



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:29 pm BST

PDB ID : 5LKJ  
Title : Crystal structure of mouse CARM1 in complex with ligand SA684  
Authors : Cura, V.; Marechal, N.; Mailliot, J.; Troffer-Charlier, N.; Hassenboehler, P.;  
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Deposited on : 2016-07-22  
Resolution : 2.60 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

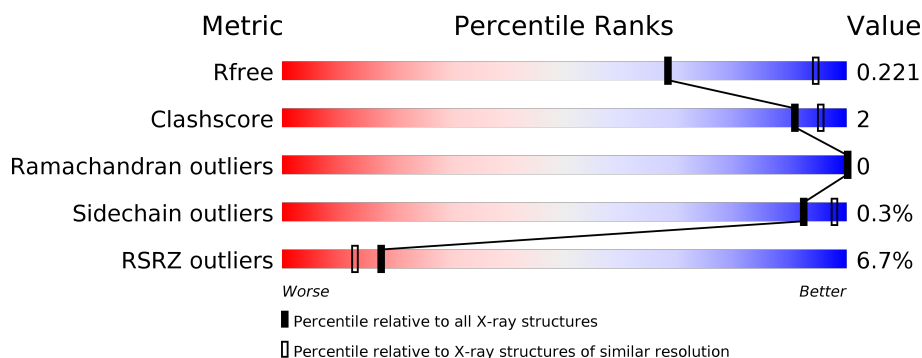
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	371	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>8%</div> </div> <div>• •</div> </div>
1	B	371	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>8%</div> </div> </div>
1	C	371	<div> <div>11%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>8%</div> </div> <div>•</div> </div>
1	D	371	<div> <div>9%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>8%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	P33	B	505	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22919 atoms, of which 11284 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.

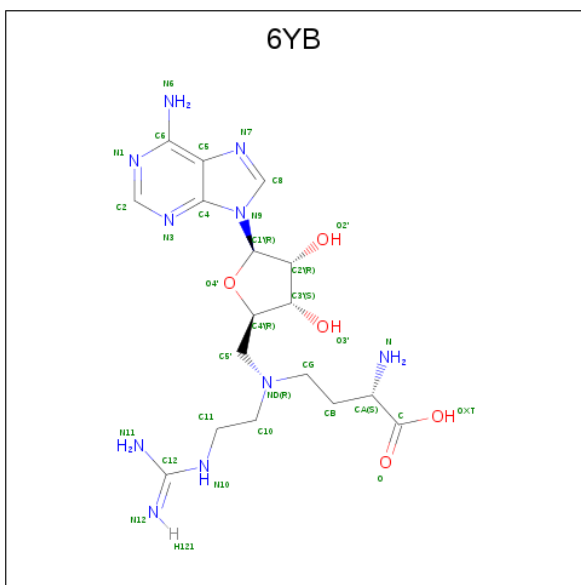
- Molecule 1 is a protein called Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	361	Total	C	H	N	O	S	0	0	0
			5687	1853	2809	475	536	14			
1	B	343	Total	C	H	N	O	S	0	2	0
			5468	1782	2707	457	508	14			
1	C	361	Total	C	H	N	O	S	0	0	0
			5687	1853	2809	475	536	14			
1	D	343	Total	C	H	N	O	S	0	0	0
			5450	1776	2699	454	507	14			

There are 12 discrepancies between the modelled and reference sequences:

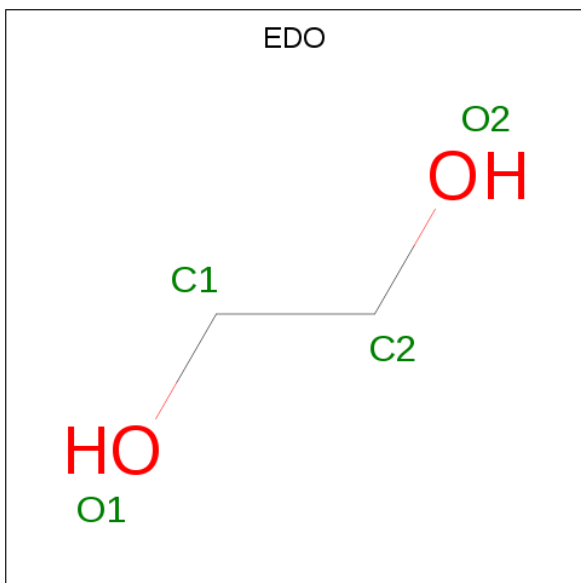
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	expression tag	UNP Q9WVG6
A	128	HIS	-	expression tag	UNP Q9WVG6
A	129	MET	-	expression tag	UNP Q9WVG6
B	127	GLY	-	expression tag	UNP Q9WVG6
B	128	HIS	-	expression tag	UNP Q9WVG6
B	129	MET	-	expression tag	UNP Q9WVG6
C	127	GLY	-	expression tag	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 (2 {S})-4-[[ (2 {R}, 3 {S}, 4 {R}, 5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl-(2-carbamimidamidoethyl)amino]-2-azanyl-butanoic acid (three-letter code: 6YB) (formula: C<sub>17</sub>H<sub>28</sub>N<sub>10</sub>O<sub>5</sub>).



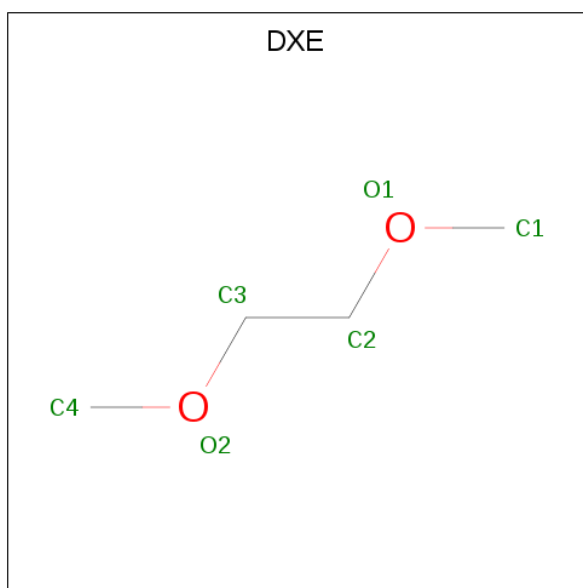
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 59	C 17	H 27	N 10	O 5	0	0
2	B	1	Total 59	C 17	H 27	N 10	O 5	0	0
2	C	1	Total 59	C 17	H 27	N 10	O 5	0	0
2	D	1	Total 59	C 17	H 27	N 10	O 5	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



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

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



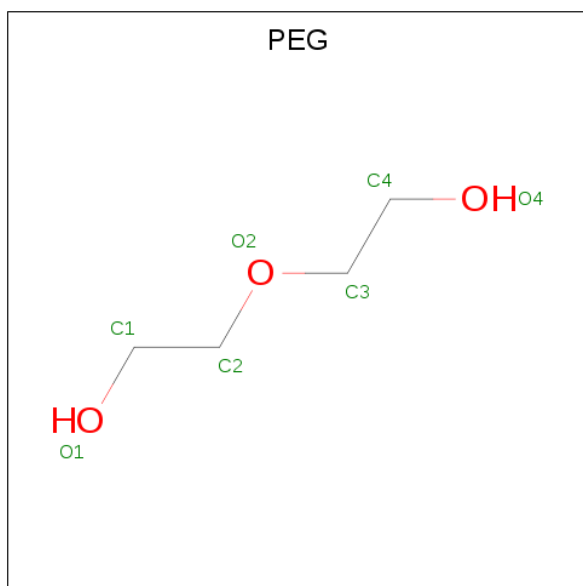
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 16 4 10 2	0	0
4	A	1	Total C H O 16 4 10 2	0	0
4	A	1	Total C H O 16 4 10 2	0	0
4	B	1	Total C H O 16 4 10 2	0	0

