



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:19 am BST

PDB ID : 5ISH  
Title : Crystal structure of mouse CARM1 in complex with inhibitor SA0765  
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Deposited on : 2016-03-15  
Resolution : 2.15 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](mailto: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.

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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

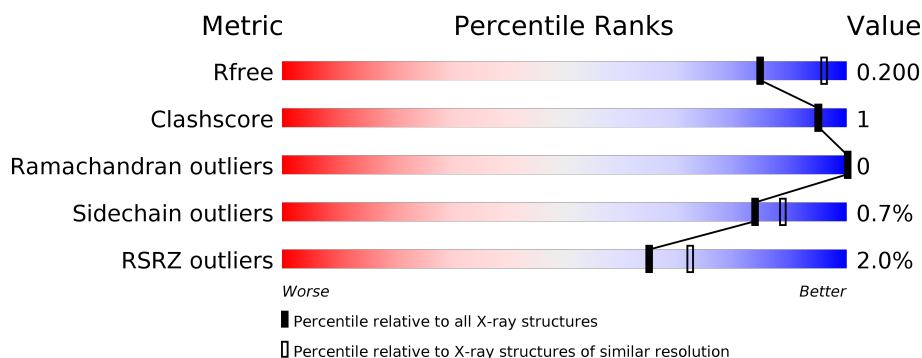
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>92%</div> <div>5%</div> </div> </div>
1	B	361	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	C	361	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	D	361	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23221 atoms, of which 11080 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.

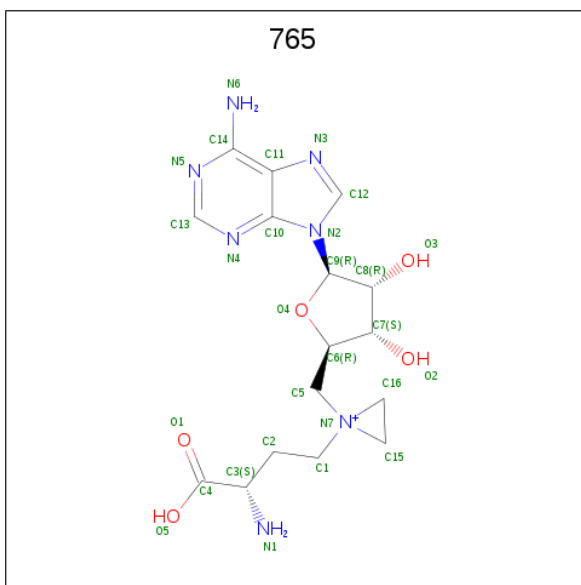
- Molecule 1 is a protein called Histone-arginine methyltransferase CARM1.

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	343	Total	C	H	N	O	S	0	2	0
			5488	1786	2718	460	510	14			
1	C	343	Total	C	H	N	O	S	0	0	0
			5450	1776	2699	454	507	14			
1	D	341	Total	C	H	N	O	S	0	0	0
			5415	1763	2683	452	503	14			

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 5'-{1-[(3S)-3-amino-3-carboxypropyl]aziridin-1-ium-1-yl}-5'-deoxyadenosine (three-letter code: 765) (formula: C<sub>16</sub>H<sub>24</sub>N<sub>7</sub>O<sub>5</sub>).



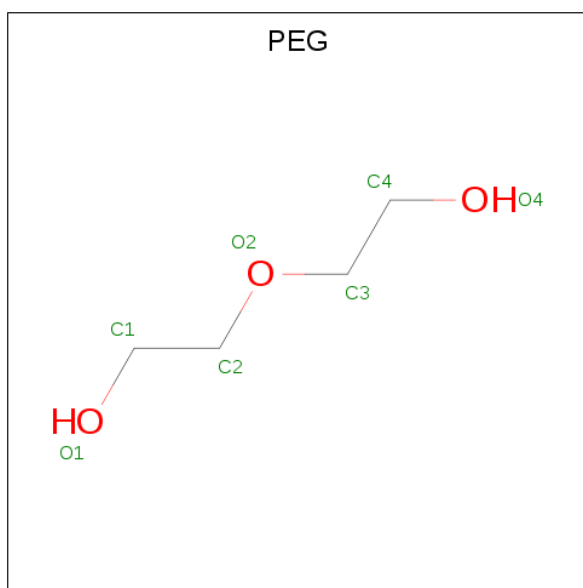
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			51	16	23	7	5		
2	B	1	Total	C	H	N	O	0	0
			51	16	23	7	5		
2	C	1	Total	C	H	N	O	0	0
			51	16	23	7	5		
2	D	1	Total	C	H	N	O	0	0
			51	16	23	7	5		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



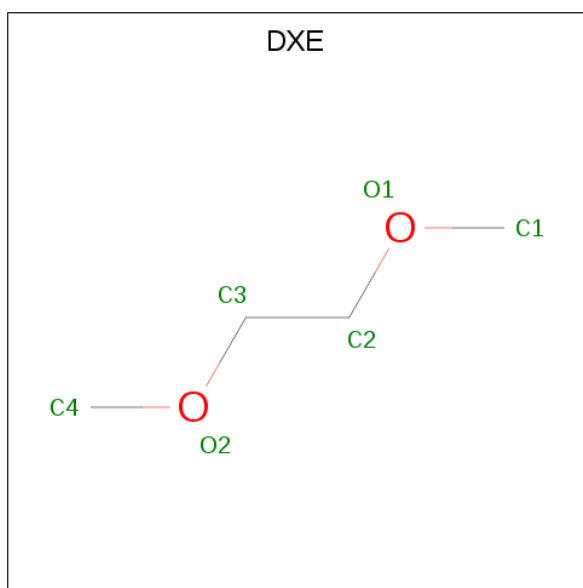
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		

