



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 10:14 am BST

PDB ID : 5LV2
Title : Crystal structure of mouse CARM1 in complex with inhibitor LH1246
Authors : Cura, V.; Marechal, N.; Troffer-Charlier, N.; Halby, L.; Arimondo, P.; Bonnefond, L.; Cavarelli, J.
Deposited on : 2016-09-12
Resolution : 2.29 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

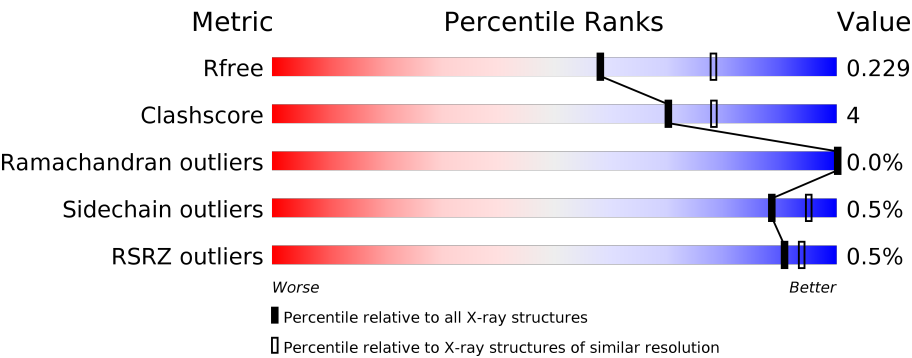
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	361	<div><div>%</div><div><div></div><div>85%</div><div>10%</div><div>5%</div></div></div>
1	B	361	<div><div>%</div><div><div></div><div>84%</div><div>11%</div><div>5%</div></div></div>
1	C	361	<div><div>%</div><div><div></div><div>88%</div><div>6%</div><div>5%</div></div></div>
1	D	361	<div><div></div><div><div></div><div>85%</div><div>9%</div><div>5%</div></div></div>
1	E	361	<div><div></div><div><div></div><div>86%</div><div>8%</div><div>5%</div></div></div>
1	F	361	<div><div></div><div><div></div><div>86%</div><div>9%</div><div>5%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	361	<div><div>%</div><div><div></div><div></div><div></div></div><div>90%5%5%</div></div>
1	H	361	<div><div>%</div><div><div></div><div></div><div></div></div><div>86%9%6%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 45590 atoms, of which 22013 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	H	N	O	S	0	0	0
			5450	1776	2699	454	507	14			
1	B	343	Total	C	H	N	O	S	0	2	0
			5479	1784	2714	460	507	14			
1	C	343	Total	C	H	N	O	S	0	2	0
			5463	1780	2704	455	510	14			
1	D	342	Total	C	H	N	O	S	0	2	0
			5461	1778	2706	457	506	14			
1	E	343	Total	C	H	N	O	S	0	2	0
			5468	1781	2709	455	508	15			
1	F	343	Total	C	H	N	O	S	0	2	0
			5478	1783	2715	458	507	15			
1	G	343	Total	C	H	N	O	S	0	2	0
			5475	1782	2713	458	508	14			
1	H	341	Total	C	H	N	O	S	0	0	0
			5415	1763	2683	452	503	14			

There are 24 discrepancies between the modelled and reference sequences:

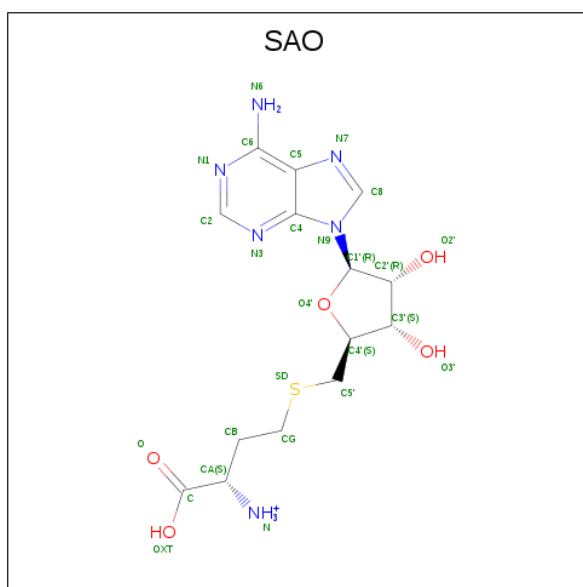
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	expression tag	UNP Q9WVG6
A	128	HIS	-	expression tag	UNP Q9WVG6
A	129	MET	-	expression tag	UNP Q9WVG6
B	127	GLY	-	expression tag	UNP Q9WVG6
B	128	HIS	-	expression tag	UNP Q9WVG6
B	129	MET	-	expression tag	UNP Q9WVG6
C	127	GLY	-	expression tag	UNP Q9WVG6
C	128	HIS	-	expression tag	UNP Q9WVG6
C	129	MET	-	expression tag	UNP Q9WVG6
D	127	GLY	-	expression tag	UNP Q9WVG6
D	128	HIS	-	expression tag	UNP Q9WVG6
D	129	MET	-	expression tag	UNP Q9WVG6
E	127	GLY	-	expression tag	UNP Q9WVG6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	128	HIS	-	expression tag	UNP Q9WVG6
E	129	MET	-	expression tag	UNP Q9WVG6
F	127	GLY	-	expression tag	UNP Q9WVG6
F	128	HIS	-	expression tag	UNP Q9WVG6
F	129	MET	-	expression tag	UNP Q9WVG6
G	127	GLY	-	expression tag	UNP Q9WVG6
G	128	HIS	-	expression tag	UNP Q9WVG6
G	129	MET	-	expression tag	UNP Q9WVG6
H	127	GLY	-	expression tag	UNP Q9WVG6
H	128	HIS	-	expression tag	UNP Q9WVG6
H	129	MET	-	expression tag	UNP Q9WVG6

- Molecule 2 is 5'-S-[(3S)-3-azaniumyl-3-carboxypropyl]-5'-thioadenosine (three-letter code: SAO) (formula: C₁₄H₂₁N₆O₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 46	C 14	H 20	N 6	O 5	S 1	0	0
2	C	1	Total 46	C 14	H 20	N 6	O 5	S 1	0	0
2	E	1	Total 46	C 14	H 20	N 6	O 5	S 1	0	0
2	G	1	Total 46	C 14	H 20	N 6	O 5	S 1	0	0

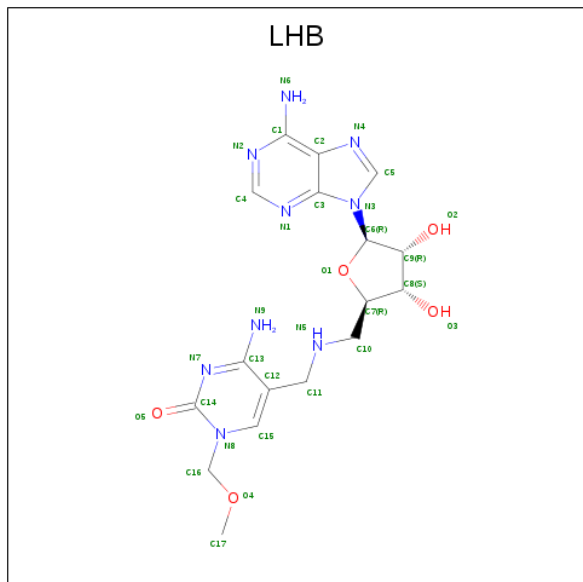
- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	E	1	Total	C	H	O	0	0
			10	2	6	2		
3	E	1	Total	C	H	O	0	0
			10	2	6	2		
3	F	1	Total	C	H	O	0	0
			10	2	6	2		
3	F	1	Total	C	H	O	0	0
			10	2	6	2		
3	G	1	Total	C	H	O	0	0
			10	2	6	2		
3	G	1	Total	C	H	O	0	0
			10	2	6	2		
3	G	1	Total	C	H	O	0	0
			10	2	6	2		
3	H	1	Total	C	H	O	0	0
			10	2	6	2		

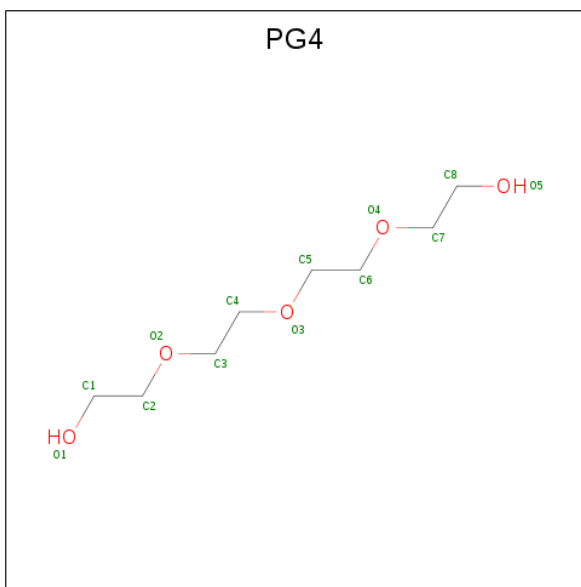
- Molecule 4 is 5-[[[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan

-2-yl[methylamino]methyl]-4-azanyl-1-(methoxymethyl)pyrimidin-2-one (three-letter code: LHB) (formula: C₁₇H₂₃N₉O₅).



