



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2022 – 06:05 PM JST

PDB ID : 7VE7  
Title : Crystal structure of KRED mutant-F147L/L153Q/Y190P/L199A/M205F/M206F  
Authors : Cui, J.; Huang, X.; Wang, B.; Zhao, H.; Zhou, J.  
Deposited on : 2021-09-08  
Resolution : 1.72 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 : 2.28.1  
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) : 2.28.1

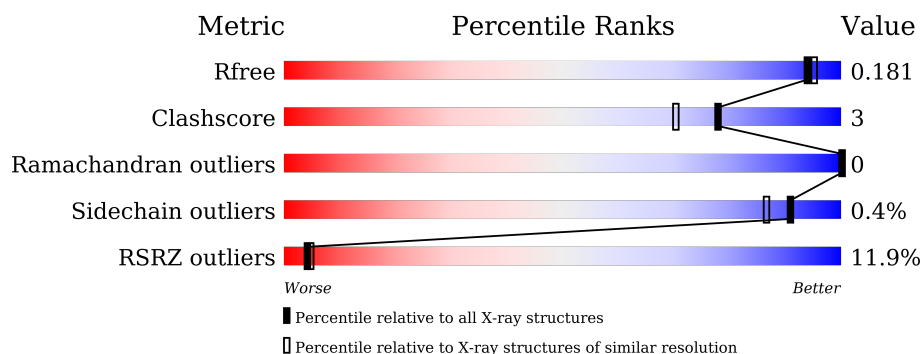
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	253	<div> <div>6%</div> <div>96%</div> <div>.</div> </div>
1	B	253	<div> <div>13%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	C	253	<div> <div>12%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	D	253	<div> <div>16%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7989 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-alpha-(Or 20-beta)-hydroxysteroid dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1873	1173	319	374	7			
1	B	250	Total	C	N	O	S	0	1	0
			1851	1159	318	368	6			
1	C	251	Total	C	N	O	S	0	0	0
			1854	1163	317	368	6			
1	D	251	Total	C	N	O	S	0	0	0
			1845	1155	316	368	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q6WVP7
A	147	LEU	PHE	engineered mutation	UNP Q6WVP7
A	153	GLN	LEU	engineered mutation	UNP Q6WVP7
A	190	PRO	TYR	engineered mutation	UNP Q6WVP7
A	199	ALA	LEU	engineered mutation	UNP Q6WVP7
A	205	PHE	MET	engineered mutation	UNP Q6WVP7
A	206	PHE	MET	engineered mutation	UNP Q6WVP7
B	0	GLY	-	expression tag	UNP Q6WVP7
B	147	LEU	PHE	engineered mutation	UNP Q6WVP7
B	153	GLN	LEU	engineered mutation	UNP Q6WVP7
B	190	PRO	TYR	engineered mutation	UNP Q6WVP7
B	199	ALA	LEU	engineered mutation	UNP Q6WVP7
B	205	PHE	MET	engineered mutation	UNP Q6WVP7
B	206	PHE	MET	engineered mutation	UNP Q6WVP7
C	0	GLY	-	expression tag	UNP Q6WVP7
C	147	LEU	PHE	engineered mutation	UNP Q6WVP7
C	153	GLN	LEU	engineered mutation	UNP Q6WVP7
C	190	PRO	TYR	engineered mutation	UNP Q6WVP7
C	199	ALA	LEU	engineered mutation	UNP Q6WVP7
C	205	PHE	MET	engineered mutation	UNP Q6WVP7
C	206	PHE	MET	engineered mutation	UNP Q6WVP7

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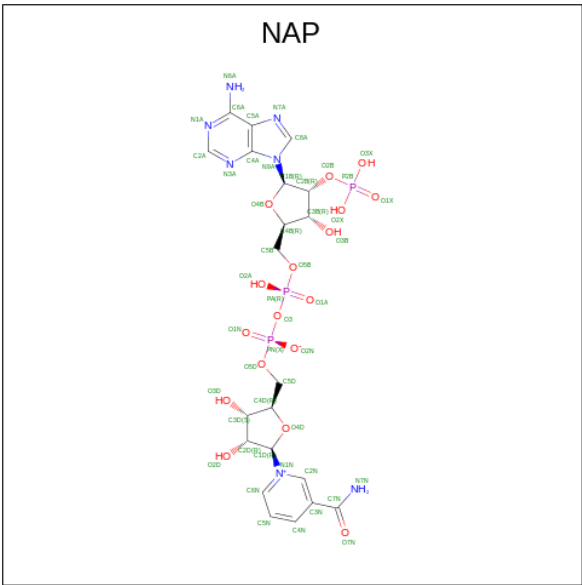
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP Q6WVP7
D	147	LEU	PHE	engineered mutation	UNP Q6WVP7
D	153	GLN	LEU	engineered mutation	UNP Q6WVP7
D	190	PRO	TYR	engineered mutation	UNP Q6WVP7
D	199	ALA	LEU	engineered mutation	UNP Q6WVP7
D	205	PHE	MET	engineered mutation	UNP Q6WVP7
D	206	PHE	MET	engineered mutation	UNP Q6WVP7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 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>) (labeled as "Ligand of Interest" by depositor).



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

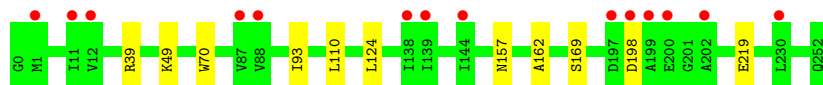
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	82	Total	O	0	0
			82	82		
4	C	84	Total	O	0	0
			84	84		
4	D	76	Total	O	0	0
			76	76		

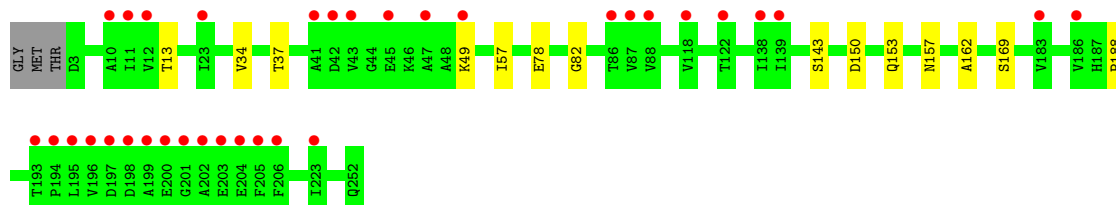
### 3 Residue-property plots [i](#)

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.

