



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 12:30 PM UTC

PDB ID : 8S3A / pdb_00008s3a
Title : Crystal structure of Medicago truncatula glutamate dehydrogenase 2 in complex with 2,6-pyridinedicarboxylic acid and NAD
Authors : Grzechowiak, M.; Ruszkowski, M.
Deposited on : 2024-02-19
Resolution : 1.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

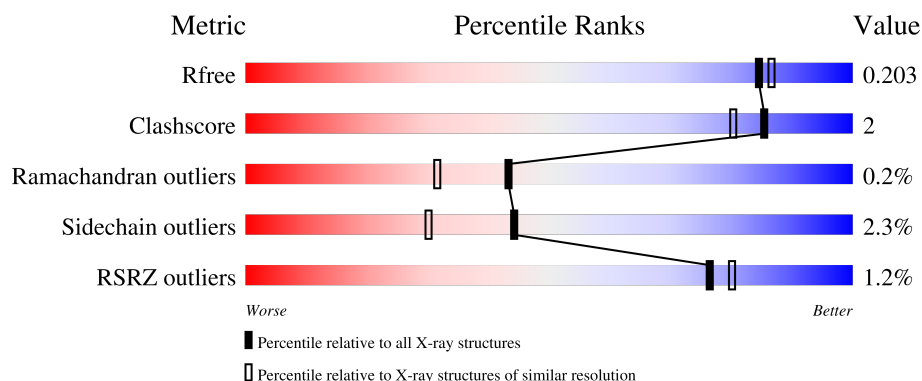
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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.



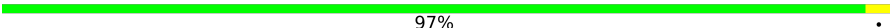
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	A	414	
1	B	414	
1	C	414	
1	D	414	
1	E	414	

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Mol	Chain	Length	Quality of chain
1	F	414	

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
9	PG4	F	605	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20309 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3126	1973	548	590	15			
1	B	409	Total	C	N	O	S	0	1	0
			3128	1975	549	589	15			
1	C	410	Total	C	N	O	S	0	0	0
			3126	1973	548	590	15			
1	D	405	Total	C	N	O	S	0	1	0
			3101	1958	543	585	15			
1	E	412	Total	C	N	O	S	0	1	0
			3150	1987	554	593	16			
1	F	413	Total	C	N	O	S	0	2	0
			3164	1994	557	597	16			

There are 18 discrepancies between the modelled and reference sequences:

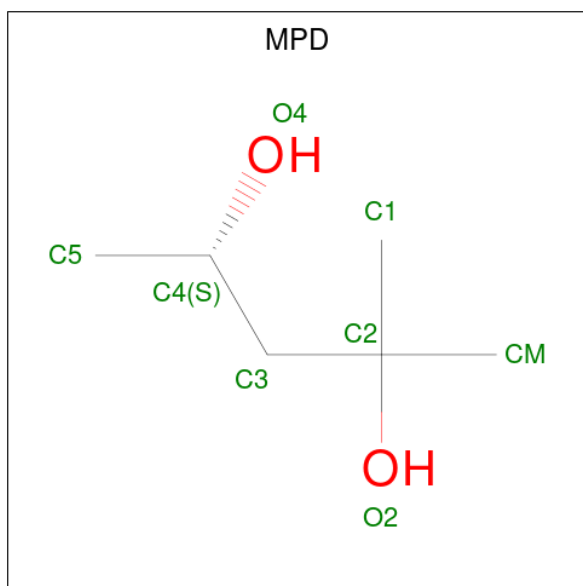
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7JYL4
A	-1	ASN	-	expression tag	UNP G7JYL4
A	0	ALA	-	expression tag	UNP G7JYL4
B	-2	SER	-	expression tag	UNP G7JYL4
B	-1	ASN	-	expression tag	UNP G7JYL4
B	0	ALA	-	expression tag	UNP G7JYL4
C	-2	SER	-	expression tag	UNP G7JYL4
C	-1	ASN	-	expression tag	UNP G7JYL4
C	0	ALA	-	expression tag	UNP G7JYL4
D	-2	SER	-	expression tag	UNP G7JYL4
D	-1	ASN	-	expression tag	UNP G7JYL4
D	0	ALA	-	expression tag	UNP G7JYL4
E	-2	SER	-	expression tag	UNP G7JYL4
E	-1	ASN	-	expression tag	UNP G7JYL4
E	0	ALA	-	expression tag	UNP G7JYL4
F	-2	SER	-	expression tag	UNP G7JYL4
F	-1	ASN	-	expression tag	UNP G7JYL4

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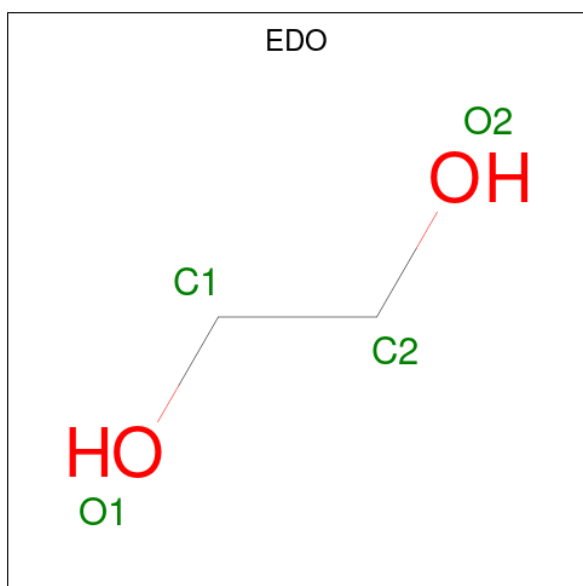
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP G7JYL4

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



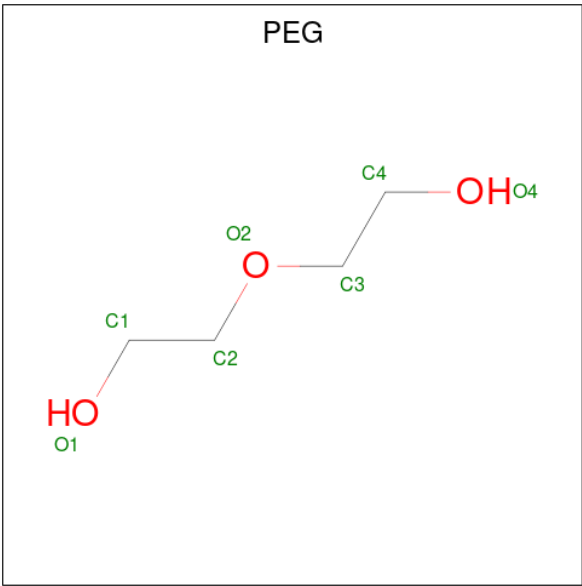
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		

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



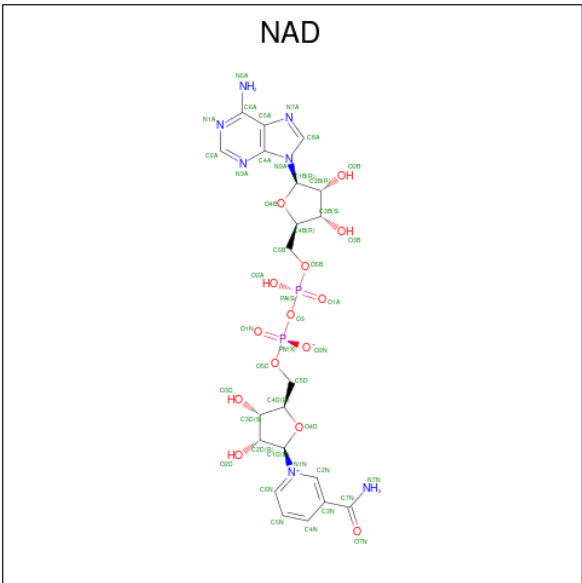
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

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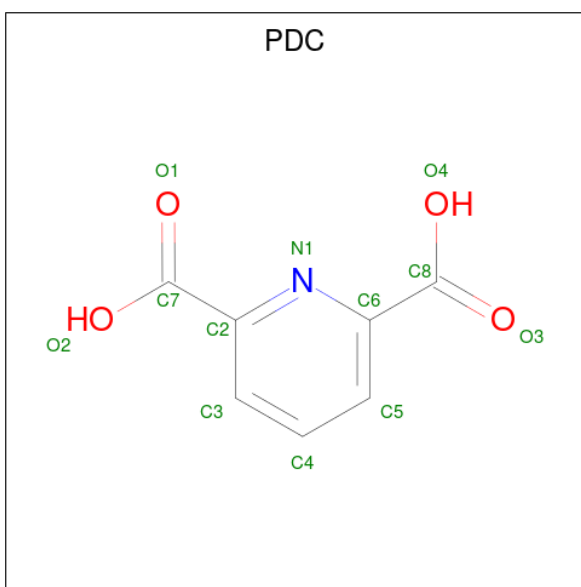
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

