



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:07 PM UTC

PDB ID : 8ZJ7 / pdb_00008zj7
Title : Terephthalate 1,2-cis-dihydrodioldehydrogenase/Decarboxylase in complex with 3,4-Dihydroxybenzoate and NAD.
Authors : Kumar, K.A.; Pahwa, D.; Kumar, P.
Deposited on : 2024-05-14
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

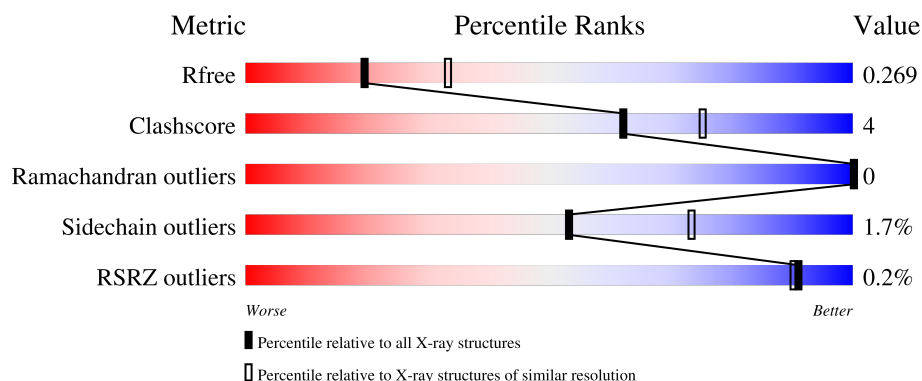
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	316	 88% 11% .
1	B	316	 90% 9% .
1	C	316	 89% 9% .
1	D	316	 88% 9% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18943 atoms, of which 9511 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.

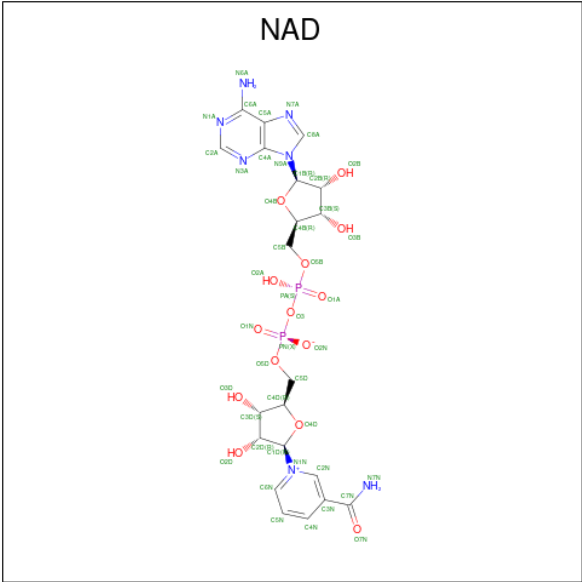
- Molecule 1 is a protein called 4-hydroxythreonine-4-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	314	Total	C	H	N	O	S	68	0	0
			4670	1445	2368	412	432	13			
1	C	315	Total	C	H	N	O	S	70	0	0
			4690	1451	2378	415	433	13			
1	D	310	Total	C	H	N	O	S	68	0	0
			4613	1427	2339	407	427	13			
1	A	313	Total	C	H	N	O	S	68	0	0
			4653	1440	2359	411	431	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP B7WRJ7
C	0	HIS	-	expression tag	UNP B7WRJ7
D	0	HIS	-	expression tag	UNP B7WRJ7
A	0	HIS	-	expression tag	UNP B7WRJ7

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

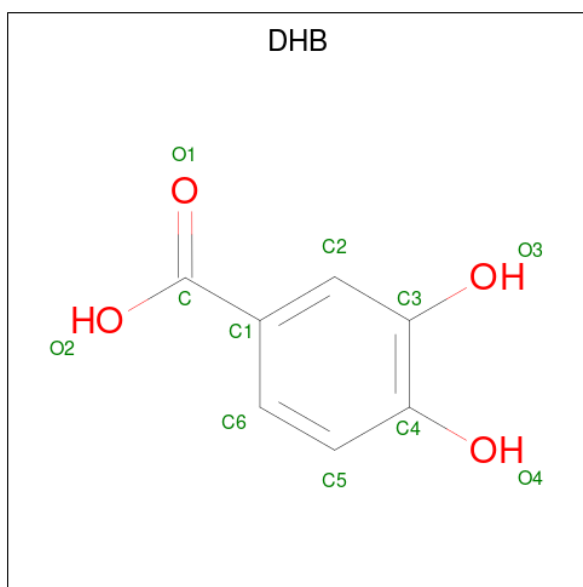


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	4	0
			70	21	26	7	14	2		
2	A	1	Total	C	H	N	O	P	4	0
			70	21	26	7	14	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is 3,4-DIHYDROXYBENZOIC ACID (CCD ID: DHB) (formula: C₇H₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	2	0
			16	7	5	4		
4	D	1	Total	C	H	O	2	0
			16	7	5	4		
4	A	1	Total	C	H	O	2	0
			16	7	5	4		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	36	Total 36	O 36	0	0
8	C	35	Total 35	O 35	0	0
8	D	19	Total 19	O 19	0	0
8	A	32	Total 32	O 32	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.

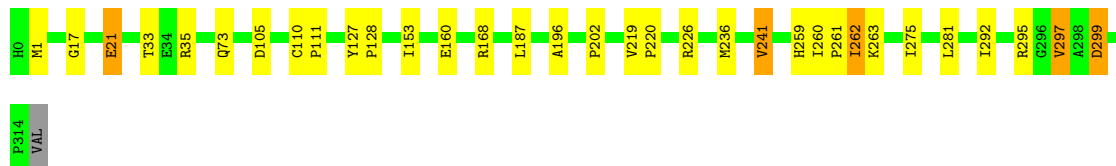
- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase

Chain B:  90% 9% .



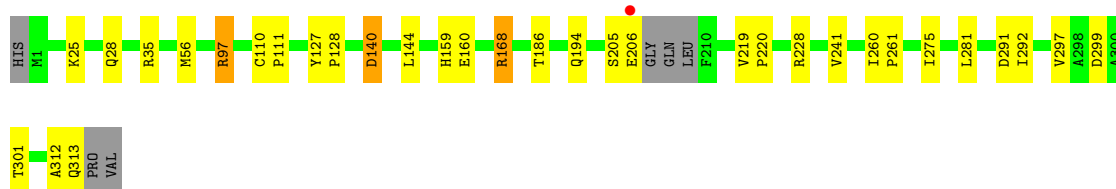
- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase

Chain C:  89% 9% .



- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase

Chain D:  88% 9% ..



- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase

Chain A:  88% 11% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.30Å 98.15Å 168.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.00 – 2.65 24.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.00-2.65) 99.0 (24.00-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 2.64Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.181 , 0.252 (Not available) , 0.269	Depositor DCC
R_{free} test set	2135 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtrriage
Anisotropy	1.261	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18943	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.74 % 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 7.6275e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DHB, MG, ZN, CL, 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	0.62	0/2331	1.02	2/3173 (0.1%)
1	B	0.59	0/2339	1.00	2/3183 (0.1%)
1	C	0.62	0/2350	1.05	5/3198 (0.2%)
1	D	0.60	0/2309	1.04	6/3140 (0.2%)
All	All	0.61	0/9329	1.03	15/12694 (0.1%)

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	A	0	1
1	B	0	1
1	C	0	3
1	D	0	2
All	All	0	7

