



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2026 – 03:19 AM UTC

PDB ID : 9NQ5 / pdb\_00009nq5  
Title : D-Ornithine/D-lysine decarboxylase C387A complexed with HEPES, putrescine, and D-ornithine  
Authors : Phillips, R.S.; Blankenship, S.  
Deposited on : 2025-03-11  
Resolution : 1.74 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

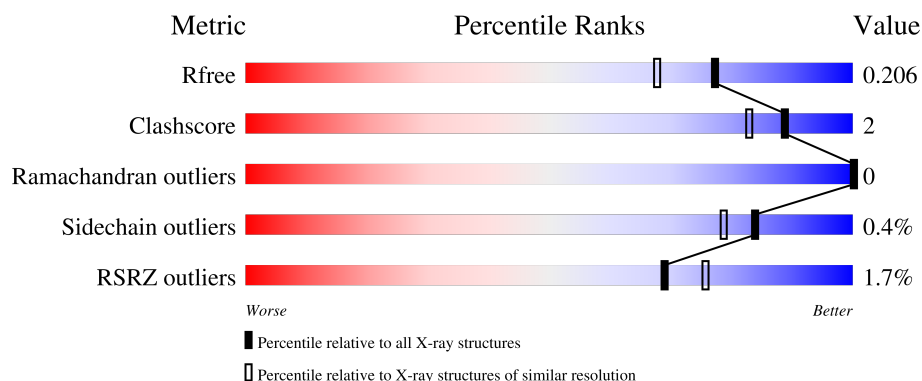
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

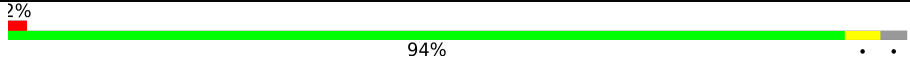
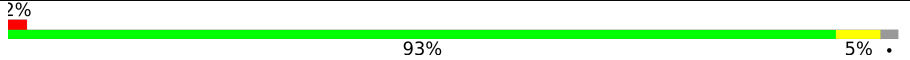
The reported resolution of this entry is 1.74 Å.

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))
$R_{free}$	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	478	
2	B	478	

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 16678 atoms, of which 7906 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
1	A	466	Total	C	H	N	O	P	S	0	43	0
			7818	2493	3882	672	747	1	23			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ALA	CYS	engineered mutation	UNP Q8ZNC4
A	466	LEU	-	expression tag	UNP Q8ZNC4
A	467	LEU	-	expression tag	UNP Q8ZNC4
A	468	ALA	-	expression tag	UNP Q8ZNC4
A	469	ALA	-	expression tag	UNP Q8ZNC4
A	470	ALA	-	expression tag	UNP Q8ZNC4
A	471	LEU	-	expression tag	UNP Q8ZNC4
A	472	GLU	-	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
A	478	HIS	-	expression tag	UNP Q8ZNC4

- Molecule 2 is a protein called D-ornithine/D-lysine decarboxylase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	469	Total	C	H	N	O	S		0	37	0
			7794	2479	3877	678	739	21				

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	387	ALA	CYS	engineered mutation	UNP Q8ZNC4
B	466	LEU	-	expression tag	UNP Q8ZNC4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	467	LEU	-	expression tag	UNP Q8ZNC4
B	468	ALA	-	expression tag	UNP Q8ZNC4
B	469	ALA	-	expression tag	UNP Q8ZNC4
B	470	ALA	-	expression tag	UNP Q8ZNC4
B	471	LEU	-	expression tag	UNP Q8ZNC4
B	472	GLU	-	expression tag	UNP Q8ZNC4
B	473	HIS	-	expression tag	UNP Q8ZNC4
B	474	HIS	-	expression tag	UNP Q8ZNC4
B	475	HIS	-	expression tag	UNP Q8ZNC4
B	476	HIS	-	expression tag	UNP Q8ZNC4
B	477	HIS	-	expression tag	UNP Q8ZNC4
B	478	HIS	-	expression tag	UNP Q8ZNC4

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

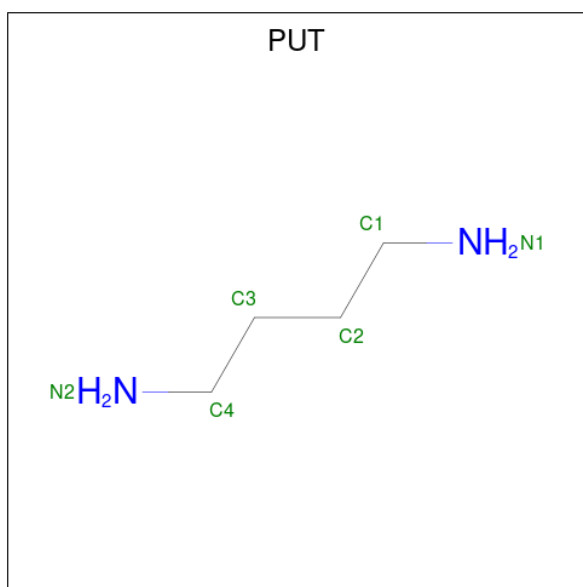
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	3	Total Cl 3 3	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



