



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:00 PM UTC

PDB ID : 5LV2 / pdb_00005lv2
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 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

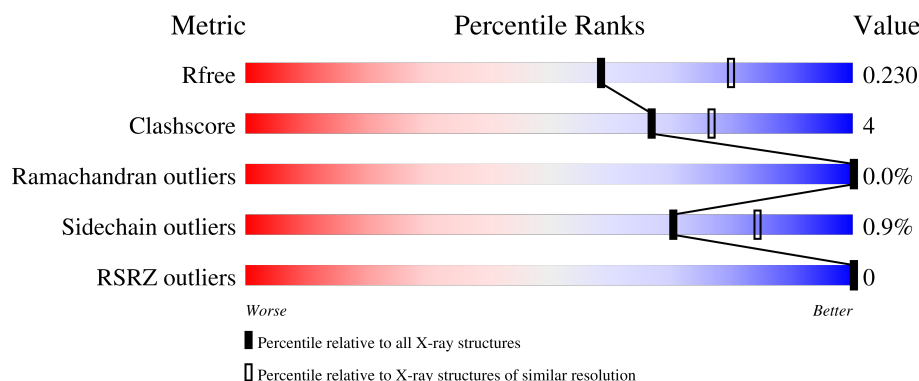
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	361	
1	B	361	
1	C	361	
1	D	361	
1	E	361	

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Mol	Chain	Length	Quality of chain
1	F	361	 86% 8% • 5%
1	G	361	 89% 6% 5%
1	H	361	 84% 9% • 6%

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:

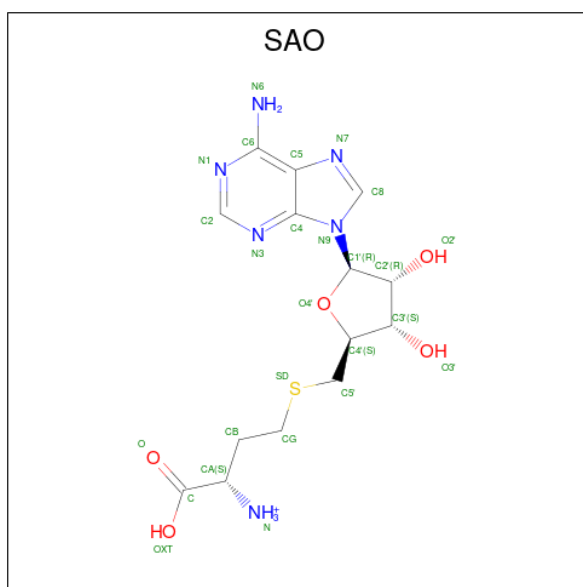
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	expression tag	UNP Q9WVG6
A	128	HIS	-	expression tag	UNP Q9WVG6
A	129	MET	-	expression tag	UNP Q9WVG6
B	127	GLY	-	expression tag	UNP Q9WVG6
B	128	HIS	-	expression tag	UNP Q9WVG6
B	129	MET	-	expression tag	UNP Q9WVG6
C	127	GLY	-	expression tag	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 (CCD ID: 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

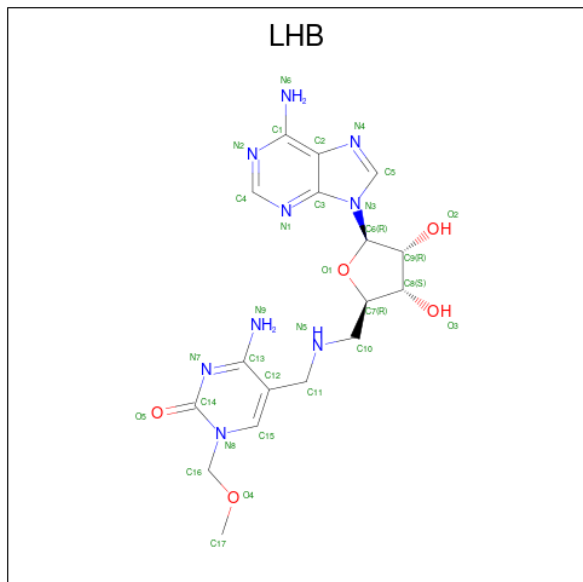
- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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		

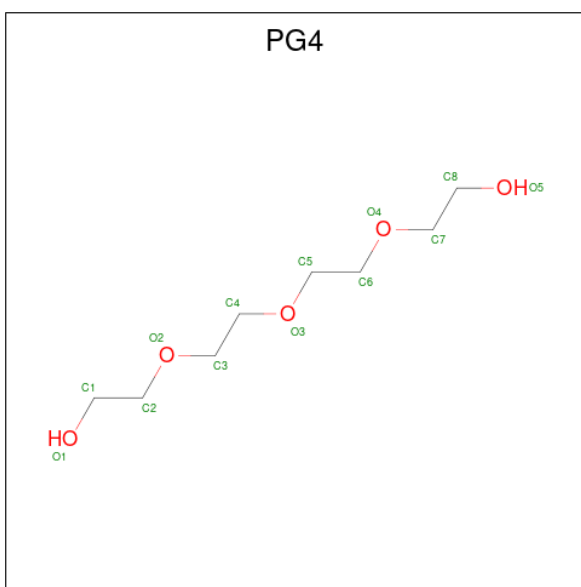
- Molecule 4 is 5-[[[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxola

n-2-yl[methylamino]methyl]-4-azanyl-1-(methoxymethyl)pyrimidin-2-one (CCD ID: LHB)
(formula: $C_{17}H_{23}N_9O_5$).



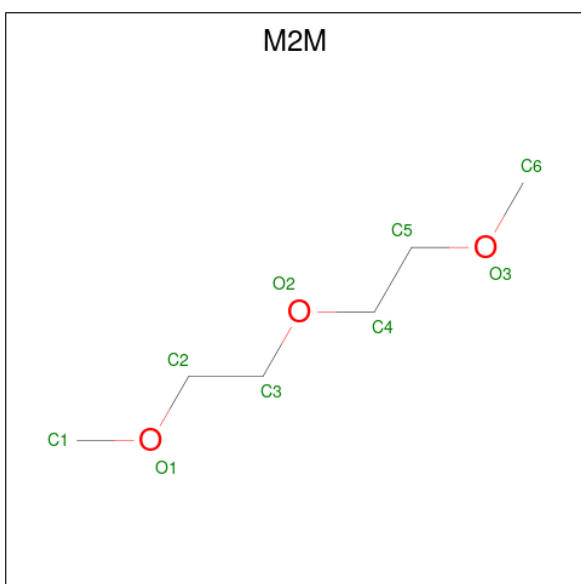
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			54	17	23	9	5		
4	D	1	Total	C	H	N	O	0	0
			54	17	23	9	5		
4	F	1	Total	C	H	N	O	0	0
			54	17	23	9	5		
4	H	1	Total	C	H	N	O	0	0
			54	17	23	9	5		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



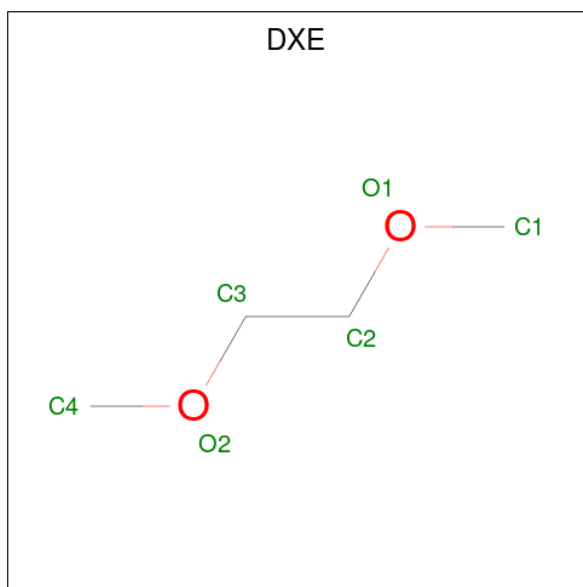
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			31	8	18	5		
5	D	1	Total	C	H	O	0	0
			31	8	18	5		
5	F	1	Total	C	H	O	0	0
			31	8	18	5		
5	F	1	Total	C	H	O	0	0
			31	8	18	5		

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



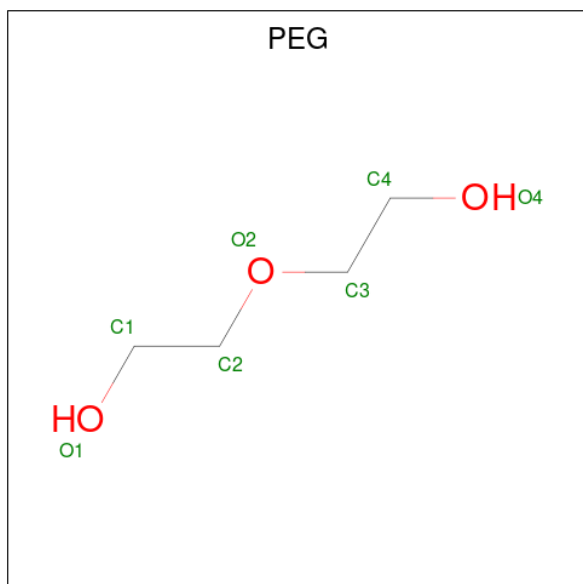
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			23	6	14	3		
6	E	1	Total	C	H	O	0	0
			23	6	14	3		

- Molecule 7 is 1,2-DIMETHOXYETHANE (CCD ID: DXE) (formula: $C_4H_{10}O_2$).