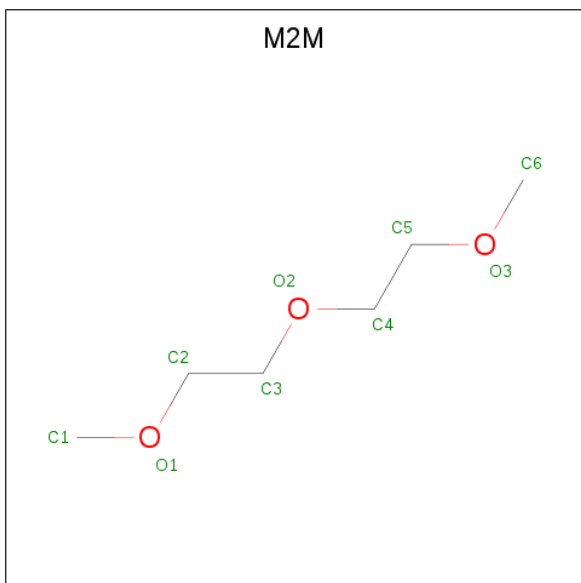
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			54	17	23	9	5		
4	D	1	Total	C	H	N	O	0	0
			54	17	23	9	5		
4	F	1	Total	C	H	N	O	0	0
			54	17	23	9	5		
4	H	1	Total	C	H	N	O	0	0
			54	17	23	9	5		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



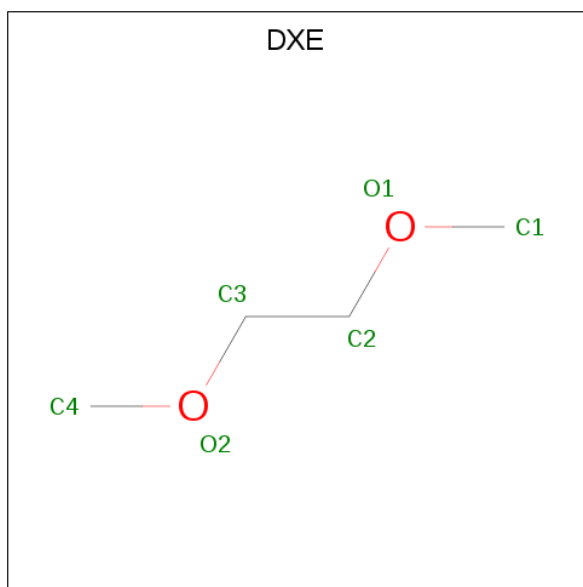
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			31	8	18	5		
5	D	1	Total	C	H	O	0	0
			31	8	18	5		
5	F	1	Total	C	H	O	0	0
			31	8	18	5		
5	F	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 6 is 1-METHOXY-2-(2-METHOXYETHOXY)ETHANE (three-letter code: M2M) (formula: $C_6H_{14}O_3$).



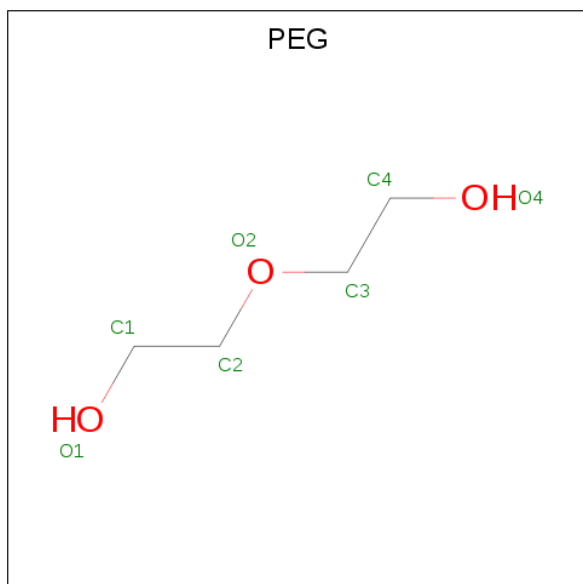
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			23	6	14	3		
6	E	1	Total	C	H	O	0	0
			23	6	14	3		

- Molecule 7 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula: C₄H₁₀O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Na	0	0
			1	1		
9	F	1	Total	Na	0	0
			1	1		

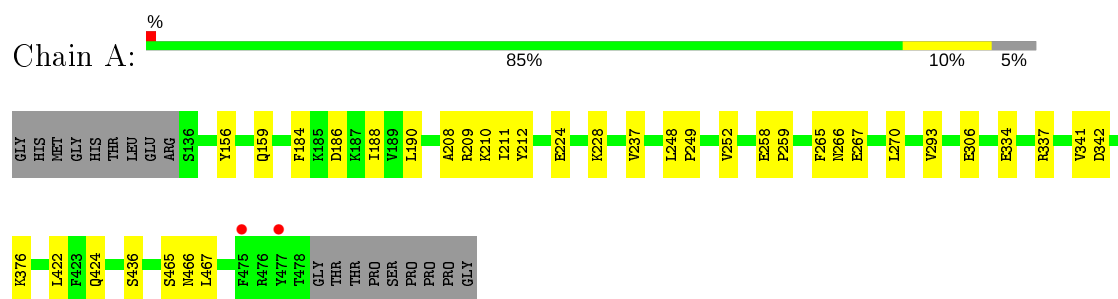
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	138	Total	O	0	0
			138	138		
10	B	115	Total	O	0	0
			115	115		
10	C	176	Total	O	0	0
			176	176		
10	D	157	Total	O	0	0
			157	157		
10	E	173	Total	O	0	0
			173	173		
10	F	163	Total	O	0	0
			163	163		
10	G	124	Total	O	0	0
			124	124		
10	H	120	Total	O	0	0
			120	120		

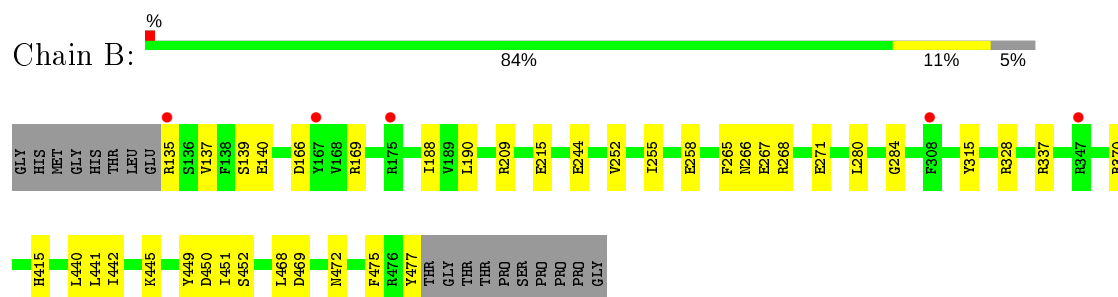
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

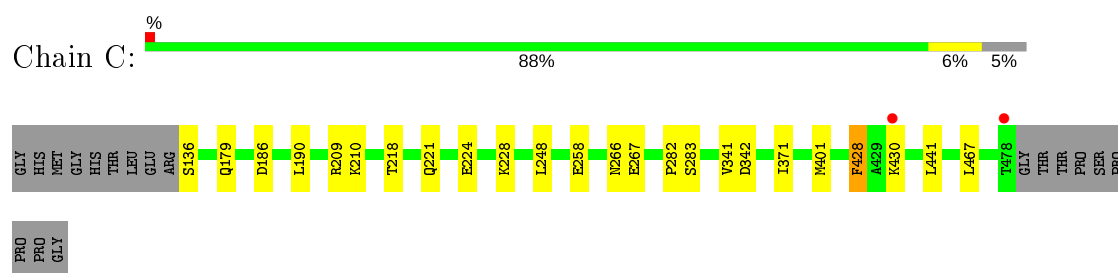
- Molecule 1: Histone-arginine methyltransferase CARM1



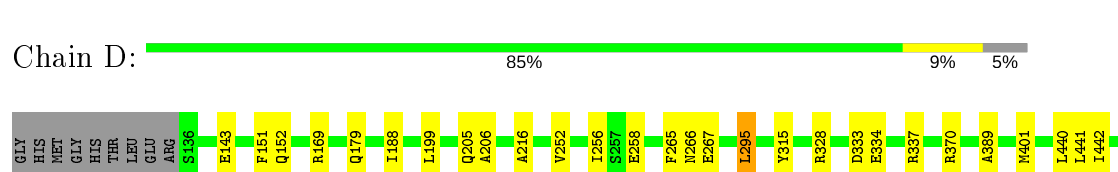
- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



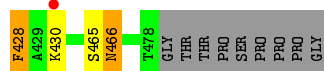
- Molecule 1: Histone-arginine methyltransferase CARM1





- Molecule 1: Histone-arginine methyltransferase CARM1

Chain E: 86% 8% 5%



- Molecule 1: Histone-arginine methyltransferase CARM1

Chain F: 86% 9% 5%



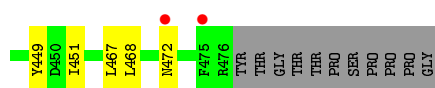
- Molecule 1: Histone-arginine methyltransferase CARM1