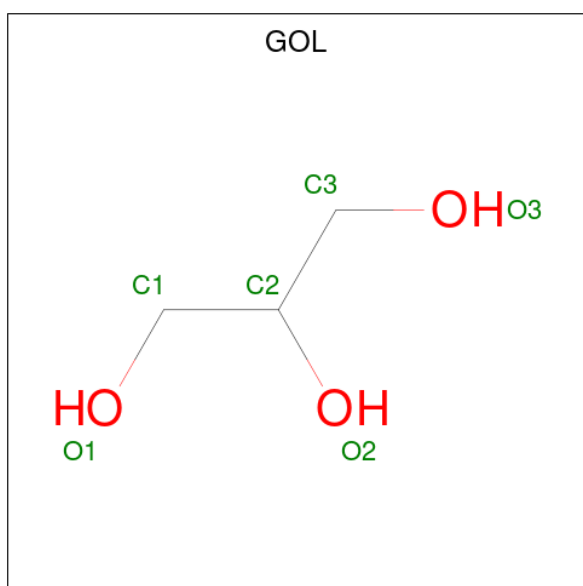
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 6 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula:  $C_4H_{12}N_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	N	0	0
			18	4	12	2		
6	B	1	Total	C	H	N	0	1
			36	8	24	4		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



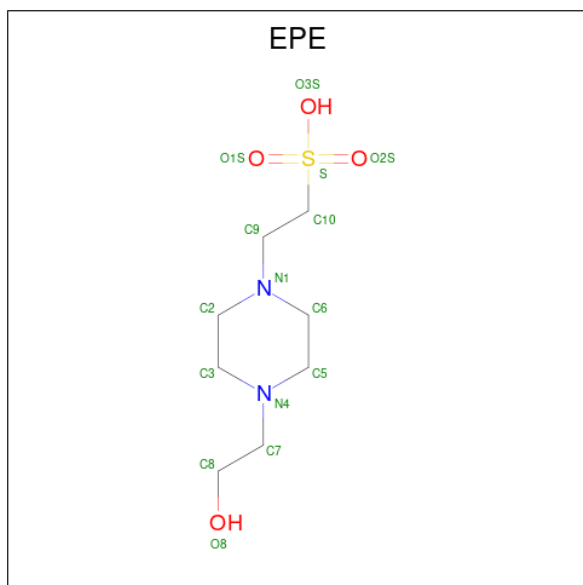
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	1
			14	3	8	3		

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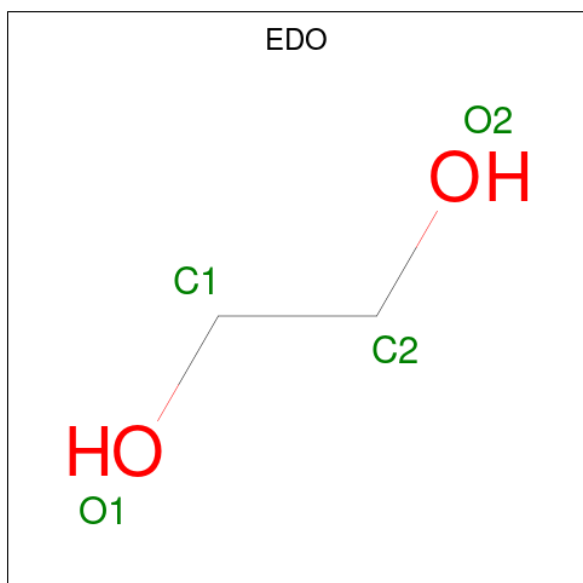
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



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

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).

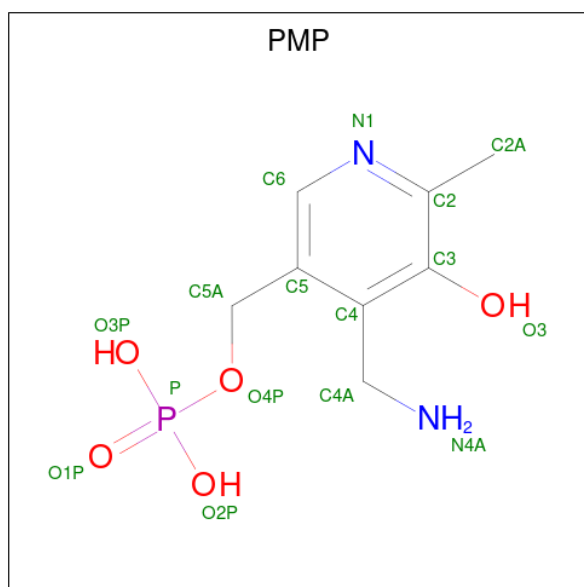


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Na	0	0
			1	1		
10	B	1	Total	Na	0	0
			1	1		

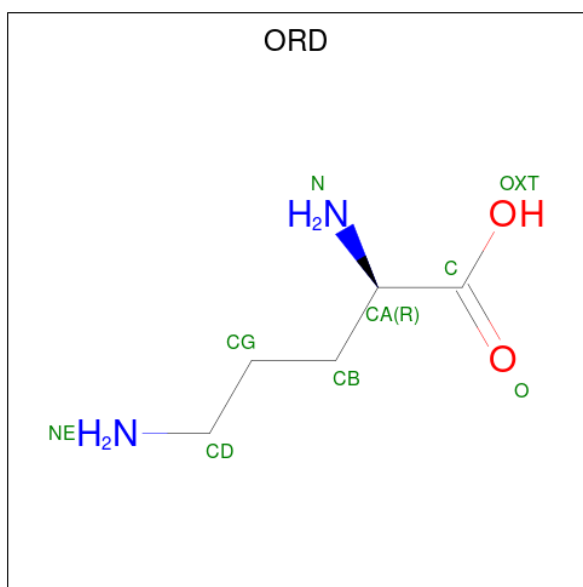
- Molecule 11 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>2</sub>O<sub>5</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	P	0	0
			27	8	11	2	5	1		

