



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2020 – 12:08 PM EDT

PDB ID : 7KF3
Title : Crystal structure of GDP-mannose 4,6-dehydratase from *Brucella abortus* (strain 2308) in complex with Guanosine-diphosphate-rhamnose
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2020-10-13
Resolution : 2.35 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 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	:	2.14.6
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)	:	2.14.6

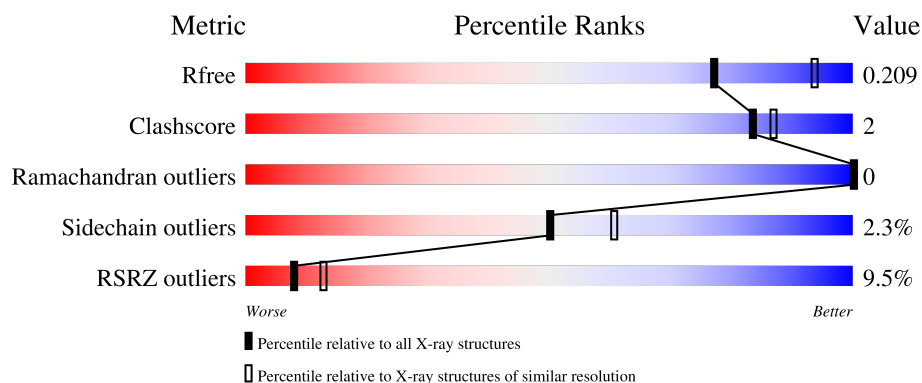
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 ≥ 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	369	<div> <div>8%</div> <div>91%</div> <div>7%</div> </div>
1	B	369	<div> <div>9%</div> <div>90%</div> <div>8%</div> </div>
1	C	369	<div> <div>9%</div> <div>91%</div> <div>7%</div> </div>
1	D	369	<div> <div>12%</div> <div>91%</div> <div>7%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12289 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 GDP-mannose 4,6-dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2841	1806	492	535	8			
1	B	362	Total	C	N	O	S	0	1	0
			2843	1807	492	536	8			
1	C	362	Total	C	N	O	S	0	2	0
			2848	1814	492	534	8			
1	D	362	Total	C	N	O	S	0	1	0
			2843	1808	493	534	8			

There are 28 discrepancies between the modelled and reference sequences:

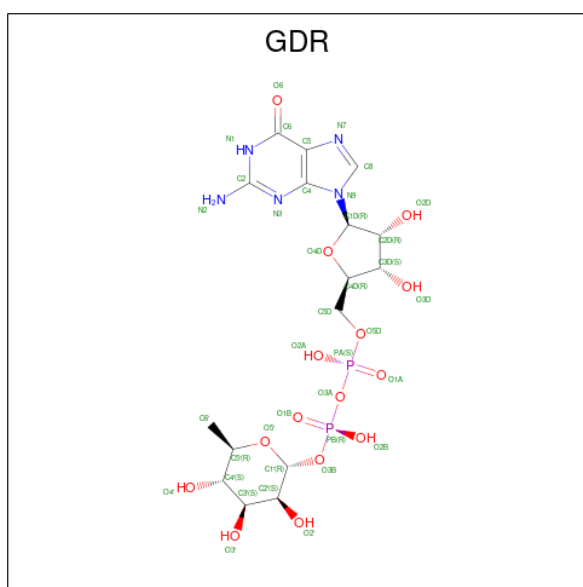
Chain	Residue	Modelled	Actual	Comment	Reference
A	363	GLY	-	expression tag	UNP Q2YMP3
A	364	HIS	-	expression tag	UNP Q2YMP3
A	365	HIS	-	expression tag	UNP Q2YMP3
A	366	HIS	-	expression tag	UNP Q2YMP3
A	367	HIS	-	expression tag	UNP Q2YMP3
A	368	HIS	-	expression tag	UNP Q2YMP3
A	369	HIS	-	expression tag	UNP Q2YMP3
B	363	GLY	-	expression tag	UNP Q2YMP3
B	364	HIS	-	expression tag	UNP Q2YMP3
B	365	HIS	-	expression tag	UNP Q2YMP3
B	366	HIS	-	expression tag	UNP Q2YMP3
B	367	HIS	-	expression tag	UNP Q2YMP3
B	368	HIS	-	expression tag	UNP Q2YMP3
B	369	HIS	-	expression tag	UNP Q2YMP3
C	363	GLY	-	expression tag	UNP Q2YMP3
C	364	HIS	-	expression tag	UNP Q2YMP3
C	365	HIS	-	expression tag	UNP Q2YMP3
C	366	HIS	-	expression tag	UNP Q2YMP3
C	367	HIS	-	expression tag	UNP Q2YMP3
C	368	HIS	-	expression tag	UNP Q2YMP3
C	369	HIS	-	expression tag	UNP Q2YMP3

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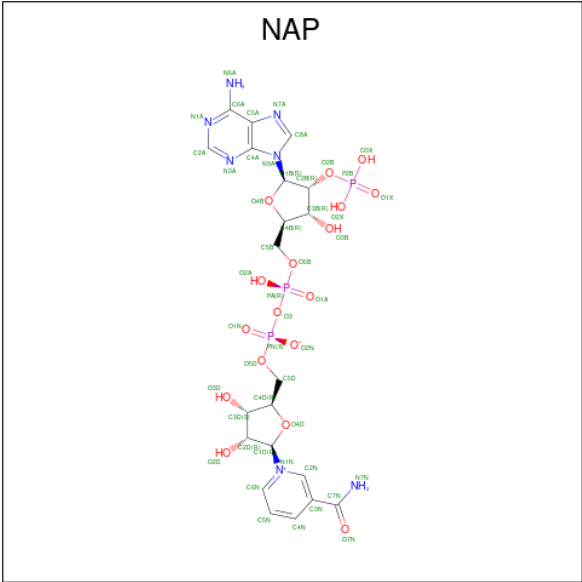
Chain	Residue	Modelled	Actual	Comment	Reference
D	363	GLY	-	expression tag	UNP Q2YMP3
D	364	HIS	-	expression tag	UNP Q2YMP3
D	365	HIS	-	expression tag	UNP Q2YMP3
D	366	HIS	-	expression tag	UNP Q2YMP3
D	367	HIS	-	expression tag	UNP Q2YMP3
D	368	HIS	-	expression tag	UNP Q2YMP3
D	369	HIS	-	expression tag	UNP Q2YMP3

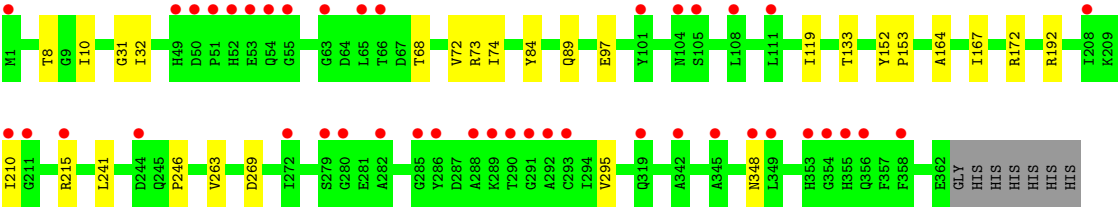
- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE-RHAMNOSE (three-letter code: GDR) (formula: $C_{16}H_{25}N_5O_{15}P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
2	B	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
2	C	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
2	D	1	Total	C	N	O	P	0	0
			38	16	5	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by author).





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.13Å 93.30Å 93.77Å 89.06° 78.91° 87.51°	Depositor
Resolution (Å)	48.35 – 2.35 48.35 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.1 (48.35-2.35) 96.1 (48.35-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.174 , 0.210 0.175 , 0.209	Depositor DCC
R_{free} test set	1975 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12289	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.87% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/2905	0.55	0/3946
1	B	0.32	0/2910	0.54	0/3954
1	C	0.33	0/2918	0.55	0/3962
1	D	0.33	0/2910	0.54	0/3953
All	All	0.33	0/11643	0.54	0/15815

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	2841	0	2745	14	0
1	B	2843	0	2742	19	0
1	C	2848	0	2770	16	0
1	D	2843	0	2749	16	0
2	A	38	0	23	0	0
2	B	38	0	23	0	0
2	C	38	0	23	0	0
2	D	38	0	23	0	0
3	A	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	25	0	0
3	C	48	0	25	1	0
3	D	48	0	25	0	0
4	A	159	0	0	3	0
4	B	134	0	0	4	0
4	C	152	0	0	0	0
4	D	125	0	0	2	0
All	All	12289	0	11198	54	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 2.

