



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:51 PM BST

PDB ID : 6DS1
Title : Crystal structure of Cj0485 dehydrogenase in complex with NADP+
Authors : Pluinage, B.; Boraston, A.B.
Deposited on : 2018-06-13
Resolution : 2.12 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 : 2.13.1
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) : 2.13.1

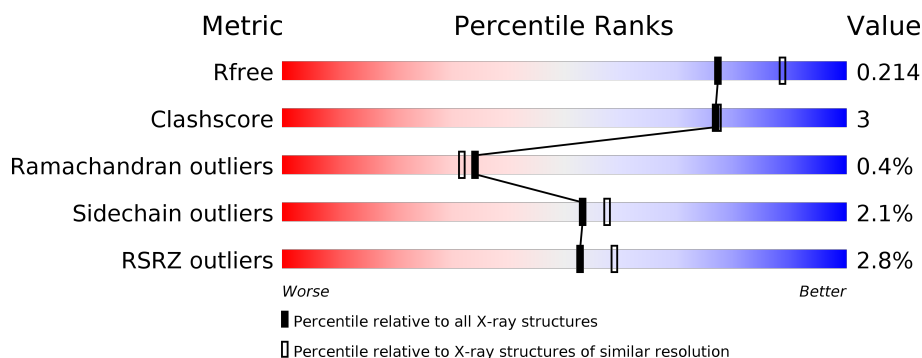
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	271	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	271	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>•</div> </div> </div>
1	C	271	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>•</div> </div> </div>
1	D	271	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>•</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8798 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 Putative oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	1	0
			2012	1285	338	380	9			
1	B	260	Total	C	N	O	S	0	2	0
			2040	1303	342	386	9			
1	C	260	Total	C	N	O	S	0	1	0
			2039	1304	342	384	9			
1	D	259	Total	C	N	O	S	0	1	0
			2022	1295	341	377	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	THR	-	expression tag	UNP Q0PB28
A	264	ARG	-	expression tag	UNP Q0PB28
A	265	GLY	-	expression tag	UNP Q0PB28
A	266	HIS	-	expression tag	UNP Q0PB28
A	267	HIS	-	expression tag	UNP Q0PB28
A	268	HIS	-	expression tag	UNP Q0PB28
A	269	HIS	-	expression tag	UNP Q0PB28
A	270	HIS	-	expression tag	UNP Q0PB28
A	271	HIS	-	expression tag	UNP Q0PB28
B	263	THR	-	expression tag	UNP Q0PB28
B	264	ARG	-	expression tag	UNP Q0PB28
B	265	GLY	-	expression tag	UNP Q0PB28
B	266	HIS	-	expression tag	UNP Q0PB28
B	267	HIS	-	expression tag	UNP Q0PB28
B	268	HIS	-	expression tag	UNP Q0PB28
B	269	HIS	-	expression tag	UNP Q0PB28
B	270	HIS	-	expression tag	UNP Q0PB28
B	271	HIS	-	expression tag	UNP Q0PB28
C	263	THR	-	expression tag	UNP Q0PB28
C	264	ARG	-	expression tag	UNP Q0PB28
C	265	GLY	-	expression tag	UNP Q0PB28

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	266	HIS	-	expression tag	UNP Q0PB28
C	267	HIS	-	expression tag	UNP Q0PB28
C	268	HIS	-	expression tag	UNP Q0PB28
C	269	HIS	-	expression tag	UNP Q0PB28
C	270	HIS	-	expression tag	UNP Q0PB28
C	271	HIS	-	expression tag	UNP Q0PB28
D	263	THR	-	expression tag	UNP Q0PB28
D	264	ARG	-	expression tag	UNP Q0PB28
D	265	GLY	-	expression tag	UNP Q0PB28
D	266	HIS	-	expression tag	UNP Q0PB28
D	267	HIS	-	expression tag	UNP Q0PB28
D	268	HIS	-	expression tag	UNP Q0PB28
D	269	HIS	-	expression tag	UNP Q0PB28
D	270	HIS	-	expression tag	UNP Q0PB28
D	271	HIS	-	expression tag	UNP Q0PB28