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



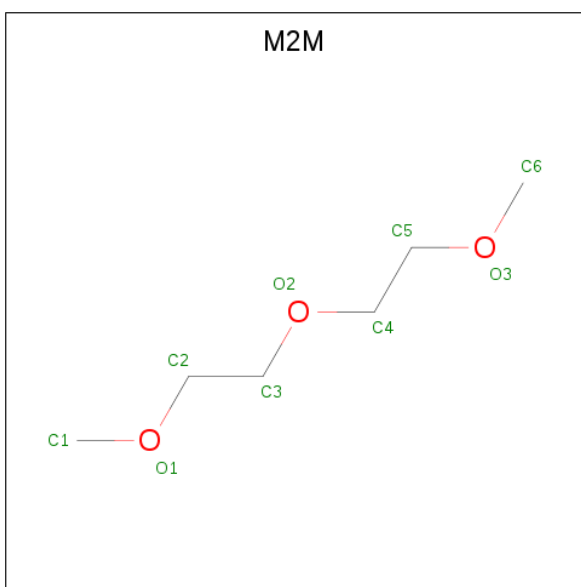
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		

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



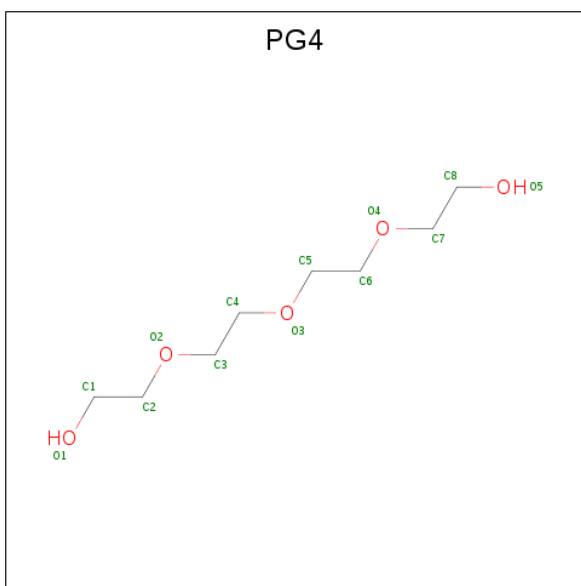
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			16	4	10	2		
5	C	1	Total	C	H	O	0	0
			16	4	10	2		
5	C	1	Total	C	H	O	0	0
			16	4	10	2		
5	C	1	Total	C	H	O	0	0
			16	4	10	2		
5	C	1	Total	C	H	O	0	0
			16	4	10	2		
5	D	1	Total	C	H	O	0	0
			16	4	10	2		

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



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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	268	Total 268	O 268	0	0
8	B	219	Total 219	O 219	0	0
8	C	219	Total 219	O 219	0	0
8	D	193	Total 193	O 193	0	0



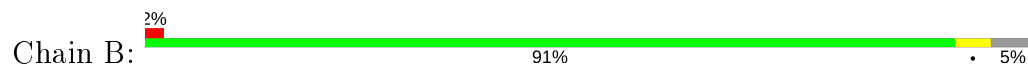
### 3 Residue-property plots [i](#)

