



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2022 – 06:22 AM JST

PDB ID : 7BY9
Title : Malate Dehydrogenase from *Geobacillus stearothermophilus* (gs-MDH) complexed with Oxaloacetic Acid (OAA) and Nicotinamide Adenine Dinucleotide (NAD)
Authors : Shimozawa, Y.; Nakamura, T.; Himiyama, T.; Nishiya, Y.
Deposited on : 2020-04-22
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.26
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) : 2.26

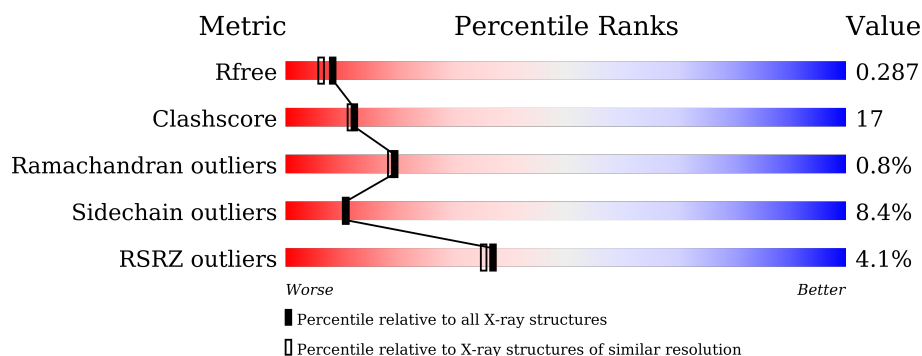
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	332	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>• 6%</div> </div> </div>
1	B	332	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>33%</div> <div>• 8%</div> </div> </div>
1	C	332	<div> <div>8%</div> <div> <div></div> <div>49%</div> <div>38%</div> <div>• 9%</div> </div> </div>
1	D	332	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>34%</div> <div>• 6%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9578 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2359	1502	391	456	10			
1	B	307	Total	C	N	O	S	0	0	0
			2327	1482	383	452	10			
1	C	302	Total	C	N	O	S	0	0	0
			2287	1461	375	442	9			
1	D	311	Total	C	N	O	S	0	0	0
			2359	1502	391	456	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A143T1U9
A	-19	GLY	-	expression tag	UNP A0A143T1U9
A	-18	SER	-	expression tag	UNP A0A143T1U9
A	-17	SER	-	expression tag	UNP A0A143T1U9
A	-16	HIS	-	expression tag	UNP A0A143T1U9
A	-15	HIS	-	expression tag	UNP A0A143T1U9
A	-14	HIS	-	expression tag	UNP A0A143T1U9
A	-13	HIS	-	expression tag	UNP A0A143T1U9
A	-12	HIS	-	expression tag	UNP A0A143T1U9
A	-11	HIS	-	expression tag	UNP A0A143T1U9
A	-10	SER	-	expression tag	UNP A0A143T1U9
A	-9	SER	-	expression tag	UNP A0A143T1U9
A	-8	GLY	-	expression tag	UNP A0A143T1U9
A	-7	LEU	-	expression tag	UNP A0A143T1U9
A	-6	VAL	-	expression tag	UNP A0A143T1U9
A	-5	PRO	-	expression tag	UNP A0A143T1U9
A	-4	ARG	-	expression tag	UNP A0A143T1U9
A	-3	GLY	-	expression tag	UNP A0A143T1U9
A	-2	SER	-	expression tag	UNP A0A143T1U9
A	-1	HIS	-	expression tag	UNP A0A143T1U9
B	-20	MET	-	initiating methionine	UNP A0A143T1U9

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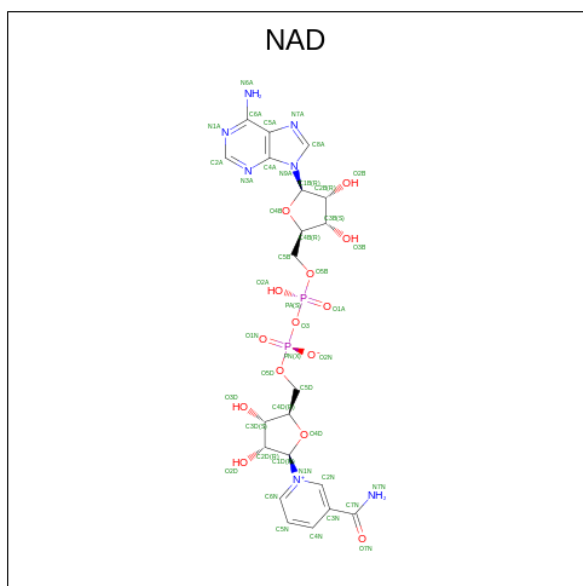
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	GLY	-	expression tag	UNP A0A143T1U9
B	-18	SER	-	expression tag	UNP A0A143T1U9
B	-17	SER	-	expression tag	UNP A0A143T1U9
B	-16	HIS	-	expression tag	UNP A0A143T1U9
B	-15	HIS	-	expression tag	UNP A0A143T1U9
B	-14	HIS	-	expression tag	UNP A0A143T1U9
B	-13	HIS	-	expression tag	UNP A0A143T1U9
B	-12	HIS	-	expression tag	UNP A0A143T1U9
B	-11	HIS	-	expression tag	UNP A0A143T1U9
B	-10	SER	-	expression tag	UNP A0A143T1U9
B	-9	SER	-	expression tag	UNP A0A143T1U9
B	-8	GLY	-	expression tag	UNP A0A143T1U9
B	-7	LEU	-	expression tag	UNP A0A143T1U9
B	-6	VAL	-	expression tag	UNP A0A143T1U9
B	-5	PRO	-	expression tag	UNP A0A143T1U9
B	-4	ARG	-	expression tag	UNP A0A143T1U9
B	-3	GLY	-	expression tag	UNP A0A143T1U9
B	-2	SER	-	expression tag	UNP A0A143T1U9
B	-1	HIS	-	expression tag	UNP A0A143T1U9
C	-20	MET	-	initiating methionine	UNP A0A143T1U9
C	-19	GLY	-	expression tag	UNP A0A143T1U9
C	-18	SER	-	expression tag	UNP A0A143T1U9
C	-17	SER	-	expression tag	UNP A0A143T1U9
C	-16	HIS	-	expression tag	UNP A0A143T1U9
C	-15	HIS	-	expression tag	UNP A0A143T1U9
C	-14	HIS	-	expression tag	UNP A0A143T1U9
C	-13	HIS	-	expression tag	UNP A0A143T1U9
C	-12	HIS	-	expression tag	UNP A0A143T1U9
C	-11	HIS	-	expression tag	UNP A0A143T1U9
C	-10	SER	-	expression tag	UNP A0A143T1U9
C	-9	SER	-	expression tag	UNP A0A143T1U9
C	-8	GLY	-	expression tag	UNP A0A143T1U9
C	-7	LEU	-	expression tag	UNP A0A143T1U9
C	-6	VAL	-	expression tag	UNP A0A143T1U9
C	-5	PRO	-	expression tag	UNP A0A143T1U9
C	-4	ARG	-	expression tag	UNP A0A143T1U9
C	-3	GLY	-	expression tag	UNP A0A143T1U9
C	-2	SER	-	expression tag	UNP A0A143T1U9
C	-1	HIS	-	expression tag	UNP A0A143T1U9
D	-20	MET	-	initiating methionine	UNP A0A143T1U9
D	-19	GLY	-	expression tag	UNP A0A143T1U9
D	-18	SER	-	expression tag	UNP A0A143T1U9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP A0A143T1U9
D	-16	HIS	-	expression tag	UNP A0A143T1U9
D	-15	HIS	-	expression tag	UNP A0A143T1U9
D	-14	HIS	-	expression tag	UNP A0A143T1U9
D	-13	HIS	-	expression tag	UNP A0A143T1U9
D	-12	HIS	-	expression tag	UNP A0A143T1U9
D	-11	HIS	-	expression tag	UNP A0A143T1U9
D	-10	SER	-	expression tag	UNP A0A143T1U9
D	-9	SER	-	expression tag	UNP A0A143T1U9
D	-8	GLY	-	expression tag	UNP A0A143T1U9
D	-7	LEU	-	expression tag	UNP A0A143T1U9
D	-6	VAL	-	expression tag	UNP A0A143T1U9
D	-5	PRO	-	expression tag	UNP A0A143T1U9
D	-4	ARG	-	expression tag	UNP A0A143T1U9
D	-3	GLY	-	expression tag	UNP A0A143T1U9
D	-2	SER	-	expression tag	UNP A0A143T1U9
D	-1	HIS	-	expression tag	UNP A0A143T1U9

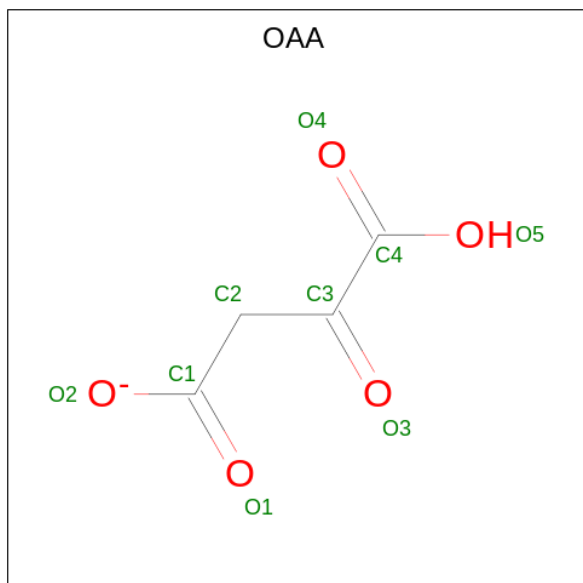
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		
3	B	1	Total	C	O	0	0
			9	4	5		
3	C	1	Total	C	O	0	0
			9	4	5		
3	D	1	Total	C	O	0	0
			9	4	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	8	Total	O	0	0
			8	8		
4	C	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	14	Total	O	0	0
			14	14		

