



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 06:21 pm BST

PDB ID : 4PIV  
Title : Human Fatty Acid Synthase Psi/KR Tri-Domain with NADPH and GSK2194069  
Authors : Williams, S.P.; Wang, L.; Brown, K.K.; Parrish, C.A.; Hardwicke, M.A.  
Deposited on : 2014-05-09  
Resolution : 2.30 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.

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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

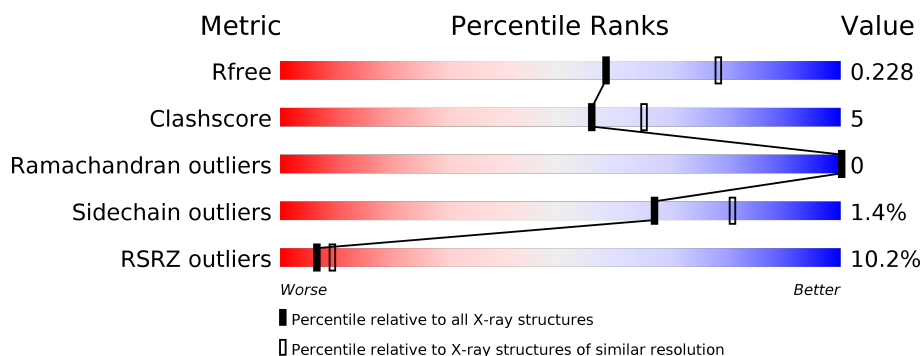
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	660	<div> <div>10%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	B	660	<div> <div>9%</div> <div>80%</div> <div>12%</div> <div>8%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9351 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.

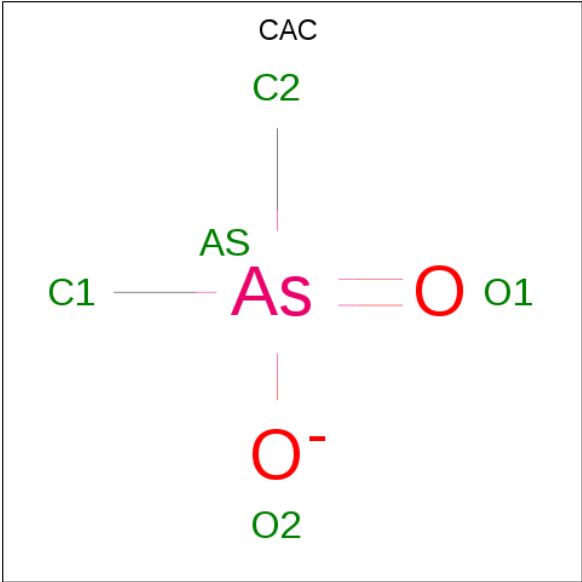
- Molecule 1 is a protein called Fatty acid synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	610	Total	C	N	O	S	0	1	0
			4462	2837	786	815	24			
1	B	610	Total	C	N	O	S	0	0	0
			4481	2847	783	827	24			

There are 16 discrepancies between the modelled and reference sequences:

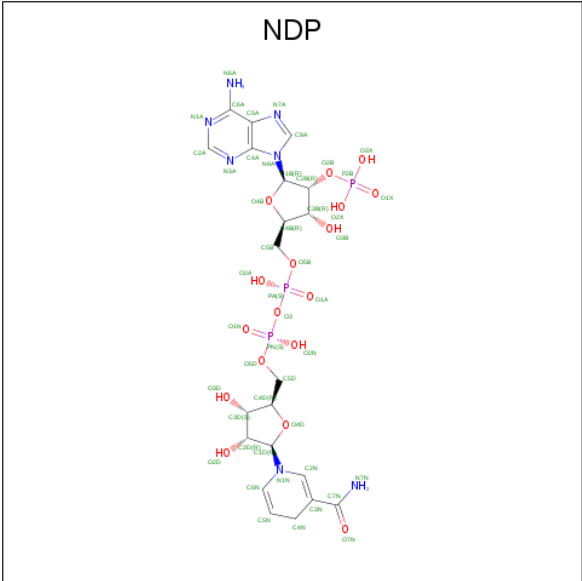
Chain	Residue	Modelled	Actual	Comment	Reference
A	1109	MET	-	initiating methionine	UNP P49327
A	1876	GLY	PRO	engineered mutation	UNP P49327
A	2115	HIS	-	expression tag	UNP P49327
A	2116	HIS	-	expression tag	UNP P49327
A	2117	HIS	-	expression tag	UNP P49327
A	2118	HIS	-	expression tag	UNP P49327
A	2119	HIS	-	expression tag	UNP P49327
A	2120	HIS	-	expression tag	UNP P49327
B	1109	MET	-	initiating methionine	UNP P49327
B	1876	GLY	PRO	engineered mutation	UNP P49327
B	2115	HIS	-	expression tag	UNP P49327
B	2116	HIS	-	expression tag	UNP P49327
B	2117	HIS	-	expression tag	UNP P49327
B	2118	HIS	-	expression tag	UNP P49327
B	2119	HIS	-	expression tag	UNP P49327
B	2120	HIS	-	expression tag	UNP P49327