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



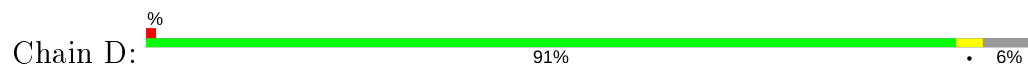
- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.67Å 98.41Å 206.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.15 29.83 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.83-2.15) 99.4 (29.83-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.72 (at 2.16Å)	Xtriage
Refinement program	PHENIX dev_1980	Depositor
R, $R_{free}$	0.164 , 0.198 0.165 , 0.200	Depositor DCC
$R_{free}$ test set	4129 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23221	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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 34.62 % 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 6.6281e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> 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: EDO, 765, 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	0.31	0/2829	0.48	0/3833
1	B	0.28	0/2840	0.46	0/3849
1	C	0.28	0/2821	0.46	0/3823
1	D	0.28	0/2801	0.45	0/3795
All	All	0.28	0/11291	0.46	0/15300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2759	2708	2707	7	0
1	B	2770	2718	2717	6	0
1	C	2751	2699	2699	6	0
1	D	2732	2683	2683	7	0
2	A	28	23	0	1	0
2	B	28	23	0	0	0
2	C	28	23	0	0	0
2	D	28	23	0	0	0
3	A	4	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	12	12	0	0
3	C	16	24	24	0	0
3	D	4	6	6	0	0
4	A	21	30	30	1	0
4	B	7	10	10	0	0
5	A	6	10	10	0	0
5	C	24	40	40	0	0
5	D	6	10	10	0	0
6	A	9	14	14	1	0
7	B	13	18	18	0	0
8	A	268	0	0	1	0
8	B	219	0	0	2	0
8	C	219	0	0	1	0
8	D	193	0	0	3	0
All	All	12141	11080	10986	26	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (26) 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:B:450:ASP:OD1	8:B:601:HOH:O	2.14	0.65
1:C:424:GLN:OE1	8:C:601:HOH:O	2.14	0.64
1:A:469:ASP:OD1	8:A:601:HOH:O	2.16	0.59
1:B:337:ARG:NH2	8:B:606:HOH:O	2.37	0.58
1:C:186:ASP:O	1:C:209:ARG:NH1	2.37	0.58
1:D:337:ARG:NH2	8:D:603:HOH:O	2.39	0.55
1:D:218:THR:O	1:D:221:GLN:HG2	2.07	0.55
1:B:186:ASP:O	1:B:209:ARG:NH1	2.42	0.52
1:A:424:GLN:HG2	6:A:507:M2M:H13	1.93	0.51
1:D:301:GLU:OE1	8:D:601:HOH:O	2.19	0.50
1:D:277:LYS:HD3	1:D:286:MET:SD	2.54	0.48
1:A:282:PRO:O	1:A:283:SER:OG	2.20	0.45
1:A:163:MET:SD	2:A:501:765:C16	3.05	0.45
1:B:266:ASN:O	1:B:267:GLU:HB2	2.18	0.44
1:C:259:PRO:HG2	1:C:270:LEU:HD23	1.99	0.44
1:C:218:THR:O	1:C:221:GLN:HG2	2.18	0.44
1:A:341:VAL:O	1:A:342:ASP:HB3	2.18	0.43
1:C:266:ASN:O	1:C:267:GLU:HB2	2.18	0.43
1:D:136:SER:N	8:D:615:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:ARG:HG2	1:D:467:LEU:O	2.19	0.43
1:D:341:VAL:O	1:D:342:ASP:HB3	2.20	0.42
1:A:399:SER:HA	4:A:504:PEG:H31	2.02	0.42
1:B:143:GLU:HG3	1:B:445:LYS:HB3	2.00	0.42
1:B:153:PHE:CE2	1:B:159:GLN:HG2	2.54	0.41
1:C:341:VAL:O	1:C:342:ASP:HB3	2.19	0.41
1:A:266:ASN:O	1:A:267:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/361 (95%)	333 (97%)	9 (3%)	0	100	100
1	B	343/361 (95%)	334 (97%)	9 (3%)	0	100	100
1	C	341/361 (94%)	331 (97%)	10 (3%)	0	100	100
1	D	339/361 (94%)	328 (97%)	11 (3%)	0	100	100
All	All	1365/1444 (94%)	1326 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	300/313 (96%)	298 (99%)	2 (1%)	84	89
1	B	301/313 (96%)	298 (99%)	3 (1%)	76	81
1	C	299/313 (96%)	298 (100%)	1 (0%)	92	95
1	D	297/313 (95%)	295 (99%)	2 (1%)	84	89
All	All	1197/1252 (96%)	1189 (99%)	8 (1%)	84	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	LEU
1	A	258	GLU
1	B	258	GLU
1	B	295	LEU
1	B	308	PHE
1	C	258	GLU
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 ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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
7	PG4	B	505	-	12,12,12	0.50	0	11,11,11	0.50	0
3	EDO	B	502	-	3,3,3	0.44	0	2,2,2	0.47	0
2	765	A	501	-	24,31,31	2.55	8 (33%)	18,47,47	1.71	4 (22%)
3	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.58	0
4	PEG	B	504	-	6,6,6	0.49	0	5,5,5	0.53	0
3	EDO	B	503	-	3,3,3	0.47	0	2,2,2	0.42	0
4	PEG	A	505	-	6,6,6	0.47	0	5,5,5	0.44	0
5	DXE	C	507	-	5,5,5	0.42	0	4,4,4	0.19	0
2	765	C	501	-	24,31,31	2.51	8 (33%)	18,47,47	1.66	4 (22%)
5	DXE	C	508	-	5,5,5	0.41	0	4,4,4	0.29	0
2	765	B	501	-	24,31,31	2.49	10 (41%)	18,47,47	1.71	5 (27%)
2	765	D	501	-	24,31,31	2.48	9 (37%)	18,47,47	1.69	4 (22%)
3	EDO	C	502	-	3,3,3	0.46	0	2,2,2	0.47	0
5	DXE	C	509	-	5,5,5	0.42	0	4,4,4	0.21	0
4	PEG	A	503	-	6,6,6	0.49	0	5,5,5	0.48	0
3	EDO	C	503	-	3,3,3	0.46	0	2,2,2	0.54	0
3	EDO	C	505	-	3,3,3	0.42	0	2,2,2	0.57	0
3	EDO	D	502	-	3,3,3	0.46	0	2,2,2	0.39	0
3	EDO	A	502	-	3,3,3	0.46	0	2,2,2	0.45	0
5	DXE	D	503	-	5,5,5	0.42	0	4,4,4	0.20	0
5	DXE	A	506	-	5,5,5	0.41	0	4,4,4	0.21	0
5	DXE	C	506	-	5,5,5	0.39	0	4,4,4	0.21	0
4	PEG	A	504	-	6,6,6	0.43	0	5,5,5	0.65	0
6	M2M	A	507	-	8,8,8	0.61	0	7,7,7	0.37	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
7	PG4	B	505	-	-	6/10/10/10	-
3	EDO	B	502	-	-	0/1/1/1	-
2	765	A	501	-	-	3/5/39/39	0/4/4/4
3	EDO	C	504	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	B	504	-	-	2/4/4/4	-
3	EDO	B	503	-	-	0/1/1/1	-
4	PEG	A	505	-	-	2/4/4/4	-
5	DXE	C	507	-	-	2/3/3/3	-
2	765	C	501	-	-	3/5/39/39	0/4/4/4
5	DXE	C	508	-	-	1/3/3/3	-
2	765	B	501	-	-	4/5/39/39	0/4/4/4
2	765	D	501	-	-	4/5/39/39	0/4/4/4
3	EDO	C	502	-	-	0/1/1/1	-
5	DXE	C	509	-	-	2/3/3/3	-
4	PEG	A	503	-	-	0/4/4/4	-
3	EDO	C	503	-	-	0/1/1/1	-
3	EDO	C	505	-	-	1/1/1/1	-
3	EDO	D	502	-	-	1/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
5	DXE	D	503	-	-	0/3/3/3	-
5	DXE	A	506	-	-	2/3/3/3	-
5	DXE	C	506	-	-	3/3/3/3	-
4	PEG	A	504	-	-	3/4/4/4	-
6	M2M	A	507	-	-	3/6/6/6	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	765	C8-C9	-7.95	1.41	1.53
2	C	501	765	C8-C9	-7.92	1.41	1.53
2	A	501	765	C8-C9	-7.88	1.41	1.53
2	D	501	765	C8-C9	-7.79	1.41	1.53
2	B	501	765	O4-C9	4.01	1.46	1.41
2	D	501	765	O4-C9	3.88	1.46	1.41
2	A	501	765	C16-N7	-3.85	1.40	1.48
2	D	501	765	C5-C6	-3.62	1.44	1.52
2	A	501	765	C8-C7	-3.60	1.43	1.53
2	D	501	765	C8-C7	-3.58	1.43	1.53
2	C	501	765	C8-C7	-3.57	1.43	1.53
2	C	501	765	O4-C9	3.56	1.46	1.41
2	A	501	765	C5-C6	-3.49	1.45	1.52
2	B	501	765	C5-C6	-3.48	1.45	1.52
2	B	501	765	C8-C7	-3.47	1.43	1.53
2	C	501	765	C5-C6	-3.46	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	765	O4-C9	3.39	1.45	1.41
2	A	501	765	O4-C6	-3.30	1.37	1.45
2	C	501	765	C16-N7	-3.20	1.41	1.48
2	C	501	765	O4-C6	-3.11	1.38	1.45
2	D	501	765	O4-C6	-3.09	1.38	1.45
2	B	501	765	O4-C6	-3.05	1.38	1.45
2	B	501	765	C16-N7	-2.81	1.42	1.48
2	C	501	765	C15-N7	-2.74	1.42	1.48
2	D	501	765	C16-N7	-2.64	1.43	1.48
2	A	501	765	C5-N7	-2.58	1.47	1.52
2	A	501	765	C15-N7	-2.58	1.43	1.48
2	B	501	765	C5-N7	-2.51	1.47	1.52
2	C	501	765	C5-N7	-2.50	1.47	1.52
2	D	501	765	C5-N7	-2.49	1.47	1.52
2	D	501	765	C15-N7	-2.42	1.43	1.48
2	B	501	765	C15-N7	-2.17	1.44	1.48
2	D	501	765	C14-N6	2.02	1.41	1.34
2	B	501	765	C13-N4	2.01	1.35	1.32
2	B	501	765	C14-N6	2.01	1.41	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	765	N4-C13-N5	-4.45	121.72	128.68
2	A	501	765	N4-C13-N5	-4.45	121.73	128.68
2	B	501	765	N4-C13-N5	-4.36	121.86	128.68
2	C	501	765	N4-C13-N5	-4.27	122.00	128.68
2	B	501	765	C9-N2-C10	-3.08	121.23	126.64
2	C	501	765	C7-C8-C9	2.99	105.48	100.98
2	B	501	765	C7-C8-C9	2.98	105.46	100.98
2	A	501	765	C9-N2-C10	-2.94	121.48	126.64
2	D	501	765	C9-N2-C10	-2.92	121.51	126.64
2	D	501	765	C7-C8-C9	2.92	105.37	100.98
2	C	501	765	C9-N2-C10	-2.84	121.65	126.64
2	A	501	765	C7-C8-C9	2.55	104.82	100.98
2	B	501	765	C10-C11-N3	-2.26	107.04	109.40
2	C	501	765	C10-C11-N3	-2.19	107.12	109.40
2	A	501	765	C8-C7-C6	2.17	106.86	102.64
2	D	501	765	C8-C7-C6	2.09	106.71	102.64
2	B	501	765	C8-C7-C6	2.00	106.53	102.64

