



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:48 pm BST

PDB ID : 5IS6
Title : Crystal structure of mouse CARM1 in complex with Sinefungin at 2.0 Angstroms resolution
Authors : Cura, V.; Marechal, N.; Mailliot, J.; Troffer-Charlier, N.; Hassenboehler, P.; Wurtz, J.M.; Bonnefond, L.; Cavarelli, J.
Deposited on : 2016-03-15
Resolution : 2.01 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 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

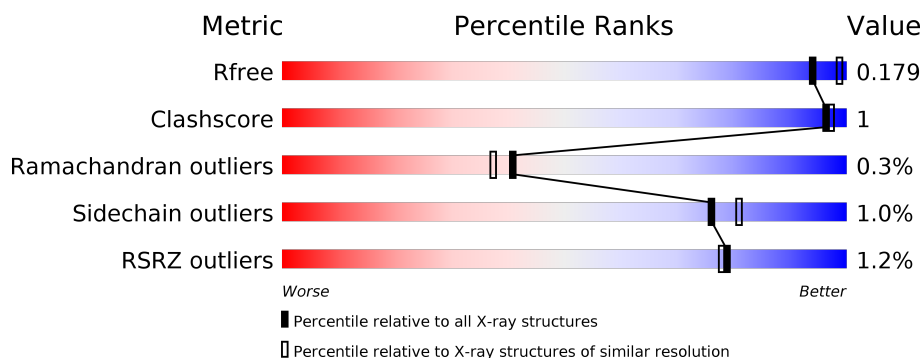
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 92% • 5% </div> </div>
1	B	361	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 92% • • 5% </div> </div>
1	C	361	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 92% • 5% </div> </div>
1	D	361	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 91%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 91% • 5% </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23412 atoms, of which 11078 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.

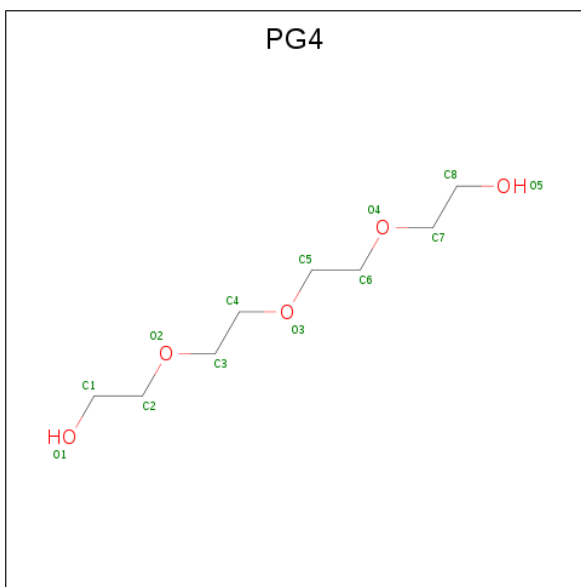
- Molecule 1 is a protein called Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	H	N	O	S	0	1	0
			5467	1781	2708	455	508	15			
1	B	344	Total	C	H	N	O	S	0	1	0
			5472	1785	2704	459	509	15			
1	C	342	Total	C	H	N	O	S	0	3	0
			5499	1796	2721	459	509	14			
1	D	342	Total	C	H	N	O	S	0	2	0
			5454	1777	2697	458	506	16			

There are 12 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

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			31	8	18	5		
2	B	1	Total	C	H	O	0	0
			31	8	18	5		
2	C	1	Total	C	H	O	0	0
			31	8	18	5		

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



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

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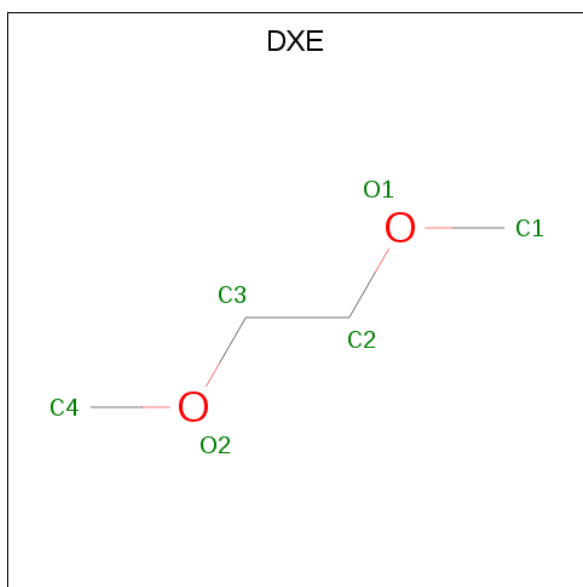
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	O		0	0
			4	2	2			
3	C	1	Total	C	O		0	0
			4	2	2			
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	O		0	0
			4	2	2			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



