



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:54 pm BST

PDB ID : 5BJY
Title : x-ray structure of the PglF 4,5-dehydratase from campylobacter jejuni, variant M405Y, in complex with UDP
Authors : Riegert, A.S.; Thoden, J.B.; Holden, H.M.
Deposited on : 2017-09-12
Resolution : 1.60 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 : 2.11
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) : 2.11

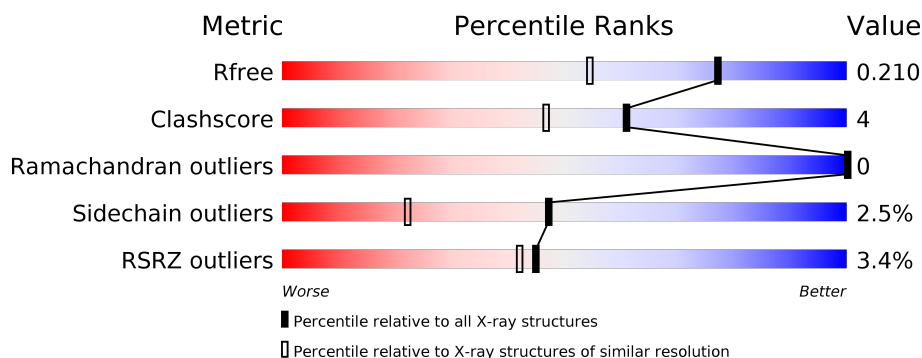
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	366	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>6% • 7%</div> </div> </div>
1	B	366	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>10% 7%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6265 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 WlaL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	7	0
			2691	1725	440	512	14			
1	B	339	Total	C	N	O	S	0	5	0
			2680	1720	440	506	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	405	TYR	MET	engineered mutation	UNP O86159
A	591	ALA	-	expression tag	UNP O86159
A	592	ALA	-	expression tag	UNP O86159
A	593	GLY	-	expression tag	UNP O86159
A	594	PHE	-	expression tag	UNP O86159
A	595	ASN	-	expression tag	UNP O86159
A	596	ARG	-	expression tag	UNP O86159
A	597	ILE	-	expression tag	UNP O86159
A	598	PRO	-	expression tag	UNP O86159
A	599	ALA	-	expression tag	UNP O86159
A	600	ALA	-	expression tag	UNP O86159
A	601	ALA	-	expression tag	UNP O86159
A	602	LEU	-	expression tag	UNP O86159
A	603	GLU	-	expression tag	UNP O86159
A	604	HIS	-	expression tag	UNP O86159
A	605	HIS	-	expression tag	UNP O86159
A	606	HIS	-	expression tag	UNP O86159
A	607	HIS	-	expression tag	UNP O86159
A	608	HIS	-	expression tag	UNP O86159
A	609	HIS	-	expression tag	UNP O86159
B	405	TYR	MET	engineered mutation	UNP O86159
B	591	ALA	-	expression tag	UNP O86159
B	592	ALA	-	expression tag	UNP O86159
B	593	GLY	-	expression tag	UNP O86159
B	594	PHE	-	expression tag	UNP O86159

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	595	ASN	-	expression tag	UNP O86159
B	596	ARG	-	expression tag	UNP O86159
B	597	ILE	-	expression tag	UNP O86159
B	598	PRO	-	expression tag	UNP O86159
B	599	ALA	-	expression tag	UNP O86159
B	600	ALA	-	expression tag	UNP O86159
B	601	ALA	-	expression tag	UNP O86159
B	602	LEU	-	expression tag	UNP O86159
B	603	GLU	-	expression tag	UNP O86159
B	604	HIS	-	expression tag	UNP O86159
B	605	HIS	-	expression tag	UNP O86159
B	606	HIS	-	expression tag	UNP O86159
B	607	HIS	-	expression tag	UNP O86159
B	608	HIS	-	expression tag	UNP O86159
B	609	HIS	-	expression tag	UNP O86159