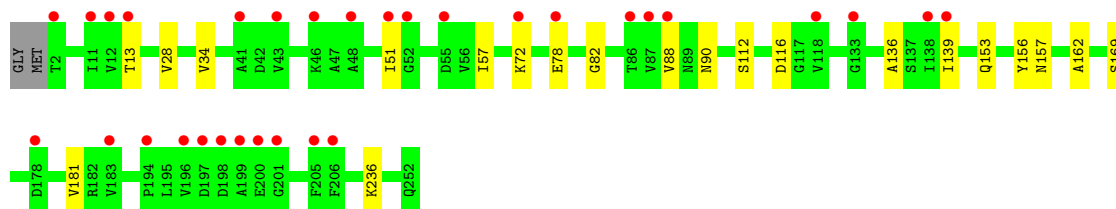
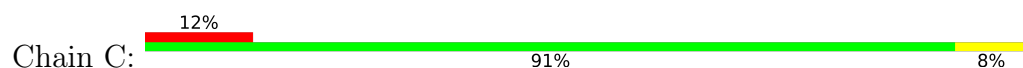
- Molecule 1: 3-alpha-(Or 20-beta)-hydroxysteroid dehydrogenase



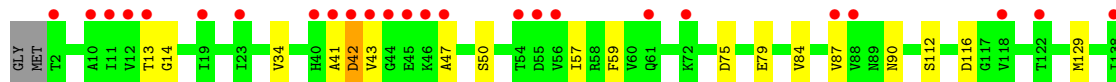
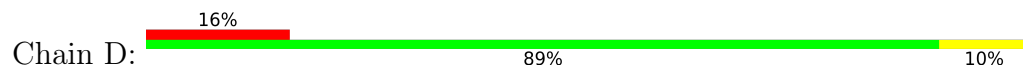
- Molecule 1: 3-alpha-(Or 20-beta)-hydroxysteroid dehydrogenase

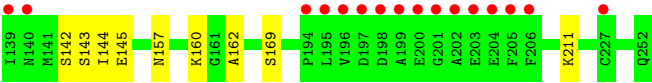


- Molecule 1: 3-alpha-(Or 20-beta)-hydroxysteroid dehydrogenase



- Molecule 1: 3-alpha-(Or 20-beta)-hydroxysteroid dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.31Å 55.57Å 128.56Å 90.00° 103.89° 90.00°	Depositor
Resolution (Å)	21.33 – 1.72 23.84 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.6 (21.33-1.72) 99.2 (23.84-1.72)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.174 , 0.210 0.177 , 0.181	Depositor DCC
$R_{free}$ test set	4683 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.7	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	7989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, MG

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	0.36	0/1903	0.56	0/2576
1	B	0.31	0/1881	0.52	0/2547
1	C	0.33	0/1884	0.52	0/2552
1	D	0.31	0/1875	0.51	0/2541
All	All	0.33	0/7543	0.53	0/10216

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 [i](#)

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	1873	0	1847	8	0
1	B	1851	0	1810	9	0
1	C	1854	0	1826	14	0
1	D	1845	0	1799	19	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	48	0	25	0	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	48	0	25	1	0
4	A	130	0	0	1	0
4	B	82	0	0	0	0
4	C	84	0	0	0	0
4	D	76	0	0	0	0
All	All	7989	0	7382	43	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 (43) 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:39:ARG:NH1	4:A:401:HOH:O	2.22	0.72
1:B:150:ASP:OD2	1:B:153[B]:GLN:NE2	2.22	0.58
1:D:84:VAL:HG12	1:D:129:MET:HE2	1.86	0.57
1:D:143:SER:OG	1:D:145:GLU:OE2	2.28	0.51
1:A:162:ALA:HB2	1:D:162:ALA:HB2	1.92	0.51
1:A:219:GLU:OE1	1:C:236:LYS:NZ	2.30	0.50
1:B:162:ALA:HB2	1:C:162:ALA:HB2	1.94	0.50
1:C:28:VAL:HG21	1:C:51:ILE:HG23	1.95	0.48
1:A:70:TRP:HB3	1:A:124:LEU:HD23	1.96	0.47
1:B:78:GLU:HA	1:B:82:GLY:O	2.15	0.47
1:D:75:ASP:O	1:D:79:GLU:HG3	2.14	0.46
1:A:157:ASN:OD1	1:D:169:SER:HB2	2.14	0.46
1:C:13:THR:O	1:C:90:ASN:HB3	2.16	0.46
1:C:34:VAL:O	1:C:57:ILE:HA	2.16	0.46
1:A:49:LYS:HD3	1:A:49:LYS:HA	1.78	0.46
1:C:112:SER:O	1:C:116:ASP:HB2	2.16	0.45
1:C:153:GLN:HB3	1:C:156:TYR:HB3	1.98	0.45
1:B:169:SER:HB2	1:C:157:ASN:OD1	2.16	0.45
1:C:28:VAL:HG21	1:C:51:ILE:CG2	2.47	0.44
1:A:93:ILE:HD11	1:A:110:LEU:HA	1.99	0.44
1:C:136:ALA:HB3	1:C:181:VAL:HG22	2.00	0.44
1:D:41:ALA:HA	1:D:59:PHE:CE2	2.52	0.44
1:D:47:ALA:O	1:D:50:SER:OG	2.28	0.44
1:D:13:THR:O	1:D:90:ASN:HB3	2.18	0.43
1:D:41:ALA:HA	1:D:59:PHE:HE2	1.83	0.43
1:A:169:SER:HB2	1:D:157:ASN:OD1	2.18	0.43
1:B:150:ASP:HB3	1:B:153[B]:GLN:HB2	2.01	0.43
1:D:144:ILE:HG13	1:D:145:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:VAL:HG23	1:D:129:MET:HE1	2.00	0.42
1:C:88:VAL:HA	1:C:139:ILE:O	2.19	0.42
1:D:87:VAL:HG23	1:D:129:MET:CE	2.49	0.42
1:B:157:ASN:OD1	1:C:169:SER:HB2	2.19	0.42
1:D:42:ASP:OD1	1:D:43:VAL:N	2.48	0.41
1:B:143:SER:HA	1:B:188:PRO:HD2	2.02	0.41
1:D:112:SER:O	1:D:116:ASP:HB2	2.19	0.41
1:D:211:LYS:HA	1:D:211:LYS:HD3	1.87	0.41
1:C:72:LYS:N	1:C:72:LYS:HD2	2.36	0.41
1:D:14:GLY:HA2	3:D:302:NAP:H1B	2.03	0.41
1:D:142:SER:HA	1:D:160:LYS:HD2	2.03	0.41
1:B:13:THR:HA	1:B:37:THR:OG1	2.21	0.40
1:C:78:GLU:HA	1:C:82:GLY:O	2.21	0.40
1:D:34:VAL:O	1:D:57:ILE:HA	2.21	0.40
1:B:34:VAL:O	1:B:57:ILE:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	251/253 (99%)	245 (98%)	6 (2%)	0	100	100
1	B	249/253 (98%)	240 (96%)	9 (4%)	0	100	100
1	C	249/253 (98%)	242 (97%)	7 (3%)	0	100	100
1	D	249/253 (98%)	240 (96%)	9 (4%)	0	100	100
All	All	998/1012 (99%)	967 (97%)	31 (3%)	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	195/197 (99%)	194 (100%)	1 (0%)	88	83
1	B	190/197 (96%)	189 (100%)	1 (0%)	88	83
1	C	192/197 (98%)	192 (100%)	0	100	100
1	D	189/197 (96%)	188 (100%)	1 (0%)	88	83
All	All	766/788 (97%)	763 (100%)	3 (0%)	91	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	B	49	LYS
1	D	42	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAP	C	301	-	45,52,52	0.83	1 (2%)	56,80,80	1.12	2 (3%)
3	NAP	B	301	-	45,52,52	0.84	2 (4%)	56,80,80	1.18	4 (7%)
3	NAP	A	302	-	45,52,52	0.82	1 (2%)	56,80,80	1.23	7 (12%)
3	NAP	D	302	-	45,52,52	0.83	2 (4%)	56,80,80	1.11	3 (5%)

