



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:32 pm BST

PDB ID : 5ISE  
Title : Crystal structure of mouse CARM1 in complex with inhibitor SA0649  
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Wurtz, J.M.; Bonnefond, L.; Cavarelli, J.  
Deposited on : 2016-03-15  
Resolution : 2.10 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

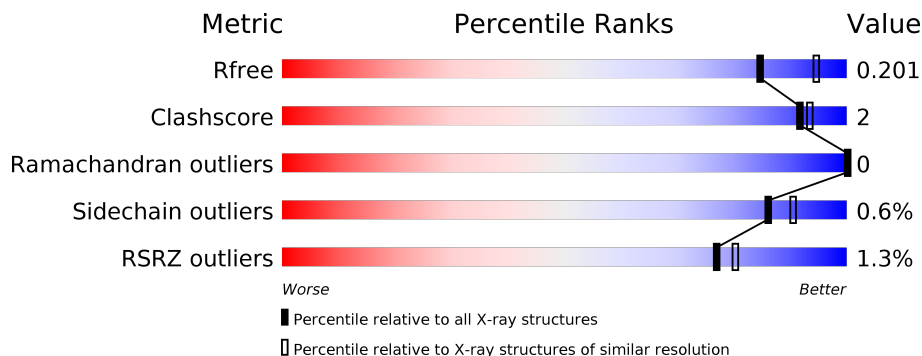
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	 92% • 5%
1	B	361	 89% 6% 5%
1	C	361	 93% • 5%
1	D	361	 89% 5% • 6%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 23211 atoms, of which 11128 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.

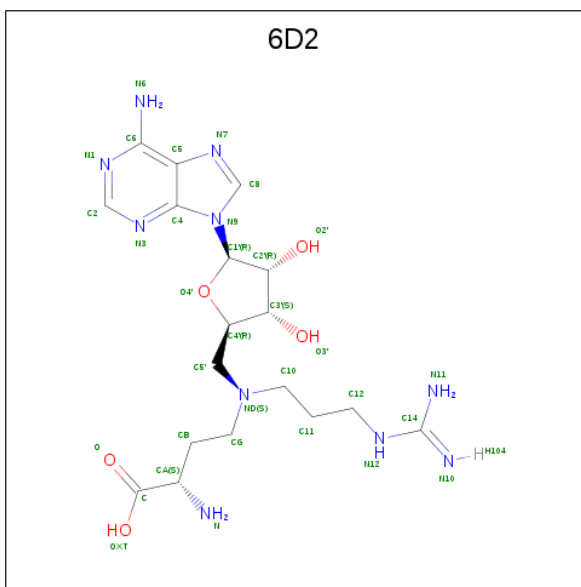
- Molecule 1 is a protein called Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	343	5504	1792	2727	459	510	16	0	6	0
1	B	343	5509	1799	2727	457	511	15	0	4	0
1	C	343	5485	1786	2717	457	510	15	0	3	0
1	D	341	5433	1768	2693	453	504	15	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

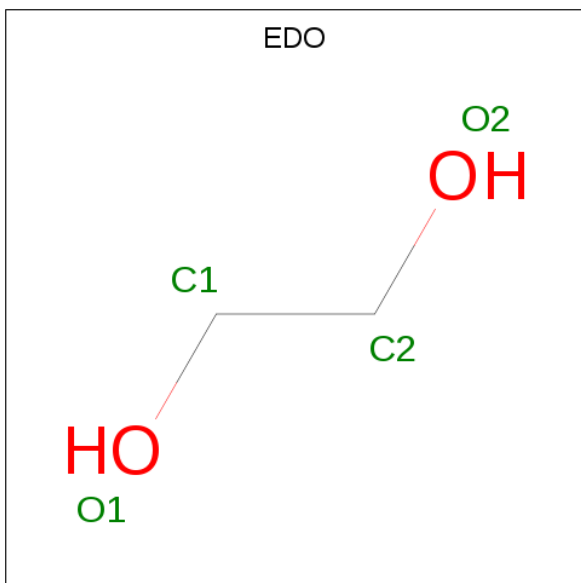
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	expression tag	UNP Q9WVG6
A	128	HIS	-	expression tag	UNP Q9WVG6
A	129	MET	-	expression tag	UNP Q9WVG6
B	127	GLY	-	expression tag	UNP Q9WVG6
B	128	HIS	-	expression tag	UNP Q9WVG6
B	129	MET	-	expression tag	UNP Q9WVG6
C	127	GLY	-	expression tag	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'-{[(3S)-3-amino-3-carboxypropyl](3-carbamimidamidopropyl)amino}-5'-deoxyadenosine (three-letter code: 6D2) (formula: C<sub>18</sub>H<sub>30</sub>N<sub>10</sub>O<sub>5</sub>).



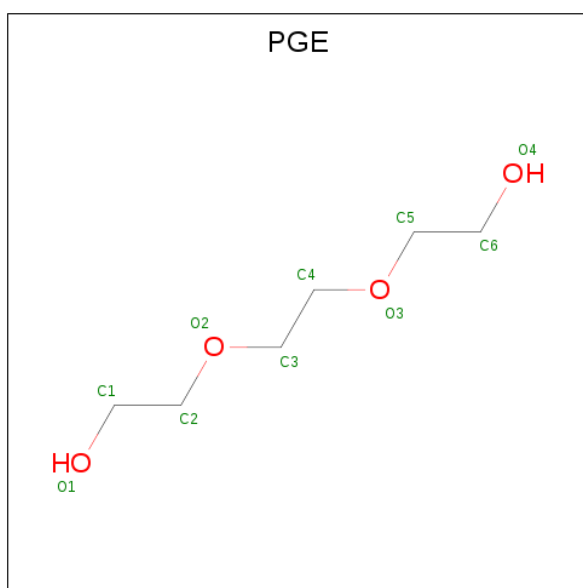
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
2	A	1	Total	C	H	N	O	0	0
			61	18	28	10	5		
2	B	1	Total	C	H	N	O	0	0
			61	18	28	10	5		
2	C	1	Total	C	H	N	O	0	0
			61	18	28	10	5		
2	D	1	Total	C	H	N	O	0	0
			61	18	28	10	5		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