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	765	N7-C5-C6-C7
2	C	501	765	N7-C5-C6-C7
2	B	501	765	C1-C2-C3-C4
2	B	501	765	N7-C5-C6-C7
2	D	501	765	C1-C2-C3-C4
2	D	501	765	N7-C5-C6-C7
2	D	501	765	N7-C5-C6-O4
7	B	505	PG4	O2-C3-C4-O3
5	C	507	DXE	O1-C2-C3-O2
7	B	505	PG4	O1-C1-C2-O2
4	B	504	PEG	O1-C1-C2-O2
3	C	505	EDO	O1-C1-C2-O2
5	C	508	DXE	O1-C2-C3-O2
7	B	505	PG4	O4-C7-C8-O5
4	A	505	PEG	O2-C3-C4-O4
4	B	504	PEG	O2-C3-C4-O4
5	C	509	DXE	C2-C3-O2-C4
5	C	506	DXE	C2-C3-O2-C4
6	A	507	M2M	C4-C5-O3-C6
4	A	504	PEG	C4-C3-O2-C2
2	B	501	765	C1-C2-C3-N1
2	D	501	765	C1-C2-C3-N1
7	B	505	PG4	C6-C5-O3-C4
5	A	506	DXE	C3-C2-O1-C1
3	C	504	EDO	O1-C1-C2-O2
2	A	501	765	N7-C5-C6-O4
2	C	501	765	N7-C5-C6-O4
2	B	501	765	N7-C5-C6-O4
6	A	507	M2M	O2-C4-C5-O3
4	A	504	PEG	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
5	C	507	DXE	C2-C3-O2-C4
4	A	504	PEG	C1-C2-O2-C3
7	B	505	PG4	C3-C4-O3-C5
7	B	505	PG4	O3-C5-C6-O4
3	D	502	EDO	O1-C1-C2-O2
2	A	501	765	C1-C2-C3-N1
2	C	501	765	C1-C2-C3-N1
4	A	505	PEG	O1-C1-C2-O2
5	C	509	DXE	O1-C2-C3-O2
5	A	506	DXE	O1-C2-C3-O2
6	A	507	M2M	O1-C2-C3-O2

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Mol	Chain	Res	Type	Atoms
5	C	506	DXE	O1-C2-C3-O2
5	C	506	DXE	C3-C2-O1-C1