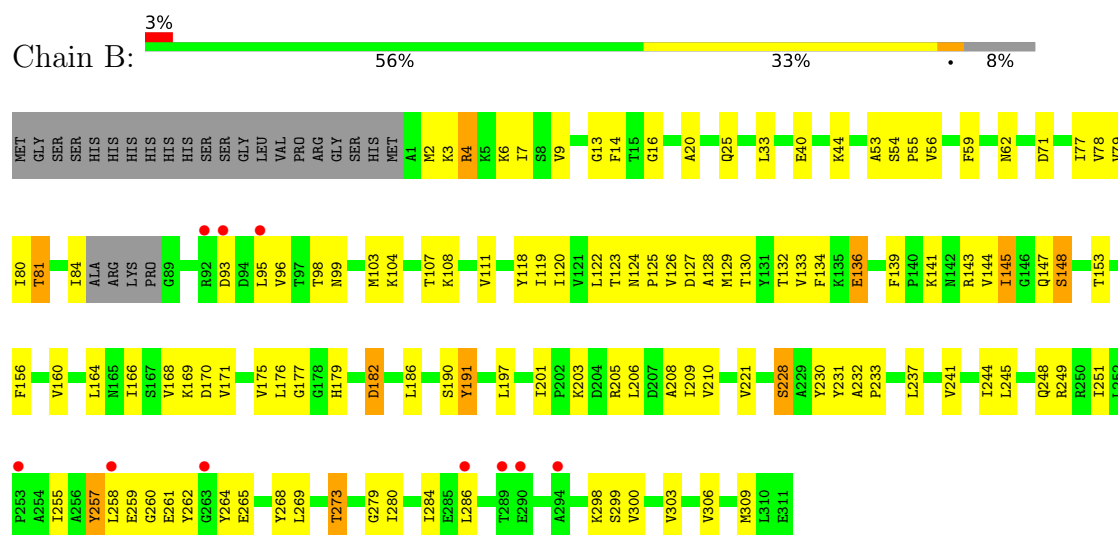
3 Residue-property plots

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: Malate dehydrogenase

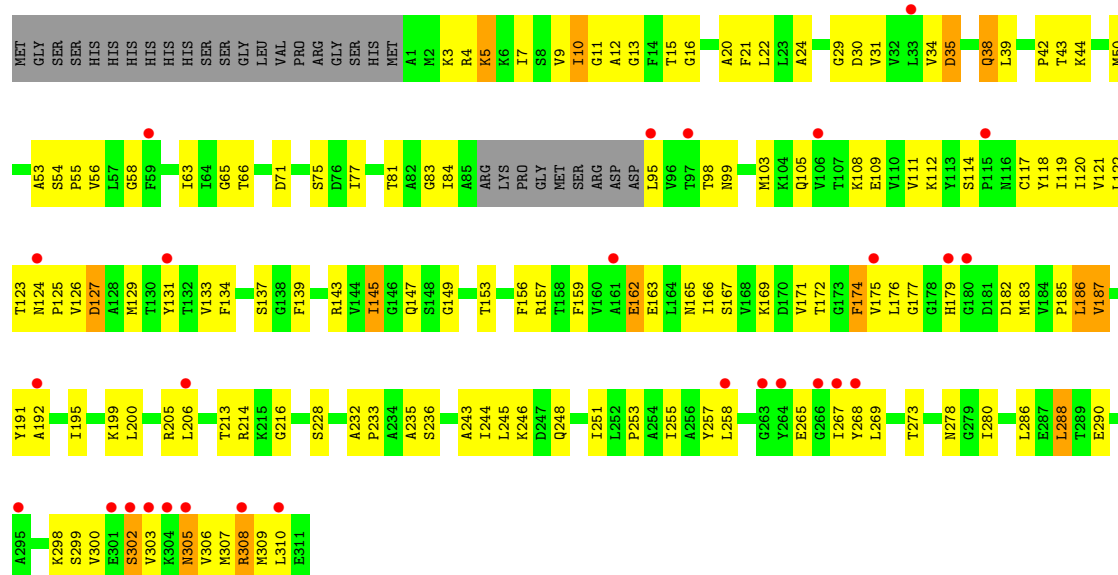


• Molecule 1: Malate dehydrogenase

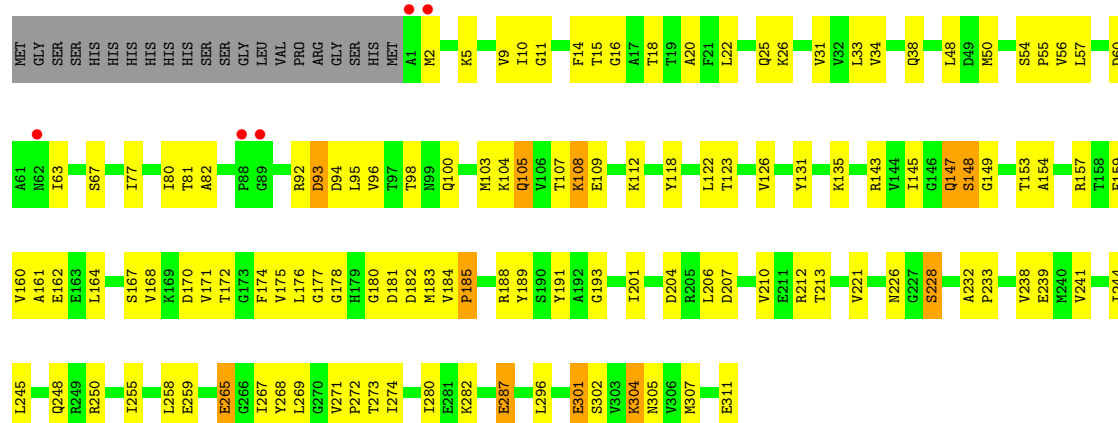


• Molecule 1: Malate dehydrogenase





• Molecule 1: Malate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.16Å 83.24Å 119.48Å 90.00° 93.42° 90.00°	Depositor
Resolution (Å)	39.39 – 2.20 39.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.39-2.20) 99.5 (39.36-2.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	279.41 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.224 , 0.285 0.234 , 0.287	Depositor DCC
R_{free} test set	3047 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9578	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OAA, 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	0.81	1/2392 (0.0%)	0.93	0/3235
1	B	0.78	0/2358	0.95	0/3188
1	C	0.77	0/2318	0.92	0/3136
1	D	0.79	1/2392 (0.0%)	0.92	0/3235
All	All	0.79	2/9460 (0.0%)	0.93	0/12794

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	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	GLU	CD-OE2	-5.80	1.19	1.25
1	D	239	GLU	CD-OE2	-5.08	1.20	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	MET	Peptide
1	C	125	PRO	Peptide

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	2359	0	2435	78	0
1	B	2327	0	2396	83	0
1	C	2287	0	2363	99	0
1	D	2359	0	2435	90	0
2	A	44	0	26	1	0
2	B	44	0	26	4	0
2	C	44	0	26	2	0
2	D	44	0	26	2	0
3	A	9	0	2	0	0
3	B	9	0	2	2	0
3	C	9	0	2	1	0
3	D	9	0	2	0	0
4	A	10	0	0	0	0
4	B	8	0	0	0	0
4	C	2	0	0	0	0
4	D	14	0	0	0	0
All	All	9578	0	9741	327	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 17.

