



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2020 – 05:21 PM BST

PDB ID : 6YPZ
Title : Promiscuous Reductase LugOII Catalyzes Keto-reduction at C1 during Lugdunomycin Biosynthesis
Authors : Xiao, X.; Elsayed, S.S.; Wu, C.; van der Heul, H.; Protá, A.; Huang, J.; Guo, R.; Abrahams, J.P.; van Wezel, G.P.
Deposited on : 2020-04-16
Resolution : 1.08 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 : 2.14.4
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) : 2.14.4

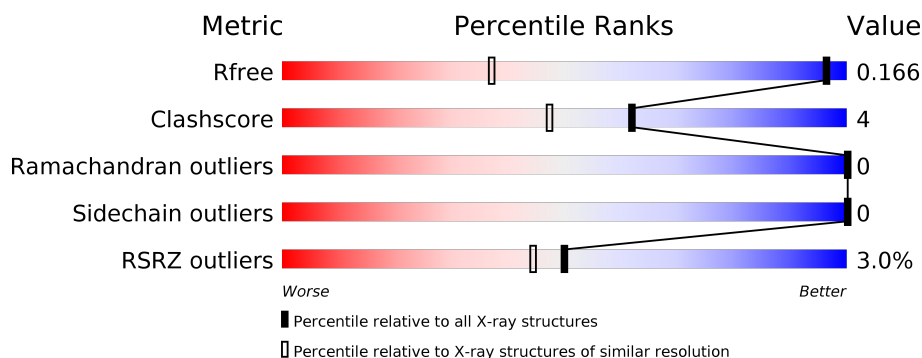
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.08 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	1386 (1.12-1.04)
Clashscore	141614	1021 (1.10-1.06)
Ramachandran outliers	138981	1381 (1.12-1.04)
Sidechain outliers	138945	1379 (1.12-1.04)
RSRZ outliers	127900	1359 (1.12-1.04)

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	AAA	255	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	BBB	255	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	BBB	303	-	-	X	-
4	PEG	BBB	306	-	-	X	-

2 Entry composition [i](#)

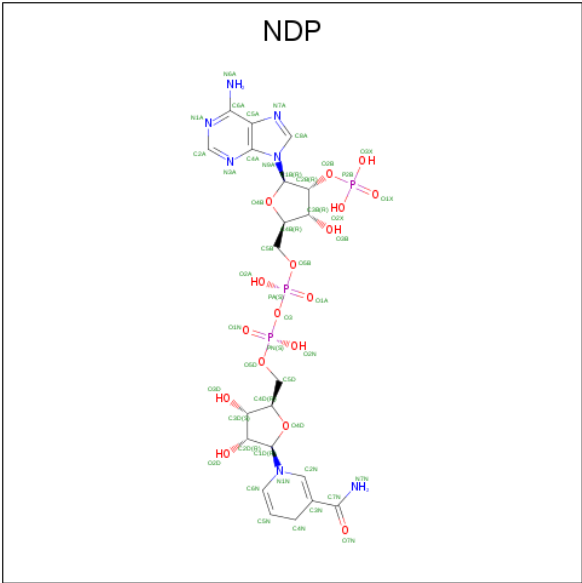
There are 5 unique types of molecules in this entry. The entry contains 4481 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	253	1908	1190	343	369	6	0	6	0
1	BBB	252	1907	1186	345	370	6	0	6	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	276	Total	O	0	0
			276	276		
5	BBB	232	Total	O	0	0
			232	232		

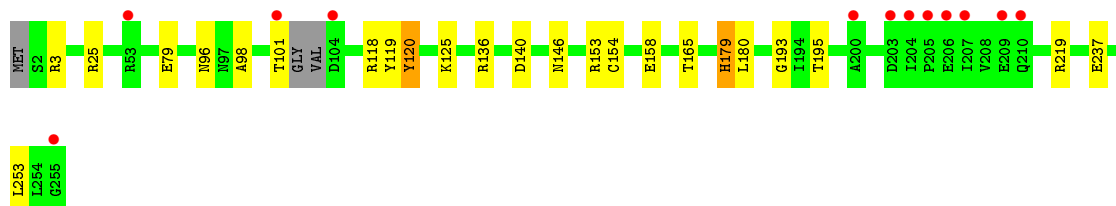
3 Residue-property plots [i](#)