Chain G: 90% 5% 5%



- Molecule 1: Histone-arginine methyltransferase CARM1

Chain H: 86% 9% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.68Å 74.83Å 206.64Å 90.00° 90.53° 90.00°	Depositor
Resolution (Å)	49.34 – 2.29 49.34 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.34-2.29) 96.8 (49.34-2.29)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_1980	Depositor
R, R_{free}	0.205 , 0.238 0.195 , 0.229	Depositor DCC
R_{free} test set	6569 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 21.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.369 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	45590	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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 33.37 % 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 8.0909e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: SAO, LHB, NA, EDO, M2M, PG4, DXE, PEG

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	0.29	0/2821	0.47	0/3823
1	B	0.30	0/2852	0.45	0/3865
1	C	0.35	1/2837 (0.0%)	0.47	0/3845
1	D	0.29	0/2833	0.48	0/3838
1	E	0.34	1/2838 (0.0%)	0.47	0/3845
1	F	0.30	0/2841	0.50	1/3847 (0.0%)
1	G	0.28	0/2841	0.48	0/3849
1	H	0.29	0/2801	0.46	0/3795
All	All	0.30	2/22664 (0.0%)	0.47	1/30707 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	428	PHE	CD2-CE2	-6.91	1.25	1.39
1	E	428	PHE	CD2-CE2	-6.89	1.25	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	295	LEU	CA-CB-CG	5.67	128.35	115.30

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	2751	2699	2699	20	0
1	B	2765	2714	2702	31	0
1	C	2759	2704	2692	13	0
1	D	2755	2706	2694	27	0
1	E	2759	2709	2702	23	0
1	F	2763	2715	2705	22	0
1	G	2762	2713	2704	11	0
1	H	2732	2683	2683	23	0
2	A	26	20	0	0	0
2	C	26	20	0	0	0
2	E	26	20	0	1	0
2	G	26	20	0	2	0
3	A	4	6	6	0	0
3	B	8	12	12	0	0
3	C	4	6	6	0	0
3	D	4	6	6	0	0
3	E	8	12	12	0	0
3	F	8	12	12	0	0
3	G	12	18	18	0	0
3	H	4	6	6	0	0
4	B	31	23	0	2	0
4	D	31	23	0	1	0
4	F	31	23	0	1	0
4	H	31	23	0	1	0
5	C	13	18	18	0	0
5	D	13	18	18	0	0
5	F	26	36	36	1	0
6	C	9	14	14	0	0
6	E	9	14	14	0	0
7	C	6	10	10	0	0
8	D	7	10	10	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
10	A	138	0	0	2	0
10	B	115	0	0	2	0
10	C	176	0	0	1	0
10	D	157	0	0	2	0
10	E	173	0	0	3	0
10	F	163	0	0	1	0
10	G	124	0	0	1	0
10	H	120	0	0	4	0
All	All	23577	22013	21779	158	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.

The worst 5 of 158 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:H:258:GLU:OE2	10:H:601:HOH:O	1.69	1.11
1:G:209:ARG:NH2	10:G:601:HOH:O	1.97	0.94
1:B:209:ARG:NH1	10:B:601:HOH:O	2.03	0.90
1:E:144:GLU:OE2	10:E:601:HOH:O	1.96	0.83
1:D:205:GLN:O	1:E:430:LYS:NZ	2.15	0.79

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	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
1	B	343/361 (95%)	334 (97%)	9 (3%)	0	100	100
1	C	343/361 (95%)	334 (97%)	9 (3%)	0	100	100
1	D	342/361 (95%)	333 (97%)	9 (3%)	0	100	100
1	E	343/361 (95%)	331 (96%)	11 (3%)	1 (0%)	41	50
1	F	343/361 (95%)	333 (97%)	10 (3%)	0	100	100
1	G	343/361 (95%)	330 (96%)	13 (4%)	0	100	100
1	H	339/361 (94%)	329 (97%)	10 (3%)	0	100	100
All	All	2737/2888 (95%)	2654 (97%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	466	ASN

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	299/313 (96%)	297 (99%)	2 (1%)	84	92
1	B	301/313 (96%)	301 (100%)	0	100	100
1	C	301/313 (96%)	298 (99%)	3 (1%)	76	87
1	D	300/313 (96%)	299 (100%)	1 (0%)	92	97
1	E	301/313 (96%)	300 (100%)	1 (0%)	92	97
1	F	301/313 (96%)	300 (100%)	1 (0%)	92	97
1	G	301/313 (96%)	300 (100%)	1 (0%)	92	97
1	H	297/313 (95%)	295 (99%)	2 (1%)	84	92
All	All	2401/2504 (96%)	2390 (100%)	11 (0%)	88	95

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	467	LEU
1	D	295	LEU
1	G	258	GLU
1	C	258	GLU
1	F	295	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	415	HIS
1	E	159	GLN
1	H	149	GLN
1	H	415	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	$\# Z > 2$
5	PG4	D	502	-	12,12,12	0.50	0	11,11,11	0.43	0
2	SAO	A	501	-	21,28,28	0.64	0	20,40,40	1.11	2 (10%)
5	PG4	F	503	-	12,12,12	0.52	0	11,11,11	0.47	0
4	LHB	D	501	-	28,34,34	0.66	0	28,49,49	1.13	3 (10%)
3	EDO	B	502	-	3,3,3	0.47	0	2,2,2	0.48	0
4	LHB	H	501	-	28,34,34	0.66	0	28,49,49	1.09	3 (10%)
8	PEG	D	504	-	6,6,6	0.48	0	5,5,5	0.46	0
5	PG4	C	502	-	12,12,12	0.51	0	11,11,11	0.49	0
3	EDO	H	502	-	3,3,3	0.47	0	2,2,2	0.50	0
3	EDO	B	503	-	3,3,3	0.49	0	2,2,2	0.33	0
3	EDO	E	503	-	3,3,3	0.49	0	2,2,2	0.44	0
4	LHB	B	501	-	28,34,34	0.80	1 (3%)	28,49,49	1.32	3 (10%)
6	M2M	E	504	-	8,8,8	0.60	0	7,7,7	0.37	0
5	PG4	F	505	-	12,12,12	0.52	0	11,11,11	0.33	0
3	EDO	G	504	-	3,3,3	0.46	0	2,2,2	0.48	0
4	LHB	F	501	-	28,34,34	0.70	0	28,49,49	1.17	4 (14%)
3	EDO	F	502	-	3,3,3	0.46	0	2,2,2	0.49	0
7	DXE	C	505	-	5,5,5	0.42	0	4,4,4	0.28	0
3	EDO	G	503	-	3,3,3	0.47	0	2,2,2	0.49	0
3	EDO	F	504	-	3,3,3	0.48	0	2,2,2	0.41	0
3	EDO	E	502	-	3,3,3	0.47	0	2,2,2	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAO	C	501	-	21,28,28	0.64	0	20,40,40	1.13	2 (10%)
2	SAO	E	501	-	21,28,28	0.65	0	20,40,40	1.22	2 (10%)
3	EDO	G	502	-	3,3,3	0.45	0	2,2,2	0.52	0
3	EDO	D	503	-	3,3,3	0.47	0	2,2,2	0.47	0
2	SAO	G	501	-	21,28,28	0.65	0	20,40,40	1.16	2 (10%)
3	EDO	A	502	-	3,3,3	0.48	0	2,2,2	0.51	0
6	M2M	C	504	-	8,8,8	0.58	0	7,7,7	0.14	0
3	EDO	C	503	-	3,3,3	0.47	0	2,2,2	0.43	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
5	PG4	D	502	-	-	5/10/10/10	-
2	SAO	A	501	-	-	0/7/31/31	0/3/3/3
5	PG4	F	503	-	-	5/10/10/10	-
4	LHB	D	501	-	-	4/8/29/29	0/4/4/4
3	EDO	B	502	-	-	1/1/1/1	-
4	LHB	H	501	-	-	2/8/29/29	0/4/4/4
8	PEG	D	504	-	-	2/4/4/4	-
5	PG4	C	502	-	-	9/10/10/10	-
3	EDO	H	502	-	-	1/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	E	503	-	-	1/1/1/1	-
4	LHB	B	501	-	-	3/8/29/29	0/4/4/4
6	M2M	E	504	-	-	6/6/6/6	-
5	PG4	F	505	-	-	0/10/10/10	-
3	EDO	G	504	-	-	1/1/1/1	-
4	LHB	F	501	-	-	4/8/29/29	0/4/4/4
3	EDO	F	502	-	-	1/1/1/1	-
7	DXE	C	505	-	-	2/3/3/3	-
3	EDO	G	503	-	-	1/1/1/1	-
3	EDO	F	504	-	-	0/1/1/1	-
3	EDO	E	502	-	-	1/1/1/1	-
2	SAO	C	501	-	-	1/7/31/31	0/3/3/3
2	SAO	E	501	-	-	1/7/31/31	0/3/3/3
3	EDO	G	502	-	-	0/1/1/1	-
3	EDO	D	503	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAO	G	501	-	-	0/7/31/31	0/3/3/3
3	EDO	A	502	-	-	0/1/1/1	-
6	M2M	C	504	-	-	4/6/6/6	-
3	EDO	C	503	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	LHB	C11-C12	2.38	1.58	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	LHB	C14-N7-C13	4.09	120.95	116.02
4	H	501	LHB	C14-N7-C13	4.02	120.87	116.02
4	F	501	LHB	C14-N7-C13	3.93	120.76	116.02
2	G	501	SAO	CB-CG-SD	-3.84	104.69	113.31
4	D	501	LHB	C14-N7-C13	3.83	120.64	116.02