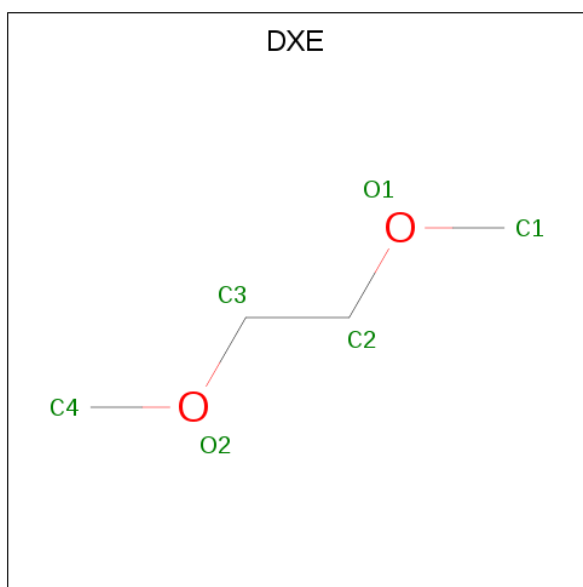
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



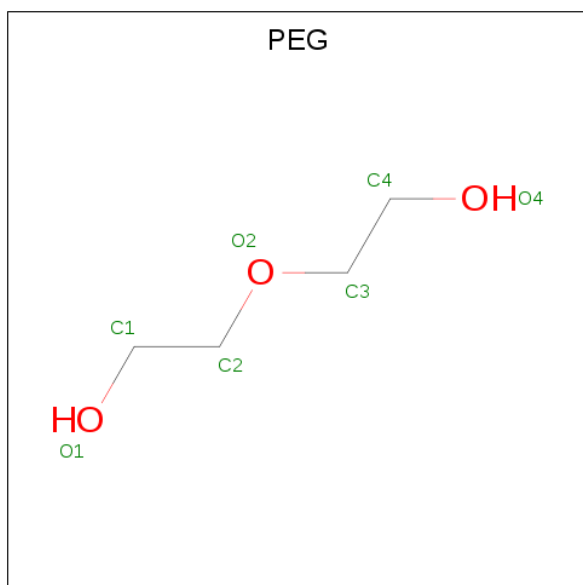
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 5 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



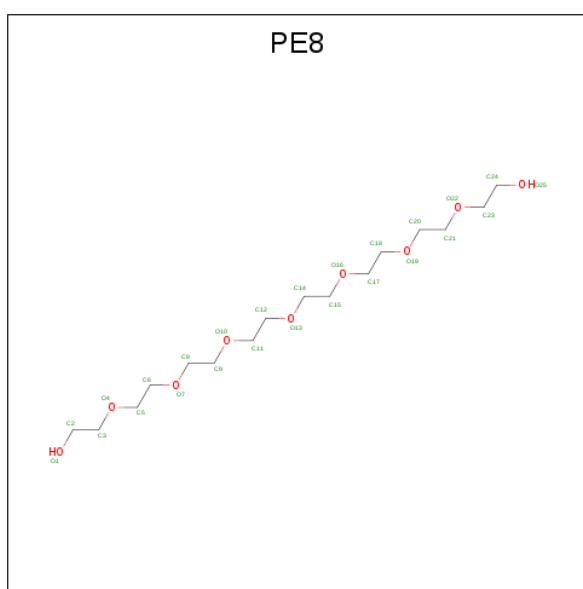
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	16	4	10	2	0	0
5	B	1	16	4	10	2	0	0
5	C	1	16	4	10	2	0	0
5	C	1	16	4	10	2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 7 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			59	16	34	9		

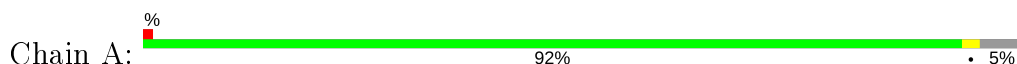
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	225	Total	O	0	4
			229	229		
8	B	192	Total	O	0	2
			194	194		
8	C	196	Total	O	0	2
			198	198		
8	D	158	Total	O	0	2
			160	160		

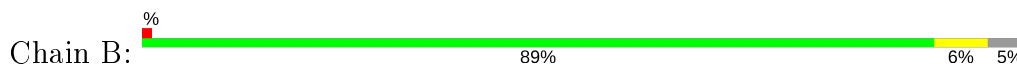
### 3 Residue-property plots [i](#)

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



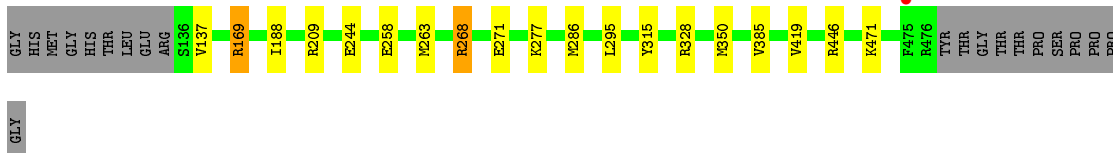
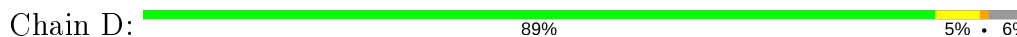
- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.74Å 98.30Å 206.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.70 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-2.10) 97.6 (29.70-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.40 (at 2.10Å)	Xtrriage
Refinement program	PHENIX dev_1839	Depositor
R, $R_{free}$	0.151 , 0.200 0.152 , 0.201	Depositor DCC
$R_{free}$ test set	4350 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtrriage
Anisotropy	0.176	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	23211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.93 % 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 7.3893e-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: 6D2, PE8, EDO, PGE, 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	0.67	1/2878 (0.0%)	0.70	1/3900 (0.0%)
1	B	0.60	0/2860	0.67	1/3874 (0.0%)
1	C	0.56	0/2847	0.67	0/3857
1	D	0.57	0/2814	0.68	2/3812 (0.1%)
All	All	0.60	1/11399 (0.0%)	0.68	4/15443 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	ASN	CB-CG	6.55	1.66	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	268	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	D	268	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	B	175	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	A	295	LEU	CA-CB-CG	5.48	127.90	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2777	2727	2703	5	0
1	B	2782	2727	2717	12	0
1	C	2768	2717	2709	4	0
1	D	2740	2693	2687	13	0
2	A	33	28	0	1	0
2	B	33	28	0	0	0
2	C	33	28	0	0	0
2	D	33	28	0	0	0
3	A	8	12	12	0	0
3	C	4	6	6	0	0
3	D	4	6	6	0	0
4	A	10	14	14	1	0
5	A	6	10	10	0	0
5	B	6	10	10	0	0
5	C	12	20	20	0	0
6	A	7	10	10	0	0
6	B	7	10	10	0	0
6	C	7	10	10	0	0
6	D	7	10	10	0	0
7	B	25	34	34	3	0
8	A	229	0	0	2	0
8	B	194	0	0	0	0
8	C	198	0	0	0	0
8	D	160	0	0	0	0
All	All	12083	11128	10968	35	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 2.