All (327) 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:D:15:THR:HG21	1:D:122:LEU:CD2	2.04	0.86
1:C:145:ILE:HG23	1:C:280:ILE:HD11	1.59	0.84
1:A:252:LEU:O	1:A:273:THR:HG22	1.79	0.83
1:D:105:GLN:HA	1:D:108:LYS:HE2	1.61	0.82
1:A:145:ILE:HG23	1:A:280:ILE:HD11	1.64	0.79
1:A:10:ILE:HG21	1:A:106:VAL:HG13	1.65	0.78
1:A:15:THR:HG21	1:A:122:LEU:CD2	2.15	0.77
1:C:175:VAL:HA	1:C:185:PRO:HA	1.66	0.77
1:D:188:ARG:NH2	1:D:287:GLU:O	2.16	0.77
1:D:153:THR:HG22	1:D:175:VAL:HG13	1.67	0.76
1:A:77:ILE:HD13	1:A:118:TYR:HB2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LEU:O	1:D:210:VAL:HG23	1.87	0.74
1:D:177:GLY:HA2	1:D:269:LEU:HD11	1.69	0.73
1:D:131:TYR:CD2	1:D:307:MET:HE3	2.24	0.72
1:B:144:VAL:C	1:B:145:ILE:HD13	2.10	0.72
1:C:119:ILE:HG21	1:C:133:VAL:HG11	1.72	0.72
1:D:94:ASP:O	1:D:98:THR:OG1	2.03	0.71
1:A:174:PHE:CZ	1:A:286:LEU:HD11	2.26	0.71
1:B:145:ILE:HG23	1:B:280:ILE:HD11	1.72	0.71
1:C:183:MET:O	1:C:214:ARG:NH2	2.24	0.71
1:A:53:ALA:HB2	1:B:232:ALA:HA	1.72	0.71
1:D:10:ILE:HG22	1:D:82:ALA:HB2	1.73	0.71
1:C:9:VAL:HG11	1:C:16:GLY:O	1.92	0.70
1:D:131:TYR:CD2	1:D:307:MET:CE	2.75	0.70
1:D:14:PHE:O	1:D:18:THR:OG1	2.06	0.70
1:A:269:LEU:HD21	1:A:296:LEU:HD11	1.73	0.69
1:B:4:ARG:NH1	1:B:62:ASN:OD1	2.25	0.69
1:D:149:GLY:O	1:D:153:THR:HG23	1.93	0.68
1:B:258:LEU:HD11	1:B:269:LEU:HD23	1.74	0.68
1:A:145:ILE:HD12	1:A:280:ILE:HG13	1.76	0.67
1:C:123:THR:O	1:C:126:VAL:HA	1.94	0.67
1:B:104:LYS:HA	1:B:136:GLU:HG2	1.76	0.67
1:A:54:SER:OG	1:A:55:PRO:HD3	1.94	0.67
1:D:258:LEU:HD21	1:D:271:VAL:HG11	1.76	0.67
1:D:145:ILE:HD12	1:D:280:ILE:HG13	1.76	0.66
1:D:232:ALA:HB3	1:D:233:PRO:HD3	1.78	0.66
1:A:64:ILE:HD11	1:A:71:ASP:HB3	1.77	0.66
1:C:111:VAL:HG12	1:C:139:PHE:CZ	2.31	0.65
1:A:7:ILE:HG21	1:A:23:LEU:HD13	1.78	0.65
1:C:186:LEU:HD13	1:C:186:LEU:N	2.12	0.65
1:C:187:VAL:HG21	1:C:206:LEU:HD21	1.78	0.65
1:B:232:ALA:HB3	1:B:233:PRO:HD3	1.77	0.65
1:C:183:MET:HE1	1:C:213:THR:HG22	1.78	0.64
1:C:121:VAL:HG21	1:C:133:VAL:HG21	1.78	0.64
1:C:182:ASP:O	1:C:299:SER:OG	2.09	0.64
1:C:127:ASP:HA	1:C:255:ILE:HG21	1.79	0.63
1:C:20:ALA:HB1	1:C:31:VAL:HG11	1.81	0.62
1:D:267:ILE:HG21	1:D:304:LYS:HD2	1.80	0.62
1:D:131:TYR:CE2	1:D:307:MET:CE	2.82	0.62
1:B:190:SER:HB2	1:B:197:LEU:HD12	1.81	0.61
1:C:145:ILE:HD13	1:C:280:ILE:HG13	1.82	0.61
1:B:99:ASN:ND2	1:B:124:ASN:O	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ALA:HB2	1:B:33:LEU:HD13	1.83	0.61
1:C:13:GLY:HA3	2:C:400:NAD:O2A	1.99	0.61
1:C:24:ALA:CB	1:C:63:ILE:HD11	2.30	0.61
1:B:251:ILE:HD11	1:C:166:ILE:HG21	1.83	0.60
1:D:50:MET:HB3	1:D:63:ILE:HD13	1.82	0.60
1:C:149:GLY:O	1:C:153:THR:OG1	2.10	0.60
1:D:25:GLN:OE1	1:D:57:LEU:HD13	2.00	0.60
1:C:159:PHE:O	1:C:162:GLU:HG3	2.02	0.60
1:A:34:VAL:HA	1:A:66:THR:O	2.02	0.60
1:B:122:LEU:HD11	2:B:400:NAD:O7N	2.02	0.60
1:A:7:ILE:HG21	1:A:23:LEU:CD1	2.32	0.59
1:B:145:ILE:HD12	1:B:280:ILE:HG13	1.84	0.59
1:C:15:THR:HG21	1:C:122:LEU:HD22	1.84	0.59
1:A:176:LEU:HD23	1:A:272:PRO:HD3	1.85	0.59
1:B:148:SER:HB2	1:B:179:HIS:CE1	2.38	0.59
1:C:153:THR:HG23	1:C:175:VAL:HG13	1.85	0.59
1:A:32:VAL:HG21	1:A:71:ASP:O	2.03	0.58
1:A:15:THR:HG21	1:A:122:LEU:HD22	1.86	0.58
1:C:192:ALA:HB3	1:C:200:LEU:HD13	1.85	0.58
1:C:84:ILE:HG22	1:C:99:ASN:OD1	2.04	0.58
1:D:31:VAL:O	1:D:63:ILE:HA	2.04	0.58
1:D:301:GLU:O	1:D:305:ASN:HB2	2.03	0.57
1:B:156:PHE:O	1:B:160:VAL:HG23	2.04	0.57
1:B:118:TYR:CE1	1:B:143:ARG:HD2	2.40	0.57
1:A:10:ILE:HG21	1:A:106:VAL:CG1	2.33	0.56
1:A:27:GLU:OE1	1:C:246:LYS:NZ	2.25	0.56
1:B:177:GLY:HA2	1:B:269:LEU:HD12	1.88	0.56
1:C:103:MET:HA	1:C:103:MET:CE	2.36	0.56
1:B:153:THR:HG23	1:B:175:VAL:HG22	1.87	0.56
1:A:100:GLN:O	1:A:103:MET:HB2	2.06	0.55
1:B:77:ILE:HG12	1:B:245:LEU:HD21	1.88	0.55
1:D:54:SER:N	1:D:55:PRO:CD	2.70	0.55
1:C:118:TYR:OH	1:C:278:ASN:HA	2.07	0.55
1:B:6:LYS:NZ	1:B:71:ASP:O	2.35	0.55
1:C:129:MET:O	1:C:133:VAL:HG23	2.05	0.55
1:B:258:LEU:O	1:B:265:GLU:HA	2.07	0.55
1:A:174:PHE:CE1	1:A:286:LEU:HD11	2.41	0.55
1:A:105:GLN:HG3	1:A:106:VAL:N	2.22	0.55
1:D:135:LYS:HE3	1:D:135:LYS:HA	1.89	0.54
1:C:149:GLY:HA3	1:C:253:PRO:HB2	1.89	0.54
1:D:103:MET:HE3	1:D:123:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ALA:HB3	1:A:233:PRO:HD3	1.90	0.54
1:A:41:ASN:HB2	1:A:42:PRO:HD3	1.89	0.54
1:C:126:VAL:HG13	1:C:255:ILE:HD11	1.89	0.54
1:A:256:ALA:CB	1:A:280:ILE:HD13	2.38	0.54
1:B:127:ASP:OD1	1:B:128:ALA:N	2.41	0.54
1:D:104:LYS:O	1:D:108:LYS:HG2	2.06	0.54
1:A:15:THR:HG21	1:A:122:LEU:HD21	1.89	0.54
1:C:54:SER:OG	1:C:55:PRO:HD3	2.08	0.54
1:B:79:VAL:HA	1:B:120:ILE:O	2.08	0.53
1:D:259:GLU:HA	1:D:265:GLU:HG2	1.91	0.53
1:A:60:ASP:OD2	1:B:169:LYS:NZ	2.40	0.53
1:A:157:ARG:NE	1:A:171:VAL:O	2.41	0.53
1:B:258:LEU:CD1	1:B:269:LEU:HD23	2.38	0.53
1:D:157:ARG:HA	1:D:171:VAL:HG11	1.89	0.53
1:B:40:GLU:HG2	1:B:44:LYS:CE	2.39	0.52
1:D:20:ALA:HB2	1:D:33:LEU:HD13	1.90	0.52
1:A:203:LYS:HE2	1:A:207:ASP:OD2	2.10	0.52
1:D:241:VAL:HG12	1:D:245:LEU:HD12	1.91	0.52
1:C:77:ILE:HG12	1:C:245:LEU:HD21	1.92	0.52
1:B:164:LEU:HD21	1:B:201:ILE:HG12	1.91	0.52
1:C:153:THR:CG2	1:C:175:VAL:HG13	2.40	0.52
1:D:185:PRO:HG3	1:D:210:VAL:HG13	1.92	0.51
1:B:107:THR:HG21	1:B:136:GLU:HB3	1.91	0.51
1:A:149:GLY:O	1:A:153:THR:HG23	2.10	0.51
1:C:153:THR:HG21	1:C:253:PRO:HG3	1.91	0.51
1:D:5:LYS:HG3	1:D:245:LEU:HD22	1.92	0.51
1:D:250:ARG:O	1:D:274:ILE:HA	2.10	0.51
1:D:269:LEU:HD21	1:D:296:LEU:HD11	1.91	0.51
1:B:260:GLY:N	1:B:265:GLU:HB3	2.24	0.51
1:D:221:VAL:HG22	1:D:228:SER:HA	1.93	0.51
1:A:153:THR:HG22	1:A:175:VAL:HG13	1.93	0.51
1:D:176:LEU:CD2	1:D:272:PRO:HD3	2.41	0.51
1:B:84:ILE:HD12	1:B:98:THR:HG21	1.92	0.50
1:A:11:GLY:N	1:A:34:VAL:O	2.42	0.50
1:C:126:VAL:HG13	1:C:255:ILE:CD1	2.41	0.50
1:D:11:GLY:N	1:D:34:VAL:O	2.42	0.50
1:D:10:ILE:HG22	1:D:82:ALA:CB	2.41	0.50
1:B:78:VAL:O	1:B:119:ILE:HA	2.11	0.50
1:A:232:ALA:HA	1:B:53:ALA:HB2	1.93	0.50
1:B:182:ASP:OD1	1:B:182:ASP:N	2.44	0.50
1:C:103:MET:HA	1:C:103:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:THR:HG21	1:D:122:LEU:HD23	1.91	0.50
1:C:53:ALA:HB2	1:D:232:ALA:HA	1.94	0.50
1:B:255:ILE:HG22	1:B:268:TYR:HD2	1.77	0.50
1:D:182:ASP:CG	1:D:302:SER:HB3	2.32	0.50
1:D:131:TYR:CG	1:D:307:MET:HE1	2.47	0.49
1:A:205:ARG:O	1:A:208:ALA:HB3	2.12	0.49
1:C:306:VAL:O	1:C:309:MET:HB2	2.11	0.49
1:D:201:ILE:HD12	1:D:206:LEU:HD13	1.95	0.49
1:A:288:LEU:HB3	1:A:292:GLU:HB2	1.94	0.49
1:B:230:TYR:CE2	1:B:231:TYR:CE2	3.01	0.49
1:D:10:ILE:HG13	1:D:80:ILE:HG12	1.95	0.49
1:A:55:PRO:HG3	1:B:168:VAL:CG1	2.42	0.49
1:A:230:TYR:C	1:A:233:PRO:HD2	2.33	0.49
1:C:183:MET:CE	1:C:213:THR:HG22	2.43	0.49
1:A:248:GLN:O	1:D:167:SER:HB2	2.13	0.49
1:B:129:MET:O	1:B:133:VAL:HG23	2.13	0.49
1:C:44:LYS:HA	1:C:65:GLY:HA3	1.95	0.49
1:B:244:ILE:HG12	1:B:279:GLY:HA2	1.95	0.49
1:D:161:ALA:CB	1:D:168:VAL:HG12	2.43	0.48
1:D:176:LEU:HD22	1:D:272:PRO:HD3	1.95	0.48
1:B:170:ASP:OD2	1:C:251:ILE:N	2.27	0.48
1:B:206:LEU:HA	1:B:209:ILE:HD12	1.95	0.48
1:B:264:TYR:CD1	1:B:300:VAL:HG11	2.48	0.48
1:C:258:LEU:HD12	1:C:267:ILE:HD11	1.95	0.48
1:D:182:ASP:OD2	1:D:302:SER:CB	2.61	0.48
1:B:145:ILE:HD13	1:B:145:ILE:N	2.28	0.48
1:A:274:ILE:HB	1:A:281:GLU:HB2	1.94	0.48
1:B:111:VAL:HG12	1:B:139:PHE:CZ	2.48	0.48
1:D:92:ARG:O	1:D:96:VAL:HG23	2.13	0.48
1:A:234:ALA:O	1:A:238:VAL:HG23	2.14	0.48
1:B:134:PHE:HB2	1:B:268:TYR:OH	2.14	0.47
1:A:96:VAL:HG11	1:A:309:MET:HB2	1.95	0.47
1:C:157:ARG:NE	1:C:171:VAL:O	2.48	0.47
1:B:237:LEU:O	1:B:241:VAL:HG23	2.15	0.47
1:C:114:SER:HB3	1:C:117:CYS:HB3	1.95	0.47
1:C:175:VAL:HA	1:C:185:PRO:CA	2.42	0.47
