



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:01 pm BST

PDB ID : 2FZD  
Title : Human aldose reductase complexed with tolrestat at 1.08 Å resolution.  
Authors : Steuber, H.; Zentgraf, M.; Gerlach, C.; Sotriffer, C.A.; Heine, A.; Klebe, G.  
Deposited on : 2006-02-09  
Resolution : 1.08 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

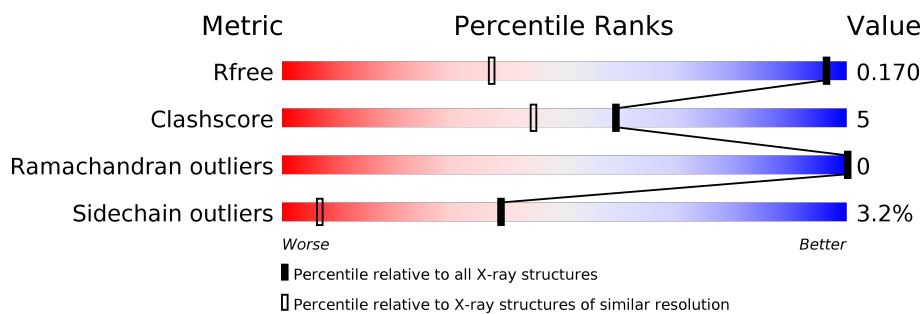
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.08 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	1386 (1.12-1.04)
Clashscore	141614	1021 (1.10-1.06)
Ramachandran outliers	138981	1381 (1.12-1.04)
Sidechain outliers	138945	1379 (1.12-1.04)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	316	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2975 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 aldose reductase.

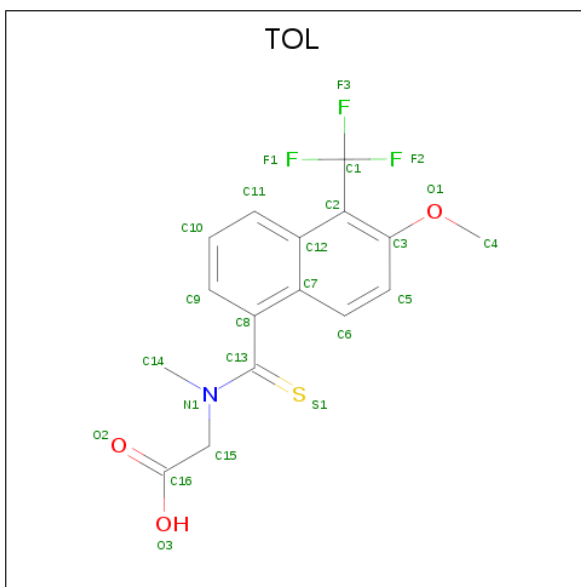
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2553	1646	426	468	13	0	13	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is TOLRESTAT (three-letter code: TOL) (formula: C<sub>16</sub>H<sub>14</sub>F<sub>3</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	
			24	16	3	1	3	1	
								0	0

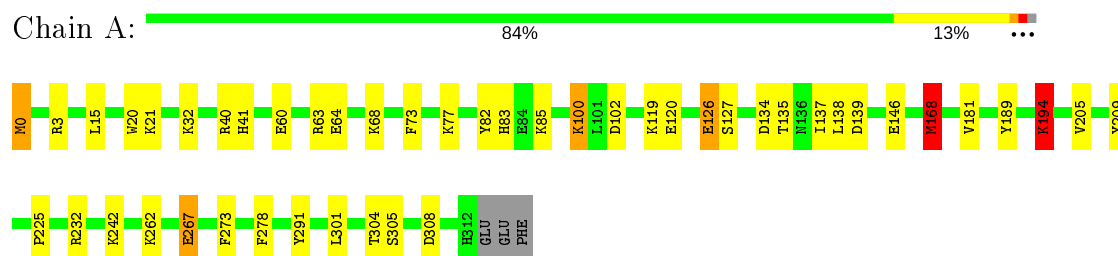
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	350	Total	O		
			350	350	0	0

### 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. 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. 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: aldose reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.45Å 66.68Å 46.06Å 90.00° 92.45° 90.00°	Depositor
Resolution (Å)	10.00 – 1.08 21.75 – 1.06	Depositor EDS
% Data completeness (in resolution range)	85.7 (10.00-1.08) 89.5 (21.75-1.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.27 (at 1.06Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.112 , 0.139 0.161 , 0.170	Depositor DCC
$R_{free}$ test set	6131 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	8.1	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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: NAP, TOL