All (35) 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:136:SER:N	8:A:602:HOH:O	2.25	0.69
1:D:263:MET:CE	1:D:419:VAL:HG11	2.29	0.63
1:B:315:TYR:HD1	1:B:328:ARG:HD3	1.70	0.56
1:B:179:GLN:NE2	1:B:401:MET:SD	2.79	0.56
1:D:350[A]:MET:SD	1:D:385:VAL:HG22	2.49	0.53
1:B:169:ARG:NE	1:B:258:GLU:OE2	2.44	0.50
1:D:137:VAL:CG2	1:D:244:GLU:HG2	2.41	0.50
1:C:190:LEU:HD13	1:C:248:LEU:HD21	1.94	0.49
1:B:241:GLY:HA3	7:B:502:PE8:H241	1.94	0.49
1:D:268:ARG:HD2	1:D:271:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:TYR:CD1	1:B:328:ARG:HD3	2.47	0.48
1:D:268:ARG:CD	1:D:271:GLU:OE2	2.62	0.48
1:C:153:PHE:CE1	1:C:159[B]:GLN:HG2	2.50	0.47
2:A:501:6D2:N11	4:A:503:PGE:H12	2.29	0.46
1:C:172:THR:HG21	1:C:405:LEU:HB2	1.97	0.46
1:D:277:LYS:HD3	1:D:286:MET:SD	2.56	0.45
1:A:143:GLU:OE1	8:A:601:HOH:O	2.21	0.45
1:D:263:MET:HE2	1:D:419:VAL:HG11	1.98	0.45
1:C:295:LEU:HG	1:C:390:PHE:CE2	2.53	0.44
1:D:169:ARG:NH2	1:D:258:GLU:OE2	2.51	0.44
1:B:262:TYR:CE2	1:B:475[A]:PHE:HE1	2.36	0.43
1:A:295:LEU:HG	1:A:390:PHE:CE2	2.52	0.43
1:D:446:ARG:NH1	1:D:471:LYS:HG2	2.33	0.43
1:B:188:ILE:HD11	1:B:209:ARG:NH1	2.34	0.43
1:D:315:TYR:HD1	1:D:328:ARG:HD3	1.84	0.43
1:D:263:MET:HE3	1:D:419:VAL:HG11	2.01	0.42
1:B:153:PHE:CE2	1:B:159:GLN:HG2	2.54	0.42
1:B:314:TRP:O	1:B:325:SER:HA	2.19	0.42
1:A:184:PHE:O	1:A:208:ALA:HA	2.20	0.42
1:B:136:SER:CB	7:B:502:PE8:H152	2.50	0.41
1:A:277:LYS:HD2	1:A:286:MET:HE2	2.02	0.41
1:B:245:GLU:HG2	7:B:502:PE8:H151	2.02	0.41
1:B:138:PHE:CE2	1:B:242:LYS:HE3	2.55	0.41
1:D:188:ILE:HD11	1:D:209:ARG:NH2	2.36	0.41
1:D:263:MET:HE2	1:D:419:VAL:CG1	2.51	0.41

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	347/361 (96%)	338 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	344/361 (95%)	335 (97%)	9 (3%)	0	100	100
1	C	344/361 (95%)	334 (97%)	10 (3%)	0	100	100
1	D	341/361 (94%)	331 (97%)	10 (3%)	0	100	100
All	All	1376/1444 (95%)	1338 (97%)	38 (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	304/313 (97%)	303 (100%)	1 (0%)	92	95
1	B	303/313 (97%)	300 (99%)	3 (1%)	76	82
1	C	302/313 (96%)	301 (100%)	1 (0%)	92	95
1	D	298/313 (95%)	296 (99%)	2 (1%)	84	88
All	All	1207/1252 (96%)	1200 (99%)	7 (1%)	86	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	GLU
1	B	169	ARG
1	B	247	SER
1	B	295	LEU
1	C	258	GLU
1	D	169	ARG
1	D	295	LEU

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

Mol	Chain	Res	Type
1	A	320	HIS

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Mol	Chain	Res	Type
1	B	466	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 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	A	502	-	3,3,3	0.46	0	2,2,2	0.75	0
7	PE8	B	502	-	24,24,24	0.57	0	23,23,23	0.63	0
3	EDO	C	502	-	3,3,3	0.41	0	2,2,2	0.46	0
5	DXE	B	503	-	5,5,5	0.42	0	4,4,4	0.34	0
2	6D2	D	501	-	28,35,35	2.05	7 (25%)	27,49,49	1.72	6 (22%)
2	6D2	A	501	-	28,35,35	1.72	5 (17%)	27,49,49	1.95	7 (25%)
5	DXE	C	503	-	5,5,5	0.45	0	4,4,4	0.44	0
6	PEG	C	505	-	6,6,6	0.45	0	5,5,5	0.53	0
6	PEG	A	506	-	6,6,6	0.59	0	5,5,5	0.34	0
2	6D2	B	501	-	28,35,35	1.94	6 (21%)	27,49,49	1.75	7 (25%)
3	EDO	D	502	-	3,3,3	0.54	0	2,2,2	0.41	0
6	PEG	D	503	-	6,6,6	0.46	0	5,5,5	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PEG	B	504	-	6,6,6	0.58	0	5,5,5	0.78	0
5	DXE	A	505	-	5,5,5	0.35	0	4,4,4	0.31	0
5	DXE	C	504	-	5,5,5	0.47	0	4,4,4	0.30	0
4	PGE	A	503	-	9,9,9	0.52	0	8,8,8	0.57	0
3	EDO	A	504	-	3,3,3	0.44	0	2,2,2	0.38	0
2	6D2	C	501	-	28,35,35	2.05	6 (21%)	27,49,49	1.52	5 (18%)