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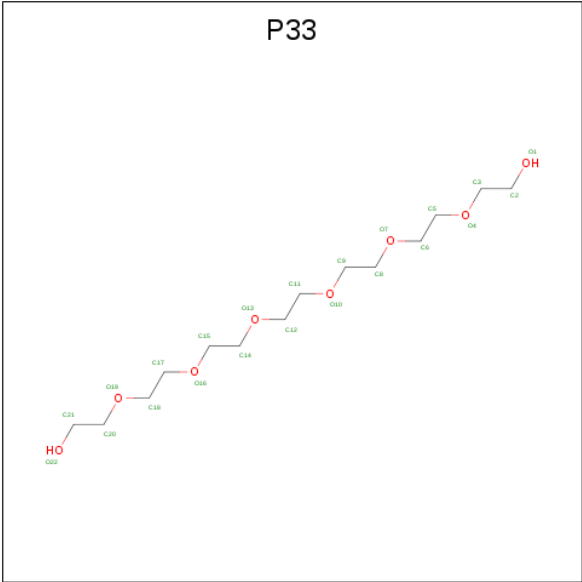
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 6 is 3,6,9,12,15,18-HEXAOSAICOSANE-1,20-DIOL (three-letter code: P33) (formula:  $C_{14}H_{30}O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			52	14	30	8		

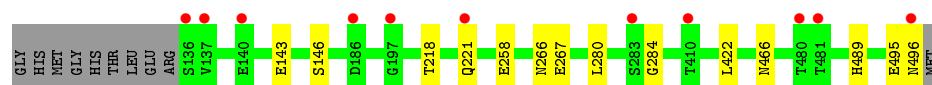
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	59	Total	O	0	0
			59	59		
7	B	45	Total	O	0	0
			45	45		
7	C	15	Total	O	0	0
			15	15		
7	D	15	Total	O	0	0
			15	15		

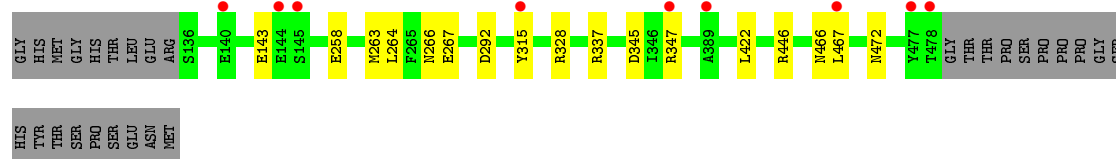
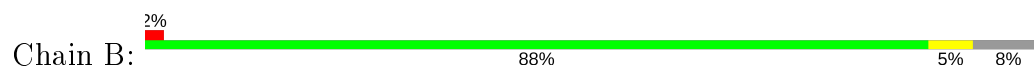
### 3 Residue-property plots [i](#)

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.

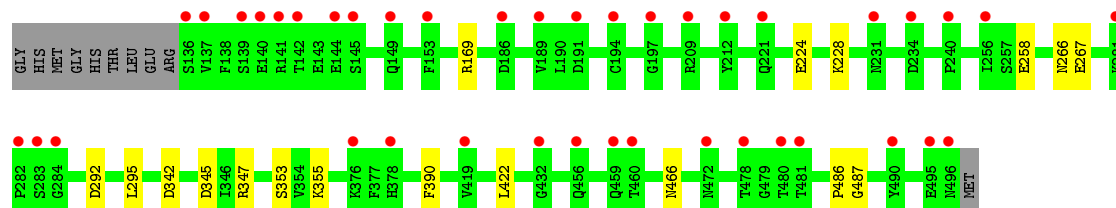
- Molecule 1: Histone-arginine methyltransferase CARM1



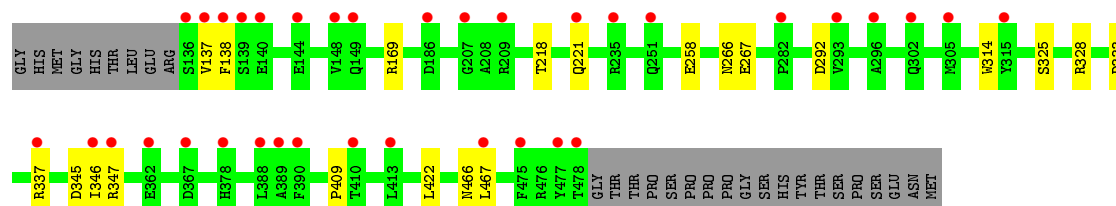
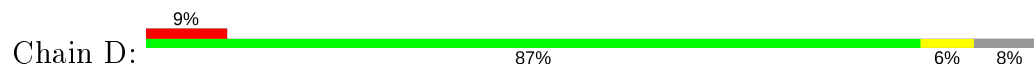
- Molecule 1: Histone-arginine methyltransferase CARM1



- 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, $\alpha$ , $\beta$ , $\gamma$	74.64 Å 98.16 Å 206.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.60 19.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.90-2.60) 99.1 (19.90-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.20 (at 2.59 Å)	Xtriage
Refinement program	PHENIX dev_1951	Depositor
R, $R_{free}$	0.189 , 0.220 0.190 , 0.221	Depositor DCC
$R_{free}$ test set	2366 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 51.5	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	0.94	EDS
Total number of atoms	22919	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	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 39.91 % 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 2.9606e-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: 6YB, P33, DXE, PEG, EDO

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	0.27	0/2955	0.45	0/4011
1	B	0.27	0/2840	0.45	0/3848
1	C	0.25	0/2955	0.42	0/4011
1	D	0.25	0/2821	0.42	0/3823
All	All	0.26	0/11571	0.44	0/15693

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	2878	2809	2809	7	1
1	B	2761	2707	2697	10	0
1	C	2878	2809	2809	11	0
1	D	2751	2699	2699	12	0
2	A	32	27	0	0	0
2	B	32	27	0	0	0
2	C	32	27	0	1	0
2	D	32	27	0	1	0
3	A	16	18	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	18	18	0	0
3	C	4	6	6	0	0
4	A	18	30	30	0	0
4	B	12	20	20	0	0
5	A	7	10	10	0	0
5	C	14	20	20	0	0
6	B	22	30	30	0	0
7	A	59	0	0	0	0
7	B	45	0	0	1	1
7	C	15	0	0	1	0
7	D	15	0	0	1	0
All	All	11635	11284	11172	39	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 2.