1:A:102:ILE:HG23	2:A:400:NAD:N6A	2.30	0.47
1:A:256:ALA:HB2	1:A:280:ILE:HD13	1.97	0.47
1:B:9:VAL:HG11	1:B:16:GLY:O	2.15	0.47
1:C:12:ALA:HB3	1:C:35:ASP:HB2	1.96	0.47
1:C:15:THR:HG21	1:C:122:LEU:CD2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:TYR:HB2	1:C:268:TYR:CE1	2.50	0.47
1:D:267:ILE:HG22	1:D:307:MET:SD	2.55	0.47
1:C:183:MET:O	1:C:214:ARG:CZ	2.63	0.47
1:C:305:ASN:O	1:C:308:ARG:N	2.45	0.47
1:A:36:ILE:HG12	1:A:39:LEU:HD12	1.96	0.46
1:A:92:ARG:O	1:A:96:VAL:HG23	2.14	0.46
1:C:75:SER:N	1:C:114:SER:OG	2.47	0.46
1:C:134:PHE:O	1:C:137:SER:OG	2.34	0.46
1:D:131:TYR:CD1	1:D:307:MET:HE1	2.51	0.46
1:A:102:ILE:O	1:A:106:VAL:HG23	2.14	0.46
1:A:294:ALA:O	1:A:297:ALA:HB3	2.14	0.46
1:B:186:LEU:O	1:B:190:SER:OG	2.33	0.46
1:B:206:LEU:O	1:B:210:VAL:HG23	2.15	0.46
1:B:176:LEU:HD12	1:B:186:LEU:HD13	1.98	0.46
1:D:160:VAL:CG1	1:D:164:LEU:HD12	2.46	0.46
1:B:81:THR:O	2:B:400:NAD:H52N	2.15	0.46
1:B:299:SER:O	1:B:303:VAL:HG23	2.16	0.46
1:D:15:THR:HG21	1:D:122:LEU:HD21	1.95	0.46
1:A:66:THR:HG21	1:A:71:ASP:HB2	1.97	0.46
1:B:80:ILE:HG21	1:B:103:MET:HE2	1.98	0.46
1:B:255:ILE:HG22	1:B:268:TYR:CD2	2.50	0.46
1:C:4:ARG:HD2	1:C:30:ASP:OD1	2.16	0.46
1:C:66:THR:HG21	1:C:71:ASP:HB2	1.98	0.46
1:D:81:THR:O	2:D:400:NAD:H4D	2.16	0.46
1:D:135:LYS:HA	1:D:135:LYS:CE	2.47	0.45
1:D:161:ALA:HB2	1:D:168:VAL:HG12	1.98	0.45
1:A:257:TYR:HA	1:A:267:ILE:O	2.16	0.45
1:C:267:ILE:HG22	1:C:307:MET:HE1	1.97	0.45
1:D:147:GLN:CD	1:D:148:SER:N	2.69	0.45
1:A:97:THR:HG21	1:A:311:GLU:OE2	2.16	0.45
1:A:251:ILE:HA	1:A:273:THR:O	2.17	0.45
1:A:95:LEU:HD13	1:A:96:VAL:N	2.31	0.45
1:B:260:GLY:H	1:B:265:GLU:HB3	1.82	0.45
1:C:39:LEU:C	1:C:42:PRO:HD2	2.36	0.45
1:C:177:GLY:HA2	1:C:269:LEU:HD11	1.99	0.45
1:D:160:VAL:HG12	1:D:164:LEU:HD12	1.97	0.45
1:B:205:ARG:O	1:B:208:ALA:HB3	2.16	0.45
1:C:54:SER:O	1:C:58:GLY:N	2.42	0.45
1:A:145:ILE:HG23	1:A:280:ILE:CD1	2.42	0.45
1:A:146:GLY:HA3	1:A:255:ILE:HB	1.98	0.45
1:D:82:ALA:HB1	2:D:400:NAD:C4A	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:VAL:HA	1:D:184:VAL:O	2.17	0.44
1:C:34:VAL:HA	1:C:66:THR:O	2.17	0.44
1:C:166:ILE:HD11	1:C:192:ALA:HB1	1.99	0.44
1:C:169:LYS:NZ	1:D:60:ASP:OD2	2.44	0.44
1:D:9:VAL:HG11	1:D:16:GLY:O	2.17	0.44
1:A:39:LEU:C	1:A:42:PRO:HD2	2.38	0.44
1:A:55:PRO:HG3	1:B:168:VAL:HG11	2.00	0.44
1:C:5:LYS:HG3	1:C:245:LEU:HD22	1.98	0.44
1:D:26:LYS:HE3	1:D:238:VAL:HG11	2.00	0.44
1:B:96:VAL:HG21	1:B:306:VAL:HG13	1.99	0.44
1:A:9:VAL:HG11	1:A:16:GLY:O	2.17	0.44
1:A:269:LEU:HD13	1:A:300:VAL:HG22	2.00	0.44
1:C:43:THR:HG22	1:C:65:GLY:CA	2.47	0.44
1:C:109:GLU:O	1:C:112:LYS:HB3	2.18	0.44
1:D:131:TYR:CD2	1:D:307:MET:HE1	2.52	0.44
1:A:35:ASP:OD1	1:A:36:ILE:N	2.47	0.44
1:C:300:VAL:O	1:C:303:VAL:HB	2.16	0.44
1:D:258:LEU:HD11	1:D:269:LEU:HD23	2.00	0.44
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.88	0.43
1:B:103:MET:HA	1:B:103:MET:CE	2.48	0.43
1:D:185:PRO:CG	1:D:210:VAL:HG13	2.48	0.43
1:A:58:GLY:O	1:B:169:LYS:HE3	2.18	0.43
1:B:54:SER:OG	1:B:55:PRO:HD3	2.18	0.43
1:B:191:TYR:CE2	1:C:191:TYR:CE2	3.06	0.43
1:D:148:SER:HB3	1:D:255:ILE:HD11	2.00	0.43
1:D:159:PHE:CE2	1:D:212:ARG:HG2	2.53	0.43
1:A:195:ILE:HA	1:D:189:TYR:CE2	2.53	0.43
1:B:108:LYS:NZ	1:B:136:GLU:OE2	2.43	0.43
1:C:118:TYR:HD1	1:C:143:ARG:HA	1.83	0.43
1:C:302:SER:O	1:C:305:ASN:ND2	2.50	0.43
1:D:109:GLU:OE2	1:D:112:LYS:NZ	2.39	0.43
1:A:14:PHE:HD2	1:A:230:TYR:CE1	2.36	0.43
1:A:167:SER:HB2	1:D:248:GLN:O	2.18	0.43
1:A:235:ALA:C	1:B:56:VAL:HG11	2.39	0.43
1:B:126:VAL:HG11	1:B:148:SER:HB3	2.01	0.43
1:B:262:TYR:OH	1:B:284:ILE:O	2.17	0.43
1:C:163:GLU:OE2	1:C:205:ARG:NE	2.37	0.43
1:A:203:LYS:CE	1:A:207:ASP:OD2	2.67	0.43
1:A:232:ALA:N	1:A:233:PRO:CD	2.81	0.43
1:B:249:ARG:NE	1:C:165:ASN:O	2.52	0.43
1:A:111:VAL:HG12	1:A:139:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:C	1:A:145:ILE:HD13	2.39	0.42
1:D:183:MET:CE	1:D:213:THR:HG22	2.48	0.42
1:C:111:VAL:HG11	1:C:137:SER:O	2.18	0.42
1:A:7:ILE:O	1:A:31:VAL:HA	2.19	0.42
1:C:10:ILE:HD12	1:C:34:VAL:HB	2.01	0.42
1:C:83:GLY:O	2:C:400:NAD:H51A	2.19	0.42
1:D:147:GLN:OE1	1:D:148:SER:N	2.52	0.42
1:A:31:VAL:O	1:A:63:ILE:HA	2.20	0.42
1:A:53:ALA:HB2	1:B:232:ALA:CA	2.45	0.42
2:B:400:NAD:H4N	3:B:401:OAA:O5	2.19	0.42
2:B:400:NAD:H4N	3:B:401:OAA:C4	2.49	0.42
1:D:255:ILE:HG22	1:D:268:TYR:HD2	1.84	0.42
1:B:25:GLN:HA	1:B:59:PHE:CG	2.54	0.42
1:B:166:ILE:HD11	1:B:171:VAL:CG2	2.50	0.42
1:B:259:GLU:N	1:B:261:GLU:OE1	2.39	0.42
1:C:186:LEU:N	1:C:186:LEU:CD1	2.79	0.42
1:C:95:LEU:HB3	1:C:98:THR:OG1	2.20	0.42
1:C:232:ALA:HB3	1:C:233:PRO:HD3	2.02	0.42
1:C:243:ALA:HA	1:C:248:GLN:HB2	2.01	0.42
1:B:249:ARG:HD3	1:C:165:ASN:O	2.19	0.42
1:D:183:MET:HE3	1:D:213:THR:HG22	2.01	0.42
1:A:195:ILE:HB	1:A:200:LEU:HD11	2.01	0.42
1:B:144:VAL:O	1:B:145:ILE:HD13	2.19	0.42
1:B:286:LEU:HD21	1:C:195:ILE:HG12	2.02	0.42
1:D:182:ASP:CG	1:D:302:SER:CB	2.88	0.42
1:C:153:THR:O	1:C:156:PHE:HB3	2.19	0.42
1:B:221:VAL:HG22	1:B:228:SER:HB3	2.01	0.42
1:C:176:LEU:HD11	1:C:286:LEU:HD12	2.02	0.42
1:B:125:PRO:CG	1:B:306:VAL:HG11	2.50	0.41
1:B:248:GLN:O	1:C:167:SER:HB2	2.21	0.41
1:D:103:MET:O	1:D:107:THR:OG1	2.27	0.41
1:D:118:TYR:CE1	1:D:143:ARG:HD2	2.55	0.41
1:C:11:GLY:HA3	1:C:81:THR:OG1	2.20	0.41
1:C:38:GLN:OE1	1:C:38:GLN:HA	2.21	0.41
1:D:131:TYR:CG	1:D:307:MET:CE	3.03	0.41
1:A:36:ILE:CG1	1:A:39:LEU:HD12	2.49	0.41
1:D:77:ILE:HD11	1:D:244:ILE:CG2	2.51	0.41
1:D:207:ASP:O	1:D:210:VAL:HB	2.20	0.41
1:A:108:LYS:HG3	1:A:136:GLU:OE2	2.20	0.41
1:A:156:PHE:HB2	1:A:213:THR:HG21	2.03	0.41
1:B:130:THR:HG22	1:B:268:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LYS:O	1:C:29:GLY:HA3	2.19	0.41
1:D:100:GLN:HE22	1:D:311:GLU:N	2.18	0.41
1:C:131:TYR:CE2	1:C:307:MET:HE2	2.56	0.41
1:C:120:ILE:HD11	1:C:244:ILE:HD12	2.03	0.41
1:C:124:ASN:ND2	3:C:401:OAA:C1	2.84	0.41
1:C:236:SER:HA	1:D:56:VAL:HG11	2.02	0.41
1:B:306:VAL:O	1:B:309:MET:HB2	2.20	0.41
1:D:170:ASP:O	1:D:193:GLY:N	2.51	0.41
1:A:26:LYS:NZ	1:A:242:GLU:OE1	2.46	0.41
1:A:147:GLN:C	1:A:147:GLN:CD	2.80	0.41
1:B:257:TYR:HD1	1:B:257:TYR:HA	1.80	0.41
1:C:7:ILE:O	1:C:31:VAL:HA	2.21	0.41
1:C:21:PHE:HE2	1:D:22:LEU:HD21	1.85	0.41
1:C:50:MET:HB3	1:C:63:ILE:HD13	2.03	0.41
1:D:267:ILE:HG21	1:D:304:LYS:CD	2.48	0.41
1:C:166:ILE:CD1	1:C:192:ALA:HB1	2.51	0.41
1:D:123:THR:O	1:D:126:VAL:HA	2.21	0.41
1:B:14:PHE:HB3	1:B:230:TYR:CG	2.55	0.40
1:B:160:VAL:HB	1:B:171:VAL:HG11	2.01	0.40
1:B:251:ILE:HA	1:B:273:THR:O	2.20	0.40
1:C:255:ILE:HG22	1:C:268:TYR:HD2	1.86	0.40
1:C:288:LEU:N	1:C:288:LEU:HD12	2.36	0.40
1:D:93:ASP:OD1	1:D:93:ASP:N	2.52	0.40
1:B:132:THR:O	1:B:136:GLU:HB2	2.21	0.40
1:C:43:THR:HG22	1:C:65:GLY:HA3	2.03	0.40
1:C:56:VAL:HG23	1:D:154:ALA:HB2	2.03	0.40
1:C:235:ALA:HB1	1:D:57:LEU:HG	2.03	0.40
1:D:48:LEU:HD12	1:D:48:LEU:HA	1.94	0.40
1:C:174:PHE:O	1:C:185:PRO:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/332 (93%)	285 (92%)	23 (7%)	1 (0%)	41	46
1	B	303/332 (91%)	285 (94%)	14 (5%)	4 (1%)	12	9
1	C	298/332 (90%)	272 (91%)	24 (8%)	2 (1%)	22	22
1	D	309/332 (93%)	285 (92%)	21 (7%)	3 (1%)	15	14
All	All	1219/1328 (92%)	1127 (92%)	82 (7%)	10 (1%)	19	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	180	GLY
1	B	13	GLY
1	B	123	THR
1	B	148	SER
1	C	216	GLY
1	D	148	SER
1	D	178	GLY
1	B	203	LYS
1	C	22	LEU
1	A	96	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/272 (93%)	237 (93%)	17 (7%)	16	18
1	B	251/272 (92%)	234 (93%)	17 (7%)	16	17
1	C	246/272 (90%)	219 (89%)	27 (11%)	6	5
1	D	254/272 (93%)	231 (91%)	23 (9%)	9	9
All	All	1005/1088 (92%)	921 (92%)	84 (8%)	11	11

