



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:42 AM UTC

PDB ID : 6YPZ / pdb_00006ypz
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 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

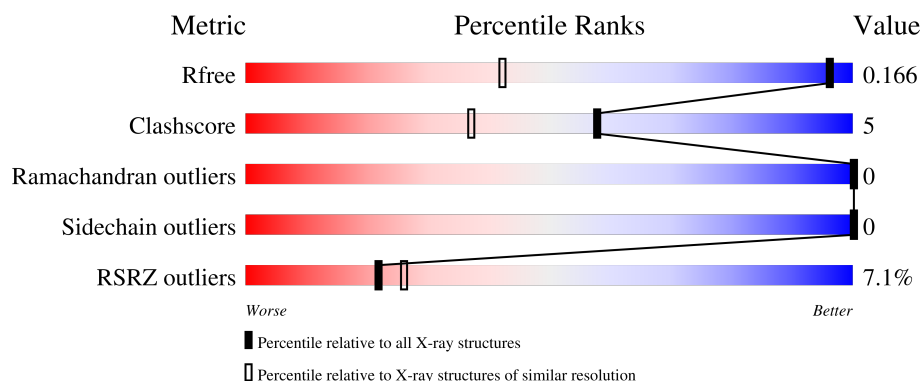
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1687 (1.10-1.06)
Clashscore	190562	1727 (1.10-1.06)
Ramachandran outliers	187476	1679 (1.10-1.06)
Sidechain outliers	187428	1676 (1.10-1.06)
RSRZ outliers	180081	1687 (1.10-1.06)

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	AAA	255	 6% 88% 11% .
1	BBB	255	 8% 89% 9% ..

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](#)

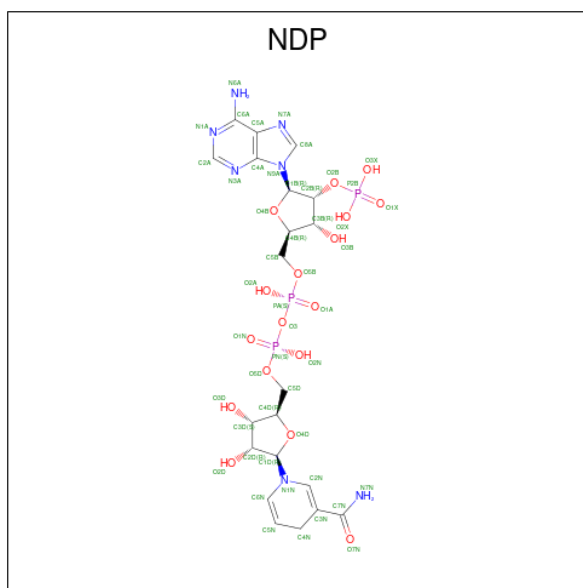
There are 5 unique types of molecules in this entry. The entry contains 4481 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	AAA	253	Total	C	N	O	S	0	6	0
			1908	1190	343	369	6			
1	BBB	252	Total	C	N	O	S	0	6	0
			1907	1186	345	370	6			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



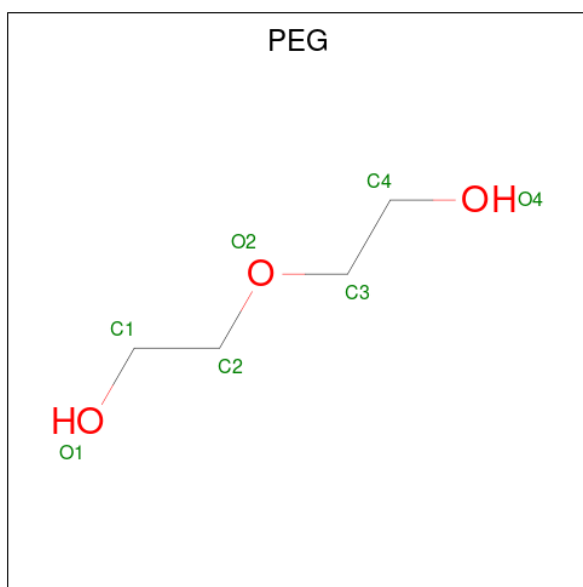
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	BBB	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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 (CCD ID: 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		