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	0.86	0/2666	1.31	28/3618 (0.8%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	0	MET	CG-SD-CE	10.89	117.62	100.20
1	A	63	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	A	60	GLU	OE1-CD-OE2	-8.84	112.69	123.30
1	A	64[A]	GLU	CG-CD-OE1	8.02	134.34	118.30
1	A	64[B]	GLU	CG-CD-OE1	8.02	134.34	118.30
1	A	40	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	168	MET	CA-CB-CG	7.57	126.17	113.30
1	A	134	ASP	CB-CG-OD1	-7.56	111.50	118.30
1	A	232	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	64[A]	GLU	OE1-CD-OE2	-7.07	114.82	123.30
1	A	64[B]	GLU	OE1-CD-OE2	-7.07	114.82	123.30
1	A	32	LYS	CG-CD-CE	7.06	133.08	111.90
1	A	194[A]	LYS	CB-CG-CD	6.92	129.59	111.60
1	A	194[B]	LYS	CB-CG-CD	6.92	129.59	111.60
1	A	102	ASP	CB-CG-OD1	6.75	124.38	118.30
1	A	3	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	3	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	308	ASP	CB-CG-OD1	-6.44	112.50	118.30
1	A	194[A]	LYS	CG-CD-CE	6.30	130.81	111.90
1	A	194[B]	LYS	CG-CD-CE	6.30	130.81	111.90
1	A	291	TYR	CG-CD1-CE1	5.92	126.03	121.30
1	A	120	GLU	OE1-CD-OE2	5.76	130.22	123.30
1	A	100	LYS	CA-CB-CG	5.46	125.42	113.40
1	A	64[A]	GLU	CA-CB-CG	5.44	125.37	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64[B]	GLU	CA-CB-CG	5.44	125.37	113.40
1	A	82	TYR	CB-CG-CD1	5.43	124.26	121.00
1	A	209	TYR	CA-CB-CG	5.32	123.51	113.40
1	A	60	GLU	CG-CD-OE2	5.01	128.32	118.30

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	2553	0	2585	25	0
2	A	48	0	25	3	0
3	A	24	0	13	0	0
4	A	350	0	0	5	0
All	All	2975	0	2623	25	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 5.

All (25) 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:83:HIS:HB3	1:A:135[B]:THR:HG21	1.78	0.64
1:A:77:LYS:NZ	2:A:316:NAP:H2N	2.15	0.61
1:A:83:HIS:CB	1:A:135[B]:THR:HG21	2.33	0.59
1:A:194[B]:LYS:HG3	4:A:601:HOH:O	2.04	0.58
1:A:137[A]:ILE:HG13	1:A:138:LEU:N	2.23	0.54
1:A:135[B]:THR:HG23	4:A:486:HOH:O	2.08	0.51
1:A:242[B]:LYS:HE3	1:A:278:PHE:CD1	2.46	0.50
1:A:262:LYS:O	2:A:316:NAP:H8A	2.12	0.50
1:A:146[A]:GLU:HG3	4:A:497:HOH:O	2.12	0.49
1:A:20:TRP:CE3	1:A:21:LYS:HE3	2.48	0.49
1:A:85[A]:LYS:HE2	1:A:139:ASP:O	2.14	0.48
1:A:77:LYS:HZ3	2:A:316:NAP:H71N	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HA	1:A:205:VAL:O	2.15	0.46
1:A:41:HIS:HA	1:A:73:PHE:O	2.15	0.46
1:A:301:LEU:HA	1:A:304:THR:HG23	1.97	0.46
1:A:189:TYR:CE2	1:A:225:PRO:HB2	2.51	0.44
1:A:146[B]:GLU:HG2	4:A:497:HOH:O	2.18	0.43
1:A:119:LYS:HG3	4:A:641:HOH:O	2.19	0.42
1:A:137[A]:ILE:HD11	1:A:168:MET:HG2	2.00	0.42
1:A:15[A]:LEU:HD21	1:A:273:PHE:HA	2.03	0.40

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	324/316 (102%)	319 (98%)	5 (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	291/281 (104%)	279 (96%)	12 (4%)	30	3

