



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2025 – 12:54 PM JST

PDB ID : 8YXY / pdb\_00008yxy  
Title : NADPH and 1-benzyl-4-methylpiperidin-3-one complex structure of Imine Reductase Mutant(M6) from Pochonia chlamydosporia 170  
Authors : Shi, M.; Zheng, G.  
Deposited on : 2024-04-03  
Resolution : 1.13 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

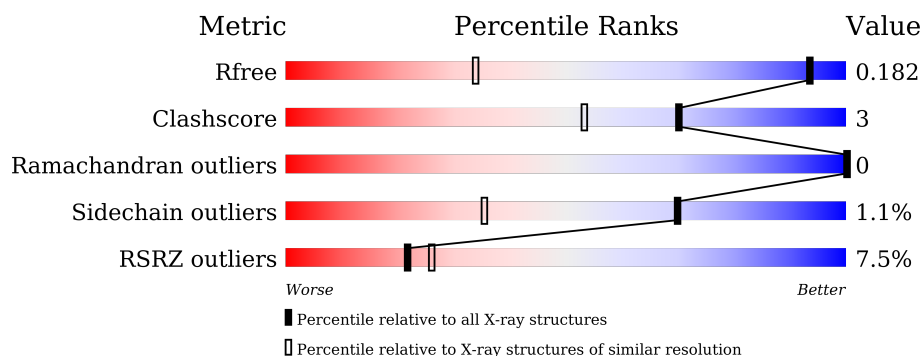
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.13 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))
$R_{free}$	164625	1652 (1.14-1.10)
Clashscore	180529	1870 (1.14-1.10)
Ramachandran outliers	177936	1828 (1.14-1.10)
Sidechain outliers	177891	1824 (1.14-1.10)
RSRZ outliers	164620	1652 (1.14-1.10)

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	293	<div> <div>7%</div> <div>92%</div> <div>6% .</div> </div>
1	B	293	<div> <div>8%</div> <div>92%</div> <div>5% ..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	A	3402	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5050 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 Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2099	1318	354	415	12			
1	B	289	Total	C	N	O	S	0	0	0
			2107	1322	356	417	12			

There are 40 discrepancies between the modelled and reference sequences:

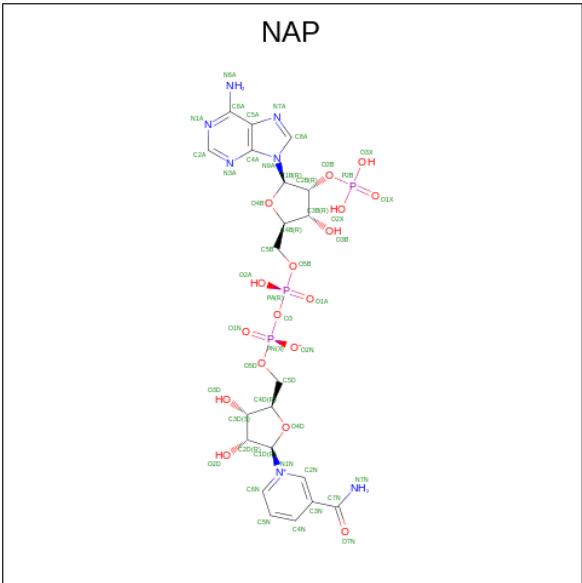
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLU	SER	conflict	UNP A0A179FZ20
A	47	PRO	ALA	conflict	UNP A0A179FZ20
A	50	ALA	VAL	conflict	UNP A0A179FZ20
A	72	ASN	SER	conflict	UNP A0A179FZ20
A	73	GLN	TYR	conflict	UNP A0A179FZ20
A	76	VAL	THR	conflict	UNP A0A179FZ20
A	124	THR	VAL	conflict	UNP A0A179FZ20
A	125	THR	PRO	conflict	UNP A0A179FZ20
A	127	GLU	ILE	conflict	UNP A0A179FZ20
A	128	TYR	LEU	conflict	UNP A0A179FZ20
A	178	VAL	ILE	conflict	UNP A0A179FZ20
A	180	SER	GLY	conflict	UNP A0A179FZ20
A	195	ALA	LYS	conflict	UNP A0A179FZ20
A	210	LEU	PHE	conflict	UNP A0A179FZ20
A	212	ALA	LYS	conflict	UNP A0A179FZ20
A	217	GLN	TRP	conflict	UNP A0A179FZ20
A	220	VAL	ARG	conflict	UNP A0A179FZ20
A	224	ARG	HIS	conflict	UNP A0A179FZ20
A	236	ILE	LEU	conflict	UNP A0A179FZ20
A	239	GLY	GLN	conflict	UNP A0A179FZ20
B	40	GLU	SER	conflict	UNP A0A179FZ20
B	47	PRO	ALA	conflict	UNP A0A179FZ20
B	50	ALA	VAL	conflict	UNP A0A179FZ20
B	72	ASN	SER	conflict	UNP A0A179FZ20
B	73	GLN	TYR	conflict	UNP A0A179FZ20