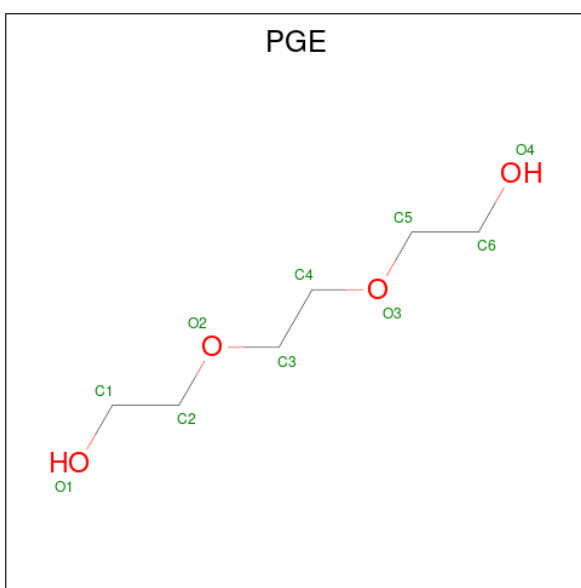
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	0
			2	2		
6	B	1	Total	Na	0	0
			1	1		
6	C	2	Total	Na	0	0
			2	2		
6	D	1	Total	Na	0	0
			1	1		
6	E	1	Total	Na	0	0
			1	1		
6	F	1	Total	Na	0	0
			1	1		

- Molecule 7 is PYRIDINE-2,6-DICARBOXYLIC ACID (CCD ID: PDC) (formula: C₇H₅NO₄) (labeled as "Ligand of Interest" by depositor).



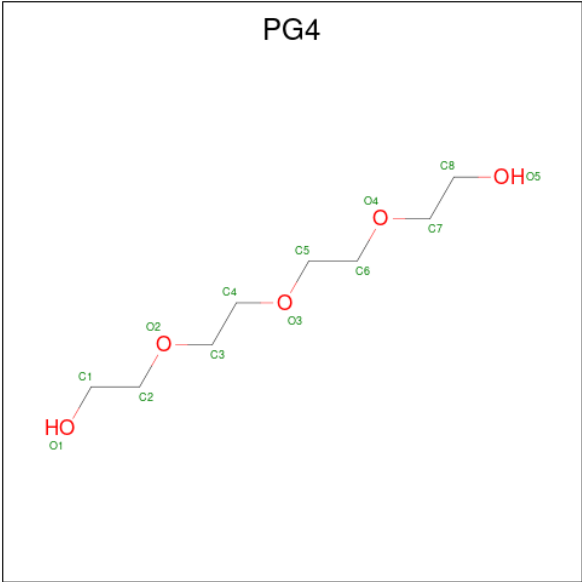
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			12	7	1	4		
7	F	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	187	Total	O	0	0
			187	187		
10	B	149	Total	O	0	0
			149	149		
10	C	151	Total	O	0	0
			151	151		
10	D	107	Total	O	0	0
			107	107		
10	E	236	Total	O	0	0
			236	236		
10	F	262	Total	O	0	0
			262	262		

3 Residue-property plots

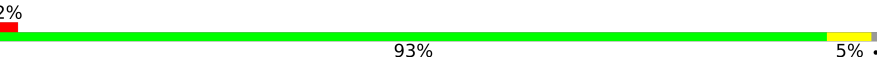
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

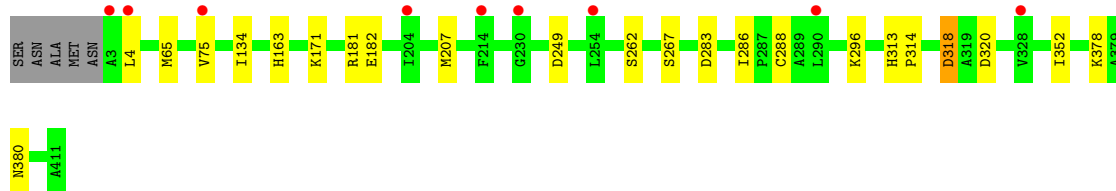
- Molecule 1: Glutamate dehydrogenase

Chain A: 



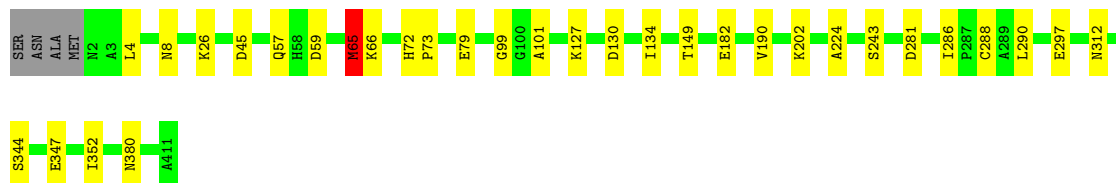
- Molecule 1: Glutamate dehydrogenase

Chain B: 



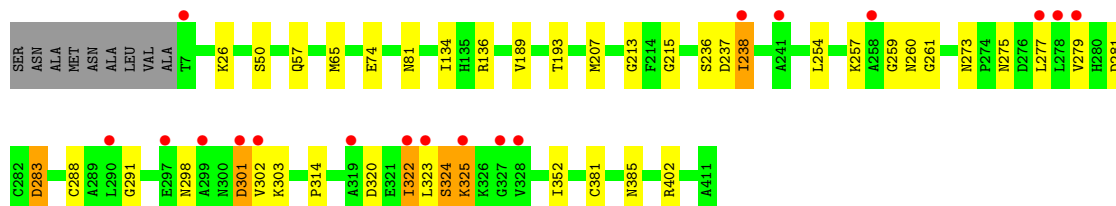
- Molecule 1: Glutamate dehydrogenase

Chain C: 



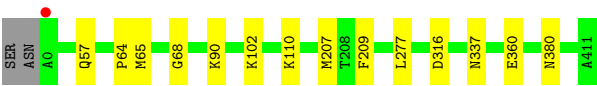
- Molecule 1: Glutamate dehydrogenase

Chain D: 



● Molecule 1: Glutamate dehydrogenase

Chain E:  96% .



● Molecule 1: Glutamate dehydrogenase

Chain F:  97% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.79Å 157.03Å 94.88Å 90.00° 99.59° 90.00°	Depositor
Resolution (Å)	46.52 – 1.85 46.52 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.52-1.85) 99.8 (46.52-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.157 , 0.199 0.165 , 0.203	Depositor DCC
R_{free} test set	2000 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20309	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: PDC, MPD, NA, PEG, NAD, PGE, PG4, 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	A	0.47	0/3188	0.61	0/4316
1	B	0.42	0/3191	0.55	0/4320
1	C	0.48	1/3188 (0.0%)	0.60	0/4316
1	D	0.44	0/3163	0.59	0/4281
1	E	0.52	0/3212	0.64	0/4347
1	F	0.53	0/3226	0.65	0/4366
All	All	0.48	1/19168 (0.0%)	0.61	0/25946

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	65	MET	SD-CE	-5.48	1.65	1.79

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	3126	0	3110	13	0
1	B	3128	0	3110	11	0
1	C	3126	0	3110	18	0
1	D	3101	0	3084	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3150	0	3139	9	0
1	F	3164	0	3149	13	0
2	A	8	0	14	0	0
3	A	20	0	30	0	0
3	B	16	0	24	0	0
3	C	8	0	12	1	0
3	D	12	0	18	0	0
3	E	20	0	30	0	0
3	F	12	0	18	0	0
4	A	7	0	10	1	0
5	A	44	0	26	0	0
5	B	44	0	26	0	0
5	C	44	0	26	0	0
5	D	44	0	26	4	0
5	E	44	0	26	0	0
5	F	44	0	26	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	E	12	0	3	0	0
7	F	12	0	3	0	0
8	E	10	0	14	0	0
9	F	13	0	18	8	0
10	A	187	0	0	2	0
10	B	149	0	0	0	0
10	C	151	0	0	5	0
10	D	107	0	0	1	0
10	E	236	0	0	1	0
10	F	262	0	0	2	0
All	All	20309	0	19052	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 85 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:F:202:LYS:HE2	9:F:605:PG4:H12	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:LYS:NZ	9:F:605:PG4:H51	1.96	0.80
1:F:202:LYS:HZ3	9:F:605:PG4:H32	1.55	0.70
1:F:202:LYS:HZ3	9:F:605:PG4:H51	1.59	0.66
1:F:202:LYS:CE	9:F:605:PG4:H12	2.27	0.64

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	408/414 (99%)	398 (98%)	10 (2%)	0	100	100
1	B	408/414 (99%)	391 (96%)	16 (4%)	1 (0%)	43	31
1	C	408/414 (99%)	397 (97%)	11 (3%)	0	100	100
1	D	404/414 (98%)	382 (95%)	19 (5%)	3 (1%)	18	8
1	E	411/414 (99%)	402 (98%)	9 (2%)	0	100	100
1	F	413/414 (100%)	401 (97%)	12 (3%)	0	100	100
All	All	2452/2484 (99%)	2371 (97%)	77 (3%)	4 (0%)	43	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	324	SER
1	B	249	ASP
1	D	260	ASN
1	D	322	ILE