- Molecule 12 is D-ORNITHINE (CCD ID: ORD) (formula: C<sub>5</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





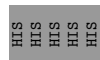
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	0	0
			20	5	11	2	2		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	400	Total	O	0	6
			400	400		
13	B	403	Total	O	0	4
			403	403		

**i**

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.99Å 104.77Å 106.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.67 – 1.74 68.67 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (68.67-1.74) 99.8 (68.67-1.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.179 , 0.207 0.181 , 0.206	Depositor DCC
$R_{free}$ test set	2003 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, EPE, CL, K, ORD, PUT, DMS, NA, LLP, GOL, PMP

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	0.47	0/4123	0.49	0/5578
2	B	0.48	0/4105	0.48	0/5552
All	All	0.48	0/8228	0.48	0/11130

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

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	3936	3882	3778	14	0
2	B	3917	3877	3806	20	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
5	A	8	12	12	0	0
5	B	16	24	24	2	0
6	A	6	12	12	0	0
6	B	12	24	24	1	0
7	A	6	8	8	0	0
7	B	12	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	15	17	18	0	0
9	A	4	6	6	0	0
9	B	4	6	6	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	B	16	11	11	0	0
12	B	9	11	11	0	0
13	A	400	0	0	1	0
13	B	403	0	0	2	0
All	All	8772	7906	7732	30	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.

The worst 5 of 30 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)
2:B:429:VAL:HB	2:B:459[B]:MET:HE1	1.68	0.75
5:B:501:DMS:H12	13:B:965:HOH:O	2.09	0.51
1:A:76:PHE:CE1	1:A:120:VAL:HG23	2.47	0.50
1:A:349:ALA:HB1	1:A:353[B]:VAL:HG21	1.95	0.49
2:B:253:LEU:HD12	2:B:253:LEU:C	2.38	0.49

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	506/478 (106%)	493 (97%)	13 (3%)	0	100	100
2	B	504/478 (105%)	490 (97%)	14 (3%)	0	100	100
All	All	1010/956 (106%)	983 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	437/405 (108%)	437 (100%)	0	100	100
2	B	431/406 (106%)	427 (99%)	4 (1%)	70	59
All	All	868/811 (107%)	864 (100%)	4 (0%)	84	75

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

Mol	Chain	Res	Type
2	B	80[A]	LYS
2	B	80[B]	LYS
2	B	101	ASN
2	B	431	ASN

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

Mol	Chain	Res	Type
1	A	359	HIS
2	B	152	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	1.15	1 (4%)	25,32,34	1.05	1 (4%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	LLP	P-OP4	4.23	1.73	1.60

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	LLP	OP3-P-OP2	2.01	115.36	107.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	80	LLP	C3-C4-C4'-NZ
1	A	80	LLP	C5-C4-C4'-NZ
1	A	80	LLP	CD-CE-NZ-C4'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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
7	GOL	A	505	-	5,5,5	0.28	0	5,5,5	0.47	0
6	PUT	B	508[A]	-	5,5,5	0.92	0	4,4,4	0.23	0
9	EDO	A	508	-	3,3,3	0.23	0	2,2,2	0.43	0
9	EDO	B	502	-	3,3,3	0.29	0	2,2,2	0.34	0
5	DMS	B	509	-	3,3,3	0.72	0	3,3,3	0.28	0
5	DMS	A	503	-	3,3,3	0.67	0	3,3,3	0.25	0
7	GOL	B	514	-	5,5,5	0.19	0	5,5,5	0.59	0
5	DMS	A	510	-	3,3,3	0.63	0	3,3,3	0.16	0
5	DMS	B	505	-	3,3,3	0.68	0	3,3,3	0.20	0
6	PUT	A	504	-	5,5,5	0.91	0	4,4,4	0.40	0
12	ORD	B	507	-	7,8,8	1.05	0	6,9,9	0.68	0
5	DMS	B	510	-	3,3,3	0.70	0	3,3,3	0.09	0
11	PMP	B	506	-	16,16,16	1.40	3 (18%)	22,23,23	1.11	2 (9%)
6	PUT	B	508[B]	-	5,5,5	0.91	0	4,4,4	0.27	0
5	DMS	B	501	-	3,3,3	0.67	0	3,3,3	0.36	0
8	EPE	A	507	-	15,15,15	0.80	1 (6%)	19,20,20	0.77	1 (5%)
7	GOL	B	513[A]	-	5,5,5	0.31	0	5,5,5	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	505	-	-	0/4/4/4	-
6	PUT	B	508[A]	-	-	1/3/3/3	-
9	EDO	A	508	-	-	1/1/1/1	-
9	EDO	B	502	-	-	0/1/1/1	-
7	GOL	B	514	-	-	2/4/4/4	-
6	PUT	A	504	-	-	0/3/3/3	-
11	PMP	B	506	-	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PUT	B	508[B]	-	-	1/3/3/3	-
12	ORD	B	507	-	-	1/8/8/8	-
8	EPE	A	507	-	-	2/9/19/19	0/1/1/1
7	GOL	B	513[A]	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	506	PMP	P-O4P	2.79	1.69	1.60
11	B	506	PMP	C6-N1	2.47	1.39	1.34
11	B	506	PMP	C2-N1	2.14	1.37	1.33
8	A	507	EPE	C10-S	2.08	1.80	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	506	PMP	C6-C5-C4	3.26	120.53	118.06
11	B	506	PMP	C5-C6-N1	-2.29	120.11	123.83
8	A	507	EPE	O2S-S-C10	-2.19	103.42	106.73

