



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:37 AM UTC

PDB ID : 4WK6 / pdb_00004wk6
Title : Crystal structure of 3-ketoacyl-(acyl-carrier-protein) reductase (FabG) (G141A) from *Vibrio cholerae* in complex with NADPH
Authors : Hou, J.; Zheng, H.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2014-10-01
Resolution : 2.21 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

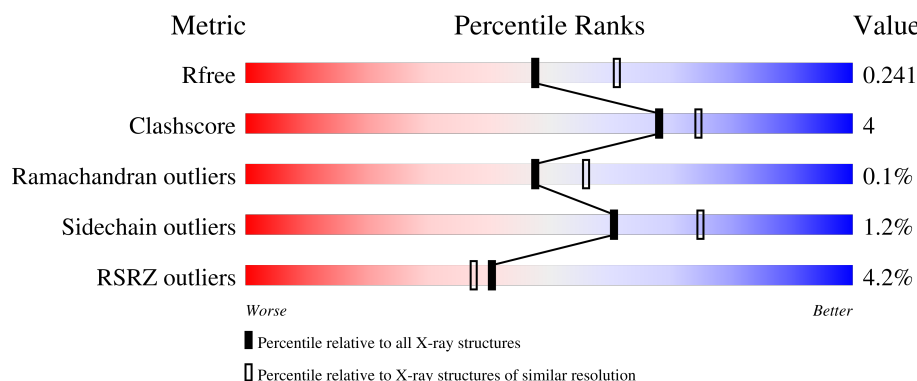
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

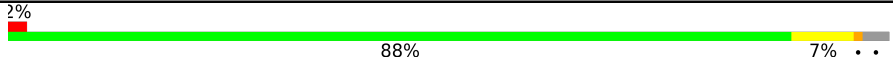
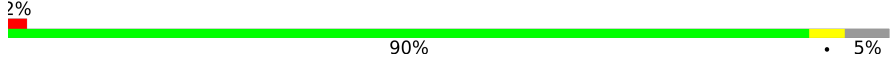
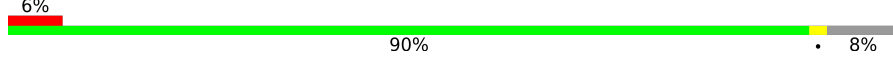
The reported resolution of this entry is 2.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 ≥ 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	251	
1	B	251	
1	C	251	
1	D	251	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6937 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 3-oxoacyl-[acyl-carrier protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1707	1059	298	340	10			
1	B	240	Total	C	N	O	S	0	1	0
			1734	1077	306	342	9			
1	C	238	Total	C	N	O	S	0	0	0
			1700	1059	299	333	9			
1	D	232	Total	C	N	O	S	0	0	0
			1569	981	275	306	7			

There are 16 discrepancies between the modelled and reference sequences:

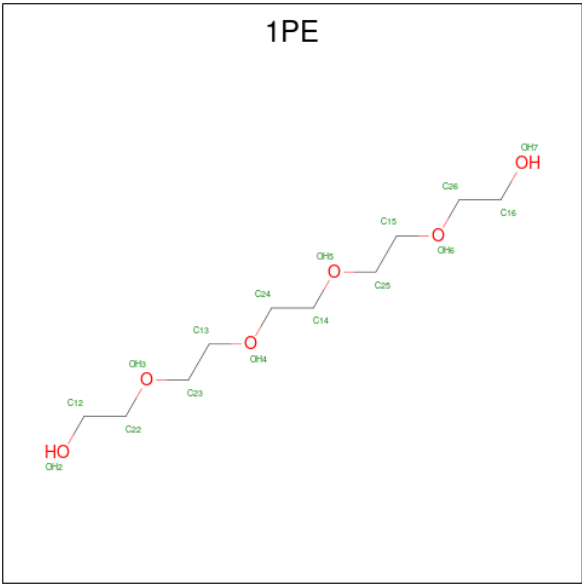
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP C2CCH9
A	-1	ASN	-	expression tag	UNP C2CCH9
A	0	ALA	-	expression tag	UNP C2CCH9
A	141	ALA	GLY	engineered mutation	UNP C2CCH9
B	-2	SER	-	expression tag	UNP C2CCH9
B	-1	ASN	-	expression tag	UNP C2CCH9
B	0	ALA	-	expression tag	UNP C2CCH9
B	141	ALA	GLY	engineered mutation	UNP C2CCH9
C	-2	SER	-	expression tag	UNP C2CCH9
C	-1	ASN	-	expression tag	UNP C2CCH9
C	0	ALA	-	expression tag	UNP C2CCH9
C	141	ALA	GLY	engineered mutation	UNP C2CCH9
D	-2	SER	-	expression tag	UNP C2CCH9
D	-1	ASN	-	expression tag	UNP C2CCH9
D	0	ALA	-	expression tag	UNP C2CCH9
D	141	ALA	GLY	engineered mutation	UNP C2CCH9

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	28	Total	O	0	0
			28	28		
4	C	29	Total	O	0	0
			29	29		
4	D	16	Total	O	0	0
			16	16		

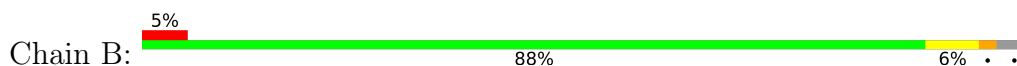
3 Residue-property plots [i](#)

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.