-
- The diagram illustrates the chemical structure of UDP (Uridine Diphosphate). It consists of a uracil base (a pyrimidine ring with two carbonyl groups at positions 2 and 4) attached to a ribose sugar (a five-membered ring with hydroxyl groups at positions 2' and 3'). The ribose sugar is linked to a diphosphate group (two phosphate groups connected by an oxygen atom). The diphosphate group is shown with various oxygen atoms labeled (O1A, O1B, O2A, O2B, O3A, O3B, O4A, O4B, O5A, O5B, O6A, O6B, O7A, O7B, O8A, O8B, O9A, O9B, O10A, O10B, O11A, O11B, O12A, O12B, O13A, O13B, O14A, O14B, O15A, O15B, O16A, O16B, O17A, O17B, O18A, O18B, O19A, O19B, O20A, O20B, O21A, O21B, O22A, O22B, O23A, O23B, O24A, O24B, O25A, O25B, O26A, O26B, O27A, O27B, O28A, O28B, O29A, O29B, O30A, O30B, O31A, O31B, O32A, O32B, O33A, O33B, O34A, O34B, O35A, O35B, O36A, O36B, O37A, O37B, O38A, O38B, O39A, O39B, O40A, O40B, O41A, O41B, O42A, O42B, O43A, O43B, O44A, O44B, O45A, O45B, O46A, O46B, O47A, O47B, O48A, O48B, O49A, O49B, O50A, O50B, O51A, O51B, O52A, O52B, O53A, O53B, O54A, O54B, O55A, O55B, O56A, O56B, O57A, O57B, O58A, O58B, O59A, O59B, O60A, O60B, O61A, O61B, O62A, O62B, O63A, O63B, O64A, O64B, O65A, O65B, O66A, O66B, O67A, O67B, O68A, O68B, O69A, O69B, O70A, O70B, O71A, O71B, O72A, O72B, O73A, O73B, O74A, O74B, O75A, O75B, O76A, O76B, O77A, O77B, O78A, O78B, O79A, O79B, O80A, O80B, O81A, O81B, O82A, O82B, O83A, O83B, O84A, O84B, O85A, O85B, O86A, O86B, O87A, O87B, O88A, O88B, O89A, O89B, O90A, O90B, O91A, O91B, O92A, O92B, O93A, O93B, O94A, O94B, O95A, O95B, O96A, O96B, O97A, O97B, O98A, O98B, O99A, O99B, O100A, O100B, O101A, O101B, O102A, O102B, O103A, O103B, O104A, O104B, O105A, O105B, O106A, O106B, O107A, O107B, O108A, O108B, O109A, O109B, O110A, O110B, O111A, O111B, O112A, O112B, O113A, O113B, O114A, O114B, O115A, O115B, O116A, O116B, O117A, O117B, O118A, O118B, O119A, O119B, O120A, O120B, O121A, O121B, O122A, O122B, O123A, O123B, O124A, O124B, O125A, O125B, O126A, O126B, O127A, O127B, O128A, O128B, O129A, O129B, O130A, O130B, O131A, O131B, O132A, O132B, O133A, O133B, O134A, O134B, O135A, O135B, O136A, O136B, O137A, O137B, O138A, O138B, O139A, O139B, O140A, O140B, O141A, O141B, O142A, O142B, O143A, O143B, O144A, O144B, O145A, O145B, O146A, O146B, O147A, O147B, O148A, O148B, O149A, O149B, O150A, O150B, O151A, O151B, O152A, O152B, O153A, O153B, O154A, O154B, O155A, O155B, O156A, O156B, O157A, O157B, O158A, O158B, O159A, O159B, O160A, O160B, O161A, O161B, O162A, O162B, O163A, O163B, O164A, O164B, O165A, O165B, O166A, O166B, O167A, O167B, O168A, O168B, O169A, O169B, O170A, O170B, O171A, O171B, O172A, O172B, O173A, O173B, O174A, O174B, O175A, O175B, O176A, O176B, O177A, O177B, O178A, O178B, O179A, O179B, O180A, O180B, O181A, O181B, O182A, O182B, O183A, O183B, O184A, O184B, O185A, O185B, O186A, O186B, O187A, O187B, O188A, O188B, O189A, O189B, O190A, O190B, O191A, O191B, O192A, O192B, O193A, O193B, O194A, O194B, O195A, O195B, O196A, O196B, O197A, O197B, O198A, O198B, O199A, O199B, O200A, O200B, O201A, O201B, O202A, O202B, O203A, O203B, O204A, O204B, O205A, O205B, O206A, O206B, O207A, O207B, O208A, O208B, O209A, O209B, O210A, O210B, O211A, O211B, O212A, O212B, O213A, O213B, O214A, O214B, O215A, O215B, O216A, O216B, O217A, O217B, O218A, O218B, O219A, O219B, O220A, O220B, O221A, O221B, O222A, O222B, O223A, O223B, O224A, O224B, O225A, O225B, O226A, O226B, O227A, O227B, O228A, O228B, O229A, O229B, O230A, O230B, O231A, O231B, O232A, O232B, O233A, O233B, O234A, O234B, O235A, O235B, O236A, O236B, O237A, O237B, O238A, O238B, O239A, O239B, O240A, O240B, O241A, O241B, O242A, O242B, O243A, O243B, O244A, O244B, O245A, O245B, O246A, O246B, O247A, O247B, O248A, O248B, O249A, O249B, O250A, O250B, O251A, O251B, O252A, O252B, O253A, O253B, O254A, O254B, O255A, O255B, O256A, O256B, O257A, O257B, O258A, O258B, O259A, O259B, O260A, O260B, O261A, O261B, O262A, O262B, O263A, O263B, O264A, O264B, O265A, O265B, O266A, O266B, O267A, O267B, O268A, O268B, O269A, O269B, O270A, O270B, O271A, O271B, O272A, O272B, O273A, O273B, O274A, O274B, O275A, O275B, O276A, O276B, O277A, O277B, O278A, O278B, O279A, O279B, O280A, O280B, O281A, O281B, O282A, O282B, O283A, O283B, O284A, O284B, O285A, O285B, O286A, O286B, O287A, O287B, O288A, O288B, O289A, O289B, O290A, O290B, O291A, O291B, O292A, O292B, O293A, O293B, O294A, O294B, O295A, O295B, O296A, O296B, O297A, O297B, O298A, O298B, O299A, O299B, O300A, O300B, O301A, O301B, O302A, O302B, O303A, O303B, O304A, O304B, O305A, O305B, O306A, O306B, O307A, O307B, O308A, O308B, O309A, O309B, O310A, O310B, O311A, O311B, O312A, O312B, O313A, O313B, O314A, O314B, O315A, O315B, O316A, O316B, O317A, O317B, O318A, O318B, O319A, O319B, O320A, O320B, O321A, O321B, O322A, O322B, O323A, O323B, O324A, O324B, O325A, O325B, O326A, O326B, O327A, O327B, O328A, O328B, O329A, O329B, O330A, O330B, O331A, O331B, O332A, O332B, O333A, O333B, O334A, O334B, O335A, O335B, O336A, O336B, O337A, O337B, O338A, O338B, O339A, O339B, O340A, O340B, O341A, O341B, O342A, O342B, O343A, O343B, O344A, O344B, O345A, O345B, O346A, O346B, O347A, O347B, O348A, O

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	B	1	Total 25	C 9	N 2	O 12	P 2	0	0

- 



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	1
			8	4	4		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Na	0	0
			3	3		
5	A	3	Total	Na	0	0
			3	3		