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	GLU	CB-CA-C	-7.95	97.60	110.79
1	D	299	ASP	CA-CB-CG	7.04	119.64	112.60
1	B	140	ASP	CA-CB-CG	6.51	119.11	112.60
1	B	241	VAL	N-CA-CB	6.01	117.58	110.55
1	D	241	VAL	N-CA-CB	5.67	117.18	110.55
1	D	97	ARG	CG-CD-NE	-5.65	99.56	112.00
1	C	105	ASP	CA-CB-CG	5.65	118.25	112.60
1	C	1	MET	CG-SD-CE	5.65	113.33	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	301	THR	CA-CB-OG1	-5.62	101.17	109.60
1	D	186	THR	CA-CB-OG1	-5.55	101.28	109.60
1	C	241	VAL	N-CA-CB	5.53	117.65	110.57
1	C	299	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	140	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	186	THR	CA-CB-OG1	-5.19	101.82	109.60
1	A	140	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	ARG	Sidechain
1	B	295	ARG	Sidechain
1	C	226	ARG	Sidechain
1	C	295	ARG	Sidechain
1	C	35	ARG	Sidechain
1	D	168	ARG	Sidechain
1	D	35	ARG	Sidechain

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	2294	2359	2345	24	0
1	B	2302	2368	2357	18	0
1	C	2312	2378	2364	20	0
1	D	2274	2339	2327	17	1
2	A	44	26	26	2	0
2	B	44	26	26	2	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	11	5	5	1	0
4	C	11	5	5	1	0
4	D	11	5	5	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
6	D	1	0	0	0	0
7	D	1	0	0	0	0
8	A	32	0	0	3	0
8	B	36	0	0	2	0
8	C	35	0	0	2	1
8	D	19	0	0	0	0
All	All	9432	9511	9460	77	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 4.

All (77) 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:C:259:HIS:NE2	4:C:401:DHB:O1	1.88	1.06
2:B:401:NAD:O1N	2:B:401:NAD:O3B	1.95	0.84
1:D:28:GLN:OE1	1:D:56:MET:HE2	1.82	0.80
1:A:110:CYS:HB3	1:A:111:PRO:HD2	1.64	0.79
1:D:110:CYS:HB3	1:D:111:PRO:HD2	1.63	0.78
1:B:236:MET:HB3	1:B:241:VAL:CG2	2.21	0.70
1:C:17:GLY:HA3	8:C:525:HOH:O	1.92	0.69
1:A:29:GLN:HG3	1:A:304:LEU:HD11	1.80	0.64
1:A:236:MET:HB2	1:A:241:VAL:CG2	2.30	0.62
1:D:159:HIS:CE1	4:D:401:DHB:H2	2.36	0.61
1:C:236:MET:HB2	1:C:241:VAL:CG2	2.32	0.59
1:D:25:LYS:HG2	1:D:56:MET:HE1	1.85	0.59
1:B:184:THR:HG21	1:B:275:ILE:HD11	1.85	0.59
1:A:147:VAL:HG11	1:A:309:LEU:HD11	1.87	0.56
1:C:261:PRO:HB3	1:A:264:LEU:HD11	1.88	0.56
1:C:202:PRO:CG	8:A:528:HOH:O	2.55	0.55
1:A:281:LEU:C	1:A:281:LEU:HD23	2.31	0.55
1:B:110:CYS:HB3	1:B:111:PRO:CD	2.37	0.54
1:C:110:CYS:HB3	1:C:111:PRO:CD	2.38	0.54
1:D:160:GLU:OE1	1:D:168:ARG:NH1	2.40	0.54
1:C:281:LEU:C	1:C:281:LEU:HD23	2.33	0.54
1:B:281:LEU:HD23	1:B:281:LEU:C	2.34	0.53
1:C:160:GLU:OE1	1:C:168:ARG:NH2	2.42	0.53
1:A:196:ALA:HB1	1:A:241:VAL:HG11	1.91	0.52
1:D:281:LEU:C	1:D:281:LEU:HD23	2.34	0.52
1:A:236:MET:HB2	1:A:241:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:MET:SD	1:B:241:VAL:HG22	2.51	0.51
1:B:184:THR:OG1	1:B:275:ILE:HD13	2.12	0.50
1:C:263:LYS:HG3	1:A:239:ASP:HB2	1.93	0.50
1:A:236:MET:CB	1:A:241:VAL:CG2	2.90	0.49
1:A:295:ARG:HG2	1:A:295:ARG:HH21	1.77	0.49
1:B:135:LEU:CD1	1:B:137:MET:HE3	2.42	0.49
1:C:73:GLN:NE2	8:C:503:HOH:O	2.46	0.49
1:A:114:GLU:HG3	2:A:401:NAD:H1D	1.94	0.48
1:C:196:ALA:HB1	1:C:241:VAL:HG11	1.95	0.48
1:B:264:LEU:HD11	1:D:261:PRO:HB3	1.96	0.48
1:B:288:SER:OG	2:B:401:NAD:H5N	2.15	0.47
1:D:205:SER:O	1:D:206:GLU:C	2.56	0.47
1:A:127:TYR:N	1:A:128:PRO:CD	2.78	0.47
1:D:110:CYS:HB3	1:D:111:PRO:CD	2.41	0.46
1:C:127:TYR:N	1:C:128:PRO:CD	2.79	0.46
1:D:312:ALA:O	1:D:313:GLN:HB2	2.15	0.46
1:B:127:TYR:N	1:B:128:PRO:CD	2.79	0.46
1:D:159:HIS:HE1	4:D:401:DHB:H2	1.81	0.46
1:D:127:TYR:N	1:D:128:PRO:CD	2.79	0.46
1:B:158:LEU:O	1:B:255:HIS:HB2	2.15	0.45
1:B:260:ILE:N	1:B:261:PRO:HD2	2.32	0.45
1:D:292:ILE:HB	1:D:297:VAL:CG2	2.47	0.45
1:A:260:ILE:N	1:A:261:PRO:HD2	2.33	0.44
1:C:292:ILE:CD1	1:C:297:VAL:HG22	2.47	0.44
1:B:178:VAL:HG22	1:B:251:VAL:HG21	2.00	0.44
1:C:260:ILE:N	1:C:261:PRO:HD2	2.33	0.44
1:C:168:ARG:O	1:C:168:ARG:HG2	2.16	0.43
1:A:145:MET:HE2	1:A:181:ALA:HB1	2.00	0.43
1:A:144:LEU:HD11	1:A:272:ALA:HB1	2.00	0.43
1:A:187:LEU:HD23	1:A:280:VAL:HG21	2.01	0.43
1:A:226:ARG:NH2	1:A:232:VAL:O	2.51	0.42
1:D:219:VAL:HB	1:D:220:PRO:HD3	2.01	0.42
1:A:110:CYS:HB3	1:A:111:PRO:CD	2.43	0.42
1:C:236:MET:SD	1:C:241:VAL:HG22	2.60	0.42
1:A:116:ALA:HB2	8:A:512:HOH:O	2.19	0.42
1:B:80:ILE:HA	8:B:524:HOH:O	2.20	0.42
1:D:260:ILE:N	1:D:261:PRO:HD2	2.34	0.41
1:C:153:ILE:HD12	1:C:262:ILE:HD13	2.01	0.41
1:C:236:MET:CB	1:C:241:VAL:CG2	2.97	0.41
2:A:401:NAD:H8A	2:A:401:NAD:O1A	2.19	0.41
1:A:236:MET:SD	1:A:241:VAL:HG22	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:HIS:HE1	1:D:159:HIS:NE2	2.19	0.41
1:C:73:GLN:N	1:C:73:GLN:OE1	2.54	0.41
1:B:230:LEU:HD23	1:B:231:THR:N	2.35	0.41
1:B:263:LYS:NZ	8:B:505:HOH:O	2.54	0.41
1:A:276:GLY:HA2	8:A:505:HOH:O	2.21	0.41
1:C:219:VAL:HB	1:C:220:PRO:HD3	2.03	0.40
1:D:144:LEU:HD11	4:D:401:DHB:O4	2.21	0.40
1:A:73:GLN:HB3	1:A:74:PRO:HD2	2.03	0.40
1:B:144:LEU:HD11	1:B:272:ALA:HB1	2.03	0.40
1:A:263:LYS:NZ	4:A:402:DHB:H5	2.36	0.40

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)
1:D:291:ASP:OD2	8:C:529:HOH:O[4_654]	2.09	0.11