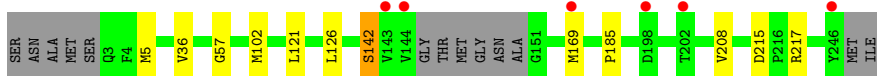
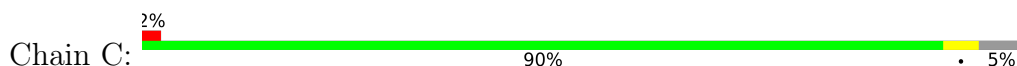
- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



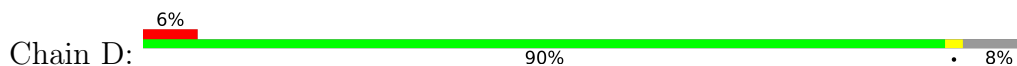
- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.90Å 110.34Å 117.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.00 – 2.21 27.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.1 (27.00-2.21) 98.5 (27.00-2.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.209 , 0.241 0.213 , 0.241	Depositor DCC
R_{free} test set	2512 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.752	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6937	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 1PE, NDP

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	0.97	1/1723 (0.1%)	0.97	4/2338 (0.2%)
1	B	0.96	1/1753 (0.1%)	0.97	4/2368 (0.2%)
1	C	0.96	0/1716	0.93	1/2322 (0.0%)
1	D	0.87	0/1583	0.89	1/2154 (0.0%)
All	All	0.94	2/6775 (0.0%)	0.94	10/9182 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	ALA	CA-C	-6.54	1.44	1.53
1	A	205	LEU	N-CA	5.03	1.52	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ALA	N-CA-C	-6.22	103.09	111.87
1	B	155	TYR	N-CA-CB	-5.85	100.68	110.39
1	B	140	VAL	CB-CA-C	5.74	119.34	110.96
1	A	204	THR	CA-C-N	5.54	129.46	120.60
1	A	204	THR	C-N-CA	5.54	129.46	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	VAL	N-CA-C	5.43	113.41	107.60
1	A	93	ILE	N-CA-C	5.30	114.23	106.55
1	B	153	ALA	N-CA-C	5.27	117.10	111.36
1	D	245	MET	N-CA-C	5.19	116.62	111.07
1	B	133	ARG	NE-CZ-NH1	-5.05	116.45	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	141	ALA	Peptide
1	C	142	SER	Peptide

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	1707	0	1672	24	0
1	B	1734	0	1724	10	0
1	C	1700	0	1683	13	0
1	D	1569	0	1490	10	0
2	A	27	0	11	3	0
2	B	31	0	11	0	0
2	C	27	0	11	0	0
2	D	27	0	11	0	0
3	D	16	0	22	0	0
4	A	26	0	0	1	0
4	B	28	0	0	0	0
4	C	29	0	0	0	0
4	D	16	0	0	0	0
All	All	6937	0	6635	48	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 4.

All (48) 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:C:5:MET:HE1	1:D:5:MET:SD	2.12	0.89
1:A:115:LEU:HD21	1:D:111:MET:HE1	1.59	0.83
1:C:5:MET:CE	1:D:5:MET:SD	2.67	0.82
1:A:93:ILE:HD12	1:A:93:ILE:H	1.52	0.75
1:B:102:MET:HE1	1:B:154:ASN:CB	2.19	0.72
1:A:245:MET:O	1:A:246:TYR:HB2	1.92	0.70
1:B:245:MET:O	1:B:246:TYR:HB2	1.93	0.69
1:B:144:VAL:HA	1:B:152:GLN:NE2	2.10	0.66
1:A:115:LEU:CD2	1:D:111:MET:CE	2.74	0.65
1:A:115:LEU:HD21	1:D:111:MET:CE	2.29	0.63
1:A:99:LEU:HD12	1:A:153:ALA:HB1	1.82	0.62
1:C:5:MET:HE3	1:D:5:MET:SD	2.39	0.61
1:A:115:LEU:CD2	1:D:111:MET:HE1	2.32	0.58
1:C:126:LEU:HD11	1:C:169:MET:HE1	1.85	0.58
1:C:126:LEU:CD1	1:C:169:MET:HE1	2.32	0.57
1:B:96:ASP:O	1:B:97:ASN:HB2	2.05	0.56
1:B:143:VAL:HG12	1:B:144:VAL:O	2.06	0.55
1:A:122:SER:HB3	1:A:169:MET:HE1	1.89	0.54
1:A:91:ALA:HB2	1:A:118:ILE:HD11	1.91	0.53
1:A:143:VAL:HG12	1:A:144:VAL:O	2.09	0.52
1:A:93:ILE:HG23	2:A:301:NDP:H51A	1.91	0.51
1:A:93:ILE:CG2	2:A:301:NDP:H51A	2.41	0.51
1:A:201:ARG:O	1:A:205:LEU:HG	2.10	0.50
1:A:21:ILE:HD12	1:A:143:VAL:CG2	2.43	0.49
1:A:21:ILE:CD1	1:A:143:VAL:CG2	2.91	0.49
1:A:92:GLY:HA2	1:A:142:SER:HB2	1.94	0.49
1:B:123:LYS:HE3	1:C:102:MET:O	2.13	0.48
1:B:102:MET:CE	1:B:154:ASN:CB	2.91	0.48
1:C:126:LEU:HD11	1:C:169:MET:CE	2.44	0.48
1:C:142:SER:HA	1:C:185:PRO:HD2	1.96	0.47
1:A:104:GLU:O	1:A:104:GLU:HG2	2.14	0.47
1:A:64:VAL:HG13	2:A:301:NDP:H2A	1.97	0.47
1:A:93:ILE:HD11	1:A:113:THR:HG22	1.97	0.46
1:A:93:ILE:HD12	1:A:93:ILE:N	2.23	0.46
1:A:21:ILE:HD12	1:A:143:VAL:HG23	1.98	0.46
1:C:36:VAL:O	1:C:57:GLY:HA3	2.16	0.45
1:D:127:ARG:HD3	1:D:127:ARG:H	1.81	0.45
1:B:142:SER:N	1:B:155:TYR:OH	2.50	0.45
1:A:115:LEU:HD23	1:D:111:MET:CE	2.47	0.45
1:B:144:VAL:HA	1:B:152:GLN:HE22	1.81	0.44
1:A:245:MET:O	1:A:246:TYR:CB	2.65	0.44
1:C:169:MET:HE3	1:C:169:MET:HB3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ASP:OD1	1:C:217:ARG:NH1	2.44	0.43
1:D:36:VAL:O	1:D:57:GLY:HA3	2.19	0.42
1:A:93:ILE:HA	4:A:426:HOH:O	2.19	0.41
1:C:102:MET:HE3	1:C:102:MET:HB2	1.98	0.40
1:B:36:VAL:O	1:B:57:GLY:HA3	2.22	0.40
1:C:126:LEU:HD13	1:C:169:MET:HE1	2.02	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	241/251 (96%)	237 (98%)	4 (2%)	0	100	100
1	B	237/251 (94%)	230 (97%)	6 (2%)	1 (0%)	30	33
1	C	234/251 (93%)	228 (97%)	6 (3%)	0	100	100
1	D	226/251 (90%)	224 (99%)	2 (1%)	0	100	100
All	All	938/1004 (93%)	919 (98%)	18 (2%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	97	ASN