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS

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Mol	Chain	Res	Type
1	A	25	GLN
1	A	38	GLN
1	A	74	ASP
1	A	86	ARG
1	A	90	MET
1	A	93	ASP
1	A	105	GLN
1	A	145	ILE
1	A	147	GLN
1	A	172	THR
1	A	175	VAL
1	A	176	LEU
1	A	190	SER
1	A	203	LYS
1	A	242	GLU
1	A	302	SER
1	B	2	MET
1	B	3	LYS
1	B	4	ARG
1	B	7	ILE
1	B	81	THR
1	B	93	ASP
1	B	95	LEU
1	B	136	GLU
1	B	141	LYS
1	B	145	ILE
1	B	147	GLN
1	B	182	ASP
1	B	191	TYR
1	B	228	SER
1	B	257	TYR
1	B	273	THR
1	B	298	LYS
1	C	3	LYS
1	C	5	LYS
1	C	10	ILE
1	C	35	ASP
1	C	38	GLN
1	C	105	GLN
1	C	108	LYS
1	C	127	ASP
1	C	145	ILE

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Mol	Chain	Res	Type
1	C	147	GLN
1	C	162	GLU
1	C	172	THR
1	C	174	PHE
1	C	179	HIS
1	C	186	LEU
1	C	187	VAL
1	C	199	LYS
1	C	228	SER
1	C	265	GLU
1	C	273	THR
1	C	288	LEU
1	C	290	GLU
1	C	298	LYS
1	C	302	SER
1	C	305	ASN
1	C	308	ARG
1	C	310	LEU
1	D	2	MET
1	D	38	GLN
1	D	67	SER
1	D	93	ASP
1	D	95	LEU
1	D	105	GLN
1	D	108	LYS
1	D	147	GLN
1	D	162	GLU
1	D	172	THR
1	D	174	PHE
1	D	181	ASP
1	D	185	PRO
1	D	191	TYR
1	D	204	ASP
1	D	226	ASN
1	D	228	SER
1	D	265	GLU
1	D	273	THR
1	D	282	LYS
1	D	287	GLU
1	D	301	GLU
1	D	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	38	GLN
1	D	179	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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	C	400	-	42,48,48	0.75	2 (4%)	50,73,73	1.28	5 (10%)
3	OAA	A	401	-	2,8,8	0.20	0	2,10,10	1.91	1 (50%)
2	NAD	D	400	-	42,48,48	1.19	2 (4%)	50,73,73	1.07	4 (8%)
2	NAD	A	400	-	42,48,48	0.59	0	50,73,73	1.20	3 (6%)
3	OAA	C	401	-	2,8,8	0.60	0	2,10,10	1.25	0
2	NAD	B	400	-	42,48,48	0.85	1 (2%)	50,73,73	1.59	6 (12%)
3	OAA	B	401	-	2,8,8	0.26	0	2,10,10	1.29	0
3	OAA	D	401	-	2,8,8	0.26	0	2,10,10	2.48	1 (50%)

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	C	400	-	-	4/26/62/62	0/5/5/5
3	OAA	A	401	-	-	1/2/8/8	-
2	NAD	D	400	-	-	16/26/62/62	0/5/5/5
2	NAD	A	400	-	-	6/26/62/62	0/5/5/5
3	OAA	C	401	-	-	2/2/8/8	-
2	NAD	B	400	-	-	15/26/62/62	0/5/5/5
3	OAA	B	401	-	-	0/2/8/8	-
3	OAA	D	401	-	-	2/2/8/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	NAD	C2N-N1N	5.56	1.41	1.35
2	D	400	NAD	O4D-C1D	3.58	1.46	1.41
2	B	400	NAD	C2N-C3N	-2.61	1.35	1.39
2	C	400	NAD	O4D-C1D	2.17	1.44	1.41
2	C	400	NAD	C8A-N7A	-2.06	1.31	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NAD	C3N-C2N-N1N	-5.87	114.69	120.43
2	B	400	NAD	O7N-C7N-C3N	-5.32	113.27	119.63
2	C	400	NAD	C6N-N1N-C2N	-3.95	118.37	121.97
2	A	400	NAD	C6N-N1N-C2N	-3.47	118.81	121.97
2	D	400	NAD	C6N-N1N-C2N	-3.24	119.02	121.97
2	C	400	NAD	C4N-C3N-C7N	3.24	129.70	121.04
2	B	400	NAD	C3N-C7N-N7N	3.15	121.53	117.75
2	A	400	NAD	C4N-C3N-C7N	3.12	129.38	121.04
2	D	400	NAD	O2B-C2B-C3B	3.11	121.89	111.82
3	D	401	OAA	C1-C2-C3	-3.11	109.97	115.51
2	D	400	NAD	O4B-C1B-C2B	-2.63	103.09	106.93
2	B	400	NAD	C5A-C6A-N6A	2.61	124.32	120.35
2	C	400	NAD	O4D-C1D-C2D	-2.58	103.16	106.93
2	B	400	NAD	C6N-N1N-C2N	-2.47	119.72	121.97
2	B	400	NAD	C5N-C4N-C3N	-2.29	117.64	120.34
3	A	401	OAA	O3-C3-C2	-2.24	117.20	120.75
2	D	400	NAD	C5A-C6A-N6A	2.22	123.73	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	NAD	C5A-C6A-N6A	2.16	123.64	120.35
2	C	400	NAD	C5A-C6A-N6A	2.06	123.47	120.35
2	C	400	NAD	C2N-C3N-C7N	-2.01	113.64	119.46

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	NAD	C5D-O5D-PN-O3
2	A	400	NAD	C5D-O5D-PN-O1N
2	A	400	NAD	C5D-O5D-PN-O2N
2	A	400	NAD	O4D-C4D-C5D-O5D
2	B	400	NAD	C5B-O5B-PA-O1A
2	B	400	NAD	C5D-O5D-PN-O1N
2	B	400	NAD	C5D-O5D-PN-O2N
2	B	400	NAD	O4D-C1D-N1N-C2N
2	B	400	NAD	O4D-C1D-N1N-C6N
2	B	400	NAD	C2D-C1D-N1N-C2N
2	C	400	NAD	O4B-C4B-C5B-O5B
2	D	400	NAD	C5B-O5B-PA-O1A
2	D	400	NAD	C5D-O5D-PN-O1N
2	D	400	NAD	C5D-O5D-PN-O2N
2	D	400	NAD	O4D-C1D-N1N-C2N
2	D	400	NAD	O4D-C1D-N1N-C6N
2	A	400	NAD	C3D-C4D-C5D-O5D
2	B	400	NAD	O4B-C4B-C5B-O5B
2	B	400	NAD	C3B-C4B-C5B-O5B
2	D	400	NAD	O4D-C4D-C5D-O5D
2	D	400	NAD	C3D-C4D-C5D-O5D
2	B	400	NAD	O4D-C4D-C5D-O5D
3	C	401	OAA	C1-C2-C3-O3
3	C	401	OAA	C1-C2-C3-C4
2	B	400	NAD	C3D-C4D-C5D-O5D
2	C	400	NAD	C4B-C5B-O5B-PA
2	B	400	NAD	PN-O3-PA-O5B
2	D	400	NAD	PN-O3-PA-O5B
2	B	400	NAD	C5B-O5B-PA-O3
2	D	400	NAD	C5B-O5B-PA-O3
2	D	400	NAD	PN-O3-PA-O1A
2	D	400	NAD	PA-O3-PN-O2N
3	D	401	OAA	C1-C2-C3-O3
3	D	401	OAA	C1-C2-C3-C4

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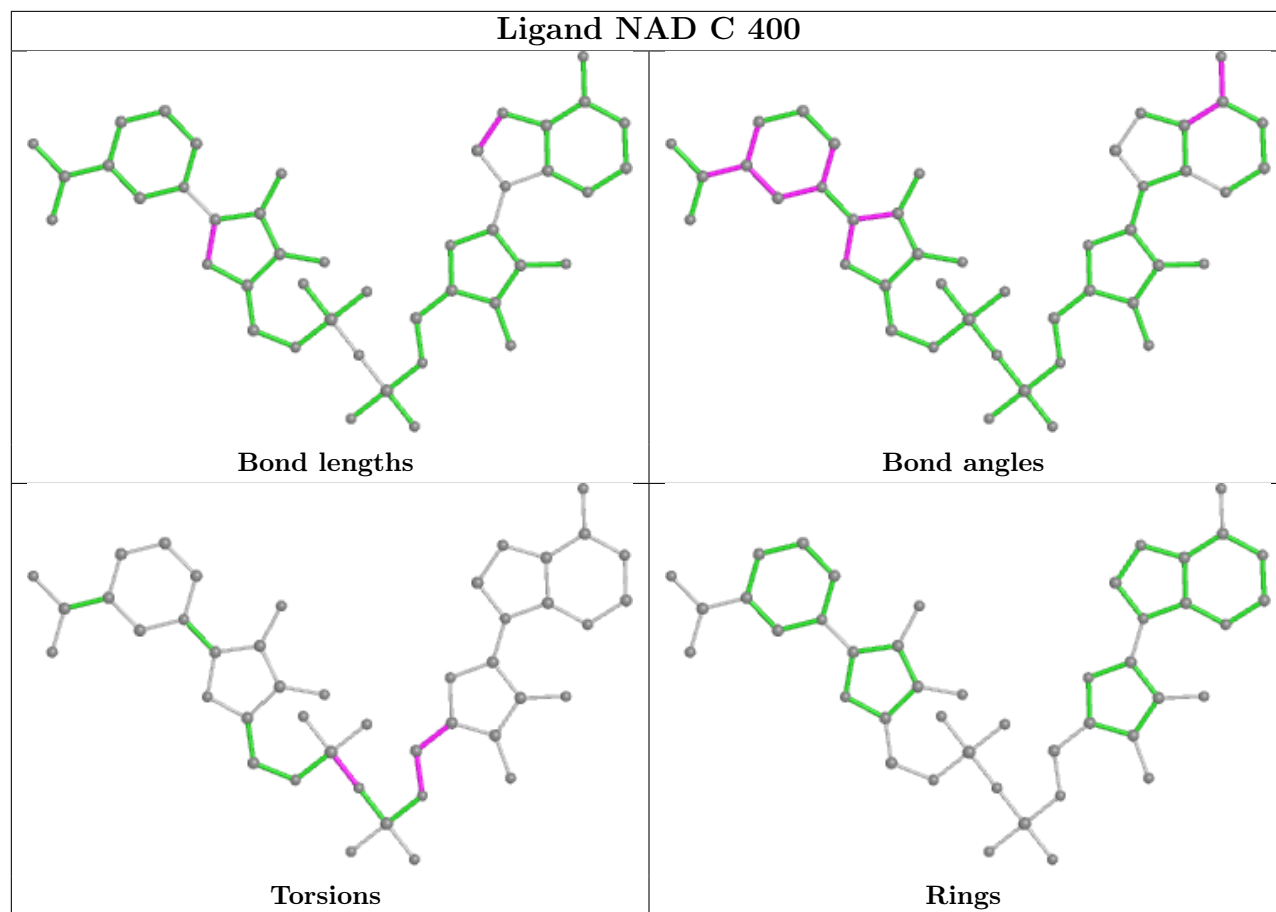
Mol	Chain	Res	Type	Atoms
2	B	400	NAD	C5B-O5B-PA-O2A
2	B	400	NAD	PA-O3-PN-O2N
2	D	400	NAD	C4B-C5B-O5B-PA
2	B	400	NAD	C5D-O5D-PN-O3
2	D	400	NAD	C5D-O5D-PN-O3
2	D	400	NAD	C2D-C1D-N1N-C2N
2	A	400	NAD	O4B-C4B-C5B-O5B
2	C	400	NAD	PA-O3-PN-O1N
2	D	400	NAD	PA-O3-PN-O1N
3	A	401	OAA	C1-C2-C3-C4
2	C	400	NAD	C3B-C4B-C5B-O5B
2	D	400	NAD	O4B-C4B-C5B-O5B