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	311/316 (98%)	305 (98%)	6 (2%)	0	100	100
1	B	129/316 (41%)	129 (100%)	0	0	100	100
1	C	297/316 (94%)	293 (99%)	4 (1%)	0	100	100
1	D	306/316 (97%)	300 (98%)	6 (2%)	0	100	100
All	All	1043/1264 (82%)	1027 (98%)	16 (2%)	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	242/245 (99%)	240 (99%)	2 (1%)	73	85
1	B	243/245 (99%)	241 (99%)	2 (1%)	73	85
1	C	244/245 (100%)	237 (97%)	7 (3%)	37	58
1	D	240/245 (98%)	235 (98%)	5 (2%)	47	69
All	All	969/980 (99%)	953 (98%)	16 (2%)	53	73

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

Mol	Chain	Res	Type
1	B	63	LEU
1	B	97	ARG
1	C	21	GLU
1	C	33	THR
1	C	187	LEU
1	C	262	ILE
1	C	275	ILE
1	C	297	VAL
1	C	299	ASP
1	D	97	ARG
1	D	140	ASP
1	D	194	GLN
1	D	228	ARG
1	D	275	ILE
1	A	28	GLN
1	A	275	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	83	GLN
1	B	118	HIS
1	B	216	GLN

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Mol	Chain	Res	Type
1	D	49	GLN
1	D	216	GLN
1	A	118	HIS

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 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	-	46,48,48	1.04	4 (8%)	64,73,73	0.74	1 (1%)
2	NAD	A	401	-	46,48,48	0.93	3 (6%)	64,73,73	0.77	2 (3%)
4	DHB	A	402	-	11,11,11	0.74	0	15,15,15	0.67	0
4	DHB	D	401	3	11,11,11	0.47	0	15,15,15	1.14	1 (6%)
4	DHB	C	401	-	11,11,11	1.03	1 (9%)	15,15,15	1.12	1 (6%)

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	-	-	7/30/62/62	0/5/5/5
2	NAD	A	401	-	-	10/30/62/62	0/5/5/5
4	DHB	A	402	-	-	0/4/4/4	0/1/1/1
4	DHB	D	401	3	-	0/4/4/4	0/1/1/1
4	DHB	C	401	-	-	0/4/4/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAD	PN-O3	3.69	1.63	1.59
2	A	401	NAD	C2N-N1N	3.66	1.39	1.35
2	B	401	NAD	PA-O3	3.64	1.63	1.59
2	B	401	NAD	C2N-N1N	3.06	1.38	1.35
2	A	401	NAD	PA-O3	2.80	1.62	1.59
2	A	401	NAD	PN-O3	2.79	1.62	1.59
2	B	401	NAD	O4D-C1D	2.14	1.43	1.40
4	C	401	DHB	O2-C	-2.09	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAD	C6N-N1N-C2N	-2.50	119.75	121.88
2	A	401	NAD	C6N-N1N-C2N	-2.36	119.87	121.88
4	D	401	DHB	O1-C-C1	-2.22	115.63	121.46
4	C	401	DHB	O3-C3-C4	2.07	123.96	118.42
2	A	401	NAD	C3B-C2B-C1B	2.03	105.30	101.46

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAD	C5D-O5D-PN-O3
2	B	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	C2D-C1D-N1N-C6N
2	A	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	PN-O3-PA-O5B
2	A	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	C5D-O5D-PN-O1N
2	A	401	NAD	C3B-C4B-C5B-O5B
2	B	401	NAD	C5D-O5D-PN-O2N
2	A	401	NAD	C5D-O5D-PN-O3

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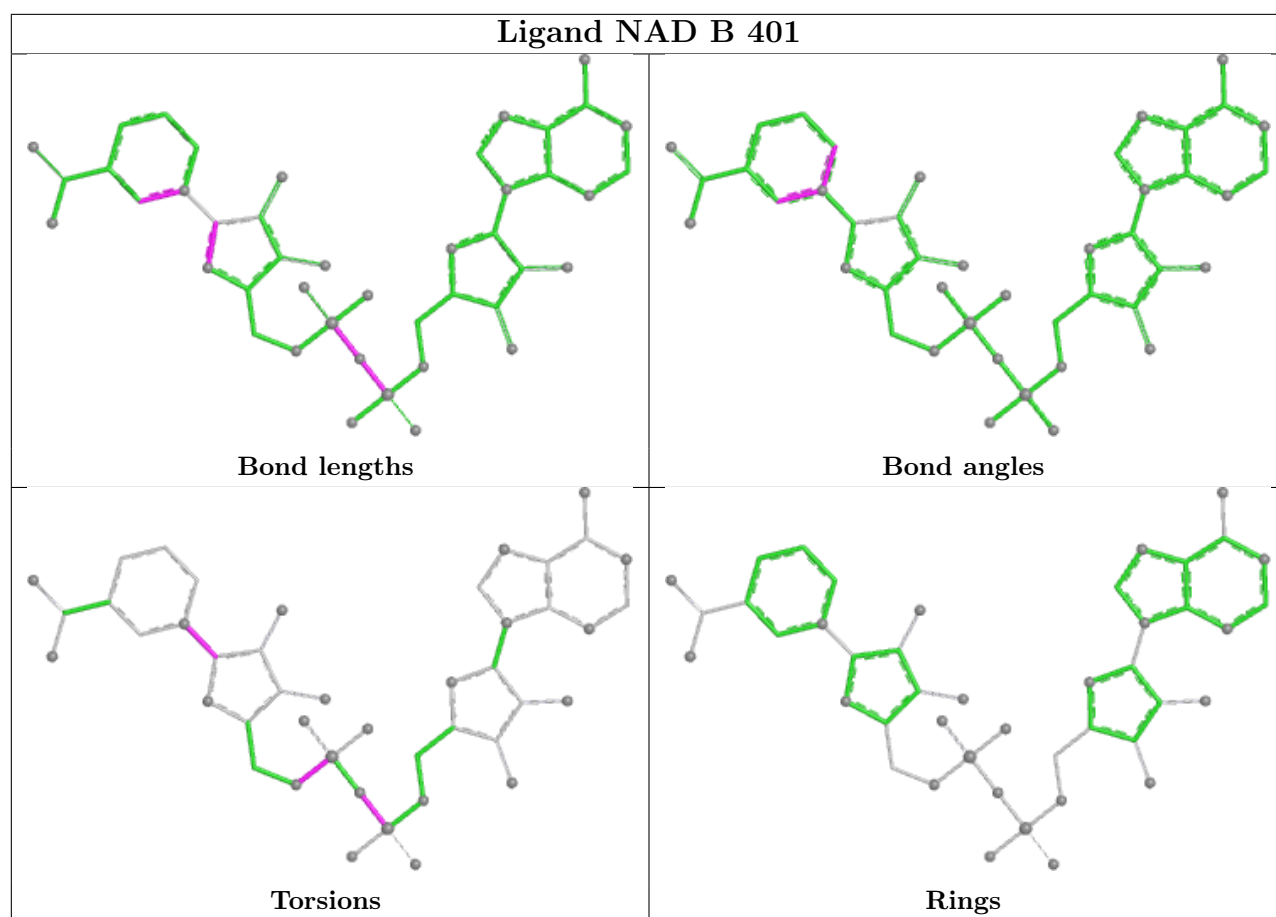
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5D-O5D-PN-O2N
2	B	401	NAD	PN-O3-PA-O1A
2	A	401	NAD	C4B-C5B-O5B-PA
2	B	401	NAD	PN-O3-PA-O2A
2	A	401	NAD	PA-O3-PN-O2N
2	A	401	NAD	PA-O3-PN-O1N