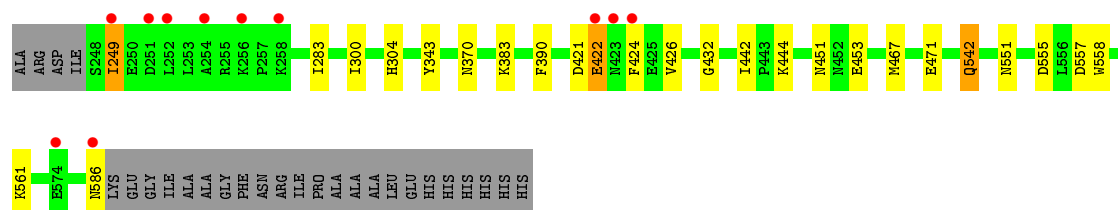
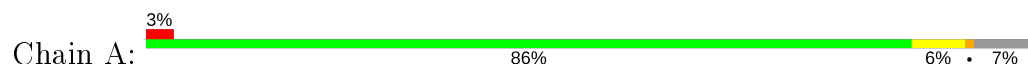
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	372	Total	O	0	0
			372	372		
6	B	354	Total	O	0	0
			354	354		

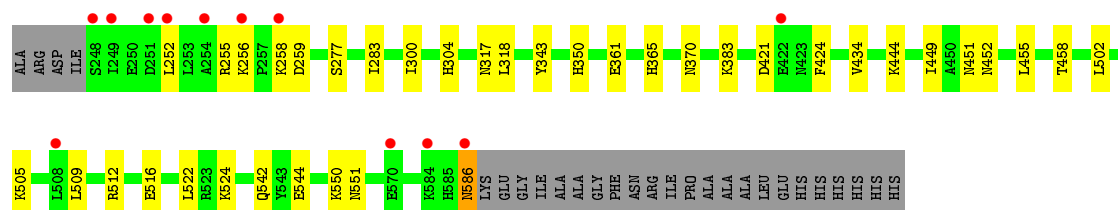
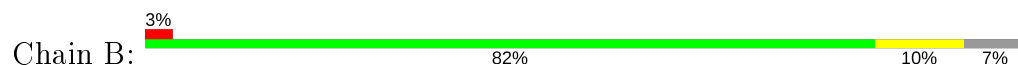
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: WlaL protein



• Molecule 1: WlaL protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.51Å 108.27Å 109.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.00 – 1.60 31.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (31.00-1.60) 94.6 (31.00-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.35 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.169 , 0.196 0.183 , 0.210	Depositor DCC
R_{free} test set	5186 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6265	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2951e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, UDP, EDO, NAD

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	0.64	0/2751	0.83	0/3714
1	B	0.64	0/2734	0.87	0/3691
All	All	0.64	0/5485	0.85	0/7405

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

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	2691	0	2796	26	0
1	B	2680	0	2796	24	0
2	A	25	0	11	0	0
2	B	25	0	11	0	0
3	A	44	0	26	4	0
3	B	44	0	26	2	0
4	A	12	0	18	1	0
4	B	12	0	18	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	372	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	354	0	0	7	0
All	All	6265	0	5702	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 4.

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:A:390:PHE:HB2	1:A:424:PHE:CZ	1.93	1.02
1:A:390:PHE:CB	1:A:424:PHE:CZ	2.54	0.91
1:A:542:GLN:H	1:A:542:GLN:HE21	1.20	0.86
1:A:390:PHE:CB	1:A:424:PHE:HZ	1.93	0.81
1:B:542:GLN:OE1	6:B:801:HOH:O	1.99	0.79
1:A:390:PHE:HB2	1:A:424:PHE:HZ	1.44	0.77
1:B:317[B]:ASN:ND2	6:B:802:HOH:O	2.20	0.75
1:B:283[A]:ILE:HD11	1:B:434:VAL:HG21	1.68	0.74
1:B:586:ASN:HD22	1:B:586:ASN:C	1.91	0.72
1:B:370:ASN:HD21	3:B:702:NAD:H61A	1.42	0.67
1:A:542:GLN:NE2	6:A:802:HOH:O	2.23	0.65
1:B:586:ASN:ND2	1:B:586:ASN:C	2.50	0.65
1:A:424:PHE:CE2	1:A:426:VAL:HG22	2.33	0.63
1:A:551:ASN:OD1	6:A:801:HOH:O	2.15	0.63
1:A:370:ASN:HD21	3:A:702:NAD:H61A	1.44	0.63
1:A:390:PHE:HB2	1:A:424:PHE:CE1	2.32	0.63
1:A:421:ASP:OD1	1:A:424:PHE:N	2.27	0.62
1:B:383:LYS:HE3	1:B:421:ASP:OD2	2.03	0.57
1:A:451[B]:ASN:ND2	1:A:453:GLU:OE2	2.18	0.57
1:A:424:PHE:CE2	1:A:426:VAL:CG2	2.89	0.56
1:B:258:LYS:HB2	1:B:544:GLU:OE1	2.06	0.56
1:A:249:ILE:HD12	1:A:442:ILE:HD13	1.90	0.54
1:B:365:HIS:HD2	6:B:840:HOH:O	1.92	0.53
1:A:390:PHE:HB3	1:A:424:PHE:CZ	2.40	0.53
1:A:370:ASN:ND2	3:A:702:NAD:H61A	2.07	0.52
1:A:432:GLY:O	3:A:702:NAD:H4N	2.11	0.51
1:B:370:ASN:ND2	3:B:702:NAD:H61A	2.07	0.51
1:A:390:PHE:CG	1:A:424:PHE:HZ	2.28	0.50
1:A:422:GLU:CD	1:A:422:GLU:H	2.14	0.50
1:B:421:ASP:OD1	1:B:424:PHE:N	2.45	0.49
1:B:255:ARG:NH2	6:B:808:HOH:O	2.40	0.49
1:B:458[B]:THR:CG2	1:B:522:LEU:HD23	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ILE:HD11	1:B:343:TYR:HB3	1.96	0.48
1:A:300[A]:ILE:HD11	1:A:343:TYR:HB3	1.95	0.48
1:B:452:ASN:OD1	1:B:512:ARG:NH1	2.49	0.45
1:A:467:MET:HG2	1:A:471:GLU:HB2	1.99	0.45
1:A:558:TRP:CE3	4:A:705:EDO:H12	2.52	0.44
1:A:283:ILE:HD12	3:A:702:NAD:O4D	2.17	0.44
1:B:252:LEU:HD13	1:B:505:LYS:HE3	1.99	0.44
1:B:318:LEU:HD12	6:B:1124:HOH:O	2.17	0.44
1:A:555:ASP:OD2	1:A:557:ASP:HB2	2.18	0.43
1:A:383:LYS:HE3	1:A:421:ASP:OD2	2.18	0.43
1:B:449:ILE:HG13	1:B:455:LEU:HD21	2.02	0.42
1:B:502:LEU:C	1:B:502:LEU:HD23	2.40	0.42
1:B:551:ASN:ND2	6:B:812:HOH:O	2.43	0.41
1:B:361:GLU:OE1	1:B:524:LYS:HE3	2.20	0.41
1:B:421:ASP:OD1	1:B:424:PHE:HB3	2.20	0.41
1:A:551:ASN:HB3	6:A:814:HOH:O	2.20	0.40
1:B:259:ASP:HB3	6:B:982:HOH:O	2.20	0.40
1:B:277:SER:OG	1:B:350:HIS:HA	2.20	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	344/366 (94%)	342 (99%)	2 (1%)	0	100	100
1	B	342/366 (93%)	339 (99%)	3 (1%)	0	100	100
All	All	686/732 (94%)	681 (99%)	5 (1%)	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	305/317 (96%)	298 (98%)	7 (2%)	50	25
1	B	303/317 (96%)	294 (97%)	9 (3%)	41	16
All	All	608/634 (96%)	592 (97%)	16 (3%)	47	21