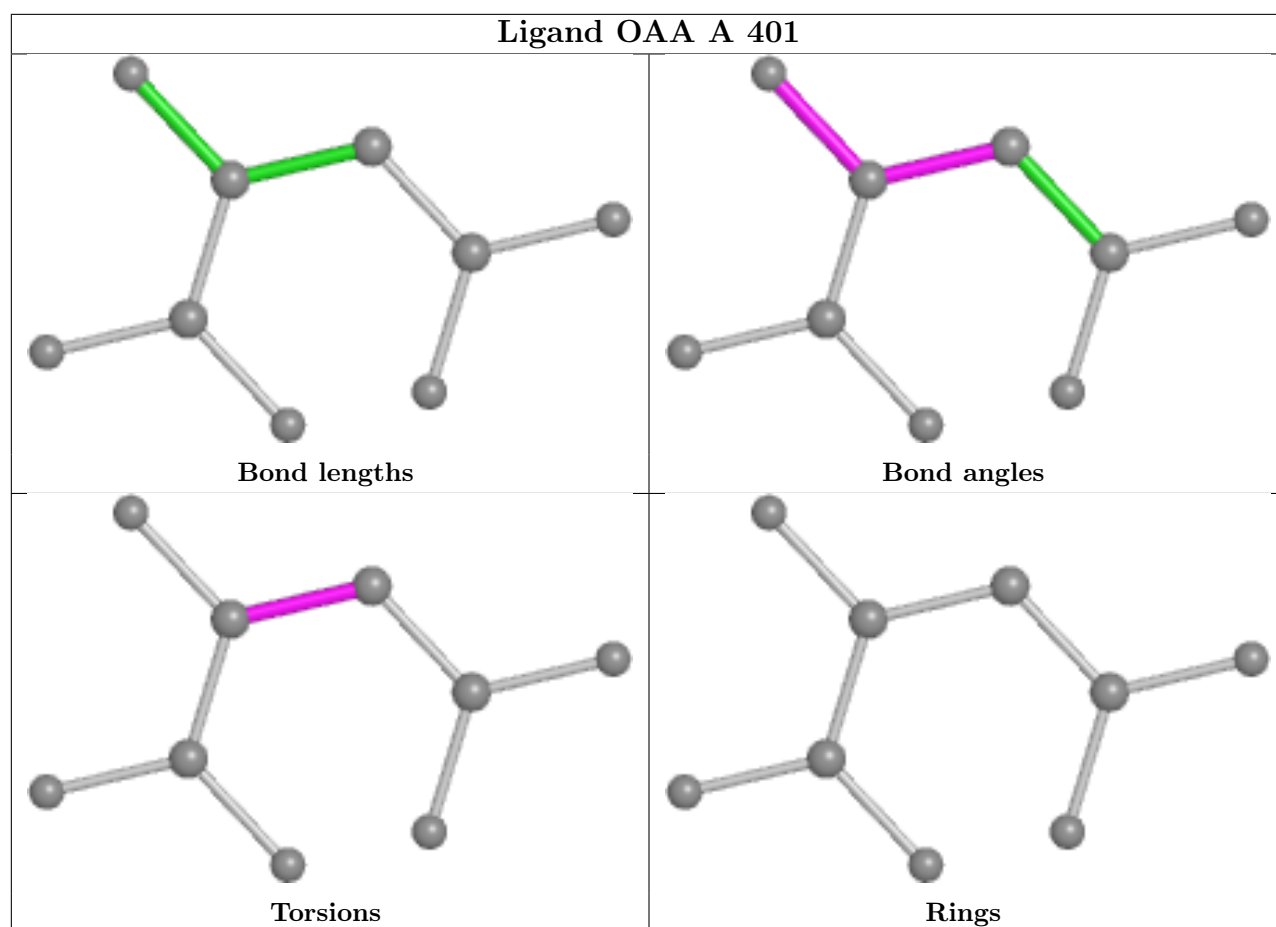
There are no ring outliers.

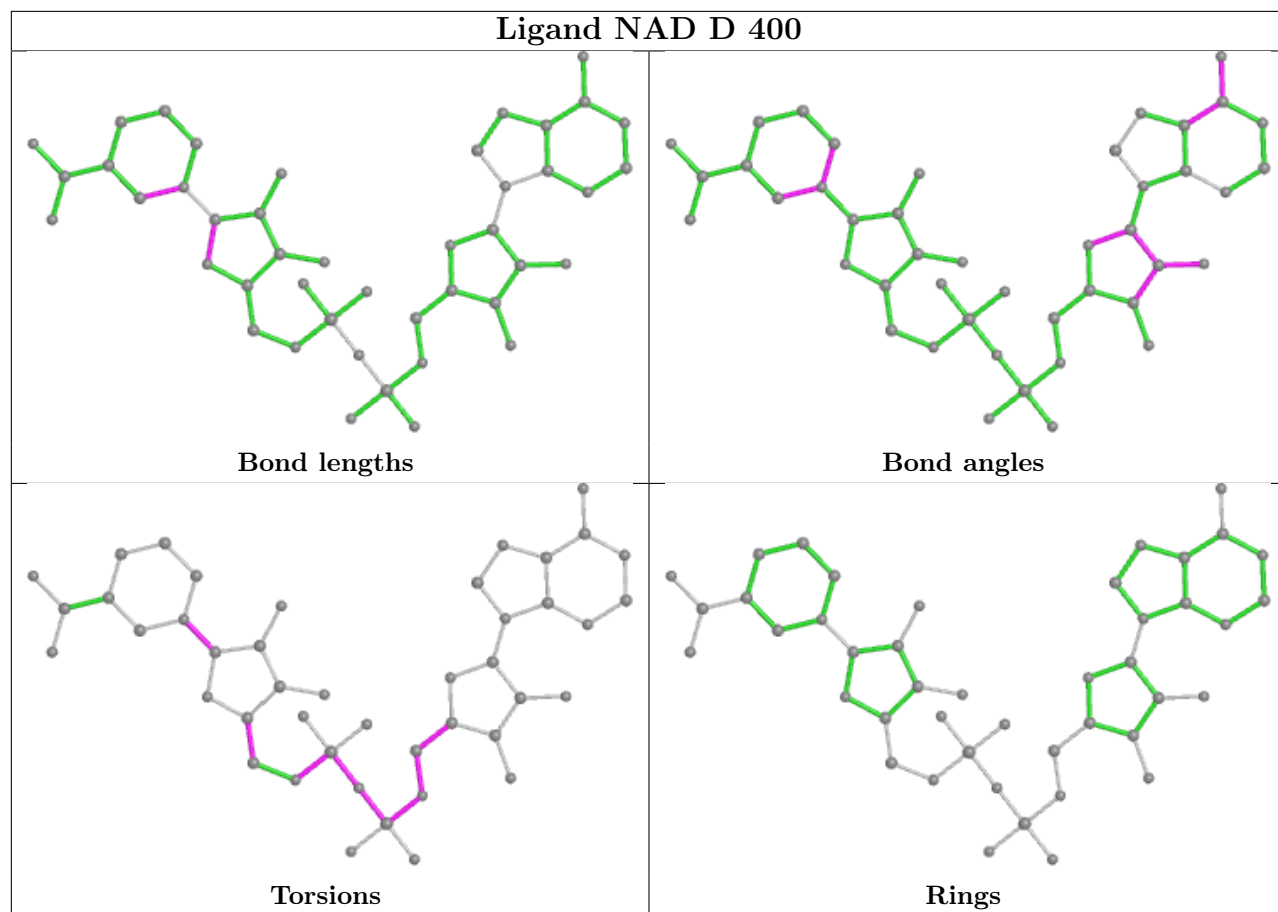
6 monomers are involved in 10 short contacts:

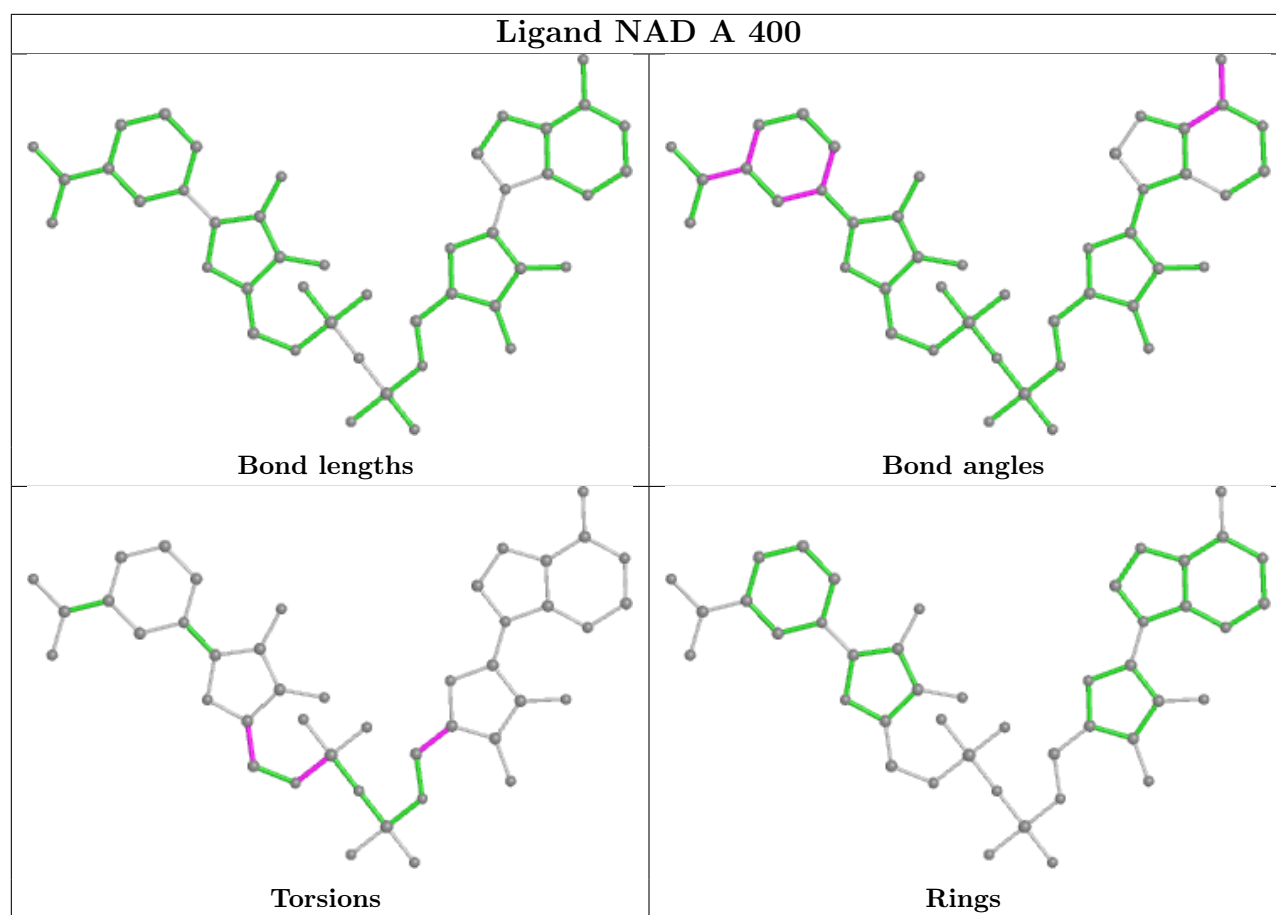
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400	NAD	2	0
2	D	400	NAD	2	0
2	A	400	NAD	1	0
3	C	401	OAA	1	0
2	B	400	NAD	4	0
3	B	401	OAA	2	0

