



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 10:01 AM EST

PDB ID : 8D4I  
Title : Structure of Y430F D-ornithine/D-lysine decarboxylase complex with putrescine  
Authors : Phillips, R.S.; Nguyen Hoang, K.N.  
Deposited on : 2022-06-02  
Resolution : 1.32 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

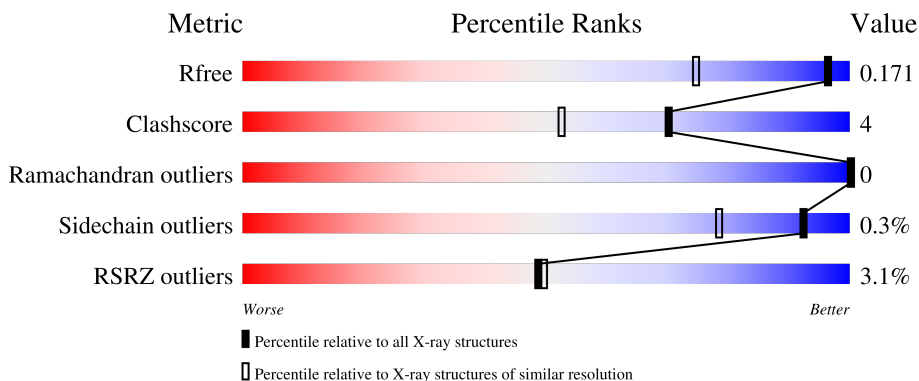
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

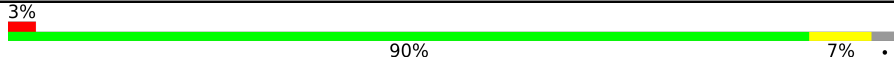
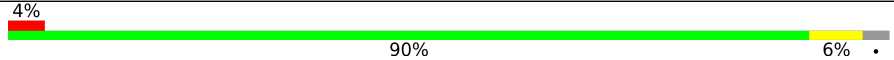
The reported resolution of this entry is 1.32 Å.

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	1611 (1.34-1.30)
Clashscore	141614	1667 (1.34-1.30)
Ramachandran outliers	138981	1615 (1.34-1.30)
Sidechain outliers	138945	1615 (1.34-1.30)
RSRZ outliers	127900	1580 (1.34-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	477	 3% 90% 7%
1	C	477	 4% 90% 6%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 17250 atoms, of which 7985 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 D-ornithine/D-lysine decarboxylase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P	S			
1	A	462	7913	2530	3932	679	747	1	24	0	55	0
1	C	462	7958	2545	3956	679	753	1	24	0	59	0

There are 26 discrepancies between the modelled and reference sequences:

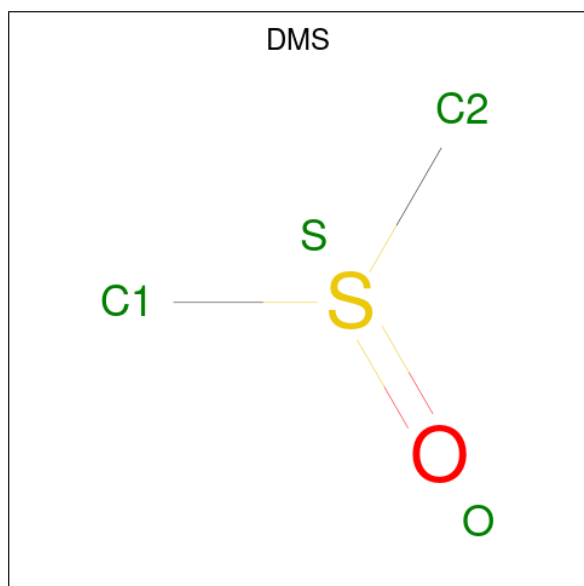
Chain	Residue	Modelled	Actual	Comment	Reference
A	430	PHE	TYR	engineered mutation	UNP Q8ZNC4
A	466	LEU	-	expression tag	UNP Q8ZNC4
A	467	ALA	-	expression tag	UNP Q8ZNC4
A	468	ALA	-	expression tag	UNP Q8ZNC4
A	469	ALA	-	expression tag	UNP Q8ZNC4
A	470	LEU	-	expression tag	UNP Q8ZNC4
A	471	GLU	-	expression tag	UNP Q8ZNC4
A	472	HIS	-	expression tag	UNP Q8ZNC4
A	473	HIS	-	expression tag	UNP Q8ZNC4
A	474	HIS	-	expression tag	UNP Q8ZNC4
A	475	HIS	-	expression tag	UNP Q8ZNC4
A	476	HIS	-	expression tag	UNP Q8ZNC4
A	477	HIS	-	expression tag	UNP Q8ZNC4
C	430	PHE	TYR	engineered mutation	UNP Q8ZNC4
C	466	LEU	-	expression tag	UNP Q8ZNC4
C	467	ALA	-	expression tag	UNP Q8ZNC4
C	468	ALA	-	expression tag	UNP Q8ZNC4
C	469	ALA	-	expression tag	UNP Q8ZNC4
C	470	LEU	-	expression tag	UNP Q8ZNC4
C	471	GLU	-	expression tag	UNP Q8ZNC4
C	472	HIS	-	expression tag	UNP Q8ZNC4
C	473	HIS	-	expression tag	UNP Q8ZNC4
C	474	HIS	-	expression tag	UNP Q8ZNC4
C	475	HIS	-	expression tag	UNP Q8ZNC4
C	476	HIS	-	expression tag	UNP Q8ZNC4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	477	HIS	-	expression tag	UNP Q8ZNC4