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	165/189 (87%)	162 (98%)	3 (2%)	51	66
1	B	171/189 (90%)	169 (99%)	2 (1%)	63	76
1	C	165/189 (87%)	164 (99%)	1 (1%)	78	88
1	D	140/189 (74%)	138 (99%)	2 (1%)	59	73
All	All	641/756 (85%)	633 (99%)	8 (1%)	61	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ILE
1	A	121	LEU
1	A	169	MET
1	B	121	LEU
1	B	140	VAL
1	C	121	LEU
1	D	121	LEU
1	D	127	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	152	GLN
1	B	89	ASN
1	B	152	GLN
1	C	89	ASN
1	C	152	GLN
1	D	89	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	NDP	D	301	-	29,29,52	1.56	5 (17%)	44,45,80	2.16	14 (31%)
2	NDP	C	301	-	29,29,52	1.59	6 (20%)	44,45,80	2.05	15 (34%)
3	1PE	D	302	-	15,15,15	0.59	0	14,14,14	0.39	0
2	NDP	A	301	-	29,29,52	1.58	5 (17%)	44,45,80	1.96	15 (34%)
2	NDP	B	301	-	32,33,52	1.57	5 (15%)	50,52,80	1.95	13 (26%)

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
2	NDP	D	301	-	-	2/15/31/77	0/3/3/5
2	NDP	C	301	-	-	2/15/31/77	0/3/3/5
3	1PE	D	302	-	-	7/13/13/13	-
2	NDP	A	301	-	-	6/15/31/77	0/3/3/5
2	NDP	B	301	-	-	4/21/37/77	0/3/3/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NDP	C5A-C4A	5.38	1.48	1.39
2	B	301	NDP	C5A-C4A	4.64	1.47	1.39
2	D	301	NDP	C5A-C4A	4.09	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NDP	PA-O3	3.92	1.63	1.59
2	C	301	NDP	C5A-C4A	3.92	1.46	1.39
2	D	301	NDP	PA-O1A	3.82	1.62	1.50
2	C	301	NDP	PA-O1A	3.61	1.61	1.50
2	C	301	NDP	C8A-N7A	3.39	1.38	1.31
2	C	301	NDP	C5A-N7A	-3.30	1.33	1.39
2	B	301	NDP	C8A-N7A	3.13	1.37	1.31
2	D	301	NDP	C8A-N7A	3.13	1.37	1.31
2	D	301	NDP	C5A-C6A	2.91	1.49	1.41
2	B	301	NDP	C5A-C6A	2.76	1.48	1.41
2	A	301	NDP	C5A-C6A	2.55	1.48	1.41
2	A	301	NDP	C8A-N7A	2.46	1.36	1.31
2	C	301	NDP	C4A-N9A	-2.38	1.32	1.37
2	A	301	NDP	C4A-N9A	-2.34	1.32	1.37
2	D	301	NDP	C4A-N9A	-2.20	1.33	1.37
2	C	301	NDP	P2B-O2B	2.18	1.63	1.59
2	A	301	NDP	C5A-N7A	-2.14	1.35	1.39
2	B	301	NDP	PN-O5D	2.03	1.62	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NDP	N3A-C2A-N1A	-5.46	120.31	128.58
2	B	301	NDP	C5A-C4A-N3A	-4.94	119.92	126.72
2	A	301	NDP	C5A-C4A-N3A	-4.92	119.95	126.72
2	D	301	NDP	C5A-C4A-N3A	-4.84	120.05	126.72
2	C	301	NDP	C5A-C4A-N3A	-4.73	120.20	126.72
2	B	301	NDP	N3A-C2A-N1A	-4.49	121.79	128.58
2	D	301	NDP	N3A-C2A-N1A	-4.48	121.81	128.58
2	B	301	NDP	N3A-C4A-N9A	4.30	134.47	127.17
2	D	301	NDP	C2A-N3A-C4A	4.29	122.30	111.83
2	A	301	NDP	N3A-C4A-N9A	4.24	134.38	127.17
2	C	301	NDP	C2A-N3A-C4A	4.00	121.59	111.83
2	B	301	NDP	C2A-N3A-C4A	3.99	121.58	111.83
2	D	301	NDP	C4A-C5A-N7A	-3.94	106.07	110.58
2	B	301	NDP	C4A-N9A-C8A	3.77	109.70	105.74
2	D	301	NDP	O3-PA-O2A	3.74	121.83	107.80
2	C	301	NDP	O3-PA-O2A	3.70	121.66	107.80
2	D	301	NDP	C6A-C5A-N7A	3.69	139.20	132.09
2	D	301	NDP	C4A-N9A-C8A	3.49	109.41	105.74
2	A	301	NDP	C4A-N9A-C8A	3.43	109.34	105.74
2	D	301	NDP	N3A-C4A-N9A	3.43	133.00	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NDP	O3X-P2B-O2X	3.37	120.43	107.80
2	C	301	NDP	O4B-C1B-N9A	3.34	114.50	108.09
2	A	301	NDP	O3-PA-O5B	-3.23	98.24	106.67
2	D	301	NDP	C2B-C1B-N9A	3.17	118.96	113.75
2	C	301	NDP	N3A-C4A-N9A	3.13	132.50	127.17
2	D	301	NDP	P2B-O2B-C2B	-3.11	115.12	123.43
2	A	301	NDP	C2A-N3A-C4A	3.08	119.36	111.83
2	A	301	NDP	C4A-C5A-N7A	-3.08	107.06	110.58
2	D	301	NDP	N9A-C8A-N7A	-3.00	109.68	113.94
2	B	301	NDP	N9A-C8A-N7A	-2.91	109.81	113.94
2	B	301	NDP	C4A-C5A-N7A	-2.91	107.26	110.58
2	B	301	NDP	C6A-C5A-N7A	2.90	137.68	132.09
2	D	301	NDP	C5A-N7A-C8A	2.82	107.88	103.45
2	B	301	NDP	O2N-PN-O1N	2.82	121.81	110.83
2	A	301	NDP	P2B-O2B-C2B	-2.78	116.00	123.43
2	A	301	NDP	N3A-C2A-N1A	-2.76	124.41	128.58
2	A	301	NDP	O4B-C1B-N9A	2.75	113.36	108.09
2	D	301	NDP	C4A-N9A-C1B	-2.66	120.40	126.63
2	D	301	NDP	O2B-P2B-O1X	-2.66	99.87	109.33
2	B	301	NDP	C5A-N7A-C8A	2.65	107.62	103.45
2	C	301	NDP	O4B-C1B-C2B	-2.60	102.11	106.59
2	C	301	NDP	C2A-N1A-C6A	2.53	122.88	118.73
2	A	301	NDP	C5A-N7A-C8A	2.38	107.19	103.45
2	C	301	NDP	C4A-C5A-N7A	-2.35	107.90	110.58
2	B	301	NDP	O3X-P2B-O2X	2.31	116.46	107.80
2	A	301	NDP	O5B-C5B-C4B	2.27	116.72	108.99
2	A	301	NDP	N9A-C8A-N7A	-2.26	110.73	113.94
2	A	301	NDP	C2B-C1B-N9A	-2.24	110.06	113.75
2	B	301	NDP	C4A-N9A-C1B	-2.24	121.39	126.63
2	C	301	NDP	C6A-C5A-N7A	2.22	136.38	132.09
2	C	301	NDP	O5B-PA-O1A	-2.20	100.50	106.44
2	C	301	NDP	O5B-C5B-C4B	2.18	116.40	108.99
2	C	301	NDP	O2X-P2B-O2B	-2.13	97.54	105.85
2	B	301	NDP	O4B-C1B-N9A	2.10	112.12	108.09
2	C	301	NDP	O2A-PA-O5B	2.07	112.07	106.67
2	A	301	NDP	C6A-C5A-N7A	2.04	136.02	132.09
2	A	301	NDP	O2A-PA-O1A	2.03	118.75	110.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