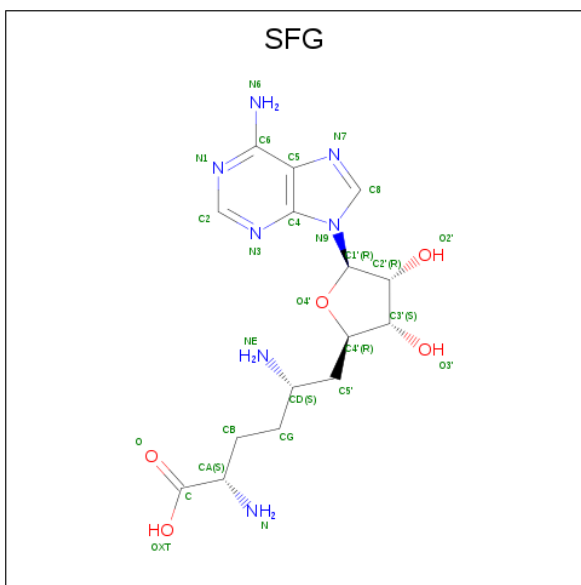
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			16	4	10	2		
5	A	1	Total	C	H	O	0	0
			16	4	10	2		
5	B	1	Total	C	H	O	0	0
			16	4	10	2		
5	B	1	Total	C	H	O	0	0
			16	4	10	2		
5	C	1	Total	C	H	O	0	0
			16	4	10	2		
5	D	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 6 is SINEFUNGIN (three-letter code: SFG) (formula: $C_{15}H_{23}N_7O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 50	C 15	H 23	N 7	O 5	0	0
6	B	1	Total 50	C 15	H 23	N 7	O 5	0	0
6	C	1	Total 50	C 15	H 23	N 7	O 5	0	0
6	D	1	Total 50	C 15	H 23	N 7	O 5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	283	Total O 283 283	0	0
7	B	242	Total O 242 242	0	0
7	C	265	Total O 265 265	0	0
7	D	246	Total O 246 246	0	0

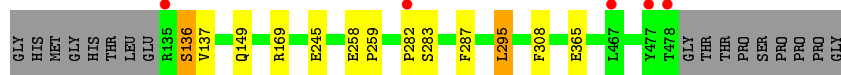
3 Residue-property plots [i](#)

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.

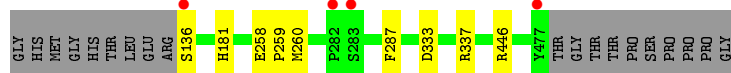
- Molecule 1: Histone-arginine methyltransferase CARM1



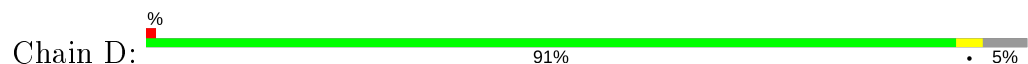
- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	74.69 Å 98.09 Å 206.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.17 – 2.01 20.17 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.17-2.01) 98.0 (20.17-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.01 Å)	Xtriage
Refinement program	PHENIX (dev_2313: ???)	Depositor
R, R_{free}	0.137 , 0.177 0.139 , 0.179	Depositor DCC
R_{free} test set	4977 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23412	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 26.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4496e-03. 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: SFG, PG4, PEG, EDO, DXE

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	0.72	3/2829 (0.1%)	0.71	2/3833 (0.1%)
1	B	0.66	1/2838 (0.0%)	0.69	3/3845 (0.1%)
1	C	0.67	0/2849	0.67	0/3858
1	D	0.67	1/2826 (0.0%)	0.69	2/3827 (0.1%)
All	All	0.68	5/11342 (0.0%)	0.69	7/15363 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	365	GLU	CB-CG	-6.62	1.39	1.52
1	B	365	GLU	CB-CG	-6.38	1.40	1.52
1	A	466	ASN	CB-CG	5.65	1.64	1.51
1	A	247	SER	C-N	-5.31	1.21	1.34
1	A	365	GLU	CB-CG	-5.30	1.42	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	VAL	CG1-CB-CG2	8.53	124.55	110.90
1	B	137	VAL	CG1-CB-CG2	8.11	123.87	110.90
1	A	454	VAL	CG1-CB-CG2	7.53	122.95	110.90
1	B	169	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	137	VAL	CA-CB-CG2	5.27	118.81	110.90
1	A	454	VAL	CA-CB-CG1	5.19	118.68	110.90
1	D	295	LEU	CA-CB-CG	5.11	127.04	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2759	2708	2707	5	0
1	B	2768	2704	2716	5	0
1	C	2778	2721	2721	5	0
1	D	2757	2697	2708	6	0
2	A	13	18	18	2	0
2	B	13	18	18	1	0
2	C	13	18	18	0	0
3	A	4	0	6	1	0
3	B	8	0	12	0	0
3	C	12	6	18	1	0
3	D	8	6	12	0	0
4	A	14	20	20	0	0
4	C	7	10	10	0	0
5	A	12	20	20	1	0
5	B	12	20	20	0	0
5	C	6	10	10	0	0
5	D	6	10	10	0	0
6	A	27	23	22	0	0
6	B	27	23	22	0	0
6	C	27	23	22	0	0
6	D	27	23	22	0	0
7	A	283	0	0	2	1
7	B	242	0	0	1	0
7	C	265	0	0	5	0
7	D	246	0	0	2	0
All	All	12334	11078	11132	23	1