-
- The chemical structure of Naphthyl Aspartate Phosphate (NAP) is shown. It consists of a naphthalene ring system (labeled N1, N2, N3, N4, N5, N6, N7, N8) connected via an amide bond to a chiral center (C1). This chiral center is also bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N9, N10, N11, N12, N13, N14, N15, N16). The phosphate group is further linked to a second chiral center (C2), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N17, N18, N19, N20, N21, N22, N23, N24). The second phosphate group is linked to a third chiral center (C3), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N25, N26, N27, N28, N29, N30, N31, N32). The third phosphate group is linked to a fourth chiral center (C4), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N33, N34, N35, N36, N37, N38, N39, N40). The fourth phosphate group is linked to a fifth chiral center (C5), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N41, N42, N43, N44, N45, N46, N47, N48). The fifth phosphate group is linked to a sixth chiral center (C6), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N49, N50, N51, N52, N53, N54, N55, N56). The sixth phosphate group is linked to a seventh chiral center (C7), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N57, N58, N59, N60, N61, N62, N63, N64). The seventh phosphate group is linked to an eighth chiral center (C8), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N65, N66, N67, N68, N69, N70, N71, N72). The eighth phosphate group is linked to a ninth chiral center (C9), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N73, N74, N75, N76, N77, N78, N79, N80). The ninth phosphate group is linked to a tenth chiral center (C10), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N81, N82, N83, N84, N85, N86, N87, N88). The tenth phosphate group is linked to an eleventh chiral center (C11), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N89, N90, N91, N92, N93, N94, N95, N96). The eleventh phosphate group is linked to a twelfth chiral center (C12), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N97, N98, N99, N100, N101, N102, N103, N104). The twelfth phosphate group is linked to a thirteenth chiral center (C13), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N105, N106, N107, N108, N109, N110, N111, N112). The thirteenth phosphate group is linked to a fourteenth chiral center (C14), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N113, N114, N115, N116, N117, N118, N119, N120). The fourteenth phosphate group is linked to a fifteenth chiral center (C15), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N121, N122, N123, N124, N125, N126, N127, N128). The fifteenth phosphate group is linked to a sixteenth chiral center (C16), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N129, N130, N131, N132, N133, N134, N135, N136). The sixteenth phosphate group is linked to a seventeenth chiral center (C17), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N137, N138, N139, N140, N141, N142, N143, N144). The seventeenth phosphate group is linked to an eighteenth chiral center (C18), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N145, N146, N147, N148, N149, N150, N151, N152). The eighteenth phosphate group is linked to a nineteenth chiral center (C19), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N153, N154, N155, N156, N157, N158, N159, N160). The nineteenth phosphate group is linked to a twentieth chiral center (C20), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N161, N162, N163, N164, N165, N166, N167, N168). The twentieth phosphate group is linked to a twenty-first chiral center (C21), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N169, N170, N171, N172, N173, N174, N175, N176). The twenty-first phosphate group is linked to a twenty-second chiral center (C22), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N177, N178, N179, N180, N181, N182, N183, N184). The twenty-second phosphate group is linked to a twenty-third chiral center (C23), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N185, N186, N187, N188, N189, N190, N191, N192). The twenty-third phosphate group is linked to a twenty-fourth chiral center (C24), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N193, N194, N195, N196, N197, N198, N199, N200). The twenty-fourth phosphate group is linked to a twenty-fifth chiral center (C25), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N201, N202, N203, N204, N205, N206, N207, N208). The twenty-fifth phosphate group is linked to a twenty-sixth chiral center (C26), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N209, N210, N211, N212, N213, N214, N215, N216). The twenty-sixth phosphate group is linked to a twenty-seventh chiral center (C27), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N217, N218, N219, N220, N221, N222, N223, N224). The twenty-seventh phosphate group is linked to a twenty-eighth chiral center (C28), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N225, N226, N227, N228, N229, N230, N231, N232). The twenty-eighth phosphate group is linked to a twenty-ninth chiral center (C29), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N233, N234, N235, N236, N237, N238, N239, N240). The twenty-ninth phosphate group is linked to a thirtieth chiral center (C30), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N241, N242, N243, N244, N245, N246, N247, N248). The thirtieth phosphate group is linked to a thirty-first chiral center (C31), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N249, N250, N251, N252, N253, N254, N255, N256). The thirty-first phosphate group is linked to a thirty-second chiral center (C32), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N257, N258, N259, N260, N261, N262, N263, N264). The thirty-second phosphate group is linked to a thirty-third chiral center (C33), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N265, N266, N267, N268, N269, N270, N271, N272). The thirty-third phosphate group is linked to a thirty-fourth chiral center (C34), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N273, N274, N275, N276, N277, N278, N279, N280). The thirty-fourth phosphate group is linked to a thirty-fifth chiral center (C35), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N281, N282, N283, N284, N285, N286, N287, N288). The thirty-fifth phosphate group is linked to a thirty-sixth chiral center (C36), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N289, N290, N291, N292, N293, N294, N295, N296). The thirty-sixth phosphate group is linked to a thirty-seventh chiral center (C37), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N297, N298, N299, N300, N301, N302, N303, N304). The thirty-seventh phosphate group is linked to a thirty-eighth chiral center (C38), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N305, N306, N307, N308, N309, N310, N311, N312). The thirty-eighth phosphate group is linked to a thirty-ninth chiral center (C39), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N313, N314, N315, N316, N317, N318, N319, N320). The thirty-ninth phosphate group is linked to a fortieth chiral center (C40), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N321, N322, N323, N324, N325, N326, N327, N328). The fortieth phosphate group is linked to a forty-first chiral center (C41), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N329, N330, N331, N332, N333, N334, N335, N336). The forty-first phosphate group is linked to a forty-second chiral center (C42), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N337, N338, N339, N340, N341, N342, N343, N344). The forty-second phosphate group is linked to a forty-third chiral center (C43), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N345, N346, N347, N348, N349, N350, N351, N352). The forty-third phosphate group is linked to a forty-fourth chiral center (C44), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N353, N354, N355, N356, N357, N358, N359, N360). The forty-fourth phosphate group is linked to a forty-fifth chiral center (C45), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N361, N362, N363, N364, N365, N366, N367, N368). The forty-fifth phosphate group is linked to a forty-sixth chiral center (C46), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N369, N370, N371, N372, N373, N374, N375, N376). The forty-sixth phosphate group is linked to a forty-seventh chiral center (C47), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N377, N378, N379, N380, N381, N382, N383, N384). The forty-seventh phosphate group is linked to a forty-eighth chiral center (C48), which is bonded to a hydroxyl group (OH), a phosphate group (PO4), and a naphthyl group (N385, N386, N387

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

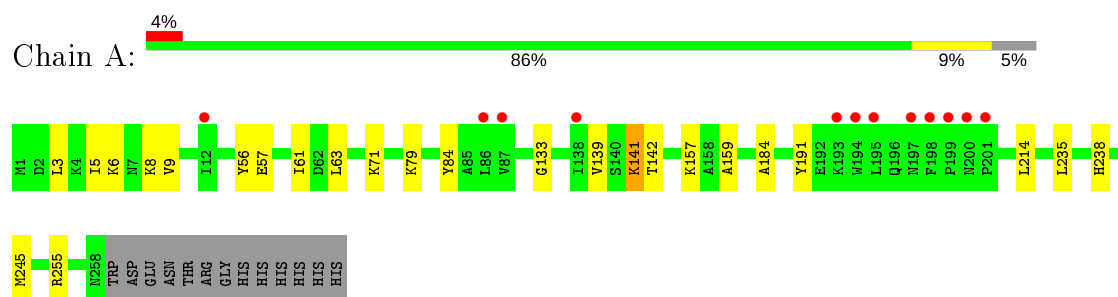
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total 119	O 119	0	0
5	B	122	Total 122	O 122	0	0
5	C	121	Total 121	O 121	0	0
5	D	109	Total 109	O 109	0	0

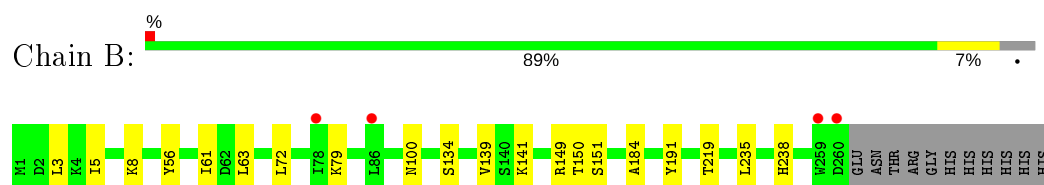
3 Residue-property plots

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.