All (54) 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:B:68:THR:HB	1:D:68:THR:HB	1.67	0.74
1:A:35:ARG:NH1	4:A:501:HOH:O	2.12	0.74
1:C:8:THR:HG22	1:C:32:ILE:HD12	1.73	0.71
1:D:97:GLU:OE1	4:D:501:HOH:O	2.11	0.68
1:A:210:ILE:HG21	1:A:348:ASN:HD21	1.59	0.68
1:B:210:ILE:HG21	1:B:348:ASN:HD21	1.59	0.68
1:A:79:ARG:NH2	4:A:505:HOH:O	2.28	0.66
1:A:8:THR:HG22	1:A:32:ILE:HD12	1.80	0.64
1:A:68:THR:HB	1:C:68:THR:HB	1.80	0.64
1:C:210:ILE:HG21	1:C:348:ASN:HD21	1.65	0.61
1:A:123:GLU:OE2	4:A:502:HOH:O	2.16	0.60
1:D:210:ILE:HG21	1:D:348:ASN:HD21	1.68	0.58
1:C:190:PRO:HB3	1:C:339:GLU:HG3	1.85	0.58
1:B:232:ASP:OD1	4:B:501:HOH:O	2.17	0.58
1:A:166:TRP:CD2	1:D:153:PRO:HD2	2.41	0.56
1:B:166:TRP:CD2	1:C:153:PRO:HD2	2.42	0.55
1:A:119:ILE:HG21	1:C:72:VAL:HG12	1.88	0.54
1:B:72:VAL:HG12	1:D:119:ILE:HG21	1.91	0.52
1:B:153:PRO:HD2	1:C:166:TRP:CD2	2.46	0.51
1:B:8:THR:HG22	1:B:32:ILE:HD12	1.91	0.51
1:D:73:ARG:NH2	4:D:502:HOH:O	2.23	0.49
1:B:119:ILE:HG21	1:D:72:VAL:HG12	1.95	0.49
1:D:8:THR:HG22	1:D:32:ILE:HD12	1.95	0.49
1:A:166:TRP:CE3	1:D:153:PRO:HD2	2.49	0.48
1:B:203[A]:ARG:NH2	4:B:504:HOH:O	2.29	0.48
1:B:203[B]:ARG:NH2	4:B:504:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PRO:HD2	1:C:166:TRP:CE3	2.50	0.47
1:B:107:ALA:HB1	1:B:163:TYR:CD1	2.52	0.45
1:B:166:TRP:CE3	1:C:153:PRO:HD2	2.52	0.45
1:B:35:ARG:NE	4:B:507:HOH:O	2.37	0.44
1:B:172:ARG:HD2	1:B:246:PRO:HG2	1.99	0.44
1:B:263:VAL:HG11	1:B:295:VAL:HG21	1.99	0.44
1:A:107:ALA:HB1	1:A:163:TYR:CD1	2.53	0.43
1:C:224:LEU:HD23	1:C:258:SER:HB3	2.00	0.43
1:A:172:ARG:HD2	1:A:246:PRO:HG2	2.00	0.43
1:B:168:THR:HG23	1:B:179:ALA:HB1	1.99	0.43
1:A:134:SER:HB3	1:A:185:PHE:CD1	2.54	0.43
1:D:84:TYR:CZ	1:D:241:LEU:HD12	2.54	0.43
1:B:129:TYR:CZ	1:B:237:GLN:HG2	2.54	0.42
1:C:190:PRO:CB	1:C:339:GLU:HG3	2.49	0.42
1:C:133:THR:HB	3:C:401:NAP:H6N	2.01	0.42
1:D:32:ILE:HG12	1:D:74:ILE:HD13	2.02	0.42
1:D:263:VAL:HG11	1:D:295:VAL:HG21	2.02	0.42
1:D:10:ILE:HG21	1:D:31:GLY:HA3	2.02	0.41
1:A:129:TYR:CZ	1:A:237:GLN:HG2	2.55	0.41
1:D:172:ARG:HD2	1:D:246:PRO:HG2	2.02	0.41
1:C:129:TYR:CZ	1:C:237:GLN:HG2	2.56	0.41
1:C:167:ILE:HA	1:C:167:ILE:HD12	1.90	0.41
1:B:6:LEU:HD11	1:B:32:ILE:HG13	2.02	0.40
1:C:198:THR:HB	1:C:262:PHE:CZ	2.55	0.40
1:D:164:ALA:HA	1:D:167:ILE:HG22	2.04	0.40
1:D:167:ILE:HD12	1:D:167:ILE:HA	1.95	0.40
1:A:263:VAL:HG11	1:A:295:VAL:HG21	2.04	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	360/369 (98%)	353 (98%)	7 (2%)	0	100	100
1	B	361/369 (98%)	354 (98%)	7 (2%)	0	100	100
1	C	362/369 (98%)	356 (98%)	6 (2%)	0	100	100
1	D	361/369 (98%)	354 (98%)	7 (2%)	0	100	100
All	All	1444/1476 (98%)	1417 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	286/306 (94%)	279 (98%)	7 (2%)	49	59
1	B	286/306 (94%)	280 (98%)	6 (2%)	53	65
1	C	288/306 (94%)	281 (98%)	7 (2%)	49	59
1	D	286/306 (94%)	280 (98%)	6 (2%)	53	65
All	All	1146/1224 (94%)	1120 (98%)	26 (2%)	50	61

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	133	THR
1	A	152	TYR
1	A	192	ARG
1	A	215	ARG
1	A	269	ASP
1	A	309	THR
1	B	89	GLN
1	B	133	THR
1	B	152	TYR
1	B	192	ARG
1	B	215	ARG
1	B	269	ASP

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Mol	Chain	Res	Type
1	C	89	GLN
1	C	152	TYR
1	C	180	CYS
1	C	192	ARG
1	C	215	ARG
1	C	268	LYS
1	C	269	ASP
1	D	89	GLN
1	D	133	THR
1	D	152	TYR
1	D	192	ARG
1	D	215	ARG
1	D	269	ASP

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

Mol	Chain	Res	Type
1	A	212	ASN
1	A	348	ASN
1	B	212	ASN
1	B	348	ASN
1	C	212	ASN
1	C	256	GLN
1	C	348	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 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	NAP	D	401	-	45,52,52	0.65	1 (2%)	56,80,80	0.70	2 (3%)
3	NAP	B	401	-	45,52,52	0.68	1 (2%)	56,80,80	0.67	2 (3%)
3	NAP	C	401	-	45,52,52	0.66	1 (2%)	56,80,80	0.72	3 (5%)
3	NAP	A	401	-	45,52,52	0.57	0	56,80,80	0.77	3 (5%)
2	GDR	A	400	-	34,41,41	0.77	1 (2%)	46,64,64	1.76	6 (13%)
2	GDR	B	400	-	34,41,41	0.78	1 (2%)	46,64,64	1.79	7 (15%)
2	GDR	C	400	-	34,41,41	0.79	1 (2%)	46,64,64	1.85	7 (15%)
2	GDR	D	400	-	34,41,41	0.75	1 (2%)	46,64,64	1.75	5 (10%)

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	D	401	-	-	10/31/67/67	0/5/5/5
3	NAP	B	401	-	-	9/31/67/67	0/5/5/5
3	NAP	C	401	-	-	8/31/67/67	0/5/5/5
3	NAP	A	401	-	-	9/31/67/67	0/5/5/5
2	GDR	A	400	-	-	3/17/57/57	0/4/4/4
2	GDR	B	400	-	-	3/17/57/57	0/4/4/4
2	GDR	C	400	-	-	3/17/57/57	0/4/4/4
2	GDR	D	400	-	-	3/17/57/57	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	GDR	C6-N1	3.27	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	GDR	C6-N1	3.25	1.38	1.33
2	D	400	GDR	C6-N1	3.09	1.38	1.33
2	A	400	GDR	C6-N1	2.96	1.38	1.33
3	B	401	NAP	P2B-O2B	2.79	1.64	1.59
3	D	401	NAP	P2B-O2B	2.45	1.63	1.59
3	C	401	NAP	P2B-O2B	2.40	1.63	1.59

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	GDR	C5-C6-N1	-8.44	111.89	123.43
2	A	400	GDR	C5-C6-N1	-8.31	112.07	123.43
2	B	400	GDR	C5-C6-N1	-8.22	112.19	123.43
2	D	400	GDR	C5-C6-N1	-8.21	112.20	123.43
2	A	400	GDR	C6-N1-C2	5.96	125.40	115.93
2	C	400	GDR	C6-N1-C2	5.94	125.38	115.93
2	B	400	GDR	C6-N1-C2	5.90	125.31	115.93
2	D	400	GDR	C6-N1-C2	5.86	125.24	115.93
2	C	400	GDR	O5'-C1'-O3B	-3.29	107.06	111.36
2	B	400	GDR	N3-C2-N1	-2.97	123.26	127.22
2	D	400	GDR	N3-C2-N1	-2.94	123.30	127.22
2	C	400	GDR	N3-C2-N1	-2.83	123.44	127.22
2	A	400	GDR	N3-C2-N1	-2.82	123.46	127.22
2	B	400	GDR	C2-N3-C4	-2.62	112.36	115.36
2	C	400	GDR	C6-C5-C4	-2.60	118.32	120.80
2	A	400	GDR	C6-C5-C4	-2.56	118.35	120.80
2	D	400	GDR	C2-N3-C4	-2.50	112.50	115.36
2	A	400	GDR	C2-N3-C4	-2.45	112.56	115.36
2	C	400	GDR	PB-O3B-C1'	2.40	129.03	119.74
2	C	400	GDR	C2-N3-C4	-2.39	112.63	115.36
2	D	400	GDR	C6-C5-C4	-2.33	118.57	120.80
3	A	401	NAP	C5A-C6A-N6A	2.32	123.87	120.35
3	C	401	NAP	C5A-C6A-N6A	2.19	123.69	120.35
2	B	400	GDR	C6-C5-C4	-2.18	118.72	120.80
3	B	401	NAP	C5A-C6A-N6A	2.16	123.64	120.35
3	D	401	NAP	C3B-C2B-C1B	-2.15	98.84	102.89
3	C	401	NAP	PN-O3-PA	-2.13	125.52	132.83
3	C	401	NAP	C3B-C2B-C1B	-2.12	98.91	102.89
3	A	401	NAP	C3B-C2B-C1B	-2.11	98.91	102.89
3	D	401	NAP	C5A-C6A-N6A	2.11	123.56	120.35
2	A	400	GDR	PB-O3B-C1'	2.11	127.90	119.74
2	B	400	GDR	O5'-C1'-O3B	-2.05	108.69	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAP	PN-O3-PA	-2.04	125.82	132.83
3	B	401	NAP	C3B-C2B-C1B	-2.03	99.06	102.89
2	B	400	GDR	PB-O3B-C1'	2.02	127.56	119.74