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	ILE
1	A	304	HIS
1	A	422	GLU
1	A	444	LYS
1	A	542	GLN
1	A	561	LYS
1	A	586	ASN
1	B	256[A]	LYS
1	B	256[B]	LYS
1	B	304	HIS
1	B	444	LYS
1	B	451	ASN
1	B	509	LEU
1	B	516	GLU
1	B	550	LYS
1	B	586	ASN

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	362	GLN
1	A	370	ASN
1	A	542	GLN
1	A	551	ASN
1	B	365	HIS
1	B	370	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	586	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	$\# Z > 2$
4	EDO	A	703	-	3,3,3	0.43	0	2,2,2	0.06	0
4	EDO	B	704[A]	-	3,3,3	0.52	0	2,2,2	0.29	0
2	UDP	A	701	-	20,26,26	1.01	0	25,40,40	0.98	1 (4%)
3	NAD	A	702	-	42,48,48	0.83	0	50,73,73	1.50	7 (14%)
3	NAD	B	702	-	42,48,48	0.81	1 (2%)	50,73,73	1.80	11 (22%)
4	EDO	B	703	-	3,3,3	0.50	0	2,2,2	0.16	0
2	UDP	B	701	-	20,26,26	1.01	1 (5%)	25,40,40	1.09	2 (8%)
4	EDO	A	705	-	3,3,3	0.44	0	2,2,2	0.54	0
4	EDO	B	704[B]	-	3,3,3	0.58	0	2,2,2	0.21	0
4	EDO	A	704	-	3,3,3	0.81	0	2,2,2	0.24	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
4	EDO	A	703	-	-	0/1/1/1	-
4	EDO	B	704[A]	-	-	0/1/1/1	-
2	UDP	A	701	-	-	3/14/32/32	0/2/2/2
3	NAD	A	702	-	-	5/26/62/62	0/5/5/5
3	NAD	B	702	-	-	6/26/62/62	0/5/5/5
4	EDO	B	703	-	-	0/1/1/1	-
2	UDP	B	701	-	-	3/14/32/32	0/2/2/2
4	EDO	A	705	-	-	0/1/1/1	-
4	EDO	B	704[B]	-	-	1/1/1/1	-
4	EDO	A	704	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	UDP	C2'-C1'	-2.80	1.49	1.53
3	B	702	NAD	O4D-C1D	2.35	1.44	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NAD	O4D-C1D-C2D	-6.06	98.07	106.93
3	A	702	NAD	O4D-C1D-C2D	-5.45	98.96	106.93
3	B	702	NAD	N3A-C2A-N1A	-4.12	122.24	128.68
3	B	702	NAD	O2D-C2D-C3D	-3.62	100.13	111.82
3	A	702	NAD	N3A-C2A-N1A	-3.54	123.14	128.68
3	A	702	NAD	C3N-C7N-N7N	3.51	121.96	117.75
3	B	702	NAD	O7N-C7N-N7N	-3.20	118.04	122.58
3	A	702	NAD	O2D-C2D-C3D	-3.04	101.99	111.82
3	B	702	NAD	C2A-N1A-C6A	2.72	123.40	118.75
3	B	702	NAD	O2D-C2D-C1D	2.66	120.68	110.85
3	A	702	NAD	C2A-N1A-C6A	2.60	123.20	118.75
3	B	702	NAD	C6N-N1N-C2N	-2.49	119.70	121.97
2	B	701	UDP	O3B-PB-O2B	2.45	116.99	107.64
3	B	702	NAD	N6A-C6A-N1A	2.44	123.65	118.57
3	A	702	NAD	C3D-C2D-C1D	2.44	104.65	100.98
2	A	701	UDP	O3B-PB-O2B	2.32	116.51	107.64
3	B	702	NAD	C3D-C2D-C1D	2.20	104.28	100.98
3	A	702	NAD	O7N-C7N-C3N	-2.14	117.07	119.63
2	B	701	UDP	O2A-PA-O1A	2.09	122.59	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NAD	C3N-C7N-N7N	2.07	120.23	117.75
3	B	702	NAD	C1B-N9A-C4A	-2.01	123.11	126.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	UDP	C2'-C1'-N1-C6
2	A	701	UDP	O4'-C1'-N1-C6
2	A	701	UDP	PB-O3A-PA-O5'
3	A	702	NAD	O4D-C1D-N1N-C2N
3	B	702	NAD	O4D-C1D-N1N-C2N
2	B	701	UDP	C2'-C1'-N1-C6
2	B	701	UDP	O4'-C1'-N1-C6
2	B	701	UDP	PB-O3A-PA-O5'
4	A	704	EDO	O1-C1-C2-O2
3	B	702	NAD	PA-O3-PN-O2N
3	A	702	NAD	O4B-C4B-C5B-O5B
3	A	702	NAD	O4D-C4D-C5D-O5D
4	B	704[B]	EDO	O1-C1-C2-O2
3	A	702	NAD	C2D-C1D-N1N-C2N
3	A	702	NAD	C2D-C1D-N1N-C6N
3	B	702	NAD	C2D-C1D-N1N-C6N
3	B	702	NAD	O4B-C4B-C5B-O5B
3	B	702	NAD	PA-O3-PN-O1N
3	B	702	NAD	O4D-C4D-C5D-O5D