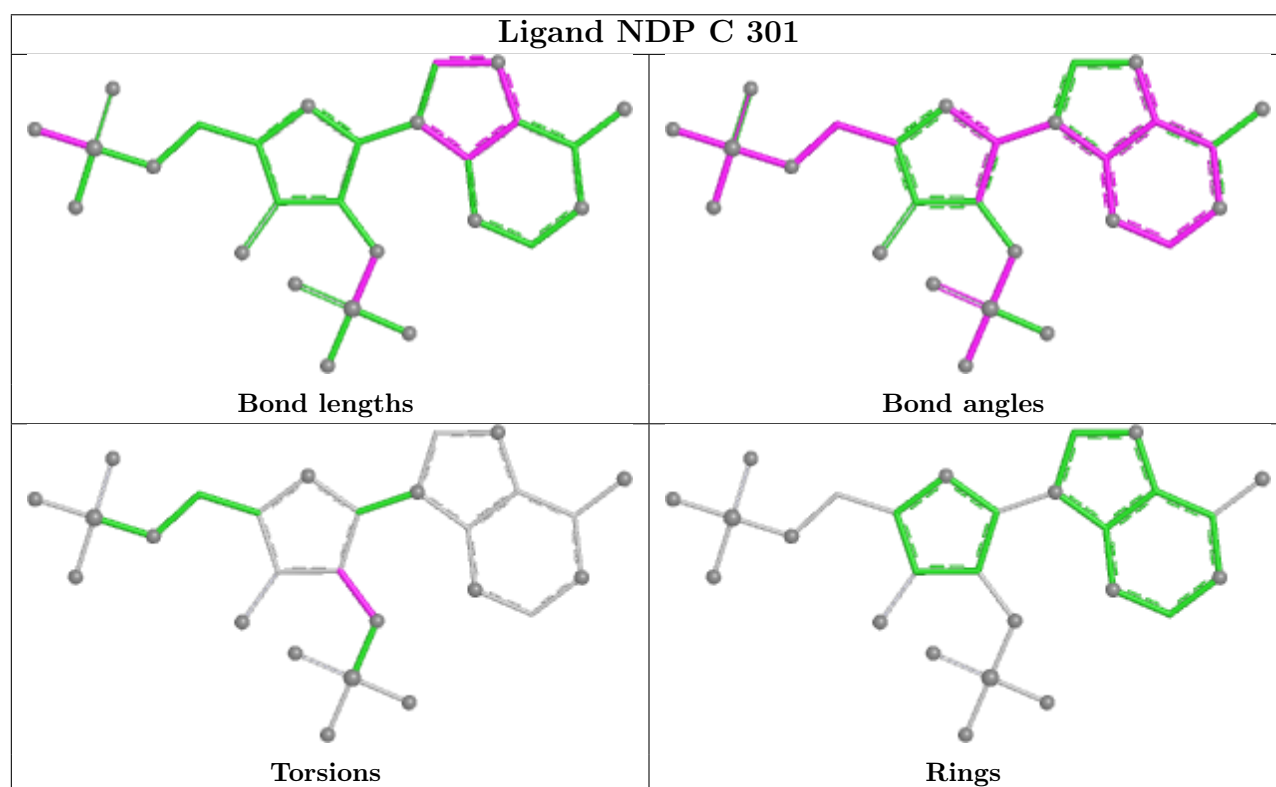
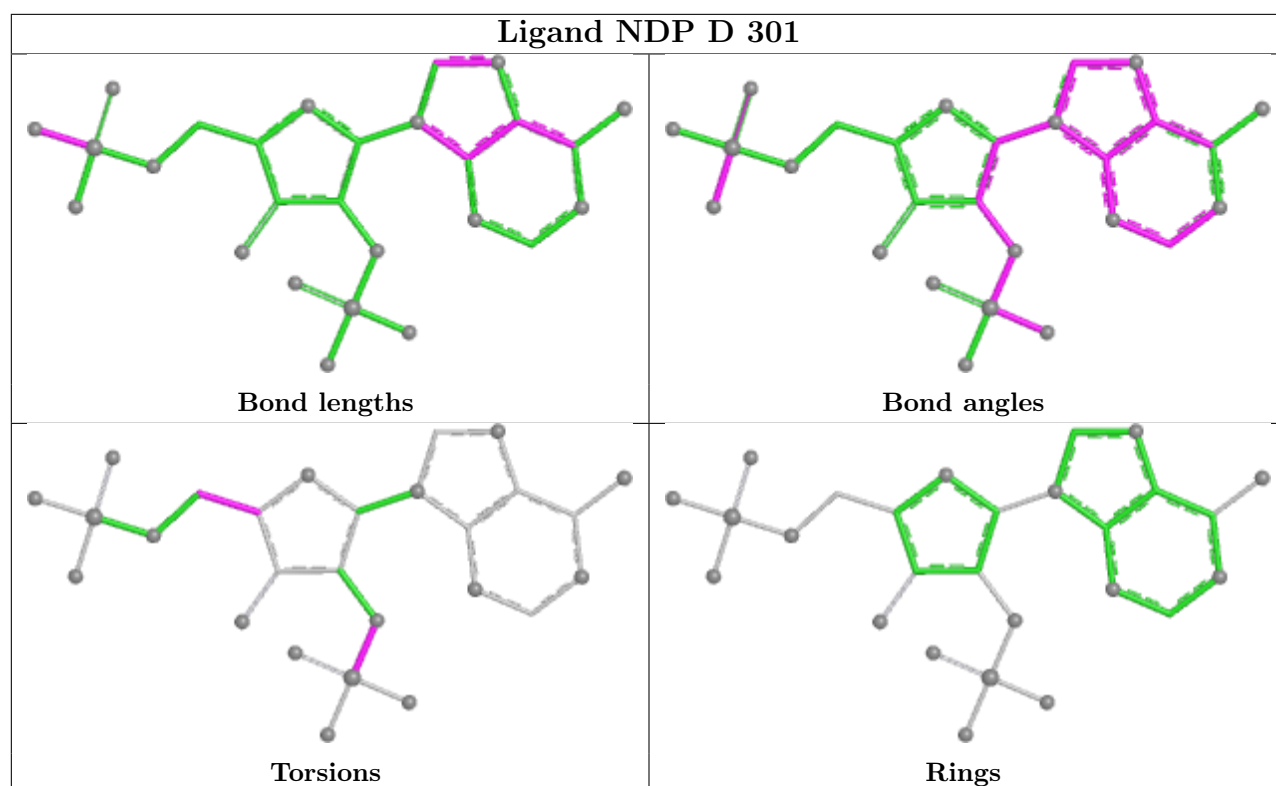
Mol	Chain	Res	Type	Atoms
3	D	302	1PE	OH6-C15-C25-OH5
3	D	302	1PE	OH4-C13-C23-OH3
2	A	301	NDP	O4B-C4B-C5B-O5B
2	A	301	NDP	C3B-C4B-C5B-O5B
3	D	302	1PE	OH2-C12-C22-OH3
2	B	301	NDP	O4B-C4B-C5B-O5B
2	B	301	NDP	C3B-C4B-C5B-O5B
3	D	302	1PE	OH5-C14-C24-OH4
2	D	301	NDP	O4B-C4B-C5B-O5B
2	A	301	NDP	C3B-C2B-O2B-P2B
2	B	301	NDP	C3B-C2B-O2B-P2B
3	D	302	1PE	C15-C25-OH5-C14
3	D	302	1PE	C23-C13-OH4-C24
2	A	301	NDP	C4B-C5B-O5B-PA
2	C	301	NDP	C1B-C2B-O2B-P2B
2	C	301	NDP	C3B-C2B-O2B-P2B
3	D	302	1PE	C16-C26-OH6-C15
2	B	301	NDP	C1B-C2B-O2B-P2B
2	A	301	NDP	C2B-O2B-P2B-O3X
2	D	301	NDP	C2B-O2B-P2B-O3X
2	A	301	NDP	C1B-C2B-O2B-P2B