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	NAP	O4D-C1D-N1N-C2N
3	D	401	NAP	O4D-C1D-N1N-C6N
3	D	401	NAP	C2D-C1D-N1N-C2N
3	D	401	NAP	C2D-C1D-N1N-C6N
3	B	401	NAP	O4D-C1D-N1N-C2N
3	B	401	NAP	O4D-C1D-N1N-C6N
3	B	401	NAP	C2D-C1D-N1N-C6N
3	C	401	NAP	O4D-C1D-N1N-C2N
3	C	401	NAP	O4D-C1D-N1N-C6N
3	C	401	NAP	C2D-C1D-N1N-C6N
3	A	401	NAP	C5D-O5D-PN-O2N
3	A	401	NAP	O4D-C1D-N1N-C2N
3	A	401	NAP	O4D-C1D-N1N-C6N
3	A	401	NAP	C2D-C1D-N1N-C6N
2	A	400	GDR	C1'-O3B-PB-O3A
2	B	400	GDR	C1'-O3B-PB-O3A
2	C	400	GDR	C1'-O3B-PB-O3A
2	D	400	GDR	C1'-O3B-PB-O3A
3	A	401	NAP	C2B-O2B-P2B-O2X
3	A	401	NAP	C5D-O5D-PN-O3
3	D	401	NAP	C5D-O5D-PN-O2N
3	B	401	NAP	C5D-O5D-PN-O2N
3	C	401	NAP	C5D-O5D-PN-O2N
2	A	400	GDR	O5'-C1'-O3B-PB
2	B	400	GDR	O5'-C1'-O3B-PB
2	C	400	GDR	O5'-C1'-O3B-PB
2	D	400	GDR	O5'-C1'-O3B-PB
3	D	401	NAP	C2B-O2B-P2B-O2X
3	D	401	NAP	C5D-O5D-PN-O3
3	B	401	NAP	C2B-O2B-P2B-O2X
3	B	401	NAP	C5D-O5D-PN-O3
3	B	401	NAP	C2D-C1D-N1N-C2N
3	C	401	NAP	C2B-O2B-P2B-O2X
3	C	401	NAP	C5D-O5D-PN-O3

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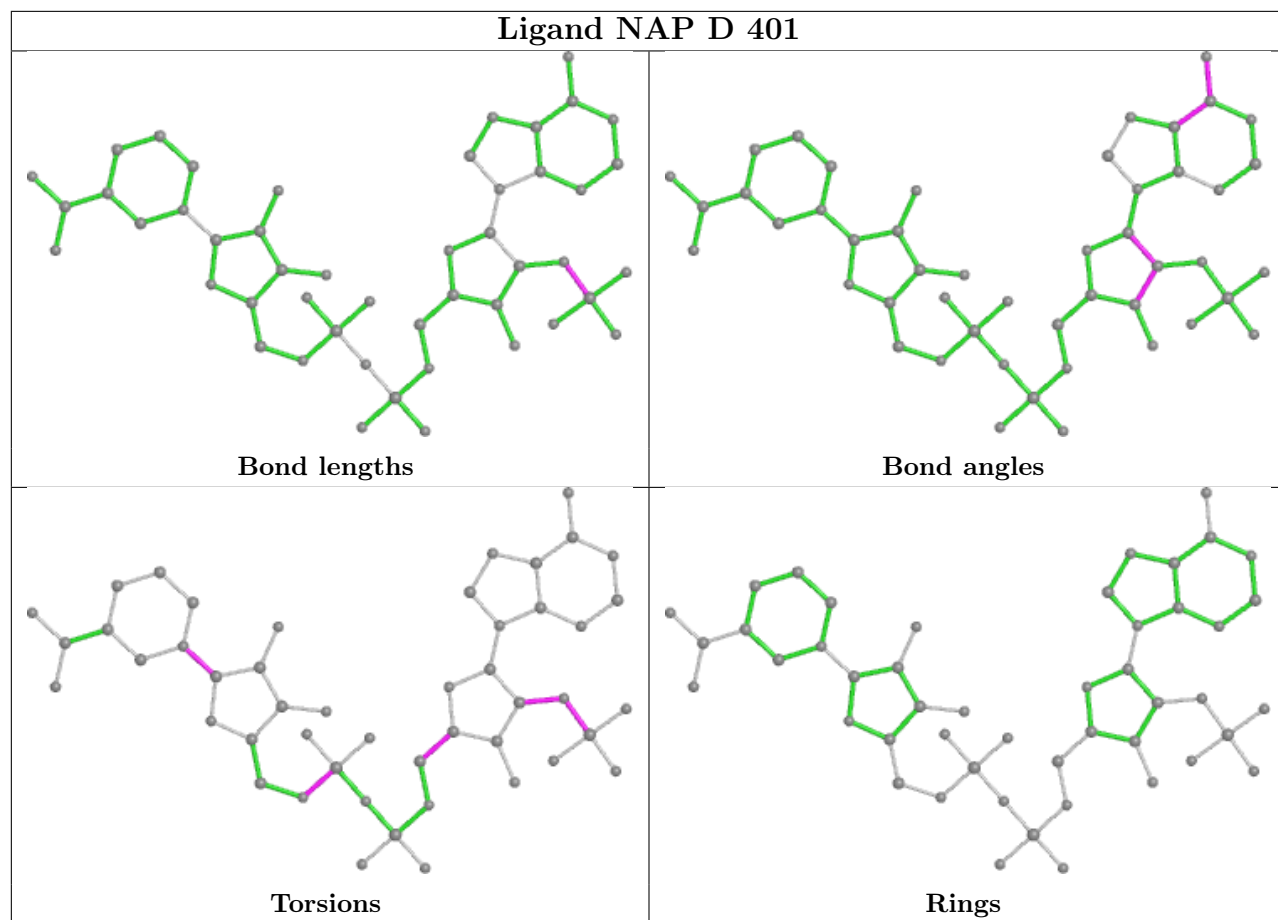
Mol	Chain	Res	Type	Atoms
3	C	401	NAP	C2D-C1D-N1N-C2N
3	A	401	NAP	C2D-C1D-N1N-C2N
3	D	401	NAP	O4B-C4B-C5B-O5B
3	C	401	NAP	O4B-C4B-C5B-O5B
2	A	400	GDR	C1'-O3B-PB-O1B
2	B	400	GDR	C1'-O3B-PB-O1B
2	C	400	GDR	C1'-O3B-PB-O1B
2	D	400	GDR	C1'-O3B-PB-O1B
3	D	401	NAP	C1B-C2B-O2B-P2B
3	D	401	NAP	C5D-O5D-PN-O1N
3	B	401	NAP	C5D-O5D-PN-O1N
3	A	401	NAP	C5D-O5D-PN-O1N
3	B	401	NAP	O4B-C4B-C5B-O5B
3	A	401	NAP	O4B-C4B-C5B-O5B

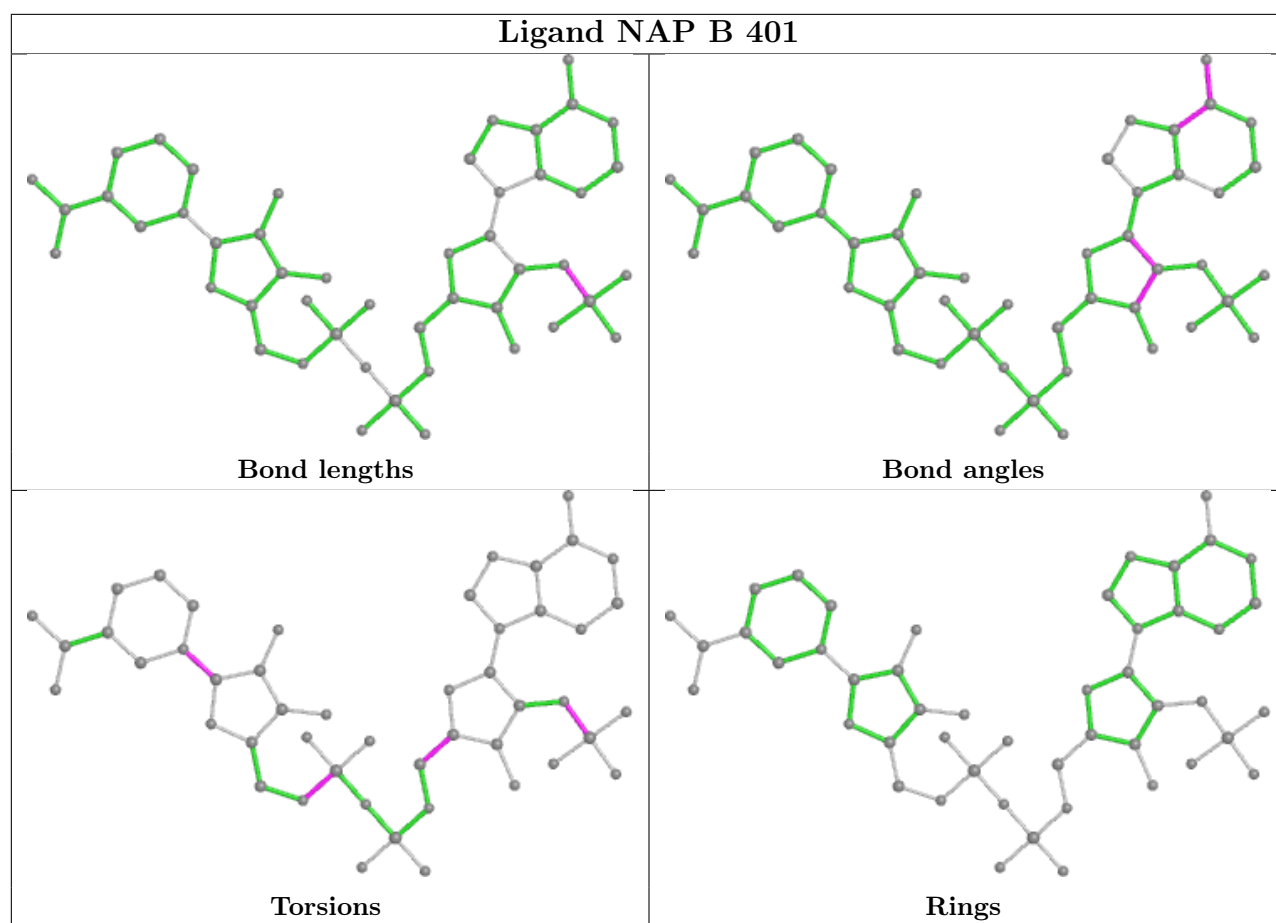
There are no ring outliers.