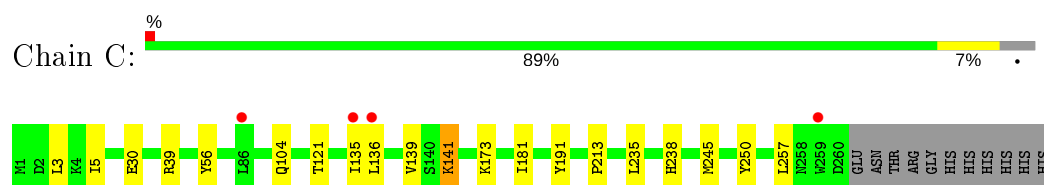
- Molecule 1: Putative oxidoreductase



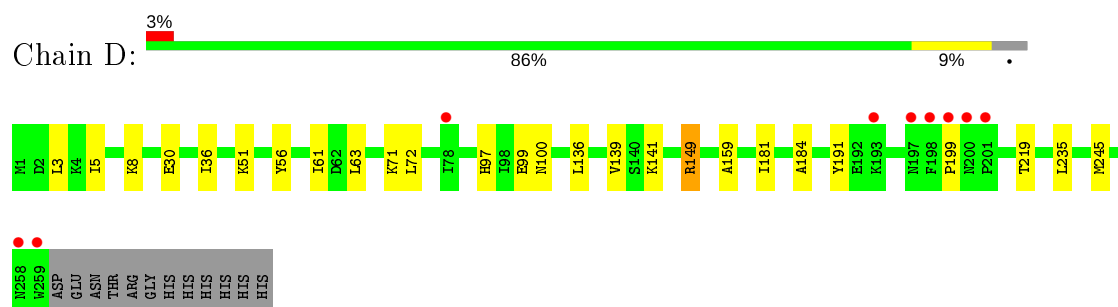
- Molecule 1: Putative oxidoreductase



- Molecule 1: Putative oxidoreductase



- Molecule 1: Putative oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.50 Å 68.46 Å 70.72 Å 89.31° 113.43° 115.67°	Depositor
Resolution (Å)	29.46 – 2.12 29.46 – 2.12	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.46-2.12) 95.1 (29.46-2.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.12 Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.159 , 0.214 0.159 , 0.214	Depositor DCC
R_{free} test set	2805 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8798	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% 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: GOL, 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	0.38	0/2055	0.53	0/2784
1	B	0.39	0/2085	0.52	0/2827
1	C	0.38	0/2084	0.53	0/2823
1	D	0.38	0/2067	0.52	0/2801
All	All	0.38	0/8291	0.52	0/11235

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	2012	0	1992	17	0
1	B	2040	0	2004	13	0
1	C	2039	0	2019	10	0
1	D	2022	0	2005	17	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
3	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	12	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	119	0	0	0	0
5	B	122	0	0	1	0
5	C	121	0	0	0	0
5	D	109	0	0	1	0
All	All	8798	0	8144	50	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 (50) 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:141:LYS:HE2	5:B:496:HOH:O	1.93	0.68
1:D:141:LYS:HG2	1:D:184:ALA:HA	1.72	0.68
1:D:8:LYS:HA	3:D:303:GOL:H31	1.76	0.67
1:C:213:PRO:HB3	1:C:257:LEU:HD23	1.77	0.66
1:A:159:ALA:HB2	1:D:159:ALA:HB2	1.79	0.65
1:D:61:ILE:HD12	1:D:72:LEU:HD12	1.79	0.64
1:B:3:LEU:HD23	1:B:235:LEU:HD22	1.82	0.61
1:C:3:LEU:HD23	1:C:235:LEU:HD22	1.86	0.58
1:A:141:LYS:HD3	1:A:184:ALA:HA	1.86	0.56
1:A:5:ILE:HA	1:A:8:LYS:HD2	1.88	0.56
1:C:136:LEU:HD11	1:C:181:ILE:HG12	1.89	0.54
1:B:61:ILE:HD12	1:B:72:LEU:HD12	1.90	0.54
1:D:3:LEU:HD23	1:D:235:LEU:HD22	1.89	0.53
1:C:5:ILE:HD11	1:C:30:GLU:HB2	1.91	0.53
1:A:61:ILE:HD13	1:A:63:LEU:HD23	1.92	0.52
1:C:39:ARG:NH2	2:C:301:NAP:O3X	2.44	0.50
1:B:3:LEU:HA	1:B:235:LEU:HD22	1.92	0.50
1:A:9:VAL:HG23	3:A:302:GOL:H2	1.94	0.49
1:D:136:LEU:HD11	1:D:181:ILE:HG12	1.95	0.48
1:D:5:ILE:HD11	1:D:30:GLU:HB2	1.96	0.47
1:B:5:ILE:HA	1:B:8:LYS:HD2	1.98	0.46
1:A:238:HIS:CE1	1:B:219:THR:HG1	2.31	0.45
1:C:238:HIS:CE1	1:D:219:THR:HG1	2.32	0.45
1:D:100:ASN:HD21	1:D:149:ARG:HH12	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ILE:HG12	1:D:56:TYR:HE1	1.81	0.45
1:A:238:HIS:ND1	1:B:219:THR:OG1	2.43	0.45
1:B:61:ILE:HD12	1:B:72:LEU:CD1	2.46	0.45
1:B:61:ILE:HD13	1:B:63:LEU:HD23	1.99	0.44
1:D:71:LYS:HB3	1:D:71:LYS:HE2	1.66	0.44
1:A:84:TYR:O	1:A:133:GLY:HA3	2.18	0.44
1:C:121:THR:HG23	1:C:135:ILE:HD13	2.00	0.44
1:D:199:PRO:HG2	5:D:481:HOH:O	2.18	0.44
1:A:255:ARG:HD2	1:C:250:TYR:O	2.18	0.44
1:B:184:ALA:O	2:B:301:NAP:H4N	2.18	0.43
1:C:141:LYS:HD2	1:C:250:TYR:CE2	2.54	0.43
1:A:8:LYS:HA	3:A:302:GOL:H31	2.01	0.43
1:D:97:HIS:CD2	1:D:99:GLU:HB2	2.53	0.43
1:D:51:LYS:HE2	1:D:51:LYS:HB3	1.83	0.42
1:A:214:LEU:HD23	1:B:238:HIS:HA	2.00	0.42
1:A:57:GLU:OE1	1:A:79:LYS:HD2	2.19	0.42
1:A:157:LYS:HD3	1:A:157:LYS:HA	1.92	0.42
1:A:3:LEU:HD23	1:A:235:LEU:HD22	2.02	0.41
1:D:72:LEU:HA	1:D:72:LEU:HD23	1.90	0.41
1:B:150:THR:HG23	1:B:150:THR:O	2.21	0.41
1:D:61:ILE:HD13	1:D:63:LEU:HD23	2.02	0.41
1:A:71:LYS:HB3	1:A:71:LYS:HE2	1.77	0.41
1:B:149:ARG:HH22	1:C:173:LYS:HE2	1.86	0.41
1:D:5:ILE:HA	1:D:8:LYS:HD2	2.03	0.41
1:A:141:LYS:HG2	1:A:142:THR:N	2.36	0.40
1:A:6:LYS:HA	1:A:6:LYS:HD2	1.79	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	257/271 (95%)	249 (97%)	7 (3%)	1 (0%)	34	32
1	B	260/271 (96%)	250 (96%)	9 (4%)	1 (0%)	34	32
1	C	259/271 (96%)	250 (96%)	8 (3%)	1 (0%)	34	32
1	D	258/271 (95%)	248 (96%)	9 (4%)	1 (0%)	34	32
All	All	1034/1084 (95%)	997 (96%)	33 (3%)	4 (0%)	34	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	D	139	VAL
1	B	139	VAL
1	C	139	VAL