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



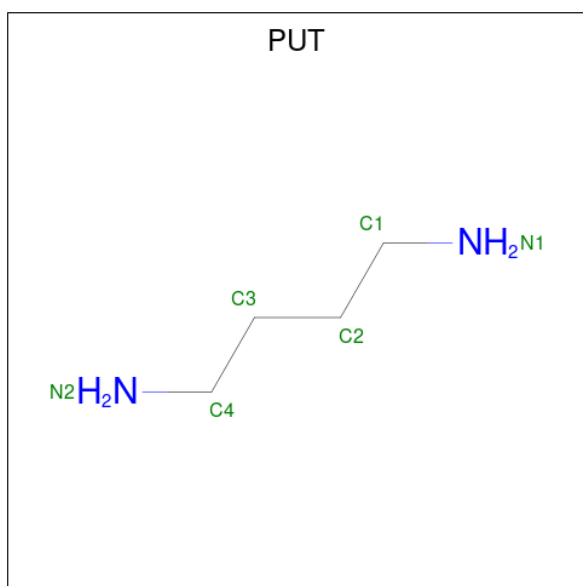
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
2	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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



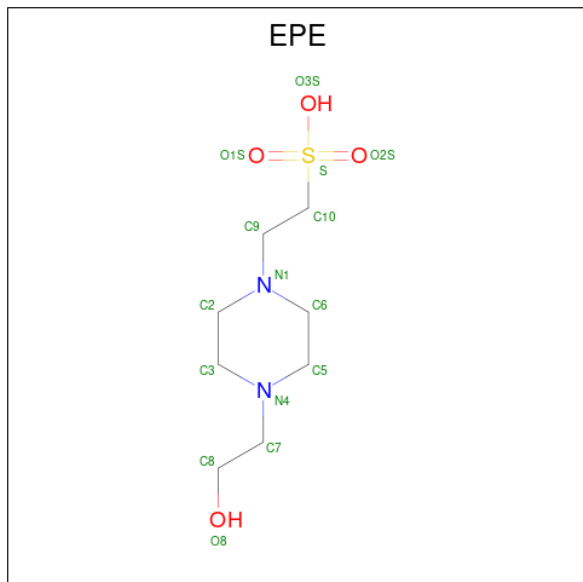
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	10	2	6	2	0	0
3	C	1	10	2	6	2	0	0

- Molecule 4 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula:  $C_4H_{12}N_2$ ) (labeled as "Ligand of Interest" by depositor).



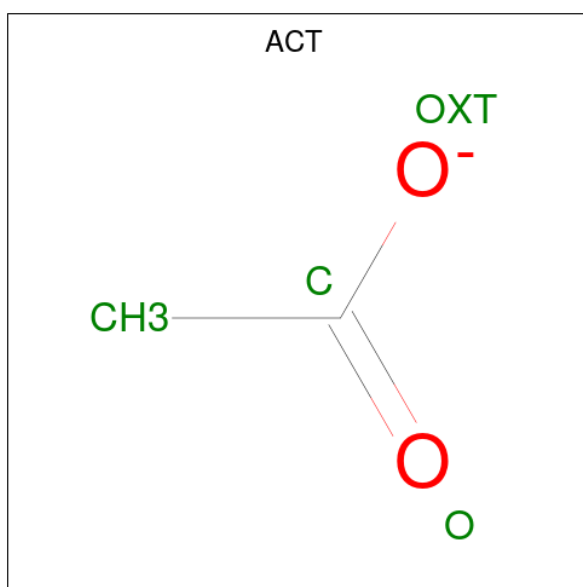
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
4	A	1	18	4	12	2	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	H	N	O			S	
5	A	1	Total	32	8	17	2	4	1	0	0
5	C	1	Total	32	8	17	2	4	1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		
7	C	1	Total	Na	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	C	1	Total	Cl	0	0
			1	1		

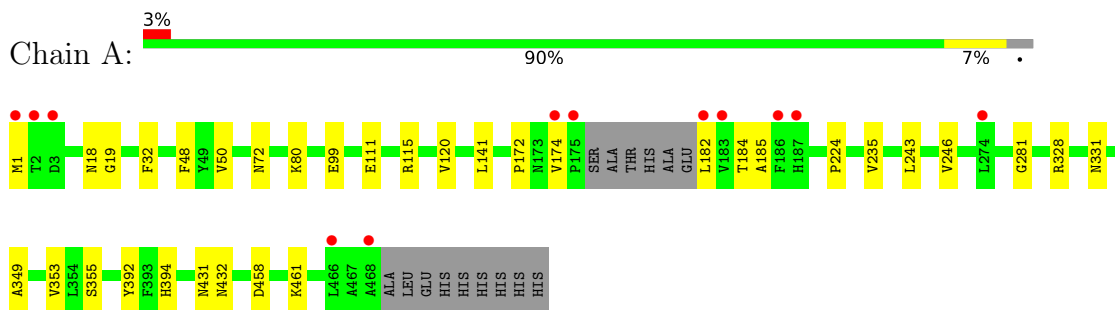
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	585	Total	O	0	68
			585	585		
9	C	621	Total	O	0	78
			621	621		