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	68	LYS
1	A	100	LYS
1	A	126[A]	GLU
1	A	126[B]	GLU
1	A	127	SER
1	A	168	MET
1	A	194[A]	LYS
1	A	194[B]	LYS
1	A	267[A]	GLU
1	A	267[B]	GLU
1	A	305	SER

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

Mol	Chain	Res	Type
1	A	200	GLN
1	A	241	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	TOL	A	317	-	21,25,25	1.11	1 (4%)	32,37,37	1.60	2 (6%)
2	NAP	A	316	-	45,52,52	1.06	4 (8%)	56,80,80	1.09	5 (8%)

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	TOL	A	317	-	-	1/18/20/20	0/2/2/2
2	NAP	A	316	-	-	4/31/67/67	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	316	NAP	C2N-C3N	-2.79	1.34	1.39
2	A	316	NAP	PA-O2A	-2.27	1.44	1.55
2	A	316	NAP	P2B-O2B	2.26	1.63	1.59
3	A	317	TOL	C1-C2	-2.08	1.49	1.52
2	A	316	NAP	PN-O2N	-2.01	1.45	1.55

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	317	TOL	C3-C2-C12	6.86	122.33	117.53
3	A	317	TOL	C5-C3-C2	-3.05	119.09	122.90
2	A	316	NAP	C5A-C6A-N6A	2.91	124.78	120.35
2	A	316	NAP	C4A-C5A-N7A	2.74	112.26	109.40
2	A	316	NAP	O3X-P2B-O2X	2.35	116.61	107.64
2	A	316	NAP	PN-O3-PA	2.28	140.64	132.83
2	A	316	NAP	C5A-C6A-N1A	-2.22	115.33	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	316	NAP	C4D-C5D-O5D-PN
2	A	316	NAP	PA-O3-PN-O5D

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Mol	Chain	Res	Type	Atoms
2	A	316	NAP	C2B-O2B-P2B-O3X
2	A	316	NAP	PN-O3-PA-O1A
3	A	317	TOL	F2-C1-C2-C3

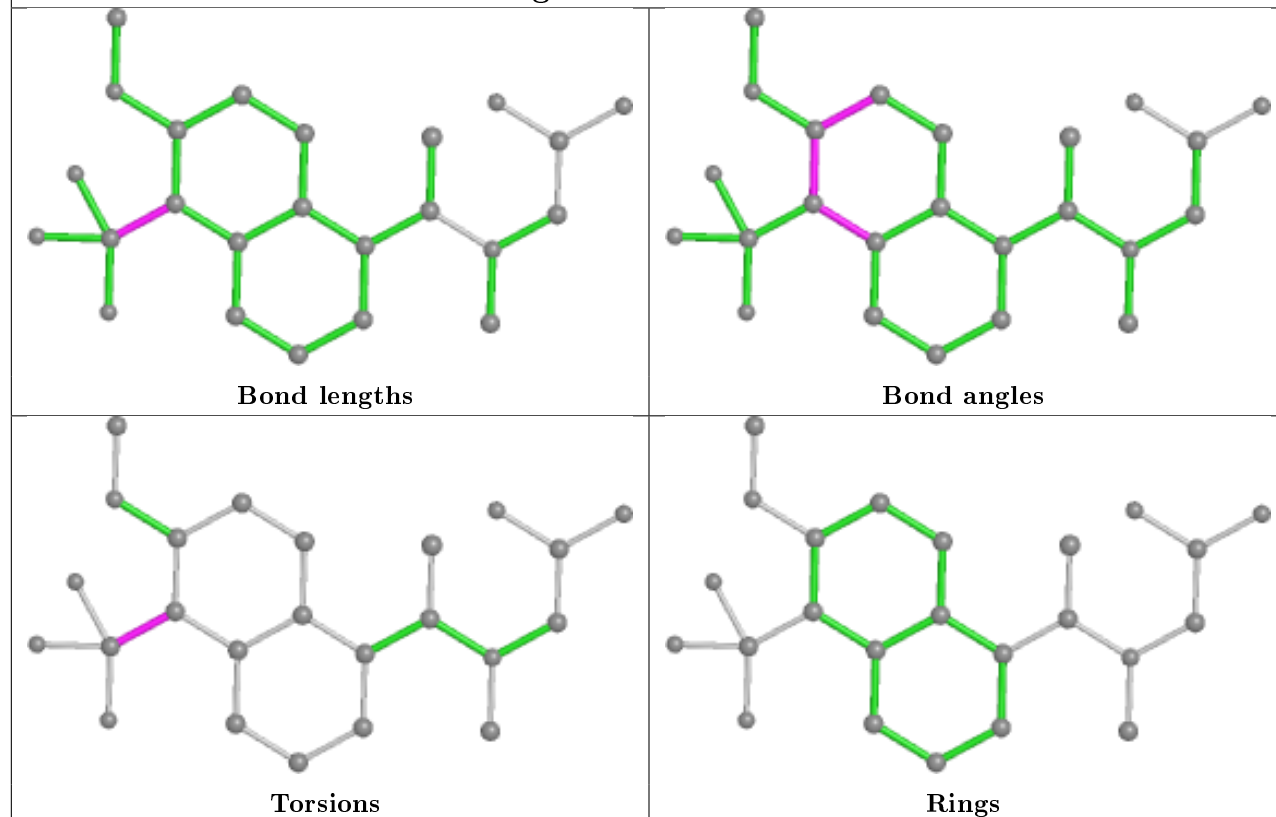
There are no ring outliers.