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Chain	Residue	Modelled	Actual	Comment	Reference
B	76	VAL	THR	conflict	UNP A0A179FZ20
B	124	THR	VAL	conflict	UNP A0A179FZ20
B	125	THR	PRO	conflict	UNP A0A179FZ20
B	127	GLU	ILE	conflict	UNP A0A179FZ20
B	128	TYR	LEU	conflict	UNP A0A179FZ20
B	178	VAL	ILE	conflict	UNP A0A179FZ20
B	180	SER	GLY	conflict	UNP A0A179FZ20
B	195	ALA	LYS	conflict	UNP A0A179FZ20
B	210	LEU	PHE	conflict	UNP A0A179FZ20
B	212	ALA	LYS	conflict	UNP A0A179FZ20
B	217	GLN	TRP	conflict	UNP A0A179FZ20
B	220	VAL	ARG	conflict	UNP A0A179FZ20
B	224	ARG	HIS	conflict	UNP A0A179FZ20
B	236	ILE	LEU	conflict	UNP A0A179FZ20
B	239	GLY	GLN	conflict	UNP A0A179FZ20

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



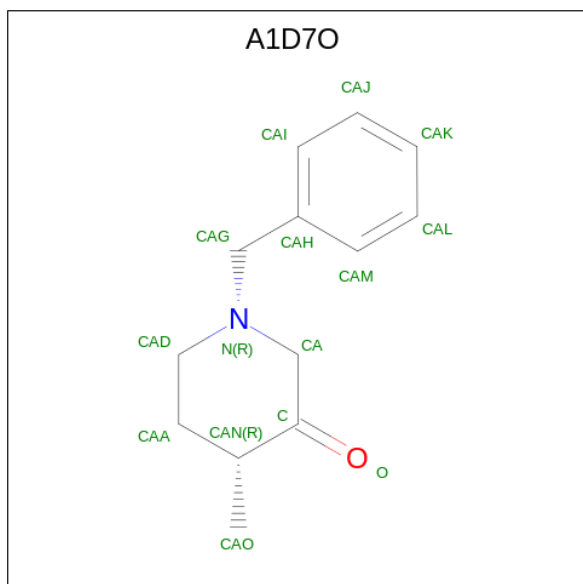
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is (4 {R})-4-methyl-1-(phenylmethyl)piperidin-3-one (CCD ID: A1D7O) (formula: C<sub>13</sub>H<sub>17</sub>NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	13	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			15	13	1	1		

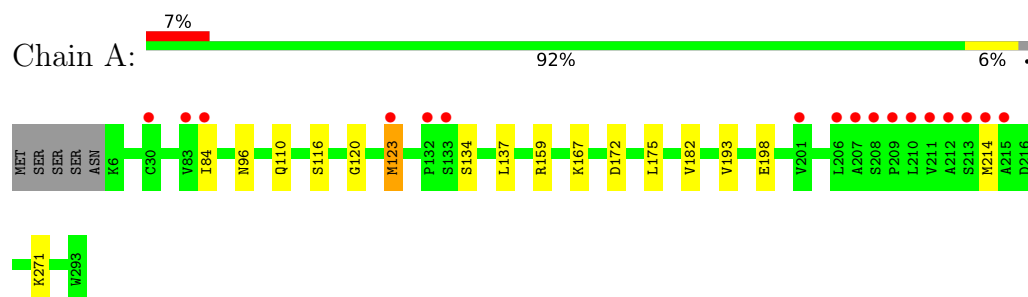
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	344	Total	O	0	0
			344	344		
5	B	360	Total	O	0	0
			360	360		

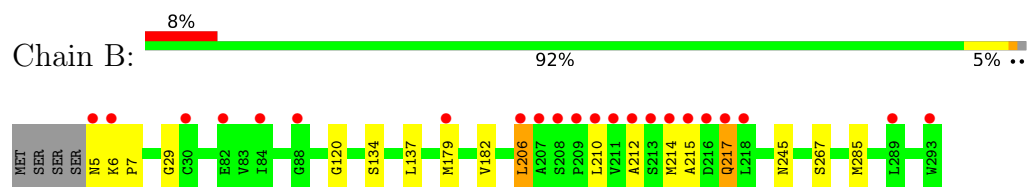
### 3 Residue-property plots [i](#)

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: Oxidoreductase



- Molecule 1: Oxidoreductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.85Å 114.45Å 62.61Å 90.00° 99.05° 90.00°	Depositor
Resolution (Å)	42.03 – 1.13 42.03 – 1.13	Depositor EDS
% Data completeness (in resolution range)	78.3 (42.03-1.13) 78.3 (42.03-1.13)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 1.13Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.154 , 0.176 0.163 , 0.182	Depositor DCC
$R_{free}$ test set	9659 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.8	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5050	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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, A1D7O, PEG

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	1.18	2/2125 (0.1%)	1.15	1/2886 (0.0%)
1	B	1.17	2/2133 (0.1%)	1.18	2/2897 (0.1%)
All	All	1.17	4/4258 (0.1%)	1.17	3/5783 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	SER	CA-CB	-6.36	1.44	1.53
1	A	123	MET	CG-SD	5.36	1.94	1.80
1	B	267	SER	CA-CB	-5.28	1.45	1.53
1	B	134	SER	CA-CB	-5.23	1.46	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	MET	N-CA-C	-6.02	104.72	111.28
1	A	172	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	7	PRO	CB-CA-C	-5.83	103.46	111.21

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	2099	0	2166	14	0
1	B	2107	0	2172	17	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
3	A	7	0	9	4	0
3	B	7	0	10	0	0
4	A	15	0	0	1	0
4	B	15	0	0	4	0
5	A	344	0	0	4	0
5	B	360	0	0	4	0
All	All	5050	0	4407	29	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 3.