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	A	329/332 (99%)	321 (98%)	8 (2%)	43	28
1	B	329/332 (99%)	321 (98%)	8 (2%)	43	28
1	C	329/332 (99%)	320 (97%)	9 (3%)	39	24
1	D	327/332 (98%)	313 (96%)	14 (4%)	26	11
1	E	331/332 (100%)	328 (99%)	3 (1%)	70	64
1	F	333/332 (100%)	329 (99%)	4 (1%)	63	55
All	All	1978/1992 (99%)	1932 (98%)	46 (2%)	44	30

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	207	MET
1	D	303	LYS
1	D	237	ASP
1	D	283	ASP
1	D	325	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	398	ASN
1	E	212	GLN
1	E	375	ASN
1	A	380	ASN
1	A	300	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 8 are monoatomic - leaving 34 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
3	EDO	A	606	-	3,3,3	0.39	0	2,2,2	0.28	0
5	NAD	F	606	-	46,48,48	0.74	3 (6%)	64,73,73	0.78	1 (1%)
5	NAD	A	608	-	46,48,48	0.71	2 (4%)	64,73,73	0.80	2 (3%)
8	PGE	E	1105	-	9,9,9	0.41	0	8,8,8	0.48	0
5	NAD	D	501	-	46,48,48	0.79	2 (4%)	64,73,73	0.74	2 (3%)
3	EDO	A	605	-	3,3,3	0.48	0	2,2,2	0.35	0
3	EDO	C	502	-	3,3,3	0.45	0	2,2,2	0.50	0
3	EDO	C	503	-	3,3,3	0.51	0	2,2,2	0.33	0
3	EDO	A	604	-	3,3,3	0.50	0	2,2,2	0.45	0
3	EDO	E	1106	-	3,3,3	0.67	0	2,2,2	0.34	0
3	EDO	B	503	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	B	502	-	3,3,3	0.59	0	2,2,2	0.41	0
3	EDO	A	602	-	3,3,3	0.41	0	2,2,2	0.72	0
3	EDO	E	1107	-	3,3,3	0.48	0	2,2,2	0.67	0
3	EDO	F	603	-	3,3,3	0.49	0	2,2,2	0.49	0
3	EDO	D	503	-	3,3,3	0.42	0	2,2,2	0.36	0
3	EDO	B	505	-	3,3,3	0.32	0	2,2,2	0.97	0
3	EDO	D	502	-	3,3,3	0.50	0	2,2,2	0.31	0
3	EDO	E	1101	-	3,3,3	0.58	0	2,2,2	0.16	0
5	NAD	C	501	-	46,48,48	0.67	1 (2%)	64,73,73	0.71	2 (3%)
3	EDO	E	1103	-	3,3,3	0.44	0	2,2,2	1.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	A	603	6	6,6,6	0.30	0	5,5,5	0.18	0
5	NAD	B	501	-	46,48,48	0.77	2 (4%)	64,73,73	0.72	1 (1%)
9	PG4	F	605	-	12,12,12	0.18	0	11,11,11	0.17	0
3	EDO	F	602	-	3,3,3	0.50	0	2,2,2	0.46	0
7	PDC	E	1102	-	12,12,12	1.18	0	16,16,16	1.14	1 (6%)
3	EDO	A	607	-	3,3,3	0.53	0	2,2,2	0.30	0
3	EDO	E	1104	-	3,3,3	0.53	0	2,2,2	0.46	0
2	MPD	A	601	-	7,7,7	0.31	0	9,10,10	1.22	1 (11%)
5	NAD	E	1108	-	46,48,48	0.59	0	64,73,73	0.75	1 (1%)
3	EDO	F	604	-	3,3,3	0.53	0	2,2,2	0.27	0
7	PDC	F	601	-	12,12,12	1.07	1 (8%)	16,16,16	0.98	0
3	EDO	D	504	-	3,3,3	0.41	0	2,2,2	0.58	0
3	EDO	B	504	-	3,3,3	0.46	0	2,2,2	0.31	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
3	EDO	A	606	-	-	1/1/1/1	-
5	NAD	F	606	-	-	3/30/62/62	0/5/5/5
5	NAD	A	608	-	-	0/30/62/62	0/5/5/5
8	PGE	E	1105	-	-	5/7/7/7	-
5	NAD	D	501	-	-	2/30/62/62	0/5/5/5
3	EDO	A	605	-	-	1/1/1/1	-
3	EDO	C	502	-	-	0/1/1/1	-
3	EDO	C	503	-	-	0/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	E	1106	-	-	1/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	A	602	-	-	0/1/1/1	-
3	EDO	E	1107	-	-	1/1/1/1	-
3	EDO	F	603	-	-	1/1/1/1	-
3	EDO	D	503	-	-	0/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-
3	EDO	D	502	-	-	0/1/1/1	-
3	EDO	E	1101	-	-	1/1/1/1	-
5	NAD	C	501	-	-	1/30/62/62	0/5/5/5
3	EDO	E	1103	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	603	6	-	0/4/4/4	-
5	NAD	B	501	-	-	1/30/62/62	0/5/5/5
9	PG4	F	605	-	-	4/10/10/10	-
3	EDO	F	602	-	-	0/1/1/1	-
7	PDC	E	1102	-	-	8/8/8/8	0/1/1/1
3	EDO	A	607	-	-	1/1/1/1	-
3	EDO	E	1104	-	-	1/1/1/1	-
2	MPD	A	601	-	-	0/5/5/5	-
5	NAD	E	1108	-	-	4/30/62/62	0/5/5/5
3	EDO	F	604	-	-	0/1/1/1	-
7	PDC	F	601	-	-	8/8/8/8	0/1/1/1
3	EDO	D	504	-	-	0/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	NAD	C2N-N1N	3.62	1.39	1.35
5	B	501	NAD	C2N-N1N	3.29	1.38	1.35
5	C	501	NAD	C2N-N1N	3.12	1.38	1.35
5	A	608	NAD	C2N-N1N	2.74	1.38	1.35
5	F	606	NAD	C2N-N1N	2.66	1.37	1.35

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	608	NAD	C6N-N1N-C2N	-3.35	119.03	121.88
5	D	501	NAD	C6N-N1N-C2N	-3.02	119.31	121.88
2	A	601	MPD	CM-C2-C1	-2.99	103.93	110.63
5	F	606	NAD	C6N-N1N-C2N	-2.93	119.38	121.88
5	B	501	NAD	C6N-N1N-C2N	-2.88	119.42	121.88

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

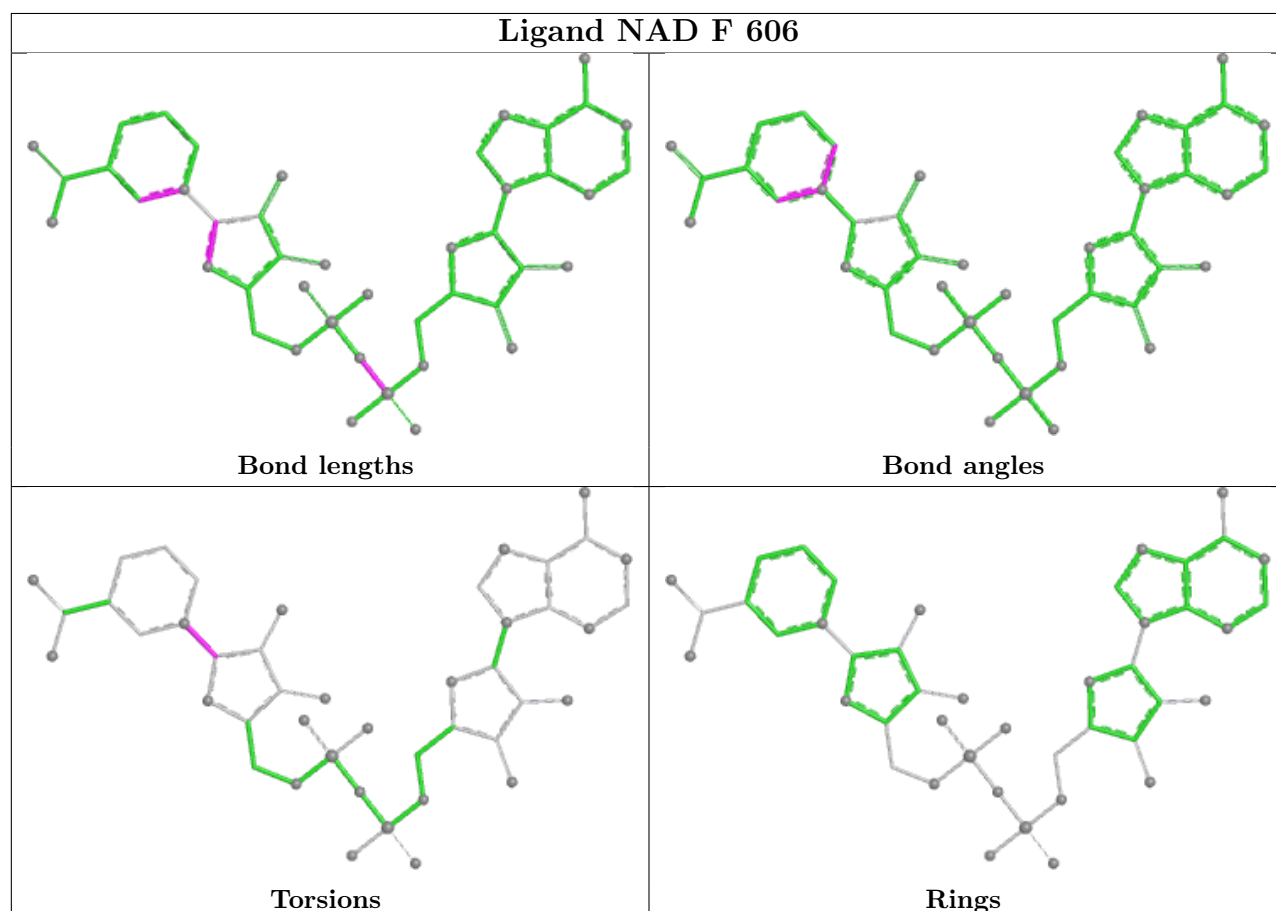
Mol	Chain	Res	Type	Atoms
5	E	1108	NAD	O4D-C1D-N1N-C2N
5	F	606	NAD	O4D-C1D-N1N-C2N
7	E	1102	PDC	N1-C2-C7-O1
7	E	1102	PDC	N1-C2-C7-O2
7	E	1102	PDC	C3-C2-C7-O1