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	211/228 (92%)	207 (98%)	4 (2%)	57	61
1	B	213/228 (93%)	207 (97%)	6 (3%)	43	46
1	C	214/228 (94%)	209 (98%)	5 (2%)	50	53
1	D	211/228 (92%)	208 (99%)	3 (1%)	67	72
All	All	849/912 (93%)	831 (98%)	18 (2%)	53	57

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	TYR
1	A	141	LYS
1	A	191	TYR
1	A	245	MET
1	B	56	TYR
1	B	79	LYS
1	B	100	ASN

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Mol	Chain	Res	Type
1	B	134	SER
1	B	151	SER
1	B	191	TYR
1	C	56	TYR
1	C	104	GLN
1	C	141	LYS
1	C	191	TYR
1	C	245	MET
1	D	149	ARG
1	D	191	TYR
1	D	245	MET

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

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 [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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
2	NAP	B	301	-	45,52,52	0.86	2 (4%)	56,80,80	1.20	3 (5%)
2	NAP	D	301	-	45,52,52	0.89	2 (4%)	56,80,80	1.14	4 (7%)
3	GOL	A	302	-	5,5,5	0.78	0	5,5,5	0.94	0
3	GOL	D	302	-	5,5,5	1.06	0	5,5,5	0.90	0
2	NAP	A	301	-	45,52,52	0.89	1 (2%)	56,80,80	1.24	5 (8%)
2	NAP	C	301	-	45,52,52	0.90	3 (6%)	56,80,80	1.12	3 (5%)
3	GOL	D	303	-	5,5,5	0.94	0	5,5,5	1.08	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	NAP	B	301	-	-	5/31/67/67	0/5/5/5
2	NAP	D	301	-	-	7/31/67/67	0/5/5/5
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	D	302	-	-	2/4/4/4	-
2	NAP	A	301	-	-	5/31/67/67	0/5/5/5
2	NAP	C	301	-	-	5/31/67/67	0/5/5/5
3	GOL	D	303	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	C5A-C4A	2.82	1.48	1.40
2	A	301	NAP	C5A-C4A	2.70	1.48	1.40
2	B	301	NAP	P2B-O2B	2.54	1.64	1.59
2	C	301	NAP	C5A-C4A	2.41	1.47	1.40
2	B	301	NAP	C5A-C4A	2.36	1.47	1.40
2	C	301	NAP	P2B-O2B	2.12	1.63	1.59
2	D	301	NAP	C2A-N3A	2.09	1.35	1.32
2	C	301	NAP	C2A-N3A	2.01	1.35	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAP	N3A-C2A-N1A	-3.54	123.15	128.68
2	B	301	NAP	N3A-C2A-N1A	-3.37	123.41	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAP	N3A-C2A-N1A	-3.11	123.82	128.68
2	D	301	NAP	N3A-C2A-N1A	-2.99	124.01	128.68
2	D	301	NAP	C4A-C5A-N7A	-2.97	106.30	109.40
2	C	301	NAP	C4A-C5A-N7A	-2.44	106.86	109.40
2	A	301	NAP	C4A-C5A-N7A	-2.42	106.88	109.40
2	B	301	NAP	C2A-N1A-C6A	2.38	122.82	118.75
2	D	301	NAP	C2A-N1A-C6A	2.36	122.79	118.75
2	A	301	NAP	C2A-N1A-C6A	2.32	122.72	118.75
2	A	301	NAP	C3N-C7N-N7N	2.27	120.48	117.75
2	C	301	NAP	C3N-C7N-N7N	2.22	120.42	117.75
2	A	301	NAP	O2A-PA-O1A	2.09	122.58	112.24
2	D	301	NAP	O2N-PN-O1N	2.04	122.33	112.24
2	B	301	NAP	O2N-PN-O1N	2.02	122.21	112.24

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	C5D-O5D-PN-O2N
2	D	301	NAP	C5D-O5D-PN-O1N
2	D	301	NAP	C5D-O5D-PN-O2N
3	D	302	GOL	C1-C2-C3-O3
2	A	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C5D-O5D-PN-O2N
3	A	302	GOL	O2-C2-C3-O3
3	A	302	GOL	C1-C2-C3-O3
3	D	303	GOL	O1-C1-C2-C3
3	D	302	GOL	O2-C2-C3-O3
2	A	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	C5D-O5D-PN-O1N
2	D	301	NAP	PA-O3-PN-O2N
3	D	303	GOL	O1-C1-C2-O2
2	B	301	NAP	C2B-O2B-P2B-O2X
2	B	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	C2B-O2B-P2B-O2X
2	D	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	C2B-O2B-P2B-O2X
2	C	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	O4B-C4B-C5B-O5B
2	A	301	NAP	O4B-C4B-C5B-O5B

