



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:58 am BST

PDB ID : 6DZ3  
Title : Crystal structure of human 5'-deoxy-5'-methylthioadenosine phosphorylase in complex with (3R,4S)-1-((4-amino-5H-pyrrolo[3,2-d]pyrimidin-7-yl)methyl)-4-(((3-(1-butyl-1H-1,2,3-triazol-4-yl)propyl)thio)methyl)pyrrolidin-3-ol  
Authors : Harijan, R.K.; Ducati, R.G.; Bonanno, J.B.; Almo, S.C.; Schramm, V.L.  
Deposited on : 2018-07-02  
Resolution : 1.91 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

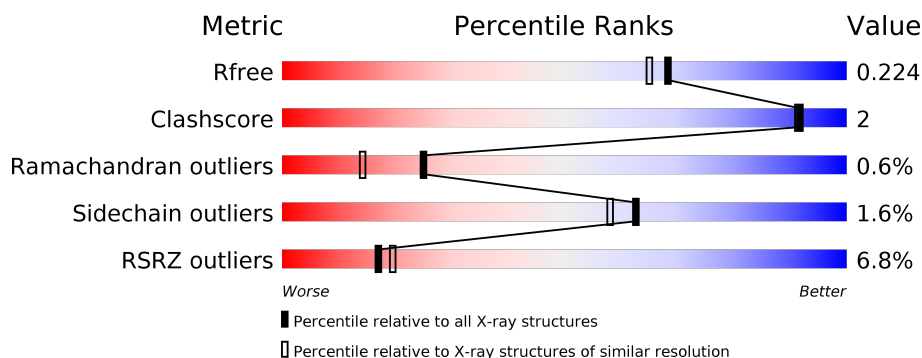
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	297	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>
1	B	297	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>
1	C	297	<div> <div>8%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6752 atoms, of which 0 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 S-methyl-5'-thioadenosine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	4	0
			2098	1330	356	394	18			
1	B	273	Total	C	N	O	S	0	3	0
			2098	1328	356	396	18			
1	C	273	Total	C	N	O	S	0	2	0
			2088	1322	357	391	18			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q13126
A	-12	HIS	-	expression tag	UNP Q13126
A	-11	HIS	-	expression tag	UNP Q13126
A	-10	HIS	-	expression tag	UNP Q13126
A	-9	HIS	-	expression tag	UNP Q13126
A	-8	HIS	-	expression tag	UNP Q13126
A	-7	HIS	-	expression tag	UNP Q13126
A	-6	GLU	-	expression tag	UNP Q13126
A	-5	ASN	-	expression tag	UNP Q13126
A	-4	LEU	-	expression tag	UNP Q13126
A	-3	TYR	-	expression tag	UNP Q13126
A	-2	PHE	-	expression tag	UNP Q13126
A	-1	GLN	-	expression tag	UNP Q13126
A	0	SER	-	expression tag	UNP Q13126
B	-13	MET	-	expression tag	UNP Q13126
B	-12	HIS	-	expression tag	UNP Q13126
B	-11	HIS	-	expression tag	UNP Q13126
B	-10	HIS	-	expression tag	UNP Q13126
B	-9	HIS	-	expression tag	UNP Q13126
B	-8	HIS	-	expression tag	UNP Q13126
B	-7	HIS	-	expression tag	UNP Q13126
B	-6	GLU	-	expression tag	UNP Q13126
B	-5	ASN	-	expression tag	UNP Q13126

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	LEU	-	expression tag	UNP Q13126
B	-3	TYR	-	expression tag	UNP Q13126
B	-2	PHE	-	expression tag	UNP Q13126
B	-1	GLN	-	expression tag	UNP Q13126
B	0	SER	-	expression tag	UNP Q13126
C	-13	MET	-	expression tag	UNP Q13126
C	-12	HIS	-	expression tag	UNP Q13126
C	-11	HIS	-	expression tag	UNP Q13126
C	-10	HIS	-	expression tag	UNP Q13126
C	-9	HIS	-	expression tag	UNP Q13126
C	-8	HIS	-	expression tag	UNP Q13126
C	-7	HIS	-	expression tag	UNP Q13126
C	-6	GLU	-	expression tag	UNP Q13126
C	-5	ASN	-	expression tag	UNP Q13126
C	-4	LEU	-	expression tag	UNP Q13126
C	-3	TYR	-	expression tag	UNP Q13126
C	-2	PHE	-	expression tag	UNP Q13126
C	-1	GLN	-	expression tag	UNP Q13126
C	0	SER	-	expression tag	UNP Q13126

