wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 09:52 AM JST

PDB ID	:	6LLA
Title	:	Crystal structure of Providencia alcalifaciens 3-dehydroquinate synthase (DHQS) in complex with Mg2+ and NAD
Authors	:	Neetu, N.; Katiki, M.; Kumar, P.
Deposited on	:	2019-12-22
Resolution	:	1.88 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 (i) 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 (i)) were used in the production of this report:

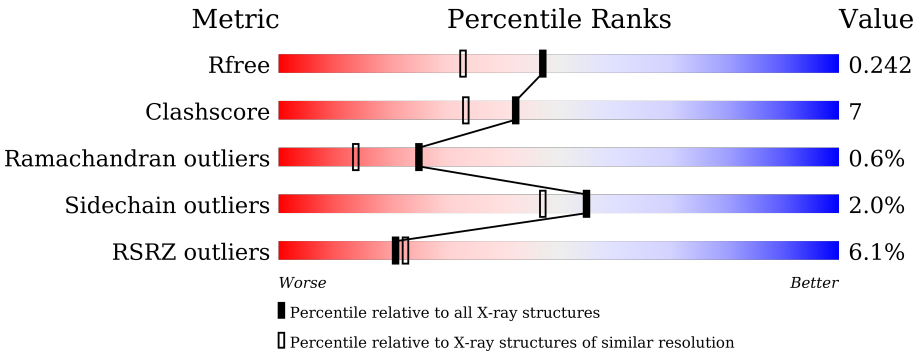
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	375	4% 84% 10%
1	B	375	3% 84% 11%
1	C	375	11% 78% 15% 6%
1	D	375	6% 83% 11% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	411	-	-	X	-
4	EDO	C	403	-	-	-	X
5	PEG	A	415	-	-	X	-
5	PEG	B	413	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12432 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 3-dehydroquinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	3	0
			2786	1769	470	528	19			
1	B	363	Total	C	N	O	S	0	3	0
			2787	1769	470	529	19			
1	C	354	Total	C	N	O	S	0	0	0
			2697	1717	453	510	17			
1	D	353	Total	C	N	O	S	0	1	0
			2701	1719	454	511	17			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP X6Q997
A	-11	HIS	-	expression tag	UNP X6Q997
A	-10	HIS	-	expression tag	UNP X6Q997
A	-9	HIS	-	expression tag	UNP X6Q997
A	-8	HIS	-	expression tag	UNP X6Q997
A	-7	HIS	-	expression tag	UNP X6Q997
A	-6	GLU	-	expression tag	UNP X6Q997
A	-5	ASN	-	expression tag	UNP X6Q997
A	-4	LEU	-	expression tag	UNP X6Q997
A	-3	TYR	-	expression tag	UNP X6Q997
A	-2	PHE	-	expression tag	UNP X6Q997
A	-1	GLN	-	expression tag	UNP X6Q997
A	0	GLY	-	expression tag	UNP X6Q997
B	-12	HIS	-	expression tag	UNP X6Q997
B	-11	HIS	-	expression tag	UNP X6Q997
B	-10	HIS	-	expression tag	UNP X6Q997
B	-9	HIS	-	expression tag	UNP X6Q997
B	-8	HIS	-	expression tag	UNP X6Q997
B	-7	HIS	-	expression tag	UNP X6Q997
B	-6	GLU	-	expression tag	UNP X6Q997
B	-5	ASN	-	expression tag	UNP X6Q997

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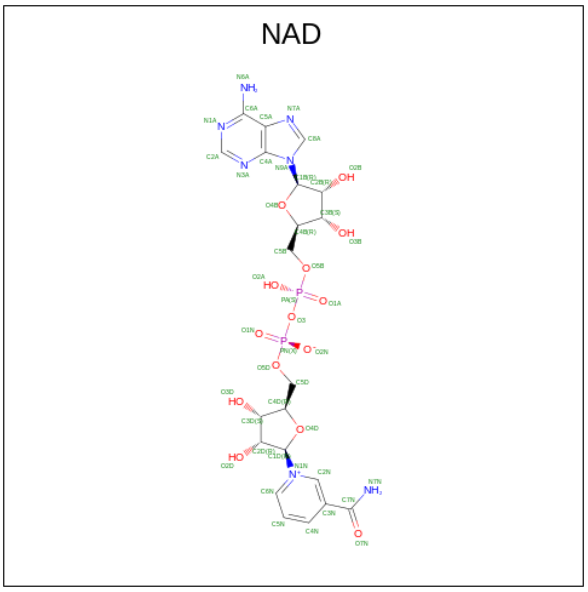
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	LEU	-	expression tag	UNP X6Q997
B	-3	TYR	-	expression tag	UNP X6Q997
B	-2	PHE	-	expression tag	UNP X6Q997
B	-1	GLN	-	expression tag	UNP X6Q997
B	0	GLY	-	expression tag	UNP X6Q997
C	-12	HIS	-	expression tag	UNP X6Q997
C	-11	HIS	-	expression tag	UNP X6Q997
C	-10	HIS	-	expression tag	UNP X6Q997
C	-9	HIS	-	expression tag	UNP X6Q997
C	-8	HIS	-	expression tag	UNP X6Q997
C	-7	HIS	-	expression tag	UNP X6Q997
C	-6	GLU	-	expression tag	UNP X6Q997
C	-5	ASN	-	expression tag	UNP X6Q997
C	-4	LEU	-	expression tag	UNP X6Q997
C	-3	TYR	-	expression tag	UNP X6Q997
C	-2	PHE	-	expression tag	UNP X6Q997
C	-1	GLN	-	expression tag	UNP X6Q997
C	0	GLY	-	expression tag	UNP X6Q997
D	-12	HIS	-	expression tag	UNP X6Q997
D	-11	HIS	-	expression tag	UNP X6Q997
D	-10	HIS	-	expression tag	UNP X6Q997
D	-9	HIS	-	expression tag	UNP X6Q997
D	-8	HIS	-	expression tag	UNP X6Q997
D	-7	HIS	-	expression tag	UNP X6Q997
D	-6	GLU	-	expression tag	UNP X6Q997
D	-5	ASN	-	expression tag	UNP X6Q997
D	-4	LEU	-	expression tag	UNP X6Q997
D	-3	TYR	-	expression tag	UNP X6Q997
D	-2	PHE	-	expression tag	UNP X6Q997
D	-1	GLN	-	expression tag	UNP X6Q997
D	0	GLY	-	expression tag	UNP X6Q997

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

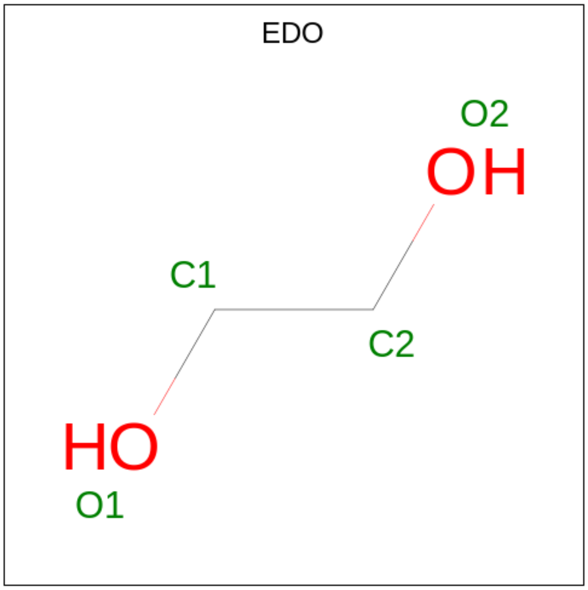


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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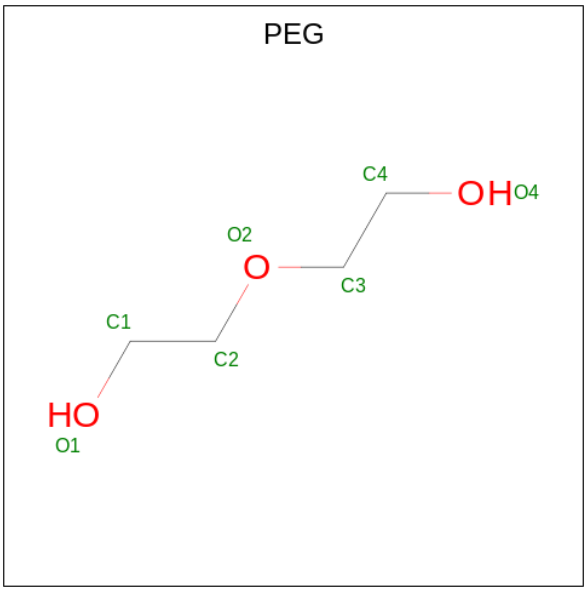
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	342	Total O 342 342	0	0
6	B	341	Total O 341 341	0	0
6	C	178	Total O 178 178	0	0