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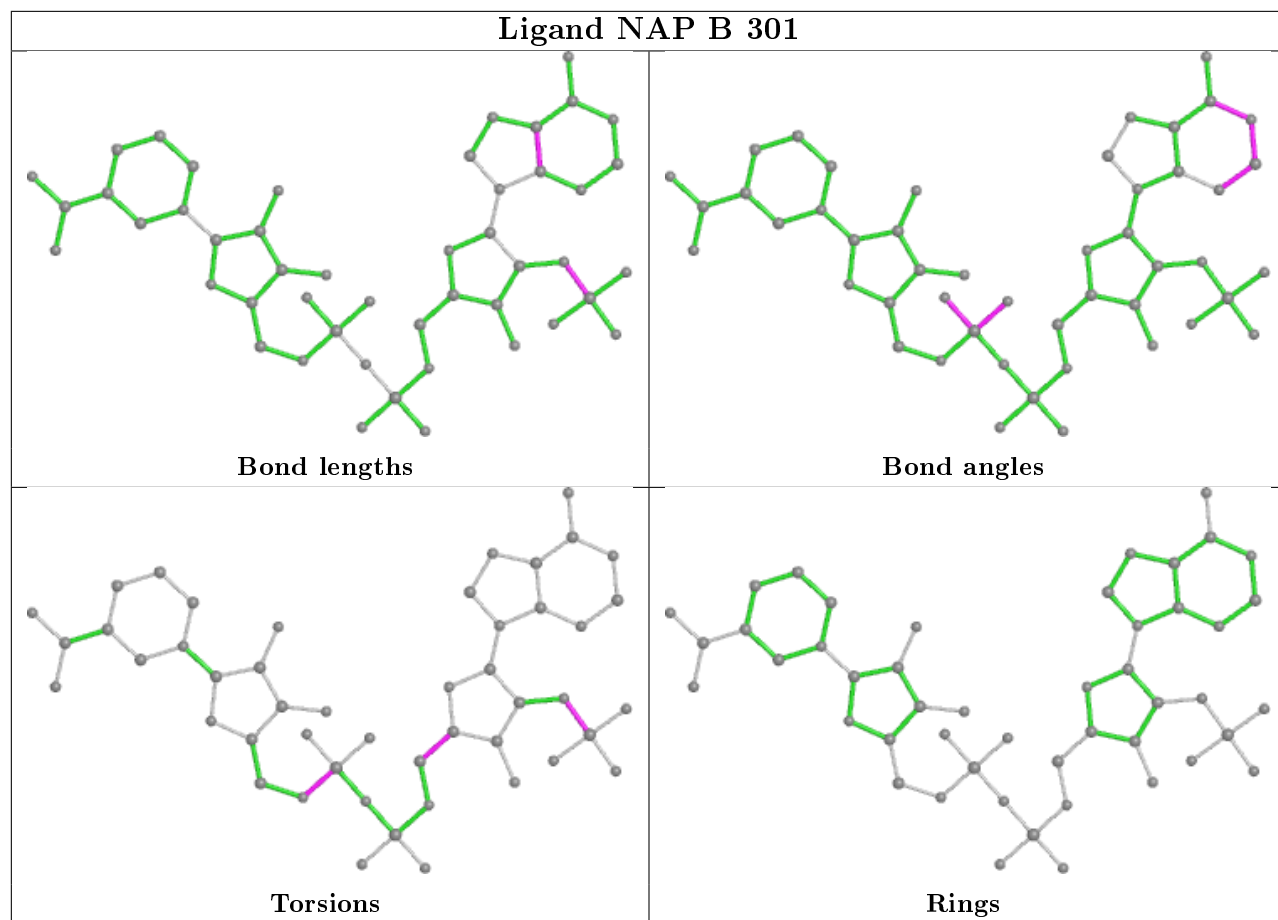
Mol	Chain	Res	Type	Atoms
2	D	301	NAP	PA-O3-PN-O1N
2	C	301	NAP	PA-O3-PN-O1N
2	D	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	O4B-C4B-C5B-O5B

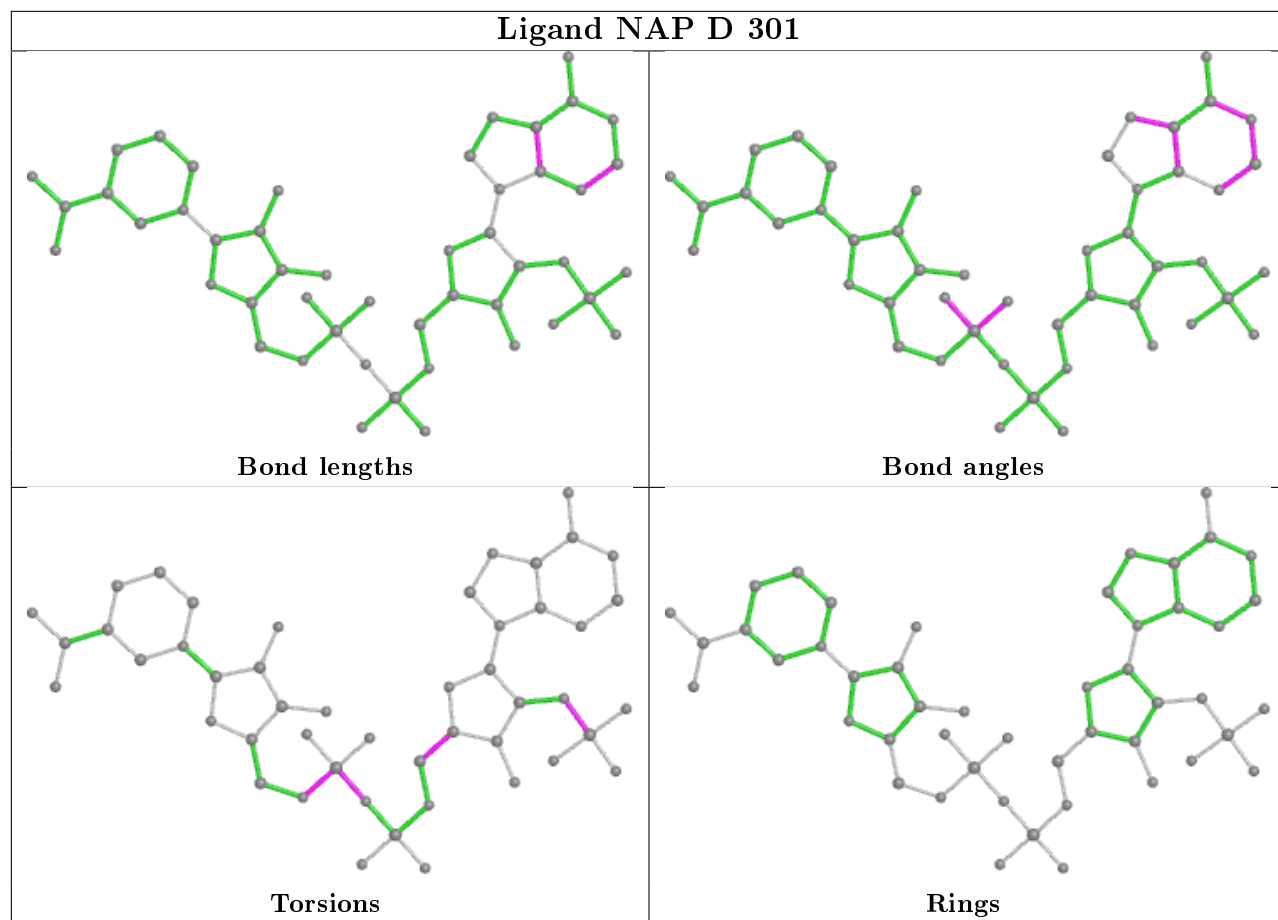
There are no ring outliers.