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

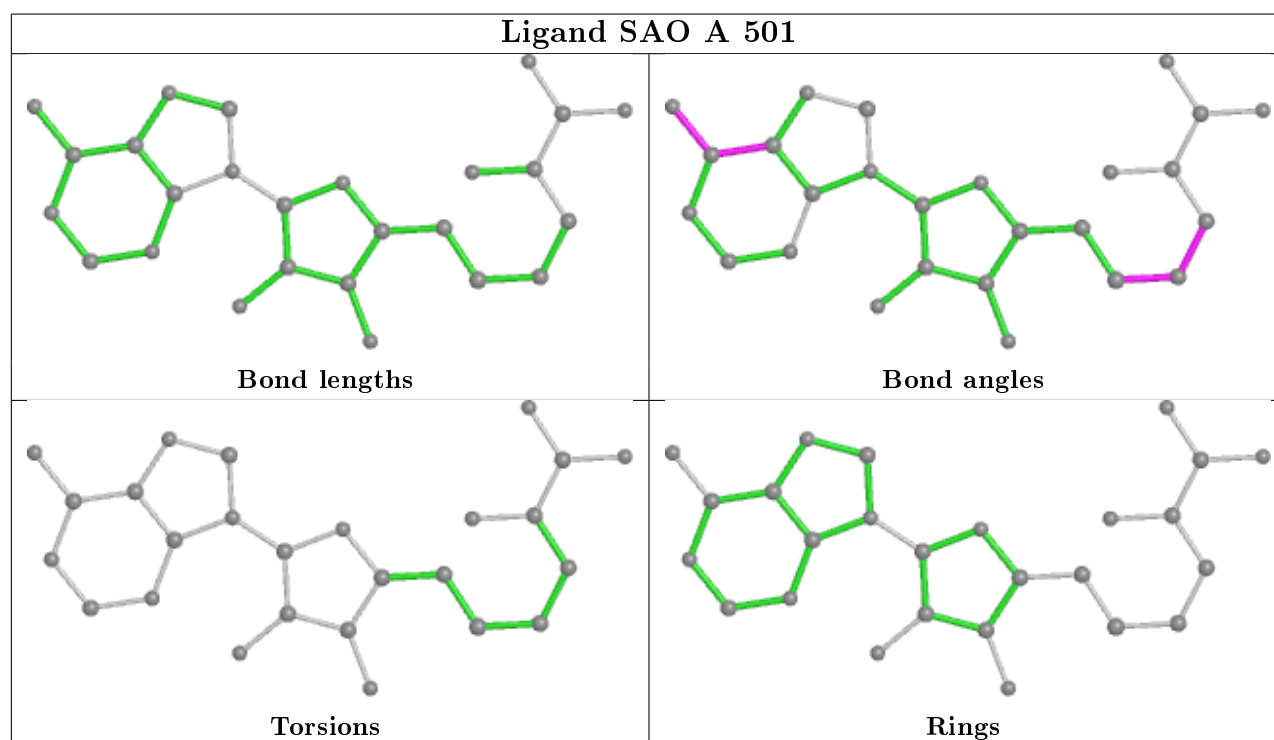
Mol	Chain	Res	Type	Atoms
4	D	501	LHB	N5-C10-C7-O1
4	D	501	LHB	N5-C10-C7-C8
4	H	501	LHB	N8-C16-O4-C17
4	B	501	LHB	O4-C16-N8-C15
5	F	503	PG4	O3-C5-C6-O4

There are no ring outliers.

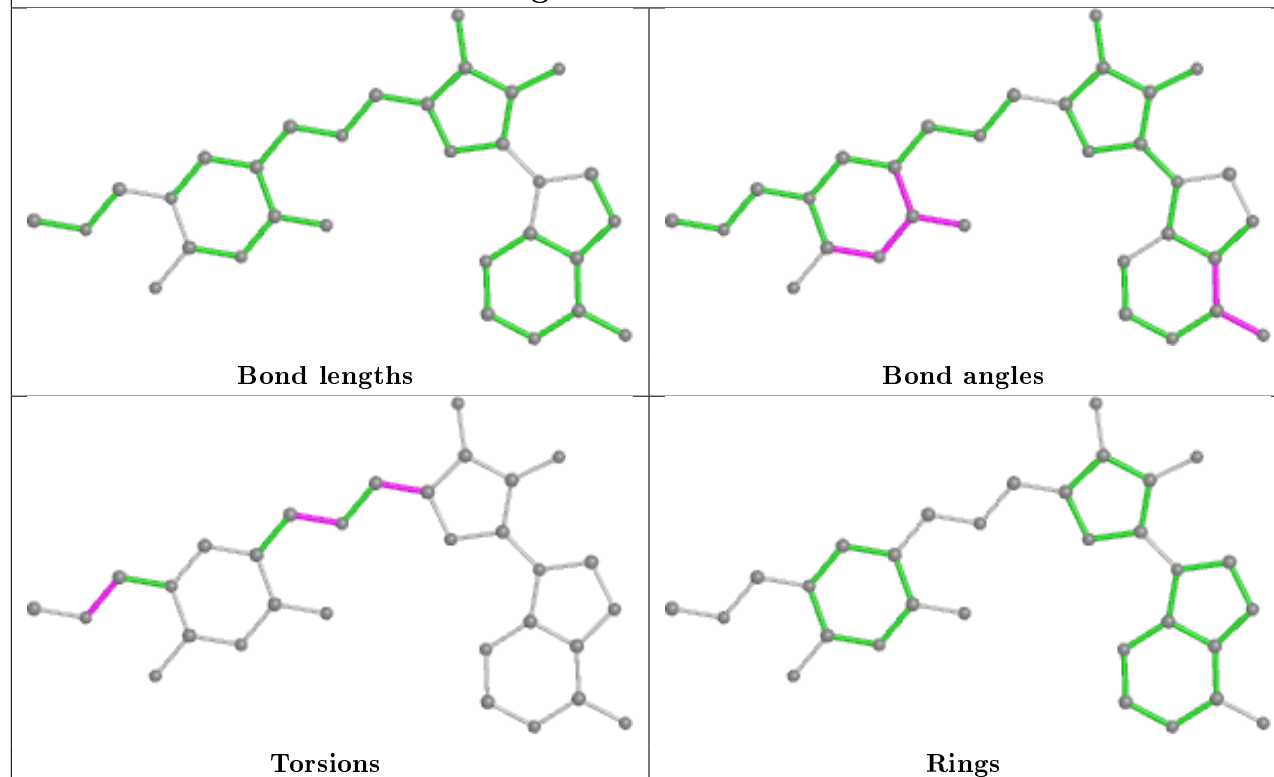
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	503	PG4	1	0
4	D	501	LHB	1	0
4	H	501	LHB	1	0
4	B	501	LHB	2	0
4	F	501	LHB	1	0
2	E	501	SAO	1	0
2	G	501	SAO	2	0

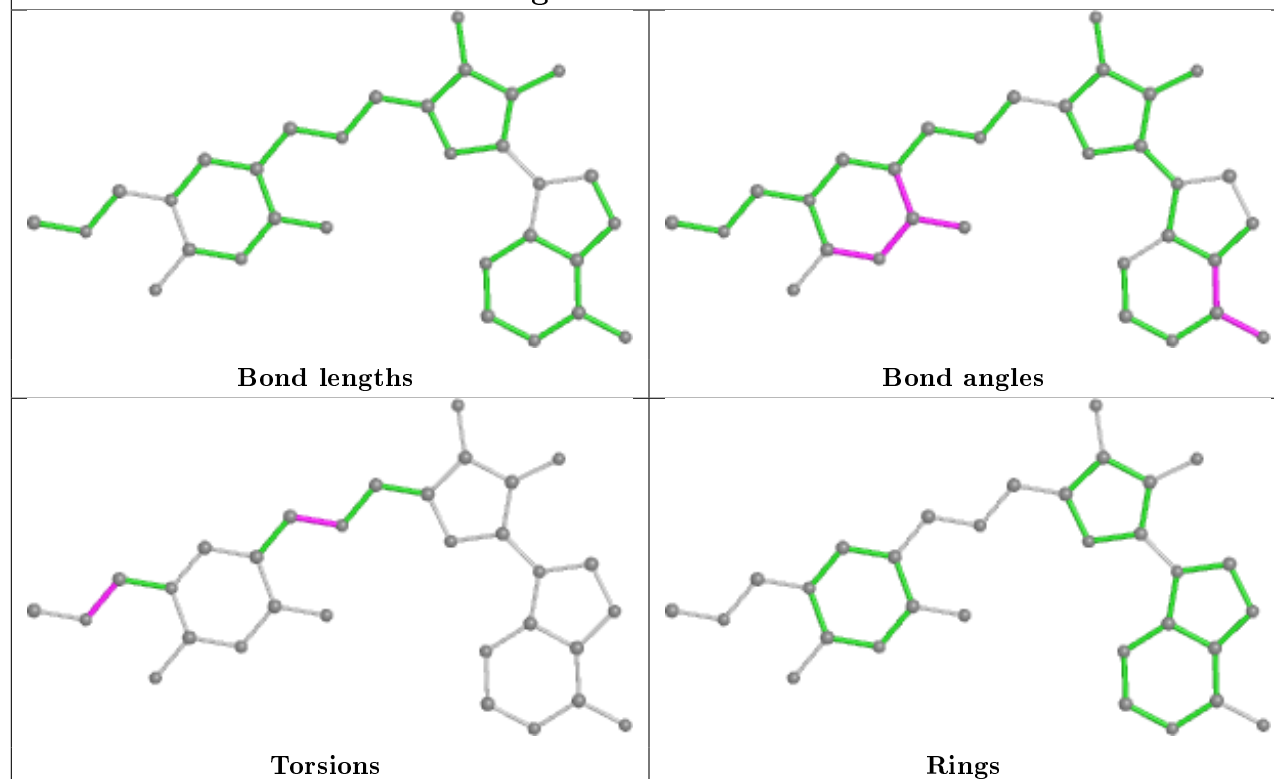
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