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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 9 is SODIUM ION (CCD ID: 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		

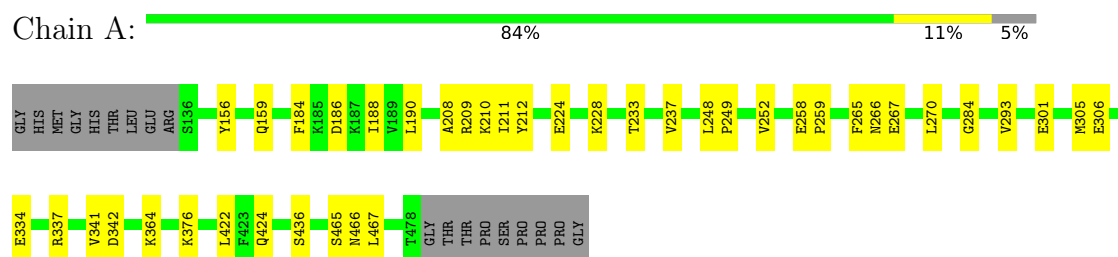
- Molecule 10 is water.

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		

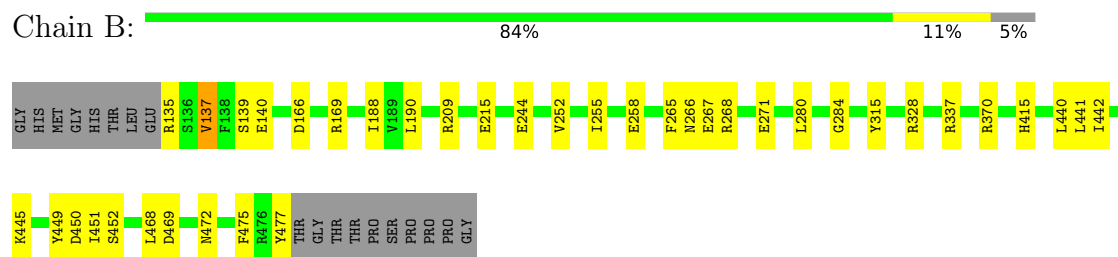
3 Residue-property plots

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

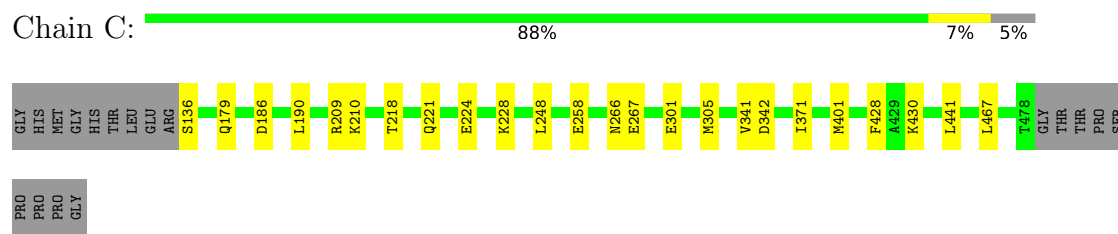
• Molecule 1: Histone-arginine methyltransferase CARM1



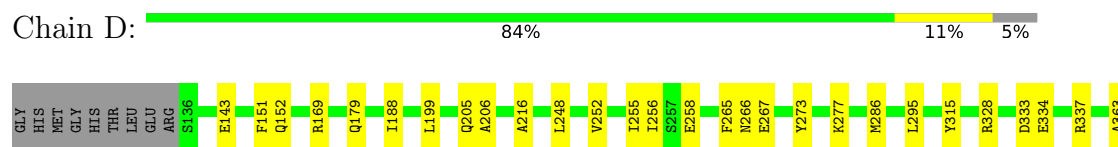
• Molecule 1: Histone-arginine methyltransferase CARM1



• Molecule 1: Histone-arginine methyltransferase CARM1



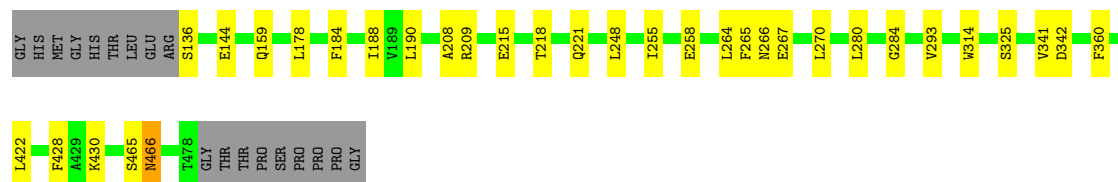
• Molecule 1: Histone-arginine methyltransferase CARM1





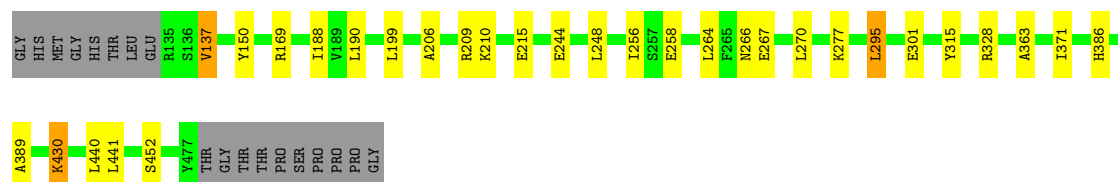
- Molecule 1: Histone-arginine methyltransferase CARM1

Chain E: 86% 9% 5%



- Molecule 1: Histone-arginine methyltransferase CARM1

Chain F: 86% 8% 5%



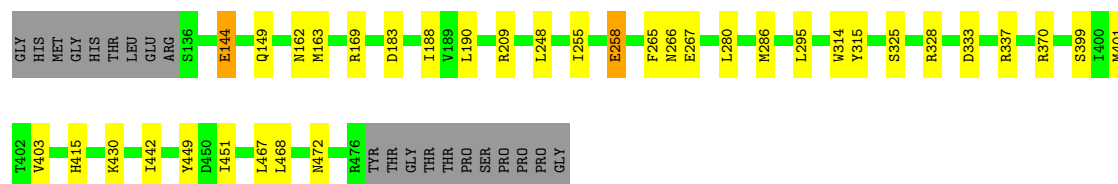
- Molecule 1: Histone-arginine methyltransferase CARM1

Chain G: 89% 6% 5%



- Molecule 1: Histone-arginine methyltransferase CARM1

Chain H: 84% 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 0.196 , 0.230	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)	0.38 , 18.4	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	0.97	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.*

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

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	0/2821	0.71	1/3823 (0.0%)
1	B	0.36	0/2852	0.67	0/3865
1	C	0.37	0/2837	0.69	0/3845
1	D	0.37	0/2833	0.70	0/3838
1	E	0.37	0/2838	0.69	0/3845
1	F	0.38	0/2841	0.72	0/3847
1	G	0.35	0/2841	0.71	0/3849
1	H	0.35	0/2801	0.68	0/3795
All	All	0.36	0/22664	0.70	1/30707 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	GLY	N-CA-C	5.01	118.96	112.54