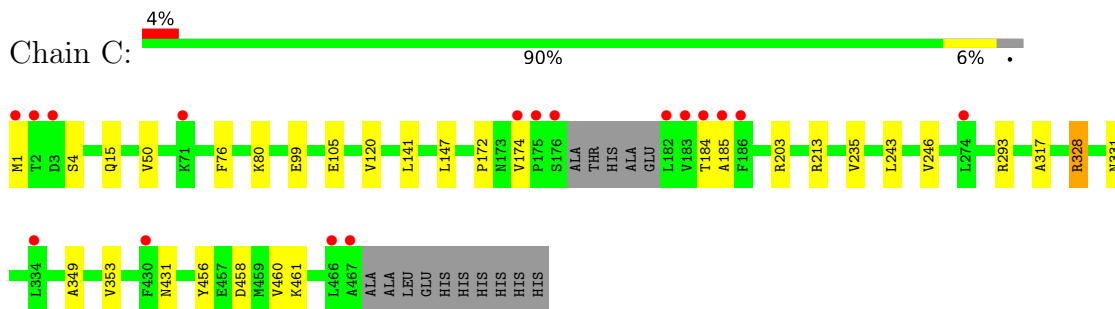
### 3 Residue-property plots [i](#)

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

- Molecule 1: D-ornithine/D-lysine decarboxylase



- Molecule 1: D-ornithine/D-lysine decarboxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.88Å 50.44Å 139.18Å 90.00° 116.93° 90.00°	Depositor
Resolution (Å)	41.36 – 1.32 41.36 – 1.32	Depositor EDS
% Data completeness (in resolution range)	96.3 (41.36-1.32) 96.3 (41.36-1.32)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 1.32Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.146 , 0.171 0.147 , 0.171	Depositor DCC
$R_{free}$ test set	2010 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtrriage
Anisotropy	0.503	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	17250	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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 78.61 % 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 6.6712e-07. 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: NA, EPE, LLP, PUT, DMS, ACT, CL, 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	0.41	0/4226	0.70	1/5711 (0.0%)
1	C	0.43	0/4252	0.71	0/5745
All	All	0.42	0/8478	0.71	1/11456 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	PHE	CB-CG-CD2	-5.33	117.07	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ARG	Sidechain
1	C	328[A]	ARG	Sidechain
1	C	328[B]	ARG	Sidechain