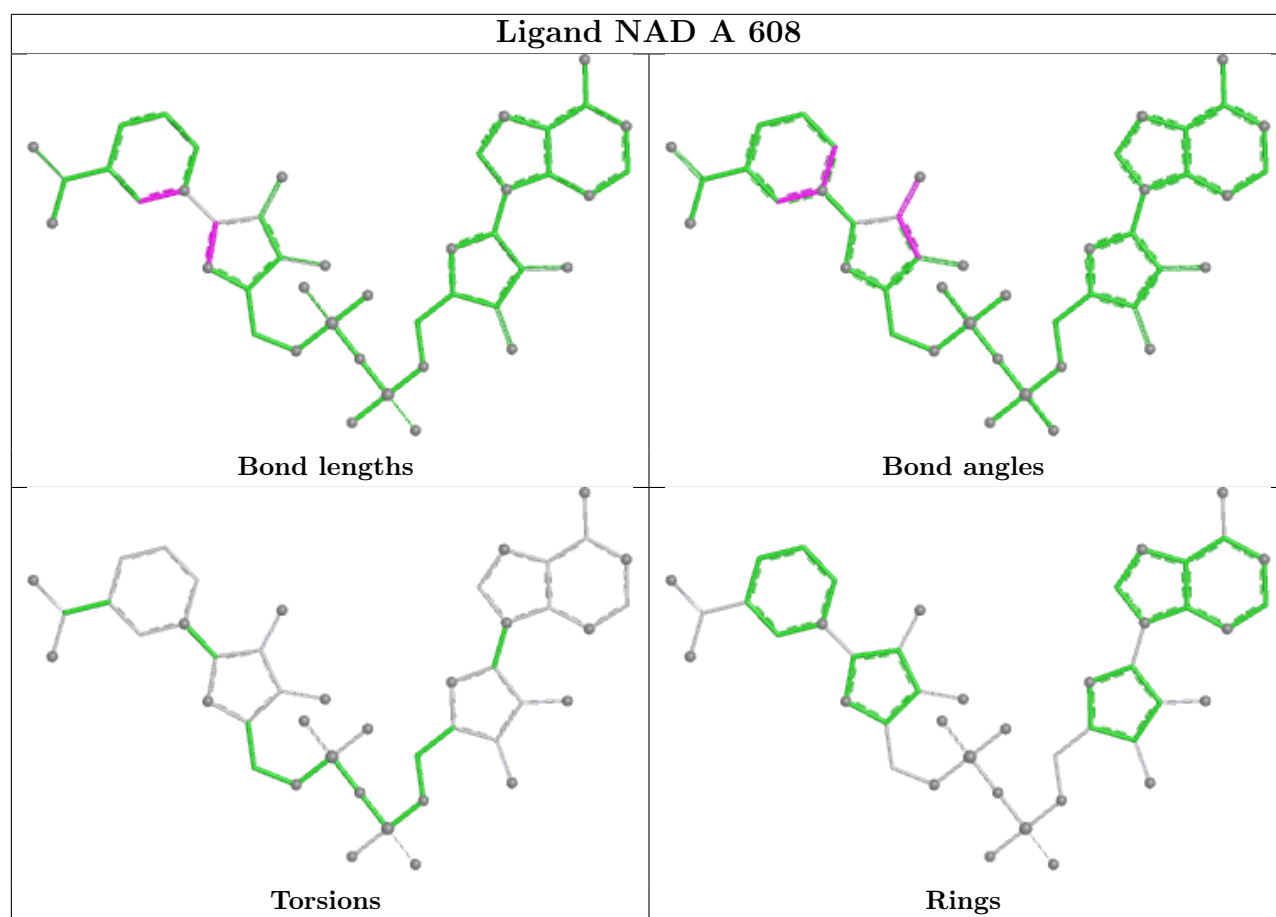
There are no ring outliers.

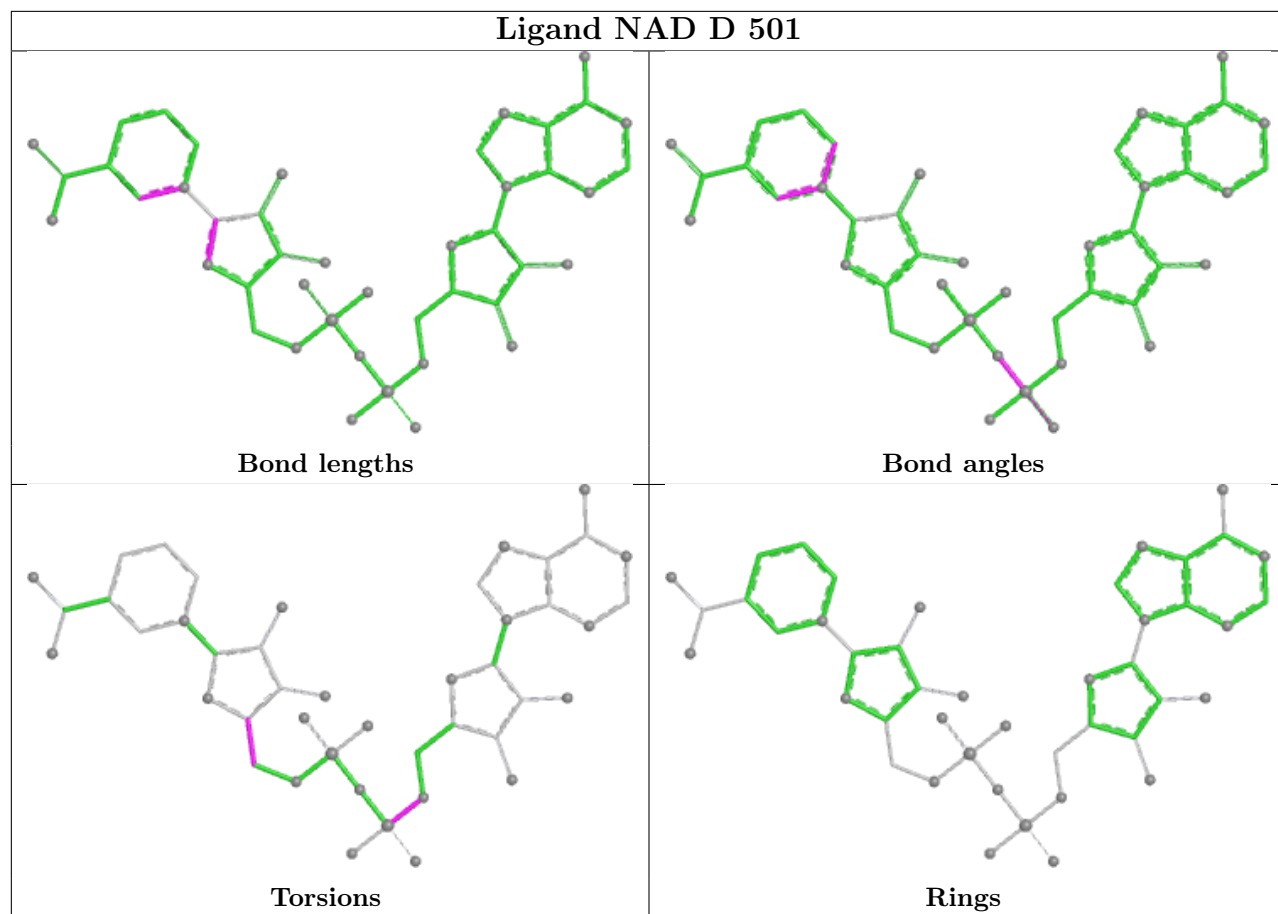
4 monomers are involved in 14 short contacts:

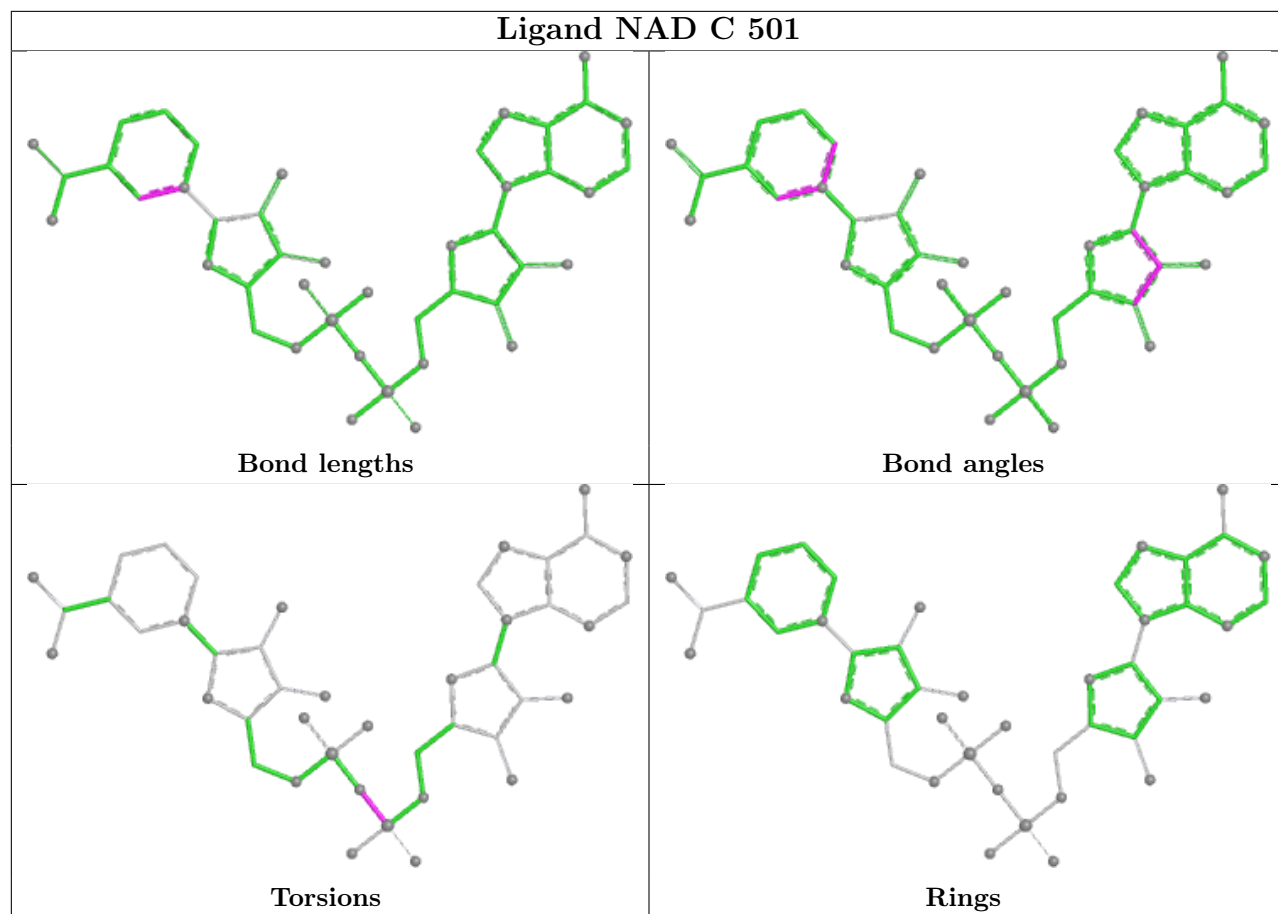
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	NAD	4	0
3	C	502	EDO	1	0
4	A	603	PEG	1	0
9	F	605	PG4	8	0

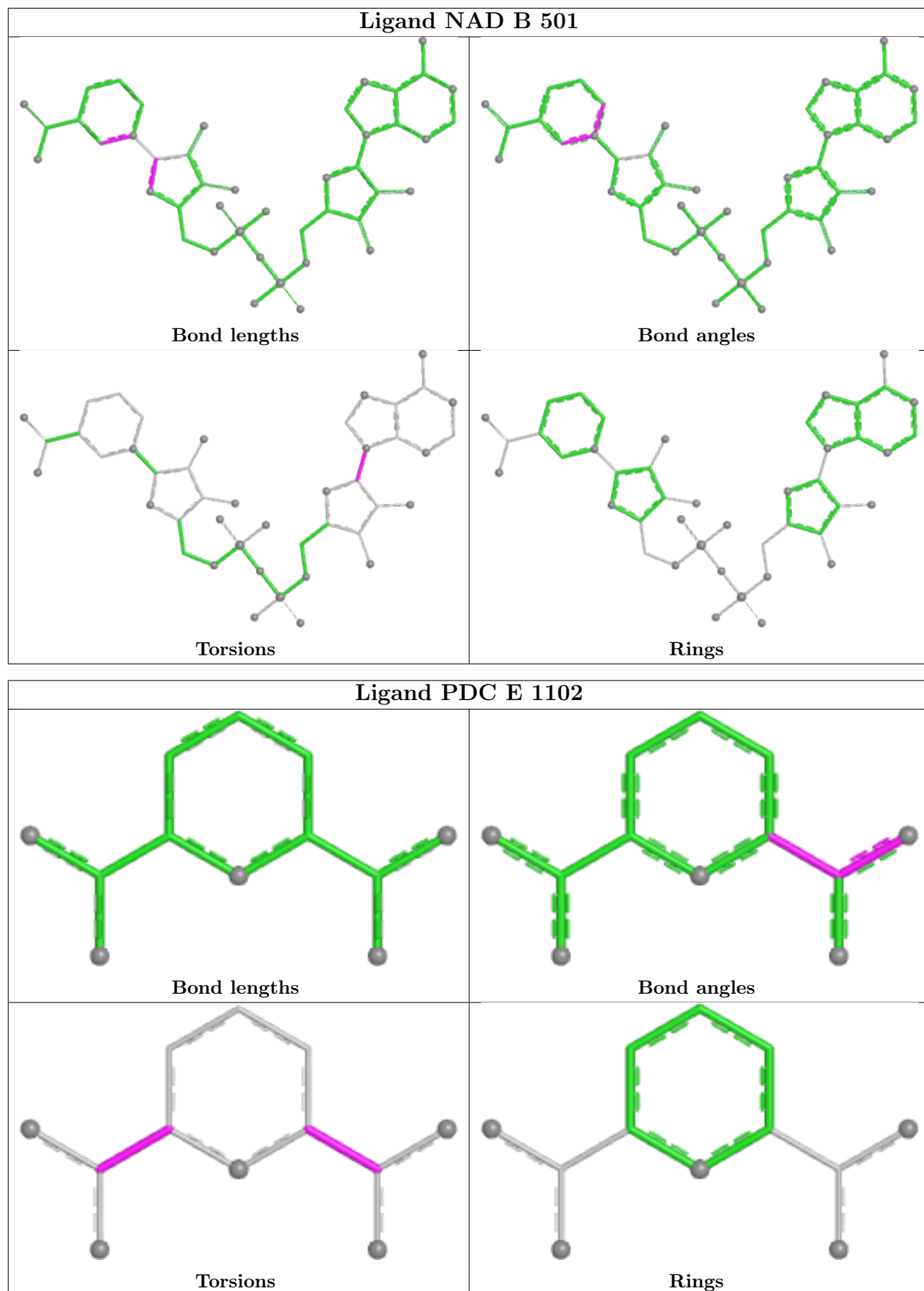
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

