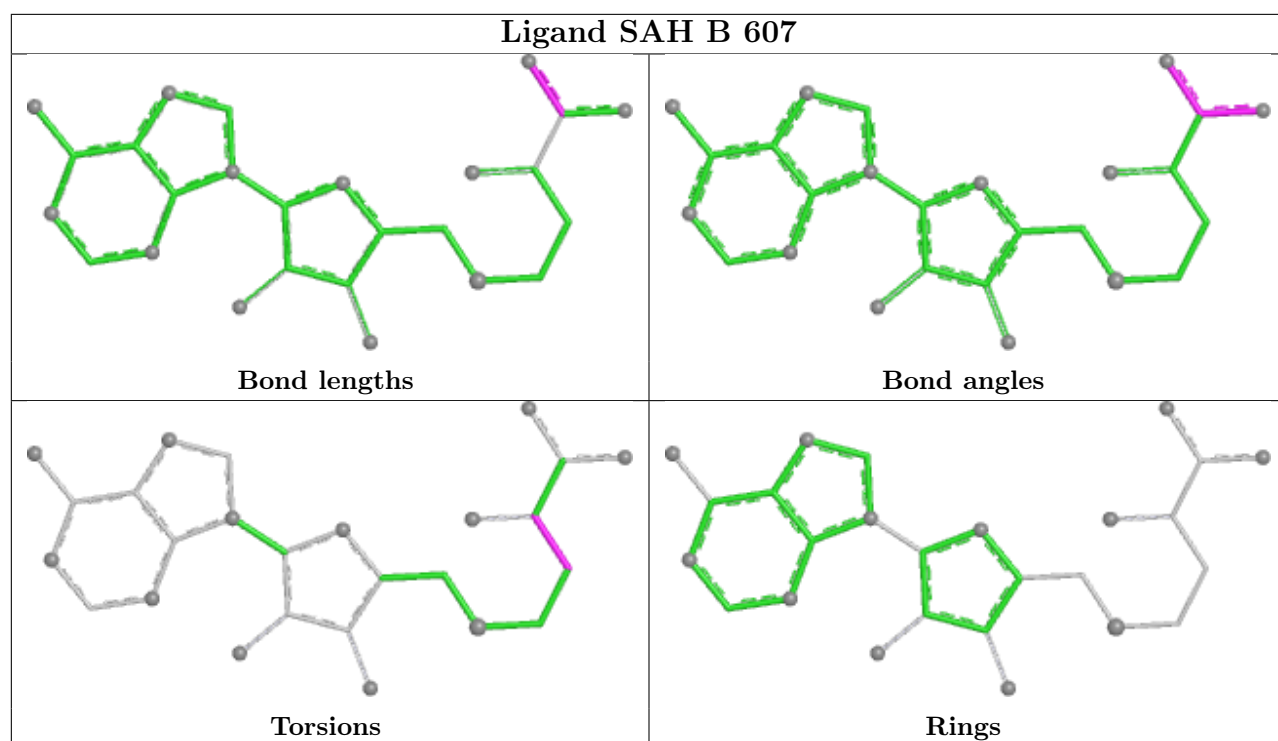
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	422/528 (79%)	0.65	50 (11%)	9 8	39, 65, 115, 166	4 (0%)
1	B	436/528 (82%)	0.54	38 (8%)	16 15	36, 59, 107, 133	2 (0%)
All	All	858/1056 (81%)	0.60	88 (10%)	12 11	36, 63, 111, 166	6 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	517	TYR	7.3
1	A	105	LEU	6.8
1	B	40	VAL	6.2
1	B	466	VAL	5.5
1	A	466	VAL	5.3
1	B	105	LEU	5.1
1	A	107	LEU	4.6
1	B	47	LYS	4.5
1	A	267	ALA	4.5
1	A	121	PRO	4.3
1	B	121	PRO	4.3
1	A	479	LEU	4.1
1	A	60	PHE	3.8
1	A	106	PRO	3.8
1	A	120	VAL	3.8
1	B	190	PHE	3.7
1	B	120	VAL	3.7
1	A	58	MET	3.6
1	A	268	HIS	3.6
1	A	92	ALA	3.6
1	B	482	ALA	3.6
1	B	467	PRO	3.6
1	B	66	VAL	3.5
1	A	156	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	92	ALA	3.4
1	B	268	HIS	3.3
1	B	107	LEU	3.3
1	A	109	LEU	3.3
1	A	249	PHE	3.3
1	B	38	LEU	3.2
1	B	73	PHE	3.1
1	A	467	PRO	3.1
1	A	34	LYS	3.0
1	B	64	TYR	2.9
1	A	118	VAL	2.9
1	B	338	ILE	2.8
1	A	37	GLY	2.8
1	B	262	GLN	2.8
1	A	481	GLY	2.8
1	A	209	LEU	2.8
1	A	91	VAL	2.8
1	A	188	HIS	2.7
1	B	523	PHE	2.7
1	A	108	GLN	2.7
1	A	27	LEU	2.7
1	B	25	THR	2.7
1	B	479	LEU	2.7
1	B	323	ALA	2.6
1	B	69	TYR	2.6
1	B	483	VAL	2.6
1	A	159	TRP	2.6
1	B	322	LEU	2.6
1	B	481	GLY	2.5
1	A	242	ILE	2.5
1	B	188	HIS	2.5
1	B	265	GLY	2.5
1	A	29	VAL	2.5
1	A	158	PRO	2.5
1	A	523	PHE	2.5
1	B	109	LEU	2.4
1	A	190	PHE	2.4
1	A	54	LEU	2.4
1	A	244	VAL	2.4
1	A	231	ILE	2.4
1	A	69	TYR	2.3
1	B	156	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	269	VAL	2.3
1	A	485	ARG	2.3
1	A	49	MET	2.3
1	A	164	ILE	2.3
1	A	70	PRO	2.3
1	A	476	ARG	2.3
1	A	250	THR	2.2
1	B	53	ARG	2.2
1	B	62	MET	2.2
1	A	247	TRP	2.2
1	B	49	MET	2.2
1	A	232	GLY	2.2
1	A	25	THR	2.2
1	A	57	MET	2.2
1	A	119	ALA	2.1
1	A	117	LEU	2.1
1	A	157	LEU	2.1
1	B	288	LYS	2.1
1	B	454	SER	2.1
1	A	115	VAL	2.1
1	B	406	LEU	2.0
1	B	26	HIS	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
5	IMD	B	606	5/5	0.88	0.21	110,111,116,120	0