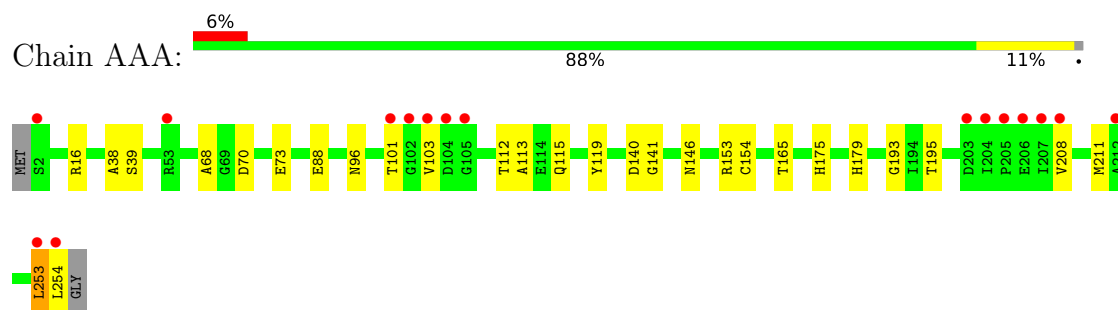
- Molecule 5 is water.

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

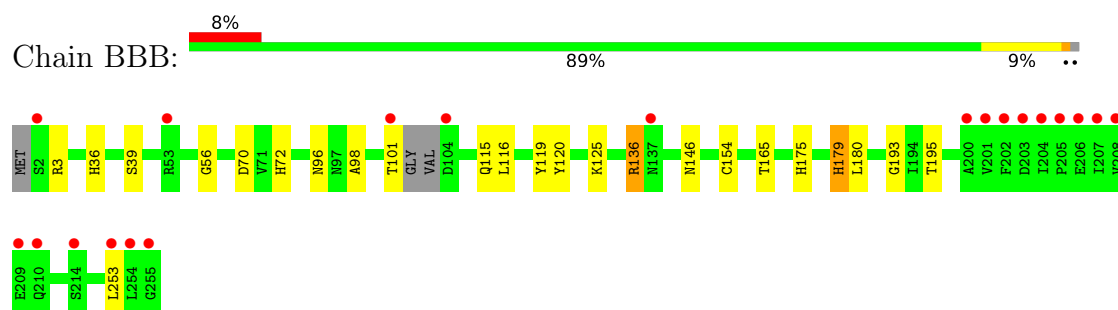
3 Residue-property plots [i](#)

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	87.83Å 59.97Å 88.43Å 90.00° 102.51° 90.00°	Depositor
Resolution (Å)	49.30 – 1.08 49.30 – 1.08	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.30-1.08) 99.9 (49.30-1.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.08Å)	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 (5.00%)	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 , 35.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NDP, 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	1.30	10/1951 (0.5%)	1.20	11/2645 (0.4%)
1	BBB	1.34	8/1946 (0.4%)	1.22	10/2635 (0.4%)
All	All	1.32	18/3897 (0.5%)	1.21	21/5280 (0.4%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	179	HIS	CE1-NE2	-12.57	1.20	1.32
1	BBB	72	HIS	CE1-NE2	-7.11	1.25	1.32
1	AAA	68	ALA	C-O	-7.08	1.15	1.23
1	BBB	116	LEU	C-O	6.68	1.31	1.24
1	AAA	115	GLN	C-O	6.33	1.31	1.24
1	AAA	253	LEU	C-O	6.13	1.32	1.24
1	AAA	253	LEU	N-CA	6.08	1.52	1.46
1	AAA	39	SER	CA-CB	-5.99	1.44	1.53
1	AAA	179	HIS	CE1-NE2	-5.94	1.26	1.32
1	AAA	103	VAL	C-O	-5.81	1.17	1.24
1	BBB	179	HIS	ND1-CE1	5.64	1.38	1.32
1	BBB	36	HIS	CE1-NE2	5.30	1.37	1.32
1	BBB	56	GLY	N-CA	5.25	1.48	1.44
1	AAA	175	HIS	CE1-NE2	5.24	1.37	1.32
1	AAA	112	THR	C-O	5.14	1.30	1.23
1	AAA	38	ALA	CA-C	-5.11	1.48	1.52
1	BBB	39	SER	CA-CB	-5.06	1.45	1.53
1	BBB	115	GLN	C-O	5.02	1.29	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	16	ARG	CG-CD-NE	7.30	128.07	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	153[A]	ARG	NE-CZ-NH1	-6.66	114.84	121.50
1	AAA	153[B]	ARG	NE-CZ-NH1	-6.66	114.84	121.50
1	BBB	101	THR	CA-CB-CG2	6.45	121.46	110.50
1	AAA	70	ASP	CA-CB-CG	6.27	118.87	112.60
1	AAA	141	GLY	CA-C-O	6.27	125.97	119.01
1	BBB	101	THR	CA-C-O	-6.15	110.34	120.80
1	AAA	101	THR	CB-CA-C	5.98	118.97	110.24
1	AAA	253	LEU	CA-C-O	-5.73	112.75	120.15
1	BBB	175	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	BBB	101	THR	CB-CA-C	-5.50	97.01	109.10
1	AAA	140	ASP	O-C-N	-5.27	116.74	123.06
1	BBB	70	ASP	CA-CB-CG	5.25	117.85	112.60
1	BBB	136[A]	ARG	CA-C-N	5.24	131.19	122.54
1	BBB	136[A]	ARG	C-N-CA	5.24	131.19	122.54
1	BBB	136[B]	ARG	CA-C-N	5.24	131.19	122.54
1	BBB	136[B]	ARG	C-N-CA	5.24	131.19	122.54
1	AAA	113	ALA	CA-C-O	-5.24	115.00	120.55
1	AAA	253	LEU	O-C-N	5.09	128.76	122.19
1	AAA	103	VAL	CA-C-O	-5.08	115.77	121.05
1	BBB	3	ARG	NE-CZ-NH2	5.05	123.75	119.20