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 (23) 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:260:MET:O	7:A:601:HOH:O	2.05	0.73
1:C:181:HIS:ND1	7:C:603:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:ASP:OD1	7:D:601:HOH:O	2.14	0.65
3:C:503:EDO:O1	7:C:601:HOH:O	2.15	0.63
5:A:506:DXE:H31	7:A:800:HOH:O	2.06	0.56
1:A:416:TRP:HE1	2:A:501:PG4:H82	1.74	0.52
1:C:333:ASP:O	1:C:337[A]:ARG:HG2	2.09	0.52
1:C:136:SER:N	7:C:611:HOH:O	2.44	0.51
1:D:350[A]:MET:SD	1:D:385:VAL:HG22	2.52	0.49
1:A:178:LEU:HD21	3:A:502:EDO:H11	1.96	0.48
1:A:416:TRP:NE1	2:A:501:PG4:H82	2.30	0.46
1:D:471:LYS:O	1:D:471:LYS:HG3	2.17	0.45
1:B:136:SER:HB2	1:B:245:GLU:HG2	2.00	0.44
1:C:446:ARG:NE	7:C:610:HOH:O	2.43	0.43
1:C:260:MET:O	7:C:602:HOH:O	2.21	0.43
1:D:364:LYS:HD3	1:D:364:LYS:N	2.33	0.43
1:D:169:ARG:HD3	1:D:415:HIS:CE1	2.54	0.43
1:D:137:VAL:HG13	7:D:689:HOH:O	2.19	0.43
1:B:149:GLN:NE2	7:B:2105:HOH:O	2.42	0.41
1:B:136:SER:CB	2:B:2001:PG4:H51	2.49	0.41
1:B:282:PRO:O	1:B:283:SER:HB2	2.20	0.41
1:A:265:PHE:HB3	1:A:449:TYR:CE1	2.56	0.41
1:B:295:LEU:HD12	1:B:295:LEU:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:828:HOH:O	7:A:828:HOH:O[2_765]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/361 (95%)	330 (96%)	11 (3%)	1 (0%)	41	37
1	B	343/361 (95%)	331 (96%)	11 (3%)	1 (0%)	41	37
1	C	342/361 (95%)	330 (96%)	11 (3%)	1 (0%)	41	37
1	D	342/361 (95%)	329 (96%)	12 (4%)	1 (0%)	41	37
All	All	1369/1444 (95%)	1320 (96%)	45 (3%)	4 (0%)	41	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	PRO
1	C	259	PRO
1	A	259	PRO
1	D	259	PRO

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	300/313 (96%)	298 (99%)	2 (1%)	84	88
1	B	301/313 (96%)	296 (98%)	5 (2%)	60	65
1	C	301/313 (96%)	299 (99%)	2 (1%)	84	88
1	D	300/313 (96%)	297 (99%)	3 (1%)	76	81
All	All	1202/1252 (96%)	1190 (99%)	12 (1%)	76	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	PHE
1	A	454	VAL
1	B	136	SER
1	B	258	GLU
1	B	287	PHE
1	B	295	LEU
1	B	308	PHE