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



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

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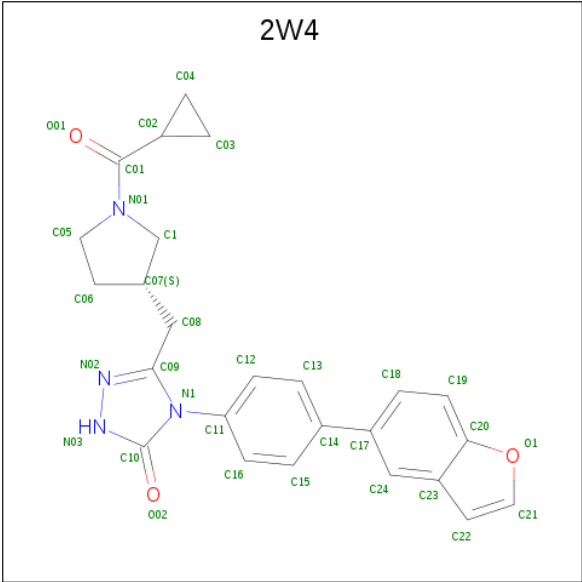
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 4-[4-(1-benzofuran-5-yl)phenyl]-5-[[ (3S)-1-(cyclopropylcarbonyl)pyrrolidin-3-yl]methyl]-2,4-dihydro-3H-1,2,4-triazol-3-one (three-letter code: 2W4) (formula: C<sub>25</sub>H<sub>24</sub>N<sub>4</sub>O<sub>3</sub>).

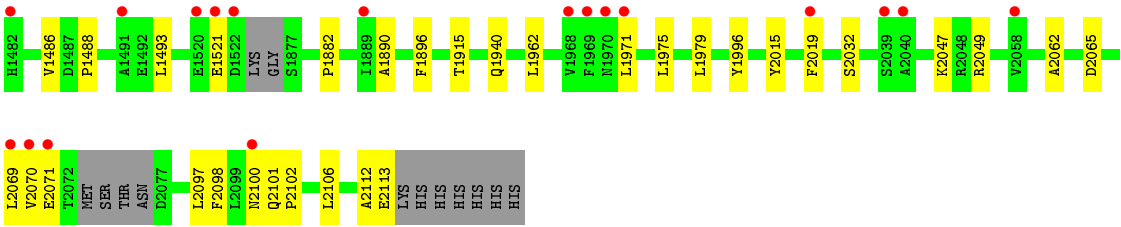


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			32	25	4	3		
5	B	1	Total	C	N	O	0	0
			32	25	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	102	Total	O	0	0
			102	102		
6	B	118	Total	O	0	0
			118	118		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.22Å 85.76Å 86.00Å 65.49° 89.96° 87.22°	Depositor
Resolution (Å)	28.55 – 2.30 28.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (28.55-2.30) 95.5 (28.55-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0109, BUSTER	Depositor
R, $R_{free}$	0.214 , 0.246 0.199 , 0.228	Depositor DCC
$R_{free}$ test set	3898 reflections (7.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9351	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: CAC, NDP, 2W4, SO4

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	0.33	0/4552	0.55	0/6200
1	B	0.33	0/4568	0.55	0/6216
All	All	0.33	0/9120	0.55	0/12416

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	4462	0	4365	39	0
1	B	4481	0	4404	51	0
2	A	4	0	0	2	0
2	B	4	0	0	2	0
3	A	48	0	26	1	0
3	B	48	0	26	1	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	32	0	24	1	0
5	B	32	0	24	2	0
6	A	102	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	118	0	0	1	0
All	All	9351	0	8869	92	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.

The worst 5 of 92 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:1110:GLN:HE22	1:A:2087:ARG:H	1.25	0.84
1:A:2062:ALA:HB1	1:A:2069:LEU:HD21	1.65	0.78
1:B:1338:GLU:HB3	1:B:1407:THR:HG22	1.66	0.75
1:B:2101:GLN:OE1	1:B:2101:GLN:HA	1.89	0.72
1:A:1110:GLN:NE2	1:A:2087:ARG:H	1.89	0.71

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	599/660 (91%)	588 (98%)	11 (2%)	0	100	100
1	B	598/660 (91%)	587 (98%)	11 (2%)	0	100	100
All	All	1197/1320 (91%)	1175 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	454/548 (83%)	450 (99%)	4 (1%)	78	89
1	B	462/548 (84%)	453 (98%)	9 (2%)	57	73
All	All	916/1096 (84%)	903 (99%)	13 (1%)	67	81