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

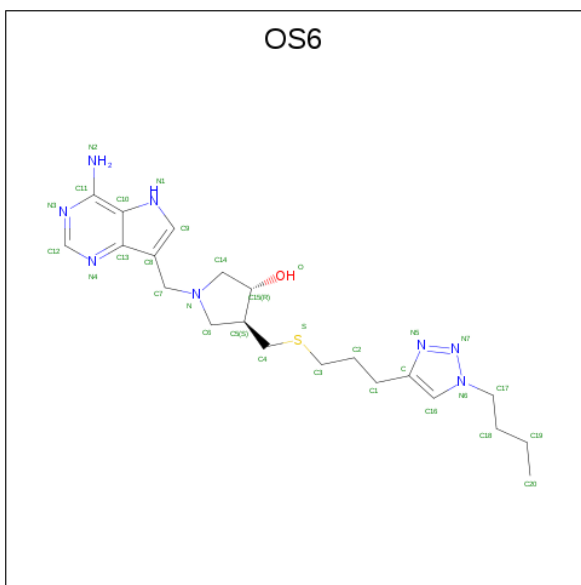
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	2	Total Cl 2 2	0	0
2	C	2	Total Cl 2 2	0	0

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



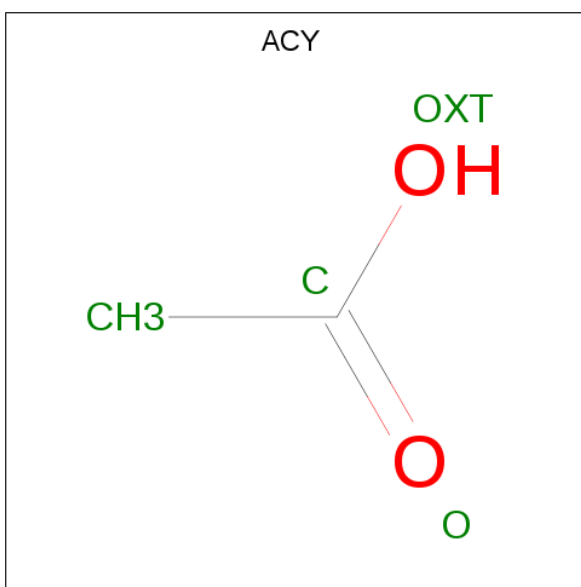
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is (3R,4S)-1-[(4-amino-5H-pyrrolo[3,2-d]pyrimidin-7-yl)methyl]-4-([3-(1-butyl-1H-1,2,3-triazol-4-yl)propyl]sulfanyl)methyl)pyrrolidin-3-ol (three-letter code: OS6) (formula: C<sub>21</sub>H<sub>32</sub>N<sub>8</sub>OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 21	N 8	O 1	S 1	0	0
4	B	1	Total 31	C 21	N 8	O 1	S 1	0	0
4	C	1	Total 31	C 21	N 8	O 1	S 1	0	0

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula:  $\text{C}_2\text{H}_4\text{O}_2$ ).



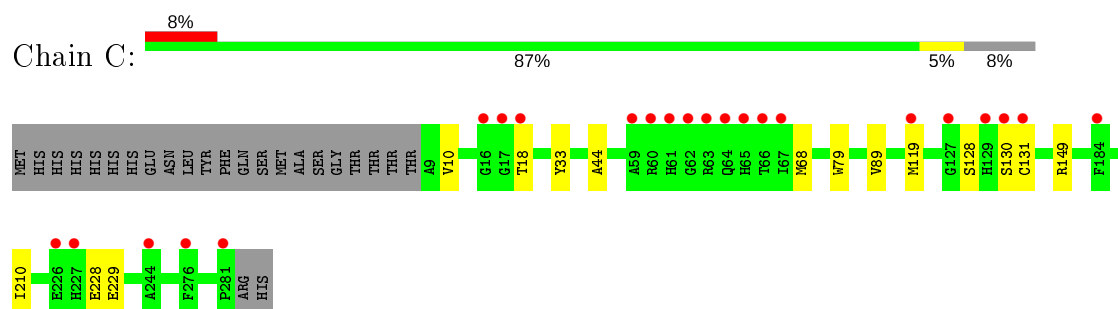
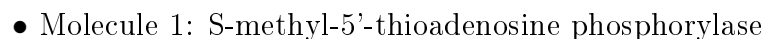
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	134	Total 134	O 134	0	0
6	B	113	Total 113	O 113	0	0
6	C	91	Total 91	O 91	0	0



- Molecule 1: S-methyl-5'-thiadenosine phosphorylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.36Å 135.13Å 158.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.43 – 1.91 79.43 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (79.43-1.91) 99.9 (79.43-1.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.197 , 0.220 0.203 , 0.224	Depositor DCC
$R_{free}$ test set	3416 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6752	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: ACY, CL, EDO, OS6

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	0/2151	0.72	2/2918 (0.1%)
1	B	0.45	0/2147	0.73	4/2912 (0.1%)
1	C	0.47	0/2133	0.73	3/2893 (0.1%)
All	All	0.46	0/6431	0.73	9/8723 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ARG	NE-CZ-NH2	7.03	123.82	120.30
1	C	149	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	A	149	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	149	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	C	68	MET	CA-CB-CG	6.07	123.62	113.30
1	C	149	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	B	162	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	60	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	60	ARG	NE-CZ-NH1	5.27	122.94	120.30