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	A	502	-	-	1/1/1/1	-
7	PE8	B	502	-	-	13/22/22/22	-
3	EDO	C	502	-	-	1/1/1/1	-
5	DXE	B	503	-	-	2/3/3/3	-
2	6D2	D	501	-	-	8/16/40/40	0/3/3/3
2	6D2	A	501	-	-	4/16/40/40	0/3/3/3
5	DXE	C	503	-	-	3/3/3/3	-
6	PEG	C	505	-	-	3/4/4/4	-
6	PEG	A	506	-	-	1/4/4/4	-
2	6D2	B	501	-	-	9/16/40/40	0/3/3/3
3	EDO	D	502	-	-	0/1/1/1	-
6	PEG	D	503	-	-	1/4/4/4	-
6	PEG	B	504	-	-	2/4/4/4	-
5	DXE	A	505	-	-	3/3/3/3	-
5	DXE	C	504	-	-	1/3/3/3	-
4	PGE	A	503	-	-	4/7/7/7	-
3	EDO	A	504	-	-	1/1/1/1	-
2	6D2	C	501	-	-	6/16/40/40	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	6D2	O4'-C1'	5.68	1.49	1.41
2	B	501	6D2	O4'-C1'	5.18	1.48	1.41
2	C	501	6D2	O4'-C1'	4.84	1.47	1.41
2	A	501	6D2	C14-N12	4.54	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	6D2	C14-N12	4.49	1.42	1.33
2	C	501	6D2	C2-N3	4.39	1.39	1.32
2	C	501	6D2	C14-N12	4.15	1.41	1.33
2	C	501	6D2	C14-N10	4.05	1.48	1.32
2	B	501	6D2	C14-N12	3.89	1.41	1.33
2	A	501	6D2	C14-N10	3.84	1.47	1.32
2	B	501	6D2	C14-N10	3.71	1.47	1.32
2	D	501	6D2	C14-N10	3.68	1.46	1.32
2	D	501	6D2	C2-N3	3.60	1.37	1.32
2	A	501	6D2	O4'-C1'	3.50	1.46	1.41
2	B	501	6D2	C2-N3	3.45	1.37	1.32
2	B	501	6D2	CA-N	-3.18	1.40	1.47
2	C	501	6D2	CA-N	-3.10	1.40	1.47
2	B	501	6D2	C5'-C4'	2.82	1.60	1.51
2	D	501	6D2	CA-N	-2.73	1.41	1.47
2	A	501	6D2	CA-N	-2.62	1.41	1.47
2	D	501	6D2	C5'-C4'	2.37	1.58	1.51
2	A	501	6D2	C5'-C4'	2.26	1.58	1.51
2	C	501	6D2	O4'-C4'	2.04	1.49	1.45
2	D	501	6D2	C3'-C4'	-2.00	1.47	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	6D2	N3-C2-N1	-5.19	120.56	128.68
2	A	501	6D2	N3-C2-N1	-5.18	120.58	128.68
2	D	501	6D2	N3-C2-N1	-4.83	121.13	128.68
2	A	501	6D2	O4'-C4'-C5'	-4.60	101.29	108.90
2	C	501	6D2	N3-C2-N1	-3.97	122.48	128.68
2	A	501	6D2	C2'-C3'-C4'	3.36	109.17	102.64
2	C	501	6D2	C4-C5-N7	-3.33	105.93	109.40
2	B	501	6D2	O4'-C1'-C2'	-3.29	102.12	106.93
2	D	501	6D2	CB-CG-ND	-3.19	103.46	113.93
2	B	501	6D2	CB-CG-ND	-3.08	103.81	113.93
2	D	501	6D2	O4'-C4'-C5'	-3.01	103.92	108.90
2	C	501	6D2	O4'-C4'-C5'	-2.95	104.01	108.90
2	B	501	6D2	C4-C5-N7	-2.70	106.59	109.40
2	A	501	6D2	N12-C14-N10	2.69	125.43	120.70
2	A	501	6D2	O3'-C3'-C4'	-2.62	103.46	111.05
2	B	501	6D2	O4'-C4'-C5'	-2.48	104.80	108.90
2	C	501	6D2	O4'-C1'-C2'	-2.40	103.42	106.93
2	B	501	6D2	C2'-C3'-C4'	2.30	107.11	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	6D2	CG-ND-C5'	-2.22	106.66	111.96
2	D	501	6D2	C2'-C3'-C4'	2.19	106.91	102.64
2	C	501	6D2	C2'-C3'-C4'	2.19	106.90	102.64
2	A	501	6D2	O4'-C1'-C2'	-2.18	103.74	106.93
2	D	501	6D2	O3'-C3'-C4'	-2.16	104.79	111.05
2	A	501	6D2	CG-ND-C10	2.08	116.39	111.44
2	B	501	6D2	CG-ND-C5'	-2.04	107.10	111.96

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	6D2	C3'-C4'-C5'-ND
2	D	501	6D2	O4'-C4'-C5'-ND
2	A	501	6D2	C11-C12-N12-C14
2	B	501	6D2	C11-C10-ND-C5'
2	B	501	6D2	C-CA-CB-CG
2	B	501	6D2	N-CA-CB-CG
2	B	501	6D2	C3'-C4'-C5'-ND
2	B	501	6D2	O4'-C4'-C5'-ND
2	D	501	6D2	C11-C10-ND-C5'
2	C	501	6D2	C11-C10-ND-C5'
2	B	501	6D2	C10-C11-C12-N12
2	A	501	6D2	C11-C10-ND-CG
5	B	503	DXE	O1-C2-C3-O2
7	B	502	PE8	O16-C17-C18-O19
5	A	505	DXE	O1-C2-C3-O2
7	B	502	PE8	O19-C20-C21-O22
2	A	501	6D2	ND-C10-C11-C12
2	D	501	6D2	C10-C11-C12-N12
7	B	502	PE8	O22-C23-C24-O25
4	A	503	PGE	O3-C5-C6-O4
7	B	502	PE8	O1-C2-C3-O4
6	B	504	PEG	O1-C1-C2-O2
6	B	504	PEG	O2-C3-C4-O4
4	A	503	PGE	O1-C1-C2-O2
5	C	504	DXE	O1-C2-C3-O2
7	B	502	PE8	O10-C11-C12-O13
2	B	501	6D2	CB-CG-ND-C10
6	C	505	PEG	O2-C3-C4-O4
3	A	504	EDO	O1-C1-C2-O2
2	B	501	6D2	CB-CG-ND-C5'