All (39) 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:292:ASP:OD2	7:B:601:HOH:O	1.92	0.85
1:D:292:ASP:OD2	7:D:601:HOH:O	2.02	0.76
1:C:342:ASP:OD1	7:C:601:HOH:O	2.07	0.71
1:D:422:LEU:O	1:D:466:ASN:ND2	2.34	0.60
1:B:337:ARG:HG2	1:B:467:LEU:O	2.03	0.57
1:B:422:LEU:O	1:B:466:ASN:ND2	2.42	0.53
1:B:345:ASP:OD2	1:B:347:ARG:NH1	2.41	0.53
1:A:495:GLU:N	1:A:496:ASN:HA	2.27	0.49
1:D:345:ASP:OD2	1:D:347:ARG:NH2	2.45	0.49
1:D:137:VAL:O	1:D:138:PHE:HB3	2.13	0.49
1:B:472:ASN:O	1:B:472:ASN:ND2	2.45	0.48
1:A:143:GLU:HG3	1:A:146:SER:H	1.79	0.48
1:B:315:TYR:HB2	1:B:328:ARG:HD2	1.96	0.48
1:C:345:ASP:OD1	1:C:347:ARG:HD3	2.14	0.48
1:C:224:GLU:HG3	1:C:228:LYS:HE3	1.96	0.47
1:A:218:THR:O	1:A:221:GLN:OE1	2.33	0.47
1:B:328:ARG:NH1	1:D:328:ARG:HH12	2.14	0.46
1:C:295:LEU:CD1	1:C:390:PHE:CE2	2.99	0.45
1:D:314:TRP:O	1:D:325:SER:HA	2.16	0.45
1:C:266:ASN:O	1:C:267:GLU:HB2	2.16	0.45
1:D:337:ARG:HG2	1:D:467:LEU:O	2.16	0.45
1:C:422:LEU:O	1:C:466:ASN:ND2	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASN:O	1:A:267:GLU:HB2	2.18	0.44
1:B:266:ASN:O	1:B:267:GLU:HB2	2.18	0.44
1:D:218:THR:O	1:D:221:GLN:OE1	2.36	0.43
1:A:422:LEU:O	1:A:466:ASN:ND2	2.41	0.43
1:C:295:LEU:O	1:C:353:SER:HA	2.19	0.43
1:D:169:ARG:NH1	2:D:501:6YB:O	2.49	0.42
1:D:266:ASN:O	1:D:267:GLU:HB2	2.19	0.42
1:C:169:ARG:NH2	2:C:501:6YB:O	2.51	0.42
1:A:495:GLU:N	1:A:496:ASN:CA	2.84	0.41
1:A:280:LEU:HD11	1:A:284:GLY:HA3	2.02	0.41
1:C:292:ASP:OD2	1:C:355:LYS:HD2	2.21	0.41
1:B:263:MET:O	1:B:264:LEU:HB3	2.20	0.41
1:B:143:GLU:OE2	1:B:446:ARG:HG2	2.21	0.41
1:D:333:ASP:O	1:D:337:ARG:HG3	2.21	0.41
1:C:486:PRO:HA	1:C:487:GLY:HA2	1.84	0.41
1:C:295:LEU:HD11	1:C:390:PHE:CE2	2.56	0.40
1:D:346:ILE:HG22	1:D:409:PRO:HG2	2.03	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)
1:A:489:HIS:HE2	7:B:602:HOH:O[2_655]	1.51	0.09

## 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	359/371 (97%)	349 (97%)	10 (3%)	0	100	100
1	B	343/371 (92%)	334 (97%)	9 (3%)	0	100	100
1	C	359/371 (97%)	350 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	341/371 (92%)	330 (97%)	11 (3%)	0	100	100
All	All	1402/1484 (94%)	1363 (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	315/323 (98%)	314 (100%)	1 (0%)	92	98
1	B	301/323 (93%)	300 (100%)	1 (0%)	92	98
1	C	315/323 (98%)	314 (100%)	1 (0%)	92	98
1	D	299/323 (93%)	298 (100%)	1 (0%)	92	98
All	All	1230/1292 (95%)	1226 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	GLU
1	B	258	GLU
1	C	258	GLU
1	D	258	GLU

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](#)

21 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$
4	DXE	A	508	-	5,5,5	0.42	0	4,4,4	0.19	0
6	P33	B	505	-	21,21,21	0.55	0	20,20,20	0.40	0
2	6YB	C	501	-	27,34,34	1.97	7 (25%)	26,48,48	1.58	4 (15%)
3	EDO	A	505	-	3,3,3	0.49	0	2,2,2	0.48	0
2	6YB	A	501	-	27,34,34	2.04	8 (29%)	26,48,48	1.43	3 (11%)
3	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.51	0
3	EDO	B	504	-	3,3,3	0.47	0	2,2,2	0.45	0
5	PEG	C	504	-	6,6,6	0.49	0	5,5,5	0.47	0
5	PEG	C	503	-	6,6,6	0.48	0	5,5,5	0.57	0
3	EDO	A	503	-	3,3,3	0.47	0	2,2,2	0.48	0
2	6YB	D	501	-	27,34,34	2.03	8 (29%)	26,48,48	1.54	4 (15%)
3	EDO	C	502	-	3,3,3	0.47	0	2,2,2	0.50	0
2	6YB	B	501	-	27,34,34	2.06	8 (29%)	26,48,48	1.34	3 (11%)
4	DXE	A	506	-	5,5,5	0.42	0	4,4,4	0.22	0
4	DXE	A	507	-	5,5,5	0.41	0	4,4,4	0.22	0
3	EDO	B	502	-	3,3,3	0.48	0	2,2,2	0.53	0
3	EDO	A	502	-	3,3,3	0.47	0	2,2,2	0.49	0
3	EDO	B	503	-	3,3,3	0.47	0	2,2,2	0.50	0
4	DXE	B	507	-	5,5,5	0.43	0	4,4,4	0.22	0
5	PEG	A	509	-	6,6,6	0.48	0	5,5,5	0.46	0
4	DXE	B	506	-	5,5,5	0.41	0	4,4,4	0.22	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
4	DXE	A	508	-	-	2/3/3/3	-
6	P33	B	505	-	-	7/19/19/19	-
2	6YB	C	501	-	-	7/15/39/39	0/3/3/3
3	EDO	A	505	-	-	0/1/1/1	-
2	6YB	A	501	-	-	7/15/39/39	0/3/3/3
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-
5	PEG	C	504	-	-	1/4/4/4	-
5	PEG	C	503	-	-	3/4/4/4	-
3	EDO	A	503	-	-	1/1/1/1	-
2	6YB	D	501	-	-	5/15/39/39	0/3/3/3
3	EDO	C	502	-	-	1/1/1/1	-
2	6YB	B	501	-	-	8/15/39/39	0/3/3/3
4	DXE	A	506	-	-	2/3/3/3	-
4	DXE	A	507	-	-	2/3/3/3	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
4	DXE	B	507	-	-	2/3/3/3	-
5	PEG	A	509	-	-	3/4/4/4	-
4	DXE	B	506	-	-	3/3/3/3	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6YB	C12-N10	6.22	1.45	1.33
2	B	501	6YB	C12-N10	6.08	1.45	1.33
2	D	501	6YB	C12-N10	6.06	1.45	1.33
2	C	501	6YB	C12-N10	5.93	1.45	1.33
2	C	501	6YB	C6-N6	4.22	1.49	1.34
2	B	501	6YB	C6-N6	4.17	1.49	1.34
2	A	501	6YB	C6-N6	4.16	1.49	1.34
2	D	501	6YB	C6-N6	4.16	1.49	1.34
2	B	501	6YB	O4'-C1'	3.90	1.46	1.41
2	D	501	6YB	O4'-C1'	3.79	1.46	1.41
2	A	501	6YB	O4'-C1'	3.67	1.46	1.41
2	C	501	6YB	O4'-C1'	3.50	1.46	1.41
2	D	501	6YB	C5'-ND	2.77	1.52	1.47
2	B	501	6YB	C5'-ND	2.75	1.52	1.47
2	B	501	6YB	C2-N3	2.64	1.36	1.32
2	A	501	6YB	C11-N10	2.62	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6YB	C5'-ND	2.62	1.52	1.47
2	D	501	6YB	C2-N3	2.54	1.36	1.32
2	D	501	6YB	C11-N10	2.52	1.51	1.46
2	B	501	6YB	C11-N10	2.51	1.51	1.46
2	A	501	6YB	C2-N3	2.46	1.36	1.32
2	C	501	6YB	C2-N3	2.44	1.36	1.32
2	D	501	6YB	C12-N11	2.40	1.44	1.34
2	C	501	6YB	C11-N10	2.38	1.51	1.46
2	C	501	6YB	C5'-ND	2.36	1.51	1.47
2	A	501	6YB	C12-N11	2.33	1.44	1.34
2	B	501	6YB	C12-N11	2.31	1.44	1.34
2	C	501	6YB	C12-N11	2.30	1.44	1.34
2	A	501	6YB	C3'-C2'	-2.14	1.47	1.53
2	B	501	6YB	C3'-C2'	-2.12	1.47	1.53
2	D	501	6YB	C3'-C2'	-2.03	1.47	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	6YB	N3-C2-N1	-4.66	121.39	128.68
2	C	501	6YB	N3-C2-N1	-4.61	121.47	128.68
2	B	501	6YB	N3-C2-N1	-4.52	121.61	128.68
2	D	501	6YB	N3-C2-N1	-4.51	121.62	128.68
2	C	501	6YB	C1'-N9-C4	-3.18	121.06	126.64
2	D	501	6YB	C1'-N9-C4	-3.06	121.27	126.64
2	D	501	6YB	C3'-C2'-C1'	2.92	105.38	100.98
2	A	501	6YB	C1'-N9-C4	-2.73	121.84	126.64
2	C	501	6YB	C3'-C2'-C1'	2.62	104.92	100.98
2	C	501	6YB	C4-C5-N7	-2.61	106.68	109.40
2	D	501	6YB	C4-C5-N7	-2.49	106.81	109.40
2	B	501	6YB	C1'-N9-C4	-2.47	122.30	126.64
2	B	501	6YB	C4-C5-N7	-2.32	106.98	109.40
2	A	501	6YB	C4-C5-N7	-2.26	107.05	109.40