All (29) 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:110:GLN:HB2	3:A:3402:PEG:H42	1.37	1.02
1:A:110:GLN:CB	3:A:3402:PEG:H42	2.19	0.68
1:A:123:MET:HE2	1:A:175:LEU:HD13	1.74	0.68
1:B:5:ASN:N	5:B:4203:HOH:O	2.28	0.66
1:A:96:ASN:ND2	1:B:245:ASN:HD22	1.94	0.65
1:B:206:LEU:HD22	1:B:206:LEU:O	1.97	0.64
1:A:193:VAL:HG13	1:A:198:GLU:HB2	1.81	0.62
3:A:3402:PEG:H11	5:A:3725:HOH:O	2.04	0.58
1:B:215:ALA:HB3	5:B:4201:HOH:O	2.08	0.53
4:A:3403:A1D7O:CAJ	5:A:3743:HOH:O	2.57	0.52
1:B:6:LYS:HB3	1:B:29:GLY:O	2.10	0.52
1:B:214:MET:HA	1:B:217:GLN:HE21	1.75	0.52
1:A:182:VAL:HG22	1:B:182:VAL:HG22	1.92	0.51
1:B:212:ALA:HA	5:B:4201:HOH:O	2.10	0.51
1:A:116:SER:HB2	5:A:3779:HOH:O	2.11	0.51
1:B:179:MET:HE1	4:B:4103:A1D7O:CAI	2.40	0.51
1:B:179:MET:HE1	4:B:4103:A1D7O:N	2.26	0.51
1:A:110:GLN:HB2	3:A:3402:PEG:C4	2.27	0.49
1:B:206:LEU:HD22	1:B:206:LEU:C	2.40	0.46
1:A:271:LYS:HD2	5:A:3519:HOH:O	2.16	0.46
1:B:179:MET:CE	4:B:4103:A1D7O:CAI	2.94	0.45
1:B:212:ALA:HB2	5:B:4460:HOH:O	2.16	0.45
1:A:120:GLY:HA2	1:A:137:LEU:O	2.18	0.44
1:A:218:LEU:N	1:A:219:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:NH1	1:B:206:LEU:HD23	2.33	0.43
1:B:120:GLY:HA2	1:B:137:LEU:O	2.19	0.43
1:B:179:MET:HE1	4:B:4103:A1D7O:CAH	2.49	0.43
1:A:218:LEU:N	1:A:219:PRO:HD2	2.35	0.42
1:A:123:MET:HE2	1:B:210:LEU:HD13	2.01	0.41

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	286/293 (98%)	283 (99%)	3 (1%)	0	100	100
1	B	287/293 (98%)	282 (98%)	5 (2%)	0	100	100
All	All	573/586 (98%)	565 (99%)	8 (1%)	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	230/235 (98%)	227 (99%)	3 (1%)	65	28
1	B	231/235 (98%)	229 (99%)	2 (1%)	75	46
All	All	461/470 (98%)	456 (99%)	5 (1%)	70	35

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	A	167	LYS
1	A	214	MET
1	B	206	LEU
1	B	217	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	48	GLN
1	A	96	ASN
1	A	131	GLN
1	A	217	GLN
1	A	245	ASN
1	B	48	GLN
1	B	96	ASN
1	B	217	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	PEG	B	4102	-	6,6,6	0.15	0	5,5,5	0.18	0
4	A1D7O	A	3403	-	15,16,16	2.08	2 (13%)	19,21,21	2.06	5 (26%)
4	A1D7O	B	4103	-	15,16,16	1.82	2 (13%)	19,21,21	1.91	5 (26%)
3	PEG	A	3402	-	6,6,6	0.83	0	5,5,5	0.20	0
2	NAP	B	4101	-	45,52,52	1.36	9 (20%)	56,80,80	1.22	5 (8%)
2	NAP	A	3401	-	45,52,52	1.33	6 (13%)	56,80,80	1.37	7 (12%)