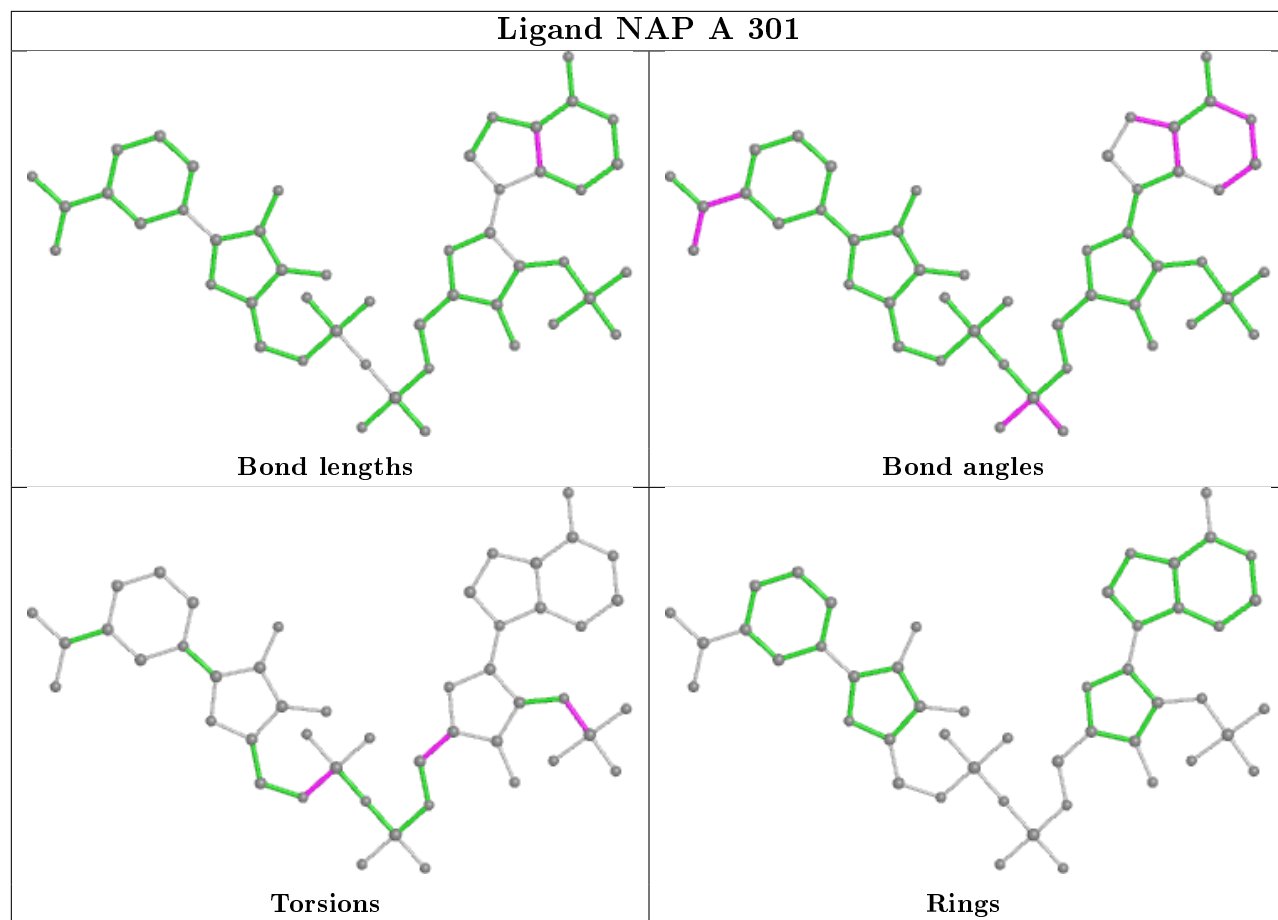
4 monomers are involved in 5 short contacts:

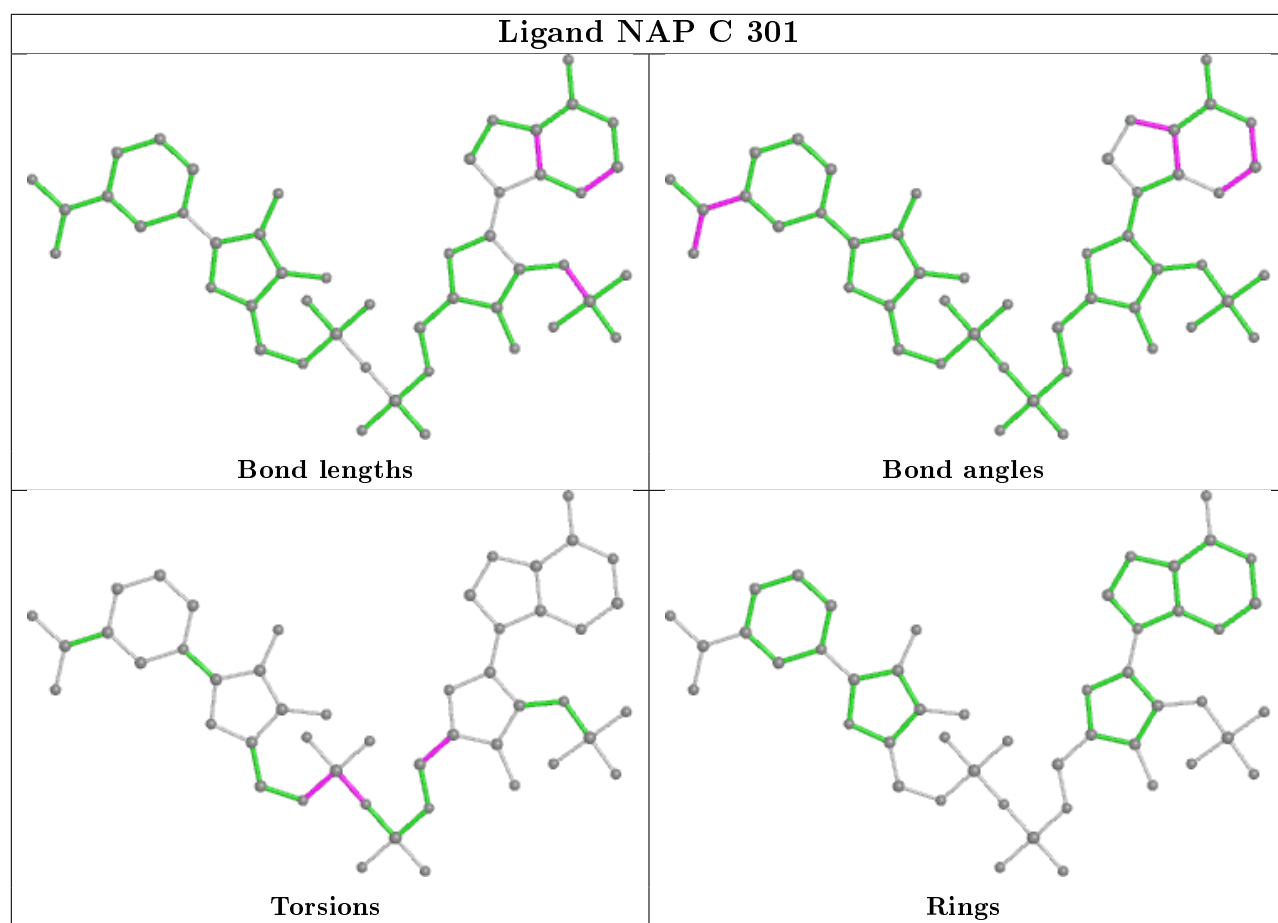
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAP	1	0
3	A	302	GOL	2	0
2	C	301	NAP	1	0
3	D	303	GOL	1	0

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	258/271 (95%)	-0.12	12 (4%) 31 36	18, 25, 41, 54	0
1	B	260/271 (95%)	-0.28	4 (1%) 73 77	19, 25, 37, 57	0
1	C	260/271 (95%)	-0.21	4 (1%) 73 77	18, 25, 38, 54	0
1	D	259/271 (95%)	-0.24	9 (3%) 44 50	17, 25, 45, 60	0
All	All	1037/1084 (95%)	-0.21	29 (2%) 53 59	17, 25, 39, 60	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	259	TRP	6.2
1	C	259	TRP	3.8
1	D	199	PRO	3.8
1	A	201	PRO	3.6
1	D	201	PRO	3.6
1	A	199	PRO	3.5
1	D	197	ASN	3.5
1	A	200	ASN	3.3
1	D	200	ASN	3.3
1	A	197	ASN	3.2
1	A	194	TRP	3.0
1	B	78	ILE	2.9
1	D	78	ILE	2.8
1	A	198	PHE	2.8
1	D	258	ASN	2.7
1	A	138	ILE	2.5
1	B	259	TRP	2.4
1	A	12	ILE	2.4
1	B	260	ASP	2.4
1	A	195	LEU	2.3
1	A	86	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	87	VAL	2.3
1	A	193	LYS	2.2
1	C	135	ILE	2.2
1	C	86	LEU	2.1
1	C	136	LEU	2.1
1	D	193	LYS	2.1
1	B	86	LEU	2.1
1	D	198	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

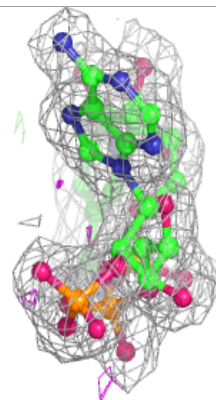
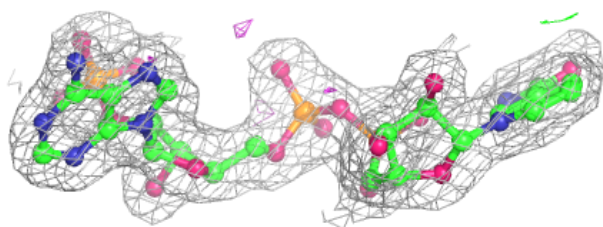
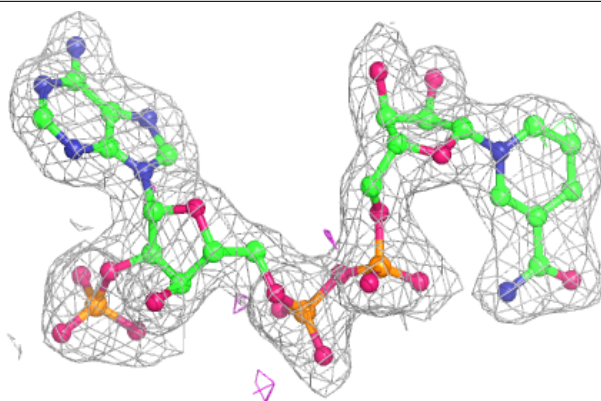
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	A	302	6/6	0.93	0.18	34,38,41,54	0
3	GOL	D	302	6/6	0.94	0.18	34,37,41,45	0
3	GOL	D	303	6/6	0.94	0.20	30,40,42,48	0
2	NAP	B	301	48/48	0.97	0.08	18,25,30,38	0
4	MG	C	302	1/1	0.98	0.12	20,20,20,20	0
2	NAP	A	301	48/48	0.98	0.08	20,27,32,36	0
2	NAP	C	301	48/48	0.98	0.07	20,26,31,37	0
2	NAP	D	301	48/48	0.98	0.07	20,27,32,40	0
4	MG	D	304	1/1	0.98	0.12	20,20,20,20	0
4	MG	B	302	1/1	0.99	0.09	23,23,23,23	0
4	MG	A	303	1/1	0.99	0.14	20,20,20,20	0