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Mol	Chain	Res	Type
1	C	258	GLU
1	C	287	PHE
1	D	137	VAL
1	D	258	GLU
1	D	295	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	D	502	-	3,3,3	0.74	0	2,2,2	0.09	0
5	DXE	B	2005	-	5,5,5	0.35	0	4,4,4	0.36	0
5	DXE	C	506	-	5,5,5	0.41	0	4,4,4	0.41	0
5	DXE	A	506	-	5,5,5	0.40	0	4,4,4	0.43	0
3	EDO	C	504	-	3,3,3	0.44	0	2,2,2	0.58	0
3	EDO	B	2003	-	3,3,3	0.47	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	A	504	-	6,6,6	0.55	0	5,5,5	0.54	0
5	DXE	D	503	-	5,5,5	0.28	0	4,4,4	0.31	0
6	SFG	B	2006	-	22,29,29	0.73	0	18,42,42	0.97	0
4	PEG	C	505	-	6,6,6	0.49	0	5,5,5	0.49	0
2	PG4	A	501	-	12,12,12	0.63	0	11,11,11	0.97	0
3	EDO	D	501	-	3,3,3	0.36	0	2,2,2	0.50	0
2	PG4	B	2001	-	12,12,12	0.63	0	11,11,11	0.66	0
2	PG4	C	501	-	12,12,12	0.52	0	11,11,11	0.43	0
6	SFG	A	507	-	22,29,29	0.70	0	18,42,42	0.95	0
5	DXE	B	2004	-	5,5,5	0.40	0	4,4,4	0.29	0
3	EDO	A	502	-	3,3,3	0.48	0	2,2,2	0.17	0
6	SFG	D	504	-	22,29,29	0.68	0	18,42,42	1.03	0
3	EDO	C	502	-	3,3,3	0.44	0	2,2,2	0.52	0
3	EDO	C	503	-	3,3,3	0.46	0	2,2,2	0.81	0
5	DXE	A	505	-	5,5,5	0.39	0	4,4,4	0.36	0
4	PEG	A	503	-	6,6,6	0.43	0	5,5,5	0.58	0
6	SFG	C	507	-	22,29,29	0.64	0	18,42,42	1.01	1 (5%)
3	EDO	B	2002	-	3,3,3	0.51	0	2,2,2	0.32	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	D	502	-	-	1/1/1/1	-
5	DXE	B	2005	-	-	1/3/3/3	-
5	DXE	C	506	-	-	2/3/3/3	-
5	DXE	A	506	-	-	2/3/3/3	-
3	EDO	C	504	-	-	0/1/1/1	-
3	EDO	B	2003	-	-	1/1/1/1	-
4	PEG	A	504	-	-	2/4/4/4	-
5	DXE	D	503	-	-	2/3/3/3	-
6	SFG	B	2006	-	-	2/9/33/33	0/3/3/3
4	PEG	C	505	-	-	1/4/4/4	-
2	PG4	A	501	-	-	6/10/10/10	-
3	EDO	D	501	-	-	0/1/1/1	-
2	PG4	B	2001	-	-	4/10/10/10	-
2	PG4	C	501	-	-	5/10/10/10	-
6	SFG	A	507	-	-	2/9/33/33	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DXE	B	2004	-	-	2/3/3/3	-
3	EDO	A	502	-	-	0/1/1/1	-
6	SFG	D	504	-	-	2/9/33/33	0/3/3/3
3	EDO	C	502	-	-	0/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
5	DXE	A	505	-	-	2/3/3/3	-
4	PEG	A	503	-	-	1/4/4/4	-
6	SFG	C	507	-	-	2/9/33/33	0/3/3/3
3	EDO	B	2002	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	507	SFG	C5-C6-N6	2.33	123.89	120.35

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2003	EDO	O1-C1-C2-O2
6	D	504	SFG	NE-CD-CG-CB
6	D	504	SFG	C5'-CD-CG-CB
6	C	507	SFG	C5'-CD-CG-CB
4	C	505	PEG	O2-C3-C4-O4
5	B	2004	DXE	O1-C2-C3-O2
2	C	501	PG4	O3-C5-C6-O4
2	B	2001	PG4	O1-C1-C2-O2
2	A	501	PG4	C8-C7-O4-C6
4	A	504	PEG	O2-C3-C4-O4
2	B	2001	PG4	O3-C5-C6-O4
5	D	503	DXE	O1-C2-C3-O2
3	D	502	EDO	O1-C1-C2-O2
2	B	2001	PG4	O2-C3-C4-O3
4	A	504	PEG	O1-C1-C2-O2
5	A	506	DXE	C3-C2-O1-C1
2	C	501	PG4	C5-C6-O4-C7
2	A	501	PG4	C4-C3-O2-C2
2	C	501	PG4	C8-C7-O4-C6
4	A	503	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	A	501	PG4	C6-C5-O3-C4
6	B	2006	SFG	NE-CD-CG-CB
6	A	507	SFG	NE-CD-CG-CB
5	A	506	DXE	O1-C2-C3-O2
6	B	2006	SFG	C5'-CD-CG-CB
6	A	507	SFG	C5'-CD-CG-CB
2	C	501	PG4	O2-C3-C4-O3
3	B	2002	EDO	O1-C1-C2-O2
5	C	506	DXE	C3-C2-O1-C1
5	D	503	DXE	C3-C2-O1-C1
5	B	2004	DXE	C3-C2-O1-C1
5	B	2005	DXE	C2-C3-O2-C4
2	A	501	PG4	C1-C2-O2-C3
2	B	2001	PG4	C1-C2-O2-C3
5	A	505	DXE	C2-C3-O2-C4
2	A	501	PG4	O3-C5-C6-O4
3	C	503	EDO	O1-C1-C2-O2
2	C	501	PG4	O4-C7-C8-O5
5	C	506	DXE	O1-C2-C3-O2
5	A	505	DXE	O1-C2-C3-O2
6	C	507	SFG	NE-CD-CG-CB
2	A	501	PG4	O2-C3-C4-O3