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	PEG	B	4102	-	-	1/4/4/4	-
4	A1D7O	A	3403	-	-	2/4/17/17	0/2/2/2
4	A1D7O	B	4103	-	-	2/4/17/17	0/2/2/2
3	PEG	A	3402	-	-	4/4/4/4	-
2	NAP	B	4101	-	-	5/31/67/67	0/5/5/5
2	NAP	A	3401	-	-	5/31/67/67	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3403	A1D7O	CAG-CAH	-6.16	1.40	1.51
4	B	4103	A1D7O	CAG-CAH	-5.24	1.42	1.51
4	A	3403	A1D7O	CAN-C	-4.00	1.40	1.50
4	B	4103	A1D7O	CAN-C	-3.72	1.41	1.50
2	B	4101	NAP	O7N-C7N	3.47	1.30	1.24
2	B	4101	NAP	C7N-N7N	-3.16	1.26	1.33
2	A	3401	NAP	C2A-N3A	2.95	1.36	1.32
2	B	4101	NAP	C4N-C3N	2.84	1.44	1.39
2	A	3401	NAP	C4A-N3A	-2.62	1.32	1.35
2	B	4101	NAP	C2A-N3A	2.60	1.36	1.32
2	A	3401	NAP	C5A-N7A	-2.52	1.30	1.39
2	B	4101	NAP	C2N-N1N	2.48	1.38	1.35
2	B	4101	NAP	P2B-O3X	-2.39	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3401	NAP	O4D-C1D	-2.36	1.37	1.41
2	B	4101	NAP	O4B-C1B	2.29	1.44	1.41
2	B	4101	NAP	C6A-N1A	-2.24	1.27	1.37
2	B	4101	NAP	C2D-C1D	-2.22	1.50	1.53
2	A	3401	NAP	C2N-C3N	-2.22	1.35	1.39
2	A	3401	NAP	P2B-O2B	2.06	1.63	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4103	A1D7O	CAA-CAD-N	-4.94	103.45	111.11
4	B	4103	A1D7O	CA-C-CAN	4.75	123.74	113.58
4	A	3403	A1D7O	CAH-CAG-N	4.65	122.15	113.12
4	A	3403	A1D7O	CAG-N-CAD	4.26	120.55	111.06
2	A	3401	NAP	C3N-C7N-N7N	4.16	122.74	117.75
4	A	3403	A1D7O	CA-C-CAN	3.53	121.13	113.58
2	B	4101	NAP	C3N-C7N-N7N	-3.52	113.52	117.75
2	B	4101	NAP	O7N-C7N-C3N	3.30	123.58	119.63
2	A	3401	NAP	N3A-C2A-N1A	-3.25	123.60	128.68
2	A	3401	NAP	C1B-N9A-C4A	-3.02	121.33	126.64
4	B	4103	A1D7O	CAG-N-CA	-2.74	106.92	110.53
2	A	3401	NAP	C2A-N1A-C6A	2.74	123.44	118.75
4	A	3403	A1D7O	CAG-CAH-CAI	-2.69	115.72	120.77
4	A	3403	A1D7O	CAG-CAH-CAM	2.49	125.44	120.77
2	B	4101	NAP	N3A-C2A-N1A	-2.46	124.84	128.68
4	B	4103	A1D7O	CAO-CAN-C	-2.45	108.52	113.05
2	A	3401	NAP	N6A-C6A-N1A	2.34	123.43	118.57
2	B	4101	NAP	O4D-C1D-C2D	-2.33	103.52	106.93
2	B	4101	NAP	C2A-N1A-C6A	2.29	122.68	118.75
2	A	3401	NAP	C6N-N1N-C2N	-2.22	119.95	121.97
4	B	4103	A1D7O	O-C-CAN	-2.11	116.09	123.00
2	A	3401	NAP	C5A-C6A-N6A	-2.07	117.20	120.35

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3401	NAP	C5D-O5D-PN-O2N
2	A	3401	NAP	O4D-C1D-N1N-C2N
2	B	4101	NAP	C2B-O2B-P2B-O3X
2	B	4101	NAP	C5D-O5D-PN-O1N
2	B	4101	NAP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
4	B	4103	A1D7O	CAH-CAG-N-CA
4	B	4103	A1D7O	CAH-CAG-N-CAD
4	A	3403	A1D7O	CAH-CAG-N-CA
4	A	3403	A1D7O	CAH-CAG-N-CAD
3	A	3402	PEG	O2-C3-C4-O4
2	A	3401	NAP	C5D-O5D-PN-O3
2	B	4101	NAP	C5D-O5D-PN-O3
3	A	3402	PEG	C1-C2-O2-C3
3	B	4102	PEG	C4-C3-O2-C2
2	A	3401	NAP	O4B-C4B-C5B-O5B
2	B	4101	NAP	O4B-C4B-C5B-O5B
3	A	3402	PEG	O1-C1-C2-O2
2	A	3401	NAP	C5D-O5D-PN-O1N
3	A	3402	PEG	C4-C3-O2-C2

There are no ring outliers.

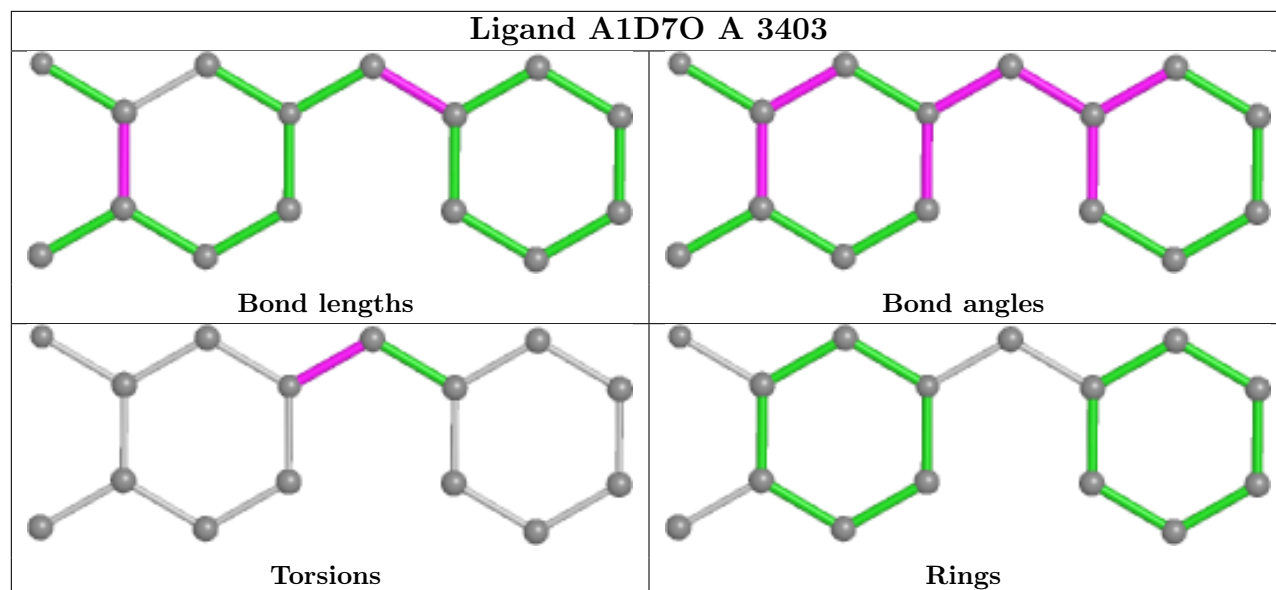
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3403	A1D7O	1	0
4	B	4103	A1D7O	4	0
3	A	3402	PEG	4	0