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1174	SER
1	B	1206	ARG
1	B	1996	TYR
1	B	1144	LEU
1	B	1896	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1110	GLN
1	A	1176	GLN
1	B	1135	GLN
1	B	1176	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

10 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
2	CAC	A	2201	1	0,3,4	0.00	-	0,3,6	0.00	-
3	NDP	B	2202	-	45,52,52	0.77	1 (2%)	53,80,80	1.66	8 (15%)
4	SO4	A	2204	-	4,4,4	0.38	0	6,6,6	0.06	0
5	2W4	A	2205	-	31,37,37	0.68	1 (3%)	36,54,54	0.80	1 (2%)
5	2W4	B	2205	-	31,37,37	0.62	1 (3%)	36,54,54	0.79	1 (2%)
3	NDP	A	2202	-	45,52,52	0.77	1 (2%)	53,80,80	1.62	8 (15%)
2	CAC	B	2201	1	0,3,4	0.00	-	0,3,6	0.00	-
4	SO4	B	2203	-	4,4,4	0.31	0	6,6,6	0.22	0
4	SO4	B	2204	-	4,4,4	0.35	0	6,6,6	0.11	0
4	SO4	A	2203	-	4,4,4	0.33	0	6,6,6	0.09	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
5	2W4	A	2205	-	-	0/20/31/31	0/6/6/6
3	NDP	B	2202	-	-	8/30/77/77	0/4/5/5
3	NDP	A	2202	-	-	8/30/77/77	0/4/5/5
5	2W4	B	2205	-	-	0/20/31/31	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2202	NDP	O4B-C1B	2.43	1.44	1.41
3	B	2202	NDP	O4B-C1B	2.32	1.44	1.41
5	A	2205	2W4	C23-C20	-2.17	1.38	1.43
5	B	2205	2W4	C23-C20	-2.11	1.39	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2202	NDP	C1D-N1N-C6N	-5.12	109.79	120.83
3	A	2202	NDP	N3A-C2A-N1A	-4.92	120.99	128.68
3	B	2202	NDP	N3A-C2A-N1A	-4.70	121.33	128.68
3	A	2202	NDP	C1D-N1N-C6N	-4.41	111.33	120.83
3	B	2202	NDP	O4D-C1D-N1N	4.13	116.13	108.06

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2202	NDP	C5D-O5D-PN-O2N
3	A	2202	NDP	C5D-O5D-PN-O2N
3	B	2202	NDP	C1B-C2B-O2B-P2B
3	B	2202	NDP	C3B-C2B-O2B-P2B
3	B	2202	NDP	C5D-O5D-PN-O3

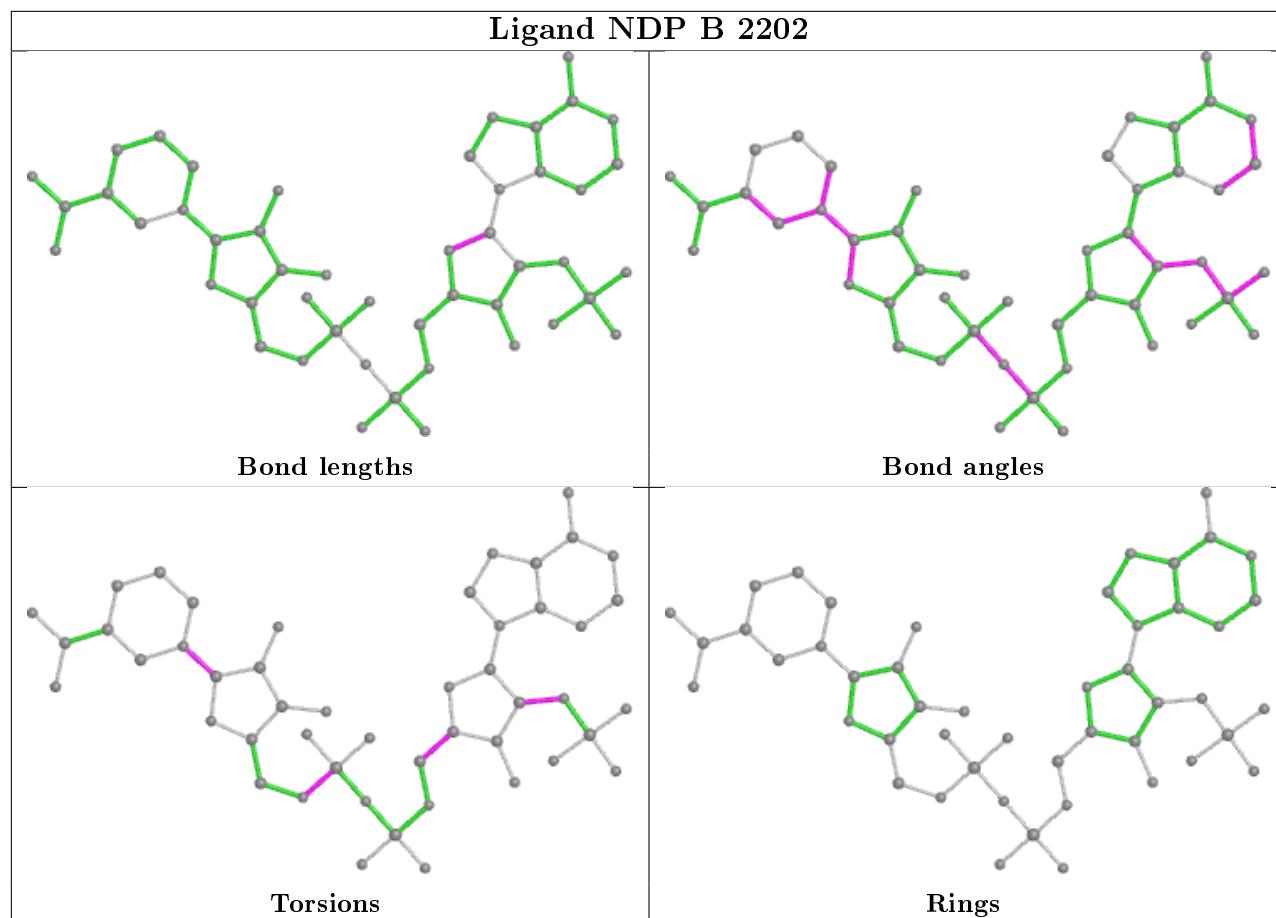
There are no ring outliers.