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	22	0
1	B	2765	2714	2702	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2759	2704	2692	13	0
1	D	2755	2706	2694	29	0
1	E	2759	2709	2702	22	0
1	F	2763	2715	2705	21	0
1	G	2762	2713	2704	12	0
1	H	2732	2683	2683	25	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	3	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	164	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 (164) 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
1:B:169:ARG:NH2	1:B:258:GLU:OE1	2.15	0.79
1:F:301:GLU:OE1	1:F:386:HIS:NE2	2.25	0.70
1:D:179:GLN:NE2	1:D:401:MET:SD	2.66	0.68
1:E:159:GLN:OE1	10:E:602:HOH:O	2.12	0.66
1:G:282:PRO:O	1:G:283:SER:OG	2.11	0.66
1:D:337:ARG:HG2	1:D:467:LEU:O	1.96	0.66
1:H:144:GLU:OE2	10:H:602:HOH:O	2.13	0.66
1:H:401:MET:HE2	1:H:403:VAL:HG22	1.79	0.65
1:B:337:ARG:HD3	1:B:469:ASP:HB2	1.79	0.64
1:E:218:THR:O	1:E:221:GLN:HG2	1.98	0.64
1:B:415[A]:HIS:NE2	4:B:501:LHB:O5	2.26	0.62
1:A:159:GLN:NE2	10:A:602:HOH:O	2.25	0.62
1:F:277:LYS:NZ	1:F:363:ALA:O	2.33	0.62
1:C:218:THR:O	1:C:221:GLN:HG2	2.01	0.61
1:F:169:ARG:HD3	1:F:258:GLU:OE1	2.01	0.61
1:B:215:GLU:OE2	4:B:501:LHB:O2	2.20	0.60
1:G:169:ARG:HH22	2:G:501:SAO:C	2.15	0.59
1:B:450:ASP:OD1	10:B:602:HOH:O	2.16	0.59
1:F:188:ILE:HD11	1:F:209:ARG:CZ	2.33	0.58
1:D:441:LEU:HD12	1:D:451:ILE:HG12	1.86	0.58
1:D:333:ASP:O	1:D:337:ARG:HG3	2.04	0.58
1:F:188:ILE:HD12	1:F:210:LYS:HB3	1.85	0.57
1:E:422:LEU:O	1:E:466:ASN:ND2	2.37	0.56
1:B:440:LEU:HB3	1:B:452:SER:OG	2.06	0.56
1:G:149:GLN:OE1	1:H:149:GLN:NE2	2.39	0.56
1:H:188:ILE:HD11	1:H:209:ARG:NH2	2.21	0.56
1:B:166:ASP:OD2	1:B:415[A]:HIS:ND1	2.39	0.55
1:C:428:PHE:HE2	1:C:430:LYS:HE2	1.72	0.55
1:H:258:GLU:O	4:H:501:LHB:N9	2.38	0.55
1:F:315:TYR:HD1	1:F:328:ARG:HD3	1.72	0.55
1:B:188:ILE:HD11	1:B:209:ARG:NH2	2.21	0.54
1:D:169:ARG:HD3	1:D:258:GLU:OE1	2.07	0.54
1:C:430:LYS:NZ	1:F:206:ALA:HA	2.22	0.54
1:H:370:ARG:HG3	1:H:442:ILE:CD1	2.39	0.53
1:B:268:ARG:HD2	1:B:271:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ALA:HA	1:E:430:LYS:NZ	2.25	0.52
1:H:163:MET:HG2	1:H:169:ARG:HH12	1.73	0.52
1:C:179:GLN:NE2	1:C:401:MET:SD	2.80	0.52
1:B:337:ARG:HG3	1:B:468:LEU:HA	1.92	0.52
1:F:430:LYS:HD3	1:G:167:TYR:CE1	2.44	0.52
1:H:315:TYR:CD1	1:H:328:ARG:NH1	2.79	0.51
1:B:370:ARG:HG3	1:B:442:ILE:CD1	2.40	0.51
1:F:188:ILE:CD1	1:F:210:LYS:HB3	2.41	0.51
1:D:315:TYR:HB2	1:D:328:ARG:HD3	1.93	0.51
1:A:306:GLU:OE2	10:A:601:HOH:O	2.19	0.51
1:E:190:LEU:HD13	1:E:248:LEU:HD21	1.93	0.51
1:E:215:GLU:OE2	2:E:501:SAO:O2'	2.28	0.50
1:G:156:TYR:OH	1:H:472:ASN:OD1	2.24	0.50
1:A:190:LEU:HD13	1:A:248:LEU:HD21	1.93	0.50
1:E:188:ILE:HD11	1:E:209:ARG:HH21	1.77	0.50
1:G:190:LEU:HD13	1:G:248:LEU:HD21	1.93	0.50
1:E:465:SER:O	1:E:466:ASN:HB2	2.11	0.50
1:E:428:PHE:HE2	1:E:430:LYS:HE2	1.77	0.49
1:D:143:GLU:HG2	1:D:445:LYS:HB3	1.93	0.49
1:A:265:PHE:CE2	1:A:293:VAL:HG21	2.46	0.49
1:B:188:ILE:HD11	1:B:209:ARG:CZ	2.42	0.49
1:D:152:GLN:NE2	10:D:611:HOH:O	2.46	0.49
1:E:428:PHE:HE2	1:E:430:LYS:CE	2.25	0.49
1:C:301:GLU:HG3	1:C:305:MET:HE2	1.94	0.49
1:D:255:ILE:HD12	1:D:286:MET:HE3	1.95	0.49
1:G:376:LYS:HG2	1:G:436:SER:CB	2.43	0.49
1:A:186:ASP:HA	1:A:209:ARG:HB2	1.95	0.48
1:G:277:LYS:NZ	1:G:363:ALA:O	2.44	0.48
1:B:328:ARG:NH2	1:D:328:ARG:HH12	2.11	0.48
1:E:136:SER:N	10:E:612:HOH:O	2.46	0.48
1:H:315:TYR:HB2	1:H:328:ARG:HD3	1.95	0.48
1:B:337:ARG:HG2	1:B:469:ASP:H	1.79	0.48
1:C:190:LEU:HD13	1:C:248:LEU:HD21	1.95	0.48
1:B:328:ARG:NH1	1:D:328:ARG:HH22	2.12	0.47
1:E:266:ASN:O	1:E:267:GLU:HB2	2.15	0.47
1:B:255:ILE:HG13	1:B:280:LEU:HD13	1.95	0.47
1:F:150:TYR:HA	5:F:503:PG4:H31	1.97	0.47
1:F:371:ILE:HB	1:F:441:LEU:HB2	1.97	0.47
1:F:215:GLU:OE2	4:F:501:LHB:O2	2.33	0.47
1:D:199:LEU:HB3	1:D:256:ILE:HD12	1.97	0.47
1:C:341:VAL:O	1:C:342:ASP:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:ASN:O	1:F:267:GLU:HB2	2.15	0.46
1:A:301:GLU:HG3	1:A:305:MET:HE2	1.98	0.46
1:H:451:ILE:O	1:H:467:LEU:HD12	2.15	0.46
1:E:255:ILE:HG13	1:E:280:LEU:HD13	1.98	0.46
1:A:190:LEU:HB2	1:A:252:VAL:HG11	1.97	0.46
1:H:183:ASP:OD1	1:H:399:SER:OG	2.19	0.46
1:H:333:ASP:O	1:H:337:ARG:HG3	2.15	0.46
1:A:259:PRO:HG2	1:A:270:LEU:HD23	1.98	0.45
1:H:169:ARG:CZ	10:H:601:HOH:O	2.64	0.45
1:D:266:ASN:O	1:D:267:GLU:HB2	2.16	0.45
1:D:440:LEU:HB3	1:D:452:SER:OG	2.17	0.45
1:D:477:TYR:O	10:D:601:HOH:O	2.21	0.45
1:G:266:ASN:O	1:G:267:GLU:HB2	2.16	0.45
1:E:341:VAL:O	1:E:342:ASP:HB3	2.16	0.45
1:C:266:ASN:O	1:C:267:GLU:HB2	2.16	0.45
1:H:451:ILE:HB	1:H:468:LEU:HB2	1.98	0.45
1:E:270:LEU:HD22	1:E:360:PHE:CE1	2.51	0.45
1:A:422:LEU:O	1:A:466:ASN:ND2	2.47	0.45
1:B:328:ARG:CZ	1:D:328:ARG:HH22	2.30	0.44
1:A:424:GLN:HG3	1:A:465:SER:O	2.17	0.44
1:B:266:ASN:O	1:B:267:GLU:HB2	2.17	0.44
1:A:156:TYR:OH	1:B:472:ASN:OD1	2.34	0.44
1:H:169:ARG:NH1	10:H:601:HOH:O	2.51	0.44
1:H:266:ASN:O	1:H:267:GLU:HB2	2.17	0.44
1:A:266:ASN:O	1:A:267:GLU:HB2	2.18	0.44
1:A:376:LYS:HG3	1:A:436:SER:HB3	2.00	0.44
1:F:295:LEU:HA	1:F:389:ALA:O	2.17	0.44
1:C:186:ASP:HA	1:C:209:ARG:HB2	2.00	0.44
1:D:295:LEU:HA	1:D:389:ALA:O	2.18	0.44
1:B:169:ARG:HD2	1:B:258:GLU:OE2	2.18	0.43
1:C:430:LYS:HE3	10:F:633:HOH:O	2.18	0.43
1:D:169:ARG:NH1	1:D:258:GLU:OE1	2.51	0.43
1:A:341:VAL:O	1:A:342:ASP:HB3	2.19	0.43
1:A:212:TYR:OH	1:A:249:PRO:HG2	2.19	0.43
1:B:475:PHE:HD1	1:B:477:TYR:HE2	1.67	0.43
1:F:190:LEU:HD13	1:F:248:LEU:HD11	2.01	0.42
1:F:199:LEU:HB3	1:F:256:ILE:HD12	2.00	0.42
1:D:370[B]:ARG:HG3	1:D:442:ILE:CD1	2.50	0.42
1:H:265:PHE:HB3	1:H:449:TYR:CE1	2.54	0.42
1:A:224:GLU:OE1	1:A:228:LYS:HE3	2.20	0.42
1:E:184:PHE:O	1:E:208:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:LEU:HG	1:F:270:LEU:HD11	2.02	0.42
1:H:255:ILE:HG13	1:H:280:LEU:HD13	2.01	0.42
1:B:135:ARG:HB3	1:B:139:SER:OG	2.20	0.42
1:B:190:LEU:HB2	1:B:252:VAL:HG11	2.02	0.42
1:B:280:LEU:HD11	1:B:284:GLY:HA3	2.00	0.42
1:D:334:GLU:HA	1:D:337:ARG:CZ	2.49	0.42
1:D:273:TYR:CE1	1:D:286:MET:HE2	2.55	0.42
1:D:258:GLU:O	4:D:501:LHB:N9	2.52	0.42
1:D:277:LYS:NZ	1:D:363:ALA:O	2.51	0.42
1:A:208:ALA:HB3	1:A:211:ILE:HD11	2.02	0.42
1:B:137:VAL:HG22	1:B:244:GLU:HG2	2.01	0.41
1:E:280:LEU:HD11	1:E:284:GLY:HA3	2.02	0.41
1:B:440:LEU:HB3	1:B:452:SER:HG	1.84	0.41
1:G:341:VAL:O	1:G:342:ASP:HB3	2.19	0.41
1:H:190:LEU:HD13	1:H:248:LEU:HD11	2.02	0.41
1:A:188:ILE:HG22	1:A:252:VAL:HG12	2.03	0.41
1:H:314:TRP:O	1:H:325:SER:HA	2.20	0.41
1:B:140:GLU:O	1:B:445:LYS:HE3	2.20	0.41
1:B:265:PHE:HB3	1:B:449:TYR:CE1	2.55	0.41
1:C:224:GLU:OE2	1:C:228:LYS:NZ	2.41	0.41
1:D:188:ILE:HG22	1:D:252:VAL:HG12	2.01	0.41
1:E:265:PHE:CE2	1:E:293:VAL:HG21	2.56	0.41
1:E:314:TRP:O	1:E:325:SER:HA	2.21	0.41
1:F:137:VAL:HG22	1:F:244:GLU:HG2	2.02	0.41
1:E:264:LEU:HG	1:E:270:LEU:HD11	2.03	0.41
1:B:315:TYR:CD1	1:B:328:ARG:NH1	2.89	0.41
1:C:136:SER:N	10:C:614:HOH:O	2.53	0.41
1:C:371:ILE:HB	1:C:441:LEU:HB2	2.03	0.41
1:H:255:ILE:HD12	1:H:286:MET:HE3	2.01	0.41
1:A:334:GLU:HA	1:A:337:ARG:NH2	2.36	0.41
1:F:328:ARG:NH1	1:H:328:ARG:HH21	2.19	0.41
1:D:151:PHE:CE1	1:D:216:ALA:HB3	2.56	0.41
1:A:184:PHE:O	1:A:208:ALA:HA	2.21	0.40
1:A:210:LYS:HE2	1:A:237:VAL:HG23	2.03	0.40
1:B:441:LEU:CD2	1:B:451:ILE:HG12	2.52	0.40
1:D:265:PHE:HB3	1:D:449:TYR:CE1	2.57	0.40
1:A:364:LYS:NZ	10:A:615:HOH:O	2.54	0.40
1:F:440:LEU:HB3	1:F:452:SER:OG	2.21	0.40
1:G:215:GLU:OE2	2:G:501:SAO:O2'	2.40	0.40
1:H:162:ASN:OD1	1:H:415:HIS:CD2	2.74	0.40
1:D:334:GLU:HA	1:D:337:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:ILE:HD12	1:F:188:ILE:HG23	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/361 (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%)	36	46
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 [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/313 (96%)	296 (99%)	3 (1%)	68	82
1	B	301/313 (96%)	300 (100%)	1 (0%)	86	93
1	C	301/313 (96%)	298 (99%)	3 (1%)	68	82
1	D	300/313 (96%)	298 (99%)	2 (1%)	76	87
1	E	301/313 (96%)	299 (99%)	2 (1%)	76	87
1	F	301/313 (96%)	298 (99%)	3 (1%)	68	82
1	G	301/313 (96%)	298 (99%)	3 (1%)	68	82
1	H	297/313 (95%)	293 (99%)	4 (1%)	61	77
All	All	2401/2504 (96%)	2380 (99%)	21 (1%)	70	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	THR
1	A	258	GLU
1	A	467	LEU
1	B	137	VAL
1	C	210	LYS
1	C	258	GLU
1	C	467	LEU
1	D	248	LEU
1	D	441	LEU
1	E	178	LEU
1	E	258	GLU
1	F	137	VAL
1	F	295	LEU
1	F	430	LYS
1	G	143	GLU
1	G	258	GLU
1	G	290	ILE
1	H	144	GLU
1	H	258	GLU
1	H	295	LEU
1	H	430	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	ASN
1	B	161	GLN
1	B	165	GLN
1	B	381	HIS
1	C	181	HIS
1	C	369	HIS
1	D	161	GLN
1	D	415	HIS
1	E	181	HIS
1	E	320	HIS
1	E	378	HIS
1	F	162	ASN
1	F	456	GLN
1	G	181	HIS
1	G	472	ASN
1	H	149	GLN
1	H	381	HIS
1	H	415	HIS