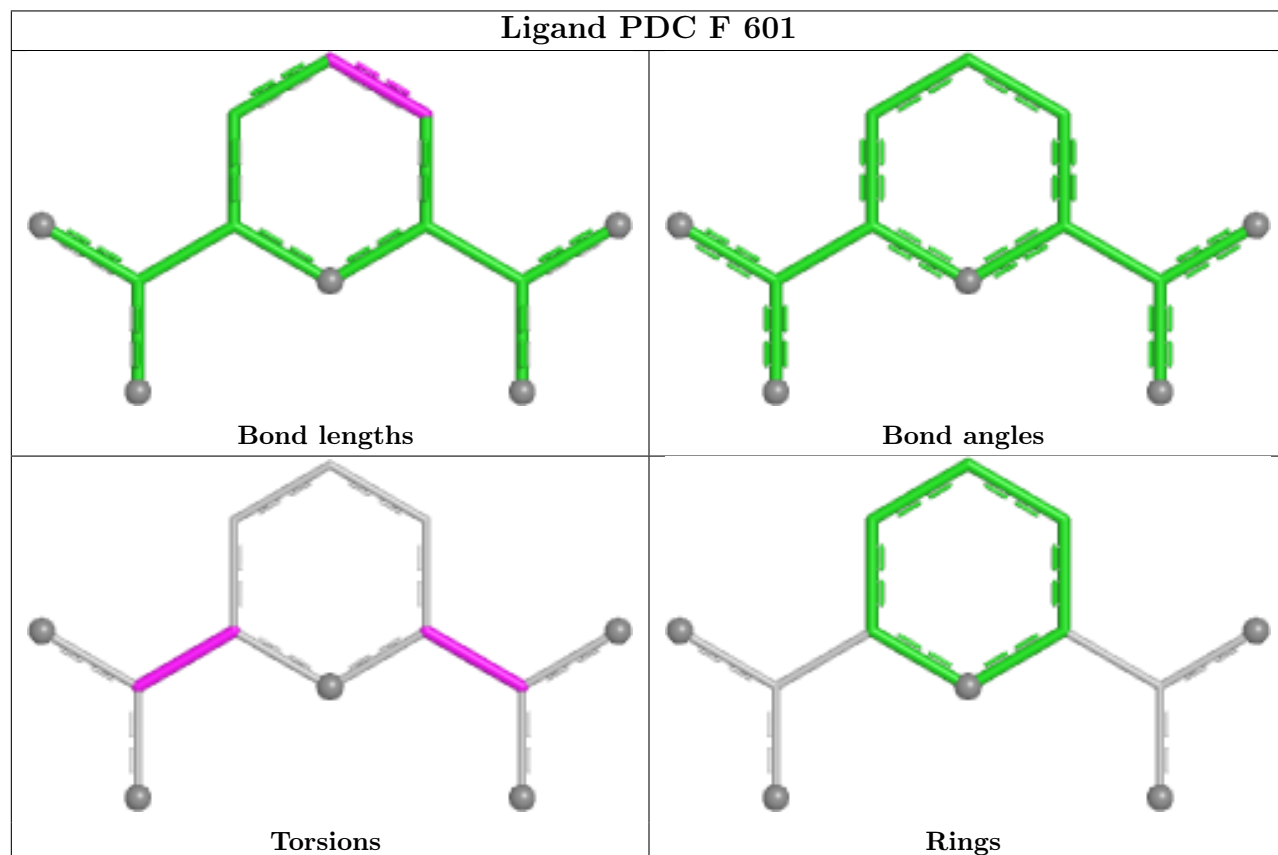
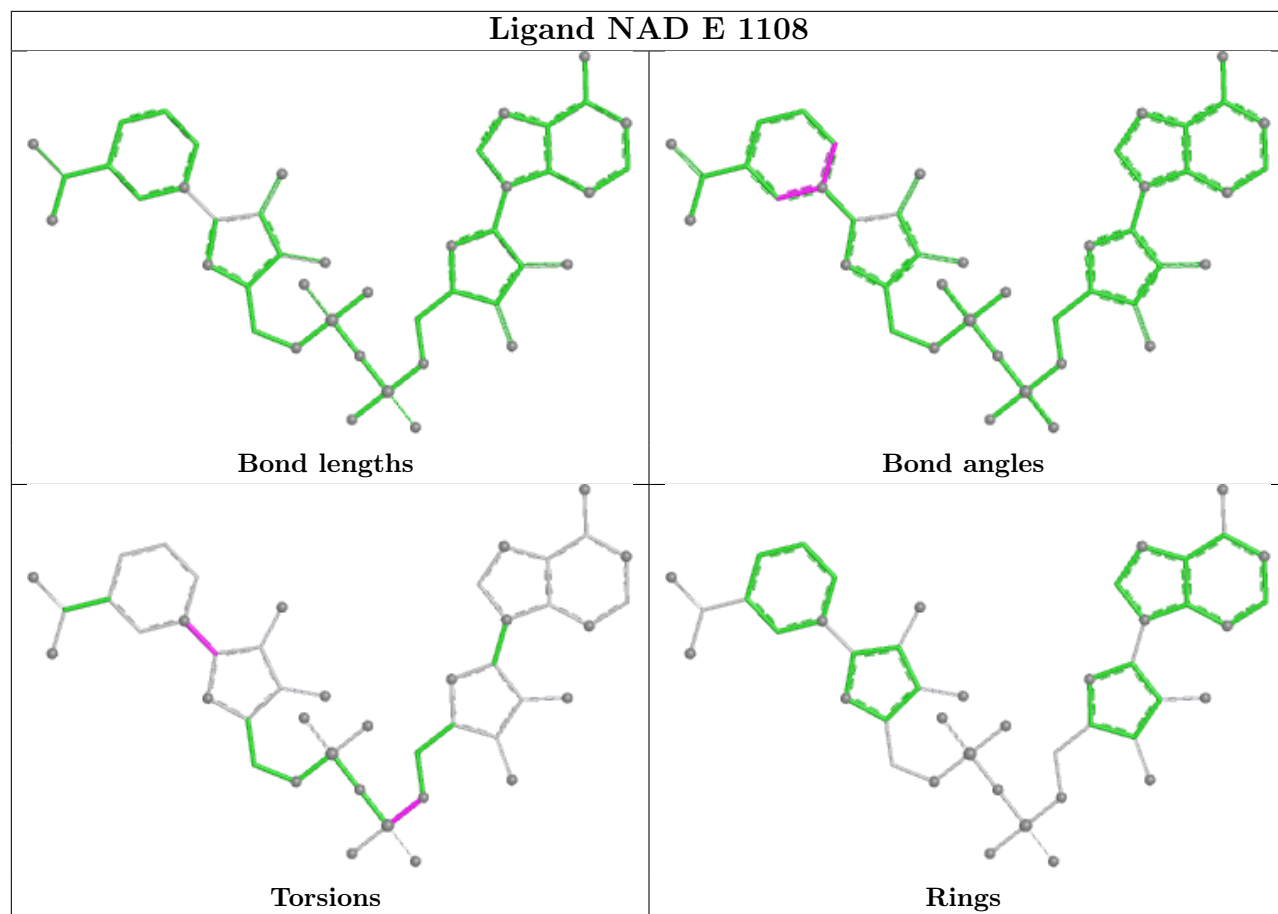












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	410/414 (99%)	-0.19	1 (0%) 91 93	24, 36, 61, 90	0
1	B	409/414 (98%)	0.17	9 (2%) 62 66	16, 46, 99, 123	1 (0%)
1	C	410/414 (99%)	-0.05	0 100 100	27, 42, 69, 92	0
1	D	405/414 (97%)	0.25	18 (4%) 39 42	13, 49, 108, 128	1 (0%)
1	E	412/414 (99%)	-0.33	1 (0%) 91 93	15, 34, 50, 81	1 (0%)
1	F	413/414 (99%)	-0.40	0 100 100	15, 32, 47, 85	2 (0%)
All	All	2459/2484 (98%)	-0.09	29 (1%) 76 80	13, 37, 86, 128	5 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	LEU	4.8
1	E	0	ALA	3.5
1	D	302	VAL	3.4
1	D	319	ALA	3.4
1	D	238	ILE	3.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