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: Monooxygenase



- Molecule 1: Monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.83 Å 59.97 Å 88.43 Å 90.00° 102.51° 90.00°	Depositor
Resolution (Å)	49.30 – 1.08 49.25 – 1.08	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.30-1.08) 99.9 (49.25-1.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.08 Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.146 , 0.165 0.147 , 0.166	Depositor DCC
R_{free} test set	9588 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	9.7	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4481	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: NDP, PEG, EDO

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	AAA	1.03	3/1951 (0.2%)	1.11	8/2645 (0.3%)
1	BBB	1.06	4/1946 (0.2%)	1.13	16/2635 (0.6%)
All	All	1.04	7/3897 (0.2%)	1.12	24/5280 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	79	GLU	CD-OE2	-8.33	1.16	1.25
1	AAA	109	GLU	CD-OE1	-7.49	1.17	1.25
1	BBB	158	GLU	CD-OE1	6.90	1.33	1.25
1	AAA	114	GLU	CD-OE2	6.82	1.33	1.25
1	BBB	237	GLU	CD-OE1	-6.51	1.18	1.25
1	AAA	39	SER	CA-CB	-5.85	1.44	1.52
1	BBB	179	HIS	CE1-NE2	-5.51	1.20	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	153[A]	ARG	NE-CZ-NH1	-10.91	114.84	120.30
1	AAA	153[B]	ARG	NE-CZ-NH1	-10.91	114.84	120.30
1	AAA	140	ASP	CB-CG-OD1	9.29	126.66	118.30
1	BBB	120[A]	TYR	CB-CG-CD1	-8.50	115.90	121.00
1	BBB	120[B]	TYR	CB-CG-CD1	-8.50	115.90	121.00
1	AAA	16	ARG	CG-CD-NE	7.75	128.07	111.80
1	AAA	140	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	BBB	3	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	BBB	153[A]	ARG	NE-CZ-NH2	6.55	123.57	120.30
1	BBB	153[B]	ARG	NE-CZ-NH2	6.55	123.57	120.30
1	BBB	153[A]	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	BBB	153[B]	ARG	NE-CZ-NH1	-6.49	117.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	101	THR	CA-CB-CG2	6.47	121.46	112.40
1	BBB	120[A]	TYR	CB-CG-CD2	6.41	124.85	121.00
1	BBB	120[B]	TYR	CB-CG-CD2	6.41	124.85	121.00
1	BBB	25	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	BBB	118	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	BBB	140	ASP	CB-CG-OD1	5.95	123.65	118.30
1	BBB	219	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	AAA	53	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	BBB	101	THR	CB-CA-C	-5.40	97.01	111.60
1	AAA	45	ASP	CB-CG-OD1	5.35	123.12	118.30
1	BBB	140	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	AAA	37	TYR	CB-CG-CD2	-5.03	117.98	121.00