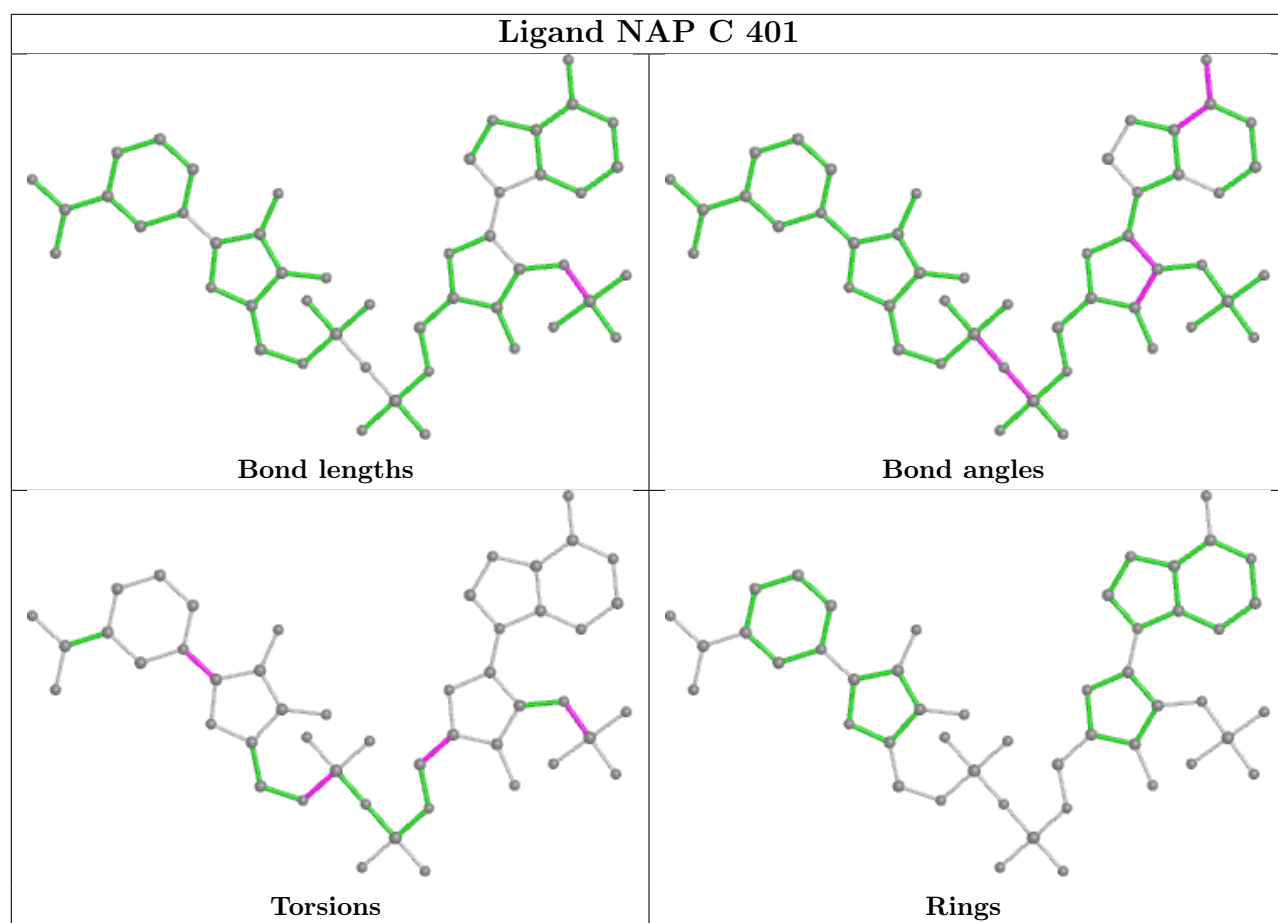
1 monomer is involved in 1 short contact:

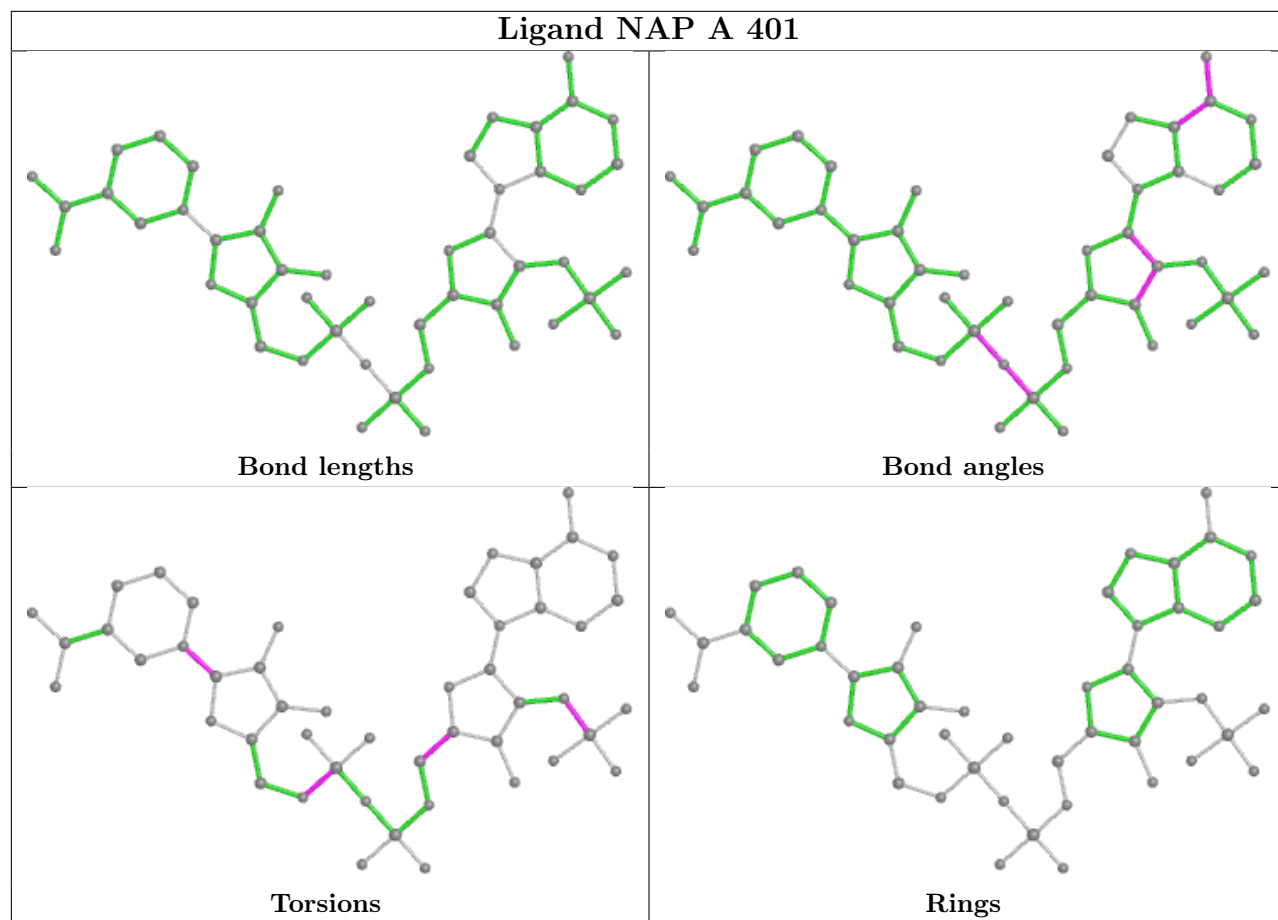
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	NAP	1	0