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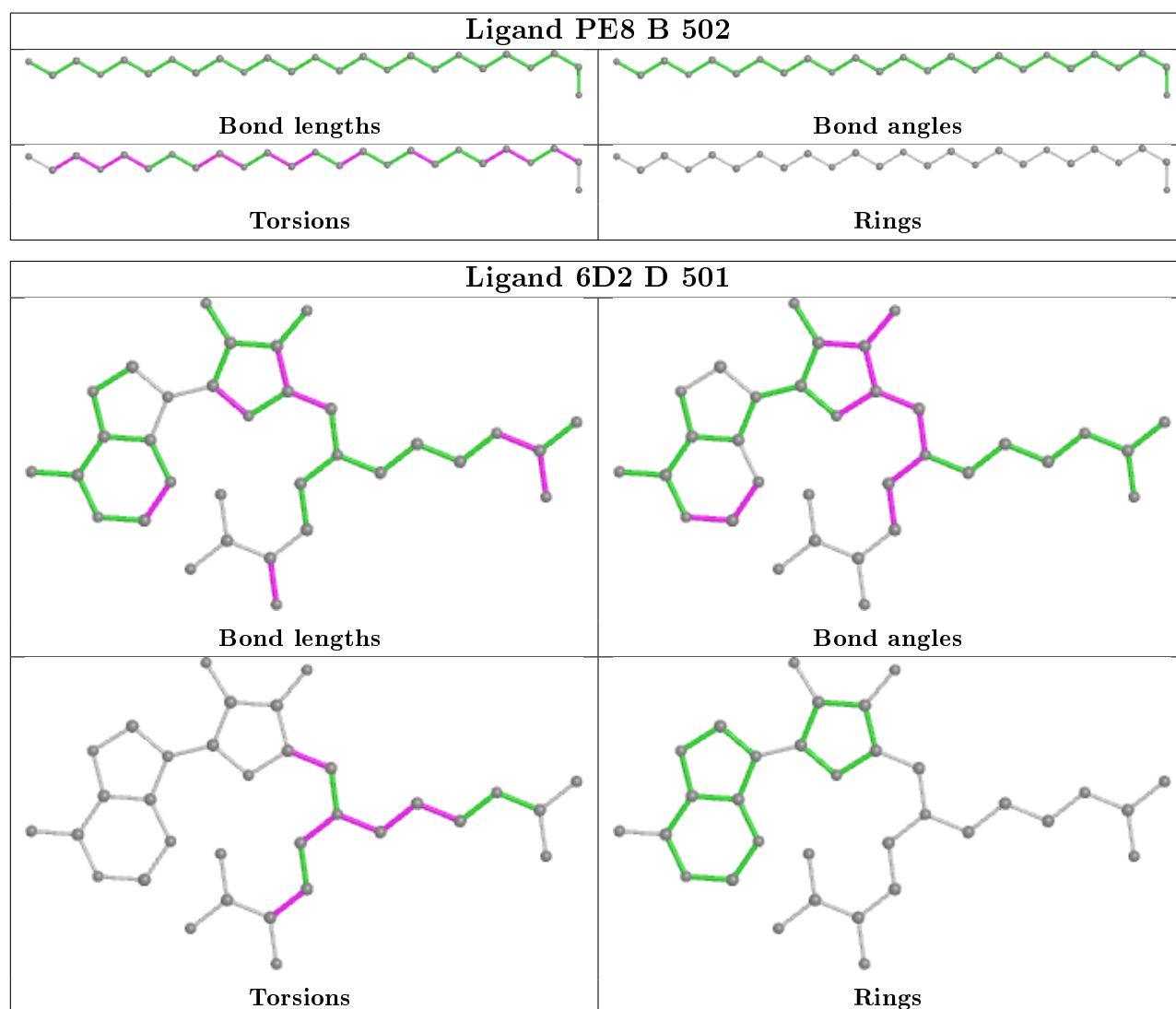
Mol	Chain	Res	Type	Atoms
2	C	501	6D2	C10-C11-C12-N12
2	B	501	6D2	C11-C10-ND-CG
7	B	502	PE8	O7-C8-C9-O10
7	B	502	PE8	C20-C21-O22-C23
5	B	503	DXE	C2-C3-O2-C4
7	B	502	PE8	C18-C17-O16-C15
3	C	502	EDO	O1-C1-C2-O2
7	B	502	PE8	C15-C14-O13-C12
5	A	505	DXE	C3-C2-O1-C1
7	B	502	PE8	O13-C14-C15-O16
2	C	501	6D2	CB-CG-ND-C5'
5	C	503	DXE	O1-C2-C3-O2
4	A	503	PGE	C1-C2-O2-C3
3	A	502	EDO	O1-C1-C2-O2
7	B	502	PE8	C24-C23-O22-C21
2	A	501	6D2	C10-C11-C12-N12
5	C	503	DXE	C2-C3-O2-C4
7	B	502	PE8	O4-C5-C6-O7
6	C	505	PEG	O1-C1-C2-O2
2	D	501	6D2	CB-CG-ND-C10
2	C	501	6D2	C11-C10-ND-CG
7	B	502	PE8	C6-C5-O4-C3
2	D	501	6D2	ND-C10-C11-C12
2	C	501	6D2	ND-C10-C11-C12
6	D	503	PEG	C1-C2-O2-C3
6	C	505	PEG	C1-C2-O2-C3
5	A	505	DXE	C2-C3-O2-C4
2	D	501	6D2	N-CA-CB-CG
5	C	503	DXE	C3-C2-O1-C1
2	C	501	6D2	CB-CG-ND-C10
4	A	503	PGE	O2-C3-C4-O3
2	D	501	6D2	CB-CG-ND-C5'
6	A	506	PEG	O2-C3-C4-O4