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	6YB	O4'-C4'-C5'-ND
2	C	501	6YB	C3'-C4'-C5'-ND
2	C	501	6YB	C-CA-CB-CG
2	C	501	6YB	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	A	501	6YB	O4'-C4'-C5'-ND
2	A	501	6YB	C3'-C4'-C5'-ND
2	A	501	6YB	C-CA-CB-CG
2	A	501	6YB	N-CA-CB-CG
2	D	501	6YB	O4'-C4'-C5'-ND
2	B	501	6YB	O4'-C4'-C5'-ND
2	B	501	6YB	C3'-C4'-C5'-ND
2	B	501	6YB	C-CA-CB-CG
2	B	501	6YB	N-CA-CB-CG
2	C	501	6YB	ND-C10-C11-N10
4	A	506	DXE	O1-C2-C3-O2
4	A	507	DXE	O1-C2-C3-O2
6	B	505	P33	O7-C8-C9-O10
5	A	509	PEG	O1-C1-C2-O2
6	B	505	P33	O19-C20-C21-O22
5	C	503	PEG	O1-C1-C2-O2
2	A	501	6YB	ND-C10-C11-N10
2	B	501	6YB	CB-CG-ND-C5'
3	B	504	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2
2	D	501	6YB	ND-C10-C11-N10
6	B	505	P33	O16-C17-C18-O19
2	B	501	6YB	CB-CG-ND-C10
2	B	501	6YB	ND-C10-C11-N10
5	C	503	PEG	O2-C3-C4-O4
5	A	509	PEG	O2-C3-C4-O4
2	C	501	6YB	CB-CG-ND-C10
2	C	501	6YB	CB-CG-ND-C5'
6	B	505	P33	O4-C5-C6-O7
4	A	508	DXE	O1-C2-C3-O2
2	A	501	6YB	CB-CG-ND-C5'
5	C	503	PEG	C4-C3-O2-C2
4	B	506	DXE	O1-C2-C3-O2
2	D	501	6YB	C3'-C4'-C5'-ND
6	B	505	P33	C2-C3-O4-C5
2	A	501	6YB	CB-CG-ND-C10
5	C	504	PEG	C1-C2-O2-C3
4	B	506	DXE	C3-C2-O1-C1
6	B	505	P33	C8-C9-O10-C11
5	A	509	PEG	C4-C3-O2-C2
3	A	503	EDO	O1-C1-C2-O2
4	A	508	DXE	C2-C3-O2-C4

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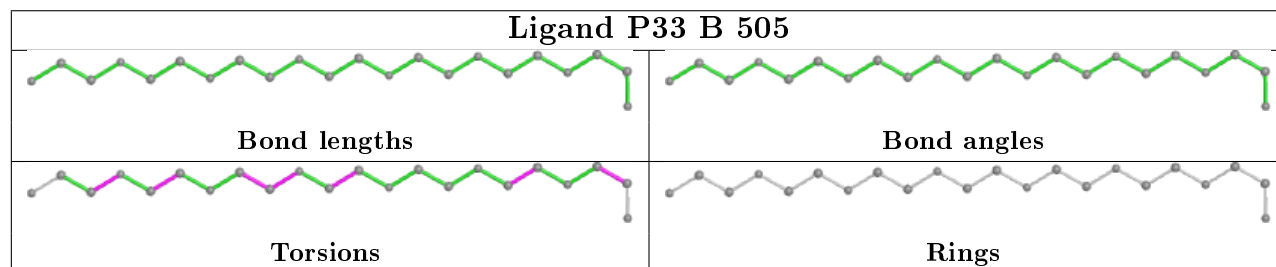
Mol	Chain	Res	Type	Atoms
4	A	506	DXE	C2-C3-O2-C4
4	B	507	DXE	C2-C3-O2-C4
2	D	501	6YB	C11-C10-ND-CG
3	A	502	EDO	O1-C1-C2-O2
2	D	501	6YB	CB-CG-ND-C5'
2	B	501	6YB	C11-C10-ND-C5'
4	B	507	DXE	O1-C2-C3-O2
4	A	507	DXE	C3-C2-O1-C1
6	B	505	P33	O10-C11-C12-O13
3	C	502	EDO	O1-C1-C2-O2
4	B	506	DXE	C2-C3-O2-C4

There are no ring outliers.