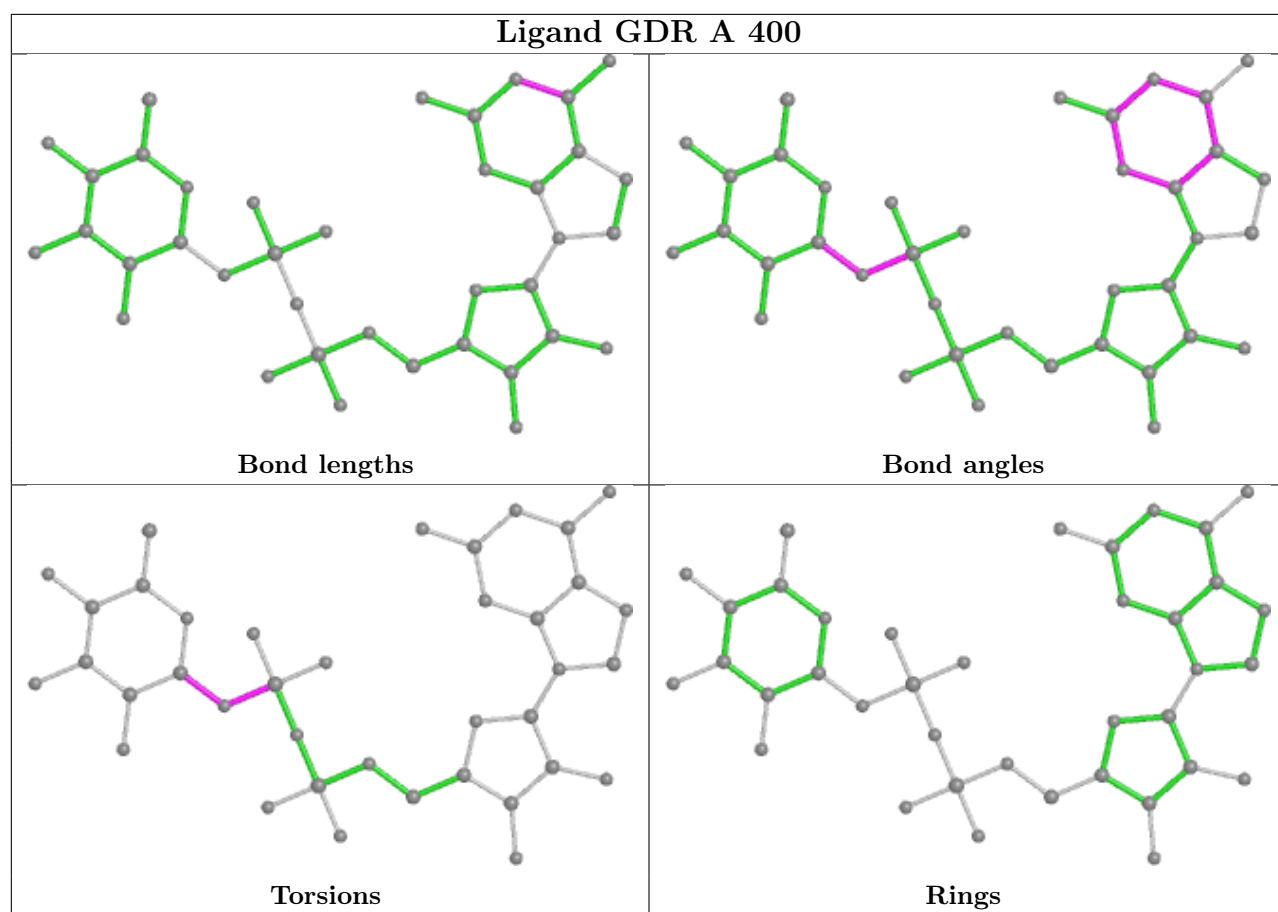
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