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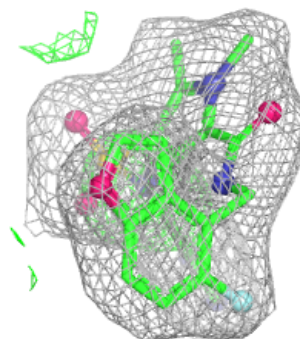
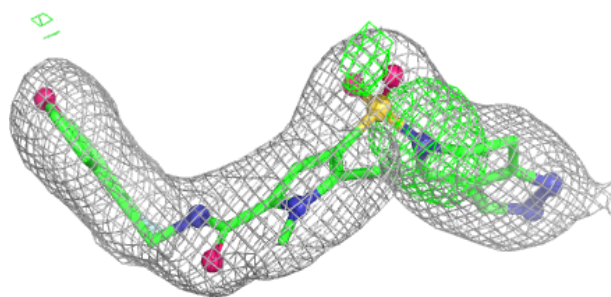
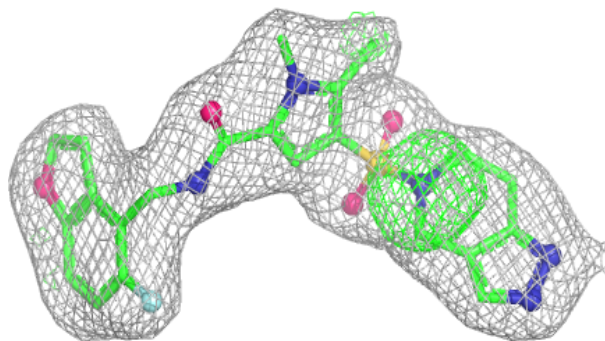
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	605	4/4	0.91	0.13	62,78,81,84	0
7	CL	B	609	1/1	0.91	0.14	86,86,86,86	0
5	IMD	B	604	5/5	0.92	0.12	72,73,74,76	0
5	IMD	B	613	5/5	0.92	0.15	73,77,79,80	0
5	IMD	B	605	5/5	0.92	0.10	64,64,67,69	0
5	IMD	A	607	5/5	0.93	0.12	60,60,62,69	0
4	EDO	A	606	4/4	0.93	0.21	64,71,72,72	0
7	CL	B	608	1/1	0.95	0.09	85,85,85,85	0
6	YDT	A	608	33/33	0.95	0.08	37,44,54,61	1
7	CL	B	610	1/1	0.95	0.10	71,71,71,71	0
3	SAH	B	607	26/26	0.96	0.07	45,50,55,59	0
7	CL	B	611	1/1	0.96	0.08	81,81,81,81	0
3	SAH	A	604	26/26	0.97	0.06	36,46,51,52	0
2	ZN	B	603	1/1	0.98	0.04	83,83,83,83	0
6	YDT	B	614	33/33	0.98	0.06	36,49,62,65	0
2	ZN	B	612	1/1	0.99	0.08	87,87,87,87	0
2	ZN	A	602	1/1	0.99	0.03	62,62,62,62	0
2	ZN	A	603	1/1	0.99	0.03	75,75,75,75	0
2	ZN	A	601	1/1	0.99	0.03	66,66,66,66	0
2	ZN	B	602	1/1	1.00	0.03	51,51,51,51	0
2	ZN	B	601	1/1	1.00	0.02	51,51,51,51	0