## 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	3981	3932	3831	33	0
1	C	4002	3956	3865	35	0
2	A	16	24	24	0	0
2	C	8	12	12	1	0
3	A	4	6	6	0	0
3	C	4	6	6	0	0
4	A	6	12	12	0	0
5	A	15	17	17	0	0
5	C	15	17	17	0	0
6	A	4	3	3	1	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	585	0	0	7	2
9	C	621	0	0	7	2
All	All	9265	7985	7793	58	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (58) 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:C:458[B]:ASP:OD1	1:C:461[B]:LYS:NZ	1.97	0.97
1:A:461[B]:LYS:HZ1	1:C:461[B]:LYS:HE3	1.50	0.76
1:C:120[B]:VAL:HG12	1:C:141:LEU:HB2	1.79	0.64
1:A:182:LEU:HD23	1:A:182:LEU:O	1.98	0.62
1:A:461[A]:LYS:HE3	1:C:461[A]:LYS:NZ	2.17	0.58
1:C:243:LEU:HA	1:C:246[A]:VAL:HG22	1.85	0.58
1:A:18[B]:ASN:OD1	1:A:19[B]:GLY:N	2.37	0.57
1:A:461[B]:LYS:HZ1	1:C:461[B]:LYS:CE	2.19	0.55
1:C:458[A]:ASP:O	1:C:461[A]:LYS:HG2	2.07	0.54
1:A:243:LEU:HA	1:A:246[A]:VAL:HG22	1.91	0.53
1:A:458[A]:ASP:OD1	1:A:461[A]:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ALA:HB1	1:A:353[A]:VAL:CG2	2.38	0.53
1:A:458[A]:ASP:O	1:A:461[A]:LYS:HE2	2.09	0.53
1:C:349:ALA:HB1	1:C:353[A]:VAL:CG2	2.39	0.52
6:A:507:ACT:H2	9:A:1087:HOH:O	2.10	0.51
1:C:184:THR:HG23	9:C:779:HOH:O	2.12	0.50
1:A:120[A]:VAL:HG12	1:A:141:LEU:HB2	1.94	0.50
1:A:172:PRO:HB3	1:A:235:VAL:HG11	1.93	0.49
1:A:1:MET:HG3	9:A:1087:HOH:O	2.13	0.48
1:A:172:PRO:HB2	1:A:174:VAL:HG23	1.96	0.47
1:C:1:MET:HG2	1:C:4:SER:H	1.79	0.47
1:A:392[B]:TYR:CZ	1:A:394:HIS:NE2	2.83	0.47
1:C:147:LEU:HD22	1:C:203[B]:ARG:HH21	1.79	0.47
1:C:458[A]:ASP:O	1:C:461[A]:LYS:HE2	2.14	0.47
1:C:76:PHE:CE2	1:C:120[A]:VAL:HG23	2.50	0.46
1:A:458[A]:ASP:HA	1:A:461[A]:LYS:CE	2.45	0.46
1:C:172:PRO:HB2	1:C:174:VAL:HG23	1.96	0.46
1:C:293[A]:ARG:NH2	9:C:615:HOH:O	2.47	0.46
1:A:461[A]:LYS:HZ1	1:C:461[A]:LYS:HE3	1.81	0.46
1:A:184:THR:HG23	9:A:787:HOH:O	2.16	0.45
1:A:461[B]:LYS:HE3	1:C:461[B]:LYS:NZ	2.31	0.45
1:C:99:GLU:HG2	1:C:120[B]:VAL:HG23	1.98	0.45
1:A:331:ASN:ND2	1:C:185[A]:ALA:HB3	2.31	0.45
1:A:331:ASN:ND2	1:C:185[B]:ALA:HB3	2.31	0.45
2:C:502:DMS:C2	9:C:1074[B]:HOH:O	2.65	0.44
1:A:461[A]:LYS:HE3	1:C:461[A]:LYS:HZ2	1.82	0.44
1:A:72[B]:ASN:ND2	9:A:607:HOH:O	2.37	0.44
1:C:293[B]:ARG:NE	9:C:626:HOH:O	2.51	0.43
1:C:141:LEU:HD21	1:C:213[B]:ARG:HD2	2.00	0.43
1:C:458[B]:ASP:HA	1:C:461[B]:LYS:HE2	2.01	0.43
1:A:355[B]:SER:HB3	9:A:873[B]:HOH:O	2.19	0.42
1:A:461[A]:LYS:NZ	1:C:461[A]:LYS:HE3	2.33	0.42
1:C:328[A]:ARG:CZ	1:C:328[A]:ARG:HB2	2.49	0.42
1:A:224:PRO:O	1:A:281:GLY:HA3	2.20	0.41
1:A:111[B]:GLU:HG3	9:A:1048:HOH:O	2.21	0.41
1:A:432[A]:ASN:HD22	1:C:105:GLU:HG3	1.85	0.41
1:A:432[B]:ASN:HB2	1:C:105:GLU:HG3	2.02	0.41
1:C:456:TYR:CZ	1:C:460[A]:VAL:HG11	2.54	0.41
1:C:15[A]:GLN:HG2	9:C:714:HOH:O	2.19	0.41
1:A:461[A]:LYS:HE3	1:C:461[A]:LYS:HZ1	1.83	0.41
1:C:293[A]:ARG:CZ	9:C:615:HOH:O	2.69	0.41
1:A:48:PHE:CE2	1:A:50[B]:VAL:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:PRO:HB3	1:C:235:VAL:HG11	2.03	0.41
1:A:115:ARG:NH1	9:A:631:HOH:O	2.54	0.40
1:A:185:ALA:HB3	1:C:331:ASN:OD1	2.20	0.40
1:A:99:GLU:HG2	1:A:120[A]:VAL:HG23	2.03	0.40
1:C:50[B]:VAL:O	1:C:317:ALA:HA	2.22	0.40

All (2) 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)
9:A:1144:HOH:O	9:C:1146:HOH:O[4_546]	2.03	0.17
9:A:1083:HOH:O	9:C:1037:HOH:O[3_545]	2.10	0.10

## 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	513/477 (108%)	503 (98%)	10 (2%)	0	100	100
1	C	516/477 (108%)	504 (98%)	12 (2%)	0	100	100
All	All	1029/954 (108%)	1007 (98%)	22 (2%)	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	447/405 (110%)	446 (100%)	1 (0%)	93	79
1	C	450/405 (111%)	449 (100%)	1 (0%)	93	79
All	All	897/810 (111%)	895 (100%)	2 (0%)	92	79

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	ASN
1	C	431	ASN

Sometimes 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](#)

2 non-standard protein/DNA/RNA residues 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
1	LLP	A	80	1	23,24,25	2.20	5 (21%)	25,32,34	1.31	3 (12%)
1	LLP	C	80	1	23,24,25	2.35	7 (30%)	25,32,34	1.30	4 (16%)

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
1	LLP	A	80	1	-	3/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	C	80	1	-	2/16/17/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	LLP	C4-C4'	6.98	1.59	1.46
1	A	80	LLP	C4-C4'	6.60	1.59	1.46
1	A	80	LLP	C4'-NZ	4.59	1.42	1.27
1	C	80	LLP	C4-C5	-4.52	1.36	1.42
1	C	80	LLP	C4'-NZ	4.50	1.42	1.27
1	A	80	LLP	C4-C5	-4.18	1.36	1.42
1	C	80	LLP	C2'-C2	2.78	1.55	1.50
1	A	80	LLP	C2'-C2	2.75	1.55	1.50
1	A	80	LLP	C6-N1	2.25	1.39	1.34
1	C	80	LLP	C5'-C5	2.22	1.56	1.50
1	C	80	LLP	C3-C2	-2.10	1.38	1.40
1	C	80	LLP	C6-N1	2.10	1.38	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	LLP	C4-C4'-NZ	-2.89	111.05	124.31
1	C	80	LLP	C5-C6-N1	-2.64	119.41	123.82
1	C	80	LLP	C4-C4'-NZ	-2.59	112.41	124.31
1	A	80	LLP	CE-NZ-C4'	-2.50	111.21	118.90
1	C	80	LLP	CE-NZ-C4'	-2.37	111.63	118.90
1	A	80	LLP	C5-C6-N1	-2.34	119.92	123.82
1	C	80	LLP	C3-C4-C5	2.23	119.97	118.26