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 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
3	EDO	G	503	-	3,3,3	0.44	0	2,2,2	0.52	0
5	PG4	F	503	-	12,12,12	0.53	0	11,11,11	0.46	0
3	EDO	A	502	-	3,3,3	0.44	0	2,2,2	0.55	0
3	EDO	F	504	-	3,3,3	0.44	0	2,2,2	0.45	0
3	EDO	B	503	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	G	504	-	3,3,3	0.43	0	2,2,2	0.51	0
8	PEG	D	504	-	6,6,6	0.49	0	5,5,5	0.46	0
3	EDO	H	502	-	3,3,3	0.43	0	2,2,2	0.53	0
3	EDO	B	502	-	3,3,3	0.44	0	2,2,2	0.51	0
5	PG4	F	505	-	12,12,12	0.53	0	11,11,11	0.33	0
4	LHB	F	501	-	33,34,34	0.27	0	41,49,49	0.66	1 (2%)
3	EDO	C	503	-	3,3,3	0.43	0	2,2,2	0.47	0
3	EDO	D	503	-	3,3,3	0.43	0	2,2,2	0.51	0
3	EDO	F	502	-	3,3,3	0.43	0	2,2,2	0.52	0
5	PG4	D	502	-	12,12,12	0.52	0	11,11,11	0.43	0
2	SAO	C	501	-	27,28,28	0.40	0	36,40,40	0.72	1 (2%)
3	EDO	G	502	-	3,3,3	0.42	0	2,2,2	0.55	0
7	DXE	C	505	-	5,5,5	0.43	0	4,4,4	0.29	0
2	SAO	G	501	-	27,28,28	0.42	0	36,40,40	0.74	1 (2%)
2	SAO	E	501	-	27,28,28	0.41	0	36,40,40	0.79	1 (2%)
4	LHB	H	501	-	33,34,34	0.18	0	41,49,49	0.48	1 (2%)
6	M2M	E	504	-	8,8,8	0.61	0	7,7,7	0.38	0
3	EDO	E	503	-	3,3,3	0.45	0	2,2,2	0.48	0
4	LHB	D	501	-	33,34,34	0.22	0	41,49,49	0.51	1 (2%)
6	M2M	C	504	-	8,8,8	0.59	0	7,7,7	0.14	0
3	EDO	E	502	-	3,3,3	0.43	0	2,2,2	0.52	0
4	LHB	B	501	-	33,34,34	0.38	0	41,49,49	0.64	1 (2%)
2	SAO	A	501	-	27,28,28	0.41	0	36,40,40	0.70	1 (2%)
5	PG4	C	502	-	12,12,12	0.52	0	11,11,11	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
3	EDO	G	503	-	-	1/1/1/1	-
5	PG4	F	503	-	-	5/10/10/10	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	F	504	-	-	0/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	G	504	-	-	1/1/1/1	-
8	PEG	D	504	-	-	2/4/4/4	-
3	EDO	H	502	-	-	1/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
5	PG4	F	505	-	-	1/10/10/10	-
4	LHB	F	501	-	-	4/12/29/29	0/4/4/4
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	D	503	-	-	0/1/1/1	-
3	EDO	F	502	-	-	1/1/1/1	-
5	PG4	D	502	-	-	5/10/10/10	-
2	SAO	C	501	-	-	1/15/31/31	0/3/3/3
3	EDO	G	502	-	-	0/1/1/1	-
7	DXE	C	505	-	-	2/3/3/3	-
2	SAO	G	501	-	-	0/15/31/31	0/3/3/3
2	SAO	E	501	-	-	1/15/31/31	0/3/3/3
4	LHB	H	501	-	-	3/12/29/29	0/4/4/4
6	M2M	E	504	-	-	6/6/6/6	-
3	EDO	E	503	-	-	1/1/1/1	-
4	LHB	D	501	-	-	5/12/29/29	0/4/4/4
6	M2M	C	504	-	-	4/6/6/6	-
3	EDO	E	502	-	-	1/1/1/1	-
4	LHB	B	501	-	-	4/12/29/29	0/4/4/4
2	SAO	A	501	-	-	0/15/31/31	0/3/3/3
5	PG4	C	502	-	-	9/10/10/10	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	SAO	CB-CG-SD	-3.92	104.69	113.45
4	F	501	LHB	C16-N8-C14	3.91	121.61	117.19
2	E	501	SAO	CB-CG-SD	-3.67	105.26	113.45
2	A	501	SAO	CB-CG-SD	-3.45	105.76	113.45
2	C	501	SAO	CB-CG-SD	-3.29	106.11	113.45
4	B	501	LHB	C16-N8-C14	2.93	120.49	117.19
4	D	501	LHB	C16-N8-C14	2.66	120.20	117.19
4	H	501	LHB	C16-N8-C14	2.63	120.16	117.19

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	LHB	O4-C16-N8-C14
4	B	501	LHB	O4-C16-N8-C15
4	D	501	LHB	N5-C10-C7-O1
4	D	501	LHB	N5-C10-C7-C8
4	D	501	LHB	C12-C11-N5-C10
4	D	501	LHB	O4-C16-N8-C14
4	F	501	LHB	N5-C10-C7-O1
4	F	501	LHB	N5-C10-C7-C8
4	F	501	LHB	C12-C11-N5-C10
4	H	501	LHB	N8-C16-O4-C17
5	F	503	PG4	O3-C5-C6-O4
7	C	505	DXE	O1-C2-C3-O2
5	C	502	PG4	O3-C5-C6-O4
6	C	504	M2M	O2-C4-C5-O3
5	D	502	PG4	O4-C7-C8-O5
6	E	504	M2M	O1-C2-C3-O2
3	E	503	EDO	O1-C1-C2-O2
3	G	504	EDO	O1-C1-C2-O2
5	D	502	PG4	O2-C3-C4-O3
5	D	502	PG4	O1-C1-C2-O2
5	F	503	PG4	O1-C1-C2-O2
8	D	504	PEG	O1-C1-C2-O2
3	E	502	EDO	O1-C1-C2-O2
3	H	502	EDO	O1-C1-C2-O2
5	C	502	PG4	O2-C3-C4-O3
3	C	503	EDO	O1-C1-C2-O2
6	C	504	M2M	C4-C5-O3-C6
5	F	503	PG4	C4-C3-O2-C2
5	C	502	PG4	C5-C6-O4-C7
5	F	503	PG4	O4-C7-C8-O5
5	D	502	PG4	C1-C2-O2-C3
5	C	502	PG4	C3-C4-O3-C5
6	E	504	M2M	O2-C4-C5-O3
6	C	504	M2M	O1-C2-C3-O2
5	C	502	PG4	O1-C1-C2-O2
5	C	502	PG4	C4-C3-O2-C2
3	G	503	EDO	O1-C1-C2-O2
4	H	501	LHB	C12-C11-N5-C10
5	C	502	PG4	C6-C5-O3-C4
7	C	505	DXE	C3-C2-O1-C1
6	C	504	M2M	C3-C2-O1-C1
4	D	501	LHB	N8-C16-O4-C17