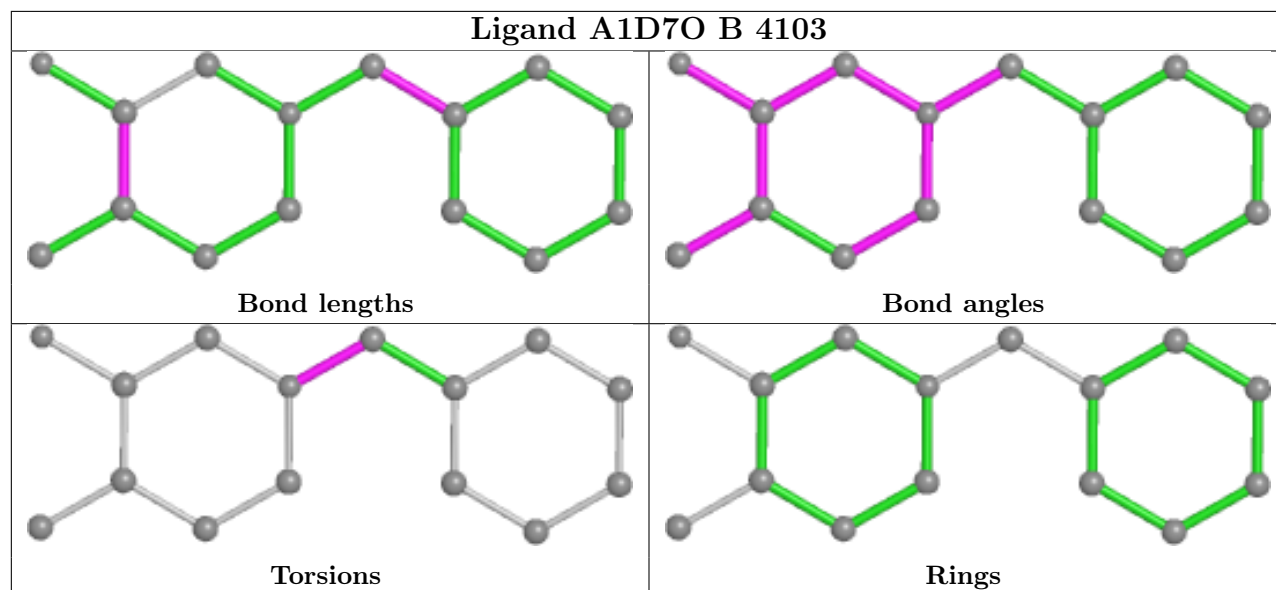
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