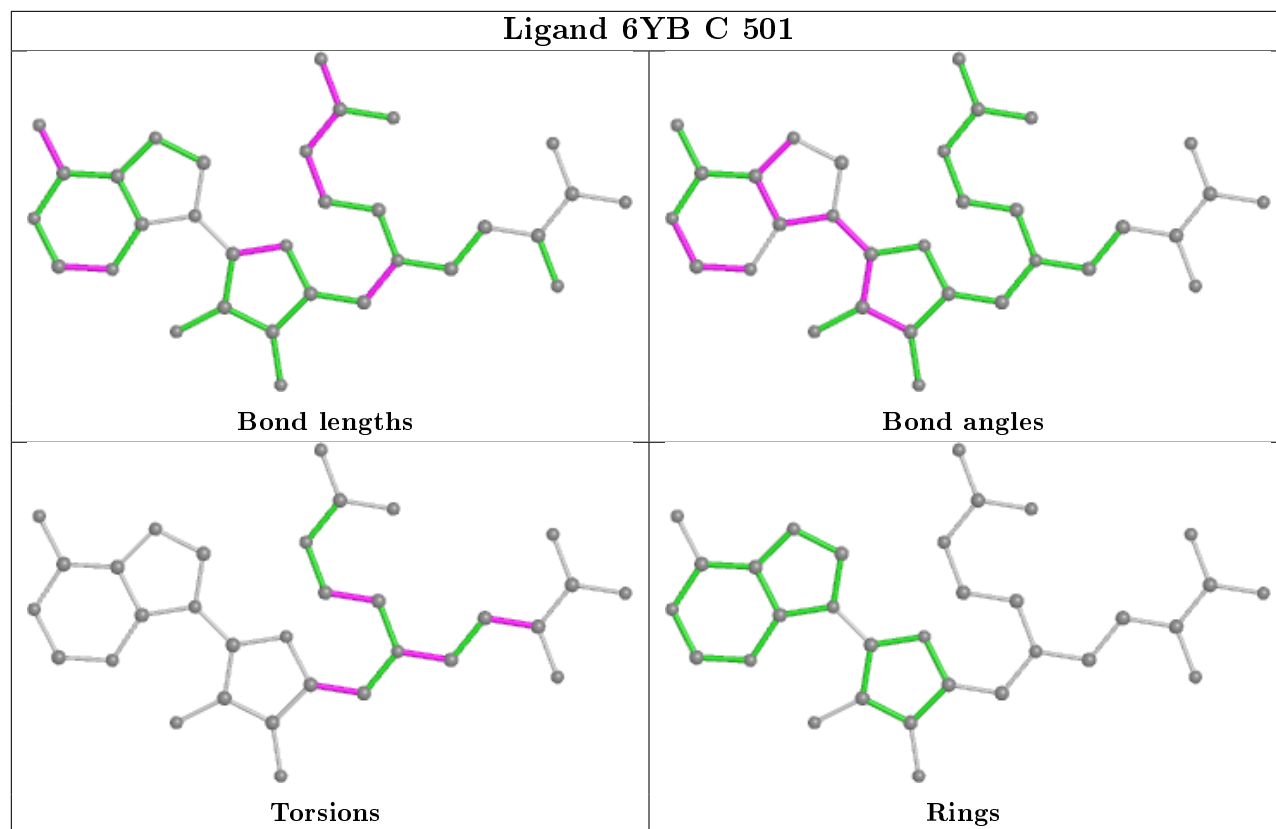
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	6YB	1	0
2	D	501	6YB	1	0

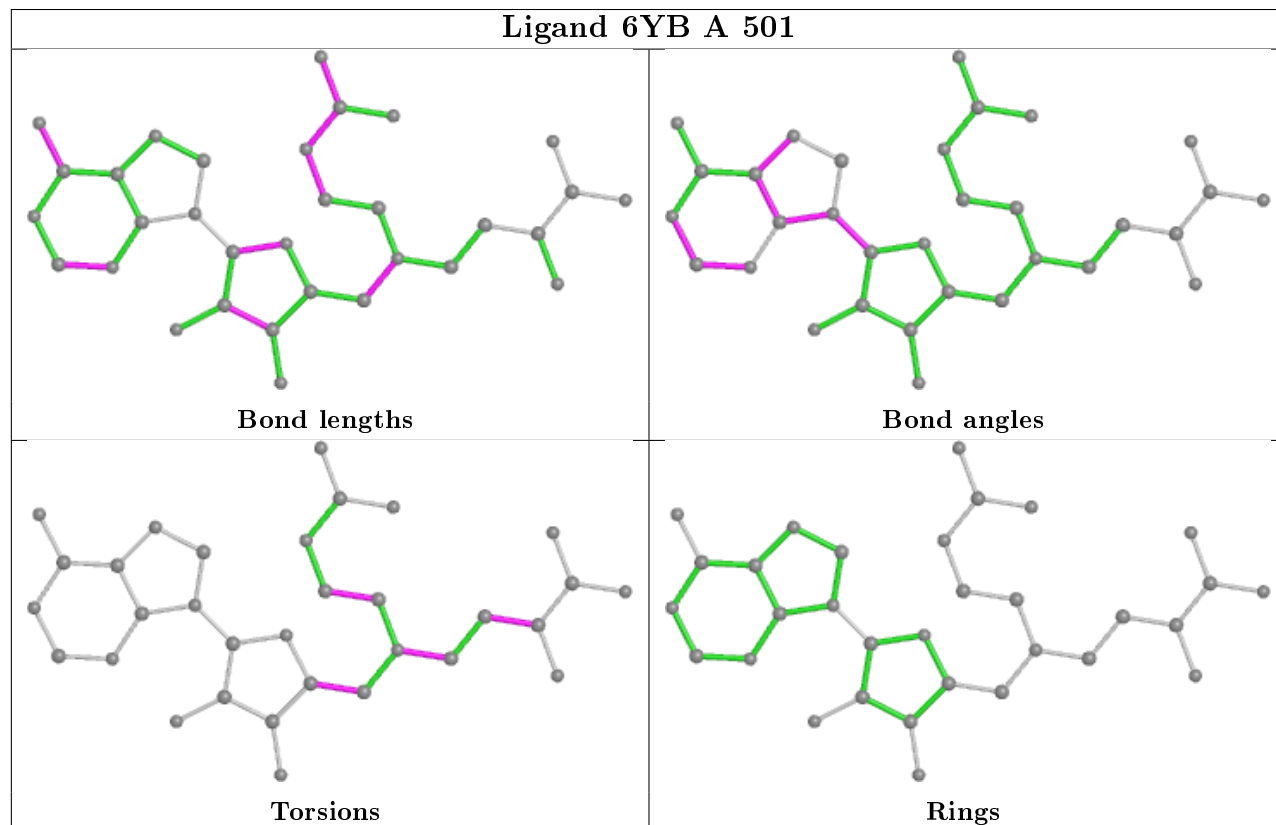
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