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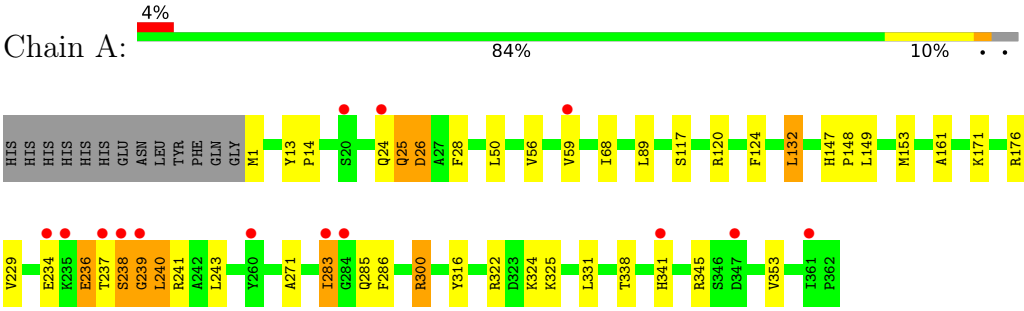
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	233	Total 233	O 233	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

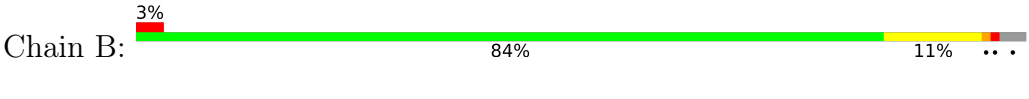
• Molecule 1: 3-dehydroquinate synthase

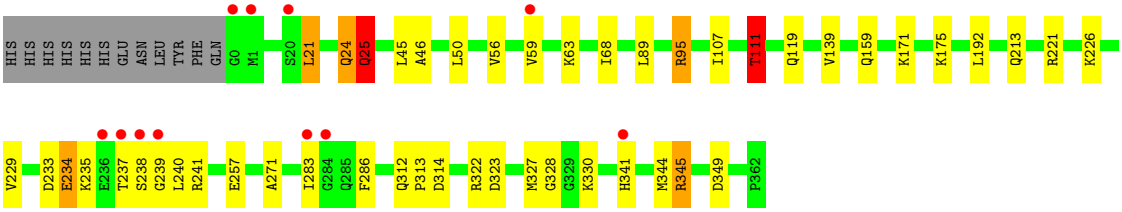
Chain A:



• Molecule 1: 3-dehydroquinate synthase

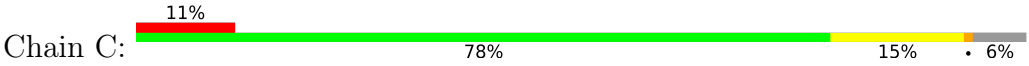
Chain B:

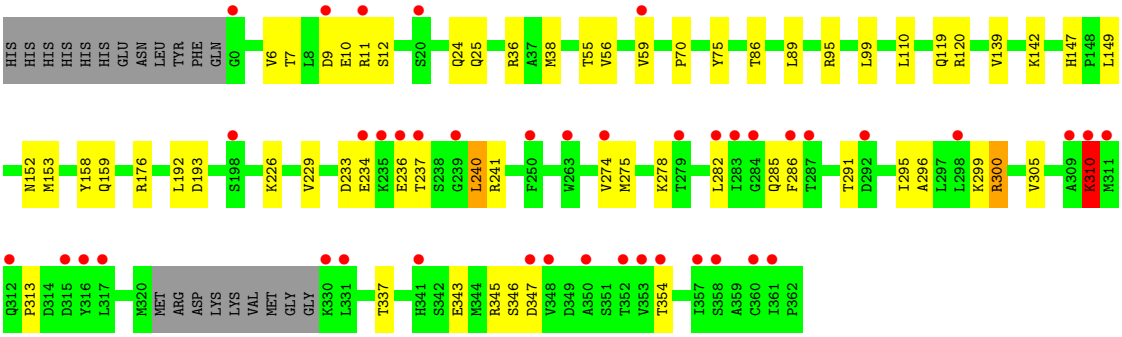




• Molecule 1: 3-dehydroquinate synthase

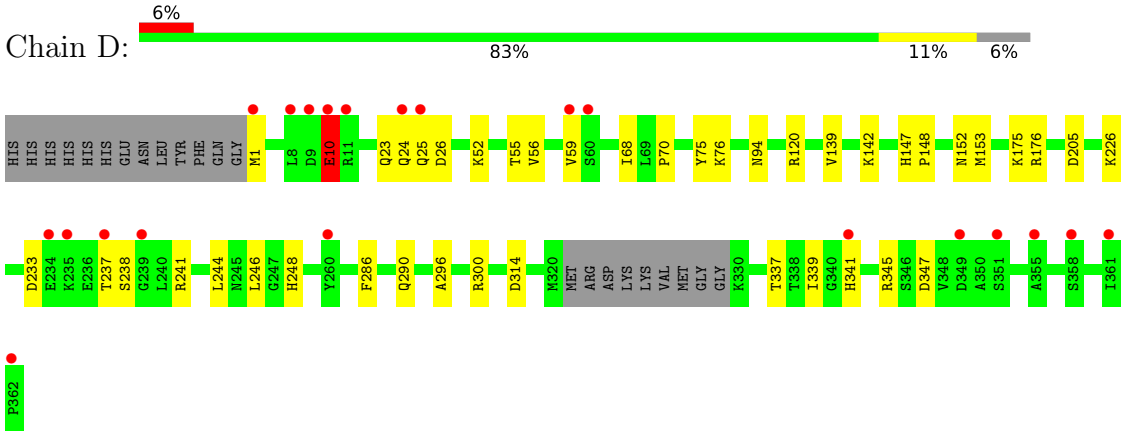
Chain C:





• Molecule 1: 3-dehydroquinate synthase

Chain D:


6%
83%
11%
6%
HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY M1 L8 D9 E10 R11 Q23 Q24 Q25 D26 K52 T55 V56 V59 S60 I68 L69 P70 Y75 K76 N94 R120 V139 K142 H147 P148 N152 M153 K175 R176 D205 K226
D233 E234 K235 E236 T237 S238 G239 L240 R241 L244 N245 L246 G247 H248 Y260 F286 Q290 A296 R300 D314 M320 MET ARG ASP LYS LYS VAL MET GLY GLY K330 T337 I338 I339 G340 H341 R345 S346 D347 V348 D349 A350 S351 A365 S358 I361
P362

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.39Å 59.92Å 143.80Å 90.00° 93.95° 90.00°	Depositor
Resolution (Å)	143.46 – 1.88 89.18 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.9 (143.46-1.88) 98.9 (89.18-1.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.173 , 0.238 0.181 , 0.242	Depositor DCC
R_{free} test set	6015 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12432	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, PEG, NAD, 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	1.05	6/2837 (0.2%)	0.91	4/3851 (0.1%)
1	B	1.09	3/2838 (0.1%)	0.96	7/3851 (0.2%)
1	C	0.81	0/2747	0.91	11/3731 (0.3%)
1	D	0.82	0/2751	0.88	7/3737 (0.2%)
All	All	0.96	9/11173 (0.1%)	0.92	29/15170 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	THR	CB-CG2	-6.69	1.30	1.52
1	B	271	ALA	CA-CB	5.93	1.65	1.52
1	A	117	SER	CB-OG	-5.72	1.34	1.42
1	A	188	TYR	CG-CD2	-5.65	1.31	1.39
1	A	271	ALA	CA-CB	5.54	1.64	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	310	LYS	CA-CB-CG	10.71	136.95	113.40
1	C	310	LYS	N-CA-CB	-10.06	92.50	110.60
1	C	310	LYS	CB-CG-CD	-9.33	87.33	111.60
1	D	314	ASP	CB-CA-C	-7.91	94.58	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	10	GLU	CA-CB-CG	-7.37	97.19	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	234	GLU	Peptide

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	2786	0	2816	48	0
1	B	2787	0	2815	42	0
1	C	2697	0	2728	48	0
1	D	2701	0	2730	28	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	44	0	66	4	0
4	B	40	0	60	5	0
4	C	16	0	24	5	0
4	D	24	0	36	5	0
5	A	42	0	60	12	0
5	B	14	0	20	6	0
5	C	7	0	10	2	0
6	A	342	0	0	10	0
6	B	341	0	0	13	1
6	C	178	0	0	5	0
6	D	233	0	0	4	1
All	All	12432	0	11469	158	1

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 7.