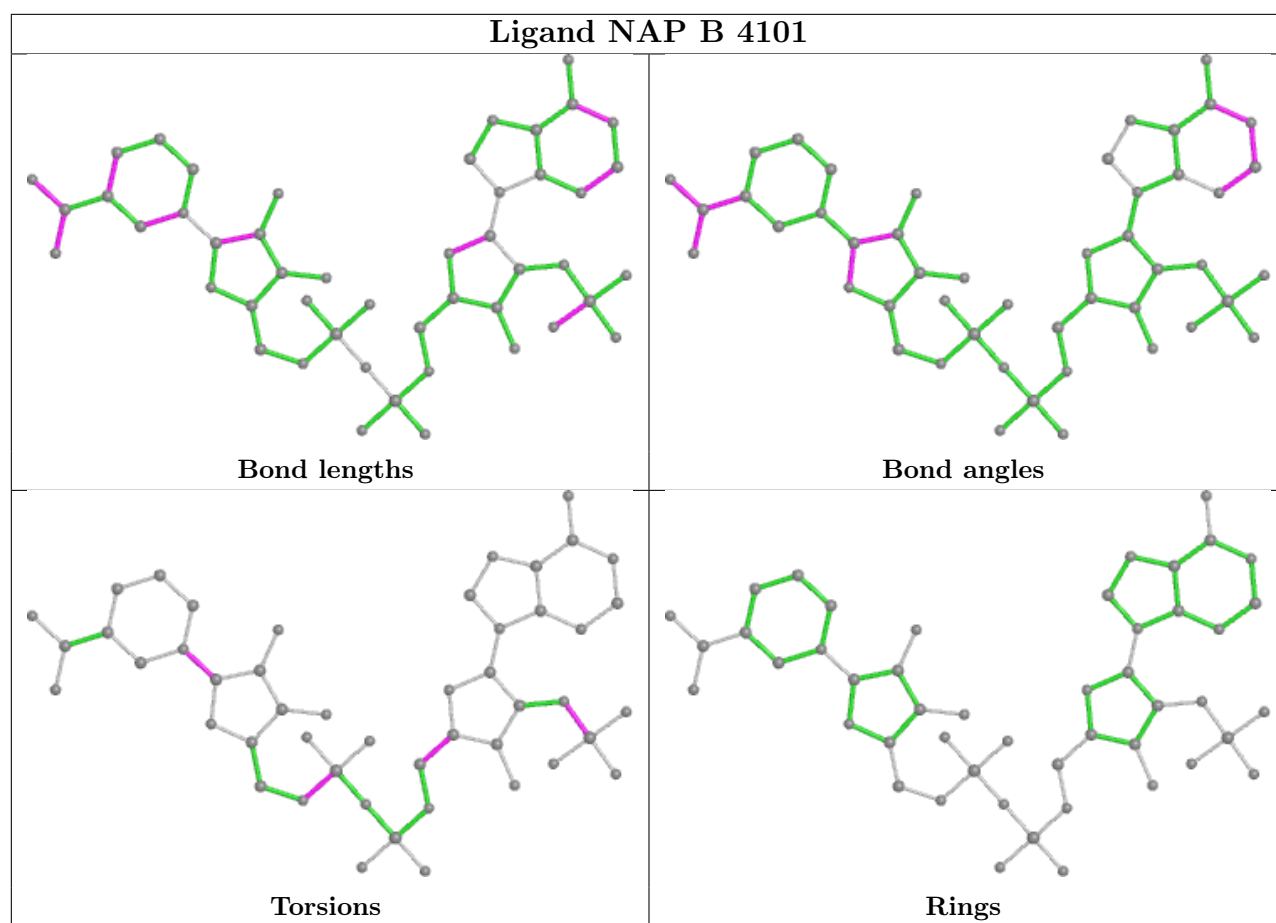


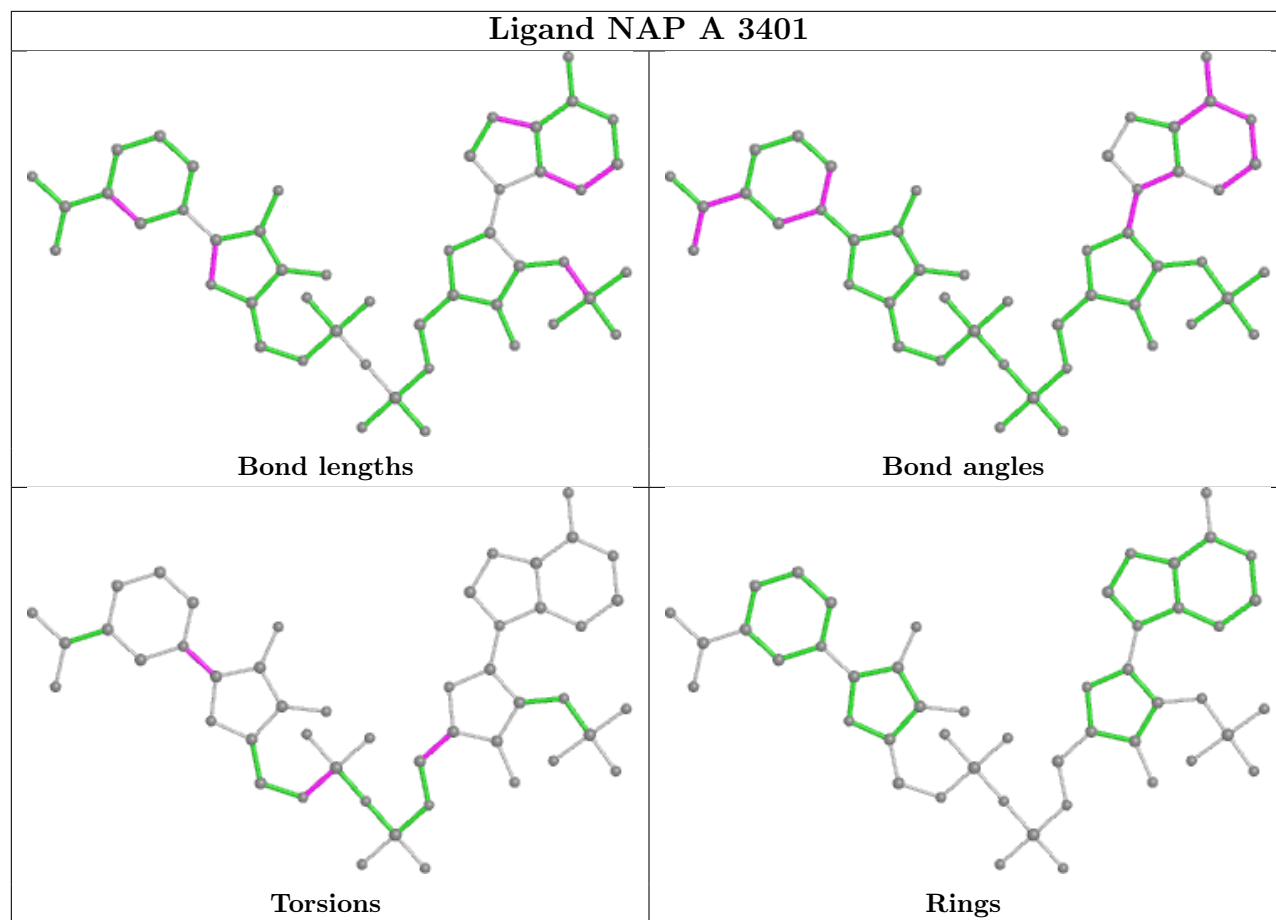
## Ligand A1D7O A 3403



## Ligand A1D7O B 4103







## 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	288/293 (98%)	0.46	21 (7%) 22 27	8, 13, 27, 39	0
1	B	289/293 (98%)	0.58	22 (7%) 21 25	9, 13, 27, 50	0
All	All	577/586 (98%)	0.52	43 (7%) 22 26	8, 13, 28, 50	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	VAL	7.7
1	B	212	ALA	5.4
1	B	210	LEU	4.8
1	B	289	LEU	4.5
1	B	206	LEU	4.3
1	B	5	ASN	3.8
1	B	215	ALA	3.8
1	B	214	MET	3.7
1	A	210	LEU	3.7
1	A	30	CYS	3.7
1	B	84	ILE	3.6
1	B	216	ASP	3.6
1	A	212	ALA	3.6
1	A	132	PRO	3.6
1	A	214	MET	3.5
1	A	208	SER	3.4
1	A	209	PRO	3.3
1	B	30	CYS	3.3
1	B	213	SER	3.2
1	A	84	ILE	3.1
1	B	207	ALA	3.0
1	A	133	SER	2.9
1	A	123	MET	2.9
1	B	6	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	208	SER	2.8
1	A	206	LEU	2.8
1	B	217	GLN	2.7
1	A	213	SER	2.5
1	B	209	PRO	2.5
1	B	179	MET	2.5
1	A	211	VAL	2.4
1	A	218	LEU	2.4
1	B	293	TRP	2.3