6 monomers are involved in 7 short contacts:

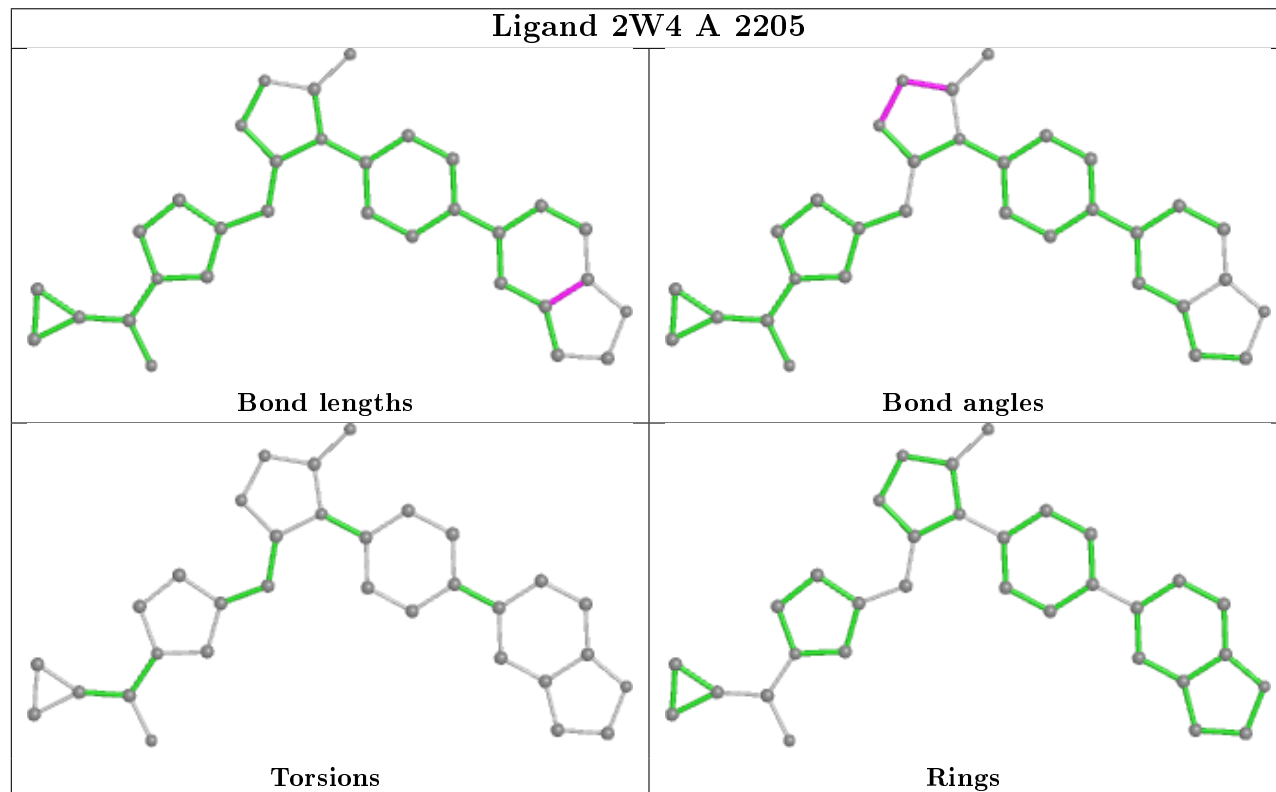
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2201	CAC	2	0
3	B	2202	NDP	1	0
5	A	2205	2W4	1	0
5	B	2205	2W4	2	0
3	A	2202	NDP	1	0
2	B	2201	CAC	2	0