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	AAA	1908	0	1932	10	0
1	BBB	1907	0	1921	18	0
2	AAA	48	0	26	3	0
2	BBB	48	0	26	2	0
3	AAA	36	0	51	3	0
3	BBB	12	0	17	1	0
4	BBB	14	0	19	12	0
5	AAA	276	0	0	4	0
5	BBB	232	0	0	6	0
All	All	4481	0	3992	35	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 (35) 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:BBB:154[B]:CYS:SG	1:BBB:253:LEU:CD2	2.55	0.94
1:BBB:179:HIS:NE2	4:BBB:303:PEG:H41	1.94	0.83
1:BBB:180:LEU:CD2	4:BBB:303:PEG:H42	2.10	0.82
1:AAA:73:GLU:HG3	5:AAA:611:HOH:O	1.79	0.82
4:BBB:306:PEG:H12	5:BBB:460:HOH:O	1.82	0.78
1:BBB:180:LEU:HD21	4:BBB:303:PEG:H42	1.63	0.77
1:BBB:154[B]:CYS:SG	1:BBB:253:LEU:HD23	2.24	0.77
4:BBB:306:PEG:C1	5:BBB:460:HOH:O	2.35	0.74
1:BBB:179:HIS:CD2	4:BBB:303:PEG:H41	2.26	0.71
1:BBB:154[B]:CYS:SG	1:BBB:253:LEU:HD22	2.30	0.71
1:AAA:88:GLU:OE1	5:AAA:401:HOH:O	2.11	0.68
1:BBB:125:LYS:HE2	4:BBB:306:PEG:H32	1.82	0.60
1:AAA:154[A]:CYS:SG	1:AAA:253:LEU:CD2	2.92	0.58
1:BBB:136[B]:ARG:NH1	5:BBB:401:HOH:O	2.37	0.57
1:BBB:180:LEU:HD23	4:BBB:303:PEG:H42	1.85	0.56
1:AAA:193:GLY:O	2:AAA:301:NDP:H42N	2.08	0.53
1:BBB:120[B]:TYR:HD2	5:BBB:588:HOH:O	1.92	0.53
1:BBB:193:GLY:O	2:BBB:301:NDP:H42N	2.09	0.52
4:BBB:306:PEG:H11	5:BBB:460:HOH:O	2.07	0.51
1:AAA:154[A]:CYS:SG	1:AAA:253:LEU:HD23	2.51	0.50
1:BBB:119:TYR:HB3	1:BBB:165:THR:HG21	1.93	0.49
3:AAA:305:EDO:H12	5:AAA:410:HOH:O	2.12	0.49
1:AAA:119:TYR:HB3	1:AAA:165:THR:HG21	1.94	0.49
1:BBB:96:ASN:HB2	1:BBB:146:ASN:HD22	1.78	0.48
1:AAA:96:ASN:HB2	1:AAA:146:ASN:HD22	1.79	0.48
1:BBB:179:HIS:CD2	4:BBB:303:PEG:C4	2.98	0.46
1:BBB:195:THR:H	2:BBB:301:NDP:H72N	1.64	0.45
1:AAA:195:THR:H	2:AAA:301:NDP:H72N	1.63	0.45
1:AAA:254:LEU:C	3:AAA:309:EDO:O2	2.55	0.44
1:AAA:73:GLU:CG	5:AAA:611:HOH:O	2.49	0.43
1:BBB:136[B]:ARG:CZ	5:BBB:401:HOH:O	2.65	0.43
2:AAA:301:NDP:H41N	3:AAA:305:EDO:C1	2.47	0.43
4:BBB:306:PEG:H11	4:BBB:306:PEG:H32	1.84	0.42
4:BBB:306:PEG:H21	4:BBB:306:PEG:H41	1.75	0.41
1:BBB:98:ALA:O	3:BBB:304:EDO:H11	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	AAA	257/255 (101%)	251 (98%)	6 (2%)	0	100	100
1	BBB	254/255 (100%)	249 (98%)	5 (2%)	0	100	100
All	All	511/510 (100%)	500 (98%)	11 (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	AAA	197/192 (103%)	197 (100%)	0	100	100
1	BBB	196/192 (102%)	196 (100%)	0	100	100
All	All	393/384 (102%)	393 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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 [i](#)

16 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	EDO	AAA	302	-	3,3,3	0.84	0	2,2,2	0.37	0
3	EDO	AAA	309	-	3,3,3	0.22	0	2,2,2	0.52	0
3	EDO	BBB	305	-	3,3,3	0.11	0	2,2,2	0.16	0
3	EDO	AAA	303	-	3,3,3	1.26	0	2,2,2	0.89	0
3	EDO	AAA	306	-	3,3,3	0.32	0	2,2,2	0.39	0
3	EDO	AAA	307	-	3,3,3	0.18	0	2,2,2	0.16	0
2	NDP	AAA	301	-	45,52,52	1.14	4 (8%)	53,80,80	0.79	1 (1%)
3	EDO	BBB	304	-	3,3,3	2.27	1 (33%)	2,2,2	1.19	0
4	PEG	BBB	306	-	6,6,6	0.89	1 (16%)	5,5,5	0.45	0
2	NDP	BBB	301	-	45,52,52	1.02	2 (4%)	53,80,80	0.91	2 (3%)
3	EDO	AAA	310	-	3,3,3	0.74	0	2,2,2	0.35	0
3	EDO	AAA	308	-	3,3,3	0.82	0	2,2,2	0.80	0
3	EDO	BBB	302	-	3,3,3	0.65	0	2,2,2	0.32	0
3	EDO	AAA	304	-	3,3,3	2.84	1 (33%)	2,2,2	1.37	0
3	EDO	AAA	305	-	3,3,3	0.61	0	2,2,2	0.83	0
4	PEG	BBB	303	-	6,6,6	1.28	1 (16%)	5,5,5	1.62	1 (20%)