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	2098	0	2111	8	1
1	B	2098	0	2108	7	2
1	C	2088	0	2101	5	2
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
3	A	12	0	18	0	0
3	C	16	0	24	0	0
4	A	31	0	0	0	0
4	B	31	0	0	0	0
4	C	31	0	0	0	0
5	B	4	0	3	1	0
6	A	134	0	0	1	0
6	B	113	0	0	1	0
6	C	91	0	0	0	0
All	All	6752	0	6365	20	4

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 (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HD11	1:A:258[A]:ILE:CD1	2.28	0.64
1:B:61:HIS:O	1:B:65:HIS:HA	2.12	0.48
1:B:17:GLY:O	1:B:20:LEU:HD23	2.13	0.48
1:C:33:TYR:CZ	1:C:44:ALA:HB2	2.49	0.48
1:C:33:TYR:CE2	1:C:44:ALA:HB2	2.50	0.47
5:B:302:ACY:H3	1:C:119:MET:HA	1.96	0.46
1:A:147:LYS:HD2	1:A:263:TRP:CZ3	2.52	0.45
1:B:33:TYR:CD1	1:B:44:ALA:HB2	2.52	0.45
1:A:31:GLU:HG3	1:A:46:ILE:HG12	1.99	0.44
1:B:245:ASN:ND2	6:B:401:HOH:O	2.51	0.44
1:A:90:ILE:HD11	1:A:258[A]:ILE:HD11	2.00	0.43
1:A:89:VAL:HG23	1:A:210:ILE:HG21	2.00	0.43
1:C:89:VAL:HG23	1:C:210:ILE:HG21	2.00	0.42
1:A:64:GLN:O	1:A:65:HIS:O	2.37	0.42
1:A:246:LYS:NZ	6:A:403:HOH:O	2.43	0.42
1:C:79:TRP:CH2	1:C:131:CYS:CB	3.03	0.42
1:B:89:VAL:HG23	1:B:210:ILE:HG21	2.02	0.41
1:B:100:GLU:OE1	1:B:225:LYS:HE3	2.21	0.41
1:A:148:THR:OG1	1:A:211[B]:CYS:SG	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TYR:CE1	1:B:44:ALA:HB2	2.56	0.40

All (4) 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:C:128:SER:O	1:C:128:SER:O[3_757]	1.09	1.11
1:A:131:CYS:CB	1:B:130:SER:CB[3_757]	1.98	0.22
1:C:130:SER:CA	1:C:130:SER:CA[3_757]	2.03	0.17
1:B:31:GLU:OE2	1:B:33:TYR:OH[3_757]	2.05	0.15

## 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	275/297 (93%)	269 (98%)	4 (2%)	2 (1%)	22	11
1	B	274/297 (92%)	266 (97%)	6 (2%)	2 (1%)	22	11
1	C	273/297 (92%)	268 (98%)	4 (2%)	1 (0%)	34	24
All	All	822/891 (92%)	803 (98%)	14 (2%)	5 (1%)	25	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	65	HIS
1	B	18	THR
1	C	18	THR
1	B	65	HIS

### 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	231/256 (90%)	225 (97%)	6 (3%)	46	37
1	B	231/256 (90%)	229 (99%)	2 (1%)	78	78
1	C	228/256 (89%)	225 (99%)	3 (1%)	69	66
All	All	690/768 (90%)	679 (98%)	11 (2%)	62	58