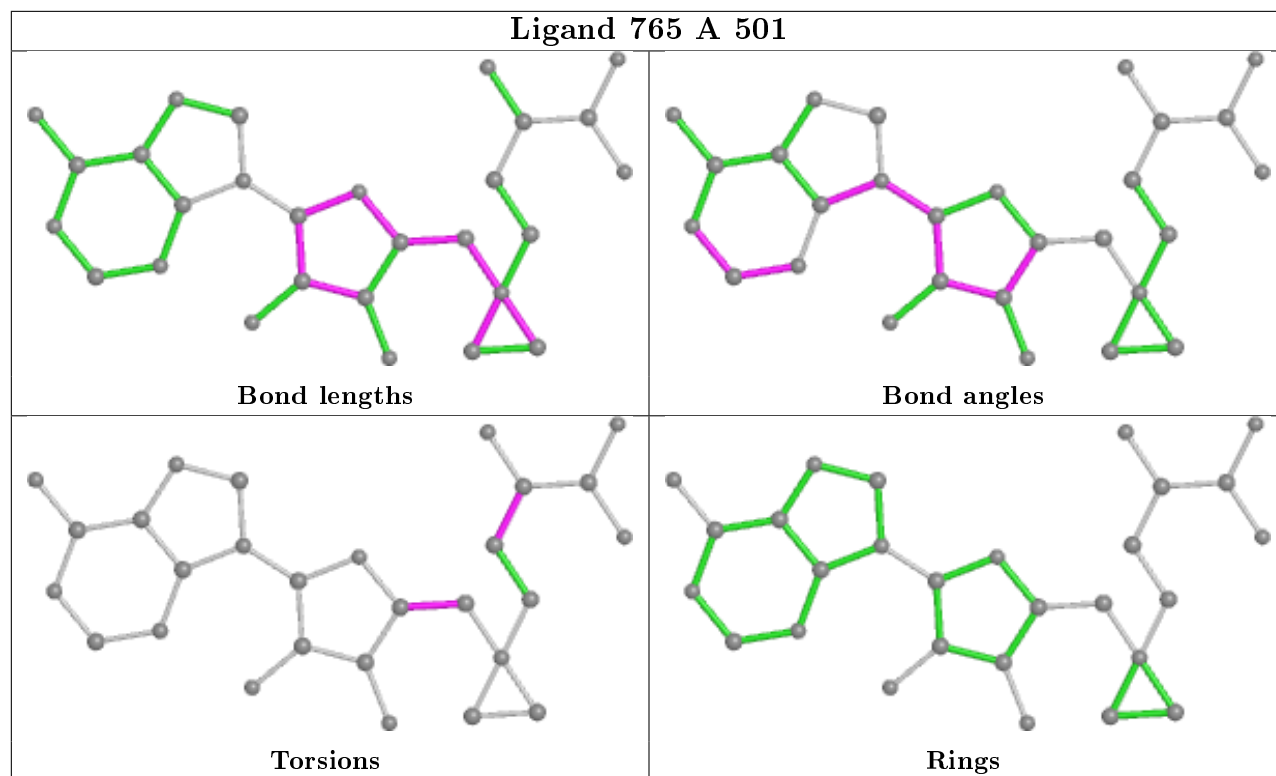
There are no ring outliers.

3 monomers are involved in 3 short contacts:

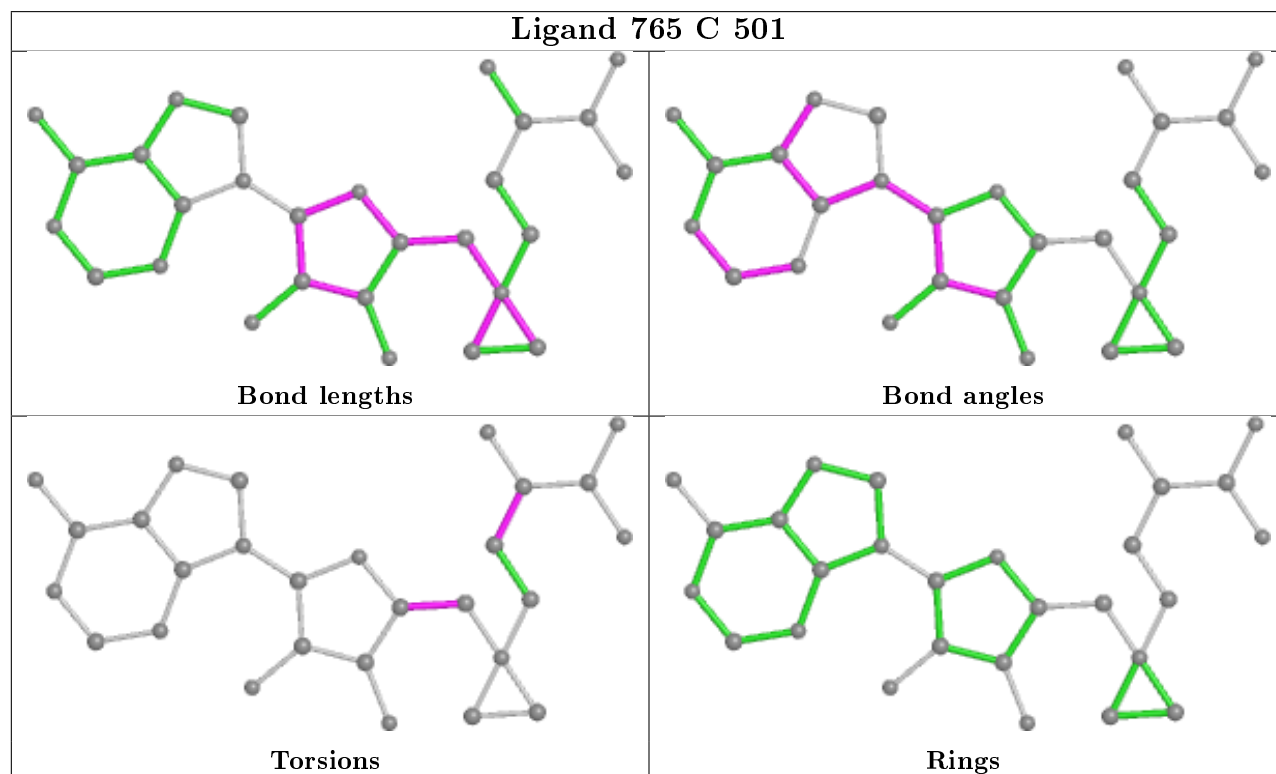
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	765	1	0
4	A	504	PEG	1	0
6	A	507	M2M	1	0