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	11	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4481	0	3992	36	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (36) 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:AAA:254:LEU:C	3:AAA:309:EDO:O2	2.55	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: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:H32	4:BBB:306:PEG:H11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:208:VAL:HA	1:AAA:211:MET:HE3	2.02	0.41
4:BBB:306:PEG:H41	4:BBB:306:PEG:H21	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 [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	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 [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	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.

Sometimes 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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	NDP	BBB	301	-	51,52,52	1.43	4 (7%)	71,80,80	0.85	2 (2%)
4	PEG	BBB	303	-	6,6,6	1.28	1 (16%)	5,5,5	1.60	1 (20%)
3	EDO	AAA	304	-	3,3,3	2.88	1 (33%)	2,2,2	1.28	0
3	EDO	AAA	303	-	3,3,3	1.24	0	2,2,2	0.79	0
3	EDO	AAA	307	-	3,3,3	0.18	0	2,2,2	0.19	0
3	EDO	BBB	305	-	3,3,3	0.10	0	2,2,2	0.19	0
3	EDO	AAA	305	-	3,3,3	0.61	0	2,2,2	0.73	0
3	EDO	AAA	302	-	3,3,3	0.85	0	2,2,2	0.41	0
3	EDO	AAA	306	-	3,3,3	0.31	0	2,2,2	0.36	0
3	EDO	BBB	302	-	3,3,3	0.66	0	2,2,2	0.32	0
4	PEG	BBB	306	-	6,6,6	0.90	1 (16%)	5,5,5	0.45	0
3	EDO	AAA	309	-	3,3,3	0.22	0	2,2,2	0.49	0
3	EDO	BBB	304	-	3,3,3	2.30	1 (33%)	2,2,2	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	AAA	310	-	3,3,3	0.70	0	2,2,2	0.28	0
3	EDO	AAA	308	-	3,3,3	0.82	0	2,2,2	0.69	0
2	NDP	AAA	301	-	51,52,52	1.21	5 (9%)	71,80,80	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	BBB	301	-	-	2/34/77/77	0/5/5/5
4	PEG	BBB	303	-	-	2/4/4/4	-
3	EDO	AAA	304	-	-	0/1/1/1	-
3	EDO	AAA	303	-	-	0/1/1/1	-
3	EDO	AAA	307	-	-	0/1/1/1	-
3	EDO	BBB	305	-	-	0/1/1/1	-
3	EDO	AAA	305	-	-	1/1/1/1	-
3	EDO	AAA	302	-	-	0/1/1/1	-
3	EDO	AAA	306	-	-	0/1/1/1	-
3	EDO	BBB	302	-	-	0/1/1/1	-
4	PEG	BBB	306	-	-	3/4/4/4	-
3	EDO	AAA	309	-	-	0/1/1/1	-
3	EDO	BBB	304	-	-	0/1/1/1	-
3	EDO	AAA	310	-	-	0/1/1/1	-
3	EDO	AAA	308	-	-	0/1/1/1	-
2	NDP	AAA	301	-	-	2/34/77/77	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	301	NDP	PA-O3	7.48	1.67	1.59
3	AAA	304	EDO	O1-C1	-4.98	1.16	1.42
3	BBB	304	EDO	O2-C2	-3.79	1.22	1.42
2	BBB	301	NDP	C4N-C5N	-3.43	1.40	1.49
2	AAA	301	NDP	PA-O3	3.39	1.63	1.59
2	AAA	301	NDP	C4N-C5N	-3.15	1.40	1.49
2	BBB	301	NDP	C4N-C3N	-3.03	1.44	1.50
2	AAA	301	NDP	C4N-C3N	-2.96	1.44	1.50
2	AAA	301	NDP	PN-O3	-2.85	1.56	1.59
2	AAA	301	NDP	O7N-C7N	2.57	1.30	1.24
2	BBB	301	NDP	PN-O3	-2.57	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	303	PEG	C2-C1	2.39	1.62	1.49
4	BBB	306	PEG	O1-C1	-2.10	1.31	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BBB	303	PEG	O1-C1-C2	2.90	128.90	111.82
2	BBB	301	NDP	O3-PA-O1A	-2.16	104.20	110.70
2	BBB	301	NDP	O2A-PA-O1A	2.11	122.27	112.44