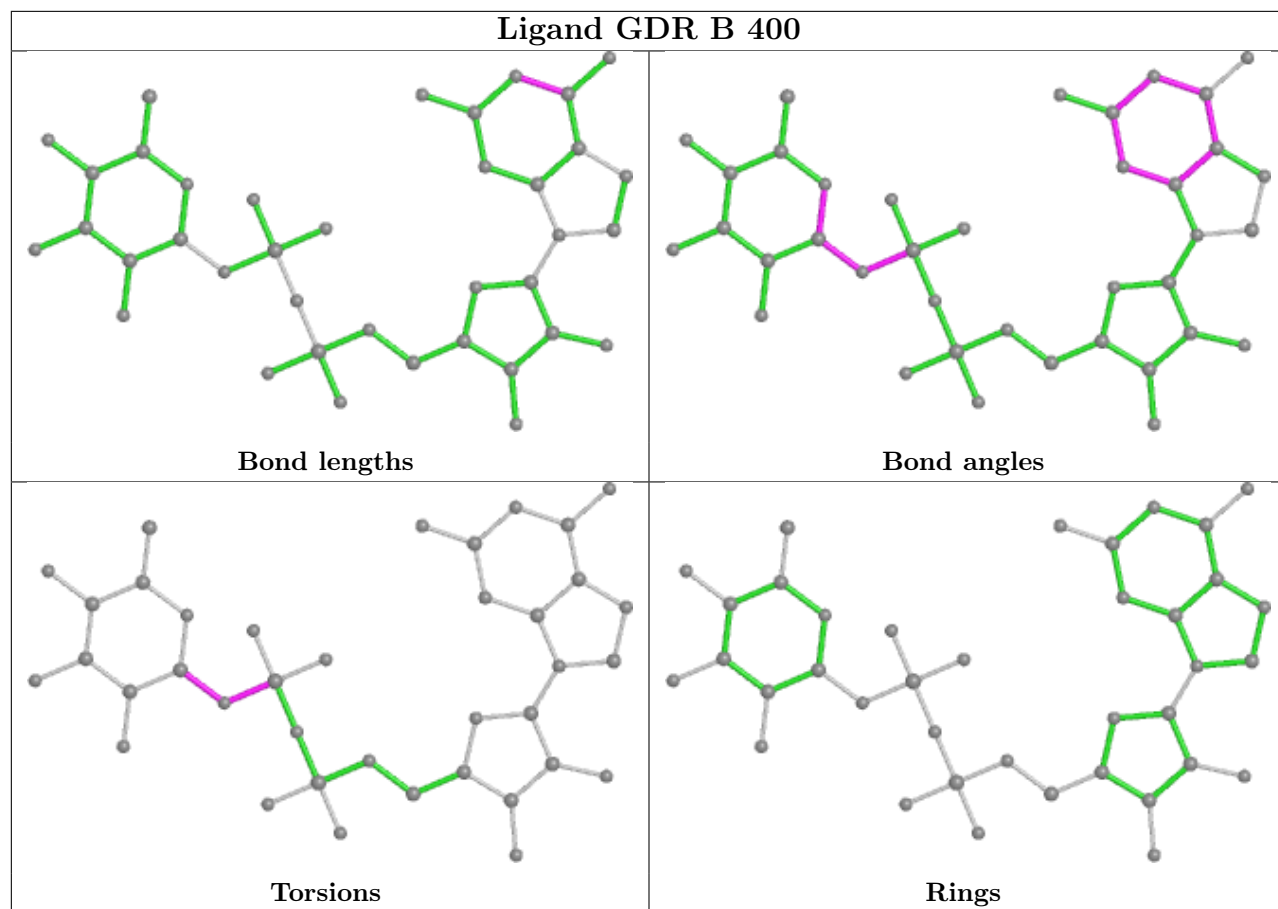


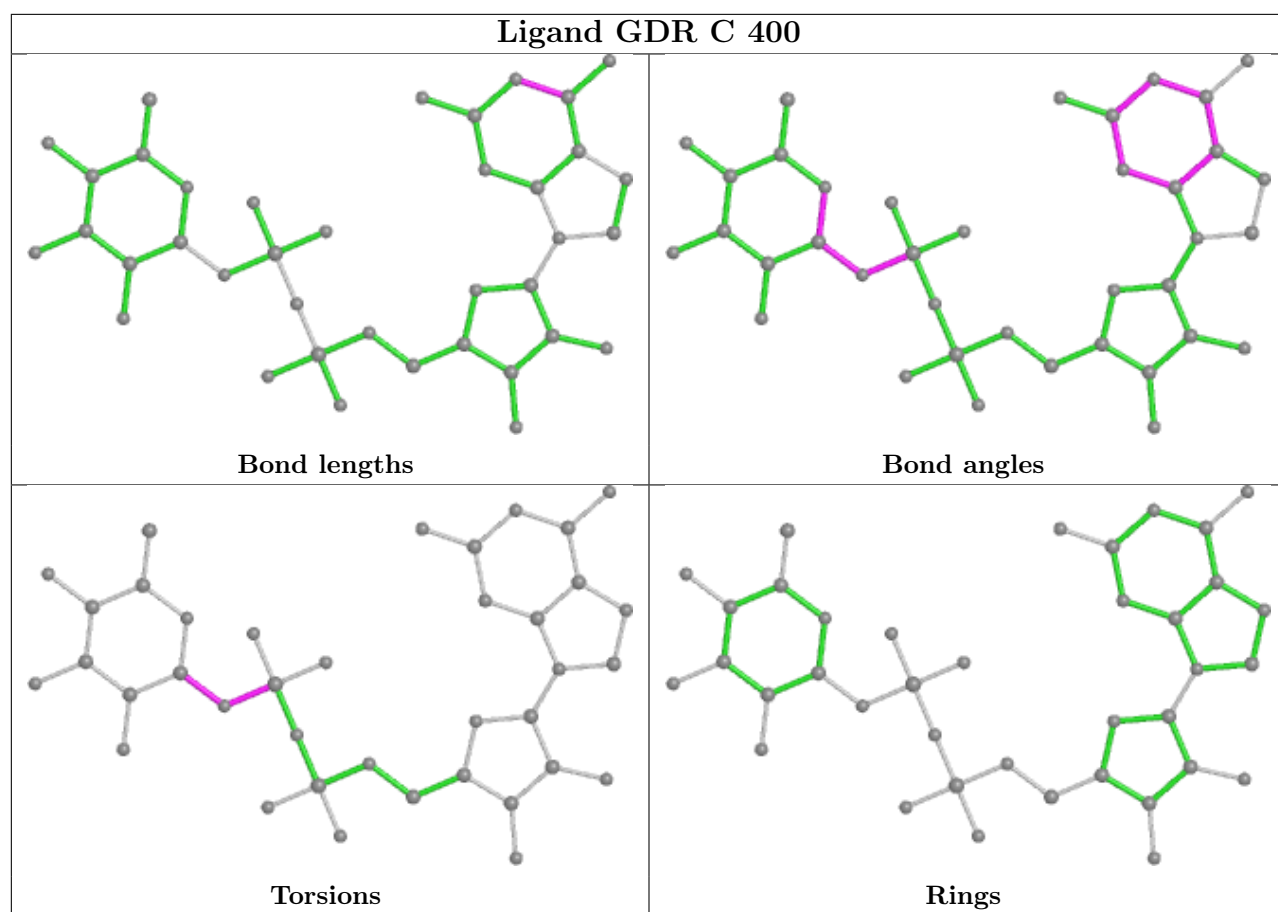


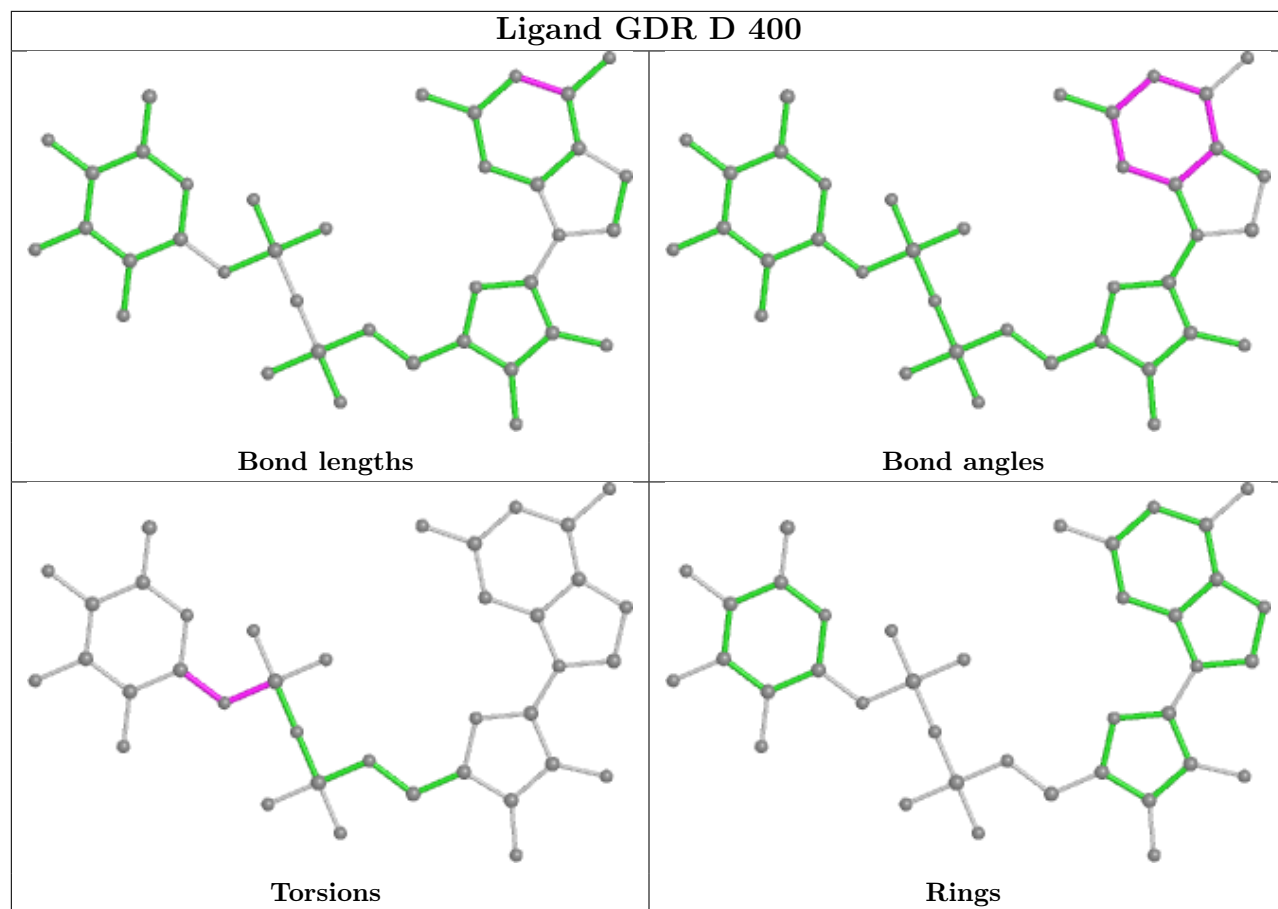












5.7 Other polymers [i](#)

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, 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	362/369 (98%)	0.47	31 (8%) 10 16	27, 43, 72, 102	0
1	B	362/369 (98%)	0.49	32 (8%) 10 15	28, 47, 81, 113	0
1	C	362/369 (98%)	0.53	32 (8%) 10 15	28, 43, 74, 108	0
1	D	362/369 (98%)	0.58	43 (11%) 4 7	27, 48, 81, 110	0
All	All	1448/1476 (98%)	0.51	138 (9%) 8 13	27, 45, 79, 113	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	353	HIS	5.4
1	D	52	HIS	5.3
1	C	211	GLY	4.9
1	A	211	GLY	4.8
1	C	52	HIS	4.7
1	C	51	PRO	4.3
1	D	288	ALA	4.2
1	A	51	PRO	4.2
1	D	1	MET	4.1
1	D	345	ALA	4.0
1	D	51	PRO	4.0
1	A	355	HIS	4.0
1	D	286	TYR	4.0
1	C	1	MET	3.9
1	A	286	TYR	3.9
1	A	1	MET	3.9
1	D	353	HIS	3.8
1	D	292	ALA	3.8
1	C	66	THR	3.8
1	A	52	HIS	3.7
1	C	108	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	65	LEU	3.7
1	C	355	HIS	3.7
1	B	286	TYR	3.7
1	A	66	THR	3.6
1	B	108	LEU	3.5
1	B	51	PRO	3.5
1	C	103	ALA	3.5
1	D	66	THR	3.5
1	D	49	HIS	3.4
1	B	49	HIS	3.4
1	D	211	GLY	3.4
1	D	349	LEU	3.4
1	A	108	LEU	3.3
1	B	349	LEU	3.3
1	D	244	ASP	3.3
1	B	282	ALA	3.3
1	C	282	ALA	3.3
1	D	355	HIS	3.3
1	A	65	LEU	3.2
1	B	211	GLY	3.2
1	D	290	THR	3.2
1	B	1	MET	3.2
1	D	55	GLY	3.2
1	B	355	HIS	3.2
1	C	291	GLY	3.2
1	B	66	THR	3.1
1	C	286	TYR	3.1
1	B	104	ASN	3.1
1	D	272	ILE	3.1
1	B	348	ASN	3.1
1	D	53	GLU	3.1
1	B	101	TYR	3.1
1	C	107	ALA	3.1
1	D	65	LEU	3.1
1	D	348	ASN	3.0
1	B	290	THR	3.0
1	D	54	GLN	3.0
1	B	291	GLY	3.0
1	A	291	GLY	3.0
1	C	88	ALA	3.0
1	C	104	ASN	2.9
1	D	282	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	49	HIS	2.9
1	B	52	HIS	2.9
1	A	354	GLY	2.9
1	C	349	LEU	2.9
1	C	318	HIS	2.9
1	B	272	ILE	2.9
1	A	353	HIS	2.9
1	B	319	GLN	2.8
1	A	352	GLU	2.8
1	C	292	ALA	2.7
1	B	215	ARG	2.7
1	D	289	LYS	2.7
1	B	54	GLN	2.7
1	D	293	CYS	2.6
1	D	358	PHE	2.6
1	B	353	HIS	2.6
1	A	292	ALA	2.6
1	D	279	SER	2.5
1	D	104	ASN	2.5
1	D	108	LEU	2.5
1	D	208	ILE	2.5
1	D	291	GLY	2.5
1	A	210	ILE	2.5
1	B	55	GLY	2.5
1	C	55	GLY	2.5
1	D	215	ARG	2.4
1	A	53	GLU	2.4
1	D	354	GLY	2.4
1	C	53	GLU	2.4
1	A	54	GLN	2.4
1	B	53	GLU	2.4
1	C	352	GLU	2.4
1	B	102	THR	2.4
1	D	63	GLY	2.4
1	A	350	LEU	2.4
1	A	272	ILE	2.4
1	D	210	ILE	2.4
1	A	348	ASN	2.4
1	D	101	TYR	2.4
1	C	101	TYR	2.3
1	C	322	GLY	2.3
1	B	65	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	109	GLY	2.3
1	D	319	GLN	2.3
1	D	111	LEU	2.3
1	A	356	GLN	2.3
1	D	50	ASP	2.3
1	C	105	SER	2.3
1	A	104	ASN	2.3
1	B	269	ASP	2.3
1	A	342	ALA	2.3
1	A	101	TYR	2.2
1	C	111	LEU	2.2
1	A	105	SER	2.2
1	D	285	GLY	2.2
1	A	88	ALA	2.2
1	C	49	HIS	2.2
1	C	68	THR	2.2
1	C	350	LEU	2.2
1	B	342	ALA	2.2
1	D	342	ALA	2.2
1	D	105	SER	2.2
1	C	342	ALA	2.1
1	B	317	ALA	2.1
1	A	107	ALA	2.1
1	A	315	THR	2.1
1	B	345	ALA	2.1
1	B	271	GLY	2.1
1	A	294	ILE	2.1
1	B	50	ASP	2.0
1	C	312	GLY	2.0
1	D	280	GLY	2.0
1	D	356	GLN	2.0
1	B	110	ALA	2.0
1	A	275	ARG	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](#)