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	EDO	AAA	302	-	-	0/1/1/1	-
3	EDO	AAA	309	-	-	0/1/1/1	-
3	EDO	BBB	305	-	-	0/1/1/1	-
3	EDO	AAA	303	-	-	0/1/1/1	-
3	EDO	AAA	306	-	-	0/1/1/1	-
3	EDO	AAA	307	-	-	0/1/1/1	-
2	NDP	AAA	301	-	-	3/30/77/77	0/5/5/5
3	EDO	BBB	304	-	-	0/1/1/1	-
4	PEG	BBB	306	-	-	3/4/4/4	-
2	NDP	BBB	301	-	-	3/30/77/77	0/5/5/5
3	EDO	AAA	310	-	-	0/1/1/1	-
3	EDO	AAA	308	-	-	0/1/1/1	-
3	EDO	BBB	302	-	-	0/1/1/1	-
3	EDO	AAA	304	-	-	0/1/1/1	-
3	EDO	AAA	305	-	-	0/1/1/1	-
4	PEG	BBB	303	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	304	EDO	O1-C1	-4.91	1.16	1.42
3	BBB	304	EDO	O2-C2	-3.74	1.22	1.42
2	BBB	301	NDP	C4N-C5N	-3.36	1.40	1.48
2	AAA	301	NDP	C4N-C5N	-3.08	1.40	1.48
2	BBB	301	NDP	C4N-C3N	-2.87	1.44	1.49
2	AAA	301	NDP	C4N-C3N	-2.81	1.44	1.49
2	AAA	301	NDP	O7N-C7N	2.53	1.30	1.24
4	BBB	303	PEG	C2-C1	2.37	1.62	1.49
2	AAA	301	NDP	C7N-N7N	-2.08	1.27	1.33
4	BBB	306	PEG	O1-C1	-2.08	1.31	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	301	NDP	C5A-C6A-N6A	3.05	124.99	120.35
4	BBB	303	PEG	O1-C1-C2	2.95	128.90	111.81
2	BBB	301	NDP	C5A-C6A-N6A	2.86	124.70	120.35
2	BBB	301	NDP	O2A-PA-O1A	2.03	122.27	112.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	303	PEG	C1-C2-O2-C3
4	BBB	303	PEG	O1-C1-C2-O2
4	BBB	306	PEG	O2-C3-C4-O4
2	AAA	301	NDP	O4D-C1D-N1N-C6N
2	BBB	301	NDP	O4D-C1D-N1N-C6N
4	BBB	306	PEG	C4-C3-O2-C2
2	AAA	301	NDP	PN-O3-PA-O2A
4	BBB	306	PEG	C1-C2-O2-C3
2	AAA	301	NDP	O4B-C4B-C5B-O5B
2	BBB	301	NDP	PN-O3-PA-O2A
2	BBB	301	NDP	O4B-C4B-C5B-O5B