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	80	LLP	C4-C4'-NZ-CE
1	C	80	LLP	C4-C4'-NZ-CE
1	C	80	LLP	CG-CD-CE-NZ
1	A	80	LLP	CG-CD-CE-NZ
1	A	80	LLP	C3-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DMS	A	503	-	3,3,3	0.65	0	3,3,3	0.39	0
2	DMS	C	502	-	3,3,3	0.60	0	3,3,3	0.32	0
2	DMS	A	506	-	3,3,3	0.65	0	3,3,3	0.66	0
6	ACT	A	507	-	3,3,3	1.29	0	3,3,3	1.54	0
3	EDO	C	501	-	3,3,3	0.36	0	2,2,2	0.61	0
2	DMS	A	501	-	3,3,3	0.63	0	3,3,3	0.13	0
4	PUT	A	504	-	5,5,5	0.11	0	4,4,4	0.30	0
2	DMS	C	504	-	3,3,3	0.62	0	3,3,3	0.55	0
2	DMS	A	508	-	3,3,3	0.62	0	3,3,3	0.26	0
5	EPE	A	505	-	15,15,15	0.76	1 (6%)	18,20,20	1.73	3 (16%)
3	EDO	A	502	-	3,3,3	0.47	0	2,2,2	0.44	0
5	EPE	C	503	-	15,15,15	0.77	1 (6%)	18,20,20	2.02	5 (27%)

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	C	501	-	-	0/1/1/1	-
4	PUT	A	504	-	-	0/3/3/3	-
5	EPE	A	505	-	-	4/9/19/19	0/1/1/1
3	EDO	A	502	-	-	1/1/1/1	-
5	EPE	C	503	-	-	6/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	EPE	C10-S	2.66	1.81	1.77
5	A	505	EPE	C10-S	2.49	1.81	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	503	EPE	C5-N4-C3	4.58	119.13	108.83
5	A	505	EPE	O3S-S-C10	3.48	111.39	105.77
5	A	505	EPE	C5-N4-C3	3.39	116.47	108.83
5	A	505	EPE	C7-N4-C3	3.29	119.66	111.23
5	C	503	EPE	O2S-S-C10	3.26	110.84	106.92
5	C	503	EPE	C7-N4-C5	2.59	117.86	111.23
5	C	503	EPE	O3S-S-C10	2.40	109.65	105.77
5	C	503	EPE	C7-N4-C3	2.21	116.90	111.23

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	EPE	C8-C7-N4-C3
5	C	503	EPE	C9-C10-S-O2S
5	C	503	EPE	C9-C10-S-O3S
5	C	503	EPE	C8-C7-N4-C5
5	C	503	EPE	C9-C10-S-O1S
5	A	505	EPE	C10-C9-N1-C6
5	C	503	EPE	C10-C9-N1-C6
5	A	505	EPE	C8-C7-N4-C5
3	A	502	EDO	O1-C1-C2-O2
5	C	503	EPE	C8-C7-N4-C3
5	A	505	EPE	C10-C9-N1-C2