1 monomer is involved in 3 short contacts:

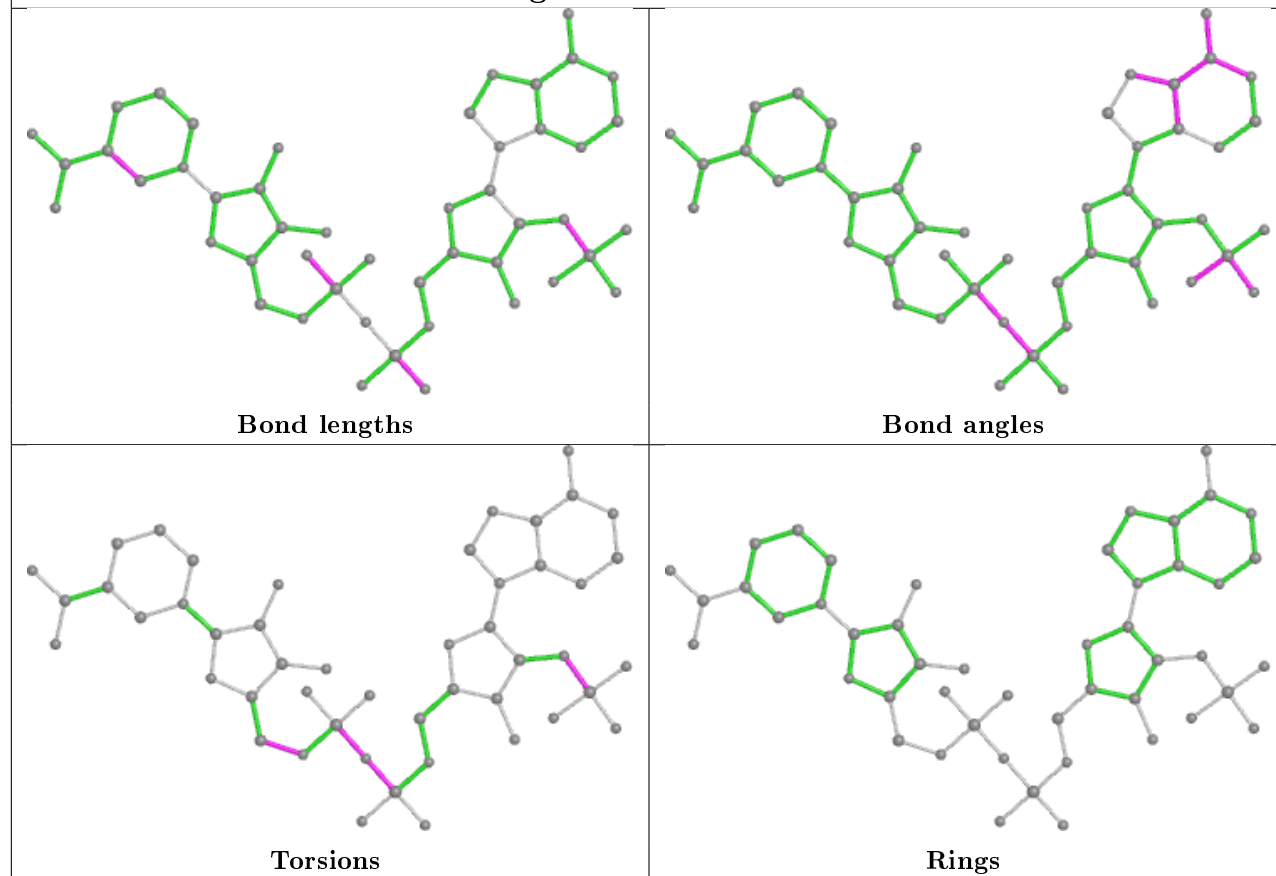
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	316	NAP	3	0