There are no chirality outliers.

All (10) 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
2	AAA	301	NDP	PN-O3-PA-O2A
4	BBB	306	PEG	C4-C3-O2-C2
4	BBB	306	PEG	C1-C2-O2-C3
2	BBB	301	NDP	PN-O3-PA-O2A
3	AAA	305	EDO	O1-C1-C2-O2

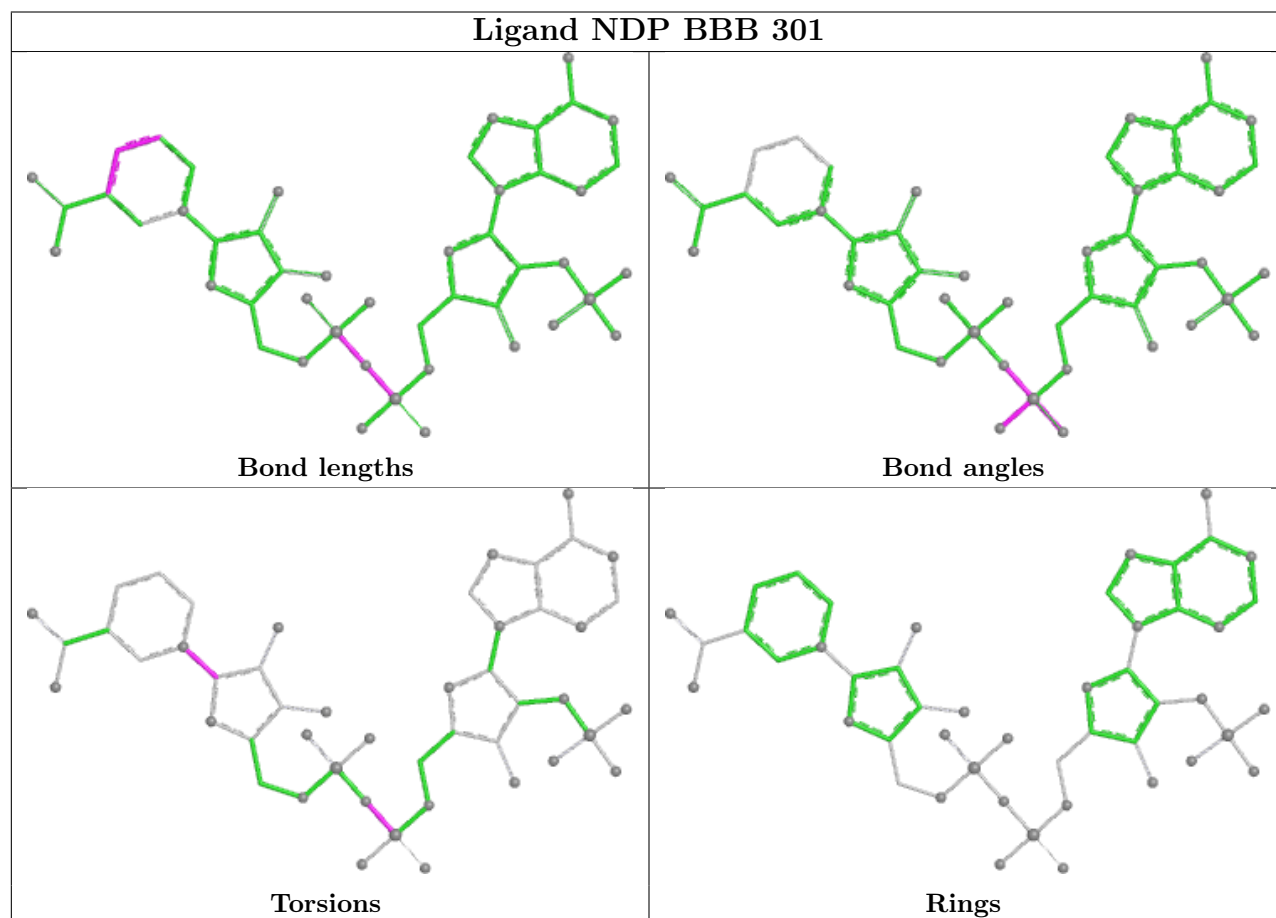
There are no ring outliers.