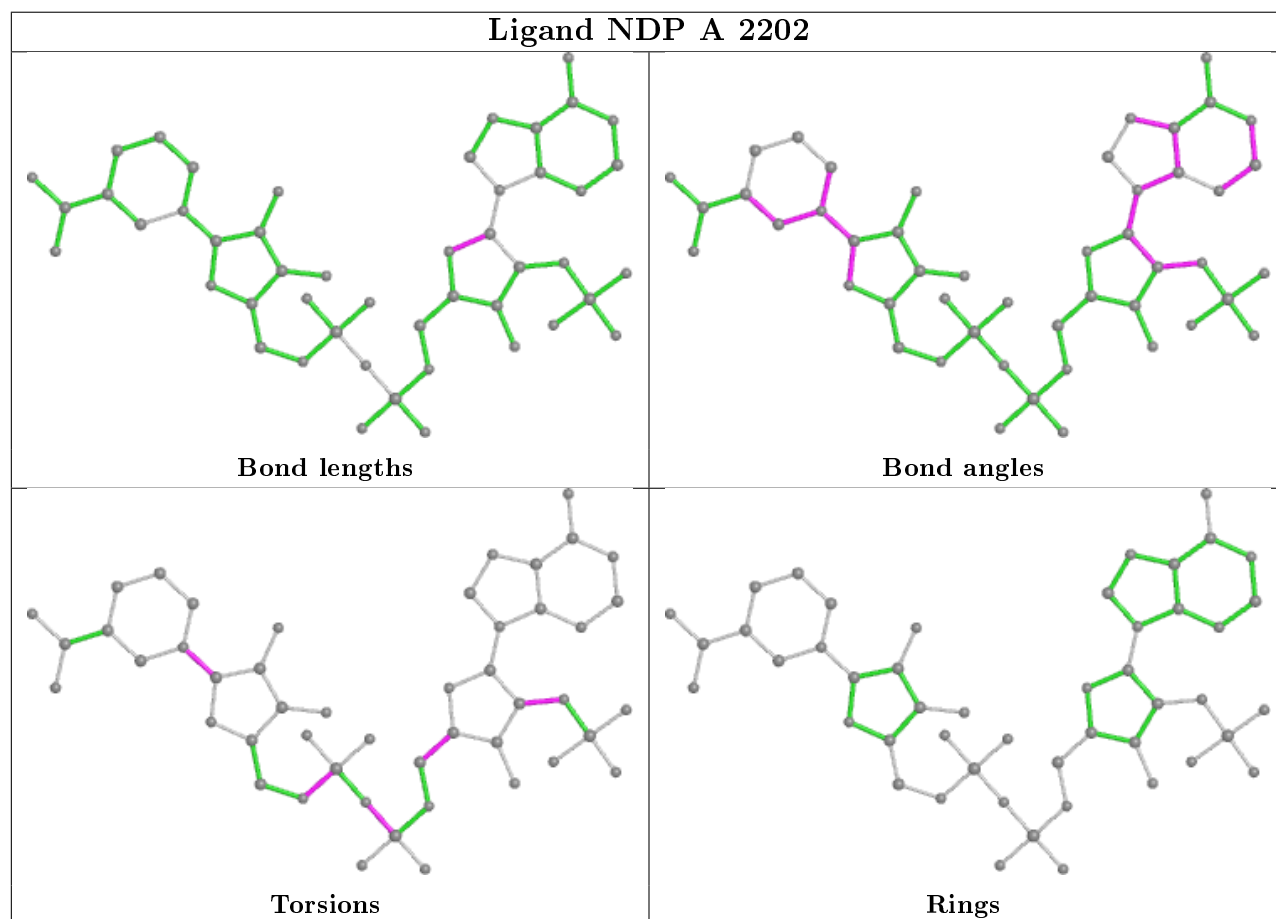
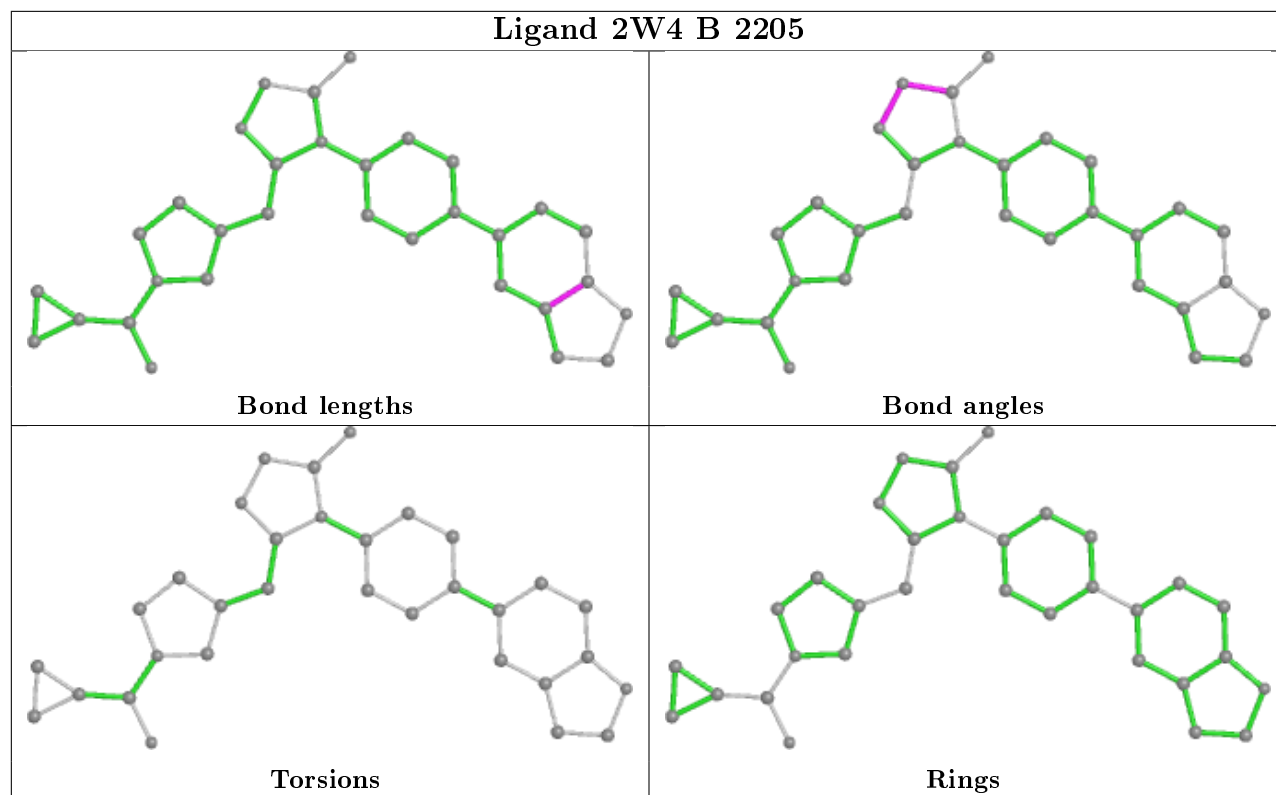
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 NDP B 2202