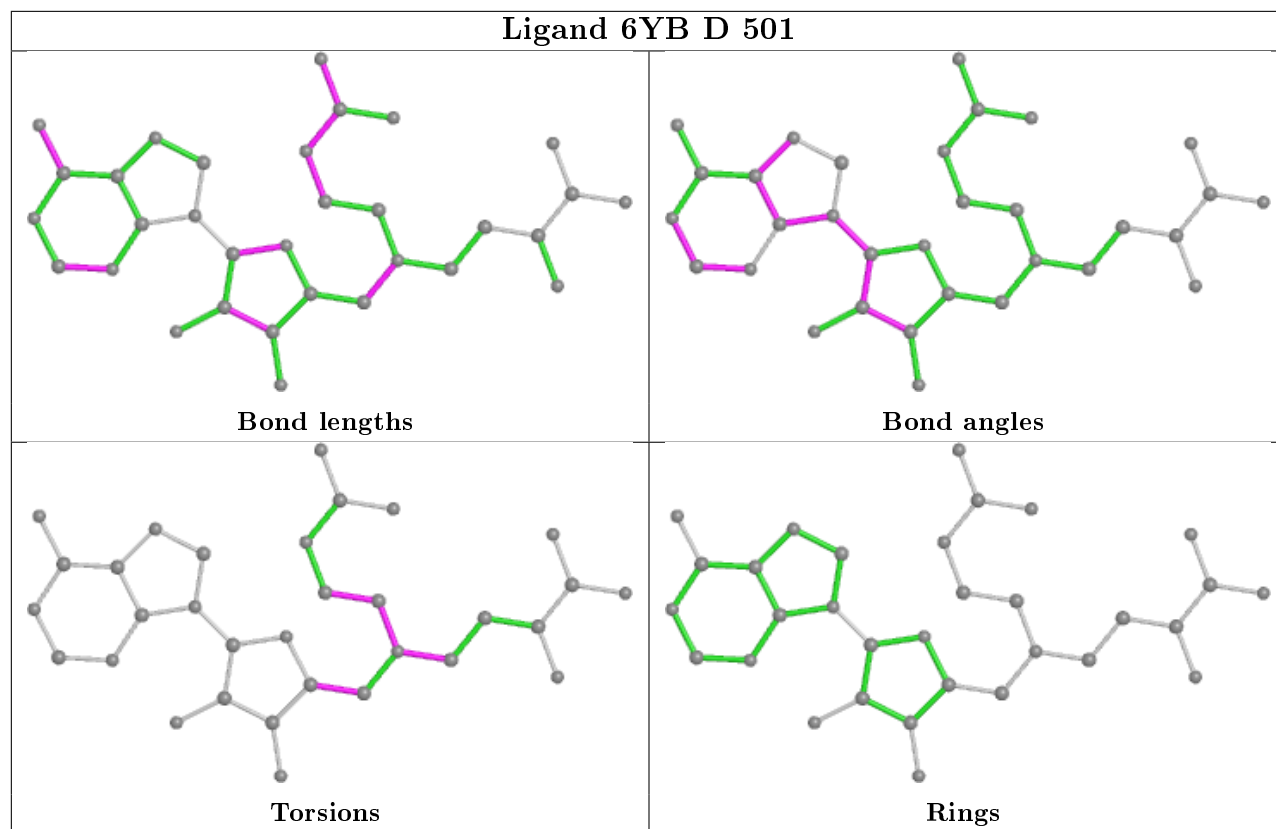
## Ligand 6YB C 501



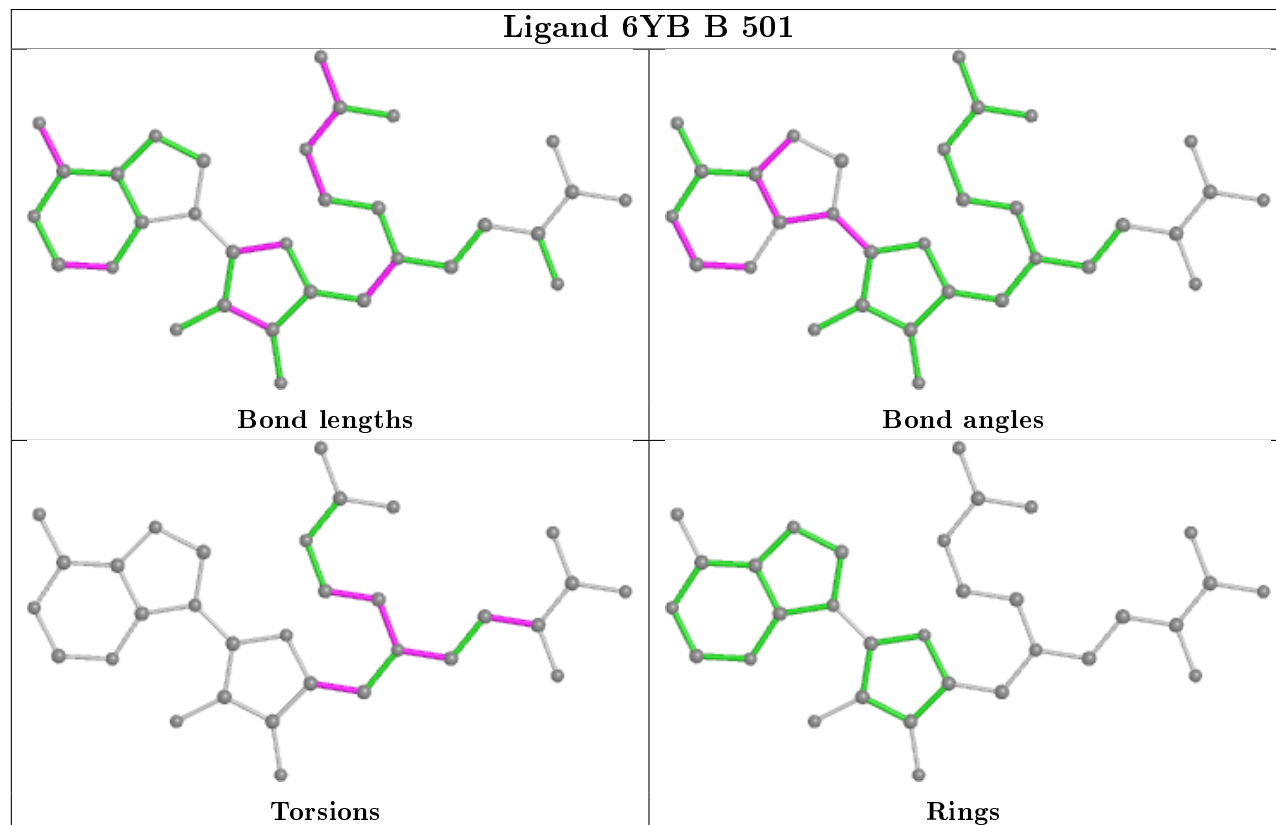
## Ligand 6YB A 501



## Ligand 6YB D 501



## Ligand 6YB B 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	361/371 (97%)	0.08	11 (3%) 50 43	21, 39, 58, 94	0
1	B	343/371 (92%)	0.18	9 (2%) 56 50	25, 43, 68, 102	0
1	C	361/371 (97%)	0.59	40 (11%) 5 3	38, 61, 94, 124	0
1	D	343/371 (92%)	0.56	35 (10%) 6 4	42, 61, 87, 121	0
All	All	1408/1484 (94%)	0.35	95 (6%) 17 13	21, 53, 86, 124	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	ASN	7.9
1	D	136	SER	7.6
1	C	496	ASN	7.0
1	C	136	SER	6.8
1	D	137	VAL	6.0
1	D	477	TYR	5.6
1	B	477	TYR	5.5
1	C	495	GLU	5.3
1	C	140	GLU	5.2
1	D	140	GLU	4.5
1	C	137	VAL	4.3
1	D	347	ARG	4.1
1	D	478	THR	4.0
1	A	186	ASP	4.0
1	B	478	THR	4.0
1	A	140	GLU	3.7
1	B	467	LEU	3.7
1	B	145	SER	3.6
1	C	480	THR	3.6
1	A	136	SER	3.5
1	C	139	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	144	GLU	3.4
1	C	282	PRO	3.4
1	A	137	VAL	3.4
1	C	256	ILE	3.3
1	D	467	LEU	3.3
1	C	284	GLY	3.3
1	D	362	GLU	3.2
1	D	389	ALA	3.2
1	D	209	ARG	3.2
1	A	283	SER	3.1
1	C	490	TYR	3.1
1	C	149	GLN	3.1
1	A	480	THR	3.1
1	D	144	GLU	3.1
1	D	302	GLN	3.0
1	C	432	GLY	3.0
1	C	186	ASP	2.9
1	D	337	ARG	2.8
1	D	388	LEU	2.8
1	C	191	ASP	2.8
1	D	235	ARG	2.8
1	A	481	THR	2.7
1	B	140	GLU	2.6
1	B	389	ALA	2.6
1	D	138	PHE	2.6
1	C	189	VAL	2.6
1	D	346	ILE	2.6
1	D	305	MET	2.6
1	C	478	THR	2.5
1	C	209	ARG	2.5
1	D	139	SER	2.5
1	C	231	ASN	2.5
1	C	240	PRO	2.4
1	C	194	CYS	2.4
1	C	153	PHE	2.4
1	D	413	LEU	2.4
1	D	475	PHE	2.4
1	D	282	PRO	2.4
1	C	221	GLN	2.4
1	C	145	SER	2.4
1	D	221	GLN	2.3
1	B	315	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	460	THR	2.3