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	NAP	C	301	-	-	5/31/67/67	0/5/5/5
3	NAP	B	301	-	-	6/31/67/67	0/5/5/5
3	NAP	A	302	-	-	7/31/67/67	0/5/5/5
3	NAP	D	302	-	-	6/31/67/67	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	NAP	C5A-C4A	2.42	1.47	1.40
3	A	302	NAP	C5A-C4A	2.34	1.47	1.40
3	C	301	NAP	C5A-C4A	2.33	1.47	1.40
3	B	301	NAP	C5A-C4A	2.32	1.47	1.40
3	B	301	NAP	O4D-C1D	2.02	1.43	1.41
3	D	302	NAP	O4D-C1D	2.00	1.43	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	NAP	N3A-C2A-N1A	-3.72	122.86	128.68
3	B	301	NAP	N3A-C2A-N1A	-3.37	123.41	128.68
3	C	301	NAP	N3A-C2A-N1A	-3.31	123.51	128.68
3	D	302	NAP	N3A-C2A-N1A	-3.16	123.73	128.68
3	D	302	NAP	C4A-C5A-N7A	-2.69	106.60	109.40
3	C	301	NAP	C4A-C5A-N7A	-2.65	106.64	109.40
3	A	302	NAP	C4A-C5A-N7A	-2.64	106.65	109.40
3	A	302	NAP	C1B-N9A-C4A	-2.51	122.24	126.64
3	B	301	NAP	C4A-C5A-N7A	-2.32	106.98	109.40
3	B	301	NAP	C3N-C7N-N7N	2.32	120.53	117.75
3	B	301	NAP	C1B-N9A-C4A	-2.30	122.59	126.64
3	A	302	NAP	C2A-N1A-C6A	2.30	122.69	118.75
3	D	302	NAP	PN-O3-PA	-2.20	125.26	132.83
3	A	302	NAP	O3X-P2B-O2X	2.14	115.82	107.64
3	A	302	NAP	C3N-C7N-N7N	2.07	120.23	117.75
3	A	302	NAP	O3D-C3D-C2D	-2.05	105.20	111.82

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	NAP	C2B-O2B-P2B-O3X
3	A	302	NAP	C5D-O5D-PN-O2N
3	A	302	NAP	O4D-C1D-N1N-C2N
3	B	301	NAP	C5D-O5D-PN-O2N
3	B	301	NAP	O4D-C1D-N1N-C2N
3	C	301	NAP	C5D-O5D-PN-O2N
3	C	301	NAP	O4D-C1D-N1N-C2N
3	D	302	NAP	C5D-O5D-PN-O2N
3	D	302	NAP	O4D-C1D-N1N-C2N
3	A	302	NAP	C5D-O5D-PN-O3
3	B	301	NAP	C2B-O2B-P2B-O3X
3	B	301	NAP	C5D-O5D-PN-O3
3	C	301	NAP	C5D-O5D-PN-O3
3	D	302	NAP	C5D-O5D-PN-O3
3	B	301	NAP	C5D-O5D-PN-O1N
3	D	302	NAP	C5D-O5D-PN-O1N
3	A	302	NAP	O4B-C4B-C5B-O5B
3	D	302	NAP	O4B-C4B-C5B-O5B
3	A	302	NAP	C2B-O2B-P2B-O2X
3	D	302	NAP	C2B-O2B-P2B-O3X
3	B	301	NAP	O4B-C4B-C5B-O5B
3	A	302	NAP	C5D-O5D-PN-O1N