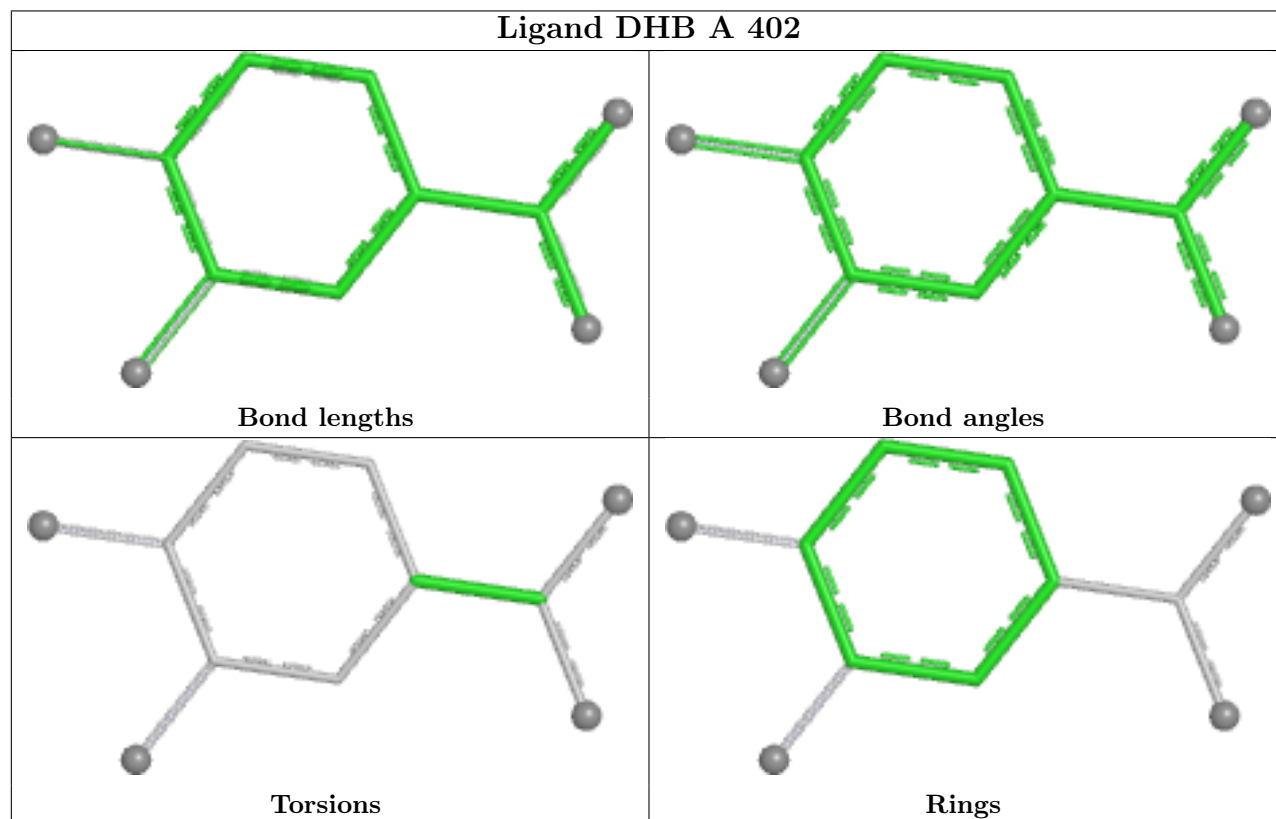
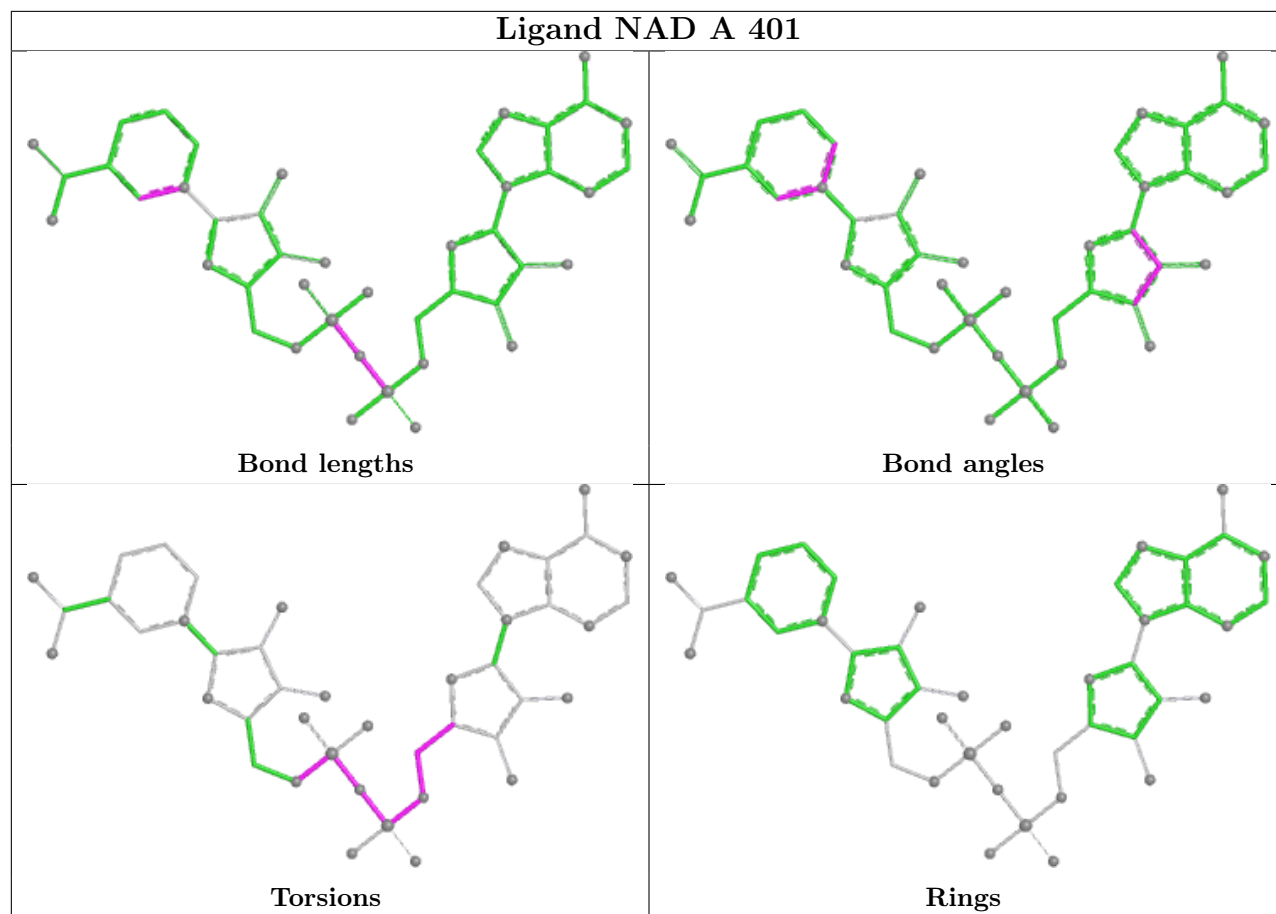
There are no ring outliers.