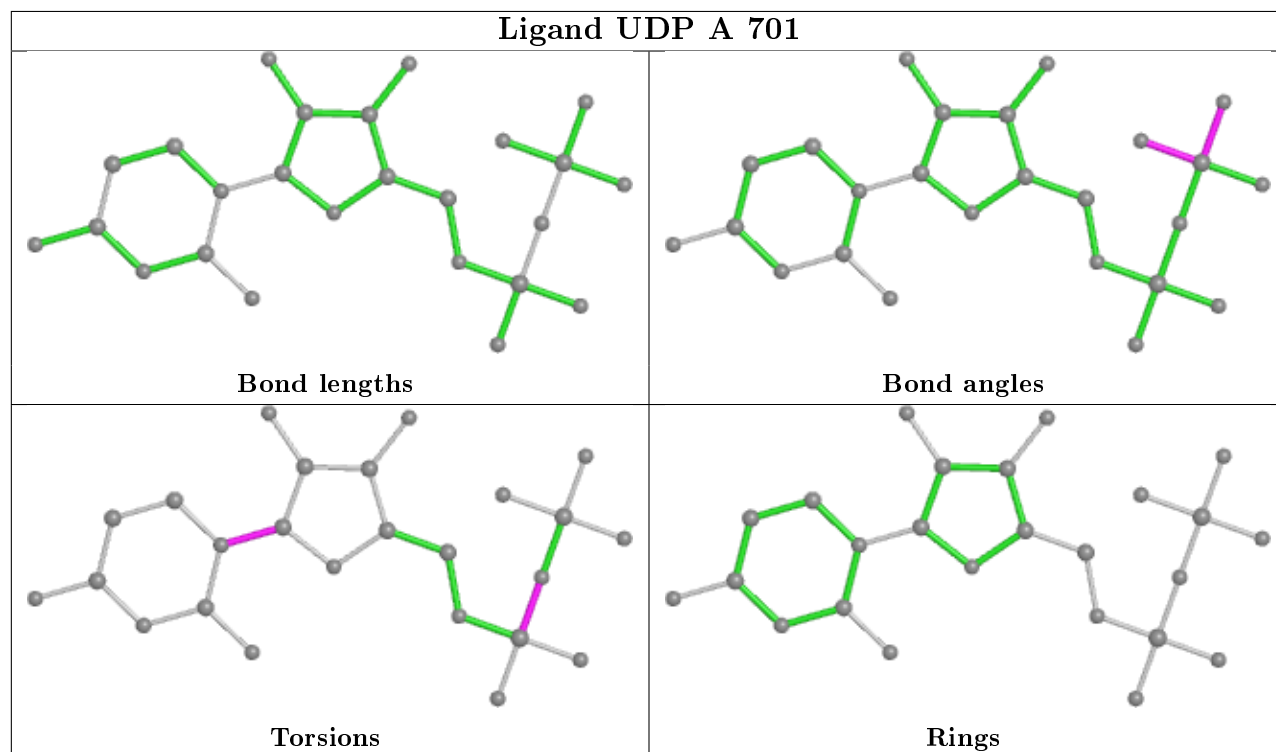
There are no ring outliers.

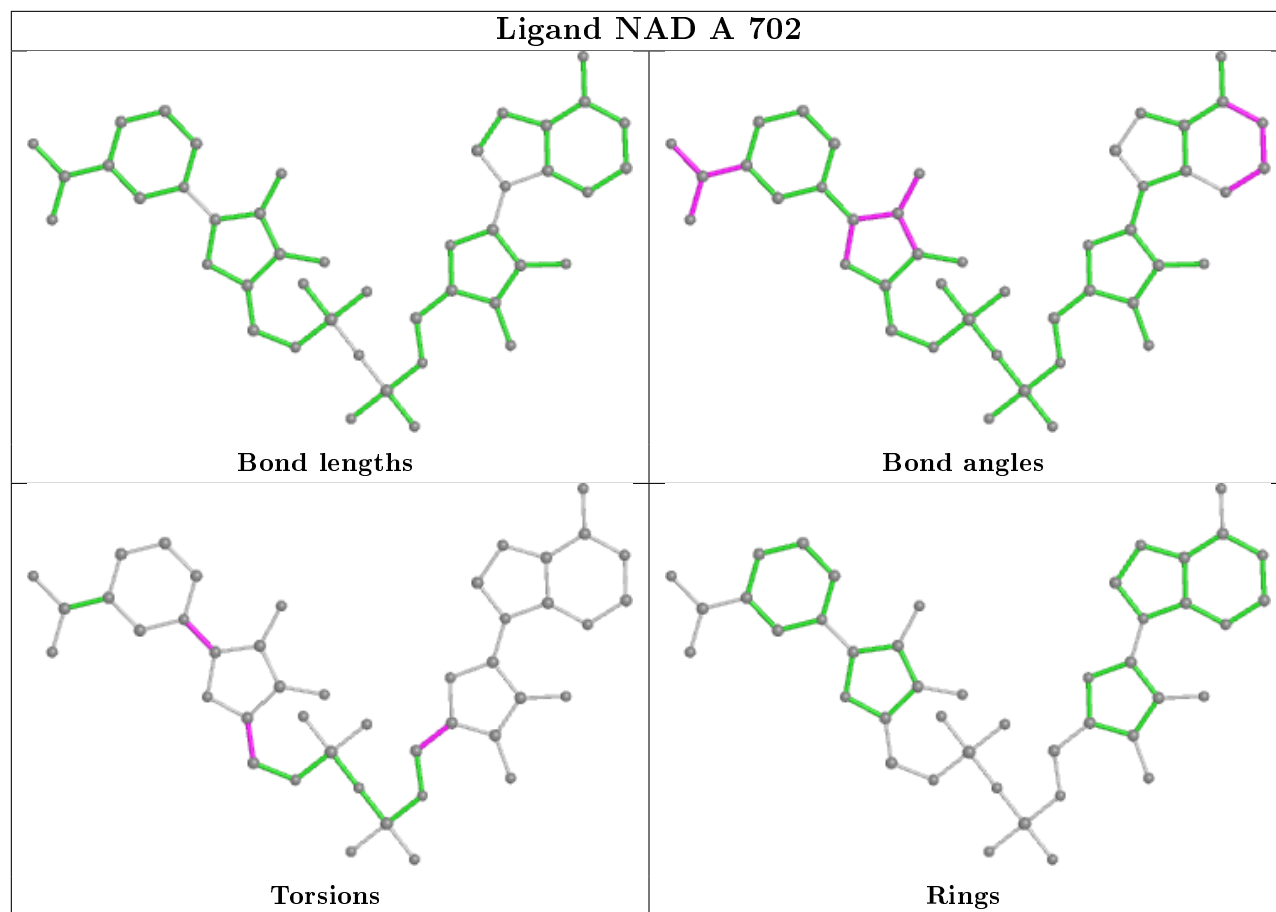
3 monomers are involved in 7 short contacts:

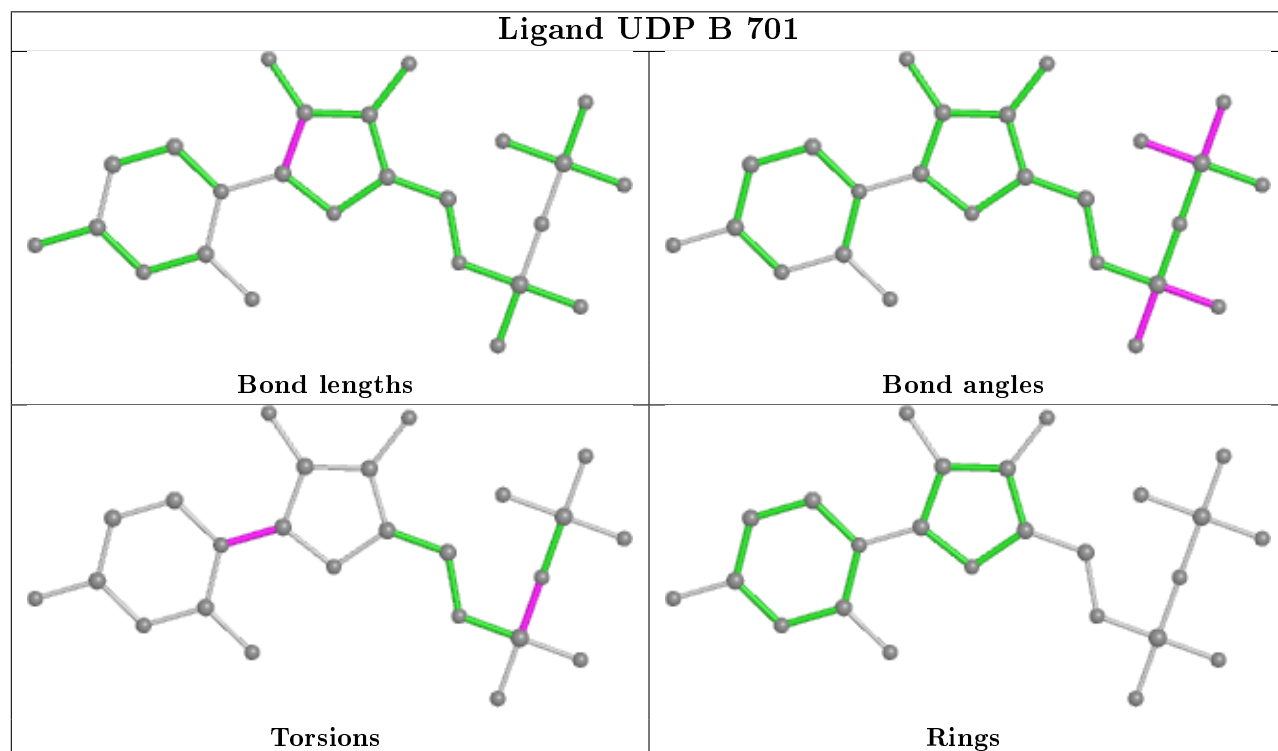
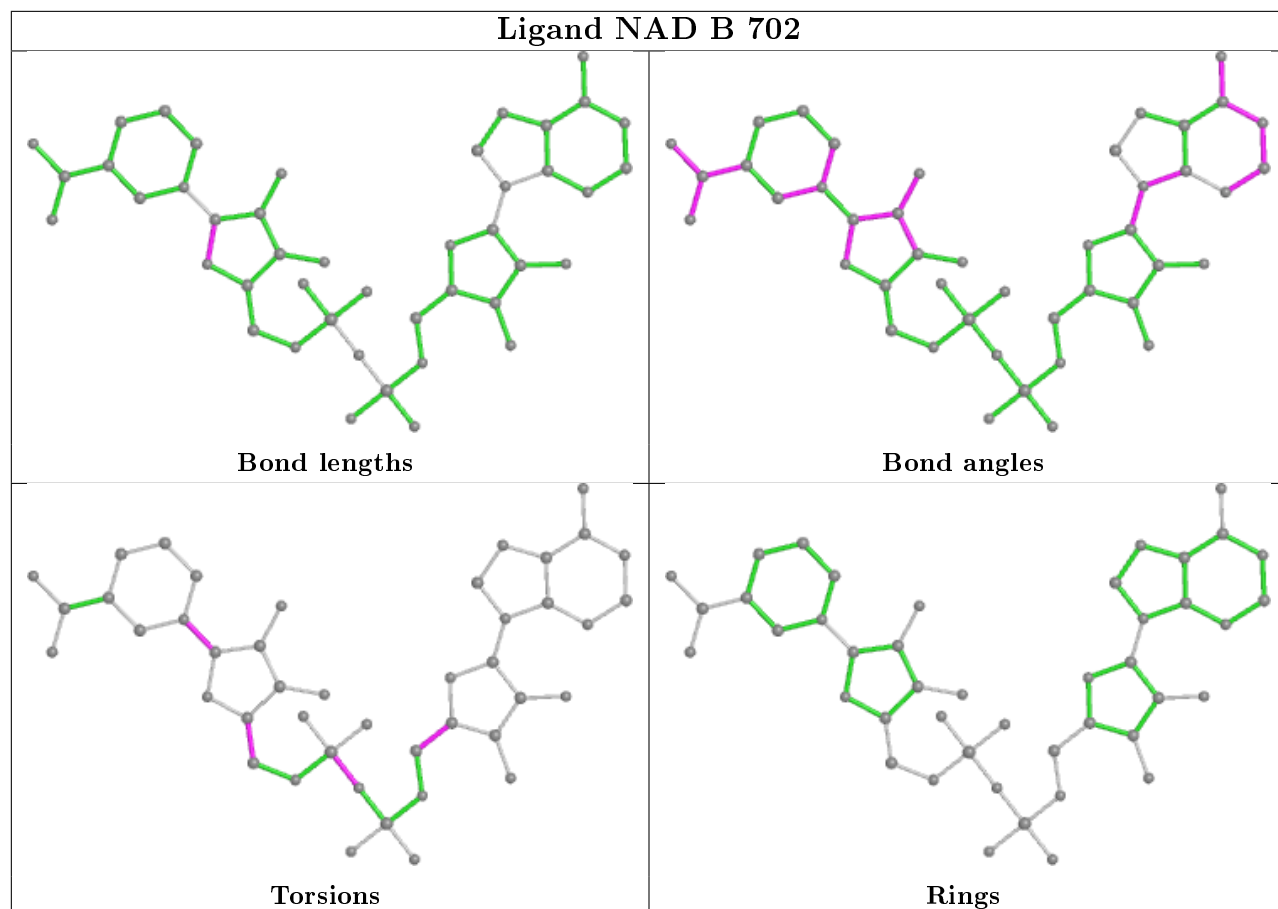
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NAD	4	0
3	B	702	NAD	2	0
4	A	705	EDO	1	0