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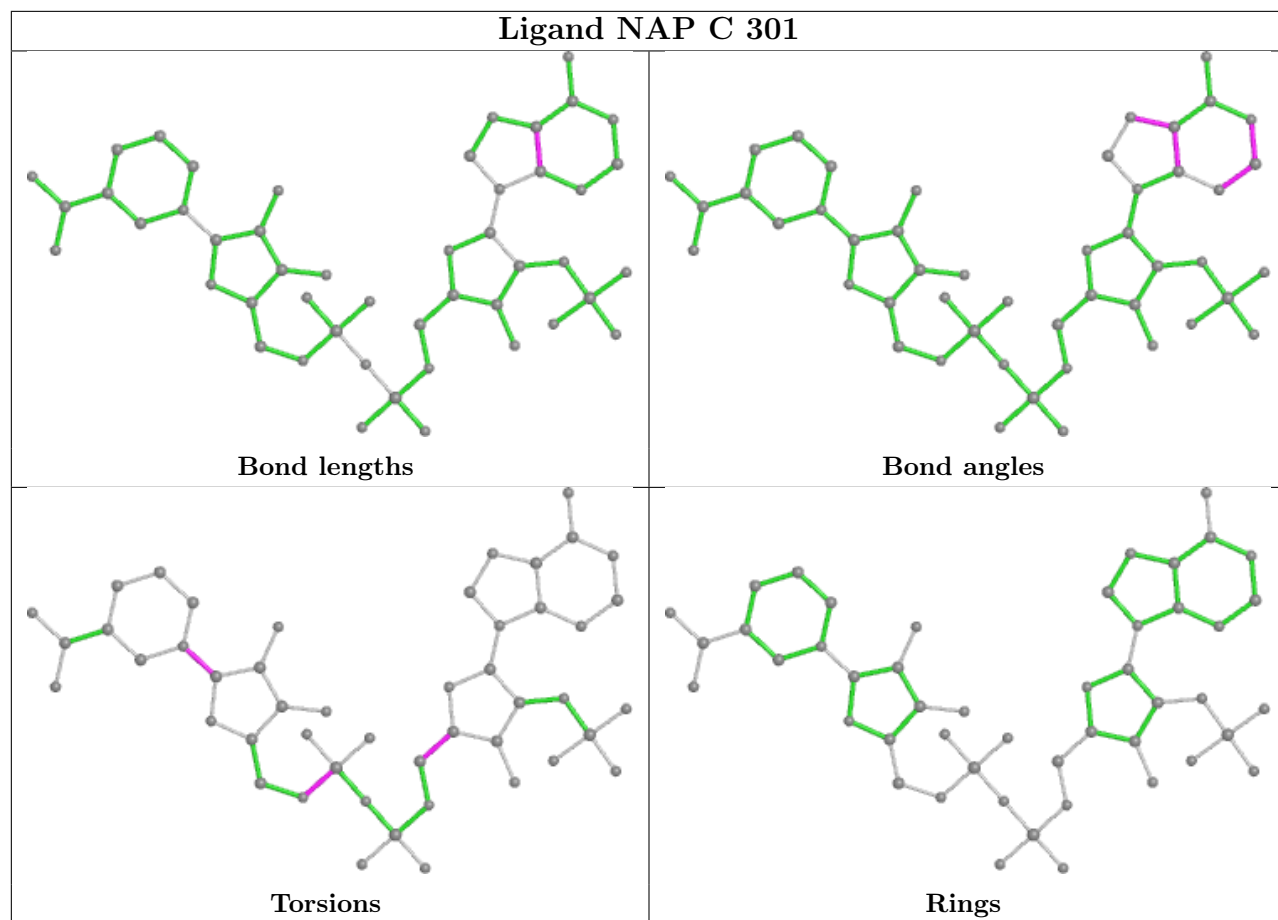
Mol	Chain	Res	Type	Atoms
3	C	301	NAP	C5D-O5D-PN-O1N
3	C	301	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

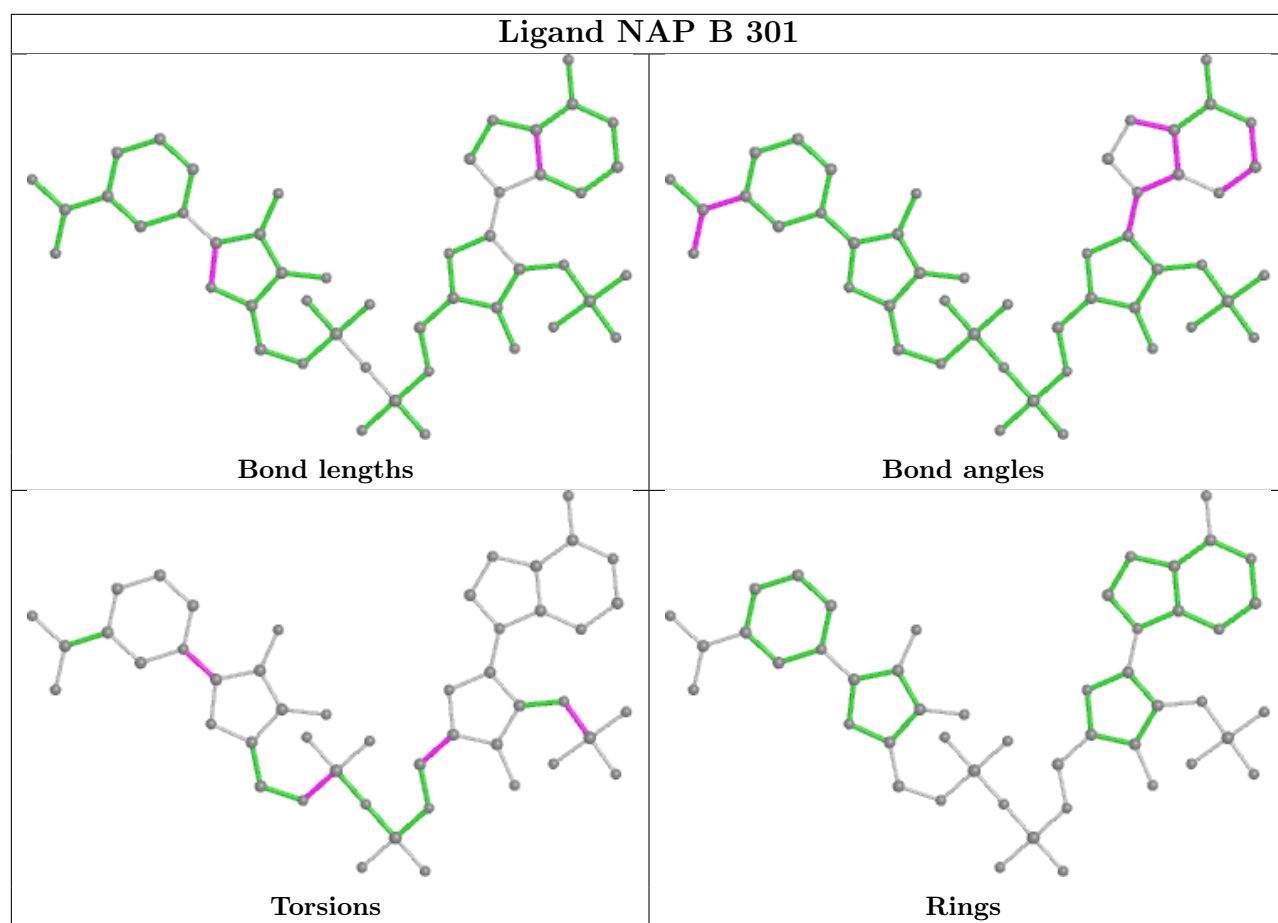
1 monomer is involved in 1 short contact:

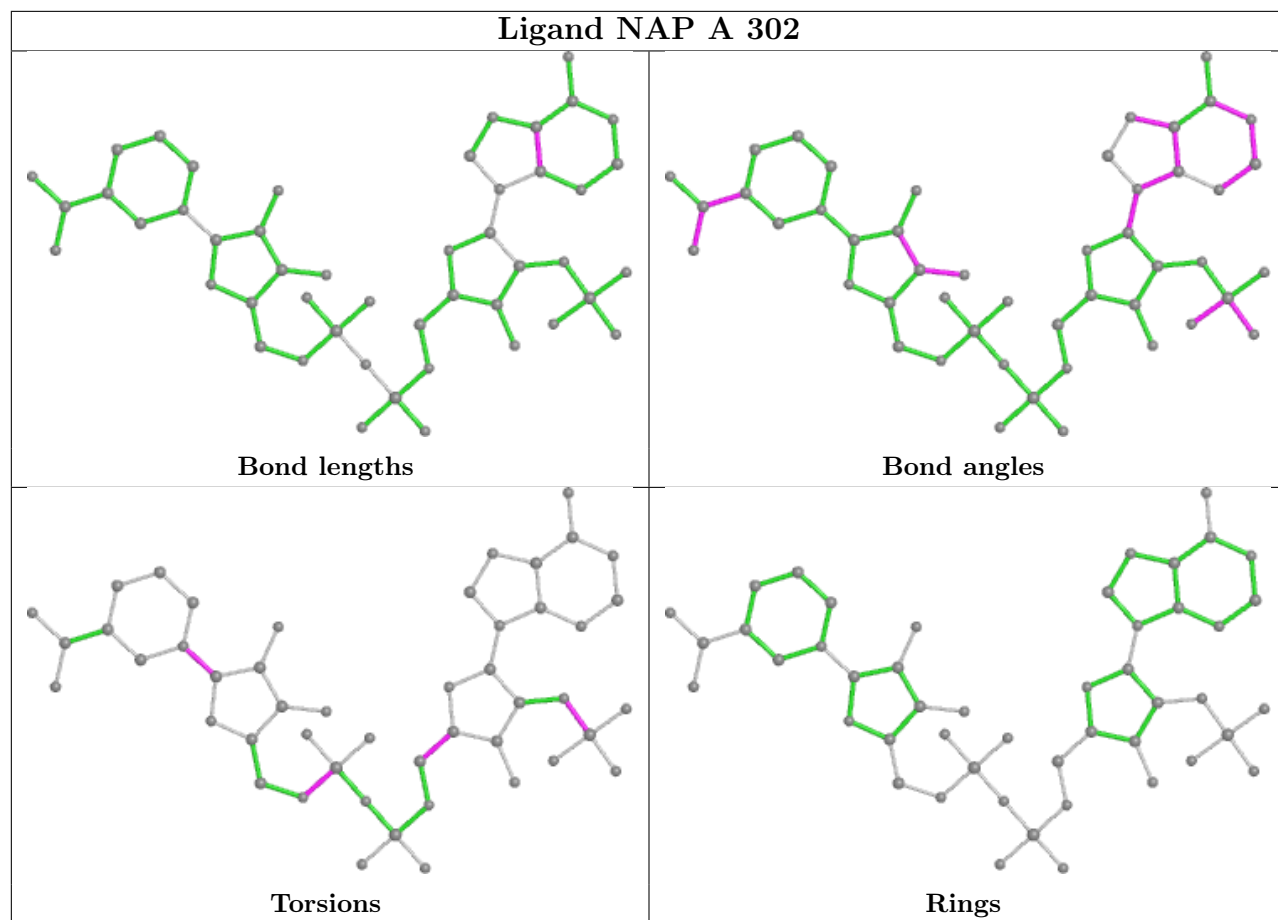
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	NAP	1	0