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	513[A]	GOL	C1-C2-C3-O3
7	B	514	GOL	C1-C2-C3-O3
7	B	513[A]	GOL	O1-C1-C2-C3
7	B	514	GOL	O2-C2-C3-O3
8	A	507	EPE	C10-C9-N1-C2

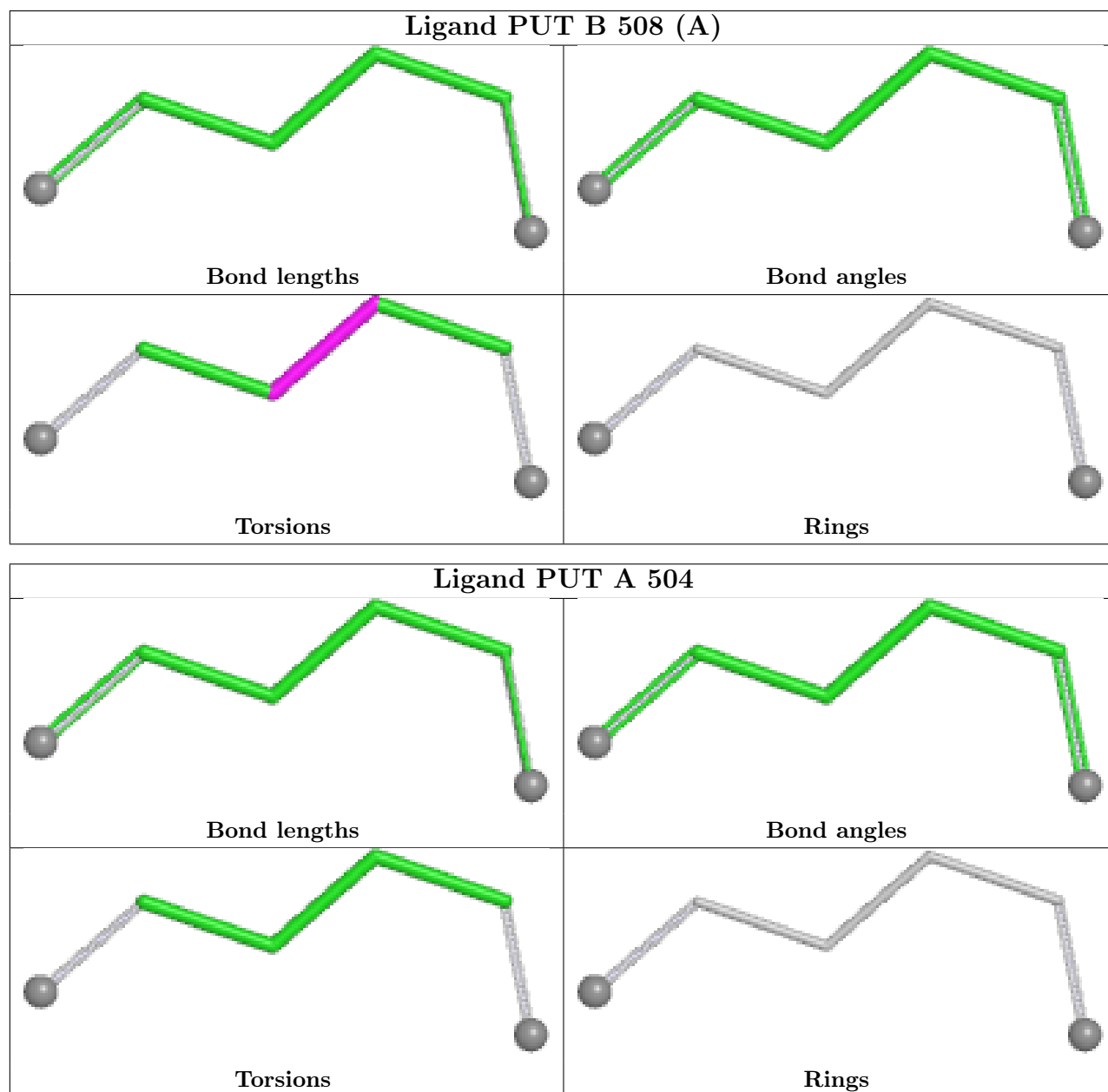
There are no ring outliers.