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	339/366 (92%)	-0.13	11 (3%) 47 44	11, 17, 38, 54	0
1	B	339/366 (92%)	-0.18	12 (3%) 44 41	10, 18, 39, 57	0
All	All	678/732 (92%)	-0.16	23 (3%) 45 42	10, 17, 39, 57	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	PHE	6.1
1	A	258	LYS	3.7
1	B	258	LYS	3.4
1	B	254	ALA	3.4
1	A	254	ALA	3.1
1	B	248	SER	3.0
1	B	422	GLU	2.9
1	A	251	ASP	2.8
1	A	423	ASN	2.8
1	B	586	ASN	2.8
1	B	584	LYS	2.7
1	B	251	ASP	2.6
1	B	256[A]	LYS	2.6
1	A	249	ILE	2.6
1	B	508	LEU	2.5
1	A	422	GLU	2.4
1	B	570	GLU	2.4
1	A	256	LYS	2.3
1	B	249	ILE	2.3
1	A	586	ASN	2.2
1	B	252	LEU	2.1
1	A	574	GLU	2.0
1	A	252	LEU	2.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

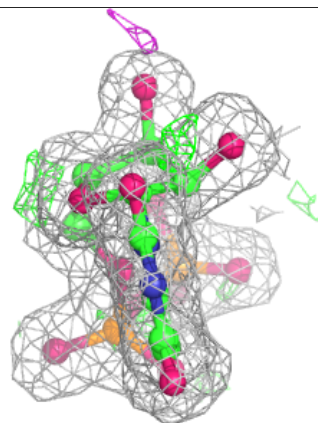
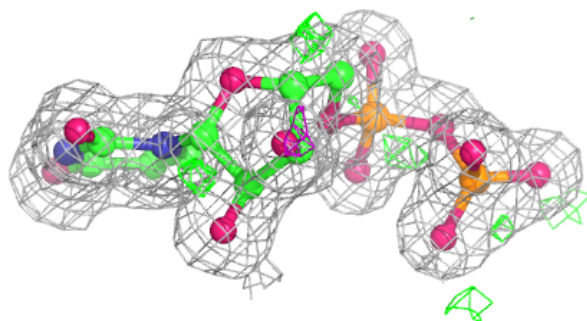
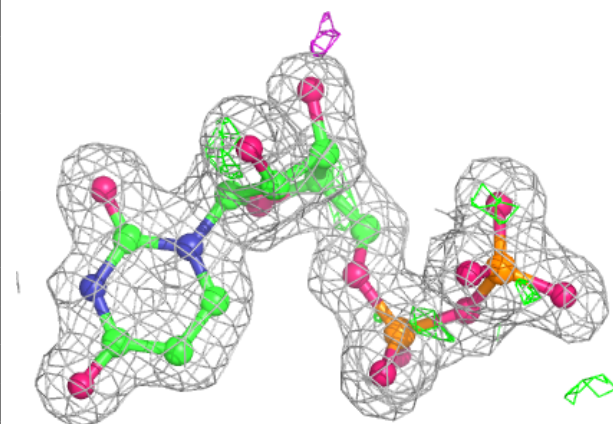
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	704	4/4	0.88	0.14	21,22,22,29	0
4	EDO	B	703	4/4	0.92	0.09	22,23,29,34	0
4	EDO	A	705	4/4	0.93	0.10	26,33,34,39	0
4	EDO	A	703	4/4	0.93	0.13	23,25,31,35	0
4	EDO	B	704[B]	4/4	0.94	0.11	18,21,21,23	4
4	EDO	B	704[A]	4/4	0.94	0.11	24,24,25,25	4
5	NA	B	706	1/1	0.96	0.14	31,31,31,31	0
5	NA	B	707	1/1	0.97	0.11	24,24,24,24	0
5	NA	B	705	1/1	0.97	0.11	27,27,27,27	0
5	NA	A	708	1/1	0.97	0.16	32,32,32,32	0
2	UDP	B	701	25/25	0.98	0.07	13,15,18,21	0
3	NAD	B	702	44/44	0.98	0.07	9,12,26,28	0
2	UDP	A	701	25/25	0.98	0.06	11,13,16,19	0
5	NA	A	706	1/1	0.98	0.18	28,28,28,28	0
3	NAD	A	702	44/44	0.98	0.07	8,12,23,26	0
5	NA	A	707	1/1	0.99	0.19	24,24,24,24	0