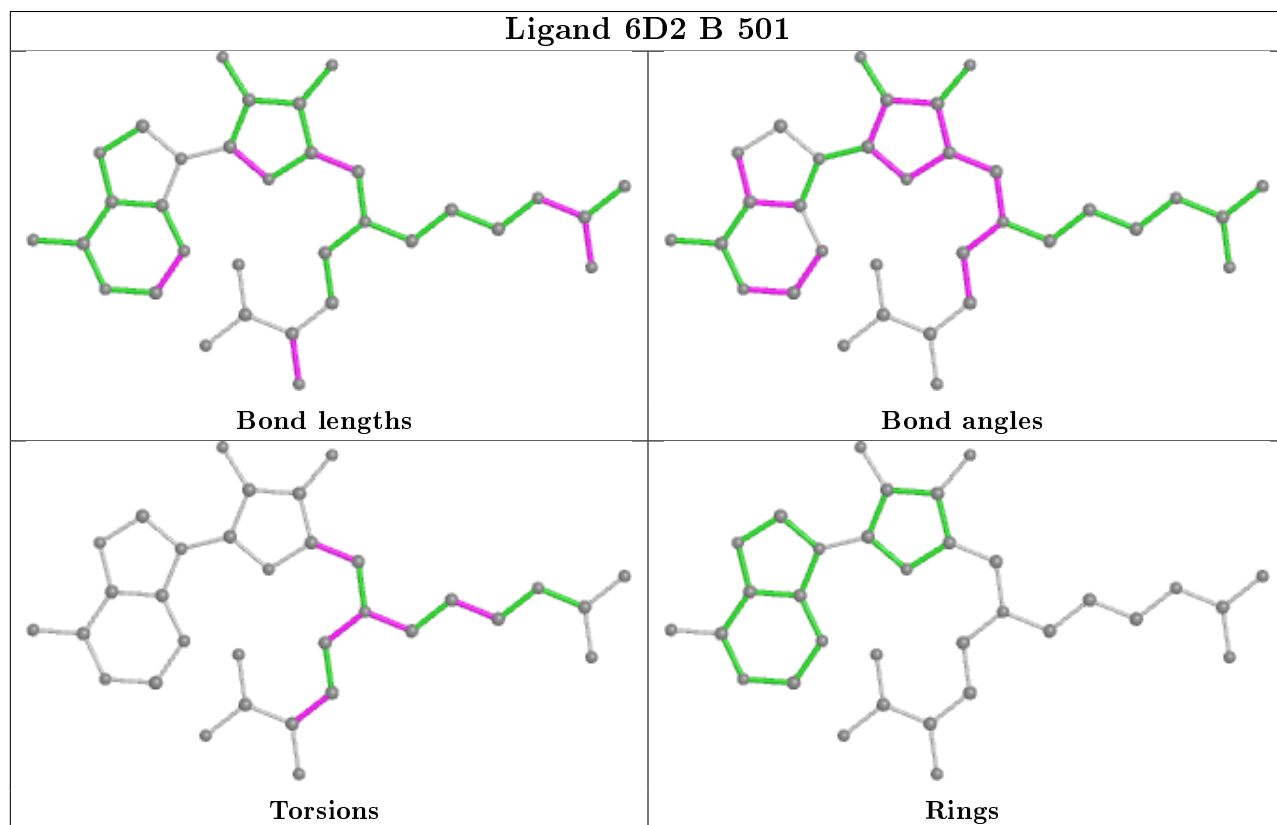
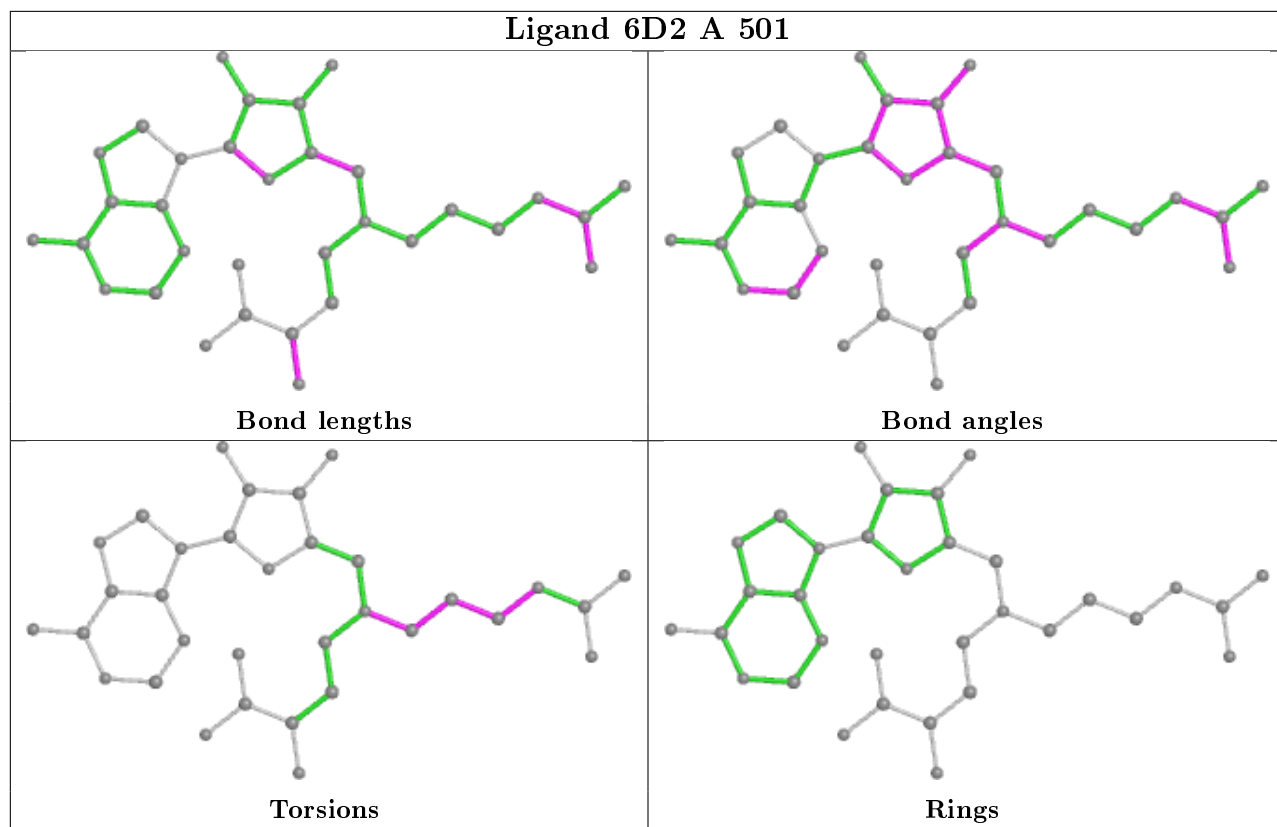
There are no ring outliers.