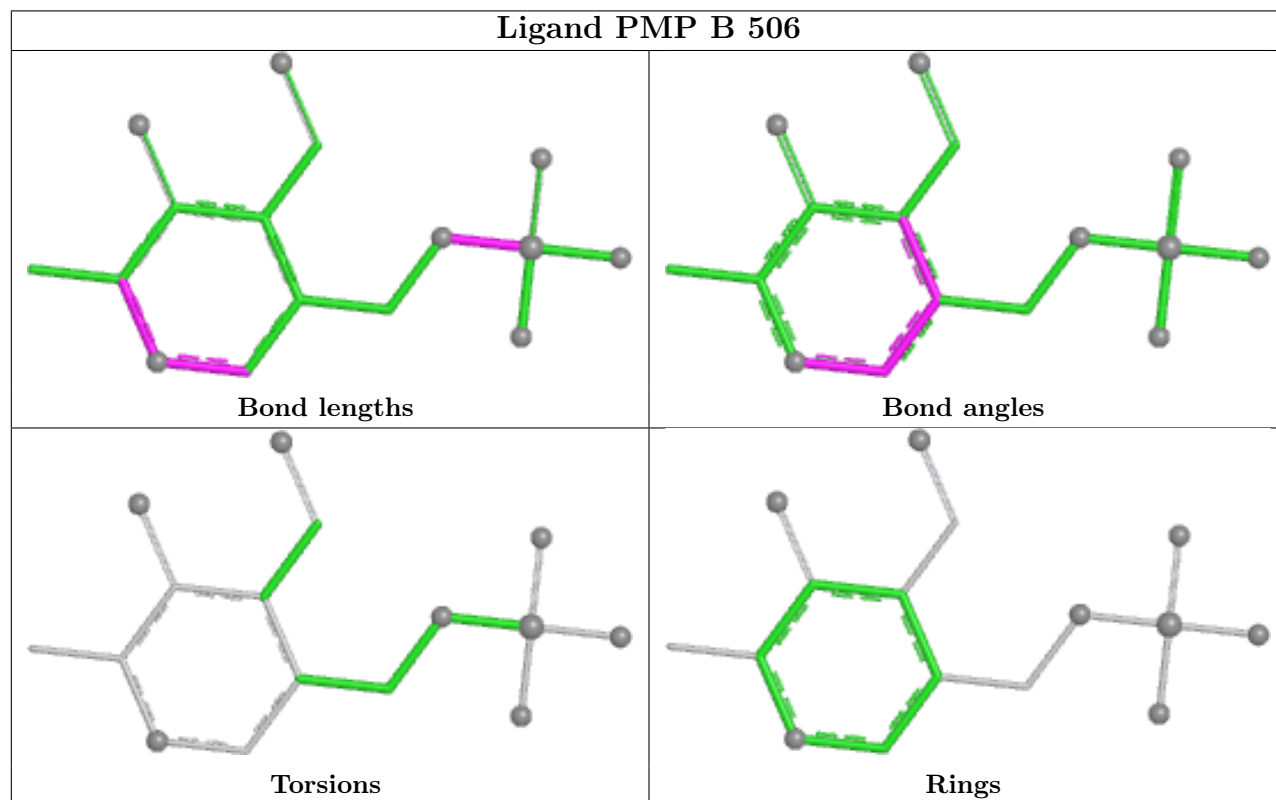
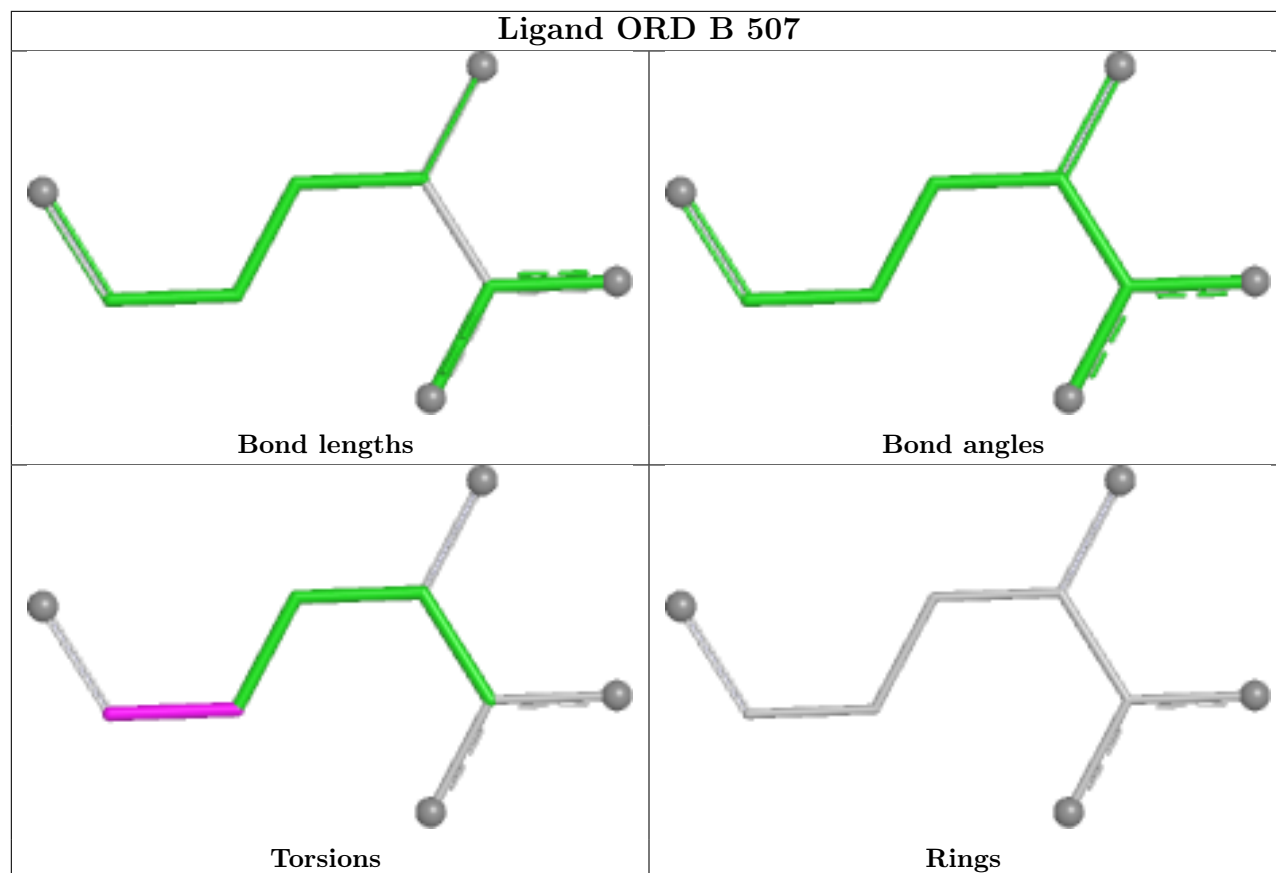
3 monomers are involved in 3 short contacts:

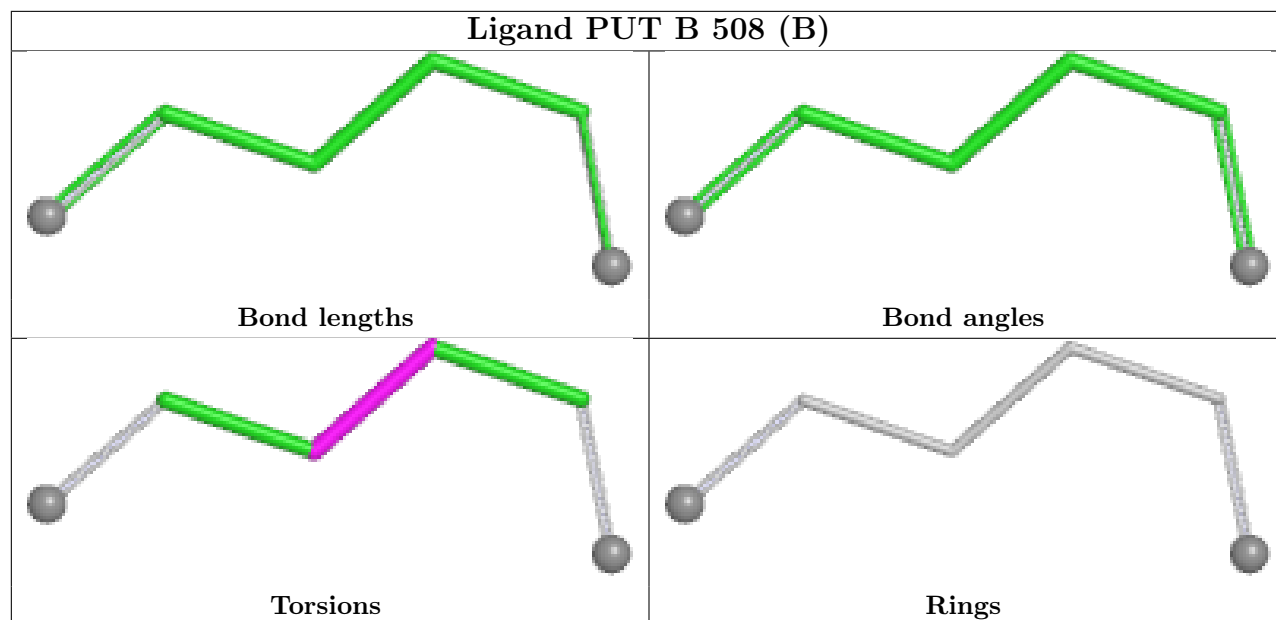
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	508[A]	PUT	1	0
5	B	509	DMS	1	0
5	B	501	DMS	1	0

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	465/478 (97%)	0.00	8 (1%) 69 76	12, 42, 82, 180	32 (6%)
2	B	469/478 (98%)	0.12	8 (1%) 69 76	20, 50, 75, 125	31 (6%)
All	All	934/956 (97%)	0.06	16 (1%) 69 76	12, 47, 78, 180	63 (6%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	LEU	3.7
2	B	467	LEU	3.4
1	A	174	VAL	3.3
2	B	469	ALA	3.2
2	B	143[A]	ASN	3.1

### 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	0.97	0.06	26,38,48,56	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