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	33	TYR
1	A	47	LEU
1	A	228	GLU
1	A	229	GLU
1	A	261	THR
1	B	10	VAL
1	B	261	THR
1	C	10	VAL
1	C	228	GLU
1	C	229	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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
4	OS6	B	303	-	32,34,34	1.22	4 (12%)	27,46,46	1.99	7 (25%)
3	EDO	A	303	-	3,3,3	0.50	0	2,2,2	0.29	0
3	EDO	C	304	-	3,3,3	0.52	0	2,2,2	0.03	0
4	OS6	A	306	-	32,34,34	1.16	4 (12%)	27,46,46	2.43	10 (37%)
3	EDO	A	305	-	3,3,3	0.45	0	2,2,2	0.39	0
4	OS6	C	307	-	32,34,34	1.29	4 (12%)	27,46,46	1.69	4 (14%)
3	EDO	C	305	-	3,3,3	0.43	0	2,2,2	0.31	0
5	ACY	B	302	-	1,3,3	1.22	0	0,3,3	0.00	-
3	EDO	C	306	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	A	304	-	3,3,3	0.57	0	2,2,2	0.11	0
3	EDO	C	303	-	3,3,3	0.49	0	2,2,2	0.32	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	OS6	B	303	-	-	3/15/28/28	0/4/4/4
3	EDO	A	303	-	-	1/1/1/1	-
3	EDO	C	304	-	-	0/1/1/1	-
4	OS6	A	306	-	-	3/15/28/28	0/4/4/4
3	EDO	A	305	-	-	0/1/1/1	-
4	OS6	C	307	-	-	4/15/28/28	0/4/4/4
3	EDO	C	305	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	306	-	-	1/1/1/1	-
3	EDO	A	304	-	-	1/1/1/1	-
3	EDO	C	303	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	307	OS6	N5-N7	3.95	1.41	1.34
4	B	303	OS6	N5-N7	3.49	1.40	1.34
4	C	307	OS6	N7-N6	3.33	1.40	1.34
4	A	306	OS6	N5-N7	3.22	1.40	1.34
4	A	306	OS6	C16-C	2.97	1.40	1.36
4	B	303	OS6	C16-C	2.81	1.40	1.36
4	B	303	OS6	N7-N6	2.81	1.39	1.34
4	C	307	OS6	C16-C	2.73	1.40	1.36
4	A	306	OS6	N7-N6	2.49	1.39	1.34
4	A	306	OS6	C12-N4	2.23	1.35	1.32
4	B	303	OS6	C12-N4	2.01	1.35	1.32
4	C	307	OS6	C-N5	2.00	1.36	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	306	OS6	C12-N4-C13	6.28	119.69	114.81
4	A	306	OS6	N4-C12-N3	-4.91	121.00	128.68
4	A	306	OS6	N5-N7-N6	-4.73	103.75	107.31
4	C	307	OS6	N4-C12-N3	-4.72	121.30	128.68
4	B	303	OS6	N4-C12-N3	-4.65	121.41	128.68
4	B	303	OS6	N5-N7-N6	-4.29	104.08	107.31
4	C	307	OS6	C12-N4-C13	4.29	118.15	114.81
4	B	303	OS6	C12-N4-C13	3.97	117.90	114.81
4	A	306	OS6	C8-C7-N	3.62	119.31	114.14
4	B	303	OS6	C8-C7-N	3.53	119.18	114.14
4	A	306	OS6	C10-C13-N4	-3.18	121.23	124.92
4	A	306	OS6	C6-N-C14	3.08	108.77	104.19
4	A	306	OS6	C4-S-C3	2.67	110.27	102.27
4	A	306	OS6	C16-C-N5	-2.63	107.44	111.34
4	C	307	OS6	N5-N7-N6	-2.61	105.35	107.31
4	A	306	OS6	C17-N6-C16	2.60	135.92	129.82
4	B	303	OS6	C4-S-C3	2.55	109.93	102.27
4	B	303	OS6	C16-C-N5	-2.54	107.57	111.34
4	C	307	OS6	C8-C7-N	2.22	117.31	114.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	OS6	C17-N6-C16	2.09	134.72	129.82
4	A	306	OS6	O-C15-C14	-2.08	106.03	110.94

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	307	OS6	N6-C17-C18-C19
4	A	306	OS6	N6-C17-C18-C19
4	B	303	OS6	N6-C17-C18-C19
3	A	304	EDO	O1-C1-C2-O2
3	C	303	EDO	O1-C1-C2-O2
4	C	307	OS6	C8-C7-N-C6
3	A	303	EDO	O1-C1-C2-O2
3	C	306	EDO	O1-C1-C2-O2
4	B	303	OS6	C-C1-C2-C3
4	A	306	OS6	C16-C-C1-C2
4	C	307	OS6	C17-C18-C19-C20
4	B	303	OS6	C2-C3-S-C4
4	C	307	OS6	C-C1-C2-C3
4	A	306	OS6	C18-C17-N6-C16