1	B	88	GLY	2.3
1	A	83	VAL	2.2
1	A	207	ALA	2.2
1	A	201	VAL	2.2
1	B	218	LEU	2.1
1	B	82	GLU	2.1
1	A	219	PRO	2.1
1	A	217	GLN	2.1
1	A	252	GLU	2.1
1	A	215	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
4	A1D7O	B	4103	15/15	0.66	0.21	47,51,54,55	0
3	PEG	B	4102	7/7	0.70	0.17	52,56,56,58	0
4	A1D7O	A	3403	15/15	0.76	0.17	43,45,47,48	0
3	PEG	A	3402	7/7	0.88	0.12	11,26,37,38	0

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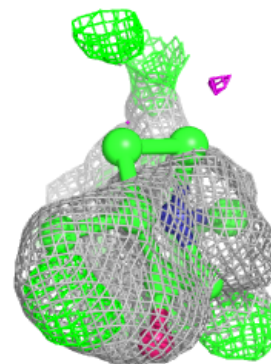
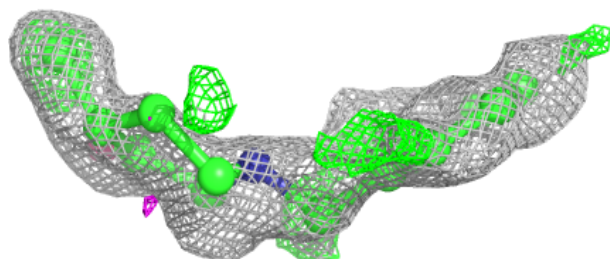
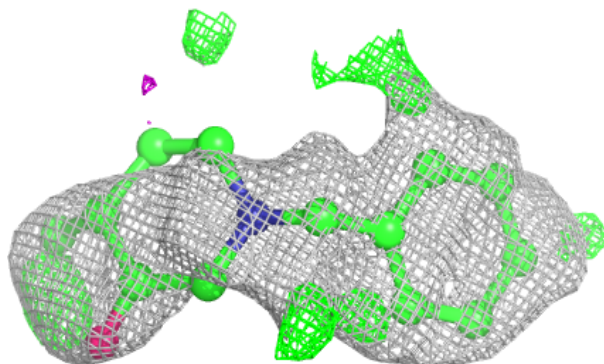
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	A	3401	48/48	0.99	0.04	8,9,12,15	0
2	NAP	B	4101	48/48	0.99	0.04	8,10,12,15	0

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.

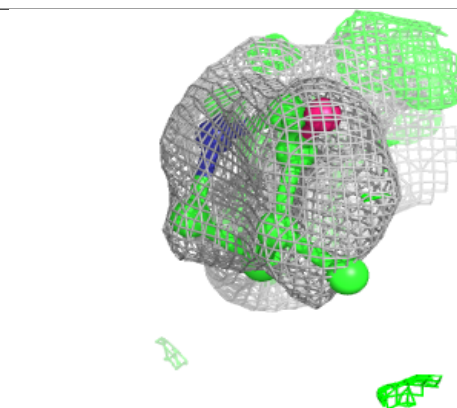
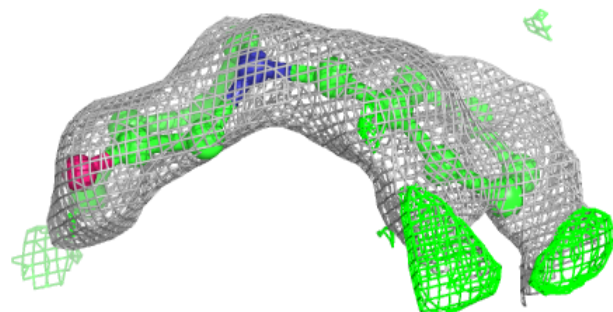
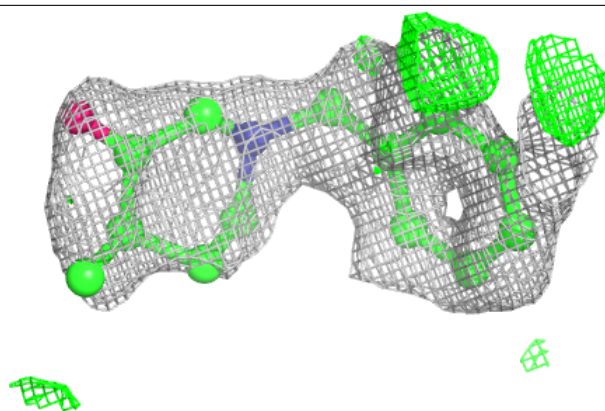
**Electron density around A1D7O B 4103:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