The worst 5 of 158 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:89:LEU:HD21	1:C:153:MET:HE2	1.13	1.09
1:A:322:ARG:NH2	6:A:501:HOH:O	1.87	1.05
1:A:89:LEU:HD21	1:C:153:MET:CE	1.93	0.98
1:B:313:PRO:HB2	5:B:413:PEG:H42	1.54	0.88
1:A:120:ARG:HH12	4:C:406:EDO:H22	1.39	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:593:HOH:O	6:D:659:HOH:O[2_545]	2.15	0.05

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	363/375 (97%)	350 (96%)	9 (2%)	4 (1%)	14 5
1	B	364/375 (97%)	355 (98%)	8 (2%)	1 (0%)	41 30
1	C	350/375 (93%)	343 (98%)	6 (2%)	1 (0%)	41 30
1	D	350/375 (93%)	339 (97%)	9 (3%)	2 (1%)	25 14
All	All	1427/1500 (95%)	1387 (97%)	32 (2%)	8 (1%)	25 14

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLN

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Mol	Chain	Res	Type
1	A	238	SER
1	C	237	THR
1	A	236	GLU
1	B	25	GLN

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	300/309 (97%)	295 (98%)	5 (2%)	60	54
1	B	300/309 (97%)	291 (97%)	9 (3%)	41	30
1	C	290/309 (94%)	284 (98%)	6 (2%)	53	45
1	D	291/309 (94%)	287 (99%)	4 (1%)	67	62
All	All	1181/1236 (96%)	1157 (98%)	24 (2%)	55	47

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	95	ARG
1	C	285	GLN
1	C	240	LEU
1	C	286	PHE
1	B	24	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	119	GLN
1	D	248	HIS
1	C	147	HIS
1	D	341	HIS
1	D	23	GLN

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 48 ligands modelled in this entry, 4 are monoatomic - leaving 44 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	NAD	B	401	-	42,48,48	1.52	6 (14%)	50,73,73	1.60	6 (12%)
4	EDO	D	407	-	3,3,3	0.49	0	2,2,2	0.54	0
4	EDO	D	408	-	3,3,3	0.68	0	2,2,2	0.19	0
4	EDO	A	411	-	3,3,3	0.64	0	2,2,2	0.28	0
2	NAD	C	401	-	42,48,48	1.62	9 (21%)	50,73,73	0.90	2 (4%)
4	EDO	C	403	-	3,3,3	0.62	0	2,2,2	0.26	0
5	PEG	A	419	-	6,6,6	0.87	0	5,5,5	0.71	0
4	EDO	D	403	-	3,3,3	0.45	0	2,2,2	0.19	0
4	EDO	A	408	-	3,3,3	0.57	0	2,2,2	0.32	0
4	EDO	B	411	-	3,3,3	0.94	0	2,2,2	0.82	0
4	EDO	B	404	-	3,3,3	0.86	0	2,2,2	0.41	0
5	PEG	C	407	-	6,6,6	0.55	0	5,5,5	0.47	0
5	PEG	A	415	-	6,6,6	0.71	0	5,5,5	0.77	0
4	EDO	A	405	-	3,3,3	0.82	0	2,2,2	0.14	0
4	EDO	D	406	-	3,3,3	0.40	0	2,2,2	0.30	0
4	EDO	B	406	-	3,3,3	0.63	0	2,2,2	0.67	0
4	EDO	A	409	-	3,3,3	0.28	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	A	401	-	42,48,48	1.67	6 (14%)	50,73,73	1.46	7 (14%)
4	EDO	B	409	-	3,3,3	0.65	0	2,2,2	0.26	0
4	EDO	A	407	-	3,3,3	0.65	0	2,2,2	0.75	0
4	EDO	C	406	-	3,3,3	0.47	0	2,2,2	1.11	0
5	PEG	A	417	-	6,6,6	0.51	0	5,5,5	0.70	0
4	EDO	A	412	-	3,3,3	0.44	0	2,2,2	0.25	0
4	EDO	C	405	-	3,3,3	0.24	0	2,2,2	0.78	0
4	EDO	A	410	-	3,3,3	0.38	0	2,2,2	0.46	0
4	EDO	B	407	-	3,3,3	0.41	0	2,2,2	0.96	0
4	EDO	A	404	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	B	405	-	3,3,3	0.58	0	2,2,2	0.55	0
4	EDO	A	403	-	3,3,3	0.51	0	2,2,2	0.44	0
4	EDO	B	412	-	3,3,3	0.35	0	2,2,2	0.48	0
4	EDO	B	410	-	3,3,3	0.51	0	2,2,2	0.80	0
4	EDO	A	406	-	3,3,3	0.43	0	2,2,2	0.77	0
4	EDO	D	404	-	3,3,3	0.37	0	2,2,2	0.96	0
2	NAD	D	401	-	42,48,48	1.61	4 (9%)	50,73,73	1.38	4 (8%)
5	PEG	A	416	-	6,6,6	0.47	0	5,5,5	0.60	0
4	EDO	B	403	-	3,3,3	0.60	0	2,2,2	0.47	0
5	PEG	A	418	-	6,6,6	0.56	0	5,5,5	0.62	0
4	EDO	C	404	-	3,3,3	0.71	0	2,2,2	1.00	0
5	PEG	A	414	-	6,6,6	0.74	0	5,5,5	0.89	0
4	EDO	A	413	-	3,3,3	0.58	0	2,2,2	0.06	0
4	EDO	B	408	-	3,3,3	0.49	0	2,2,2	0.18	0
4	EDO	D	405	-	3,3,3	0.27	0	2,2,2	0.67	0
5	PEG	B	413	-	6,6,6	0.53	0	5,5,5	1.33	1 (20%)
5	PEG	B	414	-	6,6,6	0.68	0	5,5,5	0.51	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	NAD	B	401	-	-	3/26/62/62	0/5/5/5
4	EDO	D	407	-	-	1/1/1/1	-
4	EDO	D	408	-	-	0/1/1/1	-
4	EDO	A	411	-	-	1/1/1/1	-
2	NAD	C	401	-	-	2/26/62/62	0/5/5/5
4	EDO	C	403	-	-	0/1/1/1	-
5	PEG	A	419	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	403	-	-	0/1/1/1	-
4	EDO	A	408	-	-	1/1/1/1	-
4	EDO	B	411	-	-	1/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
5	PEG	C	407	-	-	3/4/4/4	-
5	PEG	A	415	-	-	2/4/4/4	-
4	EDO	A	405	-	-	0/1/1/1	-
4	EDO	D	406	-	-	1/1/1/1	-
4	EDO	B	406	-	-	1/1/1/1	-
4	EDO	A	409	-	-	1/1/1/1	-
2	NAD	A	401	-	-	1/26/62/62	0/5/5/5
4	EDO	B	409	-	-	0/1/1/1	-
4	EDO	A	407	-	-	1/1/1/1	-
4	EDO	C	406	-	-	1/1/1/1	-
5	PEG	A	417	-	-	3/4/4/4	-
4	EDO	A	412	-	-	1/1/1/1	-
4	EDO	C	405	-	-	0/1/1/1	-
4	EDO	A	410	-	-	0/1/1/1	-
4	EDO	B	407	-	-	0/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	B	405	-	-	1/1/1/1	-
4	EDO	A	403	-	-	1/1/1/1	-
4	EDO	B	412	-	-	1/1/1/1	-
4	EDO	B	410	-	-	0/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	D	404	-	-	0/1/1/1	-
2	NAD	D	401	-	-	1/26/62/62	0/5/5/5
5	PEG	A	416	-	-	1/4/4/4	-
4	EDO	B	403	-	-	1/1/1/1	-
5	PEG	A	418	-	-	1/4/4/4	-
4	EDO	C	404	-	-	1/1/1/1	-
5	PEG	A	414	-	-	2/4/4/4	-
4	EDO	A	413	-	-	1/1/1/1	-
4	EDO	B	408	-	-	1/1/1/1	-
4	EDO	D	405	-	-	1/1/1/1	-
5	PEG	B	413	-	-	1/4/4/4	-
5	PEG	B	414	-	-	2/4/4/4	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	O4B-C1B	6.46	1.50	1.41
2	D	401	NAD	C2D-C1D	-5.69	1.45	1.53
2	C	401	NAD	O4B-C1B	4.59	1.47	1.41
2	D	401	NAD	O4B-C1B	4.56	1.47	1.41
2	C	401	NAD	C2B-C1B	-4.50	1.46	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	NAD	N3A-C2A-N1A	-6.13	119.10	128.68
2	D	401	NAD	C5A-C6A-N6A	5.17	128.21	120.35
2	A	401	NAD	N3A-C2A-N1A	-4.57	121.54	128.68
2	B	401	NAD	O7N-C7N-N7N	-4.45	116.26	122.58
2	A	401	NAD	O4B-C1B-C2B	-4.44	100.44	106.93

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C6N
5	B	413	PEG	C1-C2-O2-C3

There are no ring outliers.