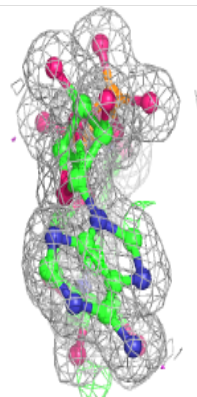
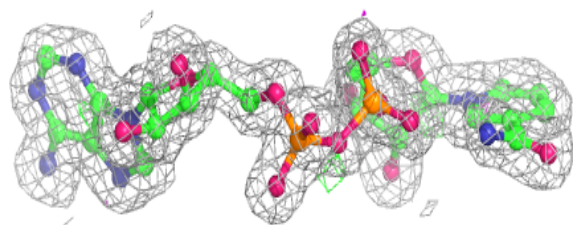
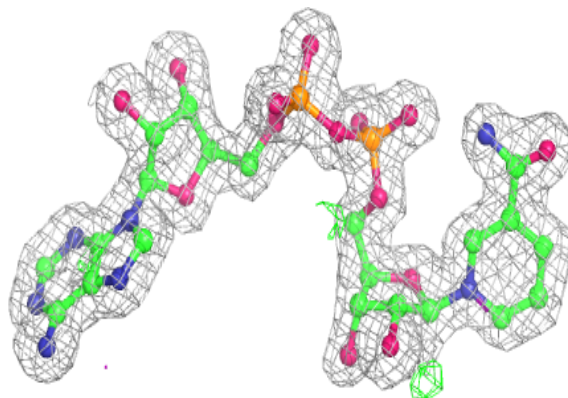
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP B 701:

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

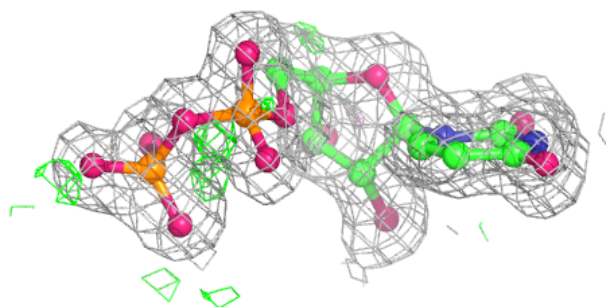
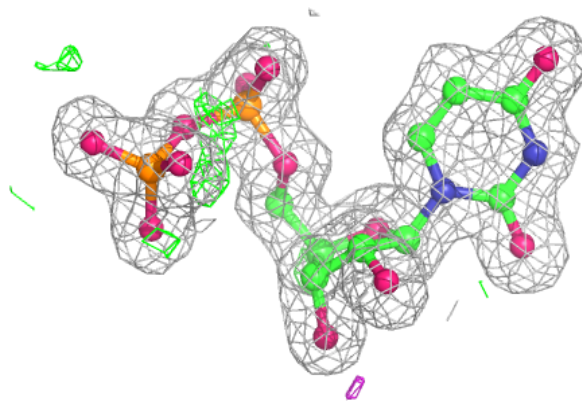
**Electron density around NAD B 702:**

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

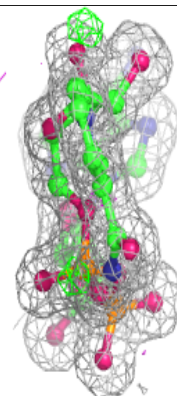
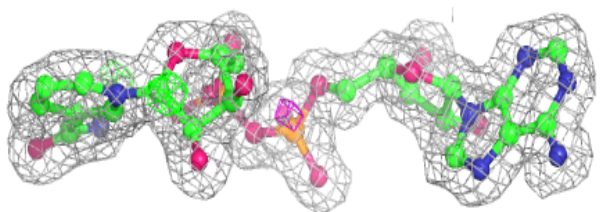
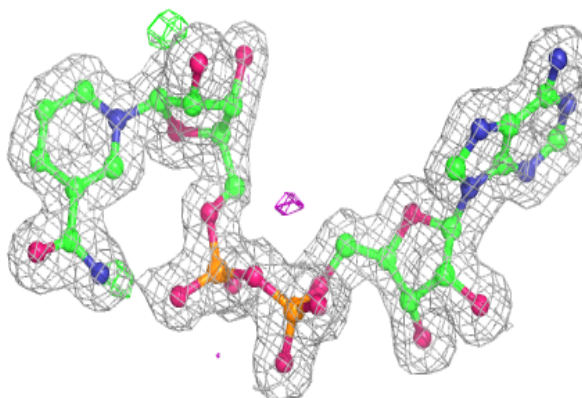


Electron density around UDP A 701:

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

**Electron density around NAD A 702:**

$2mF_o-DF_c$ (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.