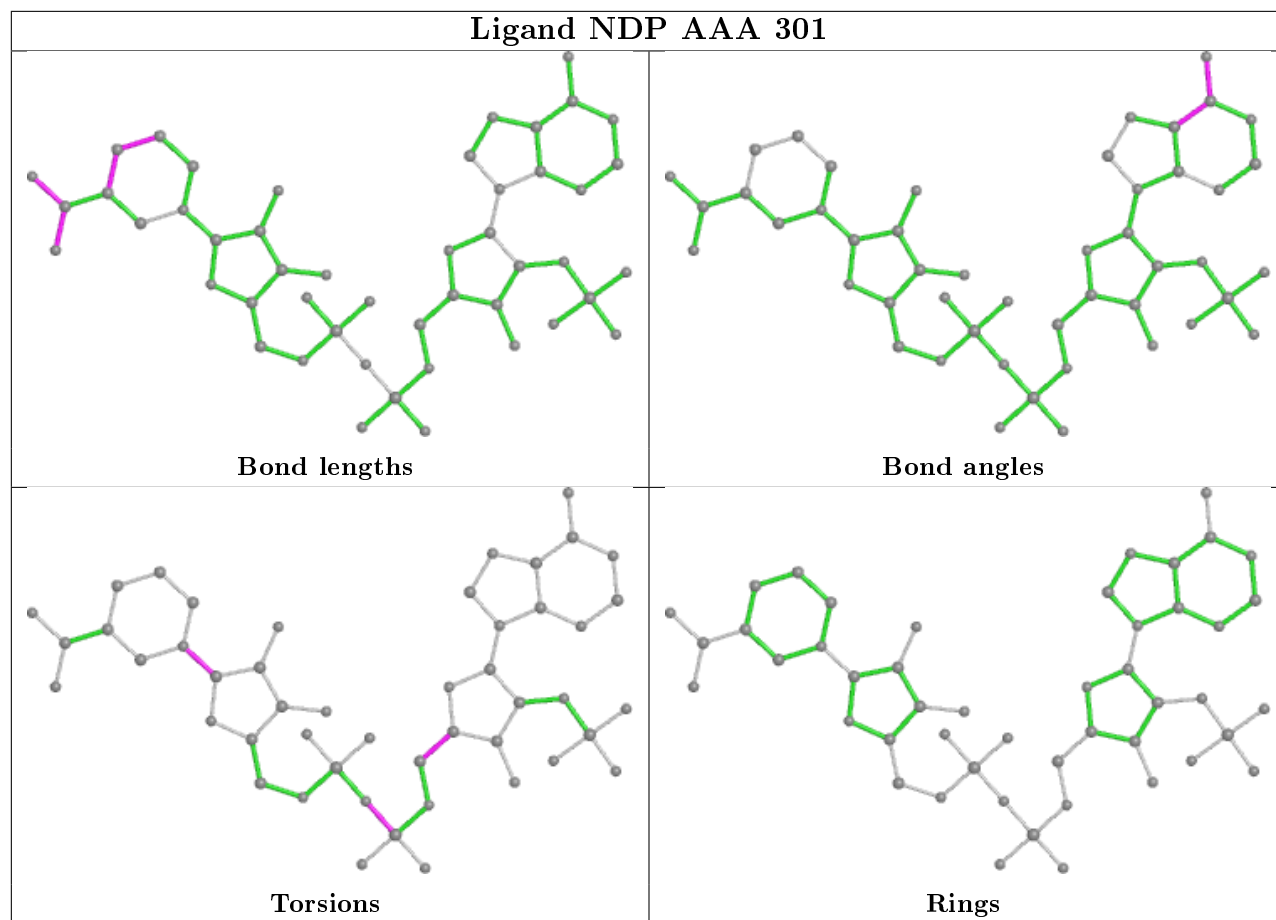
There are no ring outliers.