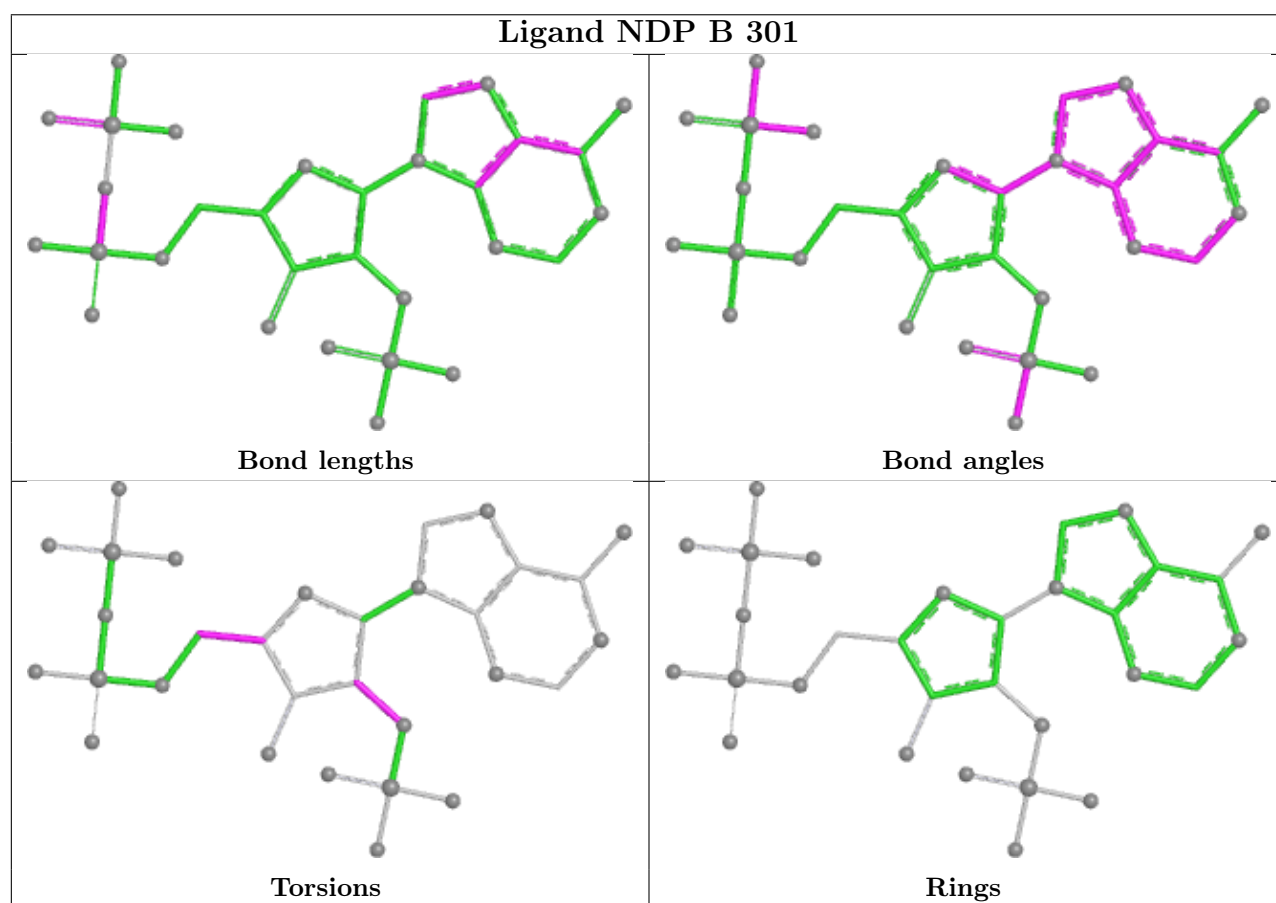
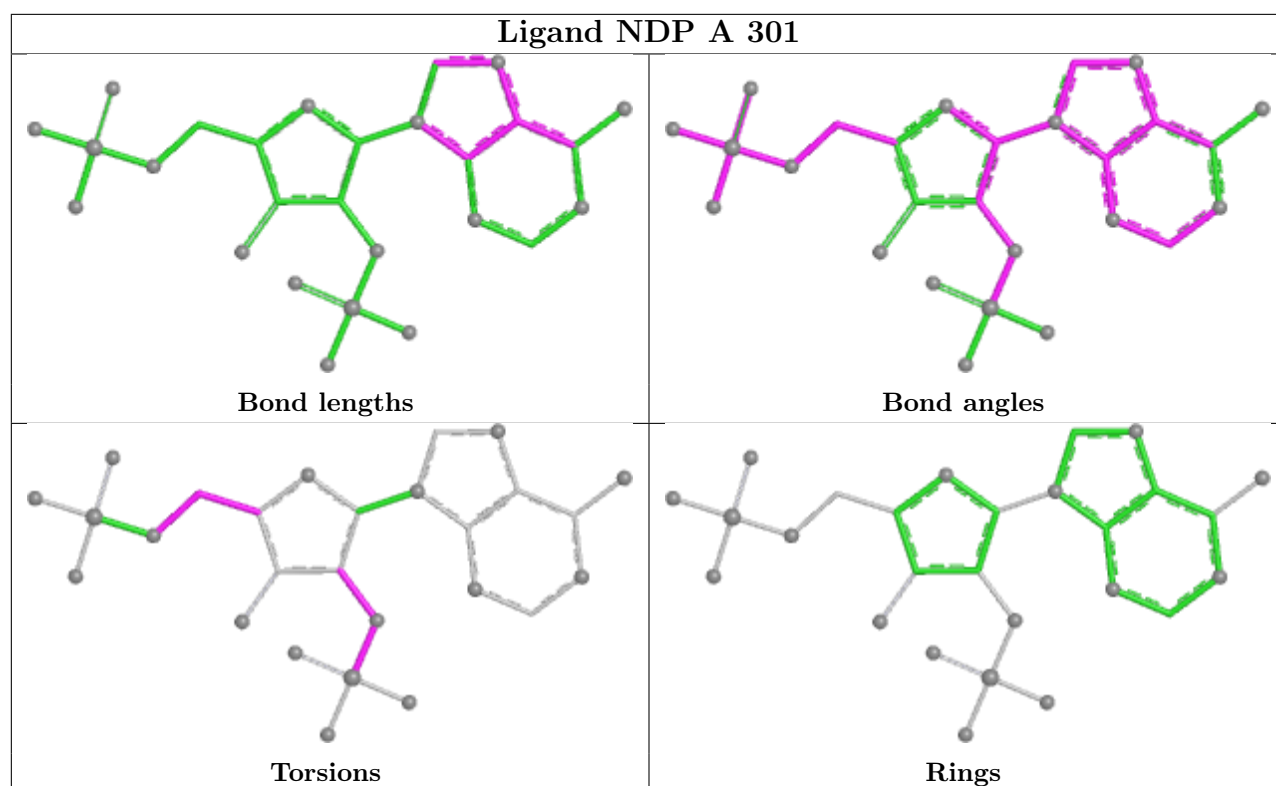
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NDP	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.