18 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	407	EDO	1	0
5	A	419	PEG	2	0
4	D	403	EDO	2	0
4	B	411	EDO	4	0
5	C	407	PEG	2	0
5	A	415	PEG	5	0
4	C	406	EDO	3	0
5	A	417	PEG	1	0
4	B	407	EDO	1	0
4	A	406	EDO	2	0
4	D	404	EDO	2	0
5	A	416	PEG	1	0
5	A	418	PEG	2	0

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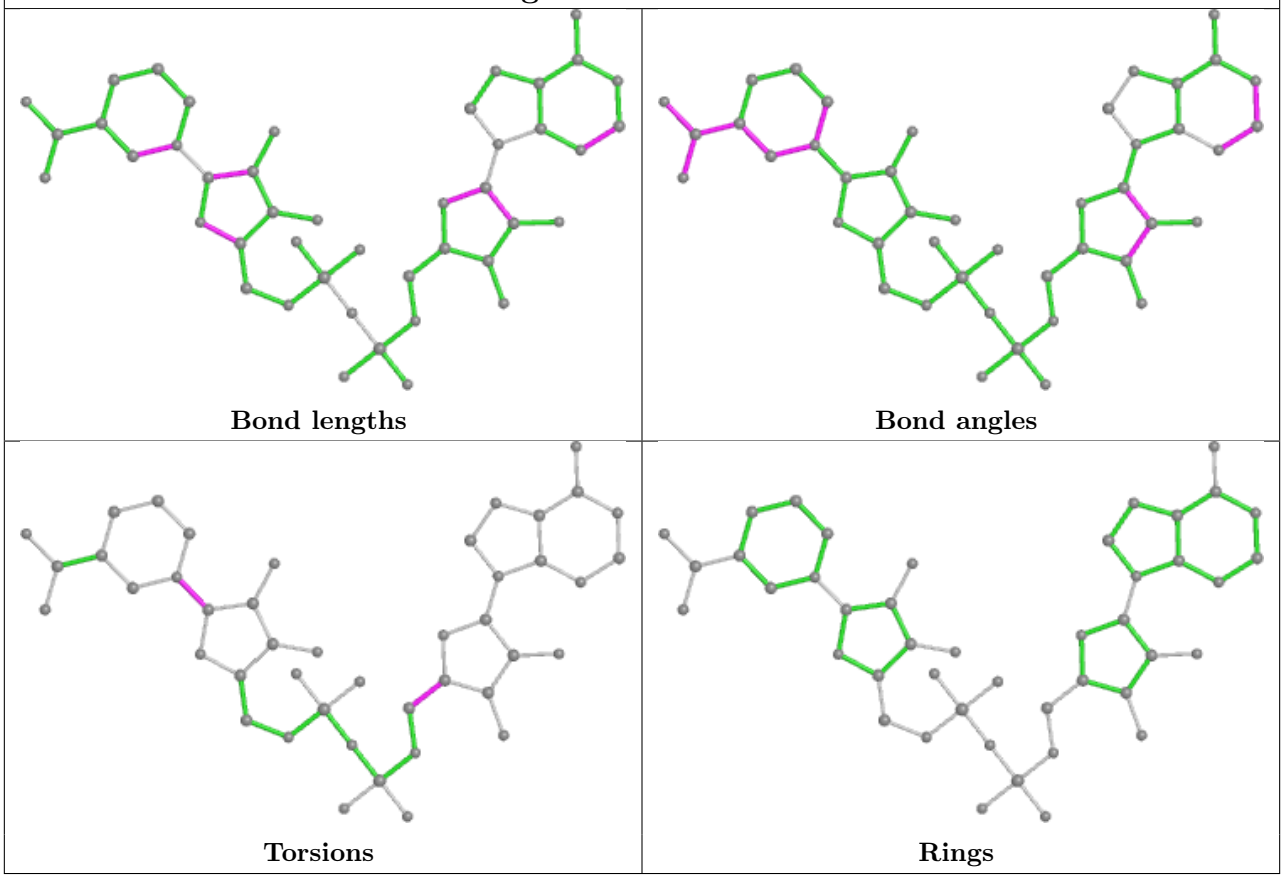
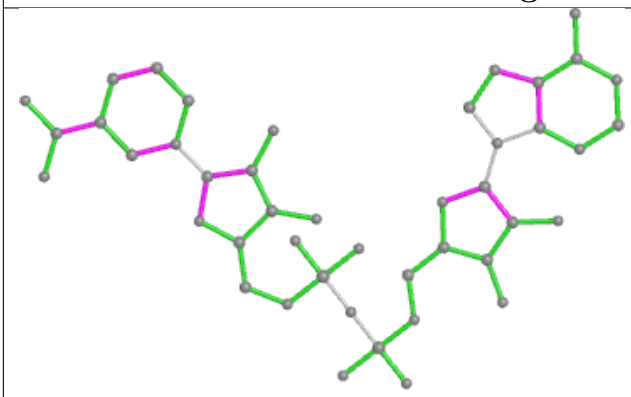
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	EDO	2	0
5	A	414	PEG	1	0
4	A	413	EDO	2	0
5	B	413	PEG	5	0
5	B	414	PEG	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