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Mol	Chain	Res	Type	Atoms
4	F	501	LHB	N8-C16-O4-C17
8	D	504	PEG	C4-C3-O2-C2
6	E	504	M2M	C4-C5-O3-C6
3	B	502	EDO	O1-C1-C2-O2
3	F	502	EDO	O1-C1-C2-O2
5	C	502	PG4	C1-C2-O2-C3
5	C	502	PG4	O4-C7-C8-O5
3	B	503	EDO	O1-C1-C2-O2
5	F	503	PG4	C5-C6-O4-C7
6	E	504	M2M	C5-C4-O2-C3
6	E	504	M2M	C2-C3-O2-C4
4	B	501	LHB	C7-C10-N5-C11
4	H	501	LHB	N5-C11-C12-C15
5	D	502	PG4	O3-C5-C6-O4
2	C	501	SAO	CB-CG-SD-C5'
2	E	501	SAO	CB-CG-SD-C5'
4	B	501	LHB	N8-C16-O4-C17
5	F	505	PG4	C1-C2-O2-C3
6	E	504	M2M	C3-C2-O1-C1

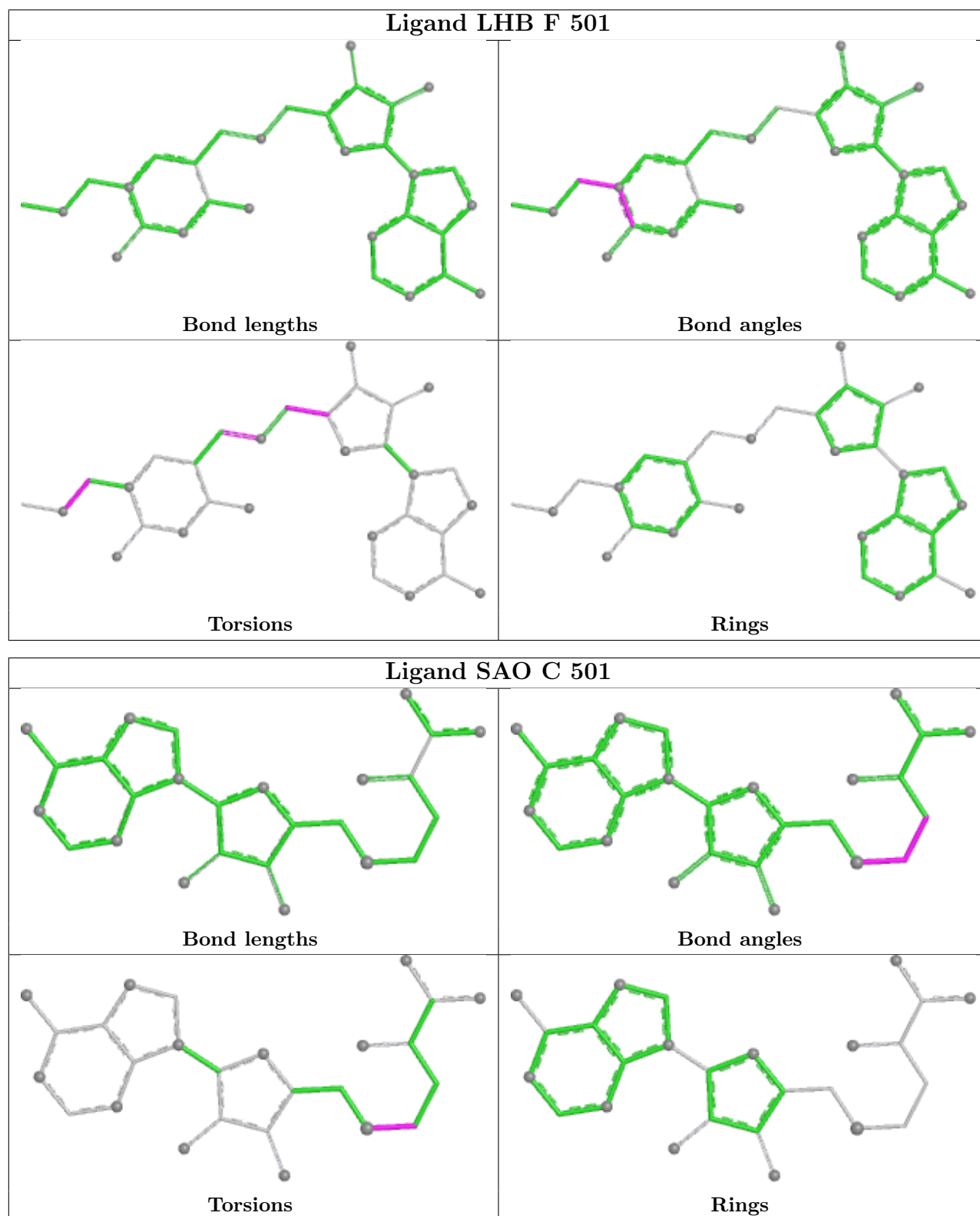
There are no ring outliers.

7 monomers are involved in 9 short contacts:

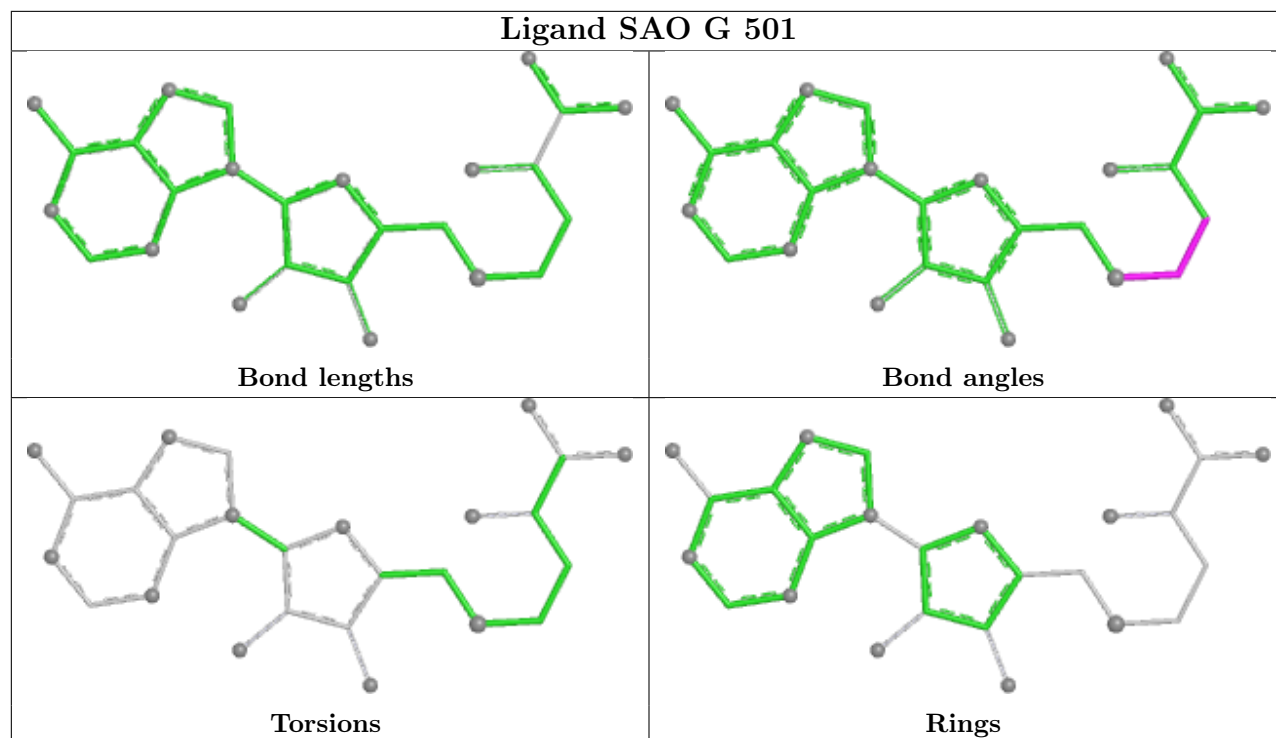
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	503	PG4	1	0
4	F	501	LHB	1	0
2	G	501	SAO	2	0
2	E	501	SAO	1	0
4	H	501	LHB	1	0
4	D	501	LHB	1	0
4	B	501	LHB	2	0

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.