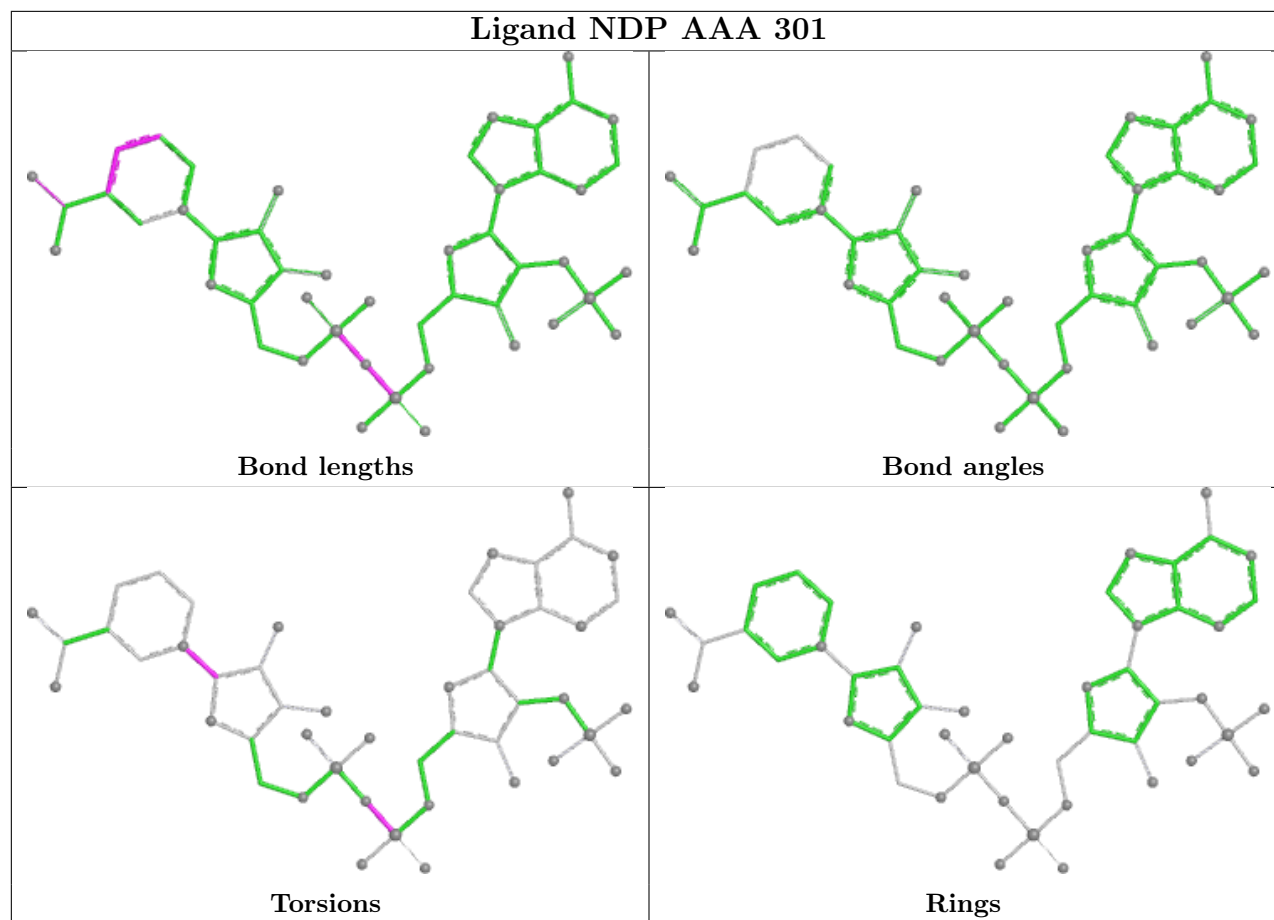
7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	301	NDP	2	0
4	BBB	303	PEG	6	0
3	AAA	305	EDO	2	0
4	BBB	306	PEG	6	0
3	AAA	309	EDO	1	0
3	BBB	304	EDO	1	0
2	AAA	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	AAA	253/255 (99%)	0.10	16 (6%)	26 30	6, 9, 21, 38	6 (2%)
1	BBB	252/255 (98%)	0.31	20 (7%)	18 23	6, 11, 24, 39	6 (2%)
All	All	505/510 (99%)	0.21	36 (7%)	22 26	6, 10, 22, 39	12 (2%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	102	GLY	5.5
1	BBB	101	THR	5.3
1	BBB	204	ILE	5.3
1	BBB	255	GLY	4.5
1	BBB	201	VAL	4.0
1	BBB	207	ILE	3.9
1	AAA	103	VAL	3.3
1	AAA	253	LEU	3.3
1	BBB	200	ALA	3.2
1	AAA	254	LEU	3.1
1	AAA	205	PRO	3.0
1	BBB	203	ASP	3.0
1	BBB	205	PRO	2.9
1	BBB	104	ASP	2.9
1	BBB	53	ARG	2.8
1	BBB	254	LEU	2.7
1	AAA	104	ASP	2.7
1	AAA	207	ILE	2.6
1	BBB	253	LEU	2.6
1	BBB	210	GLN	2.5
1	AAA	204	ILE	2.5
1	BBB	2	SER	2.5
1	BBB	206	GLU	2.4
1	AAA	2	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	BBB	208	VAL	2.4
1	AAA	101	THR	2.3
1	BBB	214	SER	2.3
1	AAA	203	ASP	2.3
1	AAA	105	GLY	2.3
1	AAA	53	ARG	2.2
1	AAA	212	ALA	2.2
1	BBB	209	GLU	2.2
1	AAA	206	GLU	2.2
1	BBB	137	ASN	2.1
1	AAA	208	VAL	2.1
1	BBB	202	PHE	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(Å ²)	Q<0.9
3	EDO	AAA	309	4/4	0.60	0.20	36,36,37,43	0
3	EDO	BBB	305	4/4	0.80	0.15	33,36,39,42	0
4	PEG	BBB	306	7/7	0.83	0.13	24,29,34,36	0
3	EDO	AAA	305	4/4	0.87	0.14	21,29,33,40	0
3	EDO	AAA	307	4/4	0.88	0.12	22,24,27,28	0
4	PEG	BBB	303	7/7	0.91	0.11	18,19,23,29	0
3	EDO	AAA	306	4/4	0.94	0.08	16,16,17,22	0
3	EDO	BBB	302	4/4	0.95	0.08	13,14,15,15	0
3	EDO	AAA	302	4/4	0.95	0.08	13,15,16,17	0
3	EDO	AAA	304	4/4	0.96	0.08	8,10,12,13	0
3	EDO	AAA	310	4/4	0.96	0.07	15,20,22,23	0