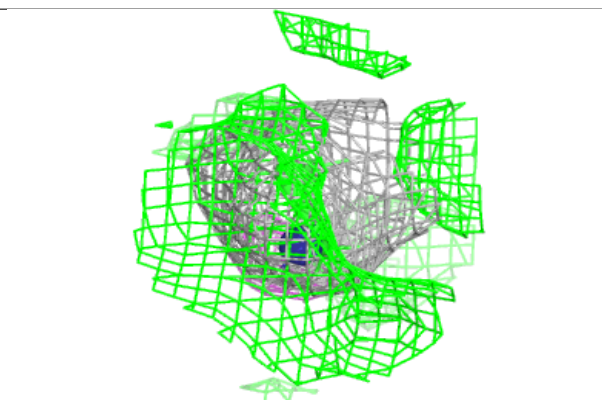
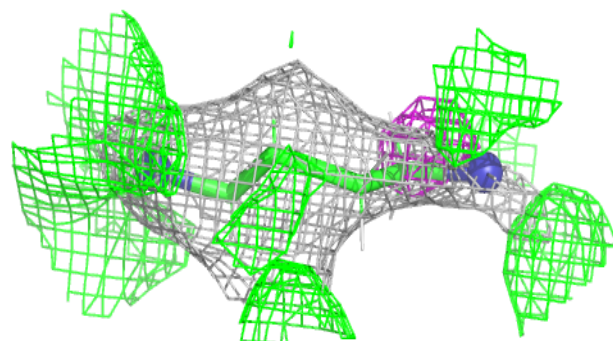
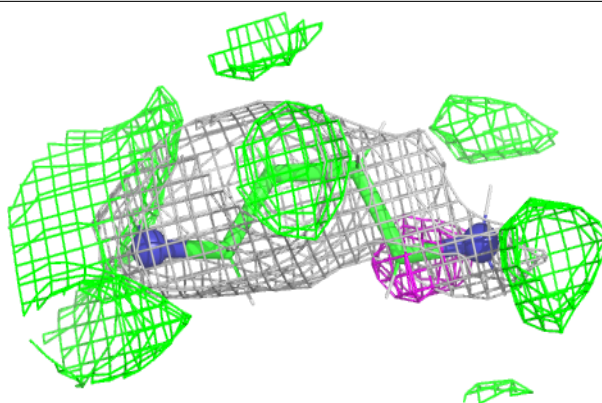
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	PUT	B	508[A]	6/6	0.71	0.25	49,62,67,67	18
6	PUT	B	508[B]	6/6	0.71	0.25	44,64,67,67	18
7	GOL	B	513[A]	6/6	0.71	0.16	72,98,113,124	0
7	GOL	B	514	6/6	0.72	0.19	47,60,71,76	0
5	DMS	A	510	4/4	0.78	0.17	68,82,91,100	0
5	DMS	B	509	4/4	0.78	0.15	47,64,77,87	0
4	CL	B	512	1/1	0.79	0.23	74,74,74,74	0
7	GOL	A	505	6/6	0.81	0.13	60,88,104,106	0
12	ORD	B	507	9/9	0.82	0.11	34,47,72,72	0
10	NA	A	509	1/1	0.83	0.11	54,54,54,54	0
5	DMS	B	501	4/4	0.83	0.15	65,78,79,91	0
8	EPE	A	507	15/15	0.86	0.13	42,58,70,81	32
4	CL	B	511	1/1	0.87	0.12	66,66,66,66	0
5	DMS	B	510	4/4	0.87	0.13	61,74,82,93	0
10	NA	B	503	1/1	0.89	0.08	53,53,53,53	1
5	DMS	B	505	4/4	0.89	0.15	74,95,109,109	0
3	K	A	501	1/1	0.91	0.09	73,73,73,73	0
9	EDO	B	502	4/4	0.92	0.11	47,66,78,79	0
4	CL	A	506	1/1	0.93	0.14	65,65,65,65	0
6	PUT	A	504	6/6	0.94	0.07	39,49,61,61	18
11	PMP	B	506	16/16	0.94	0.08	25,35,43,49	0
9	EDO	A	508	4/4	0.94	0.09	37,54,65,65	0
4	CL	A	502	1/1	0.95	0.09	42,42,42,42	1
5	DMS	A	503	4/4	0.95	0.13	53,69,100,100	0
4	CL	B	504	1/1	0.96	0.06	54,54,54,54	0

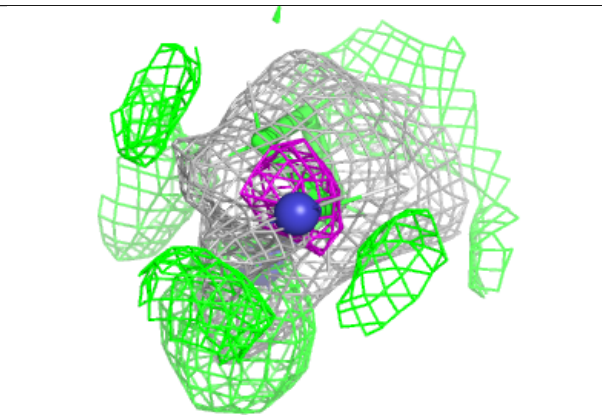
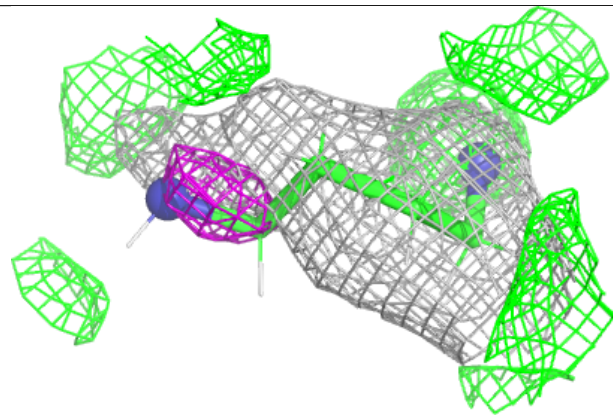
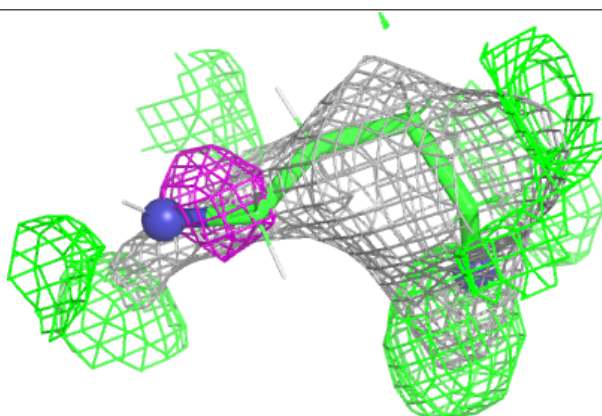
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PUT B 508 (A):**