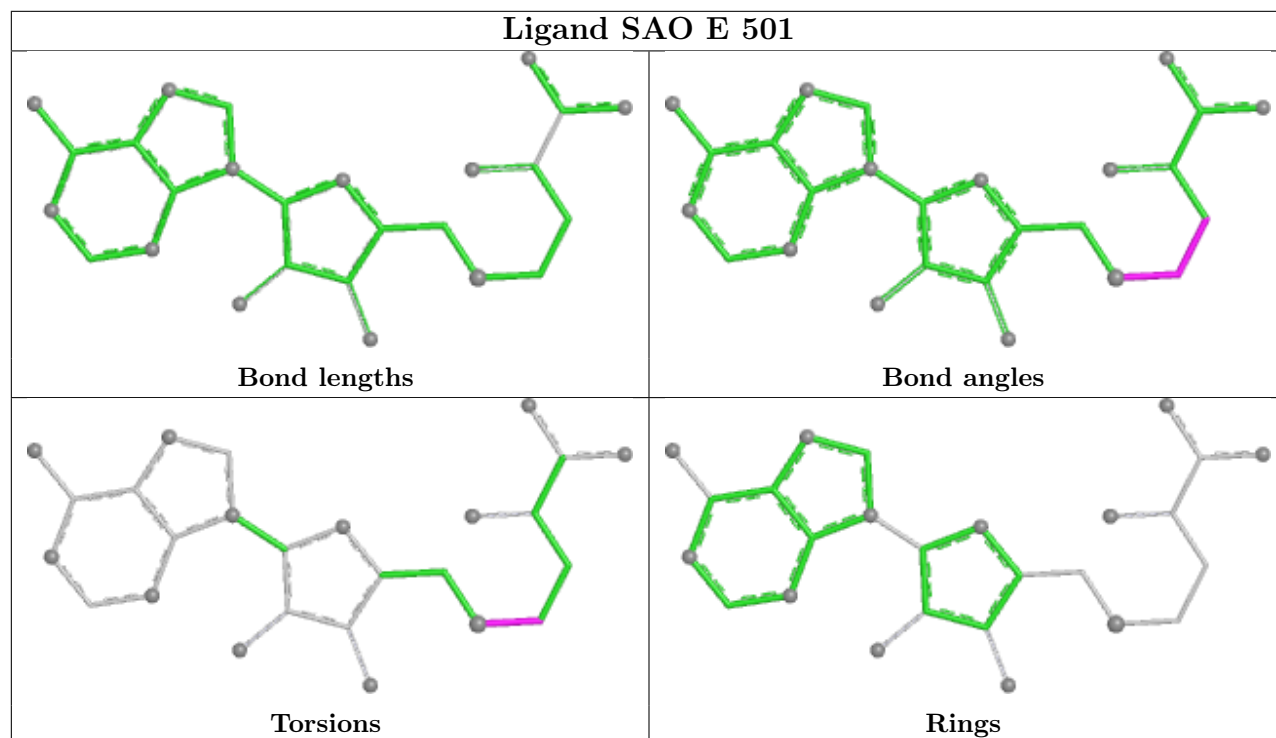
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

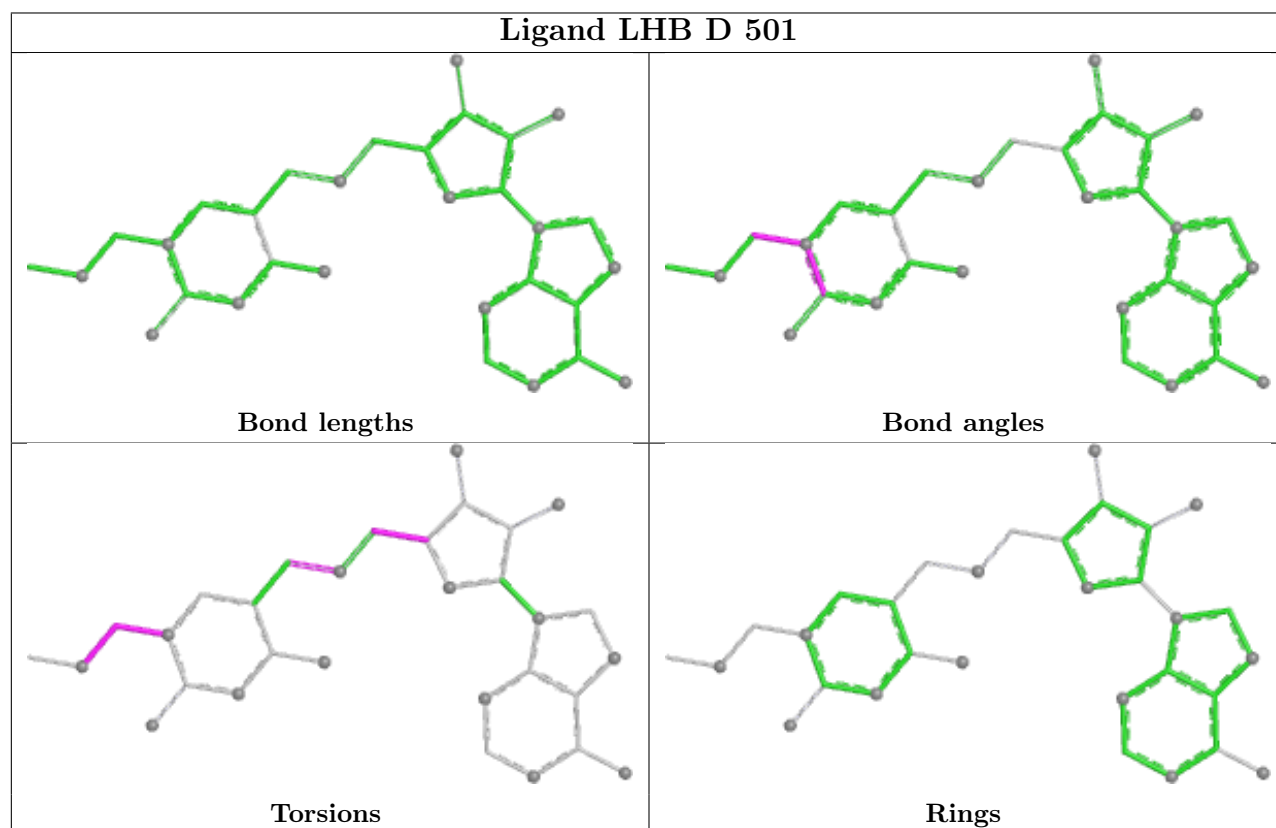
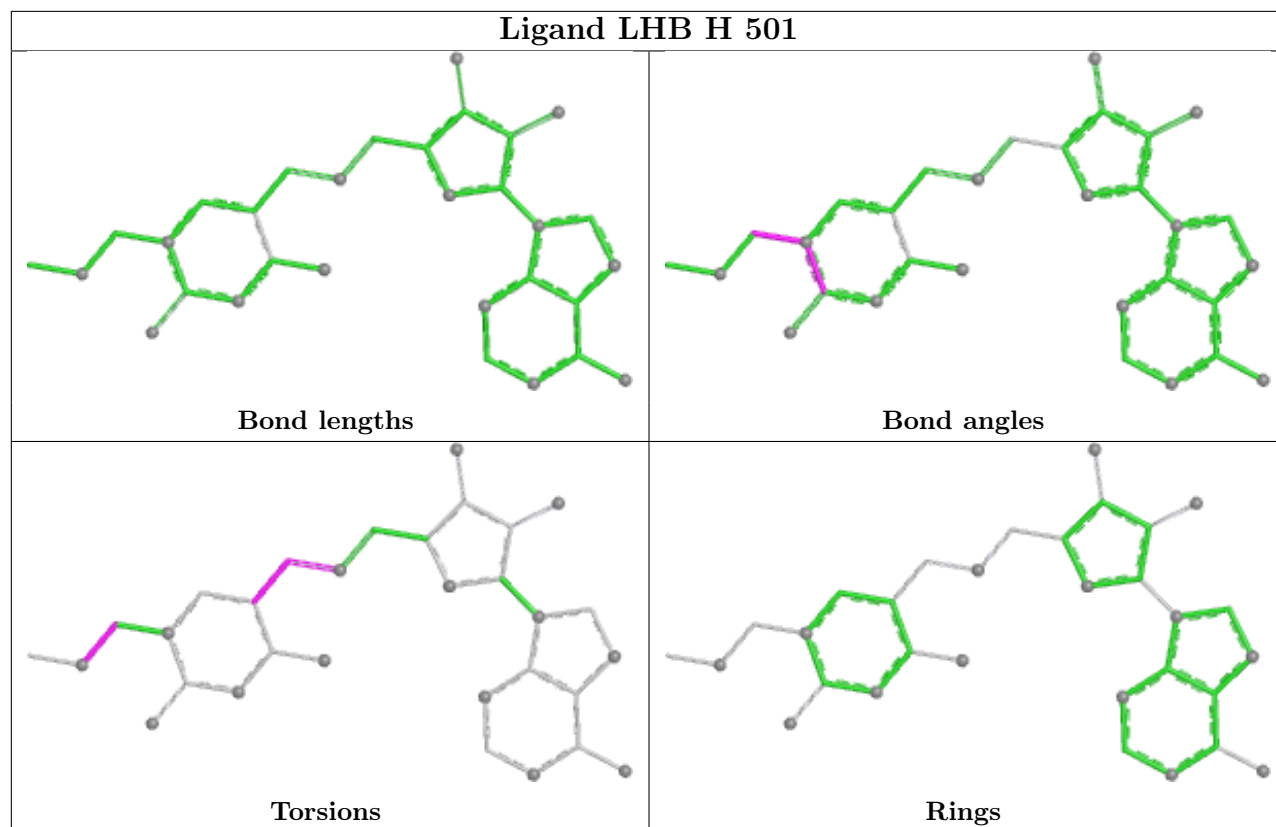