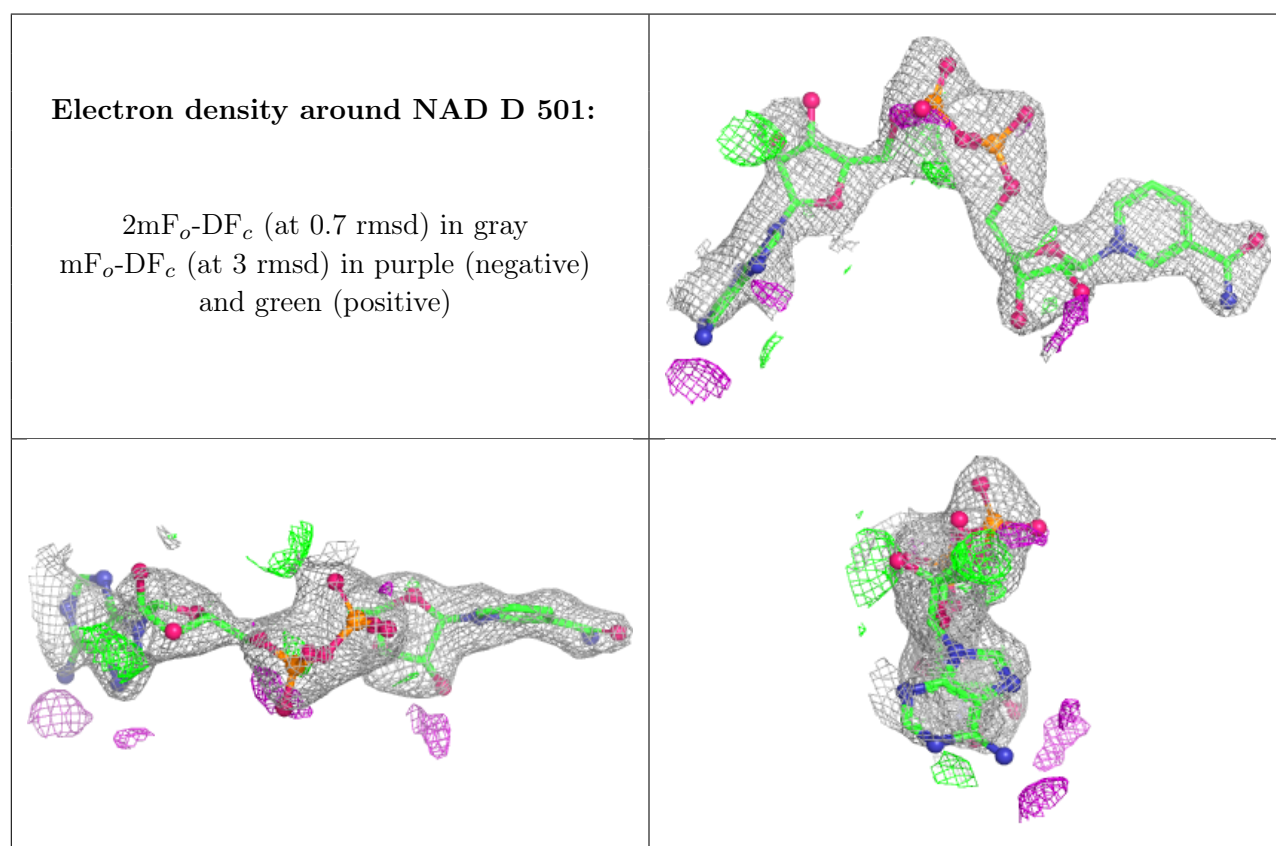
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	E	1106	4/4	0.68	0.19	44,53,55,60	0
3	EDO	A	606	4/4	0.76	0.15	46,50,52,65	0
4	PEG	A	603	7/7	0.77	0.15	53,55,59,64	0
3	EDO	B	505	4/4	0.78	0.15	49,49,51,53	0
3	EDO	F	604	4/4	0.78	0.14	48,54,59,60	0
3	EDO	D	502	4/4	0.78	0.14	52,56,58,60	0
3	EDO	C	503	4/4	0.79	0.14	53,54,58,65	0
3	EDO	D	504	4/4	0.79	0.16	46,48,52,54	0
3	EDO	E	1103	4/4	0.79	0.16	45,50,50,51	0
3	EDO	B	503	4/4	0.80	0.12	56,59,62,62	0
3	EDO	F	602	4/4	0.80	0.14	37,43,50,57	0
5	NAD	D	501	44/44	0.81	0.13	51,65,95,98	44
3	EDO	A	607	4/4	0.82	0.12	56,57,58,64	0
3	EDO	A	604	4/4	0.82	0.13	54,56,57,58	0
9	PG4	F	605	13/13	0.82	0.13	50,54,60,61	0
2	MPD	A	601	8/8	0.83	0.17	50,52,58,65	0
3	EDO	B	502	4/4	0.83	0.14	45,47,48,55	0
3	EDO	E	1101	4/4	0.84	0.12	55,57,58,61	0
8	PGE	E	1105	10/10	0.86	0.11	41,50,57,61	0
3	EDO	E	1107	4/4	0.86	0.13	50,50,51,53	0
5	NAD	B	501	44/44	0.87	0.10	55,67,81,83	0
3	EDO	E	1104	4/4	0.87	0.12	38,42,46,55	0
3	EDO	A	605	4/4	0.87	0.12	43,46,48,49	0
3	EDO	B	504	4/4	0.87	0.14	42,43,48,56	0
3	EDO	C	502	4/4	0.89	0.12	35,47,50,57	0
3	EDO	F	603	4/4	0.89	0.10	39,39,57,59	0
3	EDO	D	503	4/4	0.90	0.12	43,44,47,60	0
3	EDO	A	602	4/4	0.92	0.11	38,43,46,51	0
5	NAD	C	501	44/44	0.93	0.08	36,45,51,55	44
6	NA	C	505	1/1	0.93	0.11	57,57,57,57	0
6	NA	B	506	1/1	0.96	0.06	32,32,32,32	0
5	NAD	A	608	44/44	0.96	0.07	30,39,45,47	0
6	NA	A	609	1/1	0.96	0.11	35,35,35,35	0
6	NA	A	610	1/1	0.96	0.07	58,58,58,58	0
6	NA	C	504	1/1	0.97	0.05	35,35,35,35	0
6	NA	D	505	1/1	0.98	0.05	34,34,34,34	0
6	NA	E	1109	1/1	0.98	0.05	31,31,31,31	0

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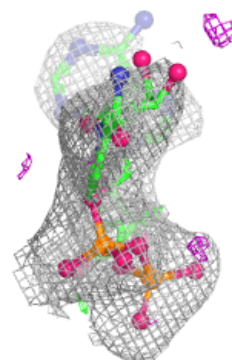
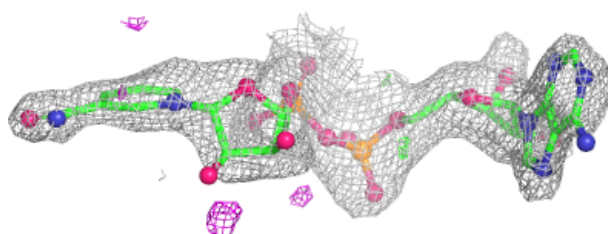
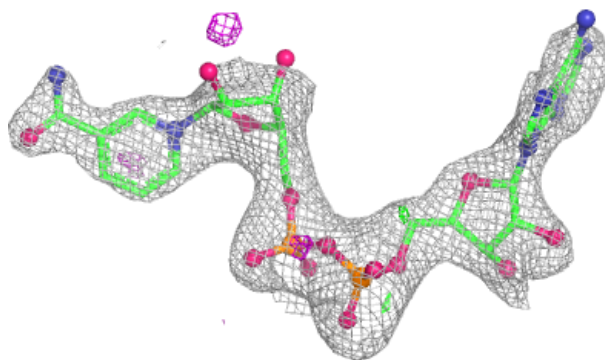
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PDC	E	1102	12/12	0.98	0.04	25,28,31,31	0
7	PDC	F	601	12/12	0.98	0.04	23,25,28,29	0
5	NAD	F	606	44/44	0.98	0.05	22,27,33,36	0
5	NAD	E	1108	44/44	0.98	0.04	24,29,34,36	0
6	NA	F	607	1/1	0.99	0.05	30,30,30,30	0

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.

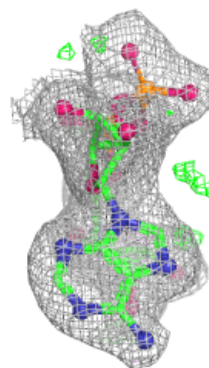
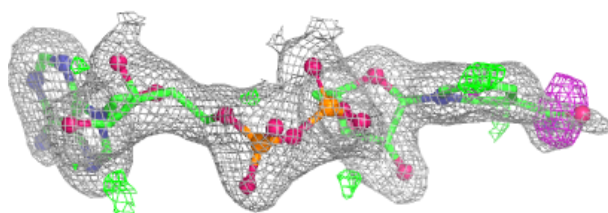
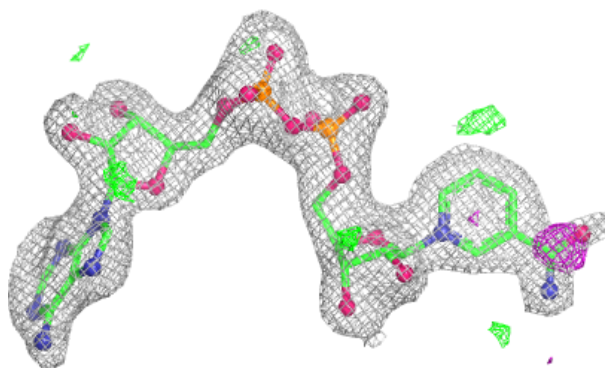


Electron density around NAD B 501:

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

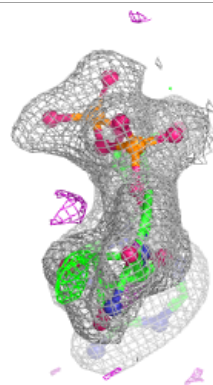
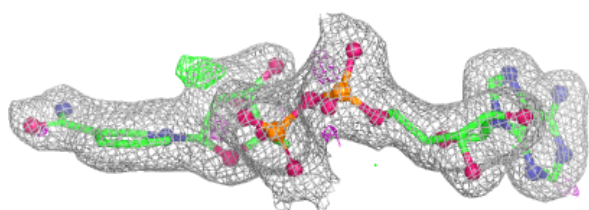
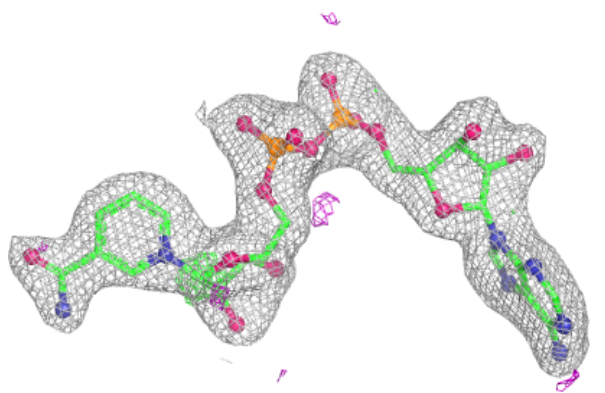
**Electron density around NAD C 501:**