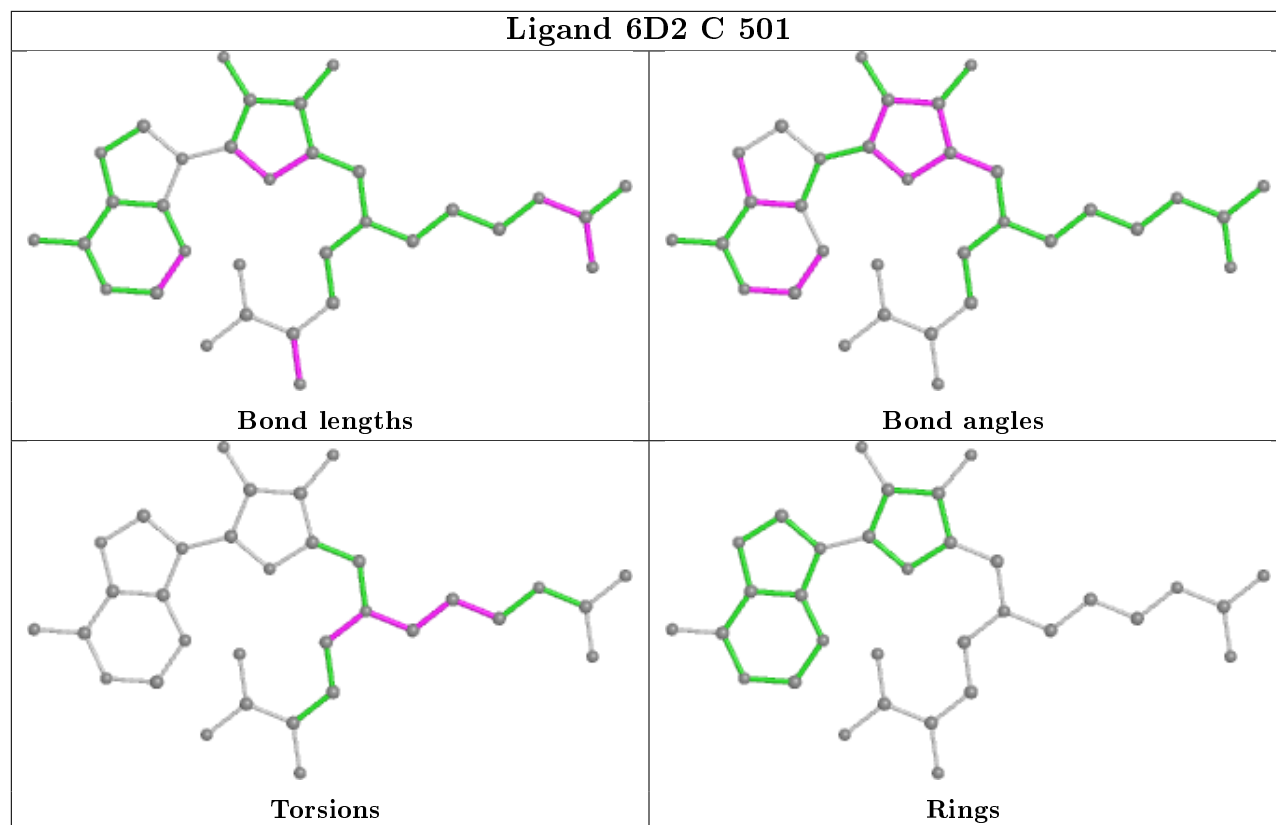
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	502	PE8	3	0
2	A	501	6D2	1	0
4	A	503	PGE	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 [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, 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%)	-0.44	5 (1%) 73 77	14, 25, 50, 76	0
1	B	343/361 (95%)	-0.46	2 (0%) 89 91	17, 30, 57, 99	0
1	C	343/361 (95%)	-0.28	10 (2%) 51 57	23, 34, 64, 91	0
1	D	341/361 (94%)	-0.40	1 (0%) 94 94	24, 34, 64, 93	0
All	All	1370/1444 (94%)	-0.40	18 (1%) 77 80	14, 32, 61, 99	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	478[A]	THR	7.2
1	C	478	THR	5.0
1	B	477[A]	TYR	3.8
1	C	477	TYR	3.5
1	D	475	PHE	3.2
1	A	478	THR	2.8
1	C	264	LEU	2.7
1	A	259	PRO	2.6
1	A	264	LEU	2.5
1	A	477	TYR	2.4
1	C	259	PRO	2.3
1	C	283	SER	2.3
1	C	257	SER	2.3
1	C	260	MET	2.1
1	C	265	PHE	2.1
1	C	231	ASN	2.1
1	A	265	PHE	2.1
1	C	144	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](#)

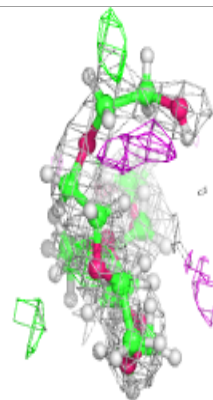
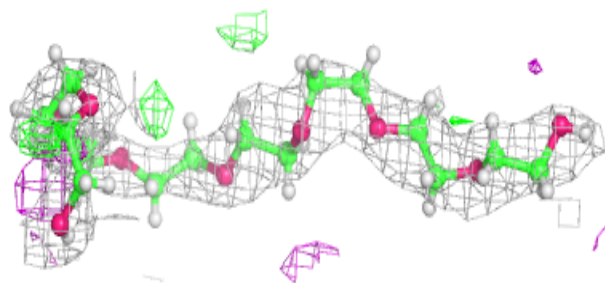
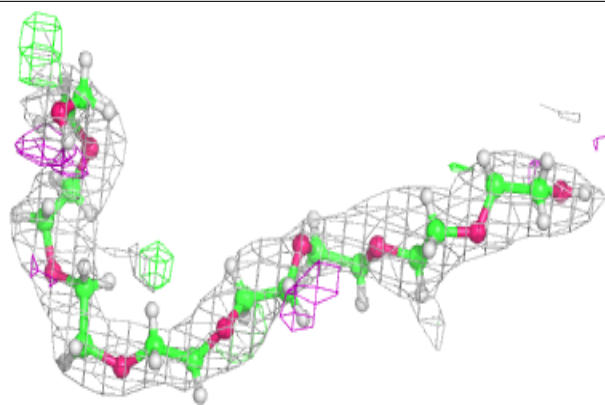
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DXE	C	504	6/6	0.50	0.19	64,88,107,107	0
7	PE8	B	502	25/25	0.73	0.23	42,85,140,149	0
6	PEG	A	506	7/7	0.76	0.24	44,65,104,104	0
5	DXE	C	503	6/6	0.78	0.17	56,68,83,83	0
6	PEG	C	505	7/7	0.85	0.15	45,62,83,83	0
5	DXE	B	503	6/6	0.86	0.14	52,63,72,72	0
4	PGE	A	503	10/10	0.86	0.20	42,68,85,87	0
3	EDO	A	504	4/4	0.87	0.11	46,57,68,71	0
6	PEG	D	503	7/7	0.91	0.14	50,62,85,88	0
3	EDO	A	502	4/4	0.91	0.22	50,61,90,100	0
3	EDO	C	502	4/4	0.91	0.12	39,53,67,75	0
6	PEG	B	504	7/7	0.92	0.17	37,52,65,65	0
3	EDO	D	502	4/4	0.93	0.13	40,48,54,54	0
5	DXE	A	505	6/6	0.95	0.10	42,51,74,74	0
2	6D2	C	501	33/33	0.95	0.16	13,35,80,92	0
2	6D2	D	501	33/33	0.95	0.16	20,38,66,79	0
2	6D2	B	501	33/33	0.96	0.15	14,34,56,61	0
2	6D2	A	501	33/33	0.97	0.17	16,26,75,102	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 PE8 B 502:**