1	A	221	GLN	2.3
1	D	315	TYR	2.3
1	C	456	GLN	2.3
1	D	378	HIS	2.3
1	C	281	LYS	2.3
1	D	296	ALA	2.3
1	C	419	VAL	2.2
1	D	148	VAL	2.2
1	D	293	VAL	2.2
1	C	142	THR	2.2
1	C	481	THR	2.2
1	C	472	ASN	2.2
1	D	251	GLN	2.2
1	D	410	THR	2.2
1	C	144	GLU	2.2
1	D	390	PHE	2.2
1	A	197	GLY	2.2
1	D	207	GLY	2.2
1	C	459	GLN	2.1
1	D	367	ASP	2.1
1	C	212	TYR	2.1
1	C	378	HIS	2.1
1	A	410	THR	2.1
1	D	186	ASP	2.1
1	D	149	GLN	2.1
1	B	347	ARG	2.1
1	C	141	ARG	2.1
1	C	234	ASP	2.0
1	C	283	SER	2.0
1	C	197	GLY	2.0
1	C	376	LYS	2.0

## 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 ⓘ

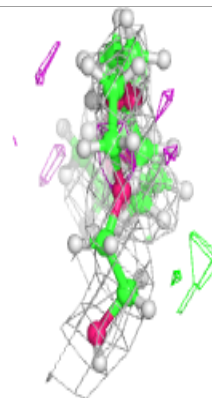
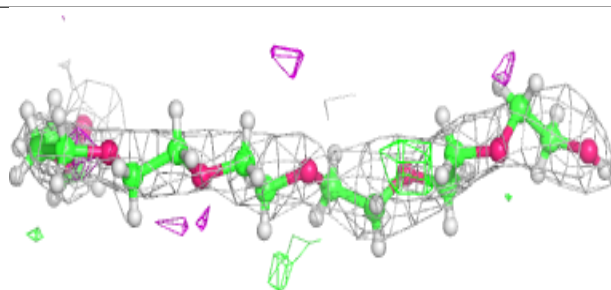
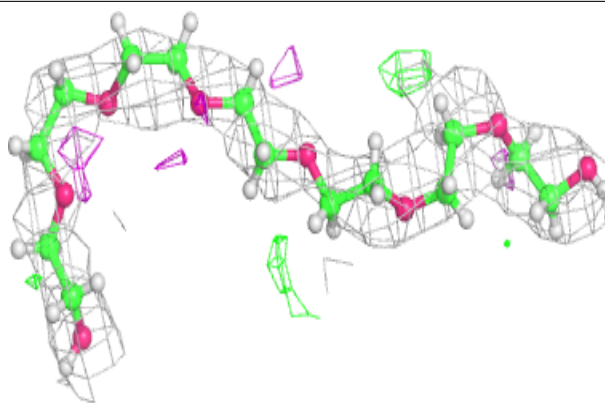
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	EDO	B	503	4/4	0.66	0.21	92,110,111,111	0
3	EDO	A	505	4/4	0.67	0.23	45,48,48,54	0
6	P33	B	505	22/22	0.76	0.42	59,75,90,90	0
4	DXE	A	508	6/6	0.77	0.24	58,70,76,76	0
5	PEG	A	509	7/7	0.79	0.26	77,93,97,97	0
4	DXE	B	506	6/6	0.80	0.38	56,71,86,86	0
3	EDO	A	504	4/4	0.82	0.26	66,79,82,84	0
3	EDO	B	504	4/4	0.83	0.36	68,82,89,89	0
3	EDO	A	502	4/4	0.85	0.17	69,83,85,87	0
4	DXE	B	507	6/6	0.85	0.16	69,83,85,85	0
4	DXE	A	506	6/6	0.86	0.16	60,72,80,80	0
5	PEG	C	504	7/7	0.86	0.22	66,79,94,95	0
3	EDO	C	502	4/4	0.87	0.10	98,117,120,122	0
3	EDO	A	503	4/4	0.88	0.36	75,91,96,97	0
5	PEG	C	503	7/7	0.89	0.17	66,79,87,87	0
3	EDO	B	502	4/4	0.90	0.17	45,55,63,69	0
2	6YB	C	501	32/32	0.90	0.19	43,67,95,104	0
2	6YB	D	501	32/32	0.90	0.20	47,64,92,107	0
4	DXE	A	507	6/6	0.91	0.26	53,64,65,65	0
2	6YB	A	501	32/32	0.94	0.19	25,52,90,102	0
2	6YB	B	501	32/32	0.94	0.16	27,54,76,91	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.