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, 95th 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 ²)	Q<0.9
1	A	243/251 (96%)	0.12	6 (2%) 58 56	42, 64, 92, 123	0
1	B	240/251 (95%)	0.09	13 (5%) 31 28	36, 60, 92, 119	1 (0%)
1	C	238/251 (94%)	-0.07	6 (2%) 58 56	39, 53, 95, 131	0
1	D	232/251 (92%)	0.29	15 (6%) 25 22	45, 69, 108, 140	0
All	All	953/1004 (94%)	0.11	40 (4%) 40 37	36, 61, 97, 140	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	MET	5.1
1	A	91	ALA	4.7
1	B	146	THR	4.0
1	A	92	GLY	3.9
1	B	246	TYR	3.8
1	D	98	LEU	3.8
1	C	143	VAL	3.6
1	B	4	PHE	3.5
1	B	94	THR	3.4
1	C	246	TYR	3.3
1	A	4	PHE	3.3
1	D	100	MET	3.2
1	C	144	VAL	3.2
1	D	3	GLN	3.2
1	D	153	ALA	3.1
1	B	99	LEU	3.1
1	B	154	ASN	3.1
1	B	3	GLN	2.8
1	B	144	VAL	2.8
1	D	193	THR	2.8
1	D	246	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	93	ILE	2.7
1	D	191	ASP	2.7
1	D	192	MET	2.5
1	D	55	ASP	2.5
1	B	100	MET	2.4
1	B	101	ARG	2.3
1	B	152	GLN	2.3
1	D	190	THR	2.3
1	D	4	PHE	2.2
1	D	202	THR	2.2
1	C	169	MET	2.2
1	A	5	MET	2.2
1	D	152	GLN	2.2
1	D	195	ALA	2.2
1	A	246	TYR	2.2
1	B	5	MET	2.2
1	C	198	ASP	2.1
1	D	99	LEU	2.1
1	C	202	THR	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, 95th 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
3	1PE	D	302	16/16	0.78	0.18	65,85,98,98	16
2	NDP	A	301	27/48	0.80	0.12	53,76,88,101	27
2	NDP	D	301	27/48	0.82	0.10	77,93,108,114	3
2	NDP	B	301	31/48	0.84	0.10	64,77,98,107	0