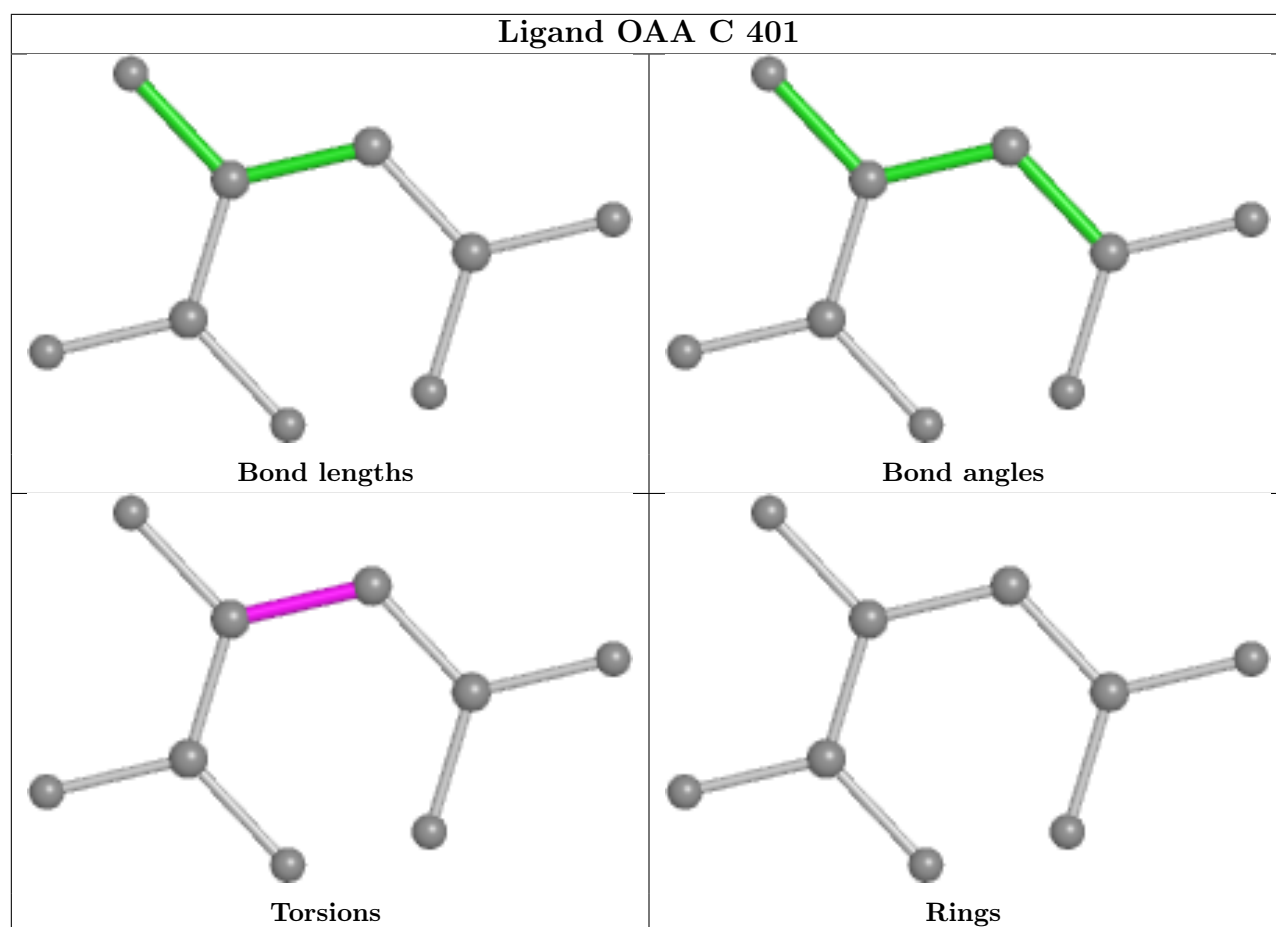
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