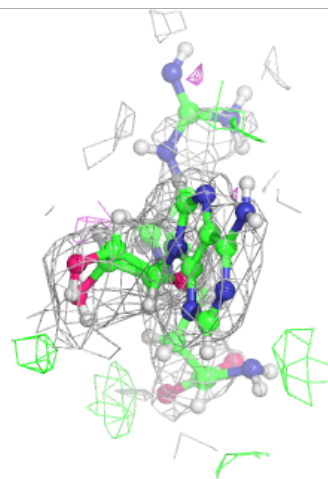
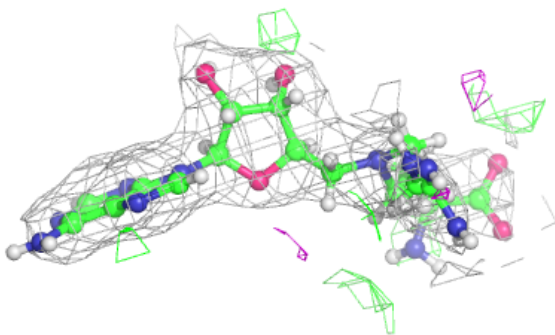
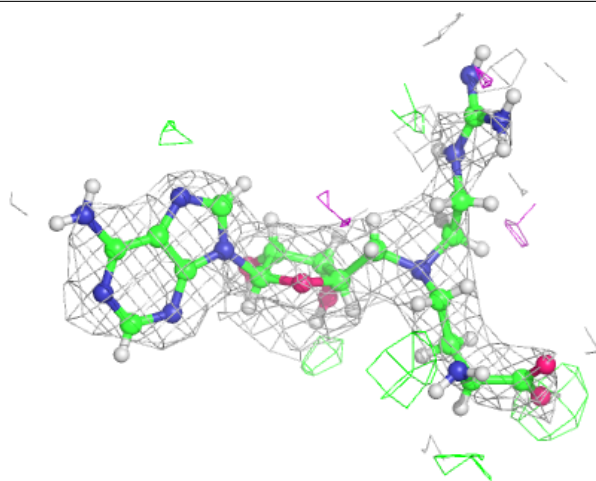
**Electron density around P33 B 505:**

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



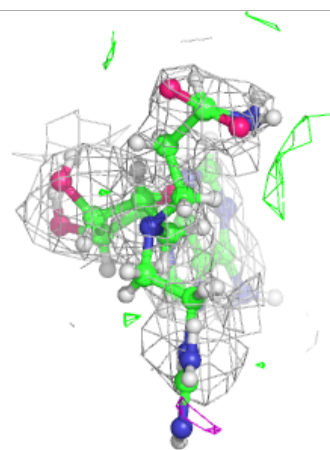
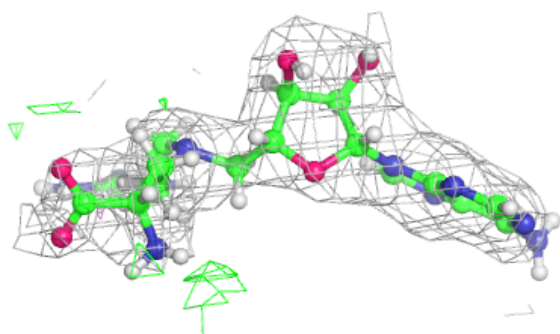
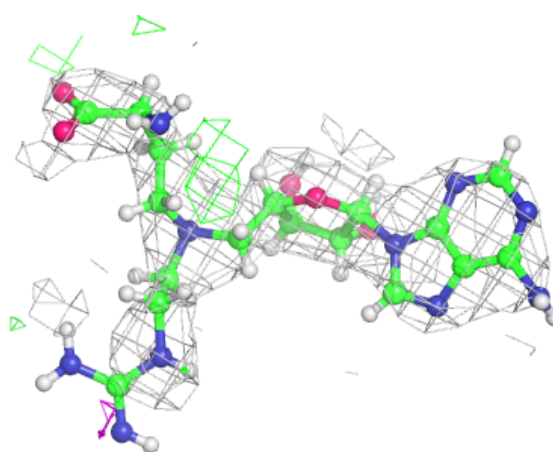
**Electron density around 6YB C 501:**

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



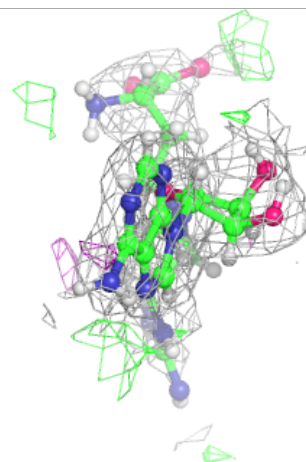
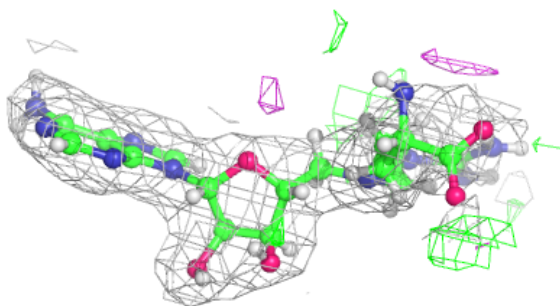
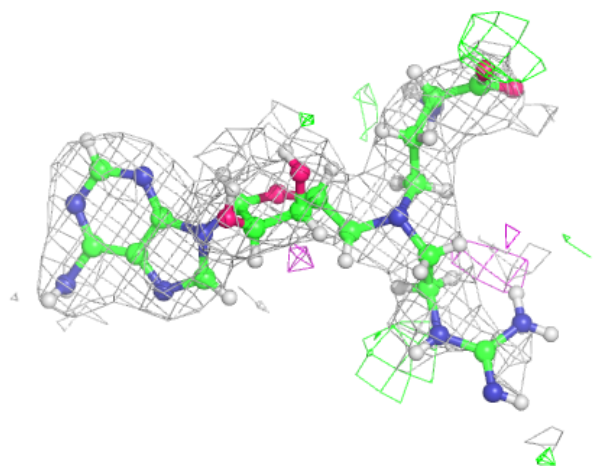
**Electron density around 6YB D 501:**

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



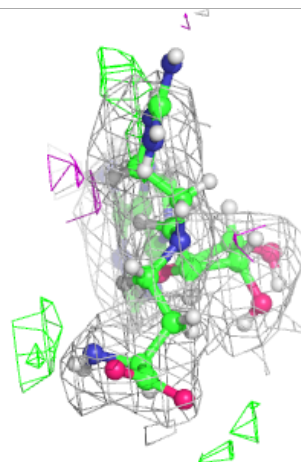
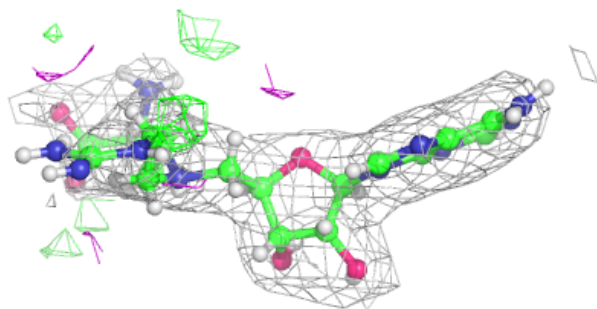
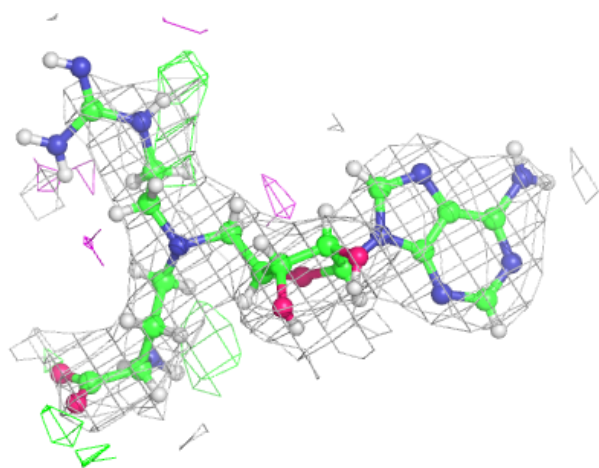
**Electron density around 6YB A 501:**

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



**Electron density around 6YB 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.