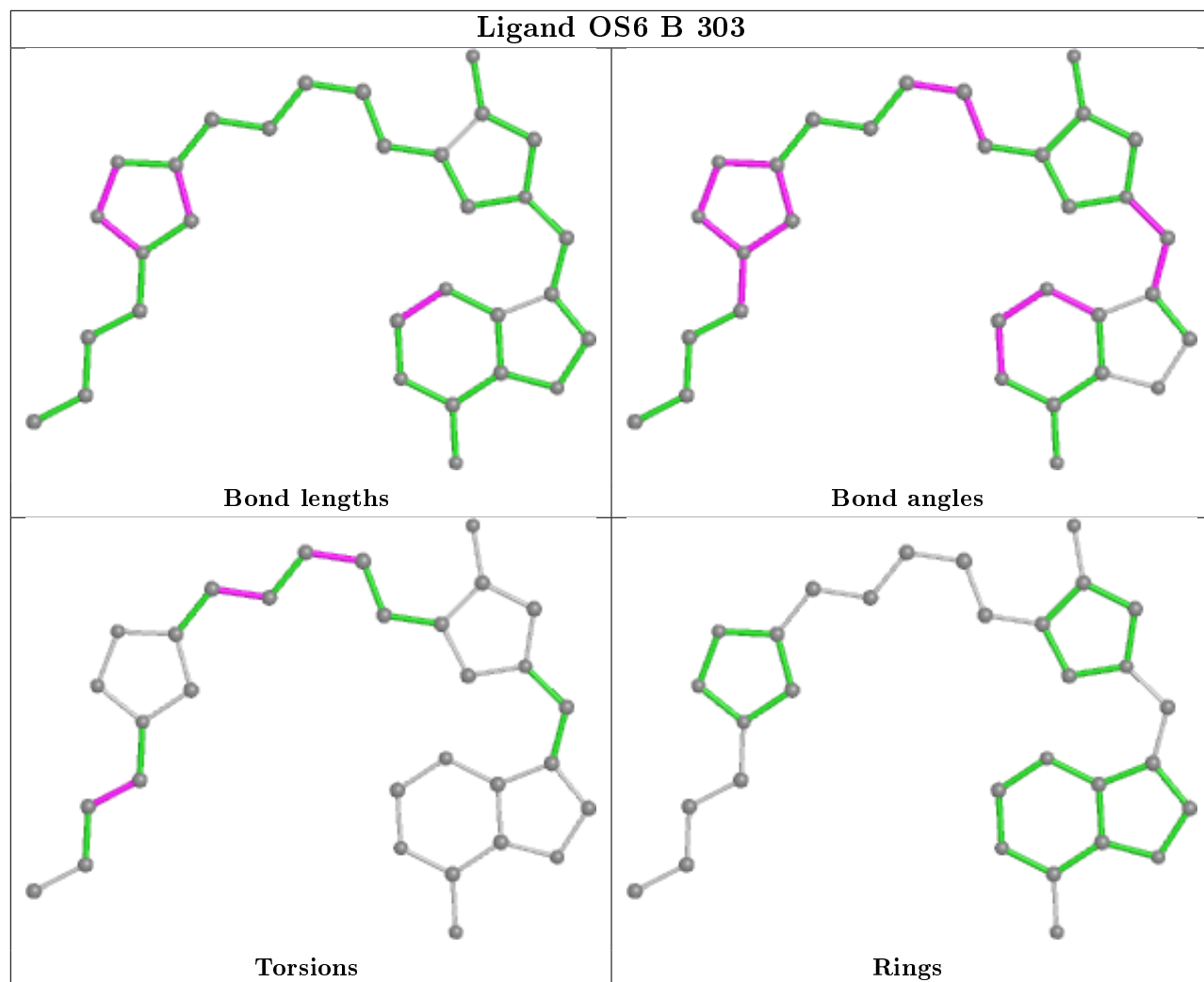
There are no ring outliers.

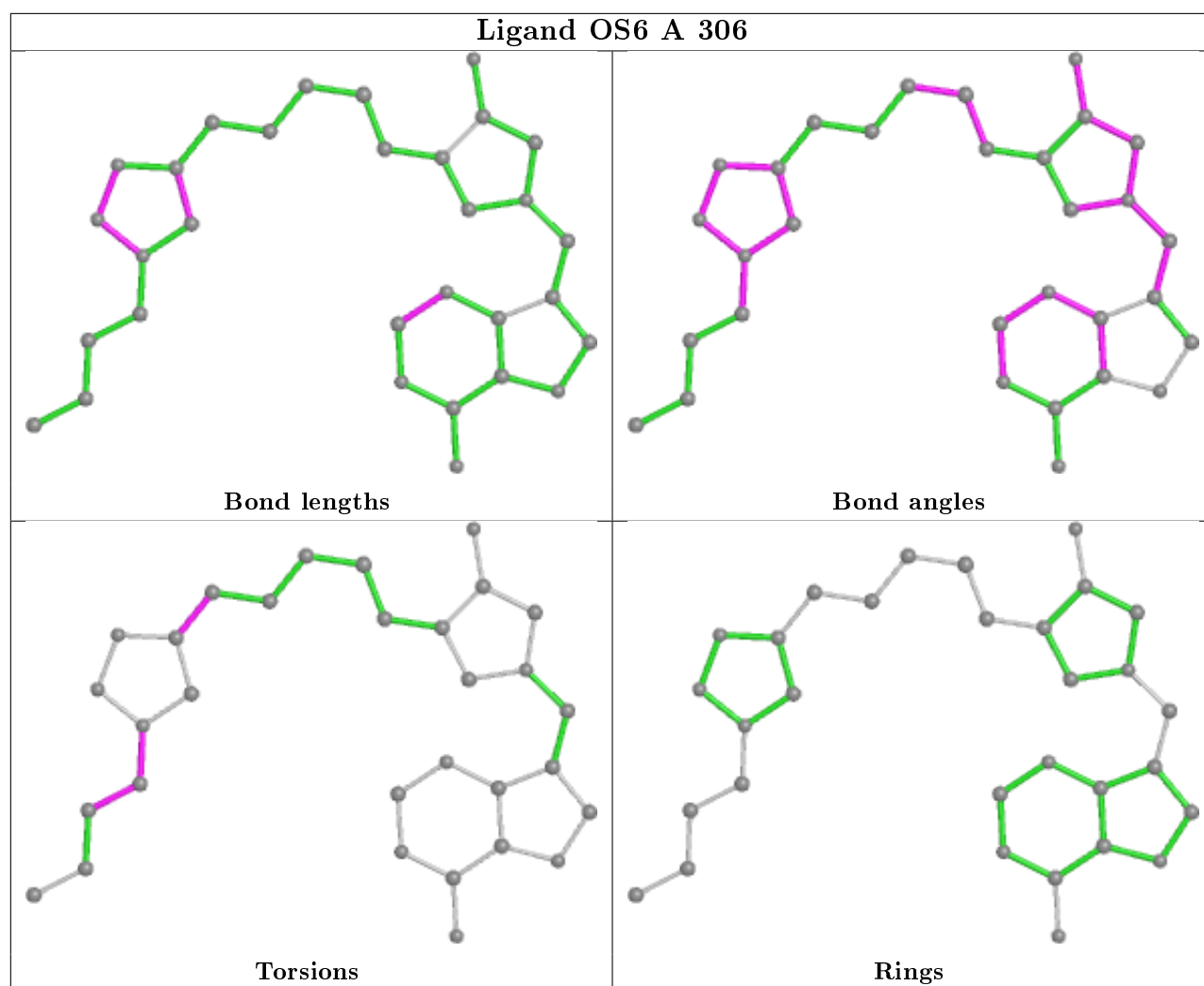
1 monomer is involved in 1 short contact:

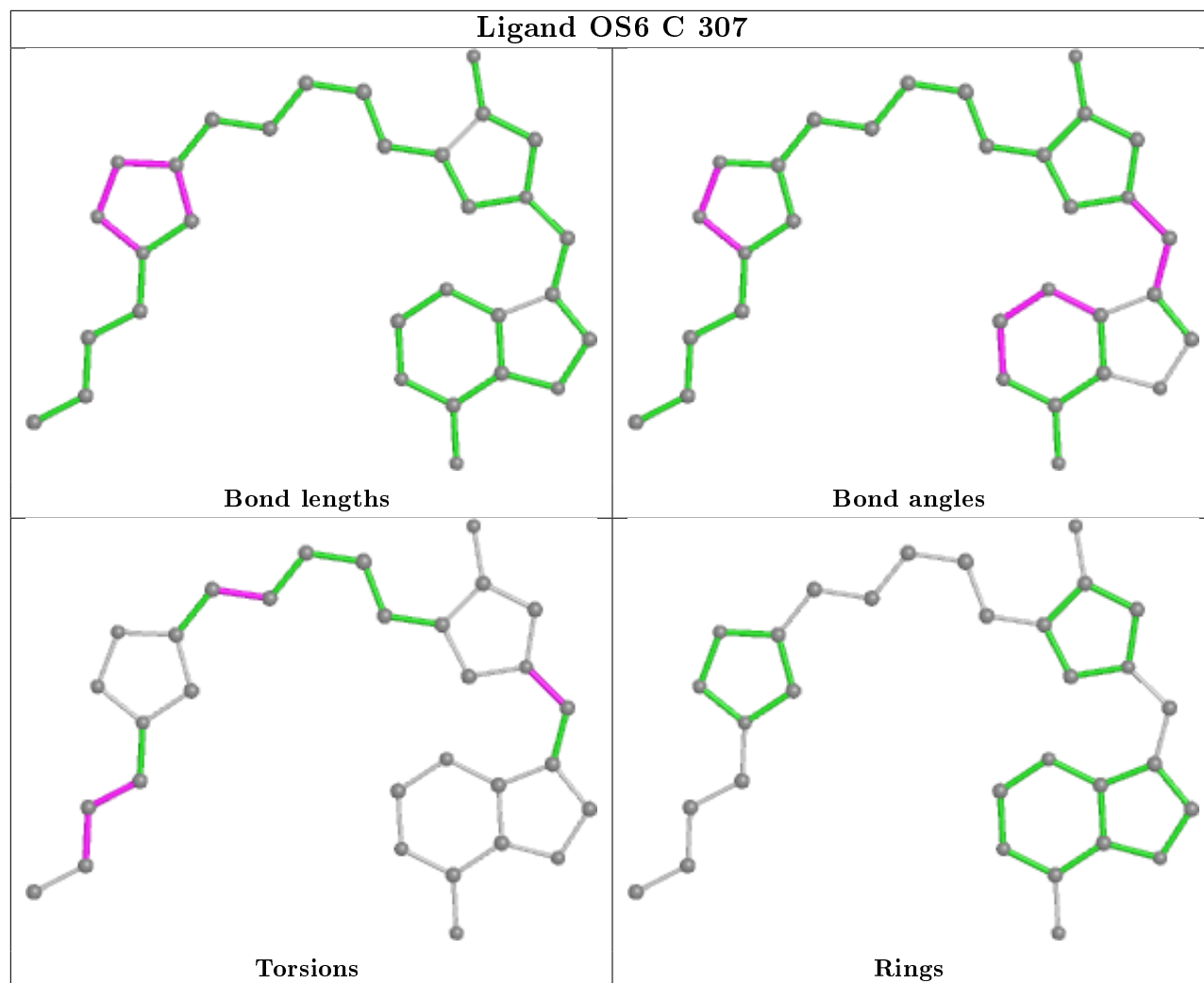
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	302	ACY	1	0