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 TOL A 317



## Ligand NAP A 316



## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

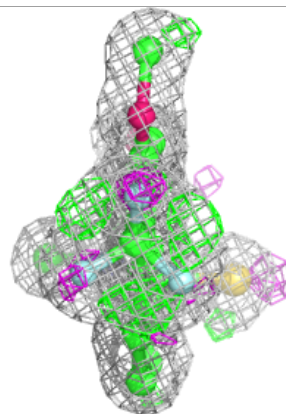
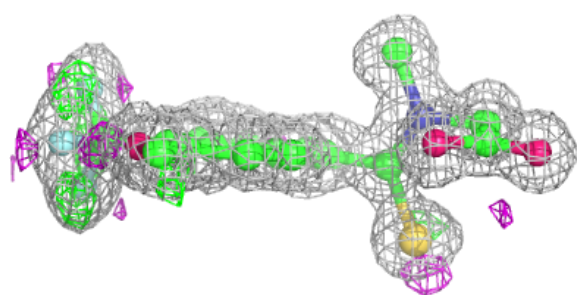
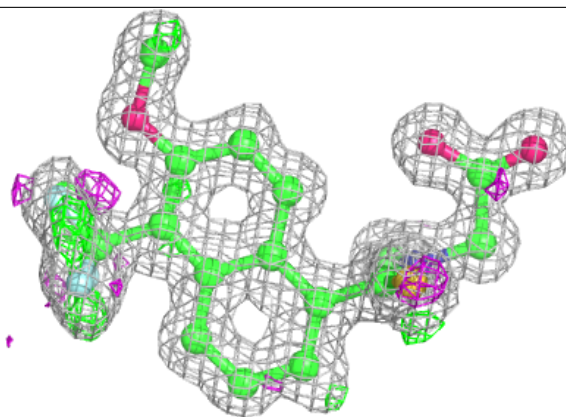
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

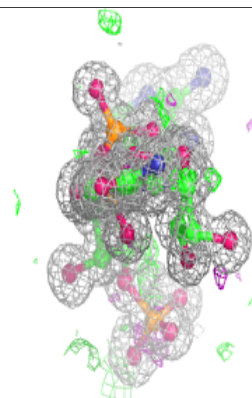
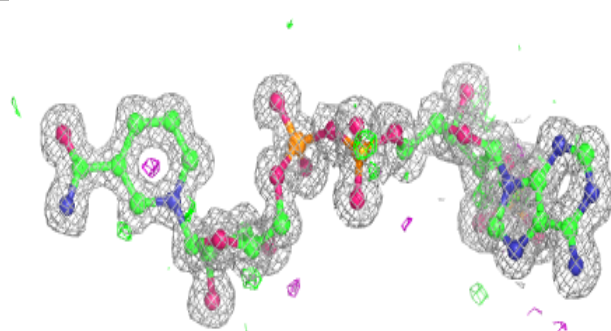
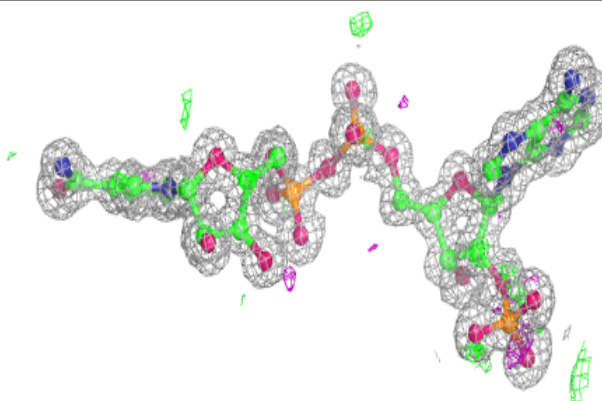
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TOL A 317:**

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

**Electron density around NAP A 316:**

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





## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.