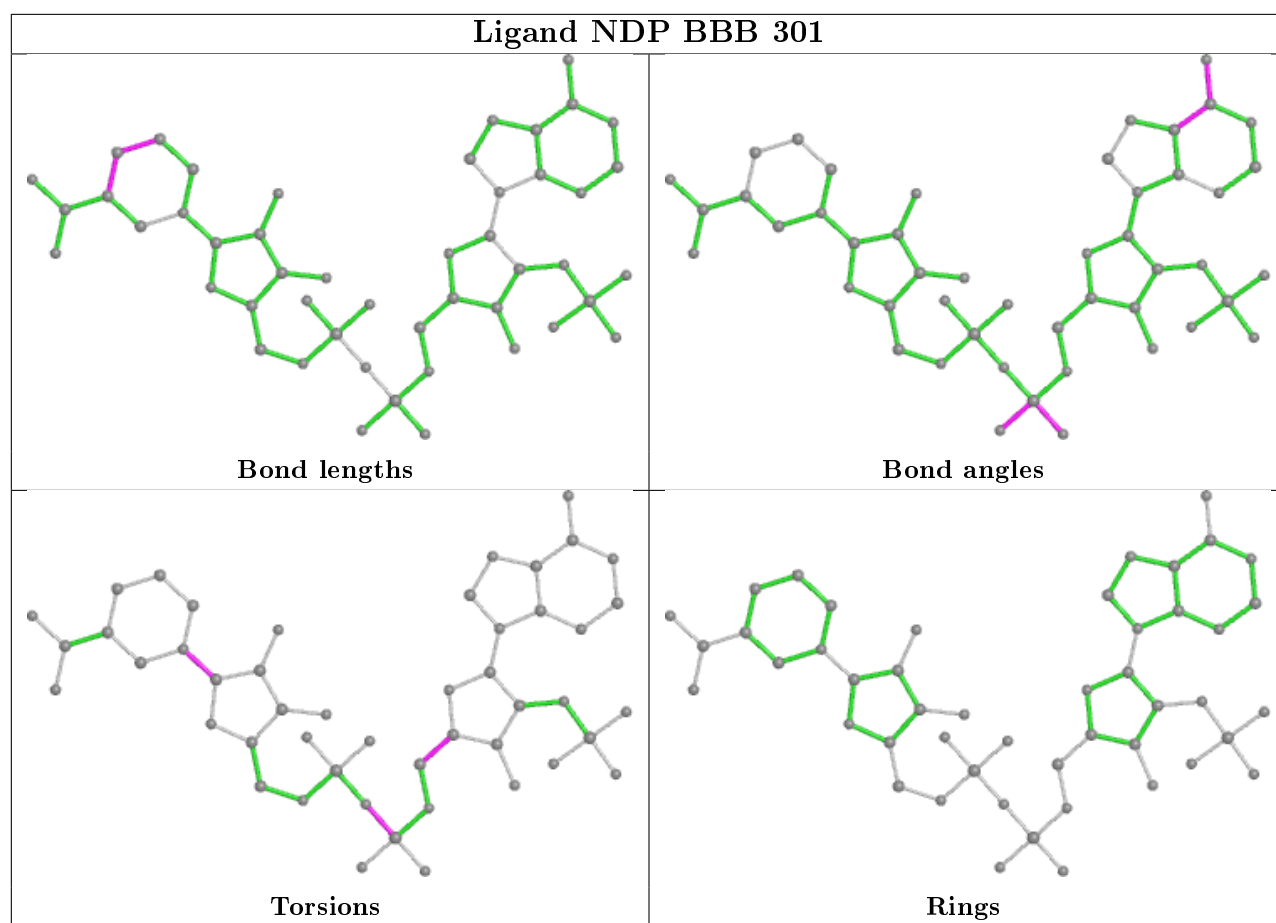
7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	309	EDO	1	0
2	AAA	301	NDP	3	0
3	BBB	304	EDO	1	0
4	BBB	306	PEG	6	0
2	BBB	301	NDP	2	0
3	AAA	305	EDO	2	0
4	BBB	303	PEG	6	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 AAA 301





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, 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	AAA	253/255 (99%)	-0.05	3 (1%) 79 74	6, 9, 21, 38	0
1	BBB	252/255 (98%)	0.03	12 (4%) 30 27	6, 11, 24, 39	0
All	All	505/510 (99%)	-0.01	15 (2%) 50 44	6, 10, 22, 39	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	255	GLY	4.7
1	AAA	102	GLY	3.9
1	BBB	203	ASP	3.4
1	BBB	207	ILE	3.3
1	BBB	101	THR	3.2
1	BBB	205	PRO	3.0
1	BBB	53	ARG	2.8
1	BBB	210	GLN	2.7
1	BBB	104	ASP	2.5
1	BBB	206	GLU	2.5
1	AAA	120[A]	TYR	2.5
1	BBB	200	ALA	2.4
1	BBB	209	GLU	2.4
1	AAA	206	GLU	2.3
1	BBB	204	ILE	2.2