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	273/297 (91%)	0.34	16 (5%) 22 25	20, 31, 59, 99	0
1	B	273/297 (91%)	0.46	17 (6%) 20 23	21, 37, 69, 95	0
1	C	273/297 (91%)	0.45	23 (8%) 11 13	20, 37, 66, 114	0
All	All	819/891 (91%)	0.41	56 (6%) 17 19	20, 35, 67, 114	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	THR	11.9
1	B	33	TYR	7.4
1	B	131	CYS	7.2
1	C	227	HIS	7.2
1	B	281	PRO	6.6
1	A	227	HIS	6.4
1	A	18	THR	6.0
1	B	64	GLN	5.8
1	A	61	HIS	5.6
1	B	18	THR	5.5
1	A	131	CYS	5.4
1	C	63	ARG	5.1
1	A	63	ARG	4.7
1	B	132	ALA	4.4
1	C	276	PHE	4.4
1	C	64	GLN	4.2
1	C	61	HIS	4.1
1	C	66	THR	4.1
1	B	17	GLY	3.9
1	B	65	HIS	3.8
1	A	226	GLU	3.8
1	C	18	THR	3.8
1	B	63	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	17	GLY	3.8
1	C	130	SER	3.7
1	C	244	ALA	3.7
1	B	66	THR	3.5
1	A	64	GLN	3.4
1	C	131	CYS	3.4
1	C	17	GLY	3.3
1	C	65	HIS	3.2
1	A	276	PHE	3.2
1	A	65	HIS	3.1
1	C	281	PRO	3.0
1	B	280	LEU	2.8
1	C	60	ARG	2.7
1	A	281	PRO	2.7
1	B	162	ARG	2.7
1	B	264	SER	2.7
1	A	59	ALA	2.6
1	B	62	GLY	2.6
1	B	24	GLU	2.6
1	C	67	ILE	2.6
1	C	226	GLU	2.5
1	C	129	HIS	2.4
1	A	67	ILE	2.4
1	C	16	GLY	2.3
1	B	276	PHE	2.2
1	A	62	GLY	2.2
1	C	119	MET	2.1
1	A	33	TYR	2.1
1	B	227	HIS	2.1
1	C	62	GLY	2.1
1	C	127	GLY	2.1
1	C	184	PHE	2.1
1	C	59	ALA	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 ⓘ

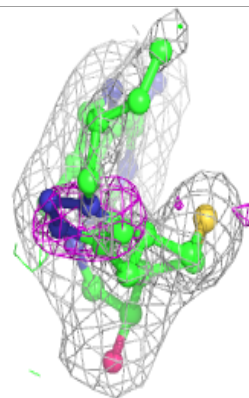
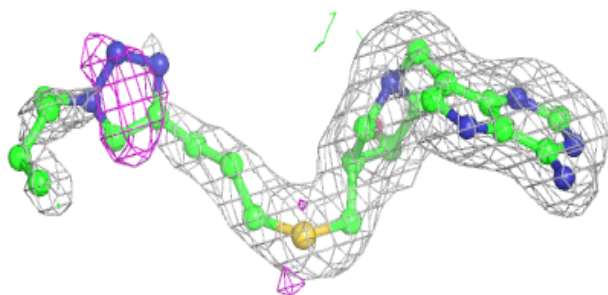
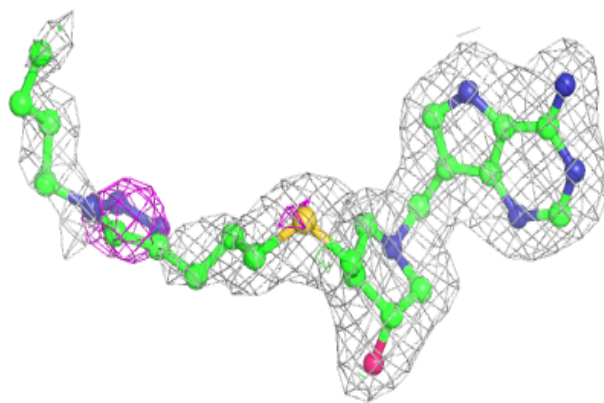
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	C	303	4/4	0.66	0.18	51,52,54,56	0
3	EDO	A	304	4/4	0.70	0.16	52,55,56,56	0
3	EDO	A	305	4/4	0.70	0.23	48,50,53,55	0
3	EDO	A	303	4/4	0.70	0.14	51,56,56,57	0
5	ACY	B	302	4/4	0.74	0.22	48,48,49,52	0
3	EDO	C	305	4/4	0.77	0.15	50,52,53,54	0
3	EDO	C	306	4/4	0.83	0.14	56,56,56,58	0
3	EDO	C	304	4/4	0.89	0.20	49,50,51,53	0
4	OS6	C	307	31/31	0.92	0.16	21,30,72,72	0
4	OS6	B	303	31/31	0.94	0.11	23,32,60,62	0
4	OS6	A	306	31/31	0.94	0.12	21,30,57,59	0
2	CL	C	301	1/1	0.98	0.12	31,31,31,31	0
2	CL	A	302	1/1	0.98	0.06	30,30,30,30	0
2	CL	B	301	1/1	0.99	0.03	30,30,30,30	0
2	CL	C	302	1/1	0.99	0.07	31,31,31,31	0
2	CL	A	301	1/1	1.00	0.08	21,21,21,21	0