## Ligand 2W4 A 2205







## 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	610/660 (92%)	0.53	63 (10%) 6 9	25, 39, 67, 86	2 (0%)
1	B	610/660 (92%)	0.49	62 (10%) 6 9	22, 37, 70, 92	3 (0%)
All	All	1220/1320 (92%)	0.51	125 (10%) 6 9	22, 38, 70, 92	5 (0%)

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2075	THR	11.5
1	A	2070	VAL	9.1
1	A	2066	VAL	7.7
1	A	1145	VAL	6.9
1	B	1150	THR	6.8

### 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](#)

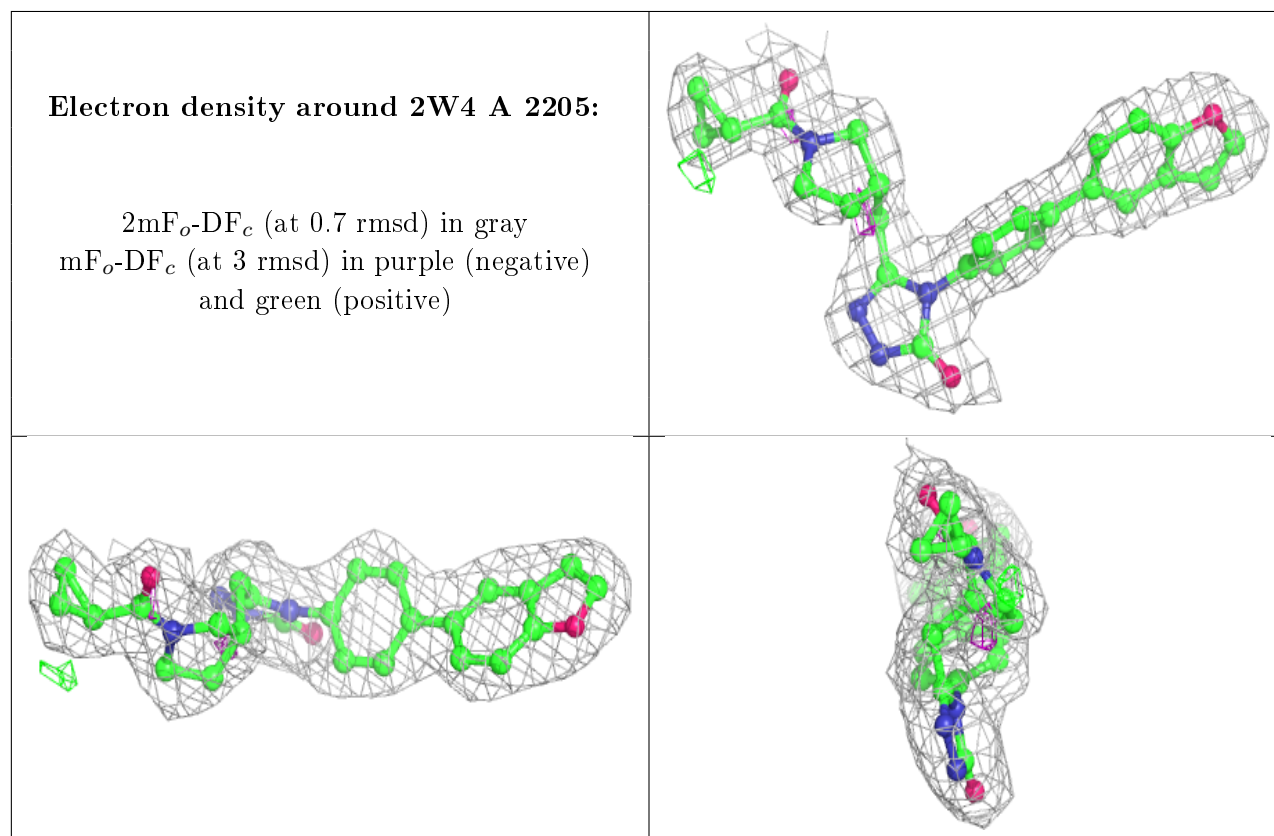
There are no carbohydrates in this entry.

### 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.

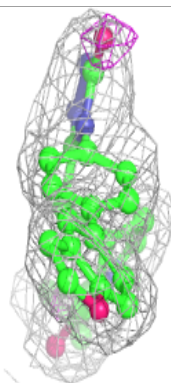
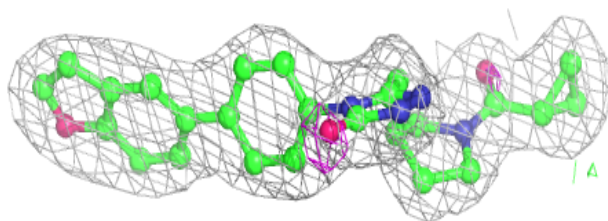
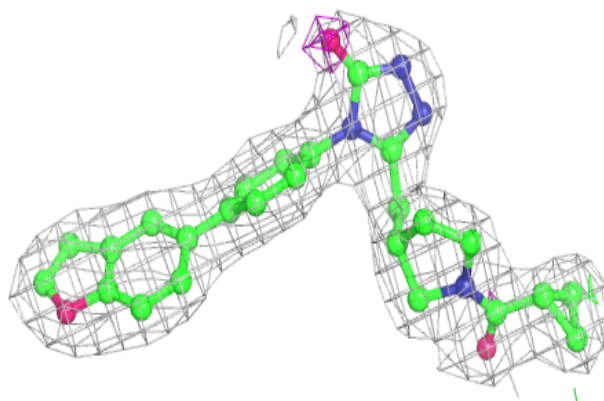
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	2204	5/5	0.88	0.18	74,74,77,78	0
5	2W4	A	2205	32/32	0.94	0.13	26,27,28,29	0
5	2W4	B	2205	32/32	0.94	0.13	24,25,28,30	0
4	SO4	B	2204	5/5	0.94	0.12	65,65,70,72	0
4	SO4	A	2203	5/5	0.94	0.23	60,63,65,66	0
3	NDP	A	2202	48/48	0.95	0.14	26,29,33,34	0
3	NDP	B	2202	48/48	0.96	0.12	24,26,30,31	0
4	SO4	B	2203	5/5	0.97	0.17	49,51,52,54	0
2	CAC	A	2201	4/5	0.97	0.15	38,38,40,41	0
2	CAC	B	2201	4/5	0.97	0.15	39,40,43,44	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.