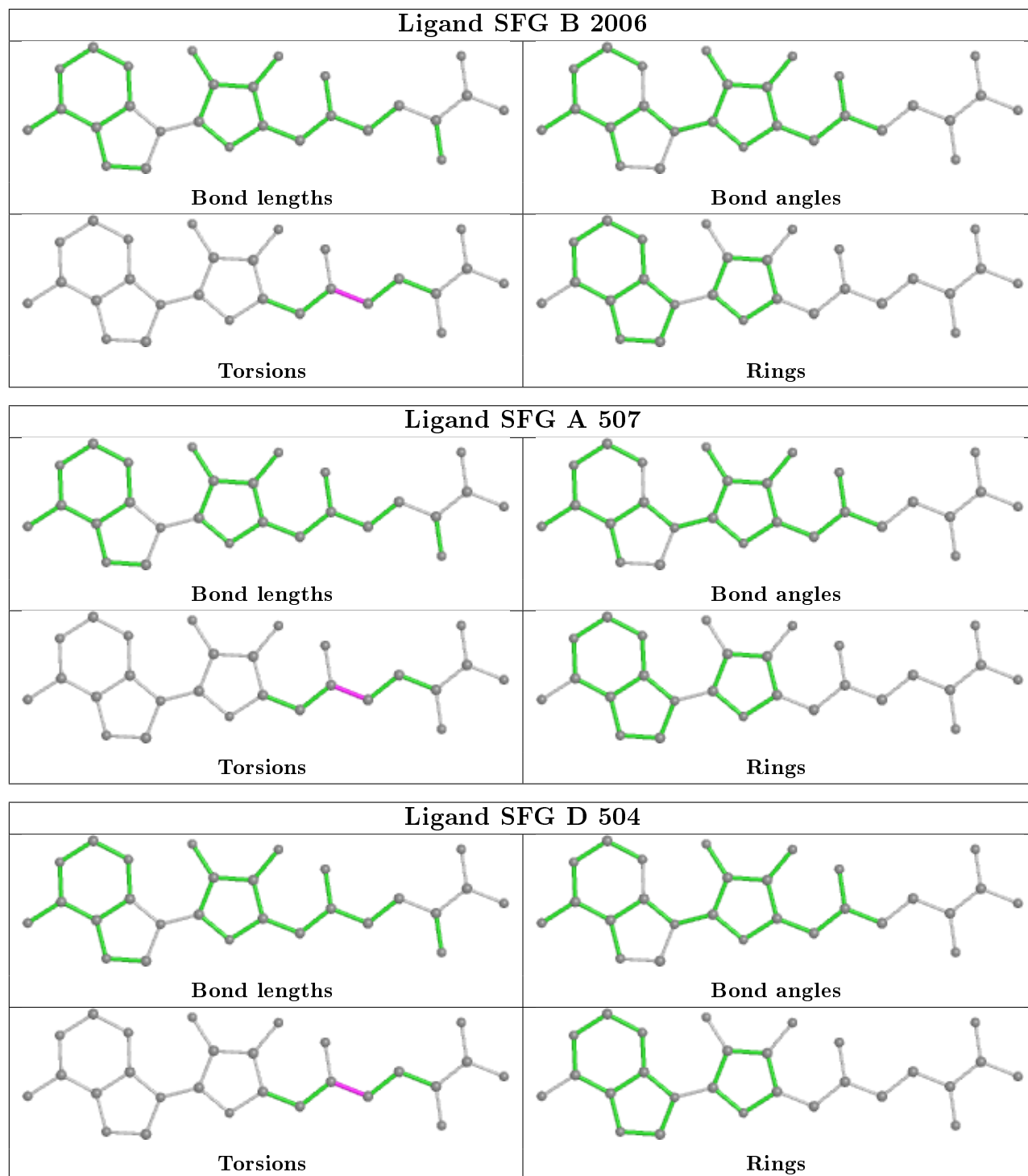
There are no ring outliers.