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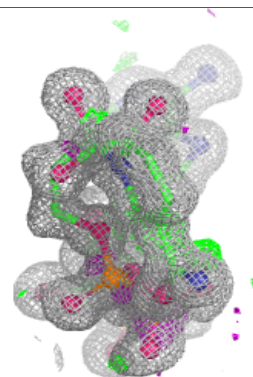
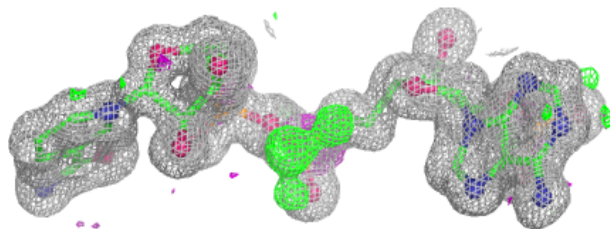
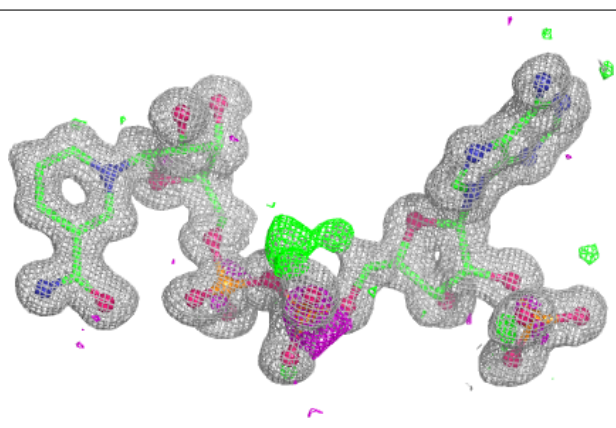
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	AAA	303	4/4	0.96	0.08	16,20,22,23	0
3	EDO	AAA	308	4/4	0.97	0.08	10,10,14,15	0
3	EDO	BBB	304	4/4	0.98	0.06	9,11,14,14	0
2	NDP	BBB	301	48/48	0.98	0.05	7,9,13,16	0
2	NDP	AAA	301	48/48	0.99	0.04	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.