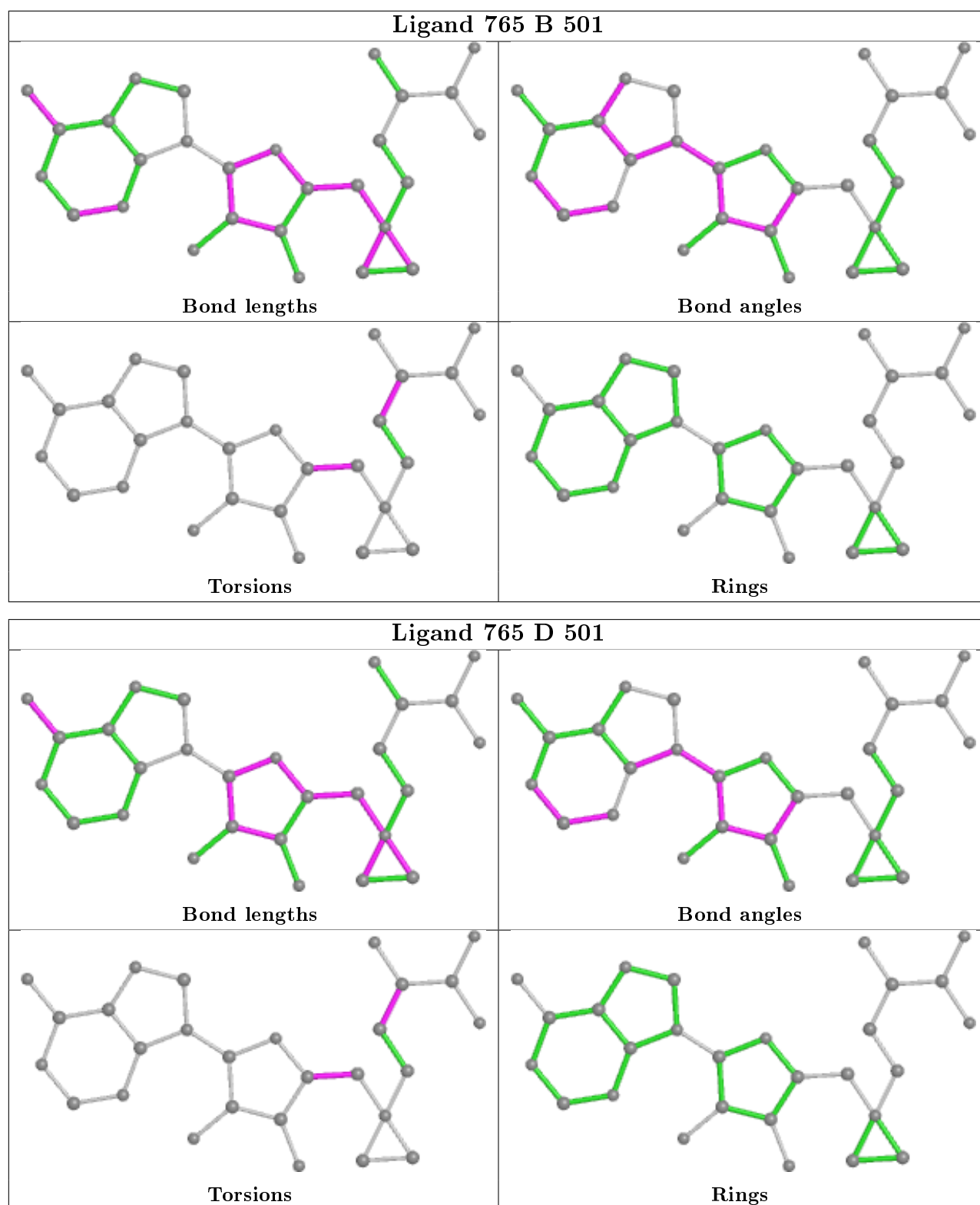
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand 765 A 501



## Ligand 765 C 501





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	343/361 (95%)	-0.24	5 (1%) 73 79	11, 24, 44, 79	0
1	B	343/361 (95%)	-0.27	7 (2%) 65 72	13, 29, 49, 102	0
1	C	343/361 (95%)	-0.10	11 (3%) 47 56	17, 30, 55, 92	0
1	D	341/361 (94%)	-0.29	5 (1%) 73 79	18, 30, 50, 66	0
All	All	1370/1444 (94%)	-0.22	28 (2%) 65 72	11, 29, 50, 102	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	478	THR	7.9
1	C	477	TYR	6.3
1	C	478	THR	6.2
1	A	478	THR	6.1
1	A	477	TYR	3.5
1	C	148	VAL	3.2
1	C	140	GLU	3.2
1	B	144	GLU	3.1
1	D	144	GLU	3.1
1	C	144	GLU	2.9
1	D	475	PHE	2.8
1	B	477	TYR	2.5
1	C	145	SER	2.5
1	B	148	VAL	2.4
1	B	283	SER	2.4
1	A	283	SER	2.2
1	B	145	SER	2.2
1	C	136	SER	2.2
1	C	191	ASP	2.2
1	D	347	ARG	2.2
1	B	136	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	282	PRO	2.1
1	C	228	LYS	2.1
1	A	144	GLU	2.0
1	D	467	LEU	2.0
1	C	192	VAL	2.0
1	D	315	TYR	2.0
1	A	140	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	M2M	A	507	9/9	0.70	0.38	48,57,61,61	0
3	EDO	C	502	4/4	0.78	0.16	38,45,49,55	0
4	PEG	A	504	7/7	0.80	0.21	34,41,45,48	0
3	EDO	A	502	4/4	0.81	0.23	41,49,54,59	0
5	DXE	C	508	6/6	0.81	0.33	35,42,45,45	0
5	DXE	C	509	6/6	0.81	0.30	29,35,39,39	0
5	DXE	D	503	6/6	0.82	0.26	36,43,45,45	0
5	DXE	C	507	6/6	0.85	0.30	35,43,48,48	0
7	PG4	B	505	13/13	0.85	0.33	40,48,51,55	0
3	EDO	D	502	4/4	0.86	0.13	33,40,44,44	0
5	DXE	A	506	6/6	0.86	0.12	36,43,50,50	0
3	EDO	B	502	4/4	0.87	0.11	31,37,39,45	0
3	EDO	C	505	4/4	0.87	0.28	30,36,42,42	0
4	PEG	A	505	7/7	0.88	0.28	30,36,41,41	0
3	EDO	B	503	4/4	0.88	0.12	42,51,52,54	0
4	PEG	A	503	7/7	0.89	0.14	38,46,51,57	0