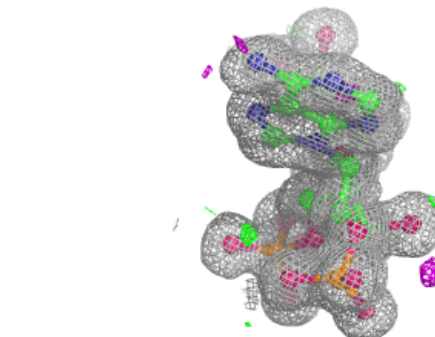
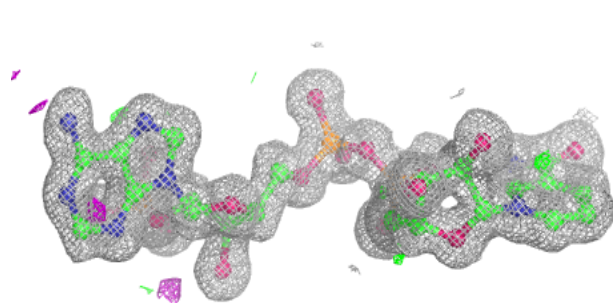
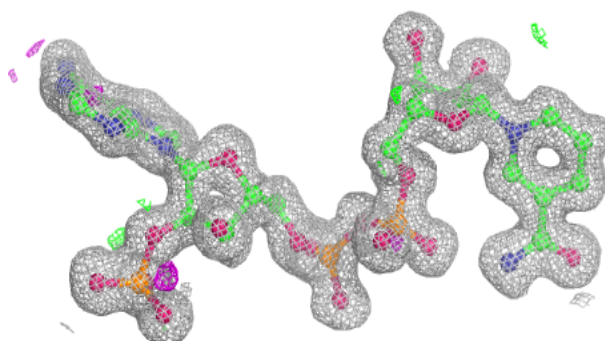


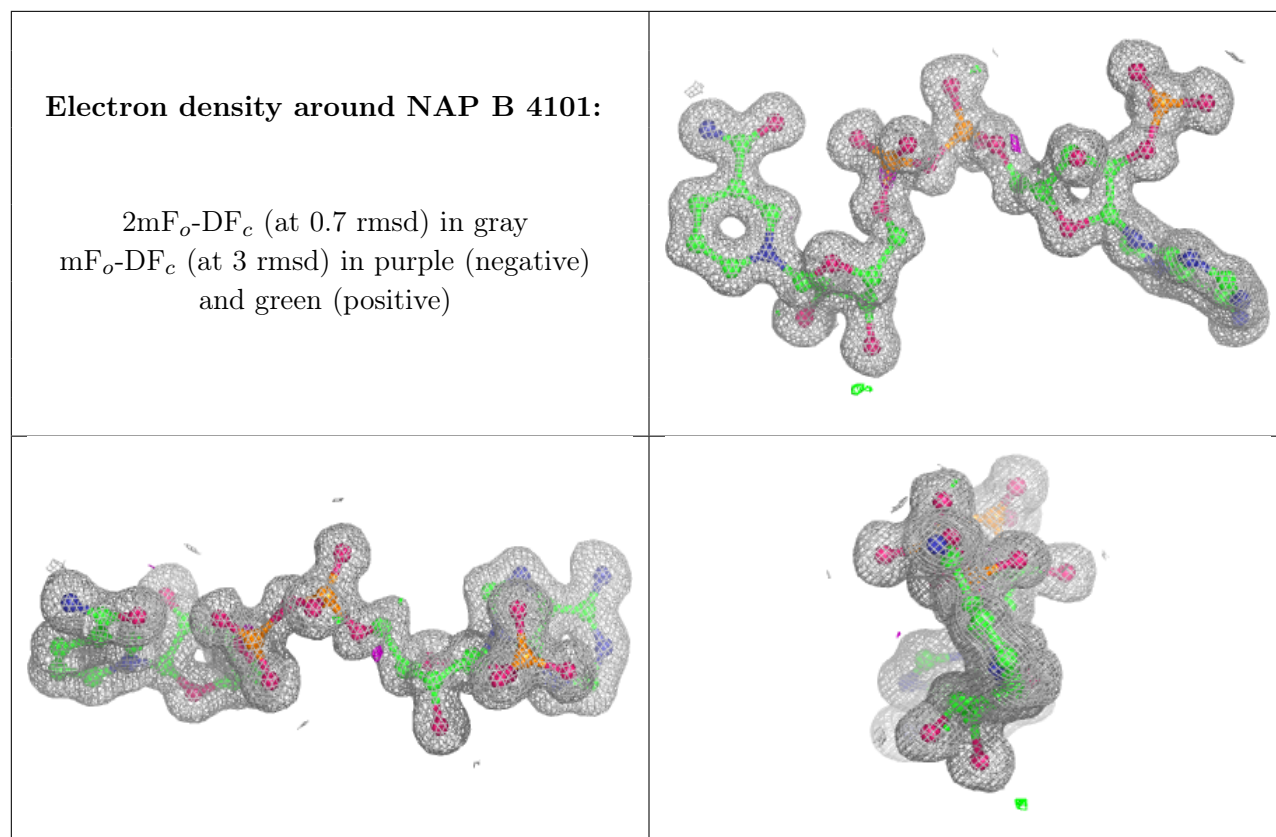
**Electron density around A1D7O A 3403:**

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

**Electron density around NAP A 3401:**

$2mF_o-DF_c$  (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.