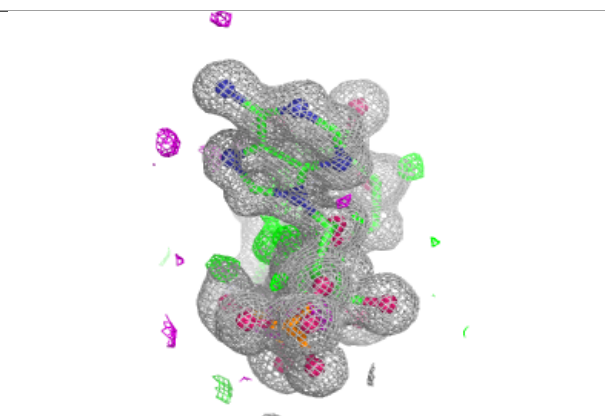
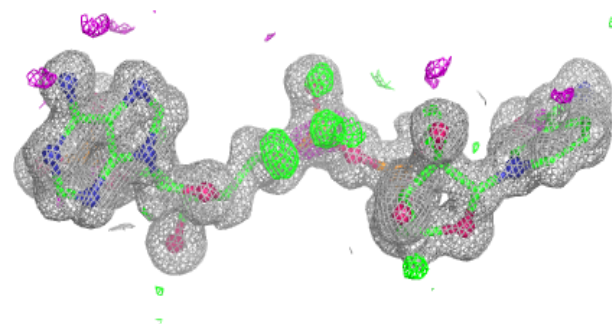
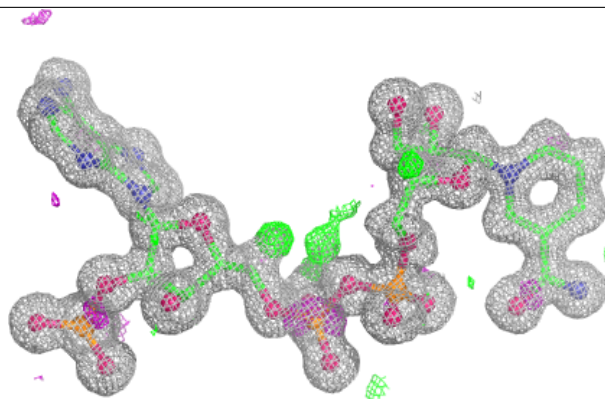
Electron density around NDP BBB 301:

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.