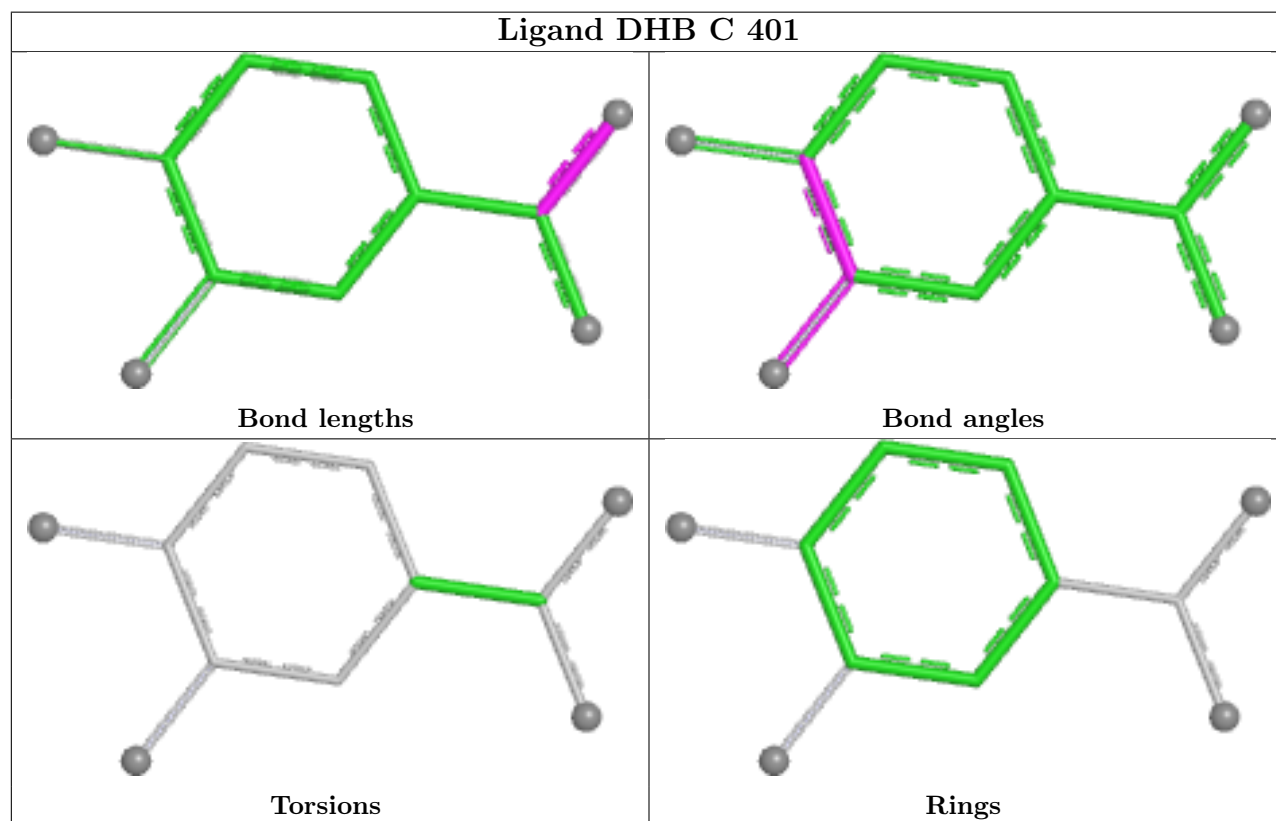
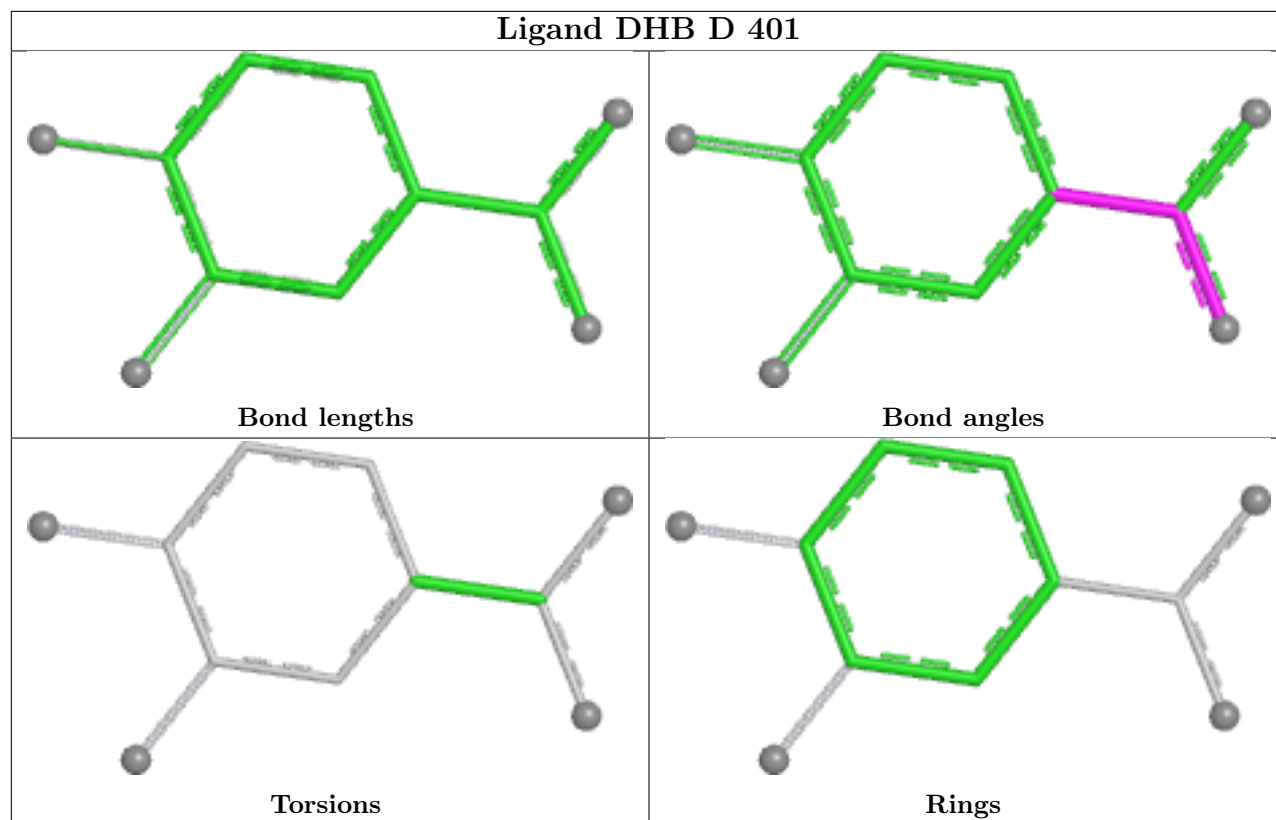
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAD	2	0
2	A	401	NAD	2	0
4	A	402	DHB	1	0
4	D	401	DHB	3	0
4	C	401	DHB	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 [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	313/316 (99%)	-0.76	0 100 100	30, 47, 70, 91	0
1	B	314/316 (99%)	-0.74	1 (0%) 90 89	29, 48, 73, 106	0
1	C	315/316 (99%)	-0.87	0 100 100	31, 45, 66, 99	0
1	D	310/316 (98%)	-0.78	1 (0%) 90 89	28, 45, 70, 111	0
All	All	1252/1264 (99%)	-0.79	2 (0%) 91 90	28, 46, 70, 111	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	206	GLU	2.4
1	B	1	MET	2.4