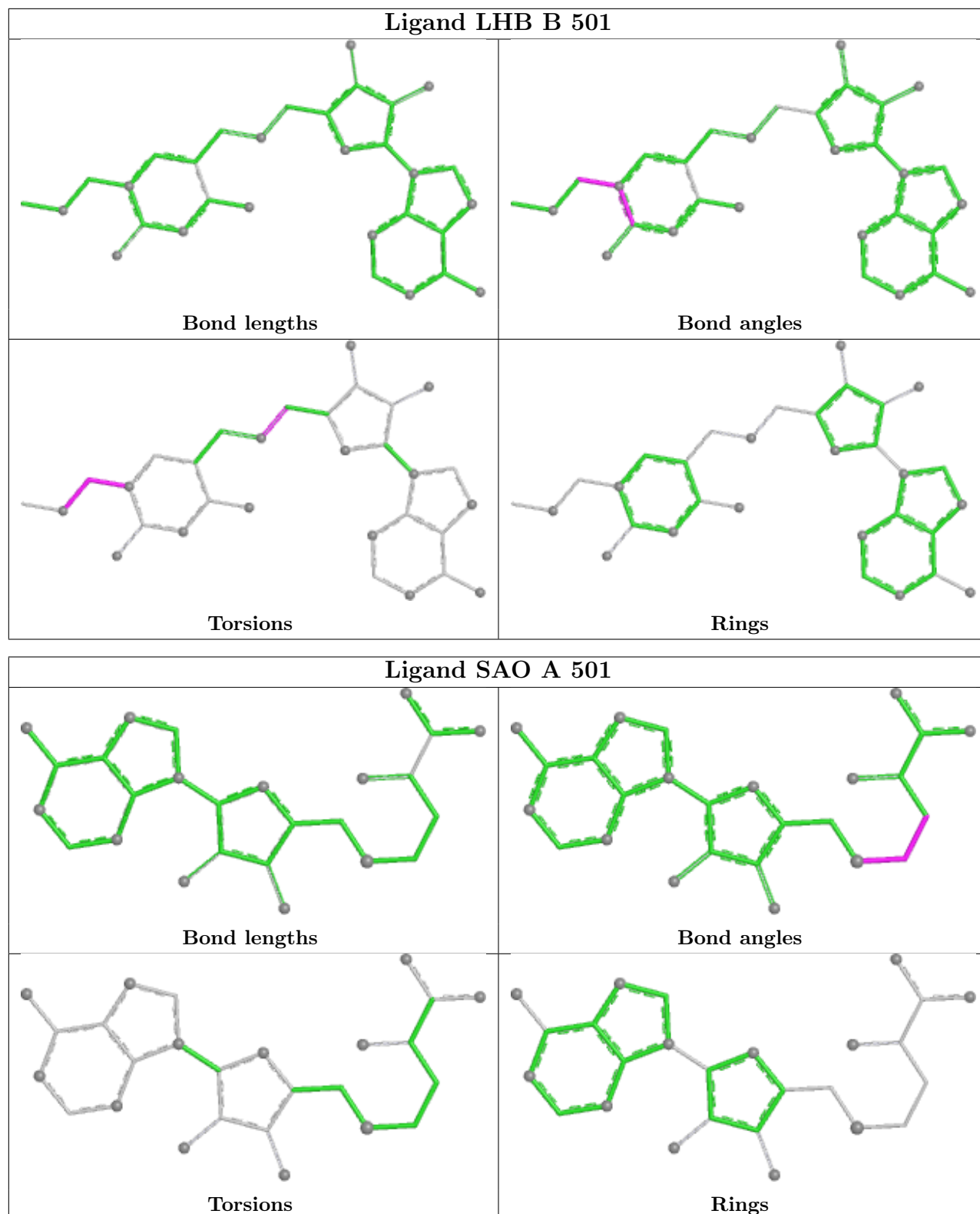
Ligand SAO G 501



Ligand SAO E 501







5.7 Other polymers [i](#)

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	343/361 (95%)	-1.49	0 100 100	30, 45, 69, 86	0
1	B	343/361 (95%)	-1.48	0 100 100	22, 45, 65, 90	1 (0%)
1	C	343/361 (95%)	-1.54	0 100 100	15, 33, 52, 75	1 (0%)
1	D	342/361 (94%)	-1.50	0 100 100	21, 38, 56, 78	1 (0%)
1	E	343/361 (95%)	-1.56	0 100 100	20, 33, 52, 66	1 (0%)
1	F	343/361 (95%)	-1.54	0 100 100	17, 37, 56, 82	1 (0%)
1	G	343/361 (95%)	-1.48	0 100 100	20, 44, 64, 79	1 (0%)
1	H	341/361 (94%)	-1.48	0 100 100	31, 44, 63, 83	0
All	All	2741/2888 (94%)	-1.51	0 100 100	15, 41, 62, 90	6 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

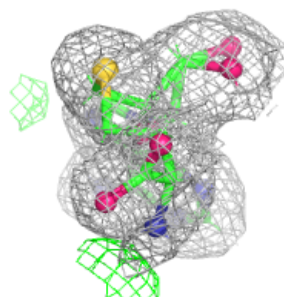
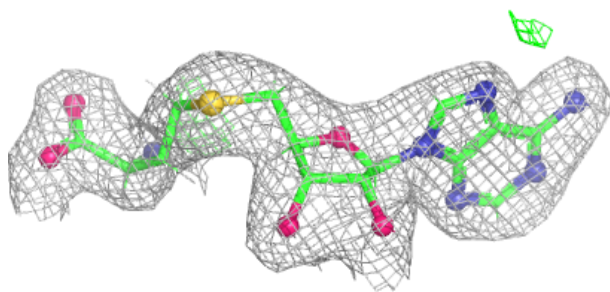
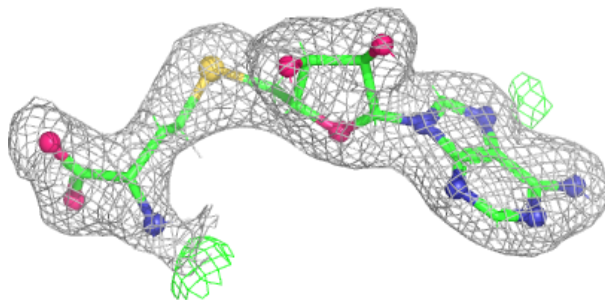
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	502	4/4	0.98	0.07	47,57,58,58	0
3	EDO	B	502	4/4	0.98	0.04	51,61,62,62	0
3	EDO	E	502	4/4	0.98	0.04	37,45,52,53	0
3	EDO	E	503	4/4	0.98	0.06	46,55,56,56	0
3	EDO	F	502	4/4	0.98	0.07	48,58,64,65	0
3	EDO	G	502	4/4	0.98	0.06	41,49,50,52	0
3	EDO	G	503	4/4	0.98	0.05	47,56,58,58	0
3	EDO	H	502	4/4	0.98	0.05	42,50,52,52	0
3	EDO	C	503	4/4	0.99	0.05	40,48,49,49	0
3	EDO	F	504	4/4	0.99	0.06	34,42,48,51	0
3	EDO	D	503	4/4	0.99	0.03	36,43,44,46	0
2	SAO	A	501	26/26	0.99	0.03	32,43,55,57	0
3	EDO	G	504	4/4	0.99	0.04	44,53,55,57	0
3	EDO	B	503	4/4	0.99	0.04	37,44,49,50	0
4	LHB	B	501	31/31	0.99	0.03	32,45,72,74	0
4	LHB	D	501	31/31	0.99	0.03	22,32,47,48	0
4	LHB	H	501	31/31	0.99	0.03	27,43,62,65	0
5	PG4	C	502	13/13	0.99	0.04	47,57,66,67	0
5	PG4	D	502	13/13	0.99	0.04	45,55,62,64	0
5	PG4	F	503	13/13	0.99	0.04	43,52,59,60	0
5	PG4	F	505	13/13	0.99	0.04	41,56,65,67	0
6	M2M	C	504	9/9	0.99	0.05	42,51,56,57	0
6	M2M	E	504	9/9	0.99	0.04	42,54,64,65	0
7	DXE	C	505	6/6	0.99	0.05	41,49,54,54	0
8	PEG	D	504	7/7	0.99	0.05	37,44,53,53	0
2	SAO	E	501	26/26	1.00	0.02	18,35,48,48	0
2	SAO	G	501	26/26	1.00	0.02	33,43,58,58	0
4	LHB	F	501	31/31	1.00	0.02	20,33,42,44	0
2	SAO	C	501	26/26	1.00	0.02	17,33,50,51	0
9	NA	D	505	1/1	1.00	0.04	38,38,38,38	0
9	NA	F	506	1/1	1.00	0.02	33,33,33,33	0