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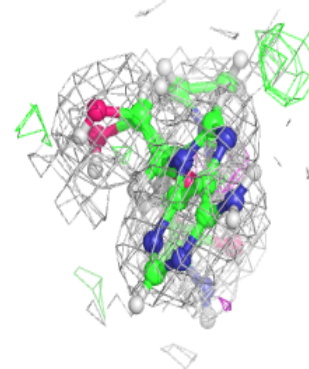
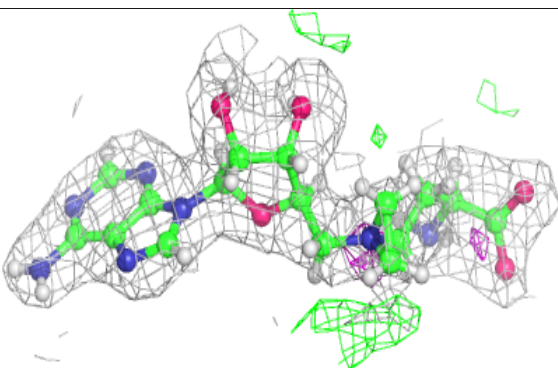
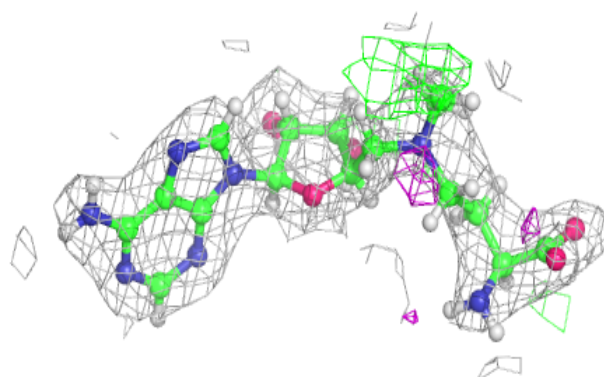
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PEG	B	504	7/7	0.89	0.29	39,47,51,55	0
3	EDO	C	504	4/4	0.90	0.35	29,35,41,43	0
2	765	B	501	28/28	0.91	0.12	22,35,45,50	0
2	765	C	501	28/28	0.92	0.12	23,32,42,44	0
5	DXE	C	506	6/6	0.92	0.18	34,41,45,45	0
2	765	D	501	28/28	0.93	0.11	24,34,45,47	0
3	EDO	C	503	4/4	0.94	0.22	29,35,41,43	0
2	765	A	501	28/28	0.95	0.12	16,24,31,34	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.

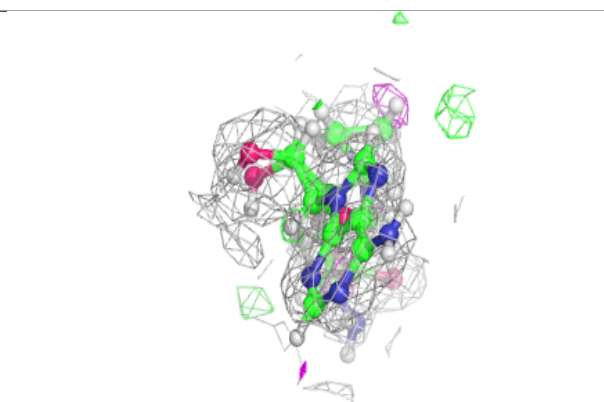
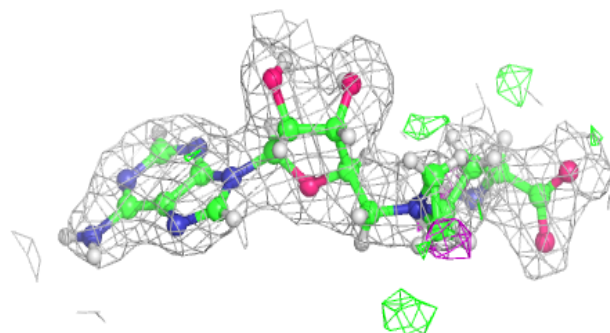
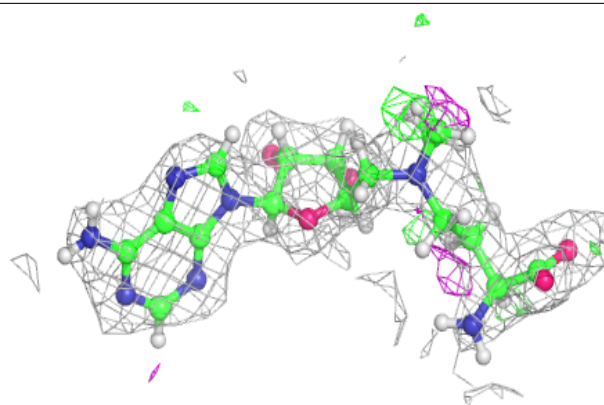
**Electron density around 765 B 501:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