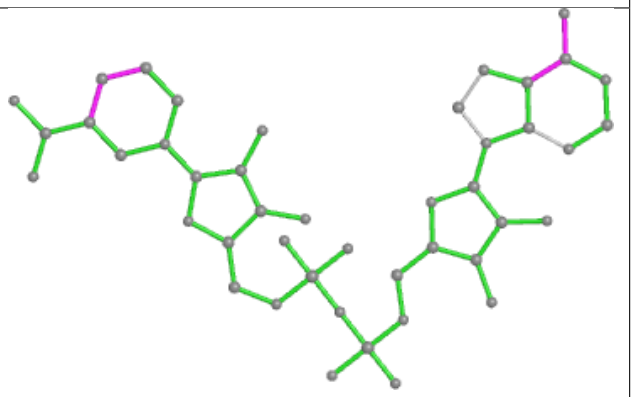
Ligand NAD B 401



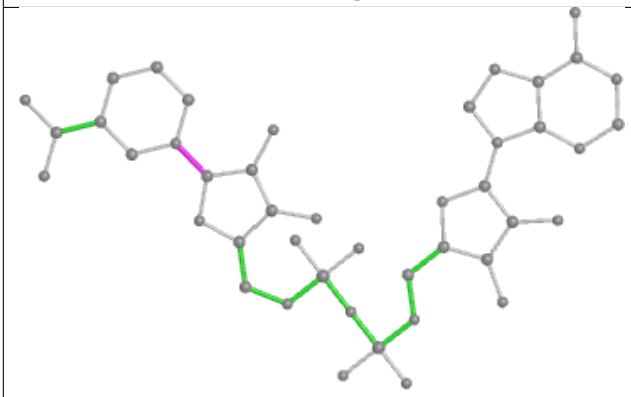
Ligand NAD C 401



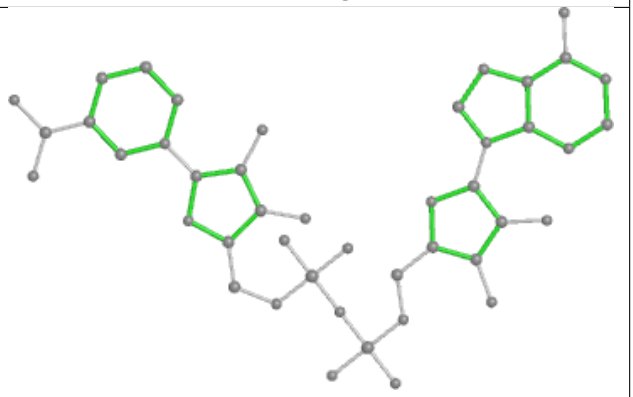
Bond lengths



Bond angles

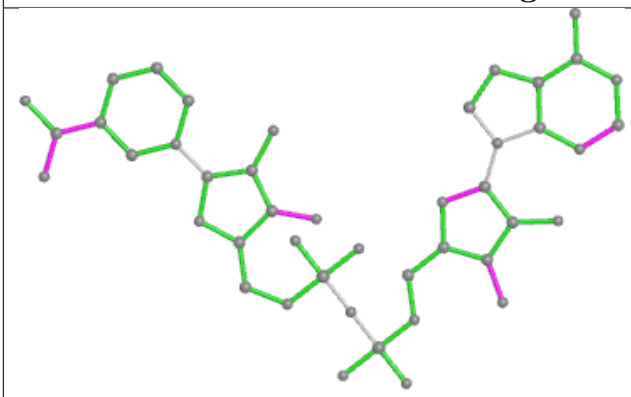


Torsions

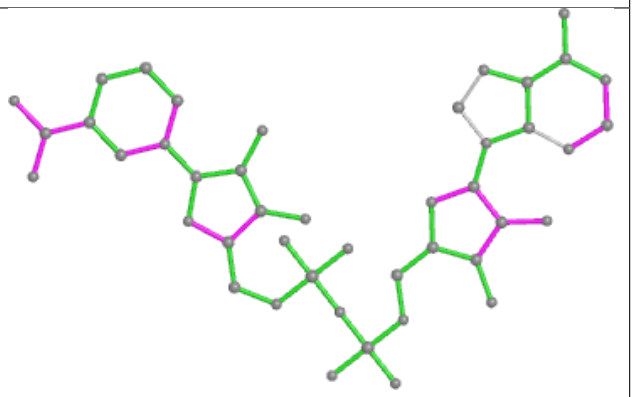


Rings

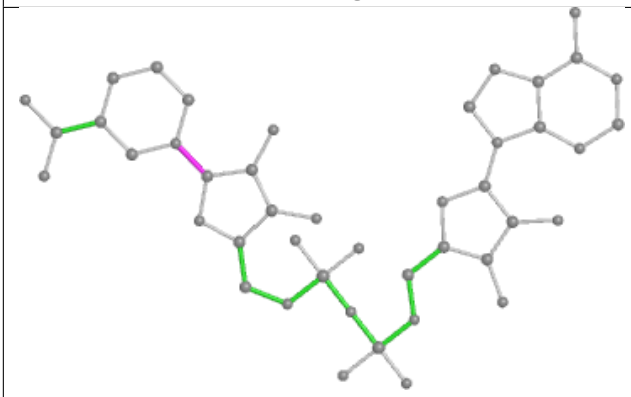
Ligand NAD A 401



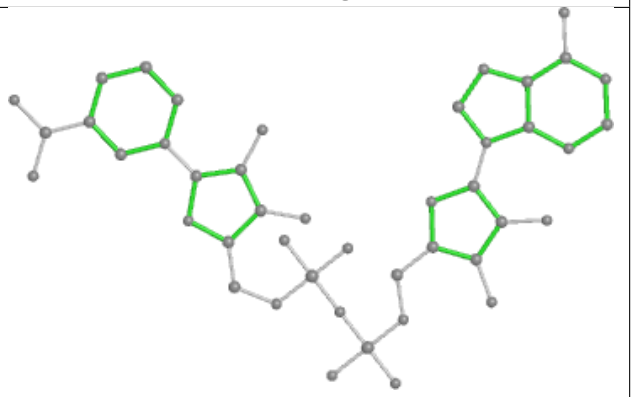
Bond lengths



Bond angles

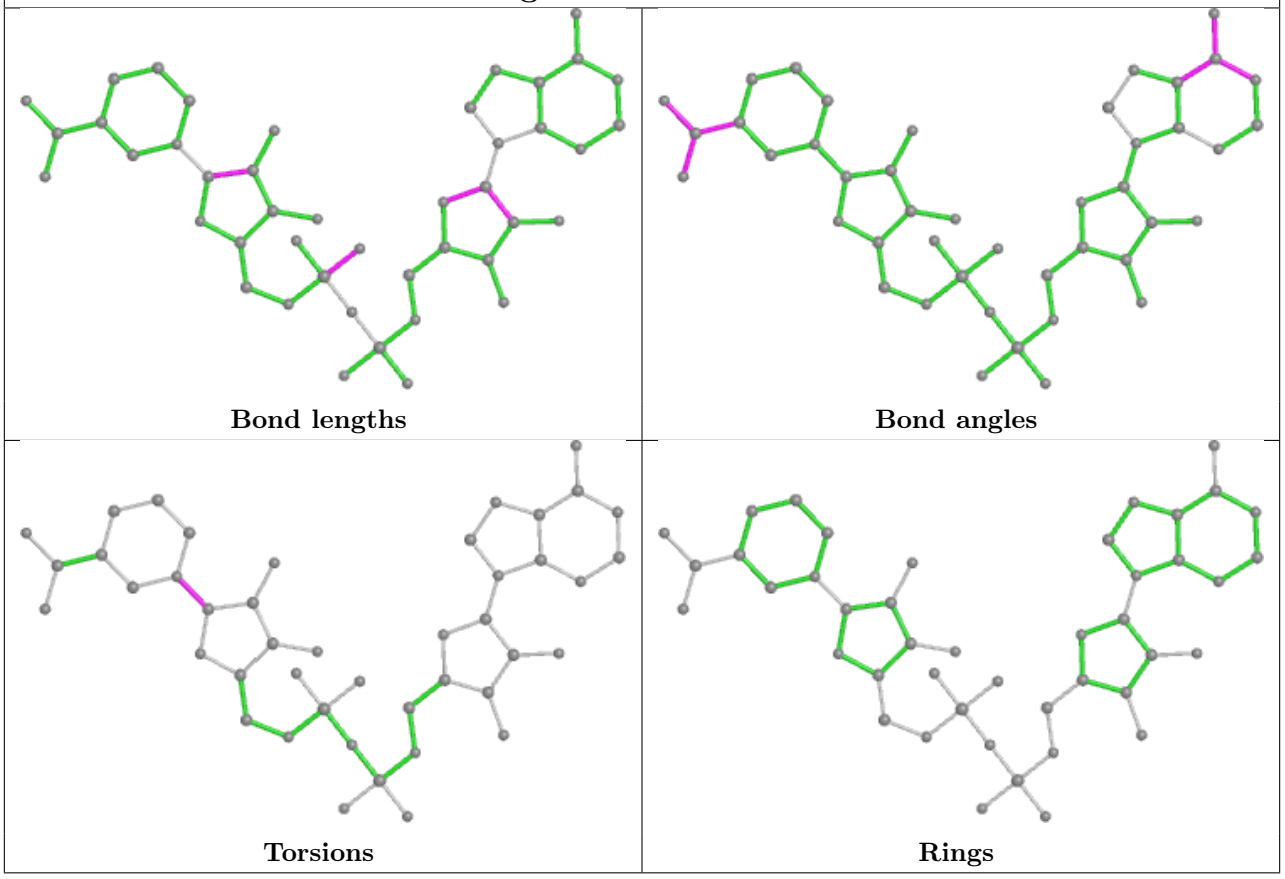


Torsions



Rings

Ligand NAD D 401



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, 95^{th} 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	362/375 (96%)	0.17	14 (3%)	39	41	20, 28, 51, 114	0
1	B	363/375 (96%)	0.14	11 (3%)	50	51	18, 27, 52, 106	0
1	C	354/375 (94%)	0.65	42 (11%)	4	4	21, 51, 101, 130	0
1	D	353/375 (94%)	0.40	21 (5%)	22	24	22, 43, 80, 110	0
All	All	1432/1500 (95%)	0.34	88 (6%)	21	22	18, 35, 87, 130	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	362	PRO	10.6
1	A	235	LYS	8.5
1	C	361	ILE	7.5
1	A	260	TYR	6.8
1	A	237	THR	6.3

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, 95^{th} 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
4	EDO	C	403	4/4	0.55	0.43	65,72,81,84	0
4	EDO	A	413	4/4	0.66	0.19	58,64,76,77	0
5	PEG	A	416	7/7	0.72	0.26	58,64,75,79	0
4	EDO	B	409	4/4	0.75	0.23	66,69,77,78	0
4	EDO	A	405	4/4	0.76	0.20	54,59,60,61	0
4	EDO	B	410	4/4	0.78	0.23	54,58,70,93	0
5	PEG	A	417	7/7	0.78	0.14	60,63,66,74	0
4	EDO	D	407	4/4	0.80	0.15	57,64,67,67	0
4	EDO	D	406	4/4	0.81	0.12	67,68,68,70	0
4	EDO	B	411	4/4	0.82	0.23	36,38,57,68	0
4	EDO	A	412	4/4	0.83	0.15	72,75,78,80	0
4	EDO	A	406	4/4	0.83	0.23	50,52,60,63	0
5	PEG	A	419	7/7	0.84	0.17	36,55,67,77	0
5	PEG	B	414	7/7	0.84	0.14	49,63,71,72	0
5	PEG	C	407	7/7	0.84	0.16	43,60,73,88	0
5	PEG	A	415	7/7	0.85	0.20	33,49,64,66	0
4	EDO	C	406	4/4	0.85	0.23	44,52,56,58	0
4	EDO	A	408	4/4	0.86	0.16	39,48,55,59	0
4	EDO	A	407	4/4	0.86	0.19	45,47,49,52	0
4	EDO	D	408	4/4	0.87	0.14	49,53,57,60	0
5	PEG	A	414	7/7	0.87	0.22	49,51,85,87	0
4	EDO	B	406	4/4	0.88	0.11	51,53,57,57	0
4	EDO	C	404	4/4	0.89	0.18	44,50,57,62	0
4	EDO	B	405	4/4	0.89	0.19	42,43,51,51	0
4	EDO	A	411	4/4	0.89	0.10	49,55,65,66	0
4	EDO	D	405	4/4	0.90	0.20	51,57,59,73	0
4	EDO	D	403	4/4	0.90	0.14	40,45,46,50	0
5	PEG	A	418	7/7	0.90	0.10	39,51,56,57	0
4	EDO	B	404	4/4	0.91	0.12	40,45,50,50	0
4	EDO	A	410	4/4	0.91	0.09	57,57,60,63	0
4	EDO	B	408	4/4	0.92	0.12	40,47,52,65	0
4	EDO	A	403	4/4	0.92	0.16	29,32,41,45	0
4	EDO	A	404	4/4	0.93	0.14	33,44,48,49	0
4	EDO	B	403	4/4	0.94	0.12	44,59,63,68	0
4	EDO	B	412	4/4	0.94	0.15	38,38,47,54	0
4	EDO	D	404	4/4	0.94	0.17	43,43,52,54	0
4	EDO	A	409	4/4	0.94	0.14	36,43,52,59	0
4	EDO	B	407	4/4	0.94	0.16	44,47,64,69	0
5	PEG	B	413	7/7	0.95	0.19	28,39,43,50	0
3	MG	C	402	1/1	0.96	0.05	41,41,41,41	0
2	NAD	A	401	44/44	0.96	0.11	17,26,33,37	0
2	NAD	B	401	44/44	0.96	0.10	18,25,29,33	0
4	EDO	C	405	4/4	0.96	0.11	58,62,69,71	0