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

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

6.3 Carbohydrates [i](#)

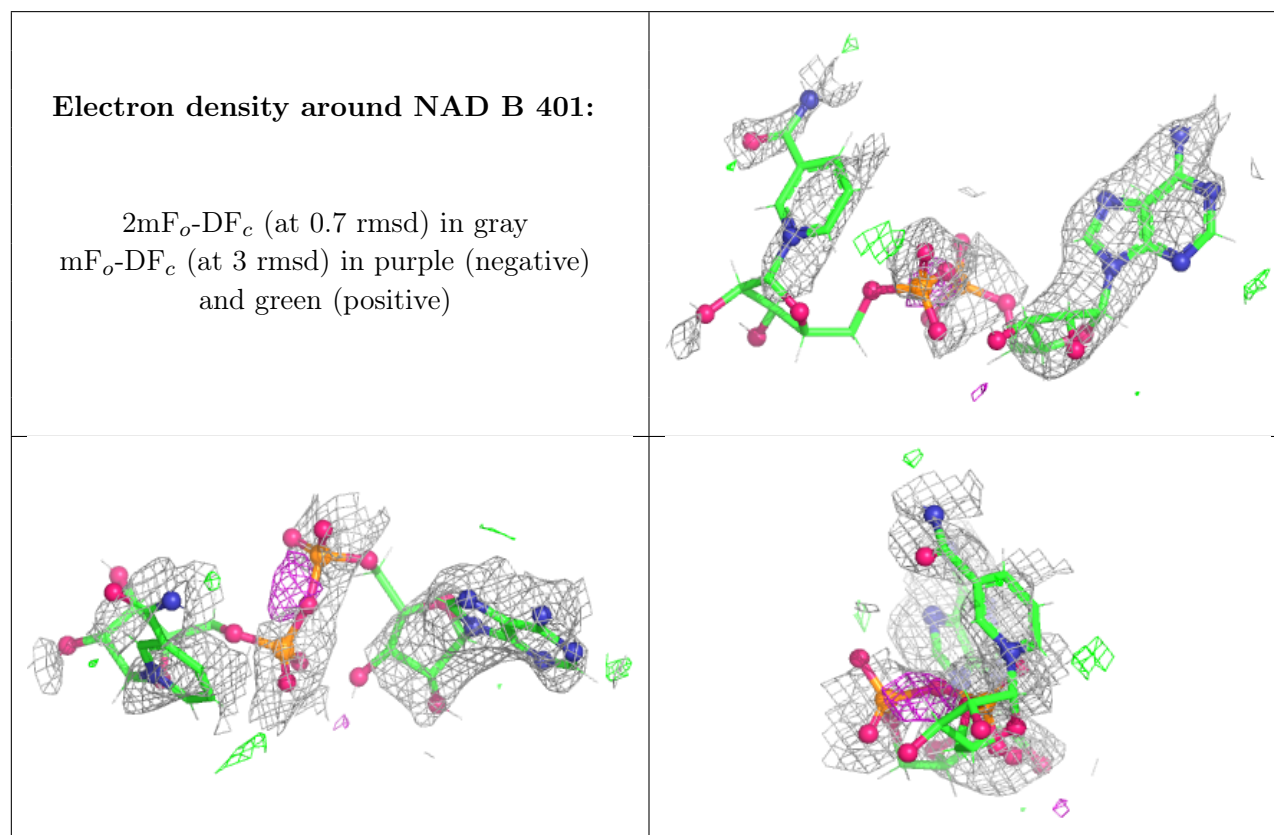
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

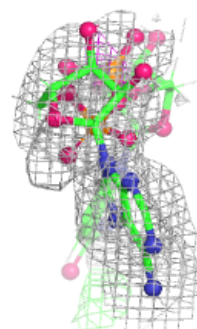
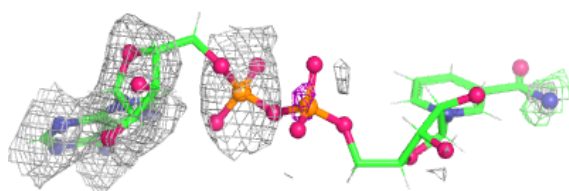
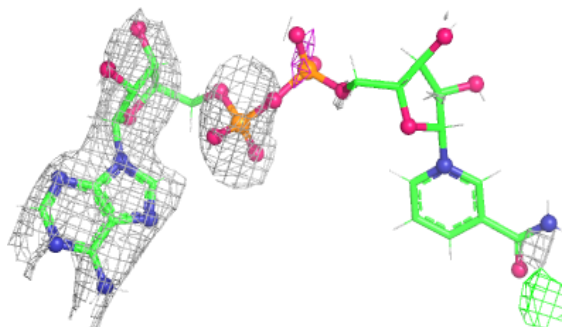
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	B	401	44/44	0.86	0.13	51,88,126,144	70
2	NAD	A	401	44/44	0.87	0.14	46,105,117,130	70
7	NA	D	404	1/1	0.87	0.28	51,51,51,51	0
4	DHB	A	402	11/11	0.91	0.10	62,73,82,85	2
4	DHB	C	401	11/11	0.95	0.08	56,70,78,80	2
4	DHB	D	401	11/11	0.96	0.08	73,81,97,108	2
5	MG	C	403	1/1	0.98	0.03	61,61,61,61	0
6	CL	D	403	1/1	0.98	0.12	64,64,64,64	0
3	ZN	B	402	1/1	0.98	0.03	94,94,94,94	0
3	ZN	D	402	1/1	0.99	0.01	67,67,67,67	0
3	ZN	C	402	1/1	1.00	0.01	54,54,54,54	0
3	ZN	A	403	1/1	1.00	0.02	63,63,63,63	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.

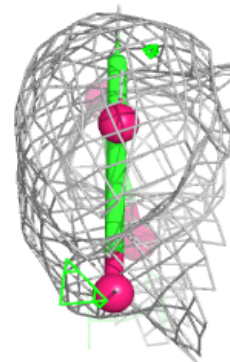
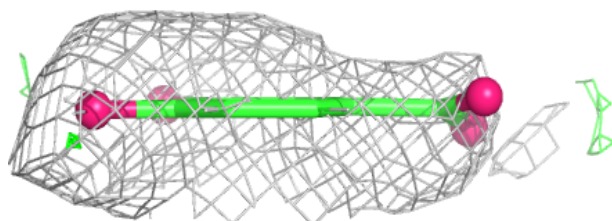
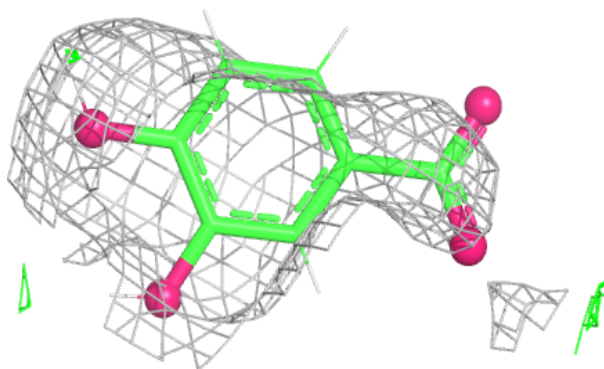


Electron density around NAD A 401:

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

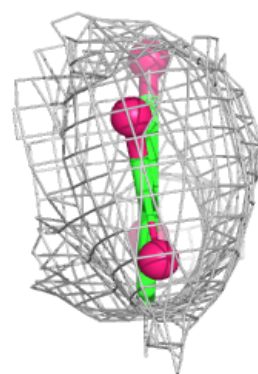
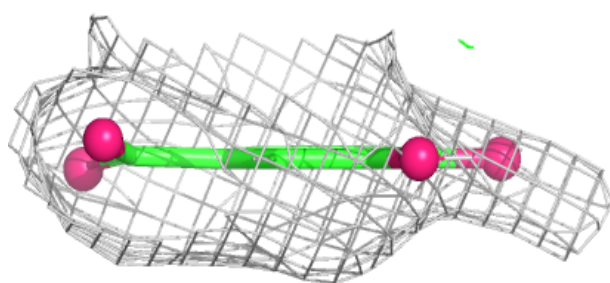
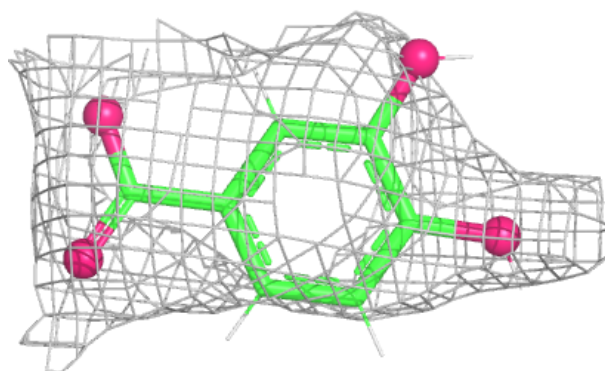
**Electron density around DHB A 402:**