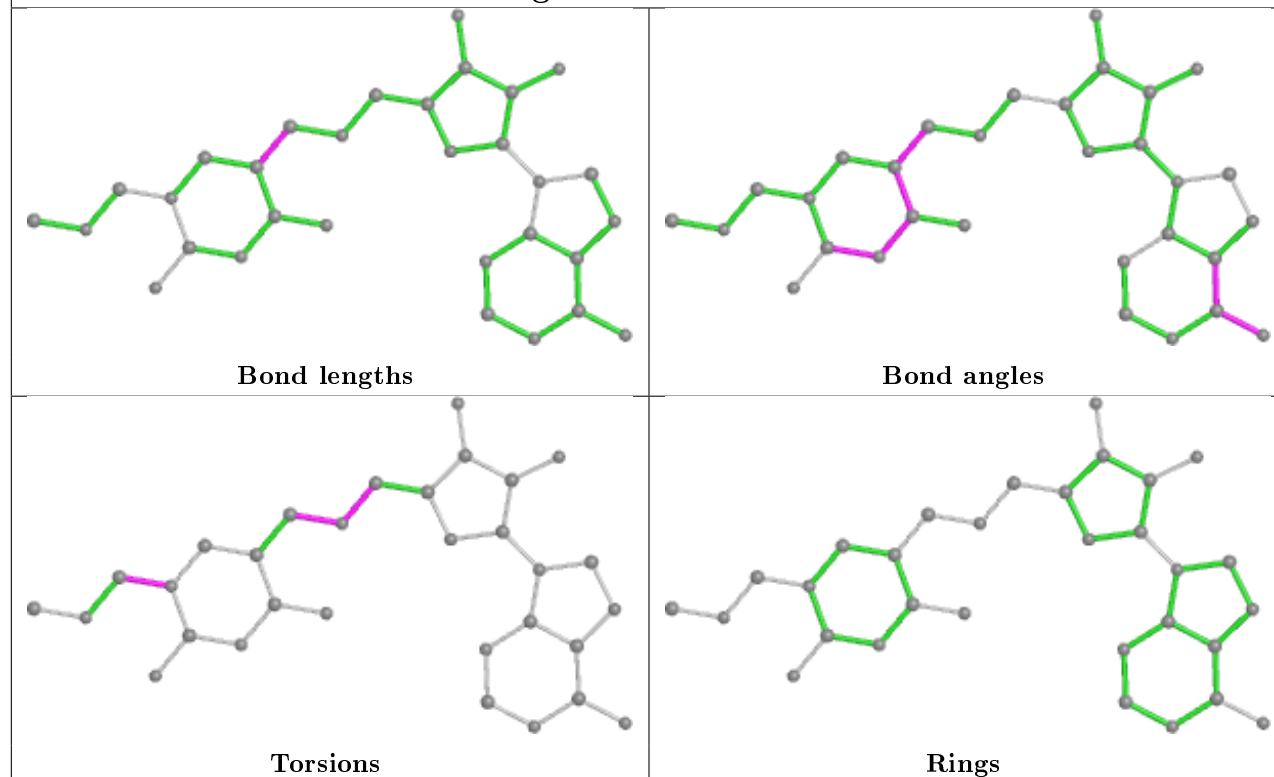
Ligand LHB D 501



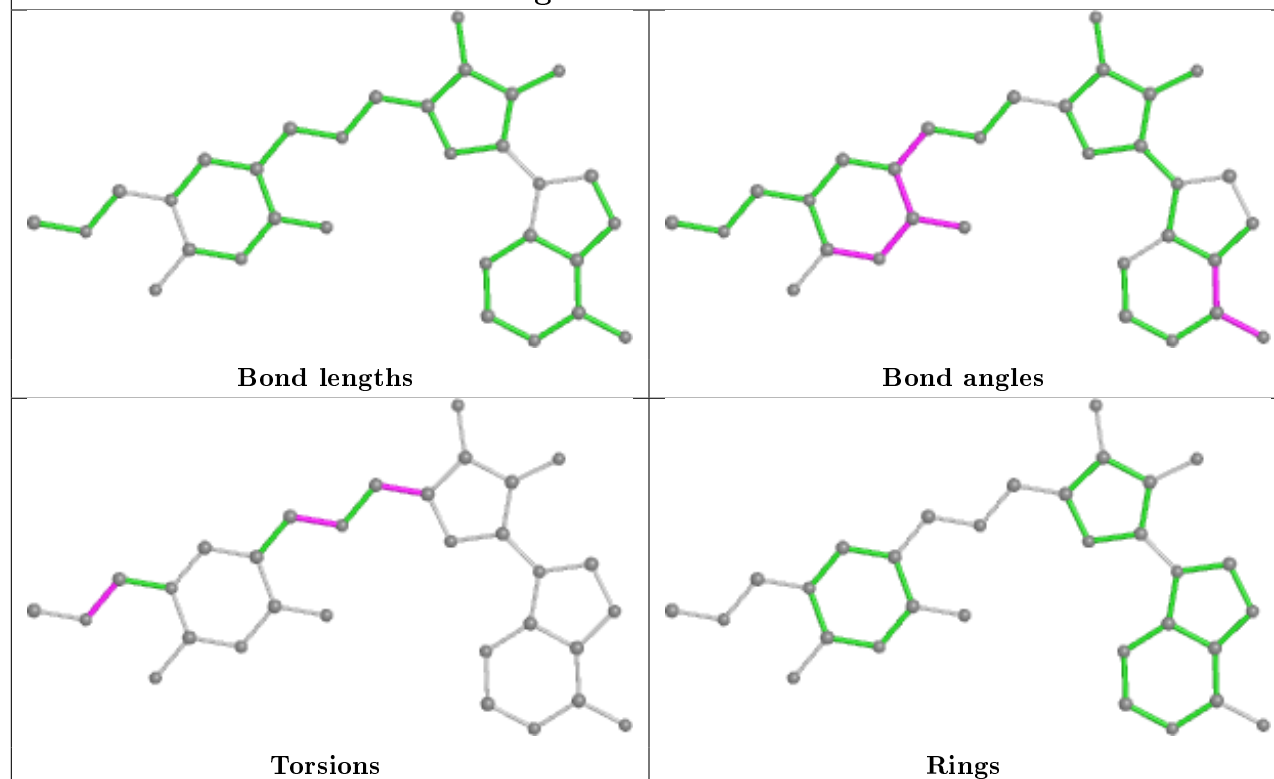
Ligand LHB H 501



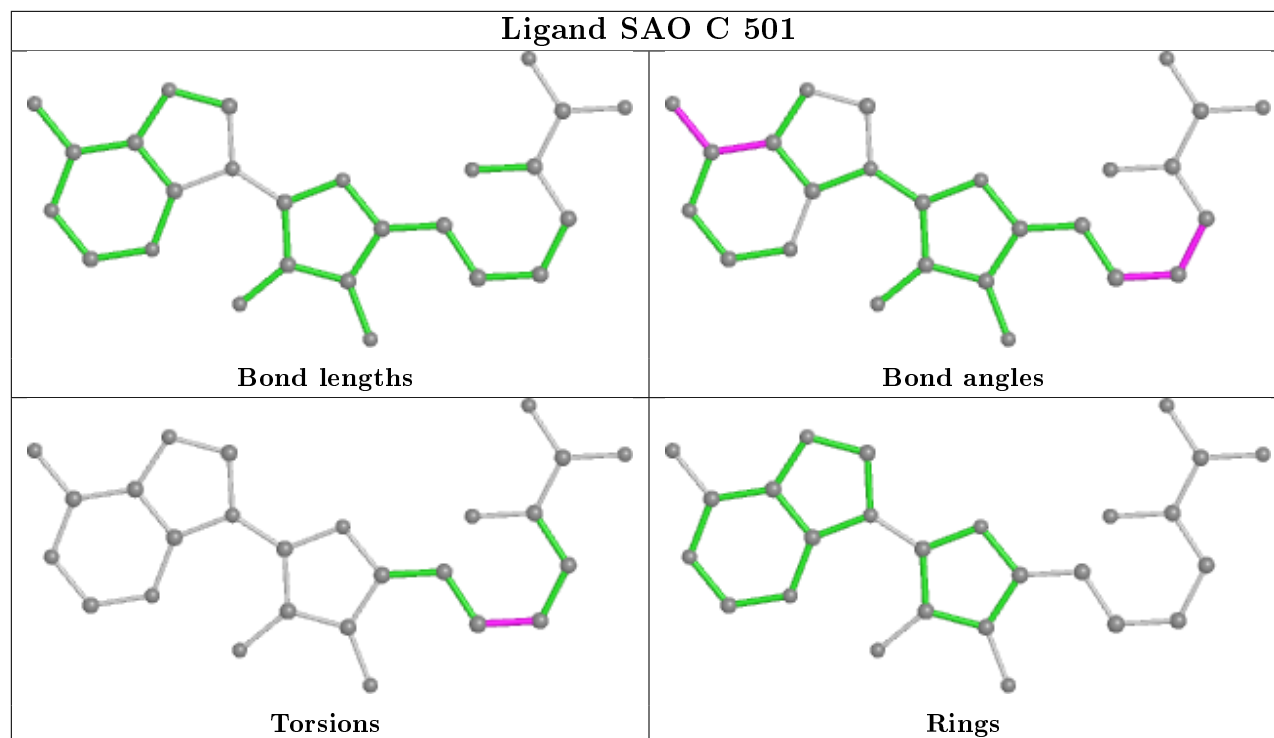
Ligand LHB B 501



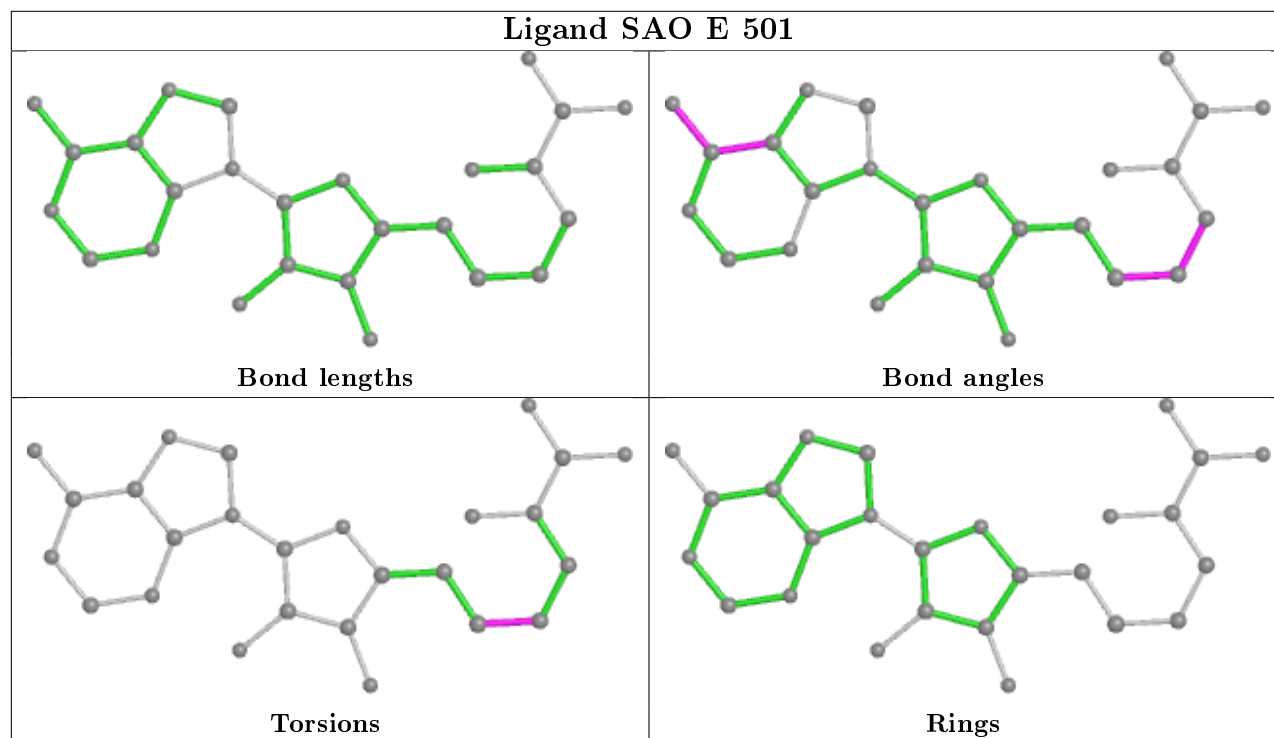
Ligand LHB F 501

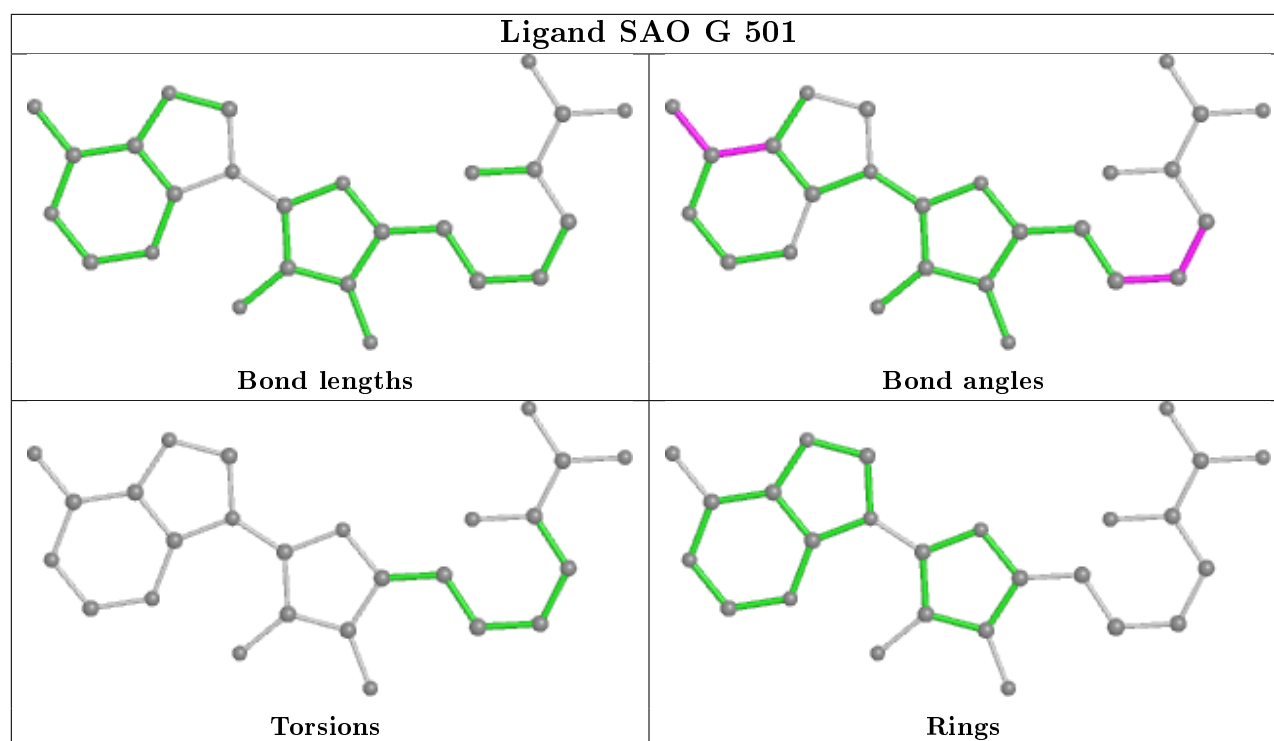


Ligand SAO C 501



Ligand SAO E 501





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	343/361 (95%)	-0.19	2 (0%) 89 92	27, 41, 61, 78	0
1	B	343/361 (95%)	-0.21	5 (1%) 73 79	30, 41, 59, 79	0
1	C	343/361 (95%)	-0.34	2 (0%) 89 92	18, 31, 46, 69	0
1	D	342/361 (94%)	-0.30	0 100 100	20, 35, 51, 67	0
1	E	343/361 (95%)	-0.36	1 (0%) 94 96	18, 30, 46, 60	0
1	F	343/361 (95%)	-0.33	0 100 100	19, 33, 50, 72	0
1	G	343/361 (95%)	-0.22	2 (0%) 89 92	28, 40, 57, 71	0
1	H	341/361 (94%)	-0.27	3 (0%) 84 88	28, 40, 57, 73	0
All	All	2741/2888 (94%)	-0.28	15 (0%) 91 94	18, 37, 56, 79	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	TYR	4.6
1	G	478	THR	3.7
1	H	475	PHE	2.9
1	H	472	ASN	2.8
1	H	315	TYR	2.5

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 carbohydrates in this entry.