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

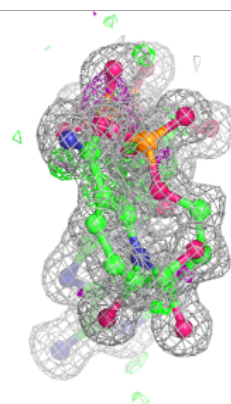
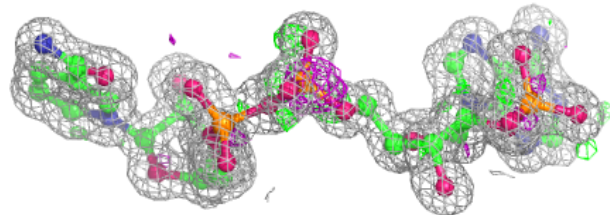
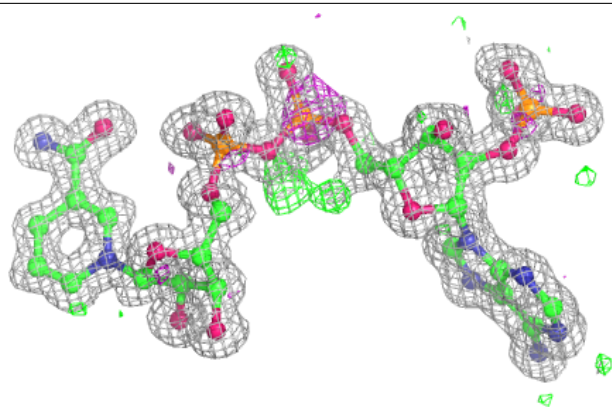
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	AAA	309	4/4	0.67	0.20	36,36,37,43	0
3	EDO	BBB	305	4/4	0.76	0.18	33,36,39,42	0
4	PEG	BBB	306	7/7	0.81	0.18	24,29,34,36	0
4	PEG	BBB	303	7/7	0.86	0.19	18,19,23,29	0
3	EDO	AAA	305	4/4	0.90	0.10	21,29,33,40	0
3	EDO	AAA	307	4/4	0.91	0.13	22,24,27,28	0
3	EDO	BBB	302	4/4	0.94	0.17	13,14,15,15	0
3	EDO	AAA	306	4/4	0.94	0.08	16,16,17,22	0
3	EDO	AAA	303	4/4	0.94	0.11	16,20,22,23	0
3	EDO	AAA	302	4/4	0.95	0.12	13,15,16,17	0
3	EDO	AAA	304	4/4	0.96	0.15	8,10,12,13	0
3	EDO	AAA	310	4/4	0.97	0.15	15,20,22,23	0
3	EDO	AAA	308	4/4	0.97	0.13	10,10,14,15	0
3	EDO	BBB	304	4/4	0.97	0.10	9,11,14,14	0
2	NDP	BBB	301	48/48	0.98	0.06	7,9,13,16	0
2	NDP	AAA	301	48/48	0.99	0.05	6,8,10,14	0

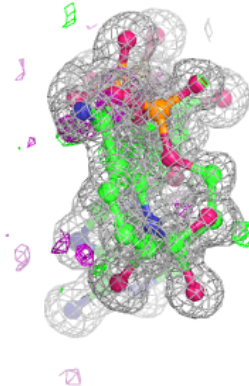
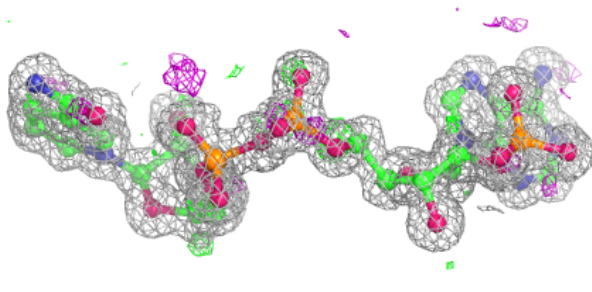
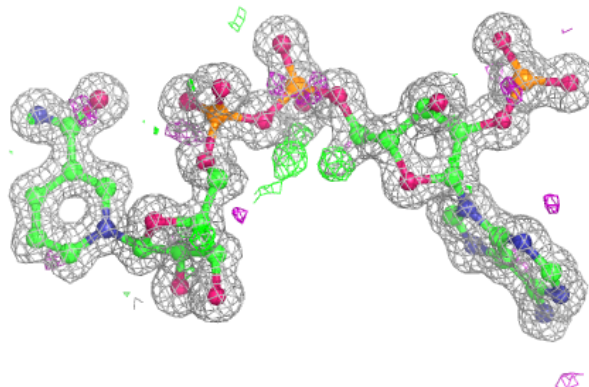
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP BBB 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 AAA 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.