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



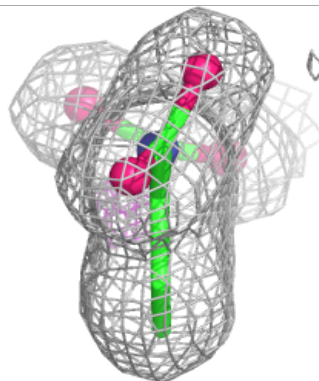
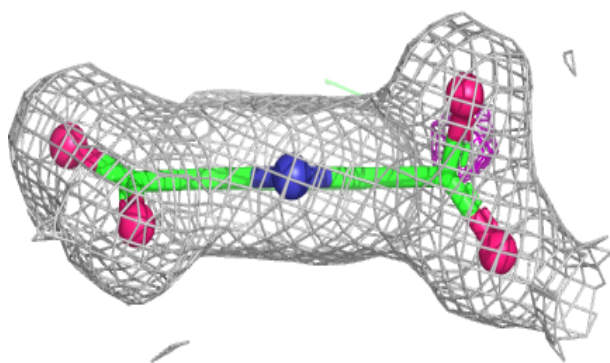
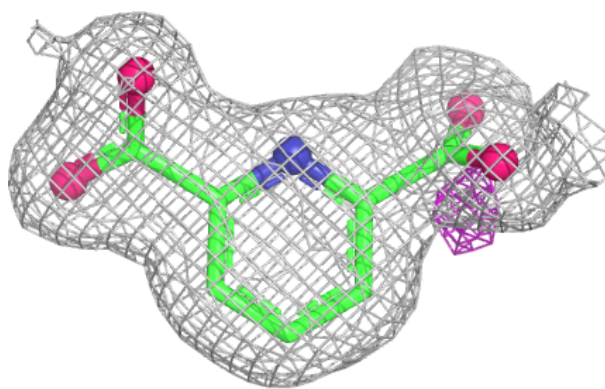
Electron density around NAD A 608:

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



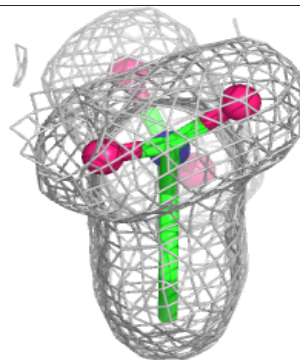
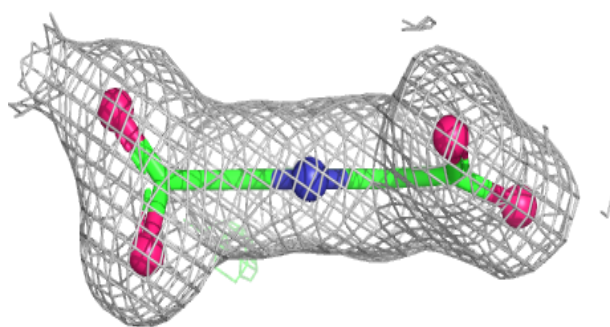
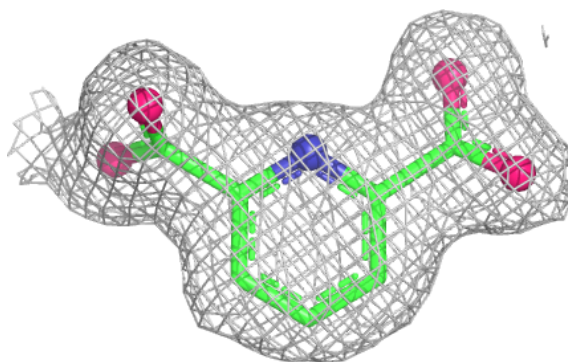
Electron density around PDC E 1102:

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

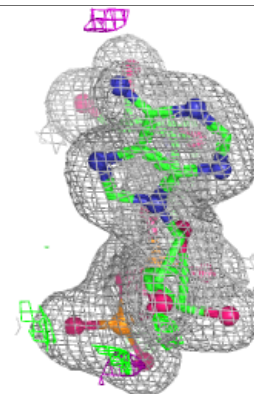
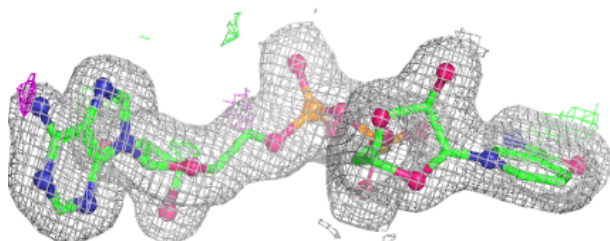
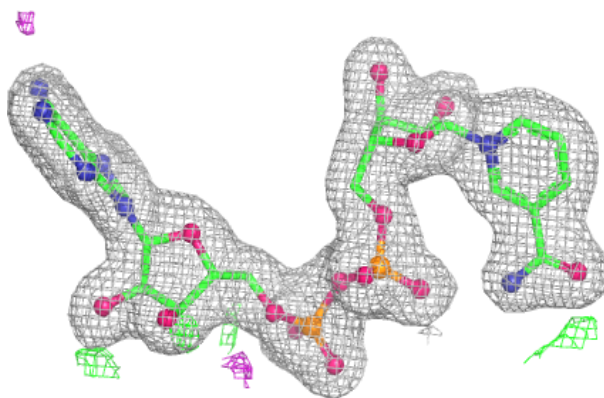


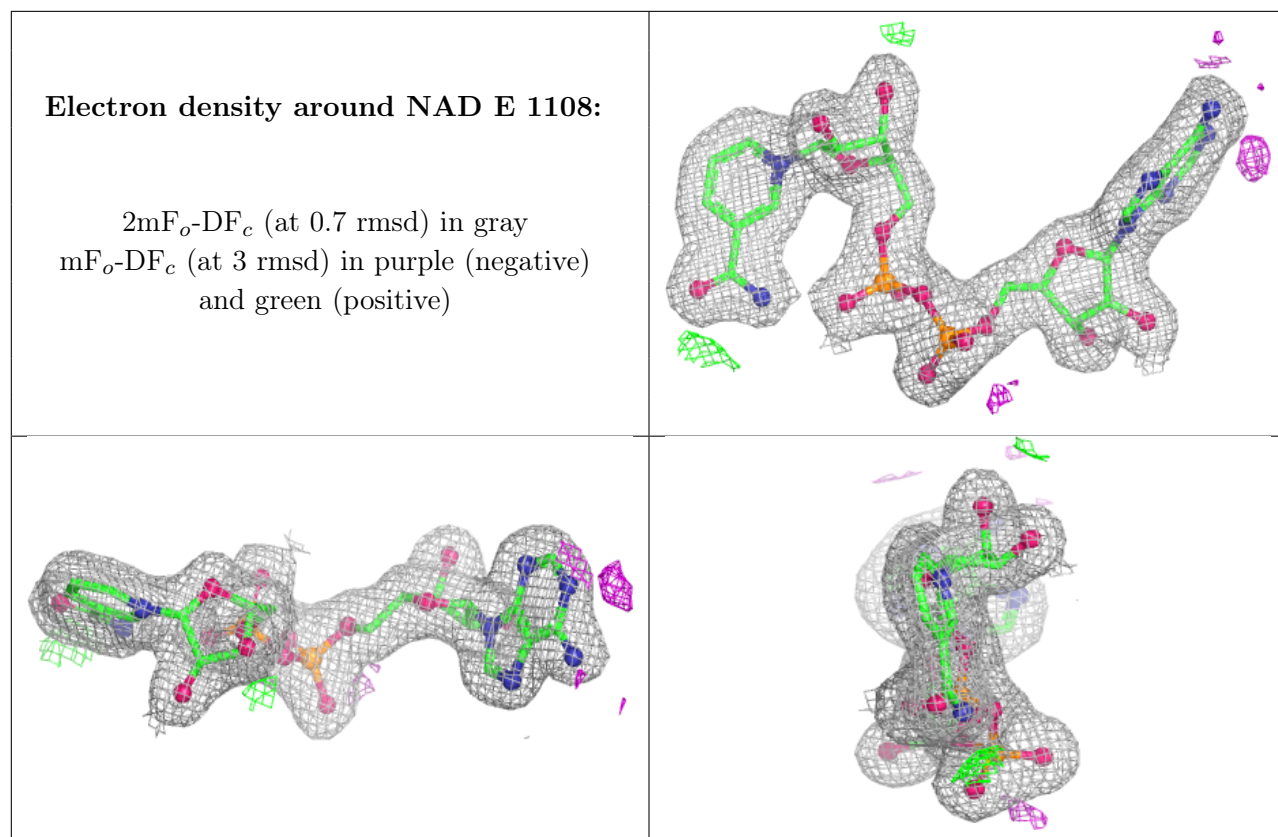
Electron density around PDC F 601:

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

**Electron density around NAD F 606:**

$2mF_o-DF_c$ (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.