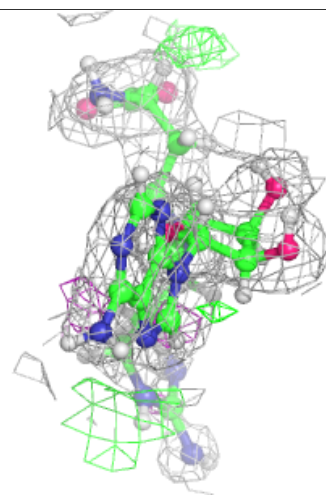
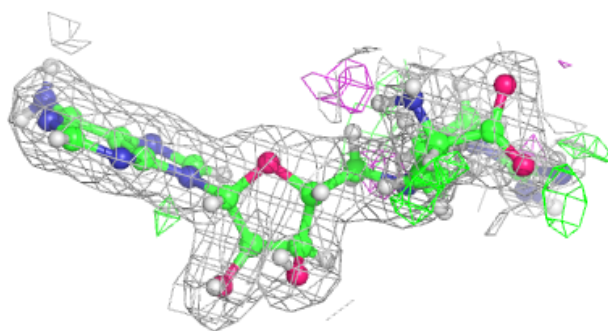
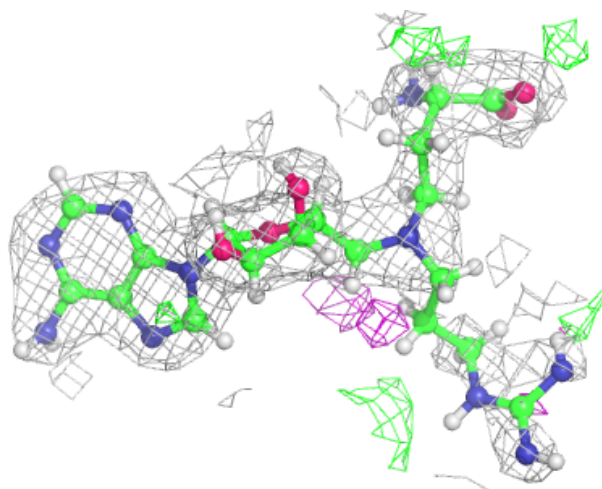
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





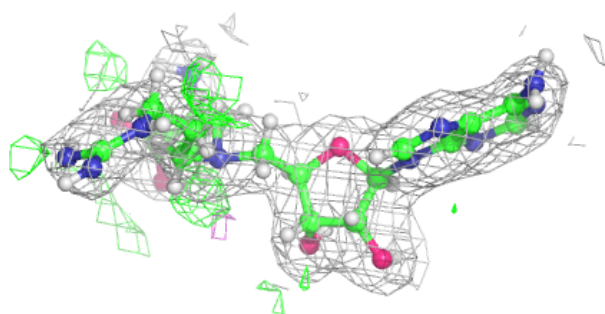
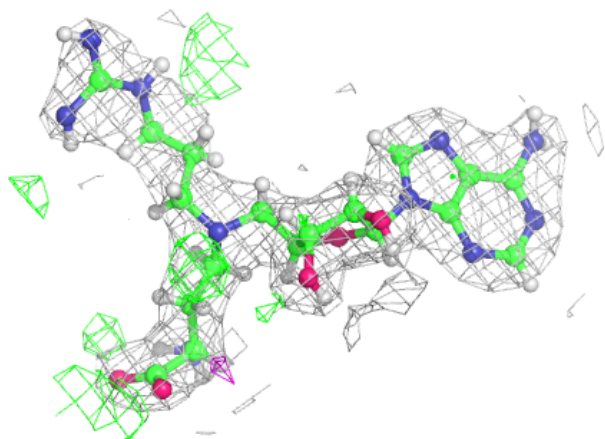
**Electron density around 6D2 C 501:**

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



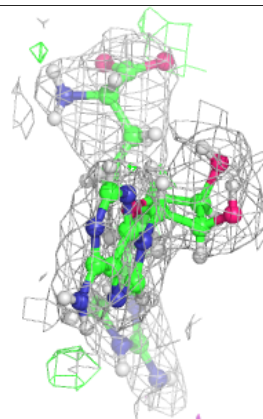
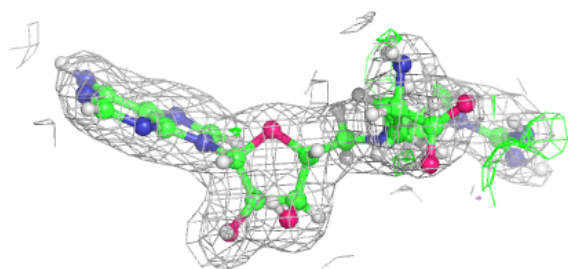
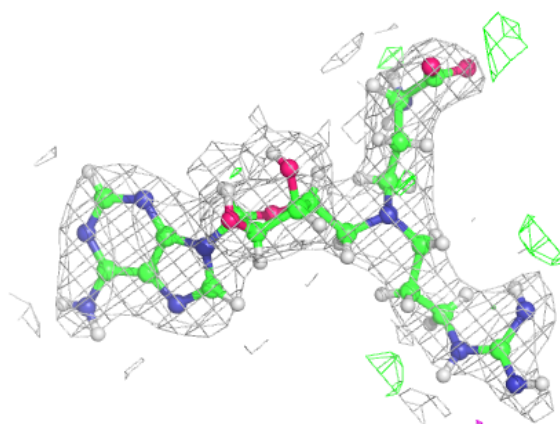
**Electron density around 6D2 D 501:**

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

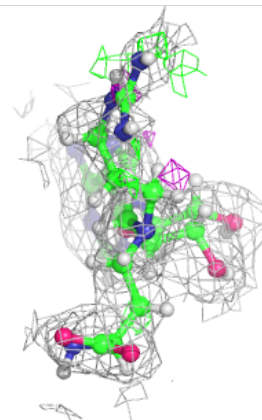
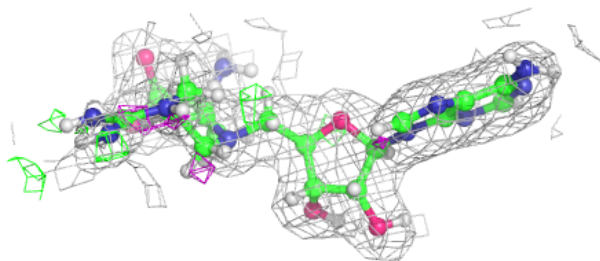
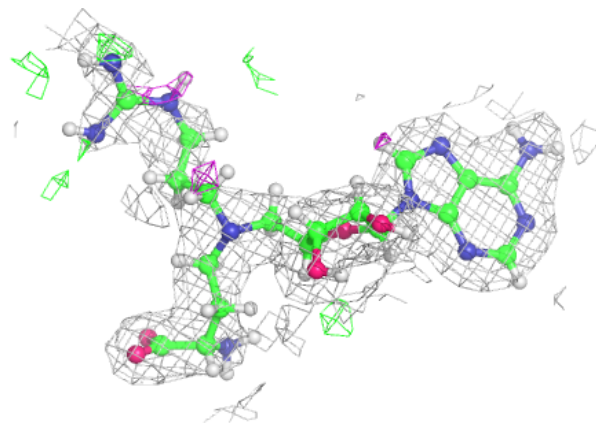


**Electron density around 6D2 B 501:**

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

**Electron density around 6D2 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)



## 6.5 Other polymers

There are no such residues in this entry.