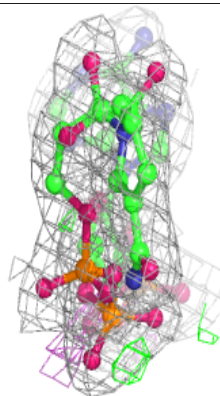
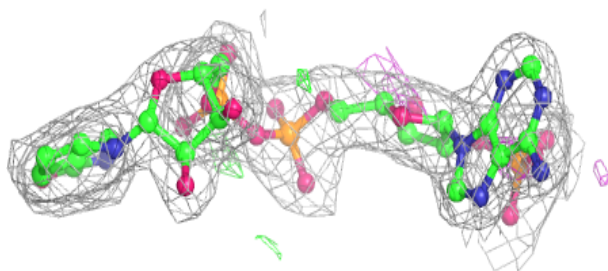
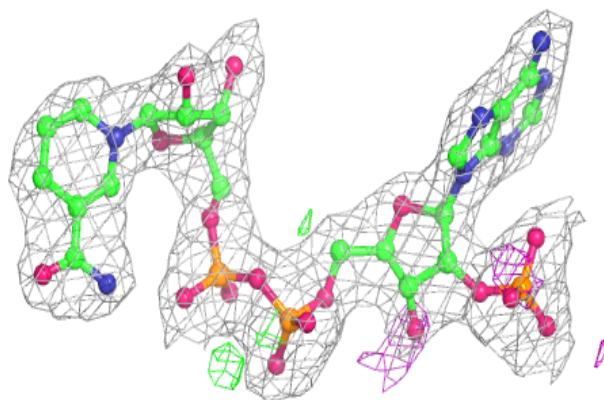


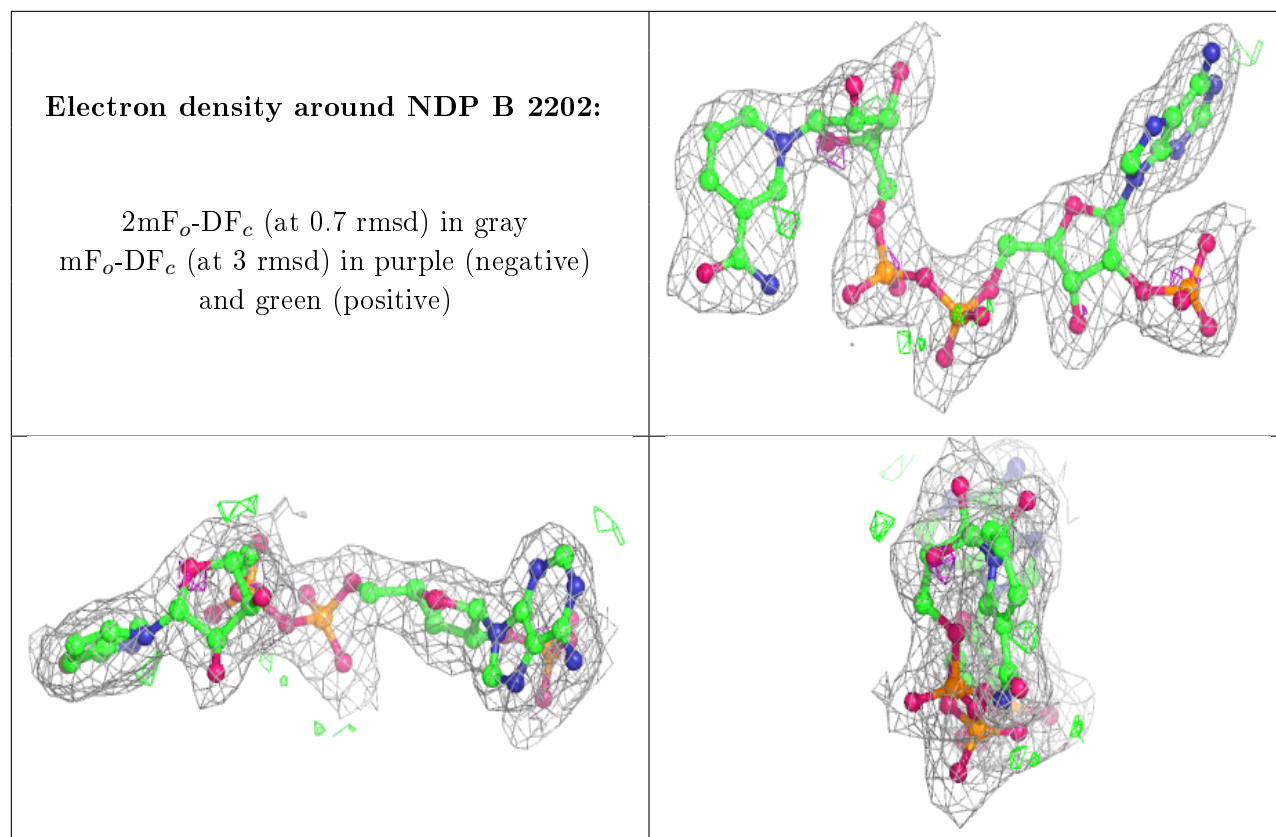
**Electron density around 2W4 B 2205:**

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

**Electron density around NDP A 2202:**

$2mF_o-DF_c$  (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.