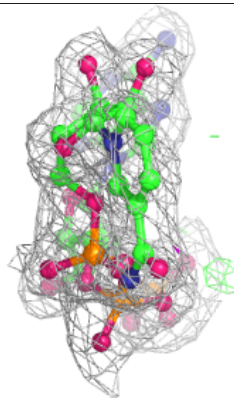
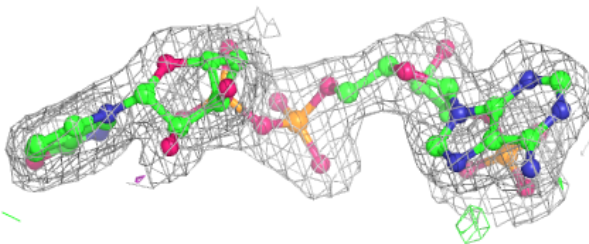
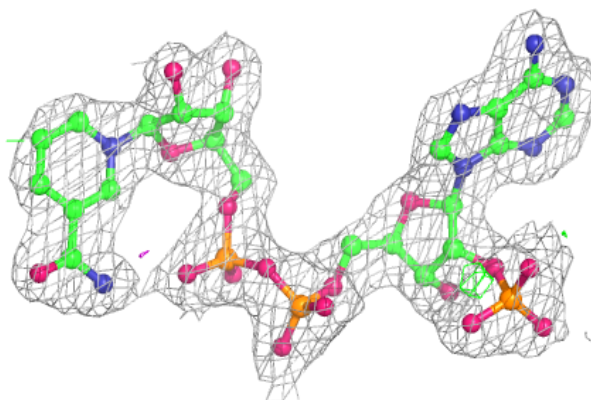
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

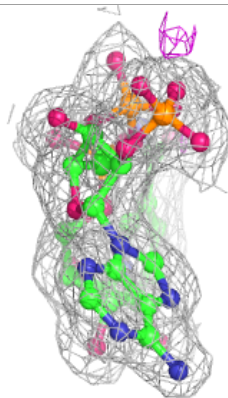
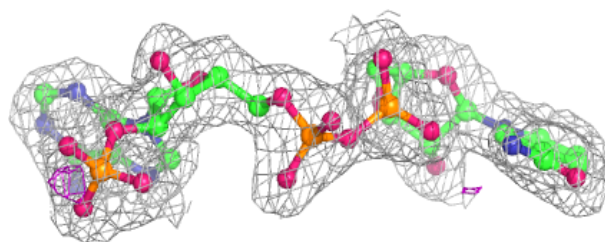
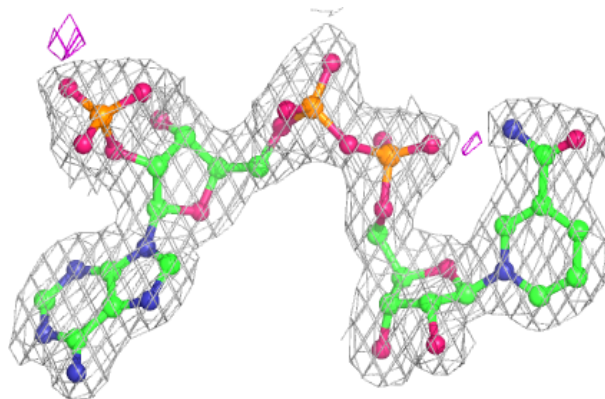
**Electron density around NAP A 301:**

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

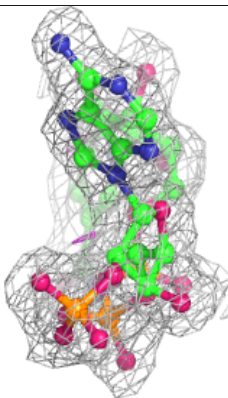
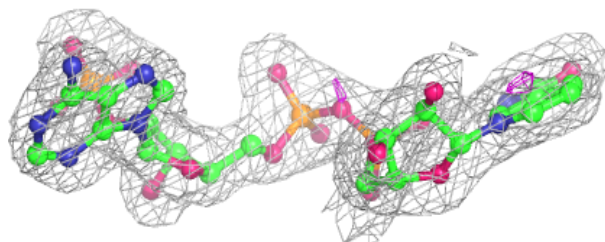
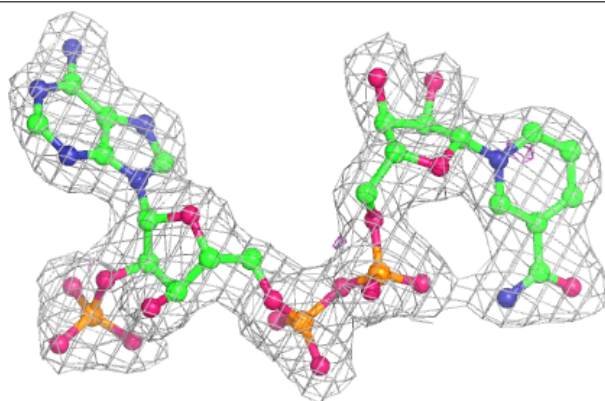


Electron density around NAP C 301:

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

**Electron density around NAP D 301:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.