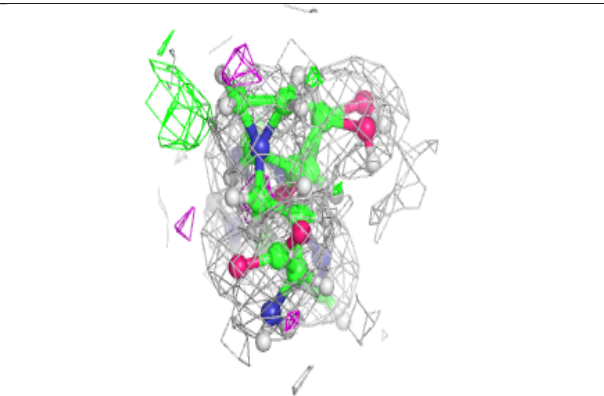
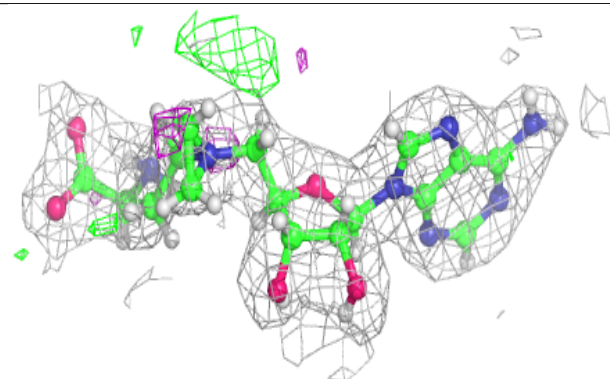
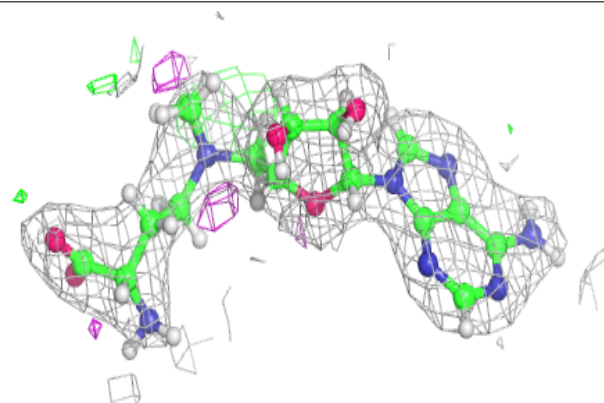


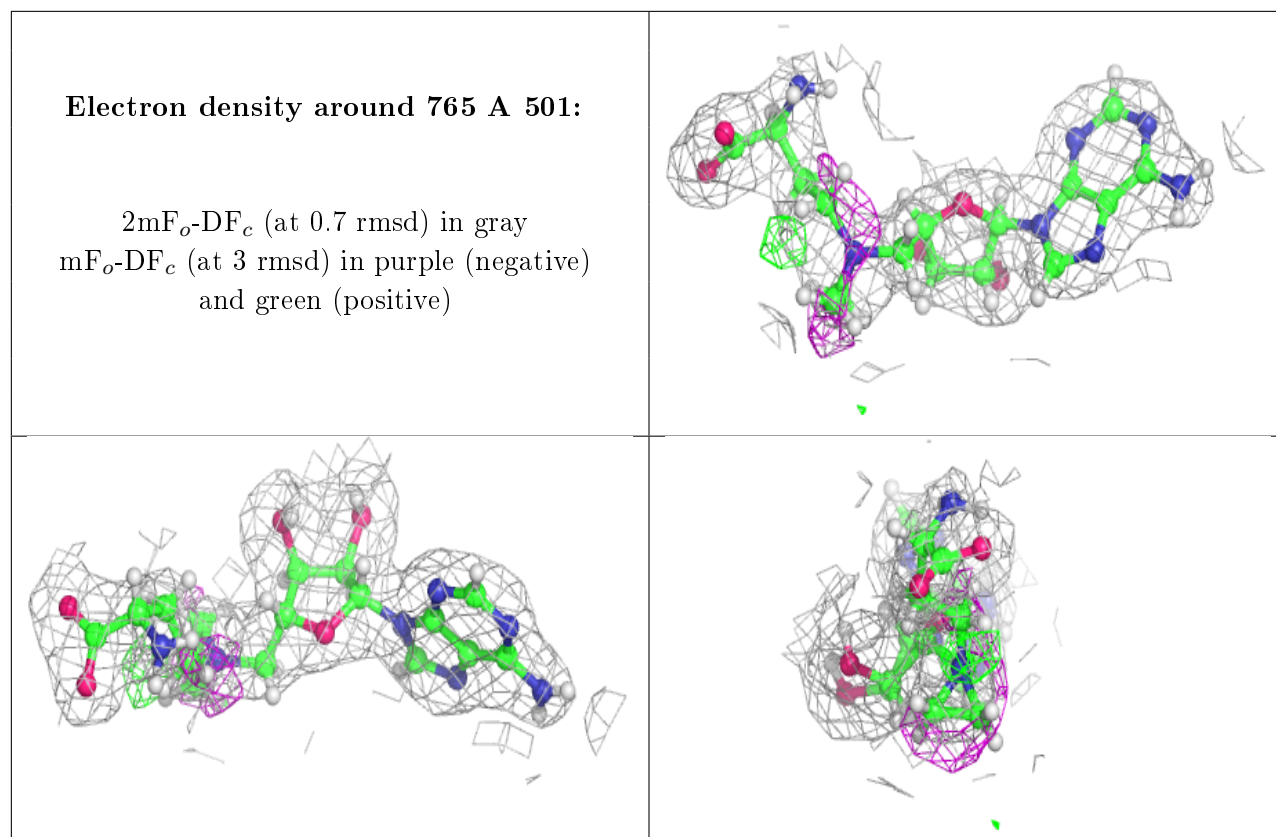
**Electron density around 765 C 501:**

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

**Electron density around 765 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.