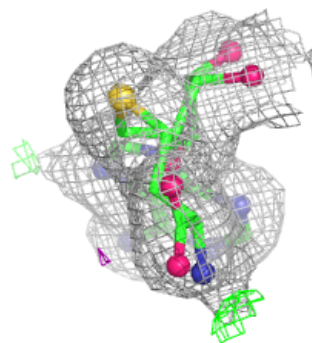
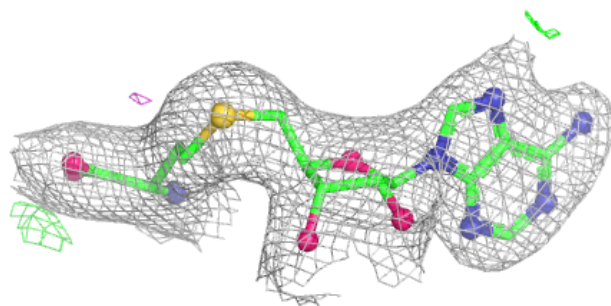
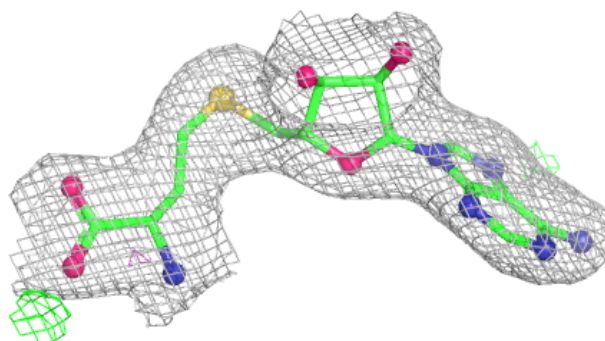
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YDT A 608:

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

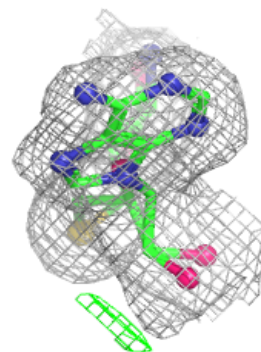
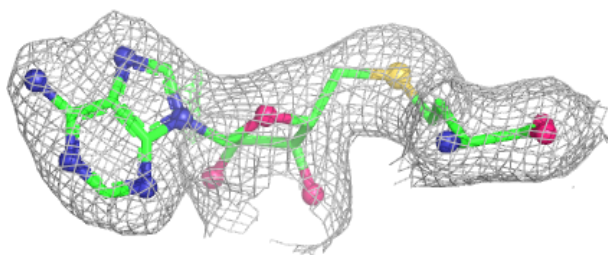
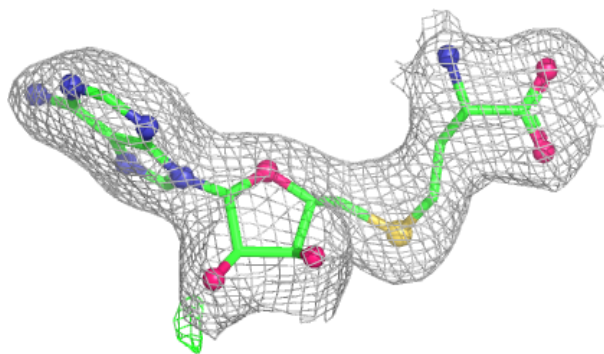
**Electron density around SAH B 607:**

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

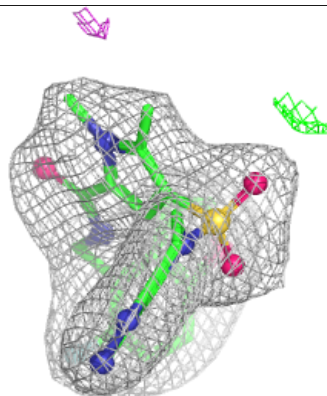
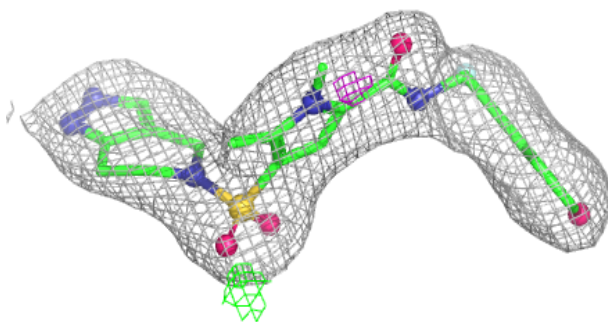
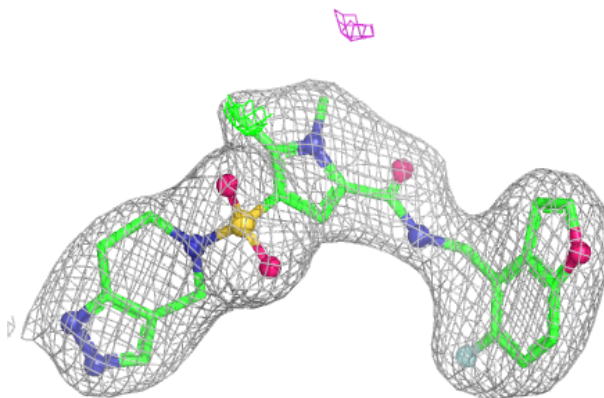


Electron density around SAH A 604:

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

**Electron density around YDT B 614:**

$2mF_o-DF_c$ (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.