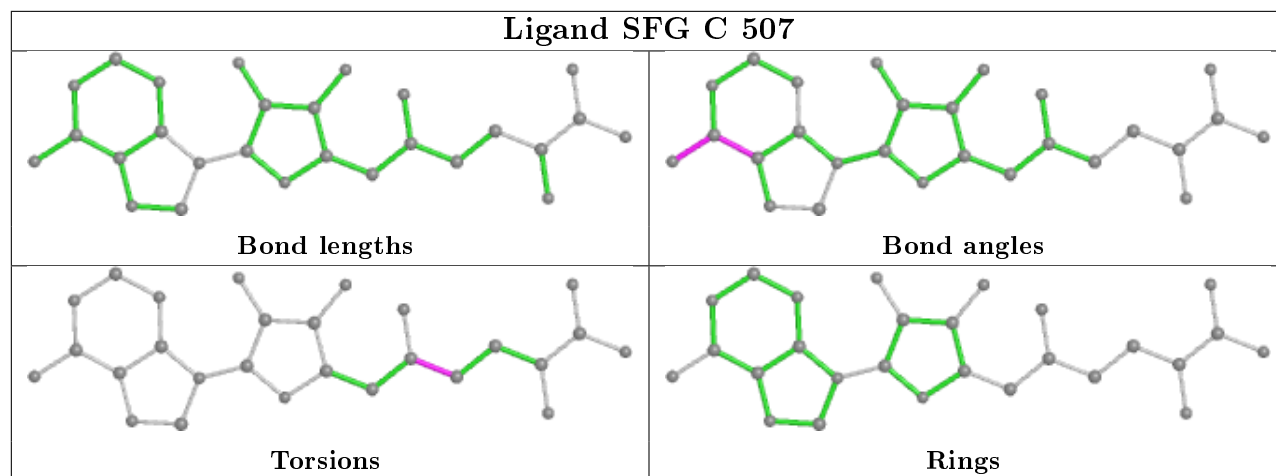
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	506	DXE	1	0
2	A	501	PG4	2	0
2	B	2001	PG4	1	0
3	A	502	EDO	1	0
3	C	503	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	-0.51	5 (1%) 73 72	13, 21, 38, 87	0
1	B	344/361 (95%)	-0.45	5 (1%) 73 72	13, 24, 45, 105	0
1	C	342/361 (94%)	-0.50	4 (1%) 79 78	15, 23, 43, 71	0
1	D	342/361 (94%)	-0.43	3 (0%) 84 83	15, 24, 43, 58	0
All	All	1371/1444 (94%)	-0.47	17 (1%) 79 78	13, 23, 43, 105	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	478	THR	6.9
1	D	135	ARG	6.8
1	A	478	THR	6.6
1	C	477[A]	TYR	3.6
1	B	135	ARG	3.3
1	B	477	TYR	3.2
1	D	475	PHE	3.1
1	A	283	SER	3.1
1	A	477	TYR	3.1
1	A	347	ARG	2.3
1	B	282	PRO	2.3
1	D	388	LEU	2.3
1	C	136	SER	2.2
1	B	467	LEU	2.2
1	C	282	PRO	2.2
1	A	234	ASP	2.2
1	C	283	SER	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