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



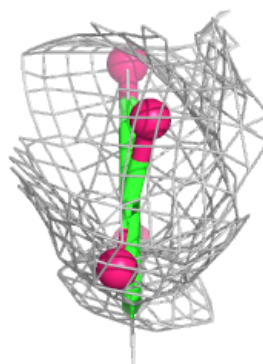
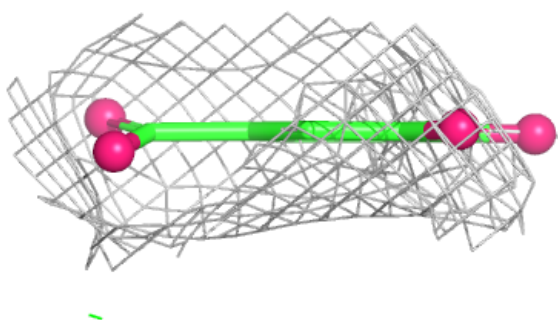
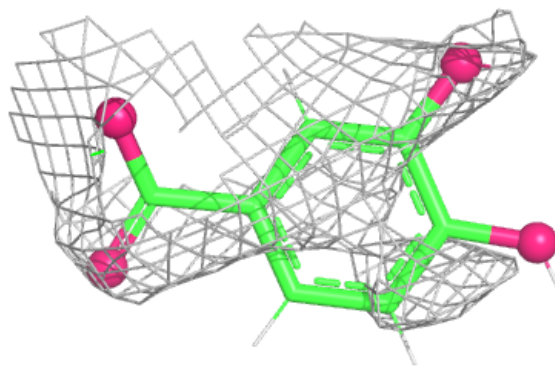
Electron density around DHB C 401:

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



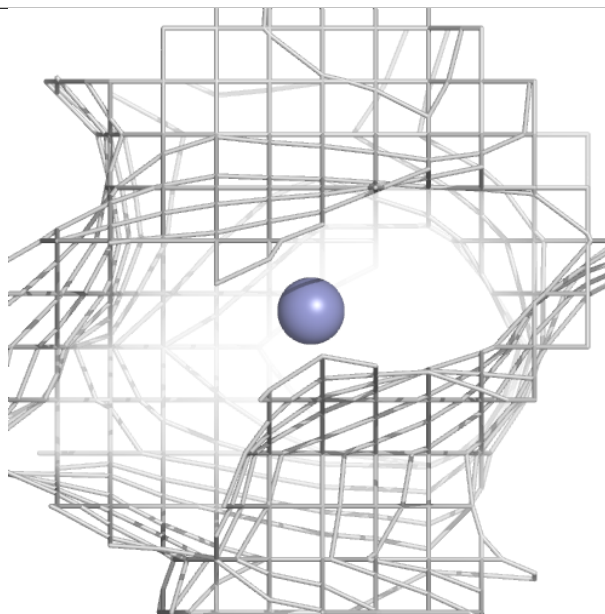
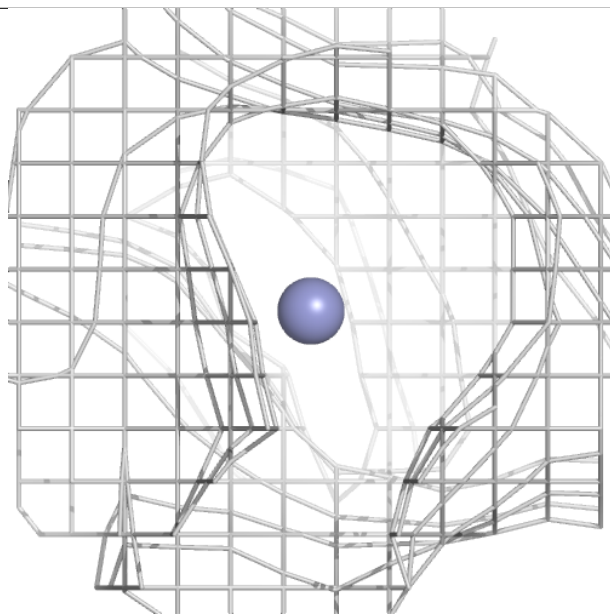
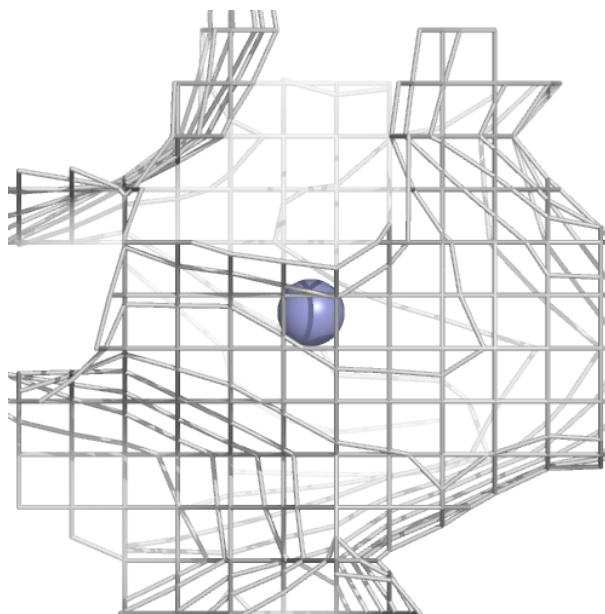
Electron density around DHB D 401:

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and green (positive)



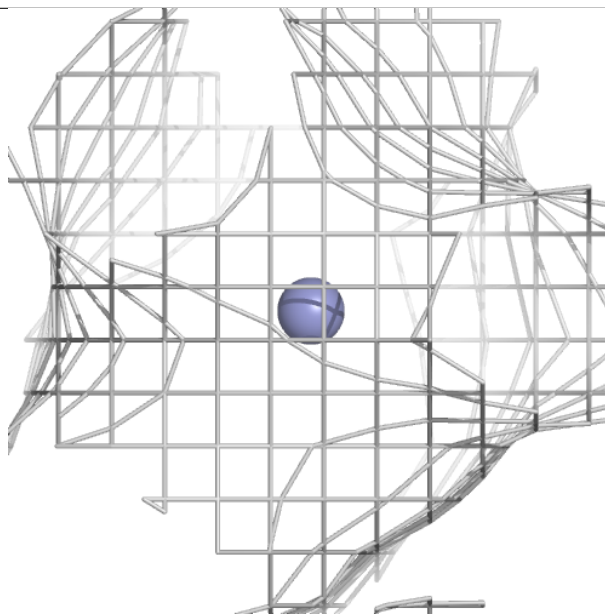
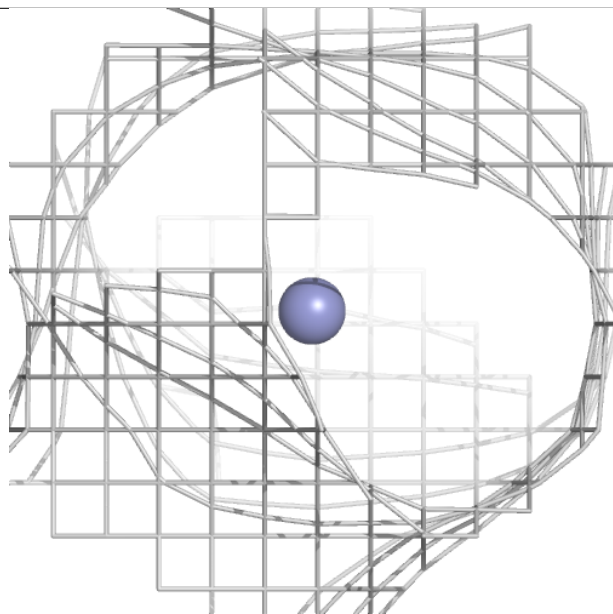
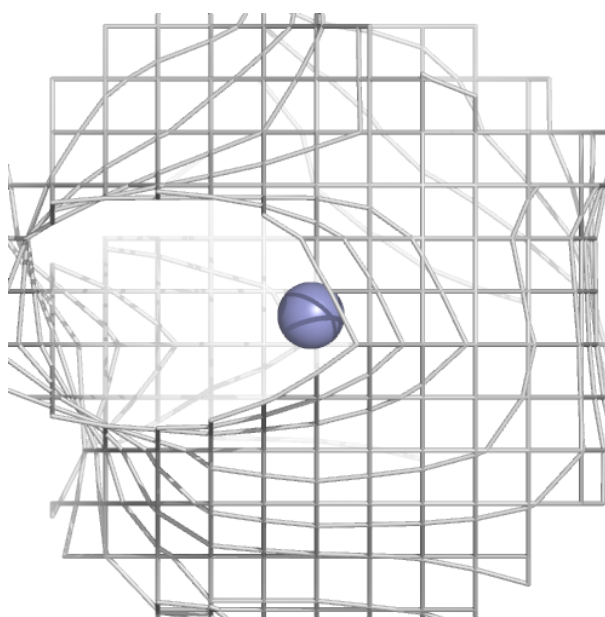
Electron density around ZN B 402:

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



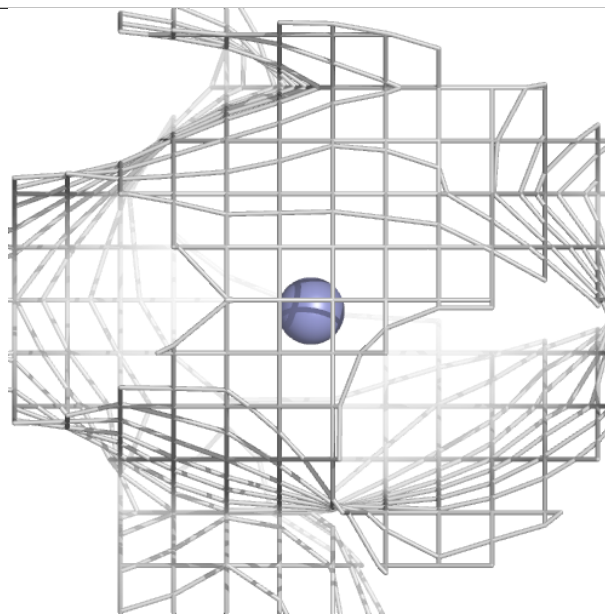
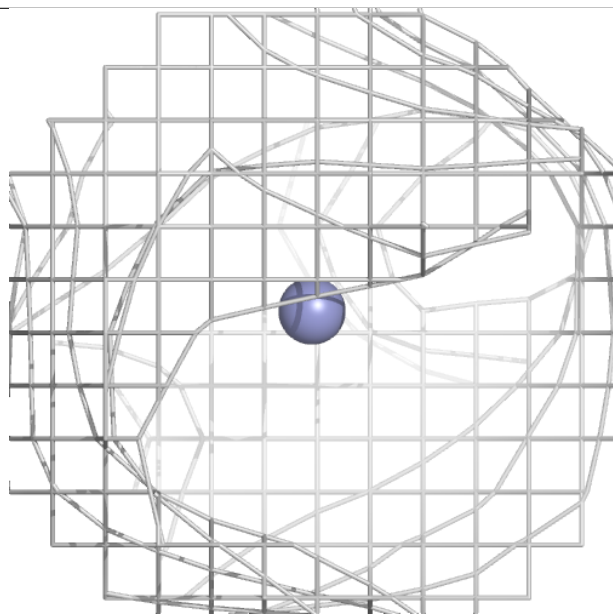
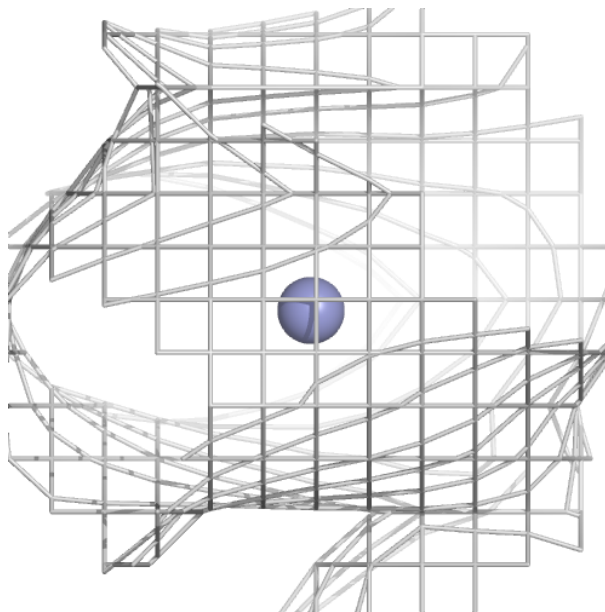
Electron density around ZN D 402:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



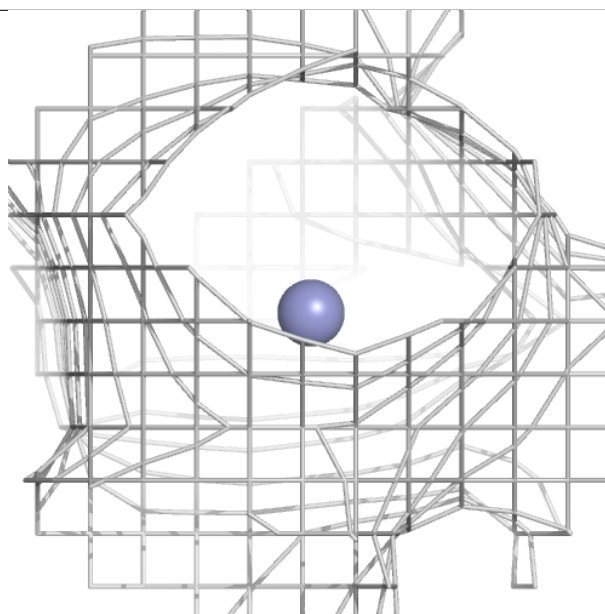
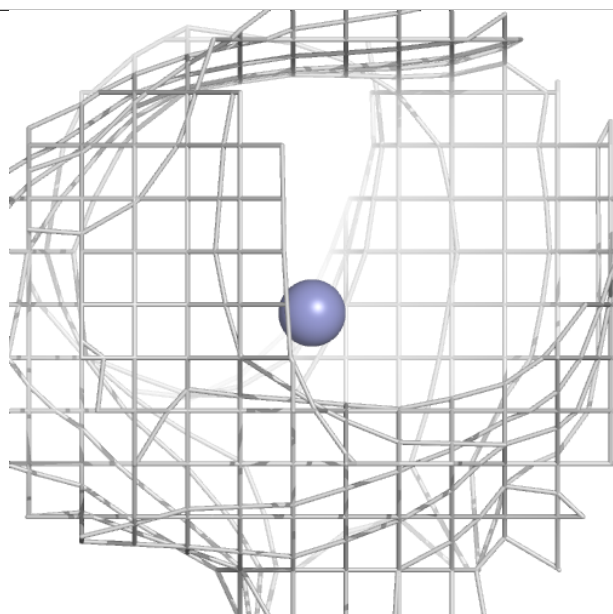
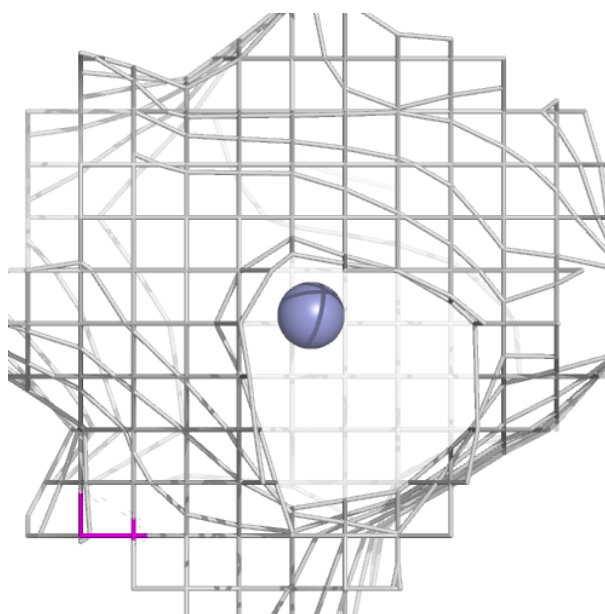
Electron density around ZN C 402:

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



Electron density around ZN A 403:

$2mF_o-DF_c$ (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.