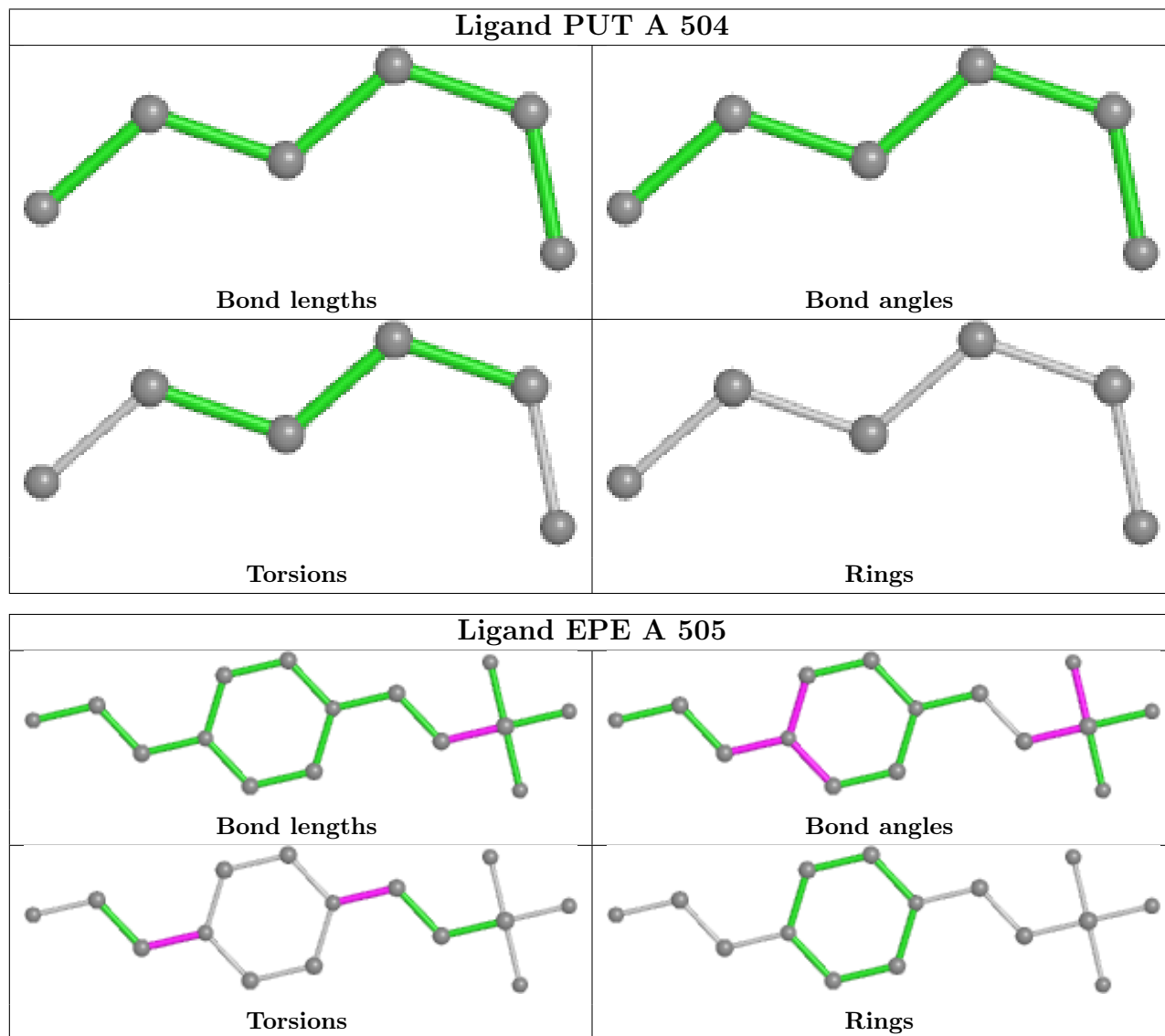
There are no ring outliers.

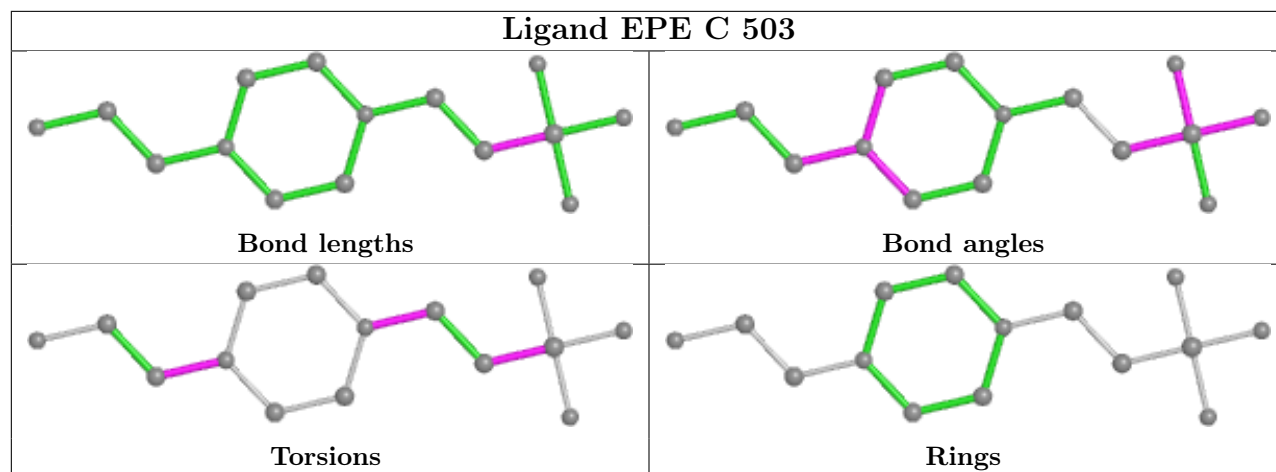
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	DMS	1	0
6	A	507	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	461/477 (96%)	-0.13	12 (2%) 56 57	12, 19, 39, 100	0
1	C	461/477 (96%)	-0.13	17 (3%) 41 42	11, 17, 41, 90	0
All	All	922/954 (96%)	-0.13	29 (3%) 49 49	11, 18, 40, 100	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	LEU	10.5
1	A	1	MET	9.9
1	A	182	LEU	8.9
1	C	176	SER	8.9
1	A	175	PRO	8.5
1	C	2	THR	8.1
1	A	2	THR	7.9
1	C	186	PHE	7.7
1	C	466	LEU	7.2
1	C	175	PRO	6.9
1	C	1	MET	6.8
1	A	468	ALA	5.8
1	C	467	ALA	5.6
1	C	183	VAL	5.5
1	C	334	LEU	4.8
1	A	186	PHE	4.8
1	A	183	VAL	3.9
1	A	174	VAL	3.6
1	C	184	THR	3.5
1	C	185[A]	ALA	3.3
1	A	466	LEU	3.1
1	A	274	LEU	2.8
1	A	3	ASP	2.5
1	C	3	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	71	LYS	2.5
1	C	174	VAL	2.4
1	C	430	PHE	2.1
1	C	274	LEU	2.0
1	A	187	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	80	24/25	0.98	0.09	12,16,25,30	0
1	LLP	C	80	24/25	0.99	0.10	10,15,25,30	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.