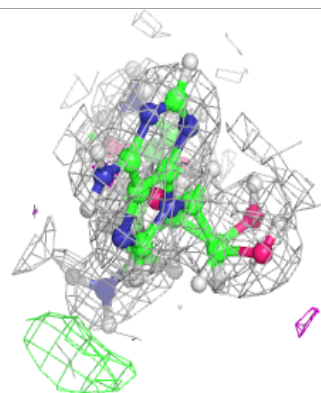
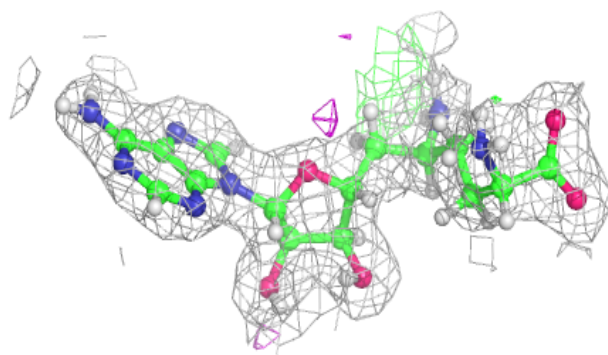
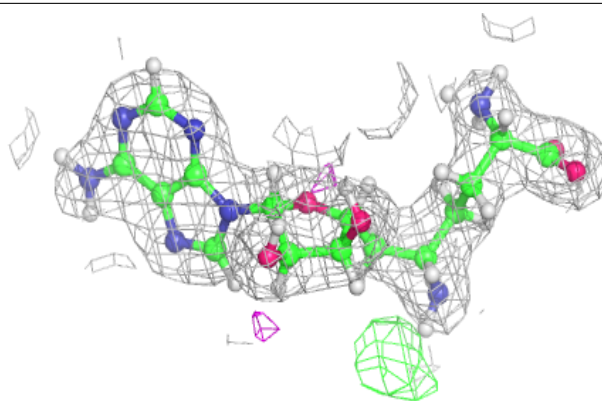
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	B	2002	4/4	0.80	0.17	46,48,51,52	0
5	DXE	B	2005	6/6	0.81	0.14	46,55,63,63	0
5	DXE	B	2004	6/6	0.82	0.17	48,58,62,62	0
5	DXE	C	506	6/6	0.82	0.15	45,55,60,60	0
3	EDO	C	504	4/4	0.84	0.15	53,54,54,55	0
2	PG4	A	501	13/13	0.84	0.25	41,54,66,67	0
4	PEG	A	504	7/7	0.85	0.24	50,60,63,64	0
2	PG4	C	501	13/13	0.86	0.23	46,59,69,70	0
5	DXE	A	506	6/6	0.86	0.21	50,60,71,71	0
4	PEG	A	503	7/7	0.86	0.13	49,59,62,62	0
3	EDO	D	502	4/4	0.86	0.26	27,27,31,32	0
3	EDO	A	502	4/4	0.88	0.12	46,47,51,54	0
5	DXE	D	503	6/6	0.89	0.16	47,57,64,64	0
5	DXE	A	505	6/6	0.89	0.14	45,54,56,56	0
3	EDO	C	503	4/4	0.90	0.10	51,52,53,54	0
4	PEG	C	505	7/7	0.90	0.23	49,59,63,64	0
2	PG4	B	2001	13/13	0.91	0.17	32,38,45,49	0
3	EDO	C	502	4/4	0.91	0.14	50,60,61,63	0
3	EDO	B	2003	4/4	0.94	0.09	45,46,46,47	0
3	EDO	D	501	4/4	0.95	0.13	44,53,55,58	0
6	SFG	D	504	27/27	0.98	0.07	15,20,24,25	0
6	SFG	B	2006	27/27	0.98	0.08	14,20,24,24	0
6	SFG	C	507	27/27	0.98	0.08	15,20,23,24	0
6	SFG	A	507	27/27	0.98	0.10	15,19,24,25	0

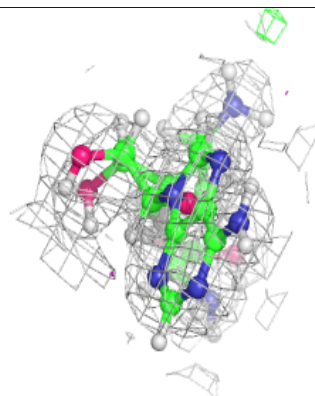
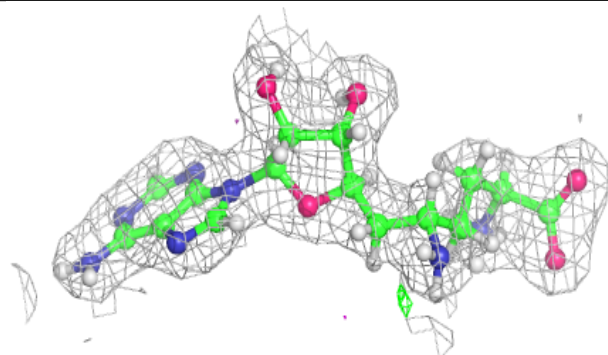
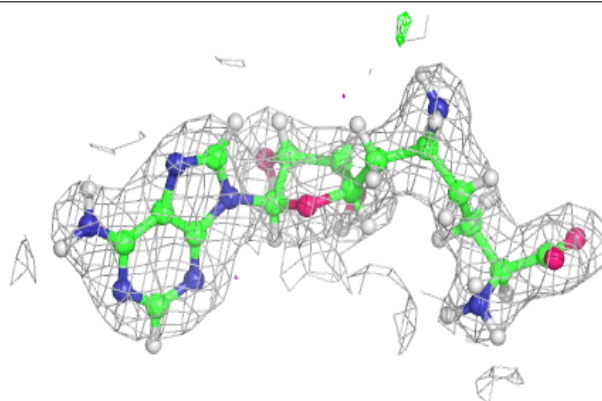
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SFG D 504:

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

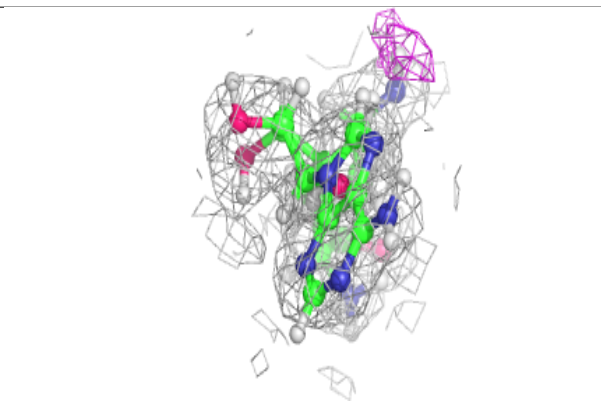
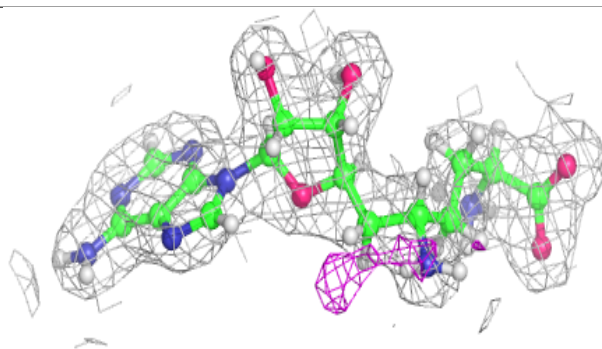
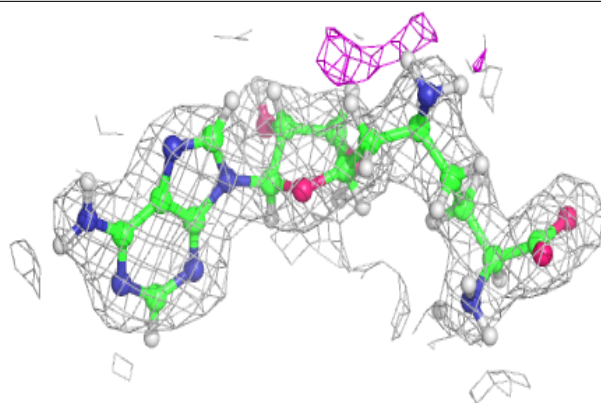
**Electron density around SFG B 2006:**

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

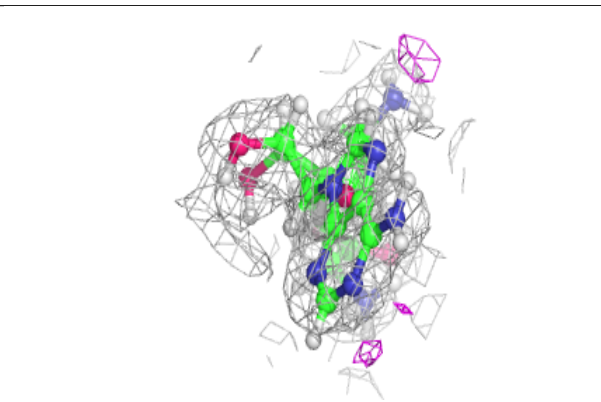
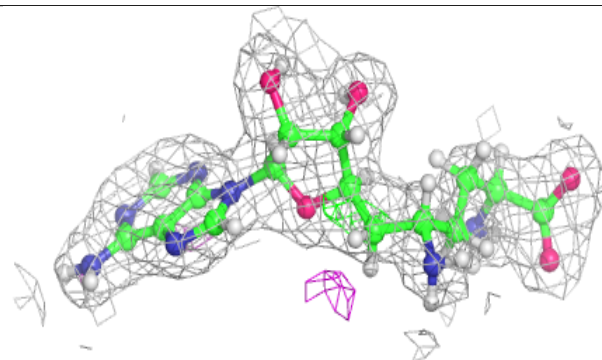
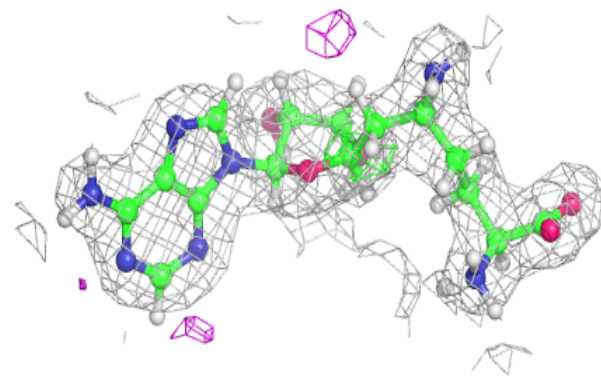


Electron density around SFG C 507:

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

**Electron density around SFG A 507:**

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



6.5 Other polymers

There are no such residues in this entry.