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

**Electron density around PUT B 508 (B):**

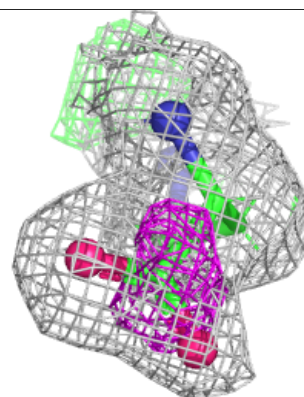
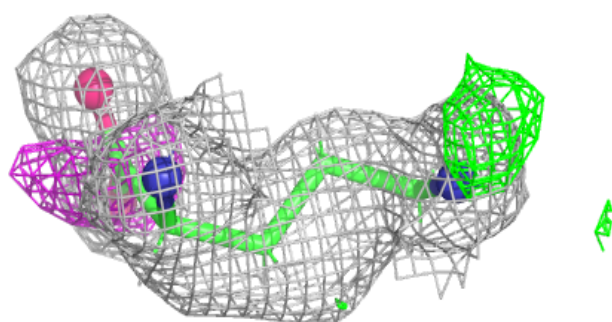
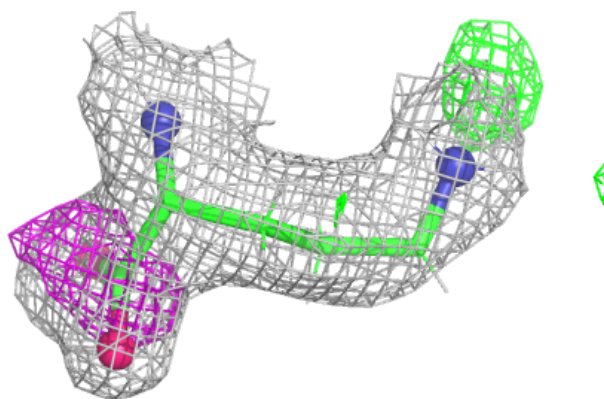
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



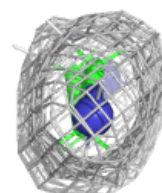
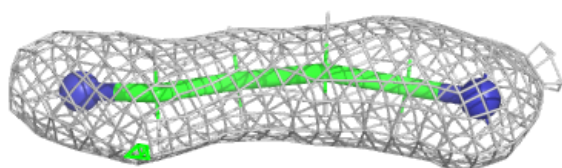
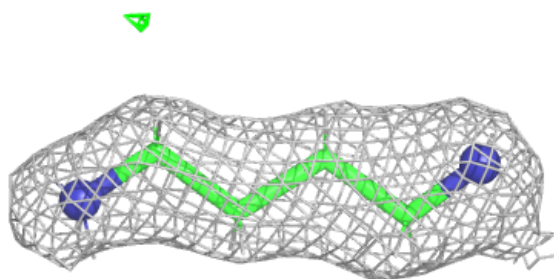


**Electron density around ORD B 507:**

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

**Electron density around PUT A 504:**

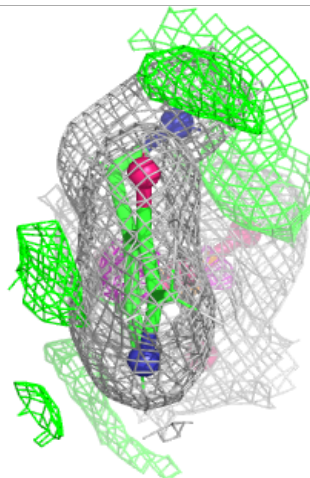
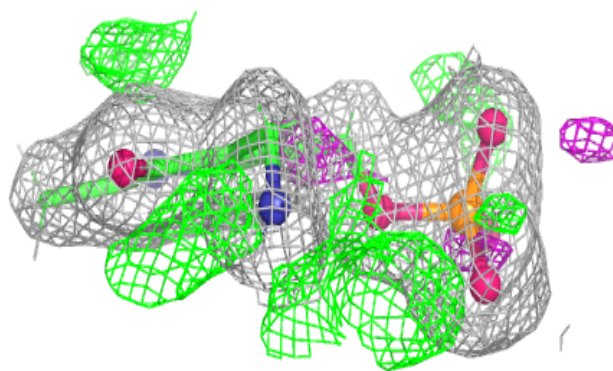
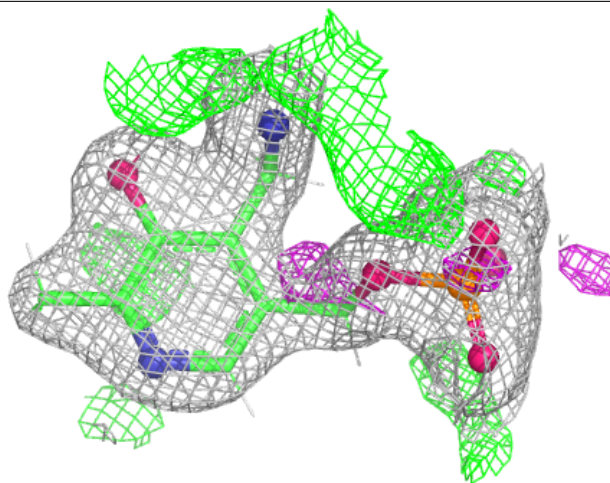
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PMP B 506:**

$2mF_o-DF_c$  (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.