6.4 Ligands ⓘ

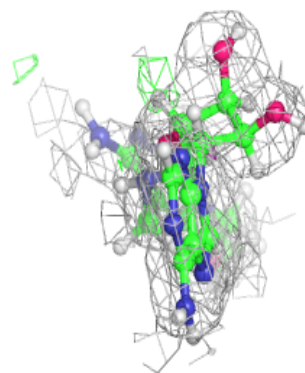
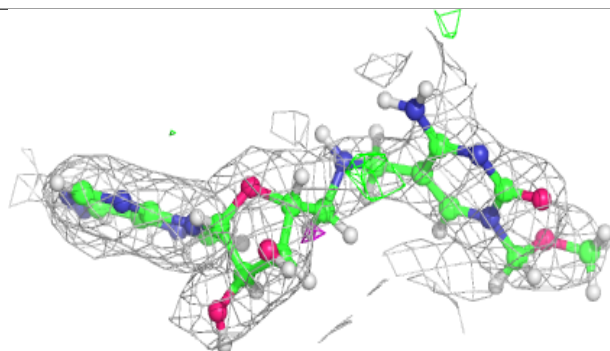
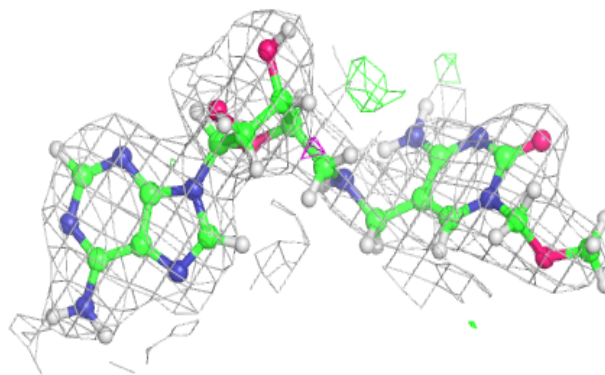
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	F	502	4/4	0.78	0.14	48,58,64,65	0
6	M2M	E	504	9/9	0.87	0.15	42,54,64,65	0
7	DXE	C	505	6/6	0.87	0.11	41,49,54,54	0
3	EDO	G	503	4/4	0.87	0.12	47,56,58,58	0
3	EDO	H	502	4/4	0.88	0.11	42,50,52,52	0
6	M2M	C	504	9/9	0.88	0.21	42,51,56,57	0
5	PG4	C	502	13/13	0.89	0.17	47,57,66,67	0
3	EDO	E	503	4/4	0.90	0.13	46,55,56,56	0
3	EDO	E	502	4/4	0.90	0.10	37,45,52,53	0
5	PG4	D	502	13/13	0.90	0.20	45,55,62,64	0
3	EDO	C	503	4/4	0.90	0.08	40,48,49,49	0
5	PG4	F	503	13/13	0.91	0.17	43,52,59,60	0
5	PG4	F	505	13/13	0.91	0.22	41,56,65,67	0
3	EDO	D	503	4/4	0.92	0.10	36,43,44,46	0
8	PEG	D	504	7/7	0.92	0.19	37,44,53,53	0
3	EDO	B	502	4/4	0.92	0.10	51,61,62,62	0
3	EDO	F	504	4/4	0.93	0.10	34,42,48,51	0
4	LHB	H	501	31/31	0.93	0.14	27,43,62,65	0
3	EDO	G	502	4/4	0.93	0.10	41,49,50,52	0
4	LHB	B	501	31/31	0.94	0.12	32,45,72,74	0
9	NA	F	506	1/1	0.94	0.10	33,33,33,33	0
3	EDO	G	504	4/4	0.95	0.12	44,53,55,57	0
2	SAO	A	501	26/26	0.95	0.10	32,43,55,57	0
3	EDO	A	502	4/4	0.95	0.07	47,57,58,58	0
3	EDO	B	503	4/4	0.95	0.07	37,44,49,50	0
2	SAO	E	501	26/26	0.95	0.10	18,35,48,48	0
2	SAO	G	501	26/26	0.96	0.11	33,43,58,58	0
9	NA	D	505	1/1	0.96	0.11	38,38,38,38	0
4	LHB	D	501	31/31	0.96	0.11	22,32,47,48	0
2	SAO	C	501	26/26	0.96	0.10	17,33,50,51	0
4	LHB	F	501	31/31	0.97	0.11	20,33,42,44	0

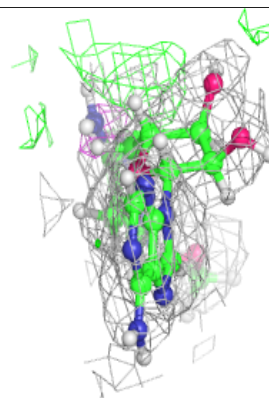
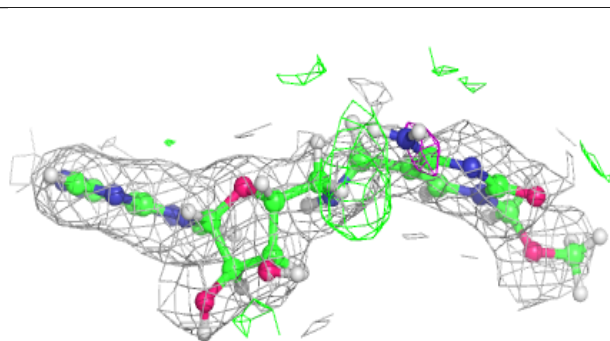
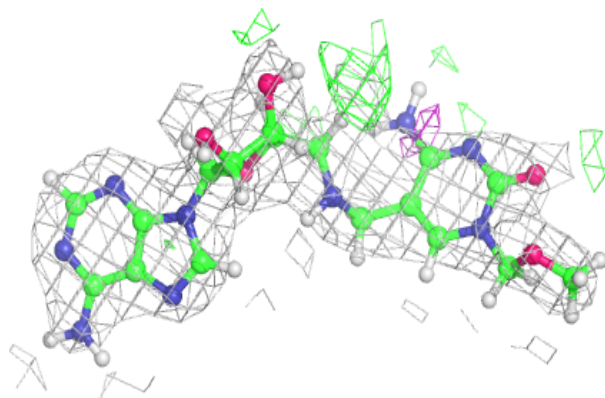
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LHB H 501:

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

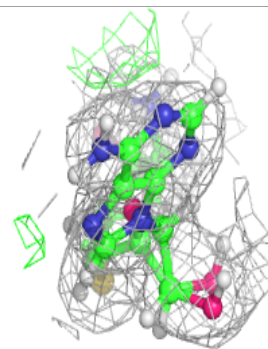
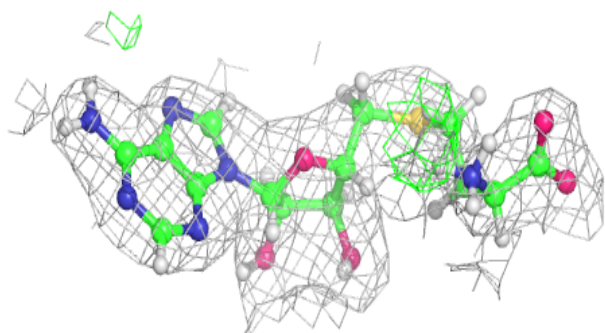
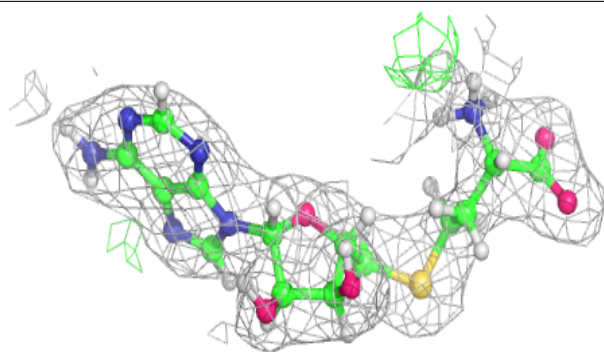
**Electron density around LHB B 501:**

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

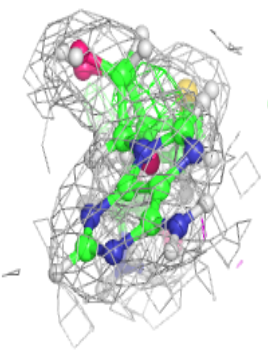
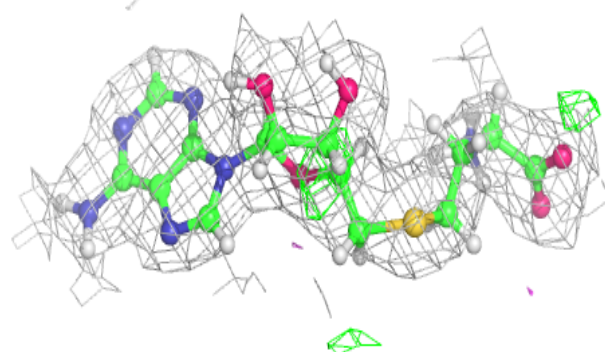
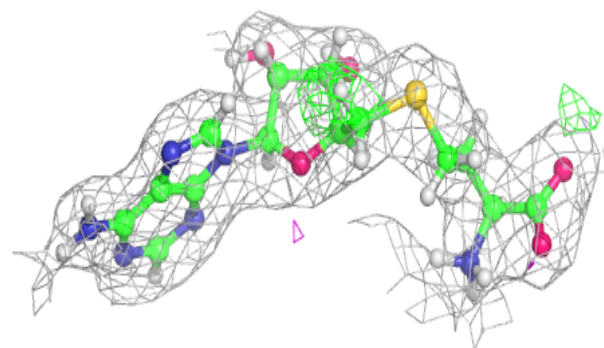