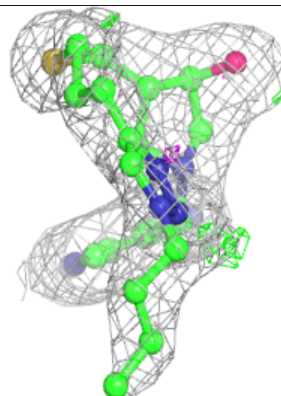
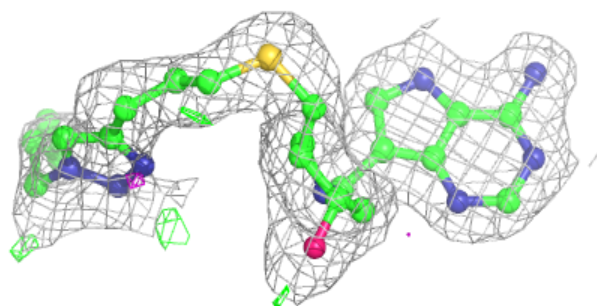
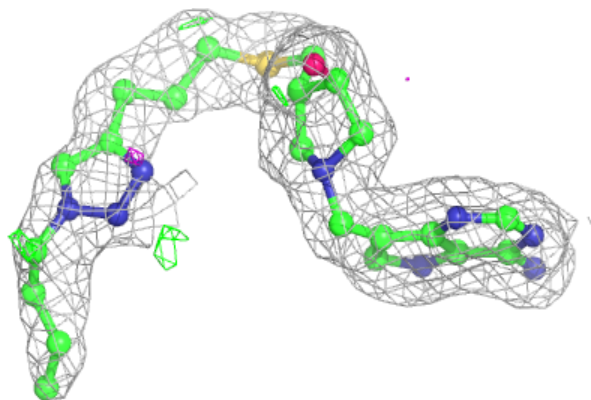
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OS6 C 307:**

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

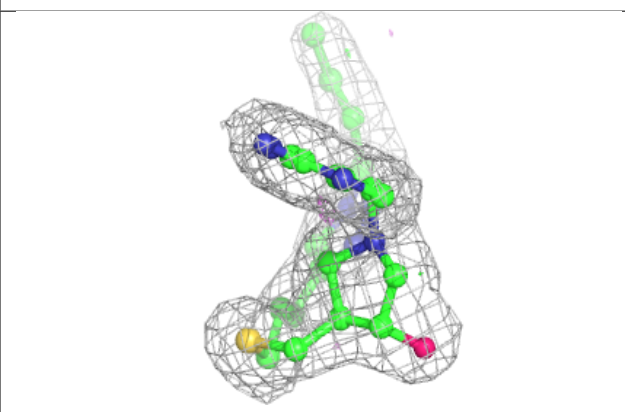
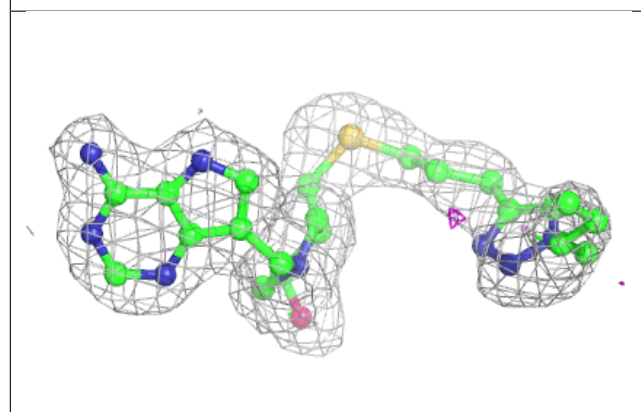
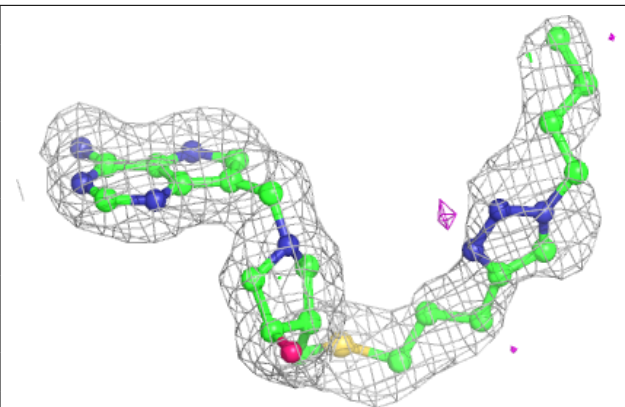
**Electron density around OS6 B 303:**

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



**Electron density around OS6 A 306:**

$2mF_o-DF_c$  (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.