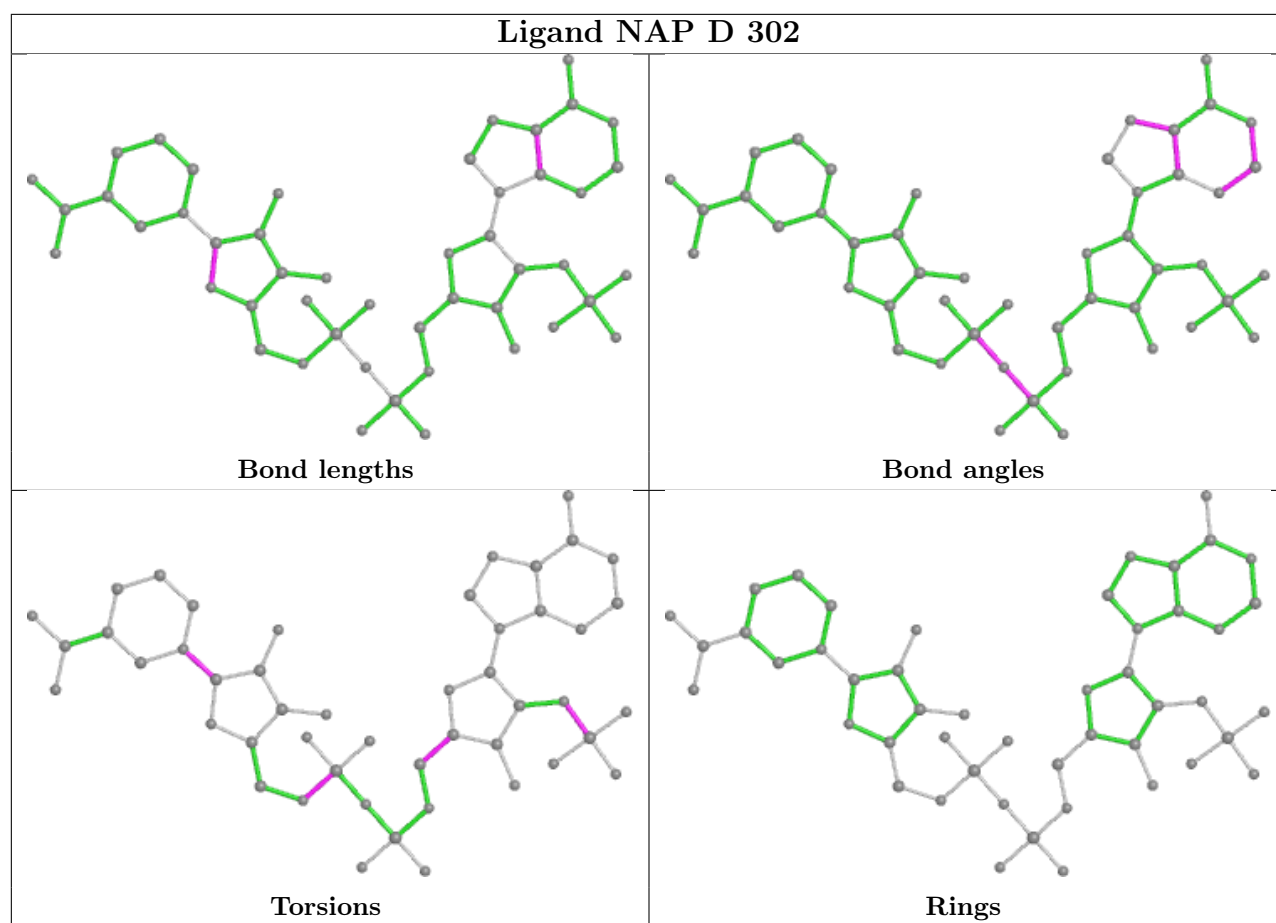
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	253/253 (100%)	0.36	14 (5%) 25 27	25, 36, 54, 71	0
1	B	250/253 (98%)	0.75	34 (13%) 3 3	28, 44, 68, 82	0
1	C	251/253 (99%)	0.66	31 (12%) 4 4	26, 41, 63, 71	0
1	D	251/253 (99%)	0.85	41 (16%) 1 1	27, 47, 75, 82	0
All	All	1005/1012 (99%)	0.65	120 (11%) 4 5	25, 41, 68, 82	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	ALA	10.5
1	D	199	ALA	8.8
1	B	196	VAL	8.0
1	D	195	LEU	7.9
1	B	195	LEU	7.6
1	B	201	GLY	7.2
1	C	199	ALA	6.5
1	D	201	GLY	6.5
1	C	2	THR	6.4
1	B	200	GLU	6.1
1	B	88	VAL	5.9
1	D	200	GLU	5.8
1	D	194	PRO	5.6
1	D	198	ASP	5.5
1	D	202	ALA	5.2
1	B	87	VAL	5.1
1	B	139	ILE	5.1
1	D	205	PHE	4.9
1	B	197	ASP	4.9
1	C	198	ASP	4.9
1	B	198	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	88	VAL	4.8
1	D	196	VAL	4.8
1	C	87	VAL	4.7
1	B	12	VAL	4.7
1	A	199	ALA	4.6
1	C	88	VAL	4.5
1	D	204	GLU	4.5
1	C	197	ASP	4.5
1	C	200	GLU	4.5
1	D	87	VAL	4.5
1	D	206	PHE	4.4
1	D	41	ALA	4.4
1	B	11	ILE	4.3
1	B	202	ALA	4.2
1	A	138	ILE	4.1
1	C	183	VAL	4.1
1	D	43	VAL	4.0
1	A	12	VAL	3.9
1	C	138	ILE	3.9
1	B	138	ILE	3.8
1	A	87	VAL	3.7
1	B	43	VAL	3.7
1	A	1	MET	3.7
1	A	88	VAL	3.7
1	C	196	VAL	3.7
1	D	45	GLU	3.6
1	C	11	ILE	3.6
1	A	200	GLU	3.6
1	D	2	THR	3.5
1	D	42	ASP	3.4
1	D	11	ILE	3.4
1	B	194	PRO	3.4
1	A	198	ASP	3.4
1	A	139	ILE	3.3
1	D	139	ILE	3.3
1	B	204	GLU	3.1
1	D	12	VAL	3.1
1	A	11	ILE	3.1
1	D	197	ASP	3.1
1	C	139	ILE	3.0
1	D	118	VAL	3.0
1	B	41	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	72	LYS	2.8
1	C	201	GLY	2.8
1	C	194	PRO	2.8
1	B	10	ALA	2.7
1	D	10	ALA	2.7
1	C	205	PHE	2.7
1	B	49	LYS	2.7
1	C	43	VAL	2.7
1	D	122	THR	2.7
1	D	44	GLY	2.6
1	B	223	ILE	2.6
1	D	19	ILE	2.6
1	D	23	ILE	2.6
1	C	13	THR	2.6
1	C	206	PHE	2.6
1	B	45	GLU	2.6
1	D	40	HIS	2.6
1	C	55	ASP	2.5
1	A	197	ASP	2.5
1	D	138	ILE	2.5
1	B	23	ILE	2.5
1	C	12	VAL	2.5
1	C	51	ILE	2.5
1	D	47	ALA	2.4
1	B	183	VAL	2.4
1	D	56	VAL	2.4
1	C	41	ALA	2.4
1	D	46	LYS	2.4
1	A	202	ALA	2.4
1	C	118	VAL	2.3
1	C	46	LYS	2.3
1	D	54	THR	2.3
1	D	203	GLU	2.3
1	D	227	CYS	2.3
1	D	61	GLN	2.3
1	B	205	PHE	2.3
1	B	86	THR	2.3
1	B	42	ASP	2.3
1	C	52	GLY	2.3
1	C	72	LYS	2.3
1	B	118	VAL	2.2
1	C	133	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	55	ASP	2.2
1	B	206	PHE	2.2
1	C	86	THR	2.2
1	C	78	GLU	2.1
1	B	203	GLU	2.1
1	A	230	LEU	2.1
1	B	122	THR	2.1
1	D	13	THR	2.1
1	B	186	VAL	2.1
1	C	48	ALA	2.1
1	A	144	ILE	2.1
1	D	140	ASN	2.1
1	B	47	ALA	2.0
1	B	193	THR	2.0
1	C	178	ASP	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 monosaccharides in this entry.