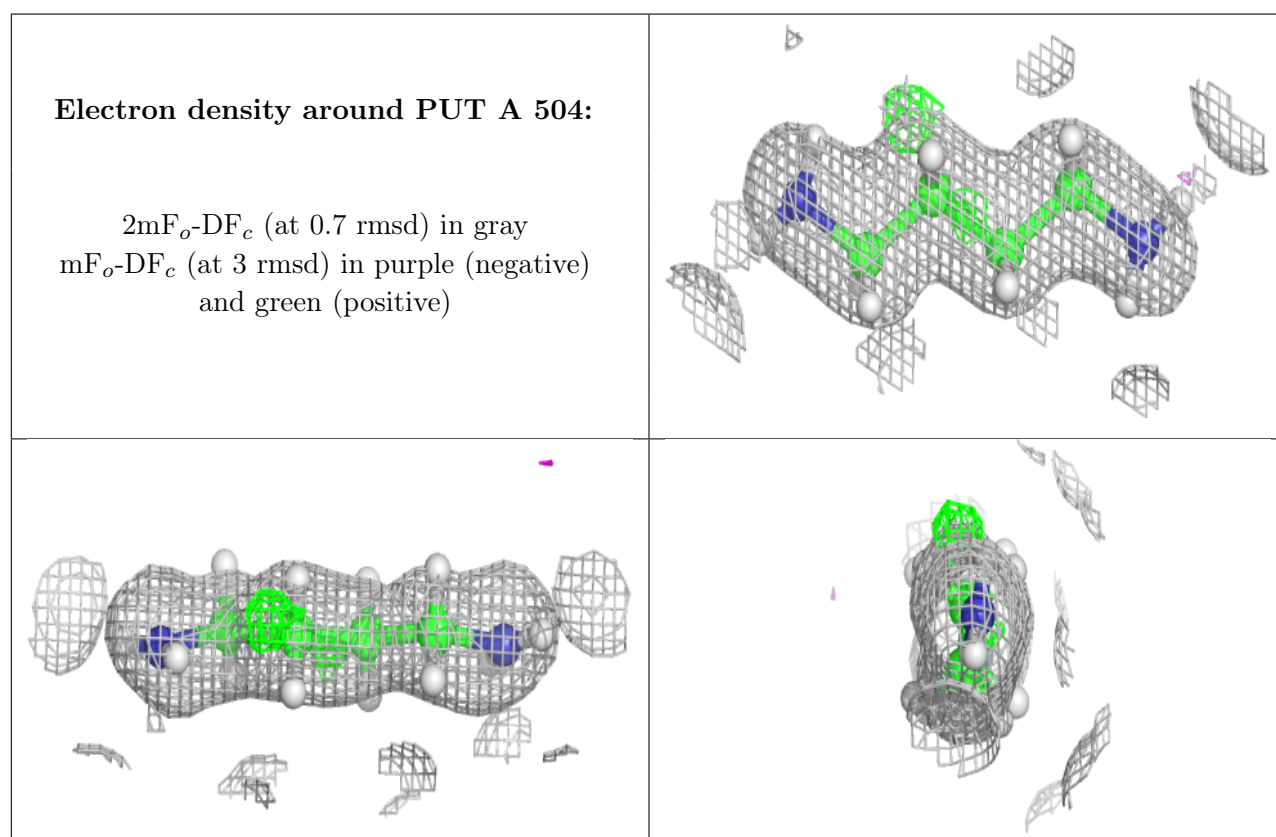
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	DMS	A	506	4/4	0.75	0.25	35,42,51,105	0
6	ACT	A	507	4/4	0.78	0.30	57,67,69,73	0
4	PUT	A	504	6/6	0.91	0.08	23,30,33,33	0
2	DMS	C	502	4/4	0.91	0.11	42,51,56,72	0
2	DMS	A	503	4/4	0.92	0.11	40,53,66,69	0
5	EPE	C	503	15/15	0.94	0.13	27,39,63,65	0
3	EDO	A	502	4/4	0.95	0.08	22,43,53,55	0
5	EPE	A	505	15/15	0.95	0.11	27,35,54,68	0
3	EDO	C	501	4/4	0.96	0.09	18,39,47,47	0
2	DMS	A	501	4/4	0.97	0.10	18,22,32,32	10
2	DMS	C	504	4/4	0.97	0.17	20,40,58,58	10