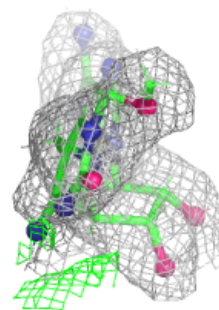
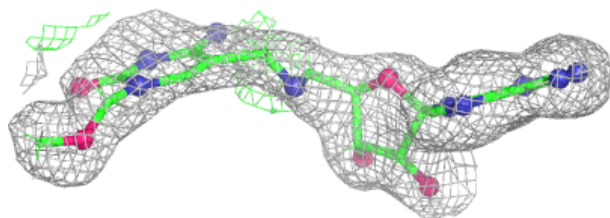
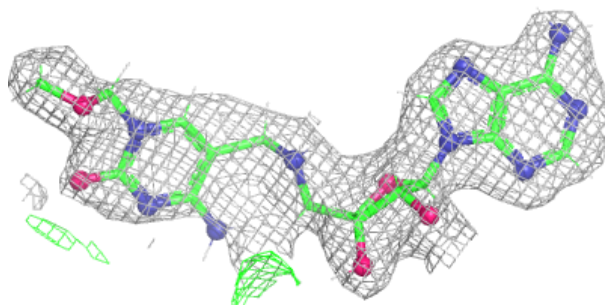
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

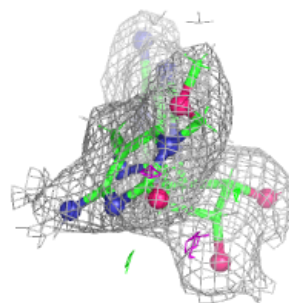
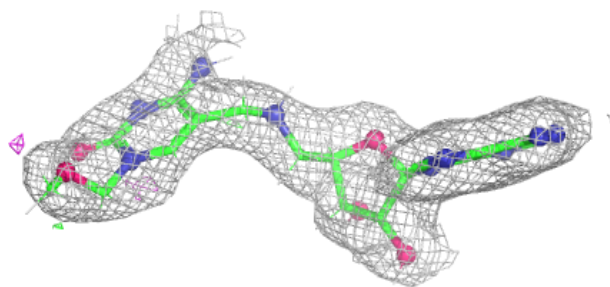
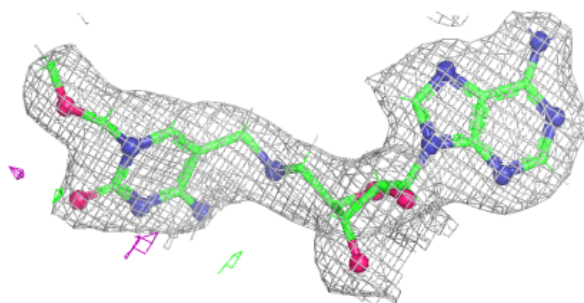
**Electron density around LHB B 501:**

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

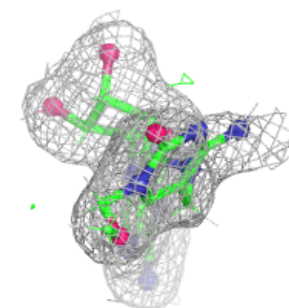
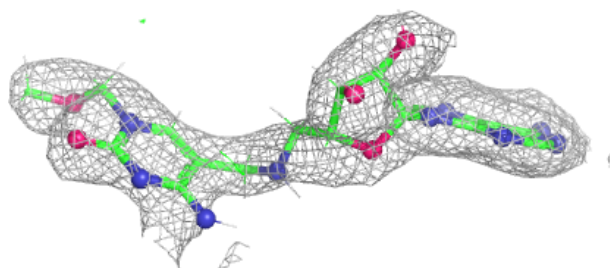
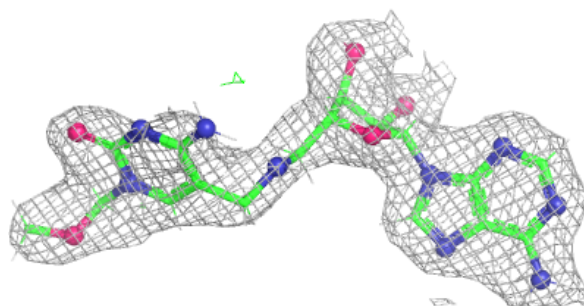


Electron density around LHB D 501:

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

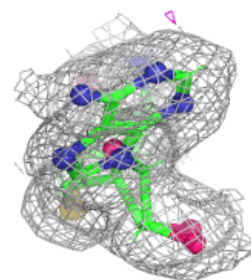
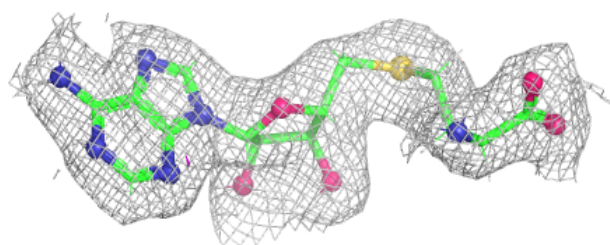
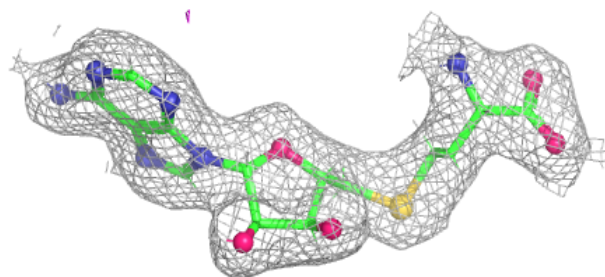
**Electron density around LHB H 501:**

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

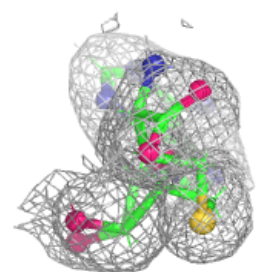
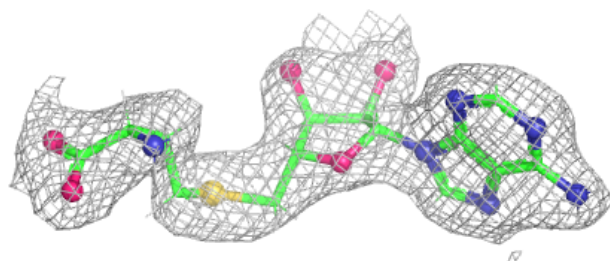
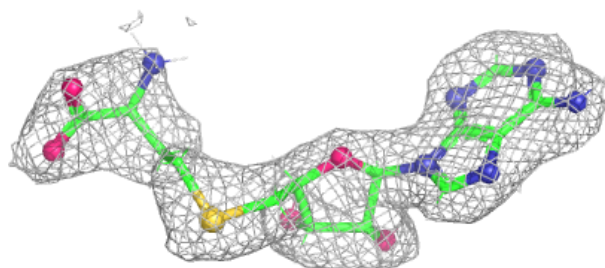


Electron density around SAO E 501:

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

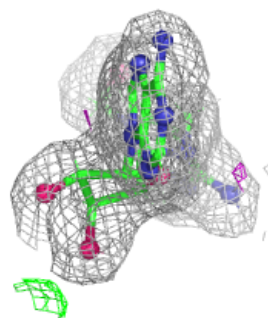
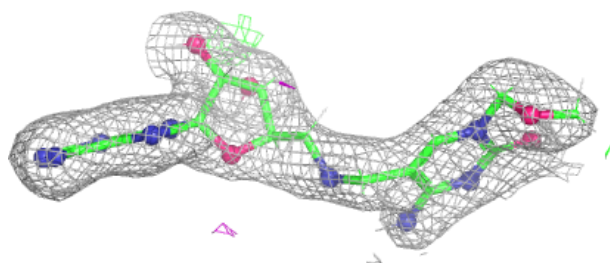
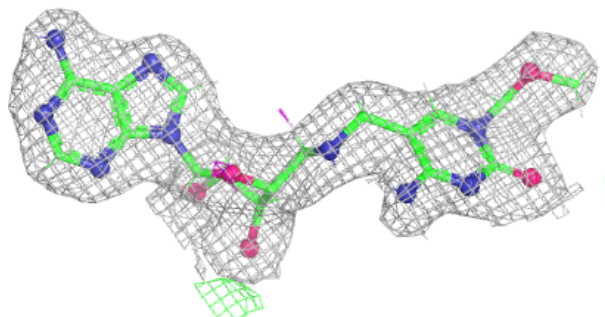
**Electron density around SAO G 501:**

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

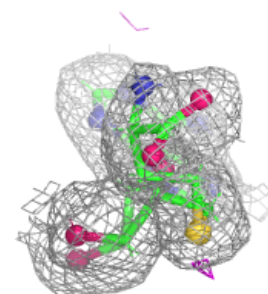
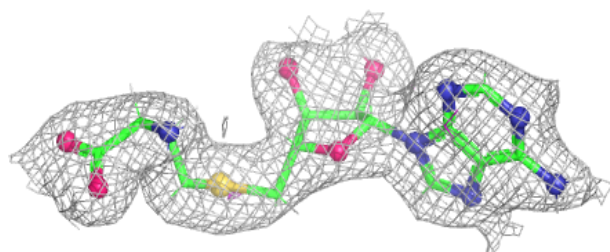
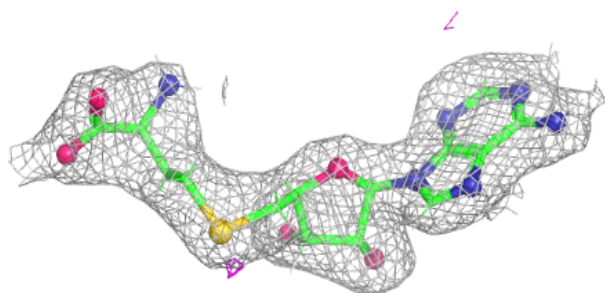


Electron density around LHB F 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.