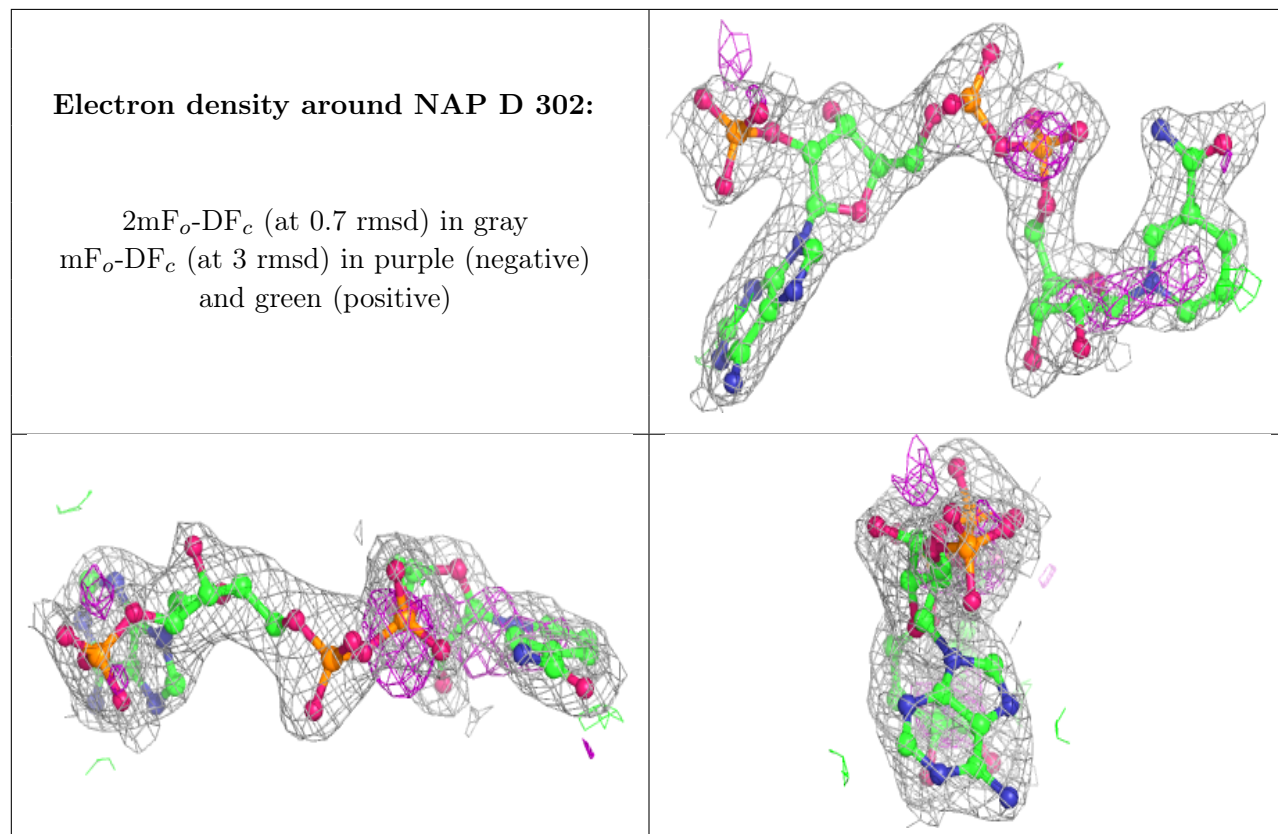
## 6.4 Ligands [i](#)

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
3	NAP	D	302	48/48	0.91	0.13	40,56,64,69	0
2	MG	A	301	1/1	0.93	0.12	28,28,28,28	0
3	NAP	B	301	48/48	0.95	0.08	37,47,55,65	0
3	NAP	C	301	48/48	0.97	0.06	32,43,52,56	0
3	NAP	A	302	48/48	0.97	0.07	27,35,41,46	0
2	MG	D	301	1/1	0.98	0.10	32,32,32,32	0

The following is a graphical depiction of the model fit to experimental electron density of all