Electron density around SAO A 501:

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

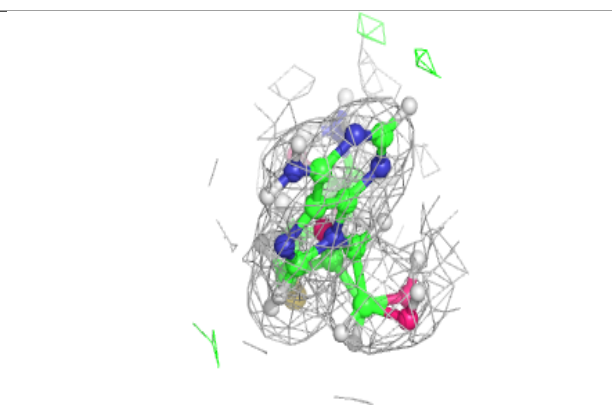
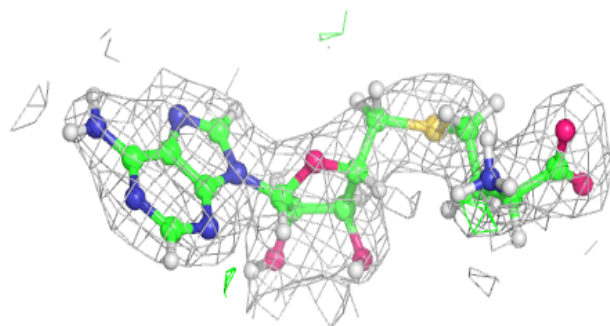
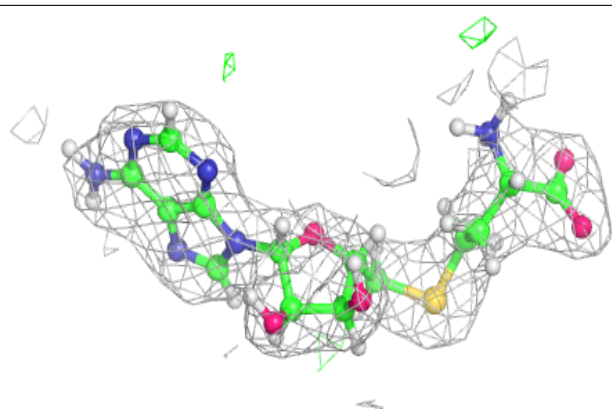
**Electron density around SAO E 501:**

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

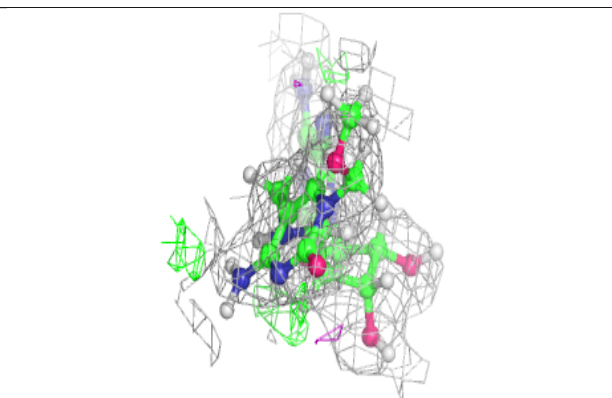
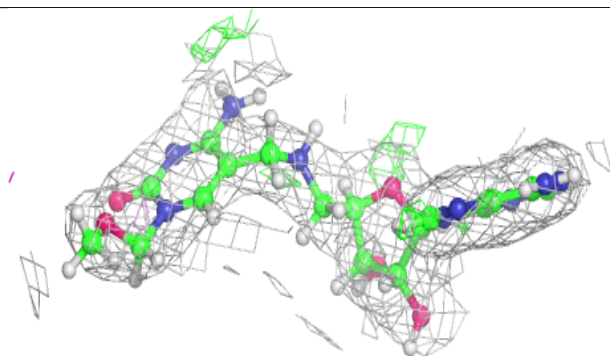
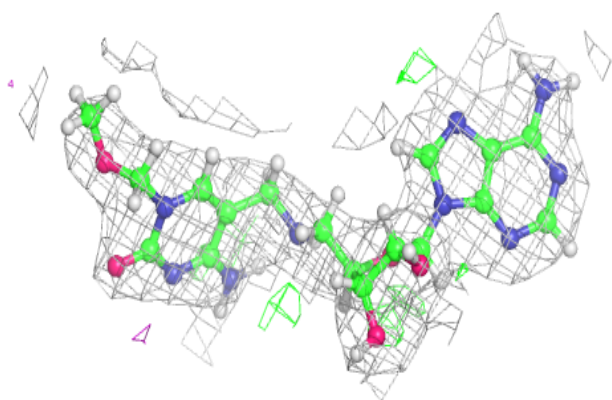


Electron density around SAO G 501:

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

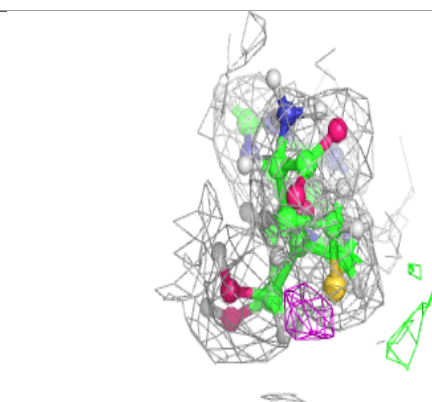
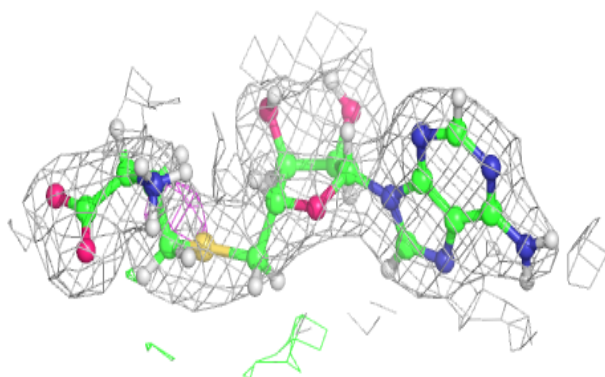
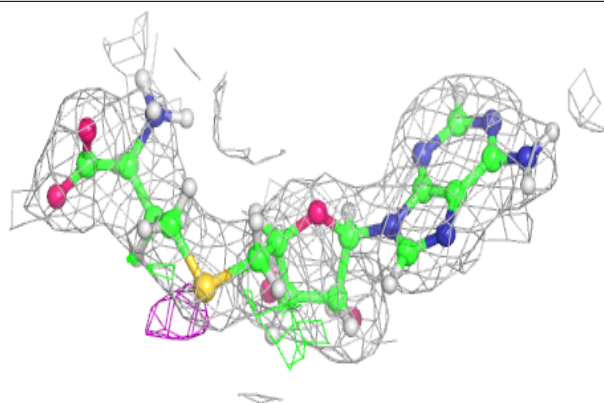
**Electron density around LHB D 501:**

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

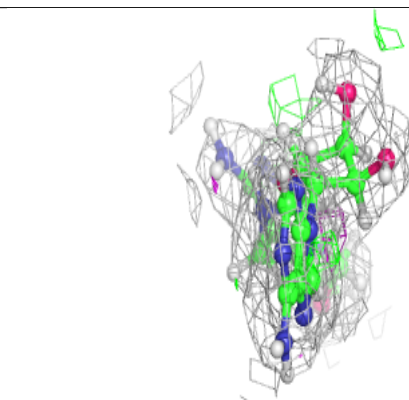
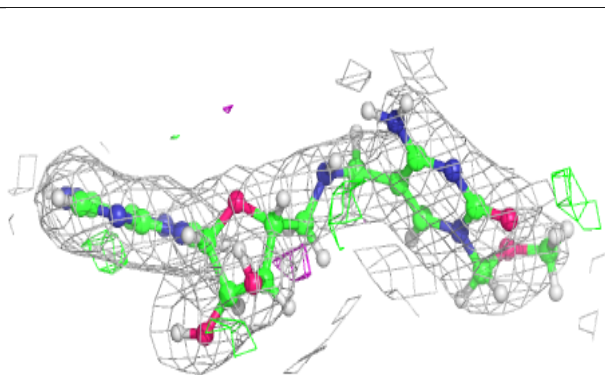
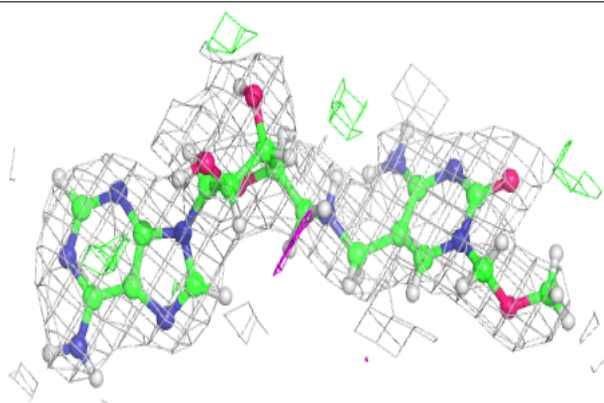


Electron density around SAO C 501:

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

**Electron density around LHB F 501:**

$2mF_o-DF_c$ (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.