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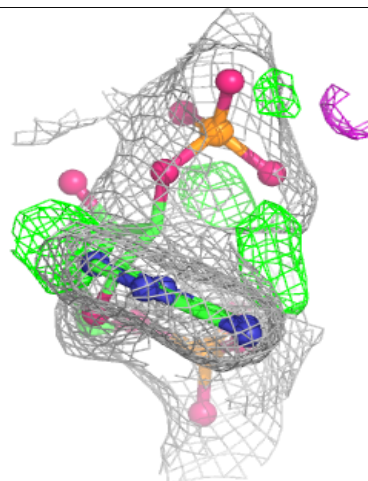
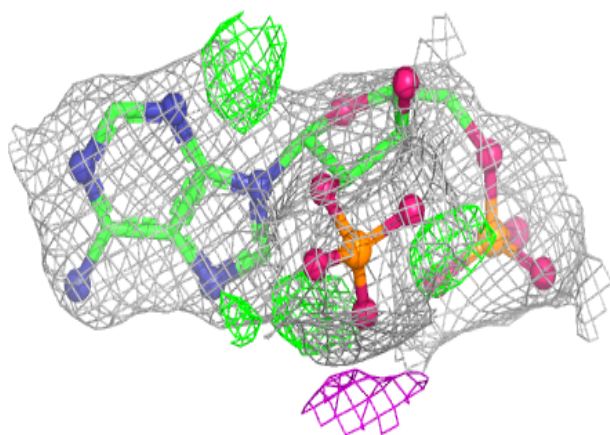
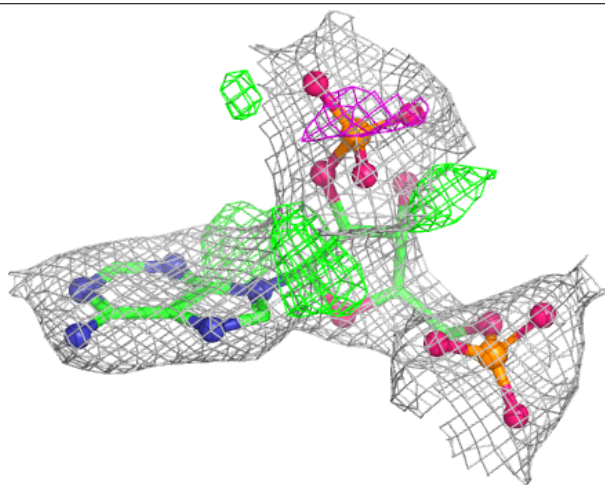
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	C	301	27/48	0.92	0.08	39,55,71,85	3

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.

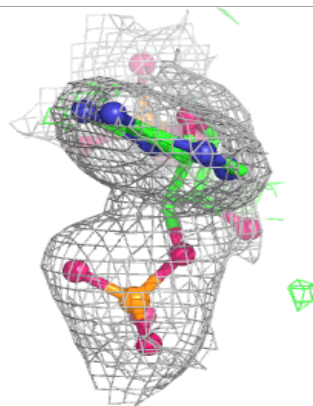
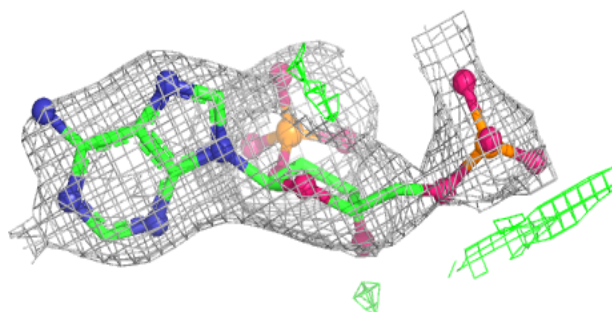
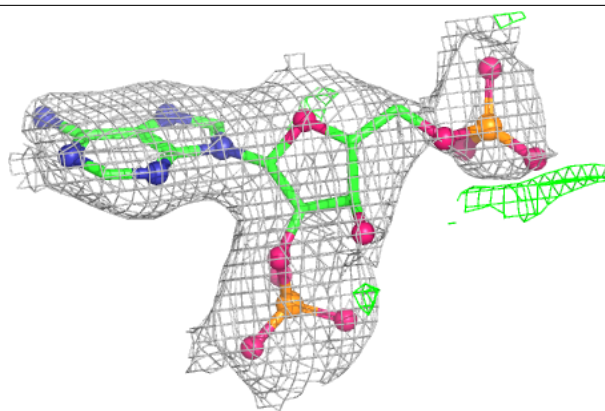
Electron density around NDP A 301:

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

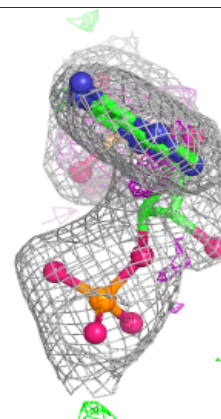
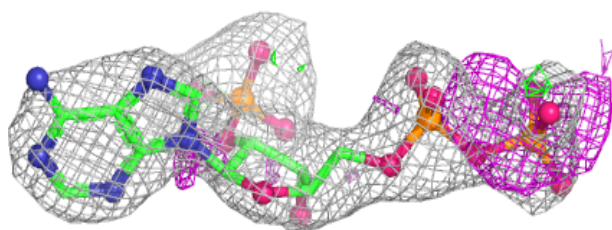
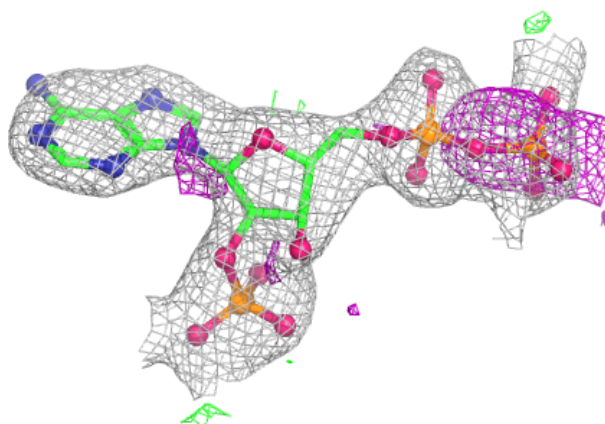


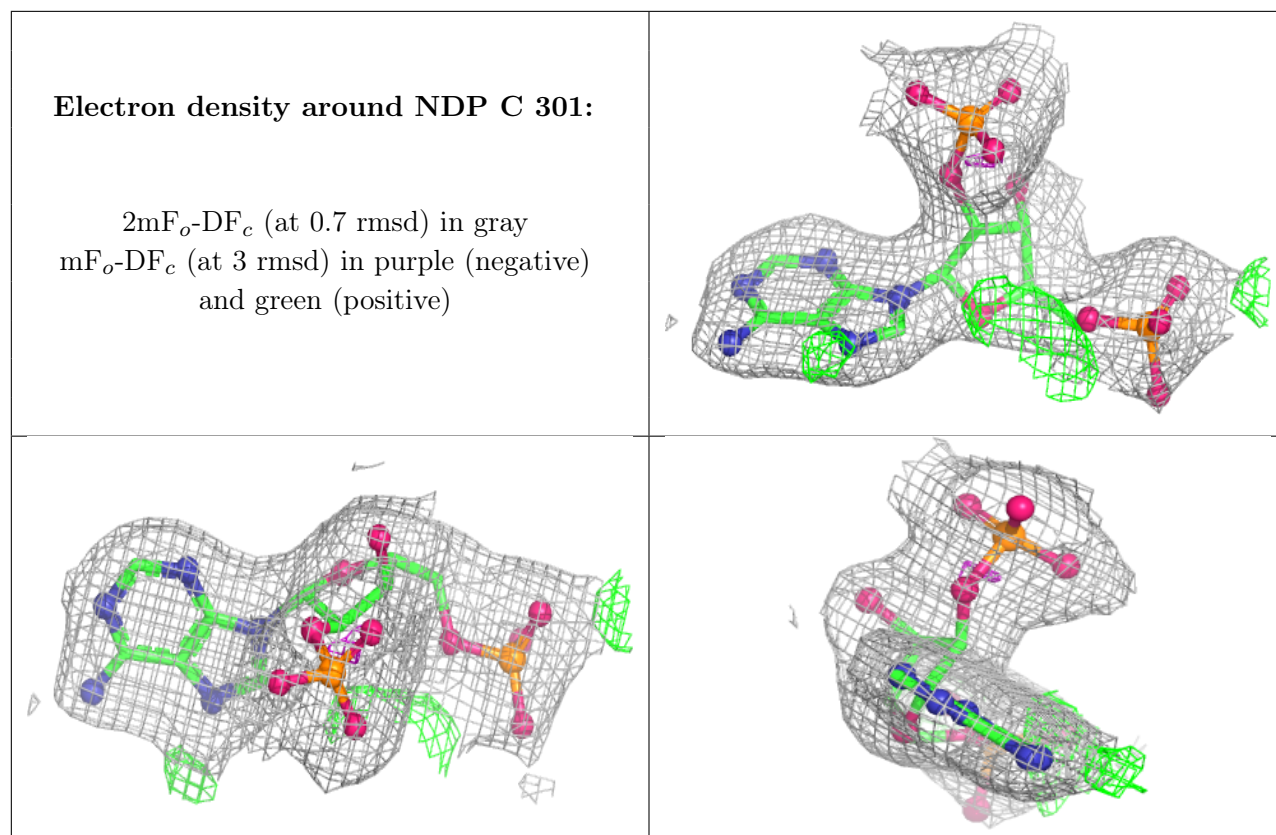
Electron density around NDP D 301:

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

**Electron density around NDP B 301:**

$2mF_o-DF_c$ (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.