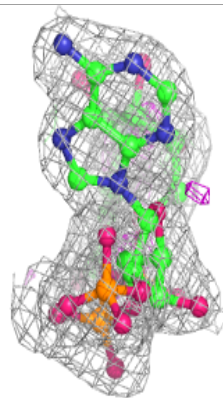
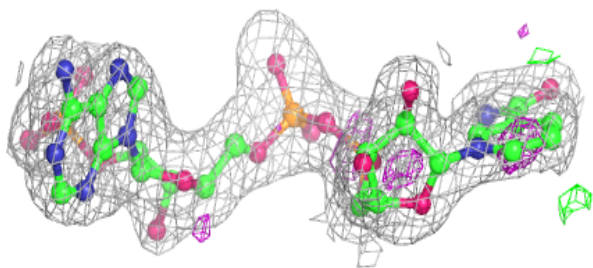
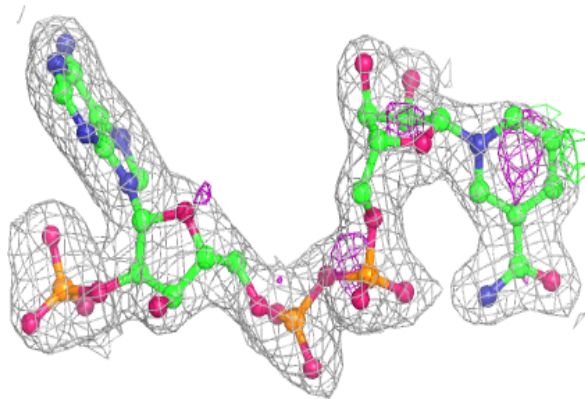
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



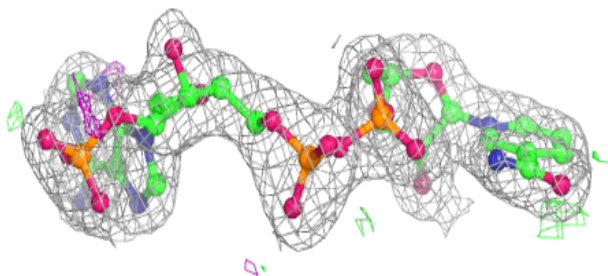
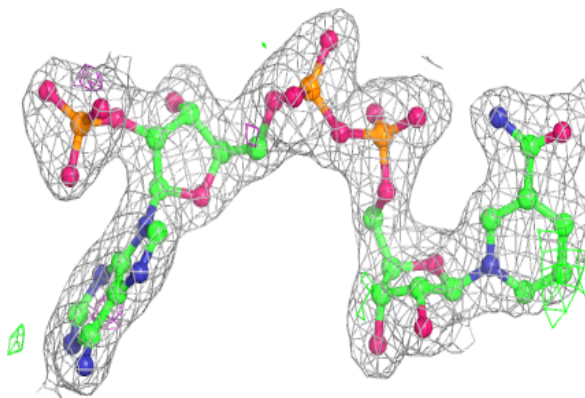


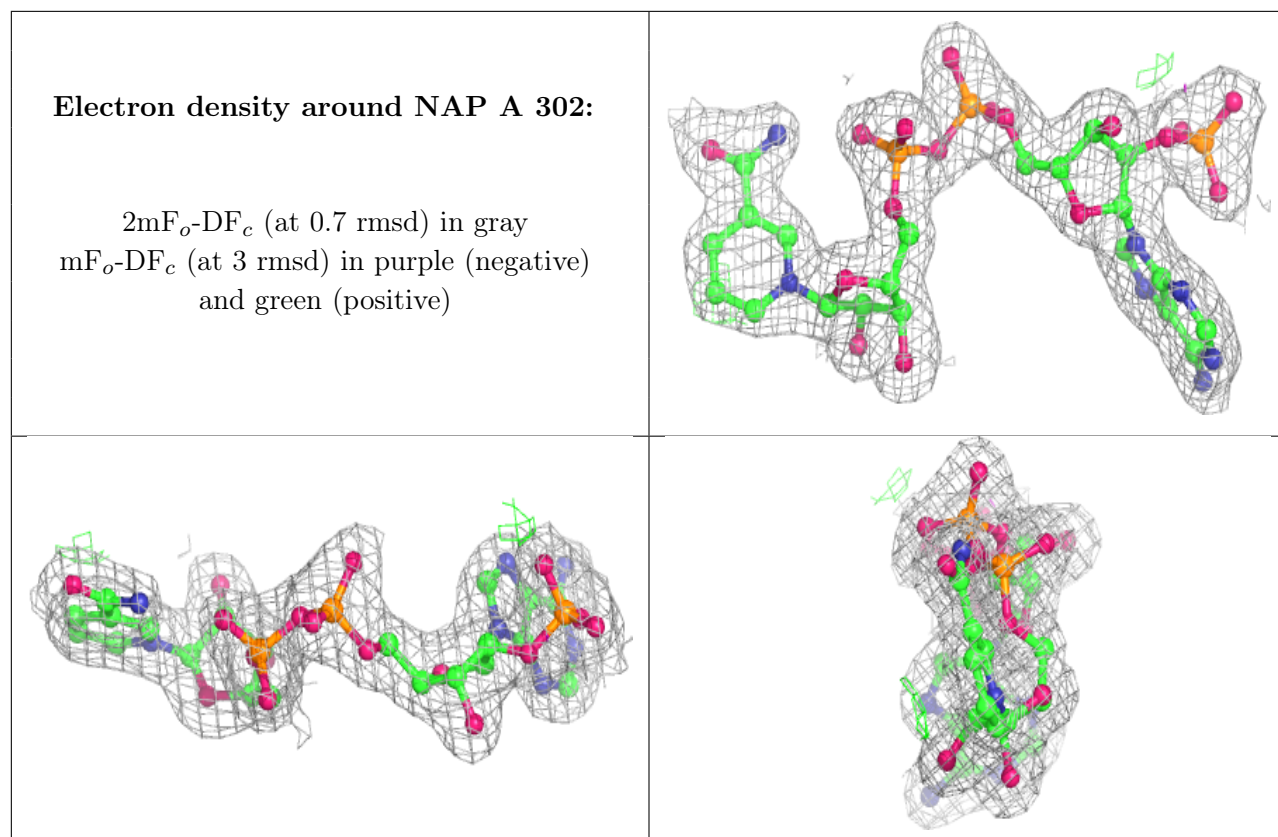
**Electron density around NAP B 301:**

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

**Electron density around NAP C 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.