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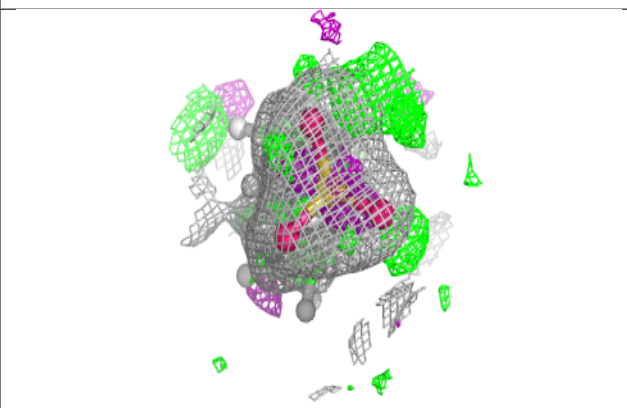
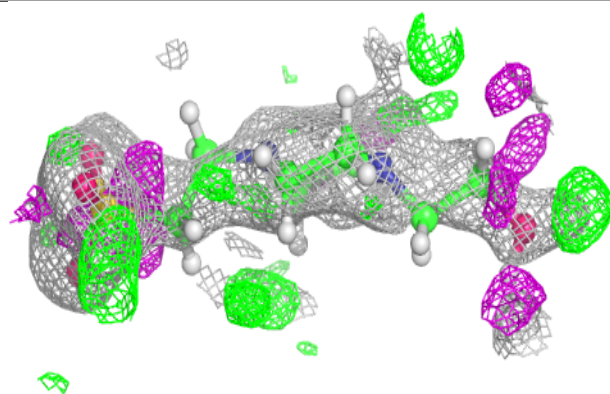
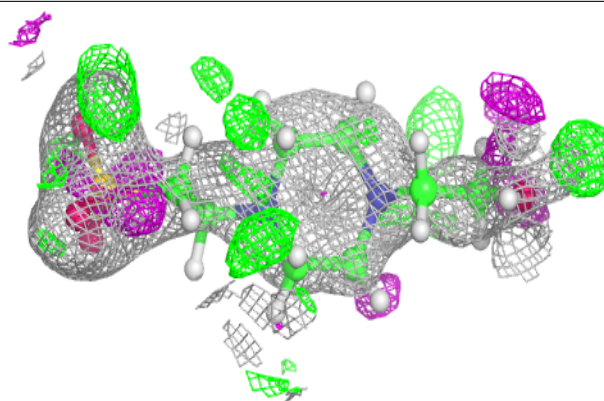
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CL	A	510	1/1	0.97	0.04	27,27,27,27	0
7	NA	C	505	1/1	0.98	0.05	18,18,18,18	0
7	NA	A	509	1/1	0.98	0.04	19,19,19,19	0
8	CL	C	506	1/1	0.98	0.04	24,24,24,24	0
2	DMS	A	508	4/4	0.99	0.11	20,26,30,30	10

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.

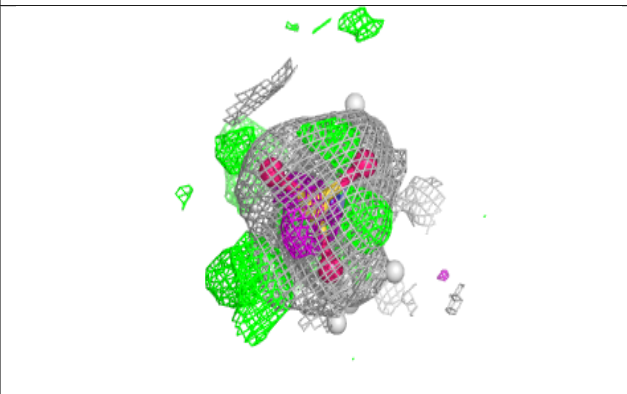
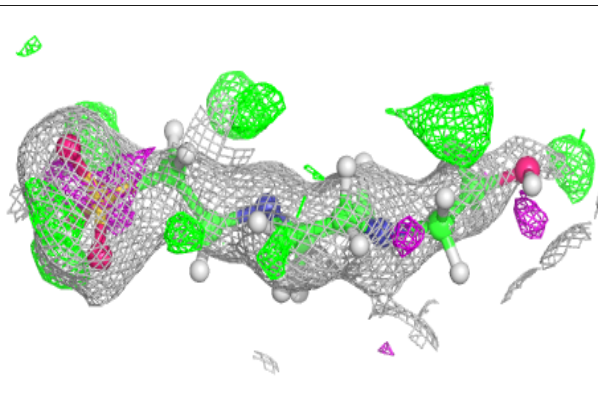
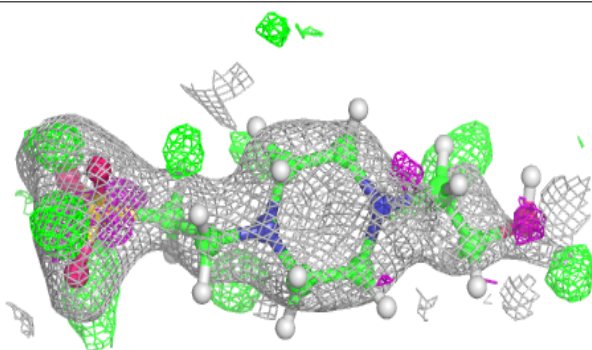


**Electron density around EPE C 503:**

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

**Electron density around EPE A 505:**

$2mF_o-DF_c$  (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.