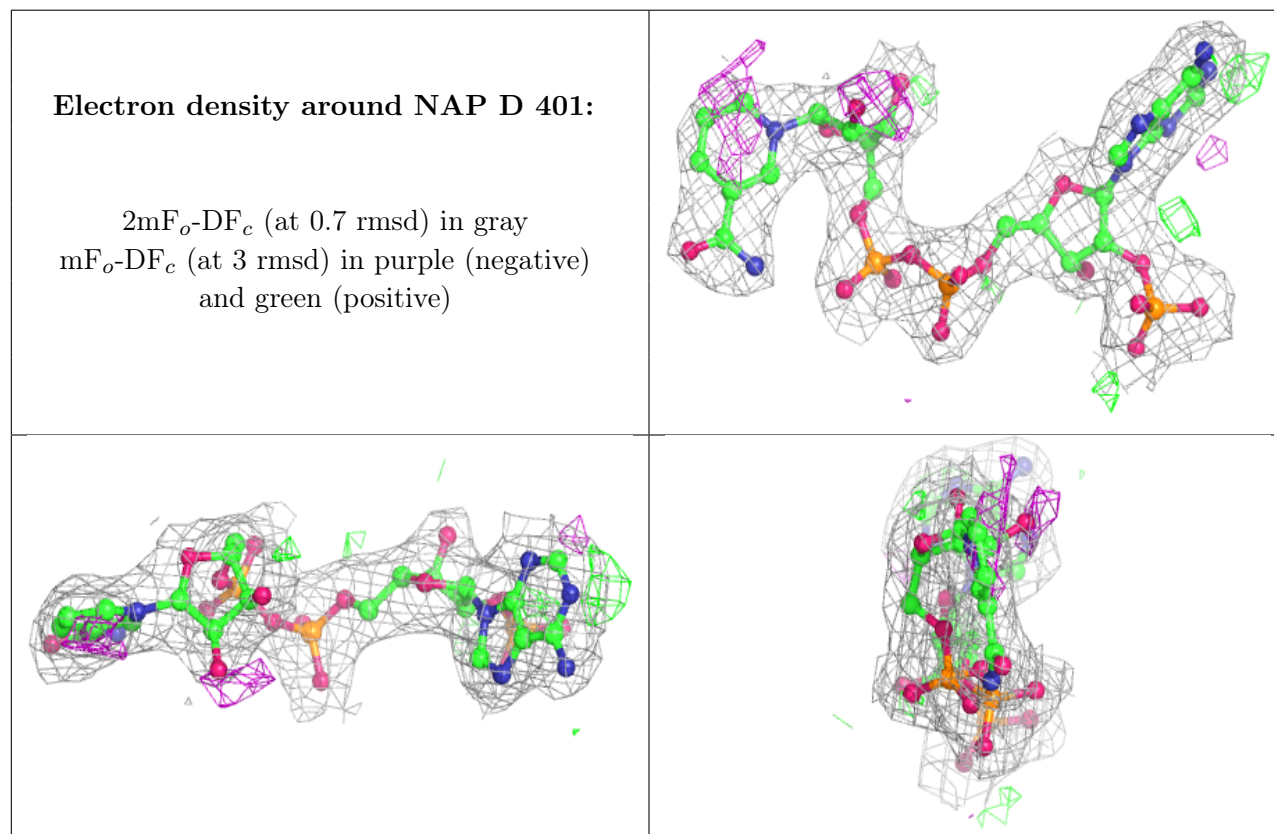
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

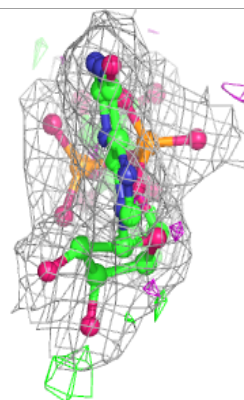
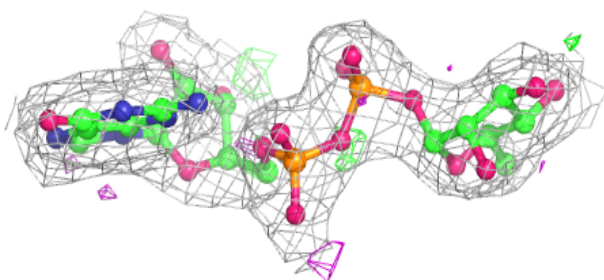
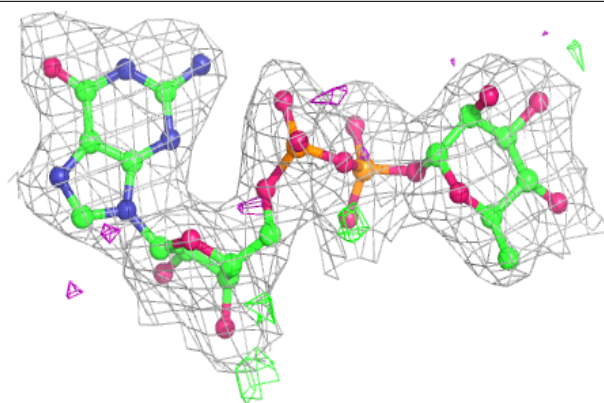
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	D	401	48/48	0.96	0.18	27,34,41,46	0
2	GDR	A	400	38/38	0.96	0.13	31,39,43,50	0
2	GDR	C	400	38/38	0.96	0.14	28,39,43,47	0
2	GDR	D	400	38/38	0.96	0.12	34,42,46,49	0
3	NAP	B	401	48/48	0.97	0.17	29,34,40,42	0
2	GDR	B	400	38/38	0.97	0.13	36,42,47,51	0
3	NAP	C	401	48/48	0.97	0.17	27,32,36,39	0
3	NAP	A	401	48/48	0.97	0.17	26,32,36,37	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.

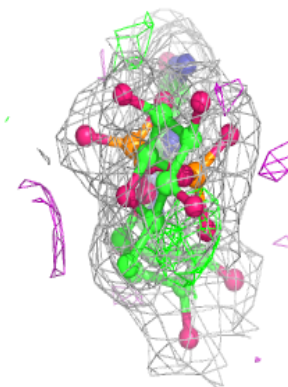
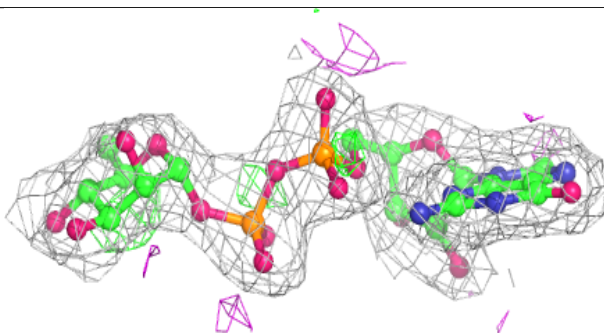
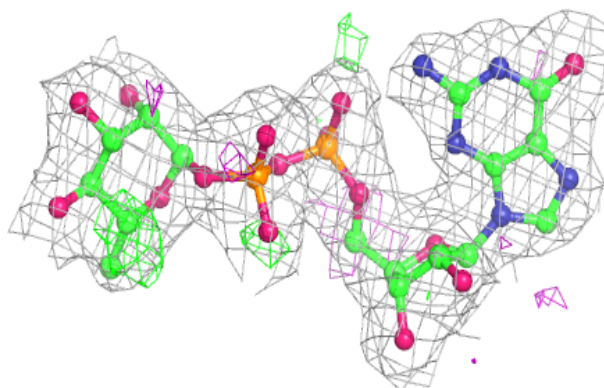


Electron density around GDR A 400:

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

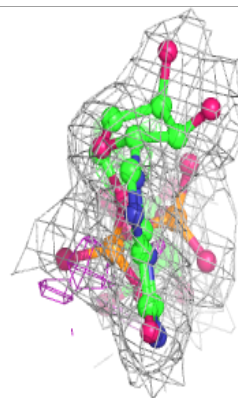
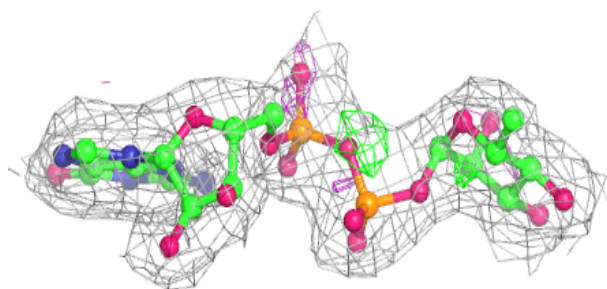
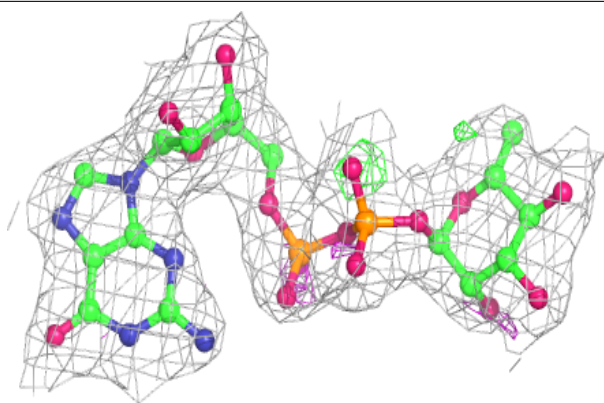
**Electron density around GDR C 400:**

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

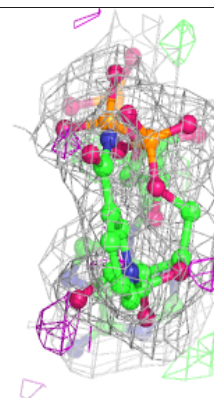
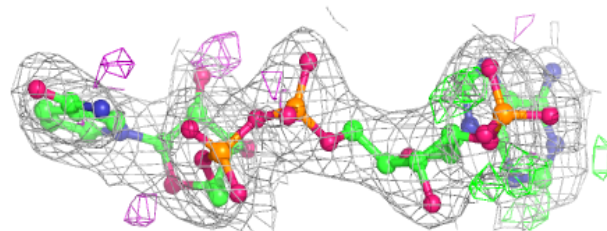
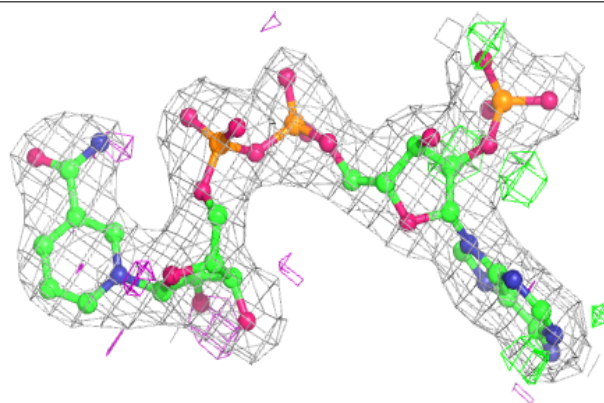


Electron density around GDR D 400:

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

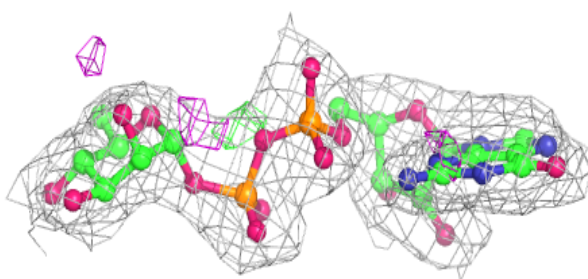
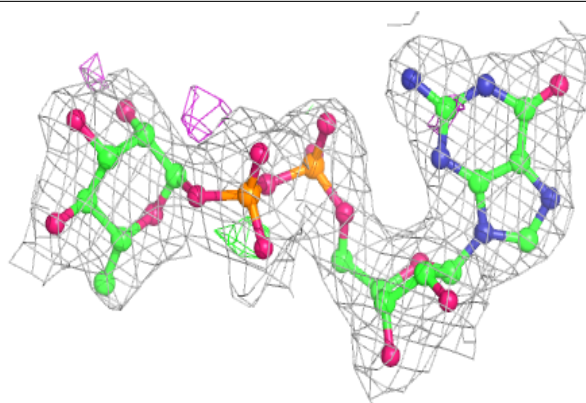
**Electron density around NAP B 401:**

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

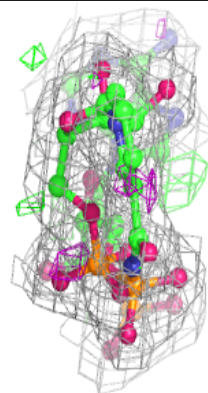
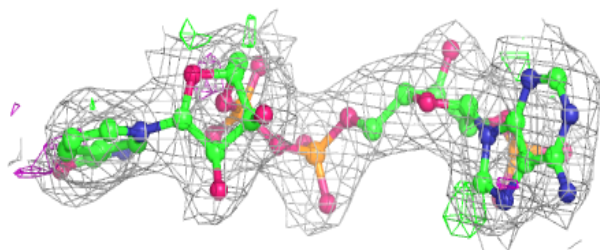
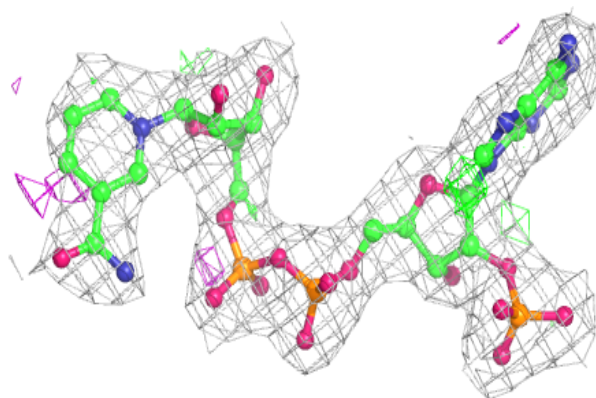


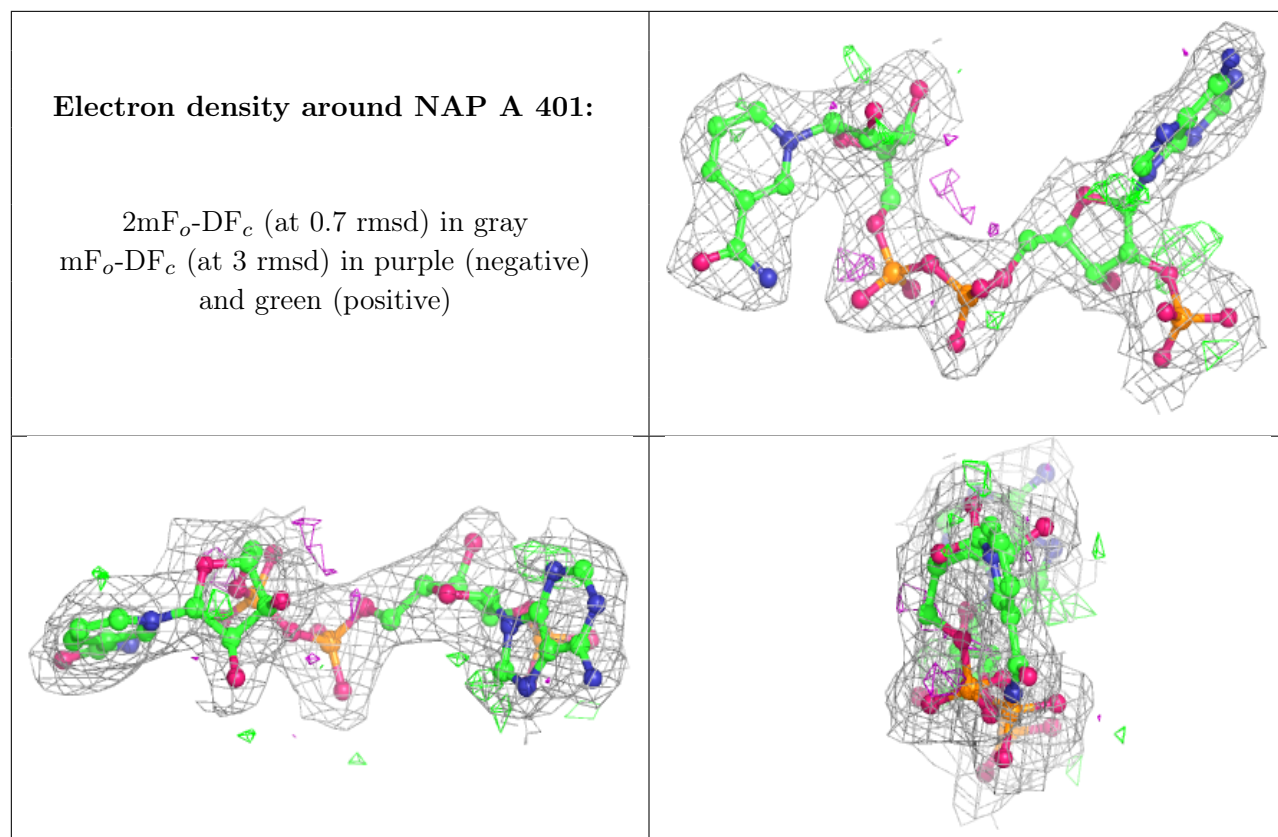
Electron density around GDR B 400:

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

**Electron density around NAP C 401:**

$2mF_o-DF_c$ (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.