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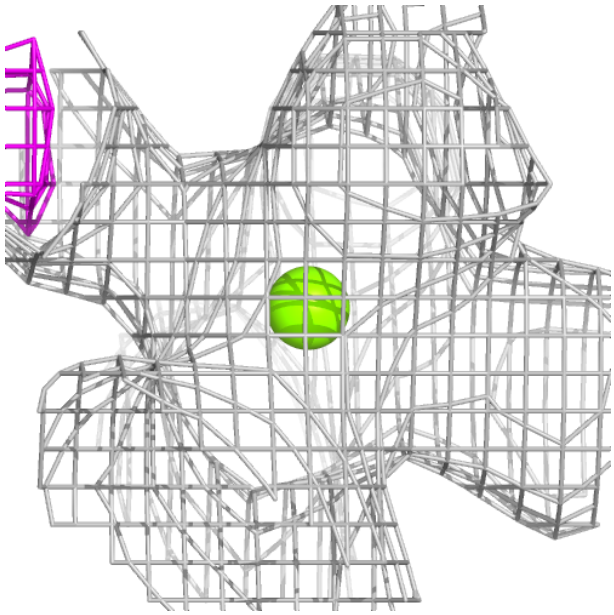
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	C	401	44/44	0.97	0.10	25,32,40,44	0
3	MG	D	402	1/1	0.97	0.06	28,28,28,28	0
2	NAD	D	401	44/44	0.98	0.10	25,28,33,39	0
3	MG	A	402	1/1	0.98	0.10	20,20,20,20	0
3	MG	B	402	1/1	0.98	0.09	21,21,21,21	0

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.

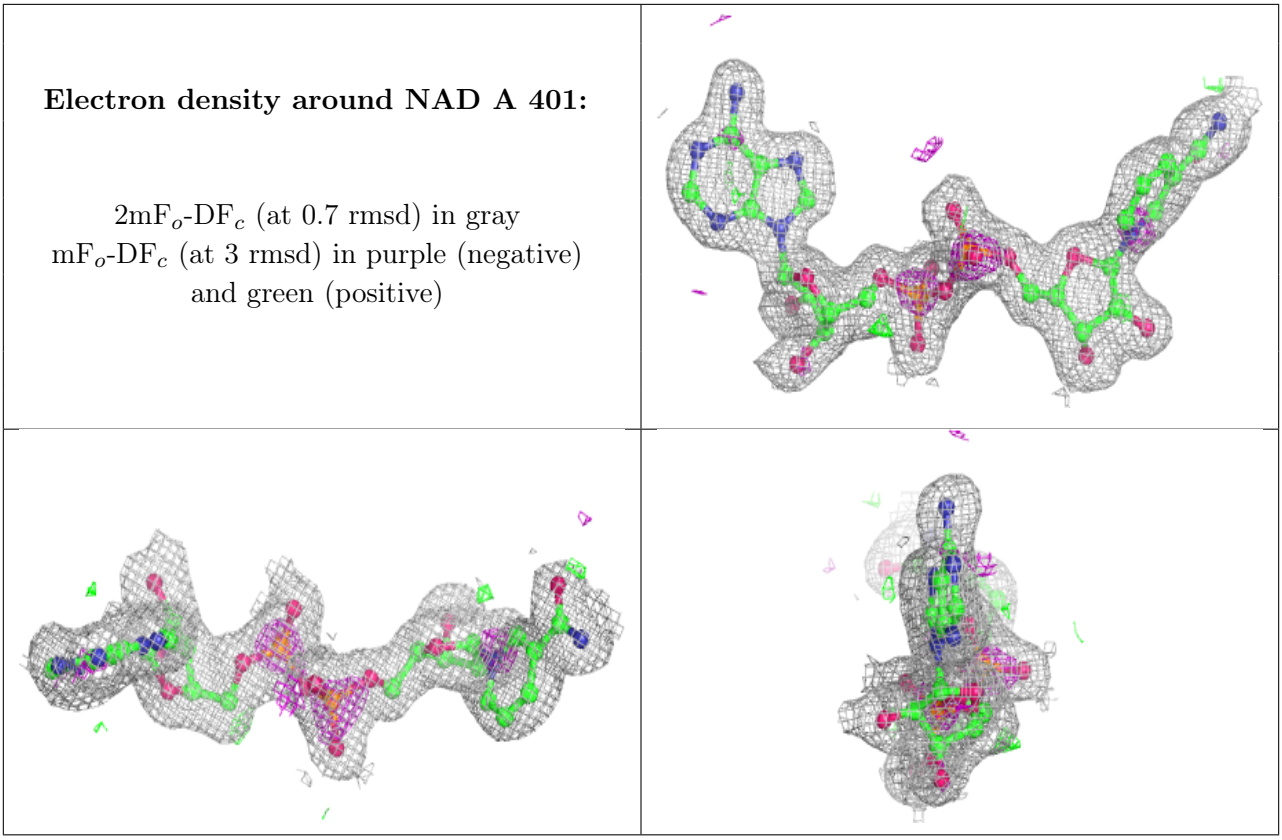
Electron density around MG C 402:

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



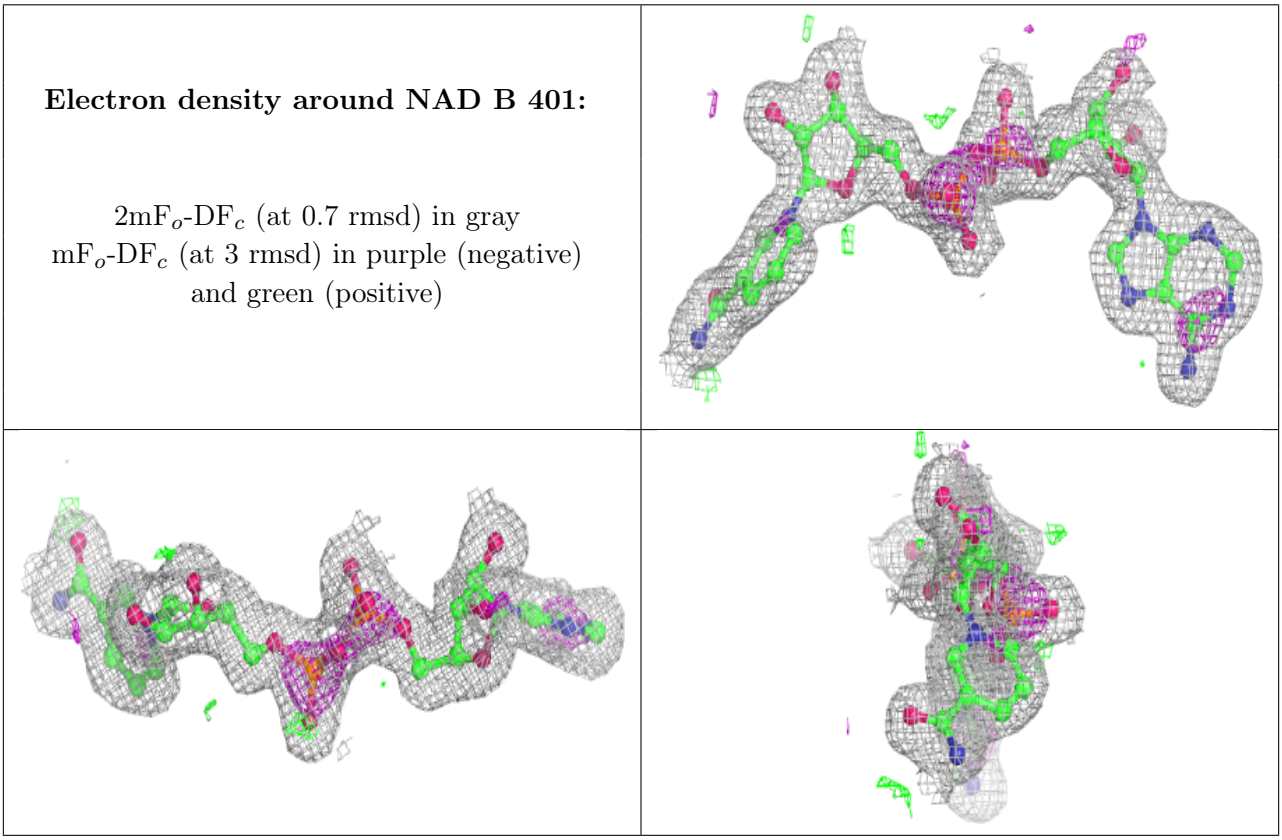
Electron density around NAD A 401:

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



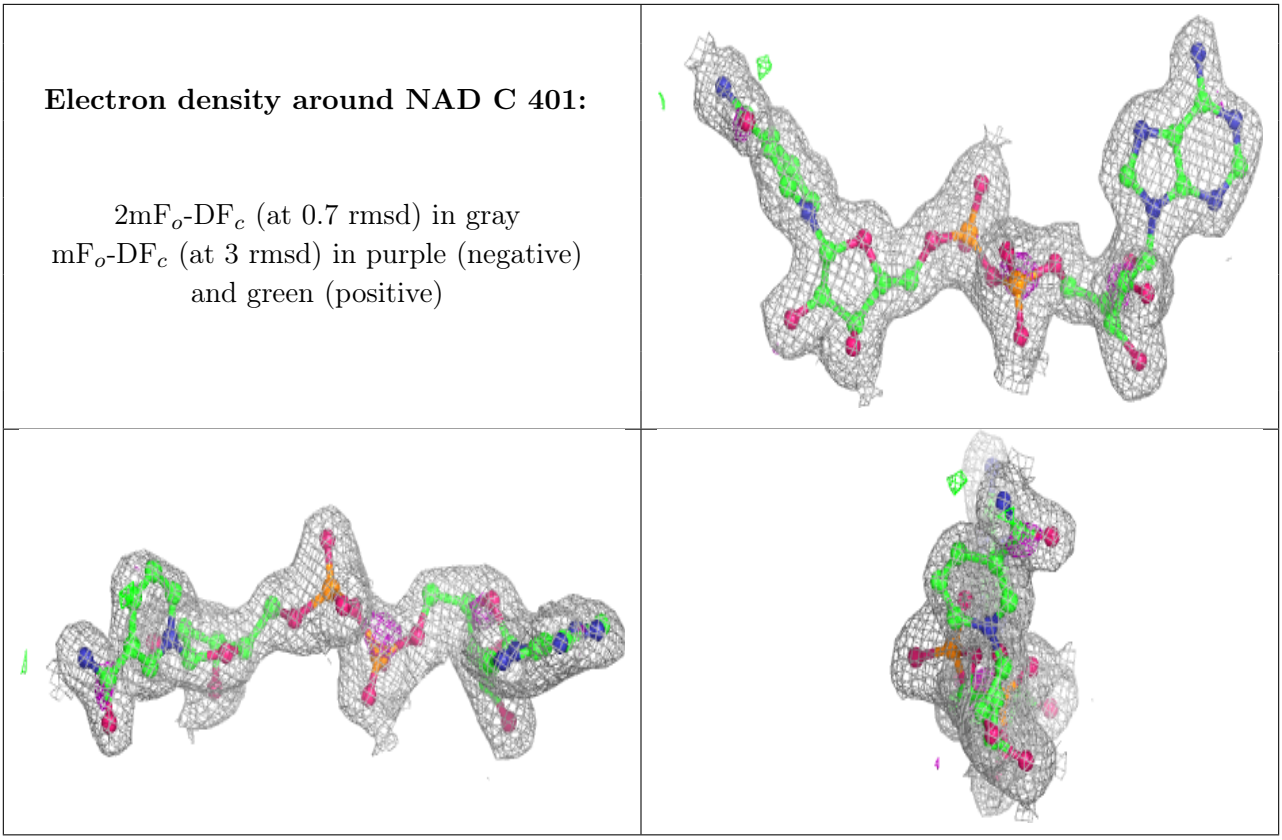
Electron density around NAD B 401:

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



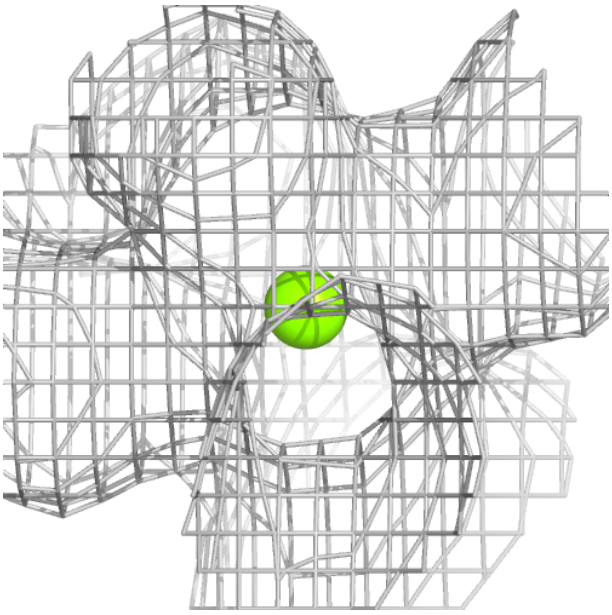
Electron density around NAD C 401:

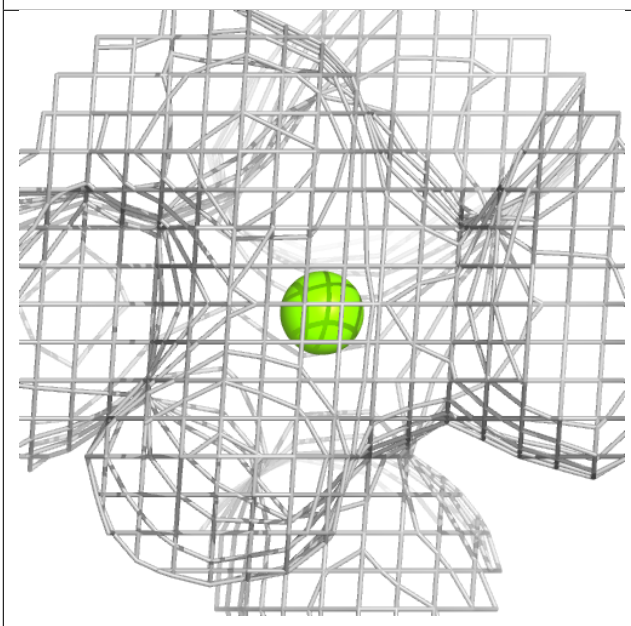
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

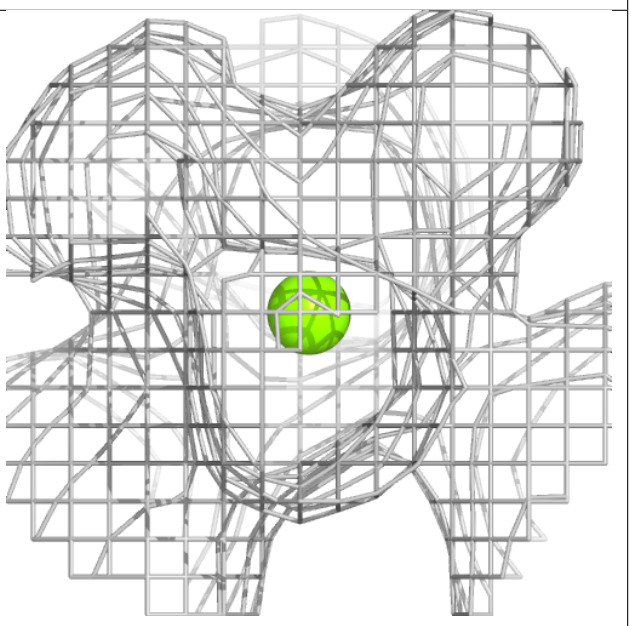


Electron density around MG D 402:

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

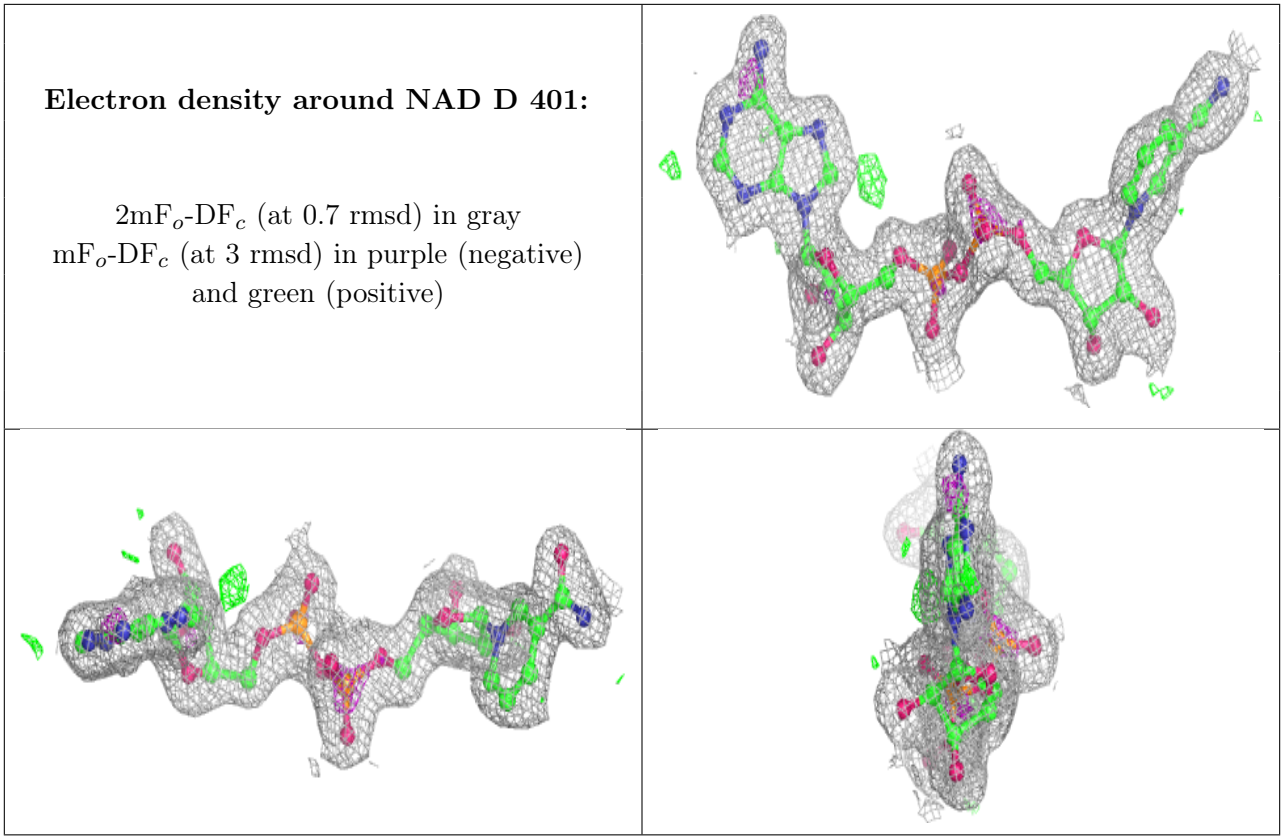






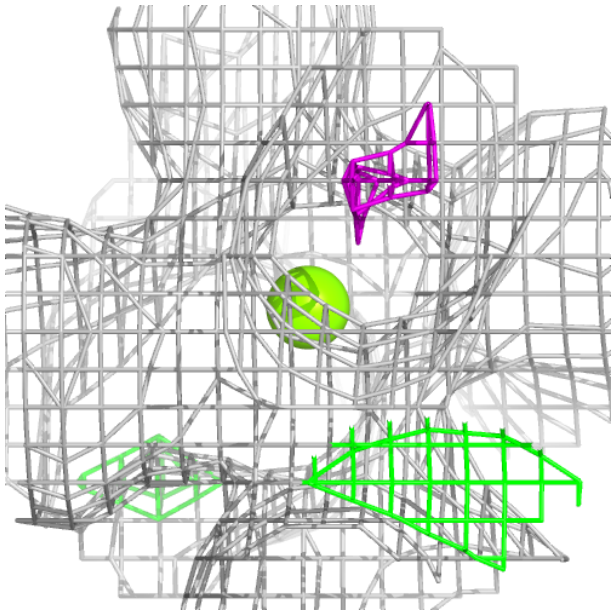
Electron density around NAD D 401:

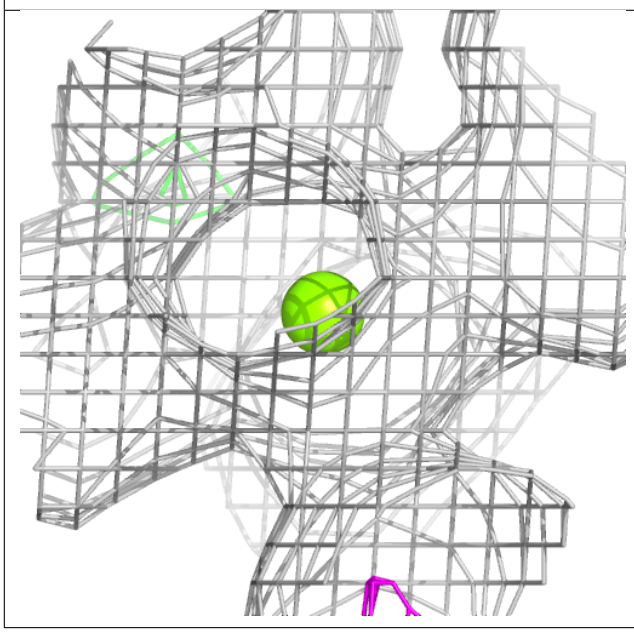
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

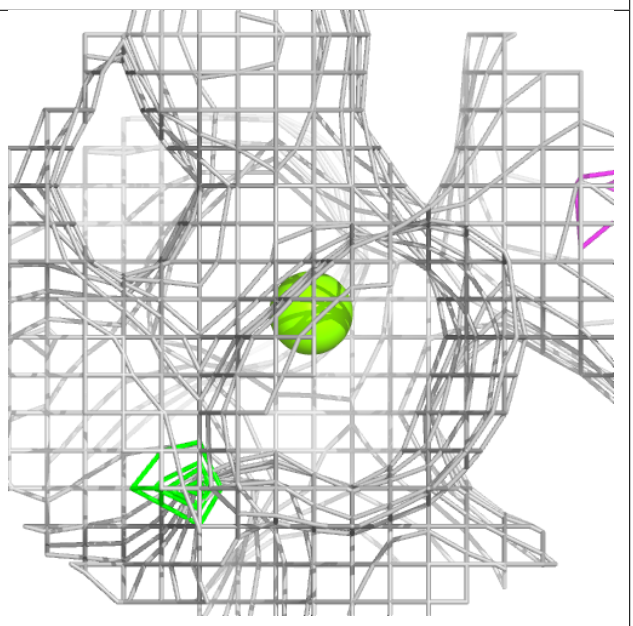


Electron density around MG A 402:

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

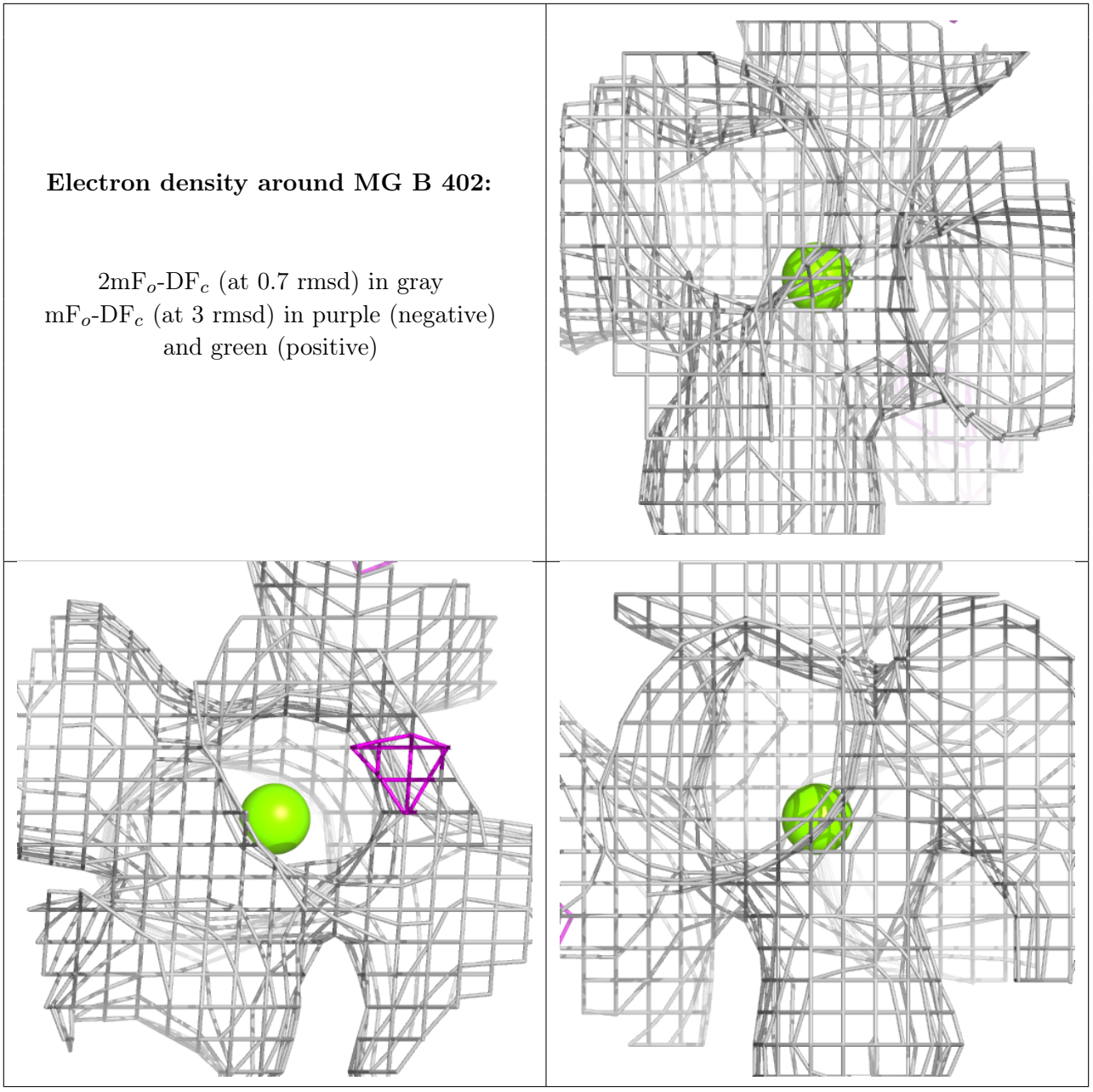






Electron density around MG B 402:

$2mF_o$-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

There are no such residues in this entry.