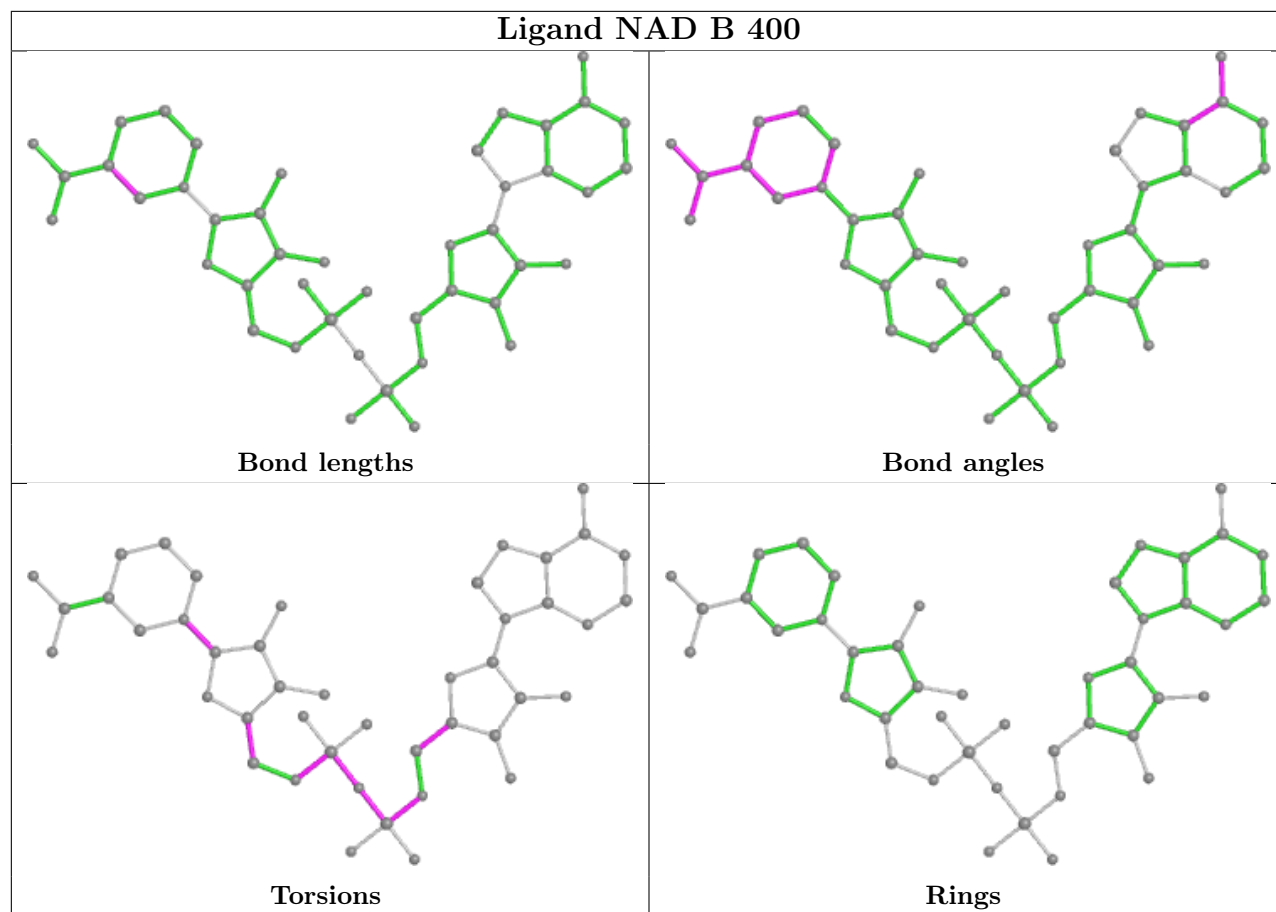


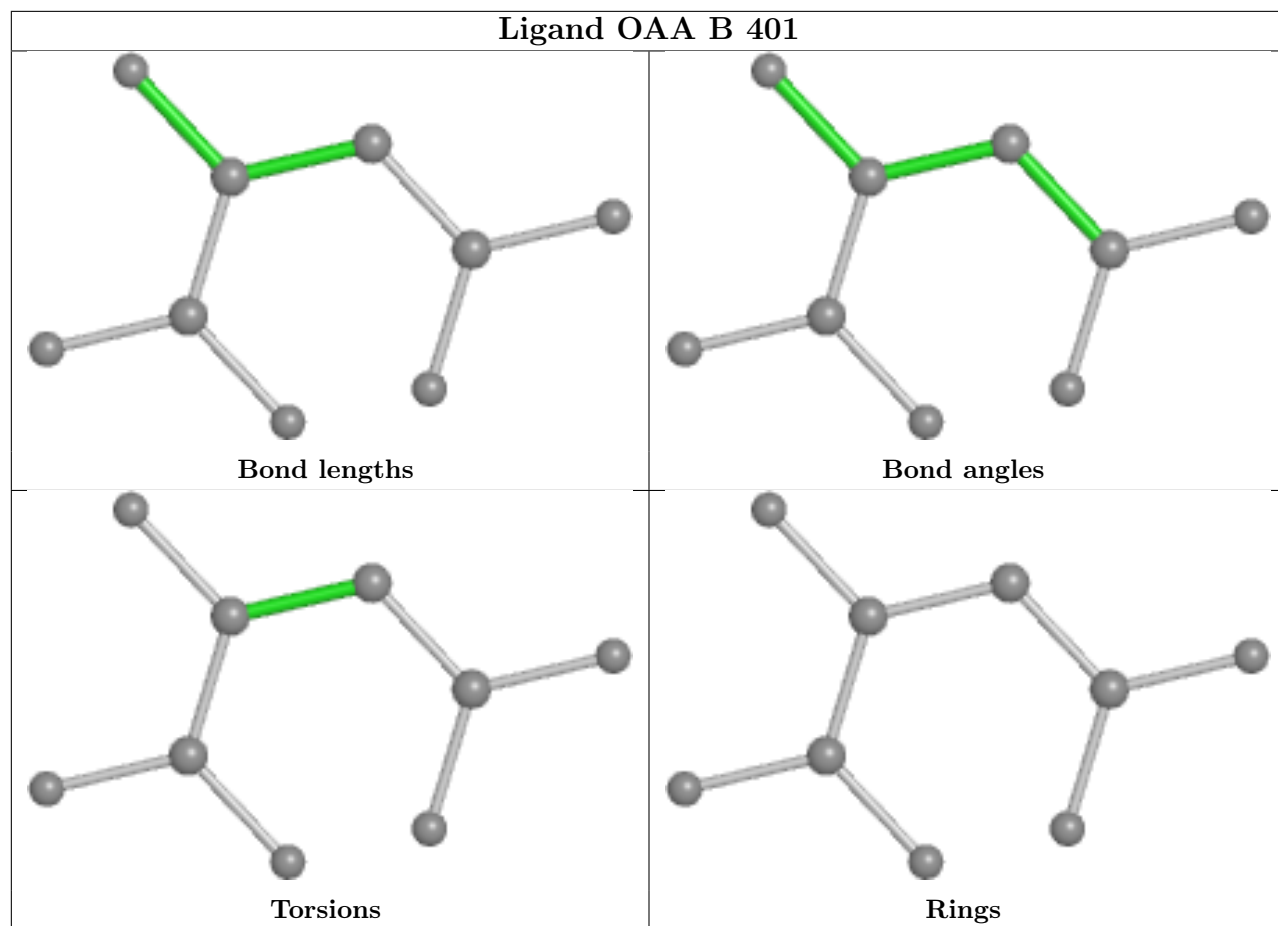


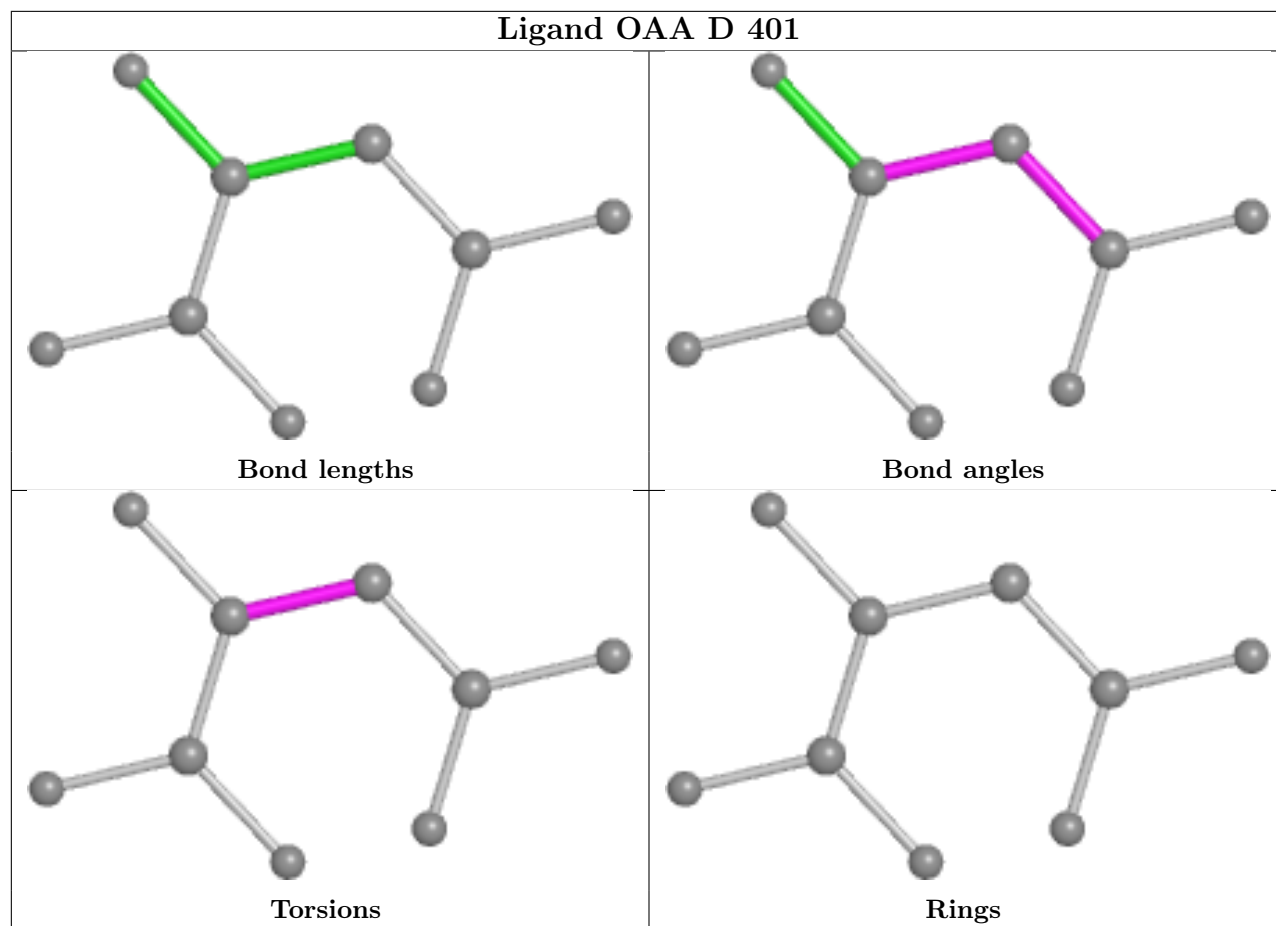












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	311/332 (93%)	0.32	8 (2%) 56 53	31, 43, 55, 81	0
1	B	307/332 (92%)	0.36	10 (3%) 46 44	28, 44, 58, 77	0
1	C	302/332 (90%)	0.57	28 (9%) 8 7	32, 47, 68, 98	0
1	D	311/332 (93%)	0.40	5 (1%) 72 70	32, 43, 62, 74	0
All	All	1231/1328 (92%)	0.41	51 (4%) 37 35	28, 44, 63, 98	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	263	GLY	5.8
1	B	263	GLY	4.5
1	D	1	ALA	4.2
1	C	266	GLY	3.8
1	C	268	TYR	3.5
1	C	295	ALA	3.4
1	B	258	LEU	3.4
1	C	124	ASN	3.2
1	D	88	PRO	3.2
1	C	258	LEU	3.2
1	D	89	GLY	3.2
1	D	62	ASN	3.1
1	C	179	HIS	3.1
1	C	33	LEU	3.0
1	C	305	ASN	3.0
1	C	308	ARG	3.0
1	C	106	VAL	2.9
1	C	267	ILE	2.9
1	B	289	THR	2.9
1	C	97	THR	2.9
1	C	303	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	95	LEU	2.8
1	A	263	GLY	2.8
1	B	290	GLU	2.8
1	C	175	VAL	2.7
1	C	131	TYR	2.7
1	C	115	PRO	2.6
1	C	161	ALA	2.6
1	C	304	LYS	2.6
1	B	93	ASP	2.5
1	C	59	PHE	2.5
1	B	294	ALA	2.5
1	B	286	LEU	2.5
1	A	38	GLN	2.5
1	A	2	MET	2.5
1	B	253	PRO	2.4
1	A	140	PRO	2.3
1	B	95	LEU	2.2
1	B	92	ARG	2.2
1	C	180	GLY	2.2
1	A	89	GLY	2.2
1	C	206	LEU	2.2
1	C	264	TYR	2.2
1	A	238	VAL	2.2
1	A	132	THR	2.1
1	A	257	TYR	2.1
1	C	301	GLU	2.1
1	C	302	SER	2.1
1	C	192	ALA	2.1
1	D	2	MET	2.0
1	C	310	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

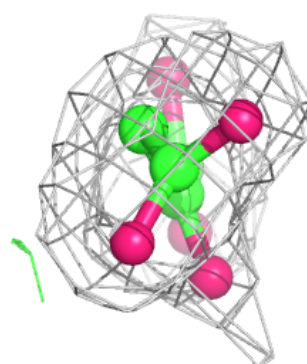
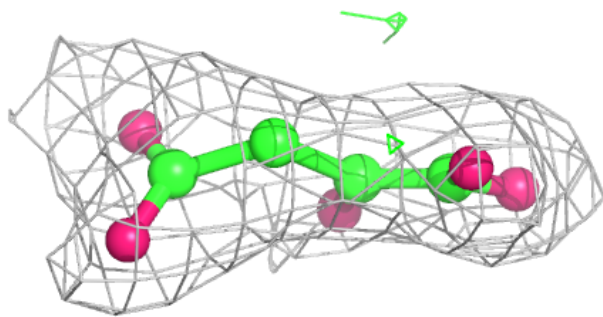
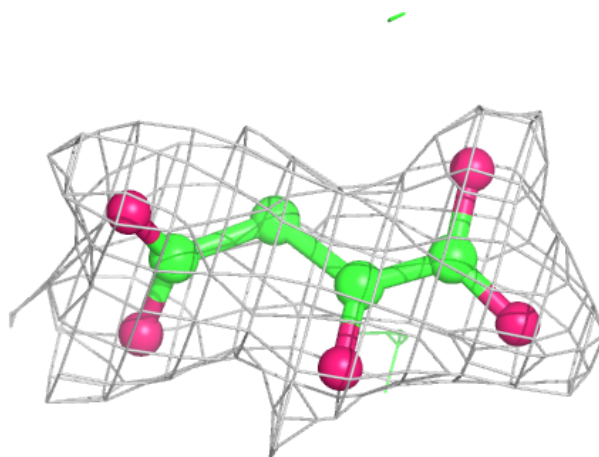
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OAA	B	401	9/9	0.77	0.16	56,62,71,72	0
3	OAA	C	401	9/9	0.84	0.14	50,55,61,61	0
2	NAD	A	400	44/44	0.88	0.17	27,43,56,60	0
3	OAA	A	401	9/9	0.89	0.16	51,56,70,72	0
3	OAA	D	401	9/9	0.90	0.16	50,54,60,60	0
2	NAD	C	400	44/44	0.91	0.17	29,42,51,56	0
2	NAD	B	400	44/44	0.92	0.15	34,46,58,69	0
2	NAD	D	400	44/44	0.93	0.14	28,35,49,54	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.

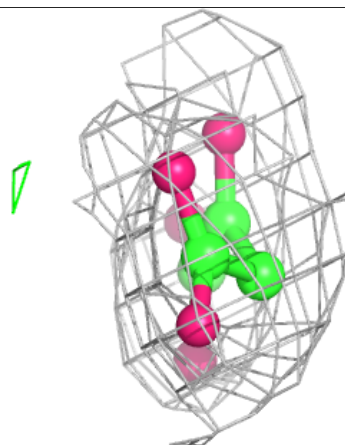
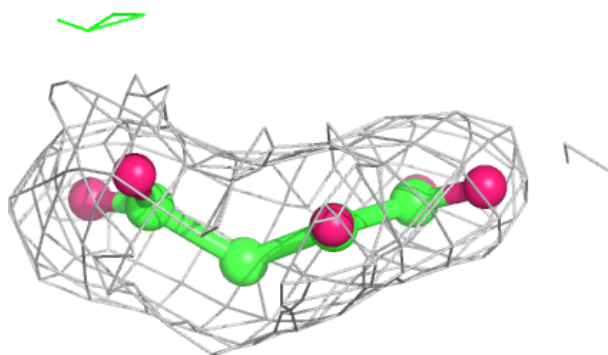
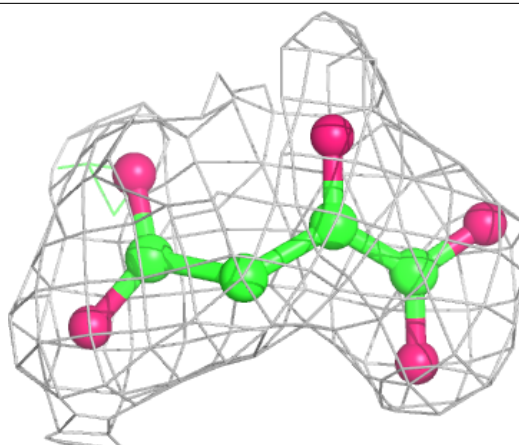
Electron density around OAA B 401:

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

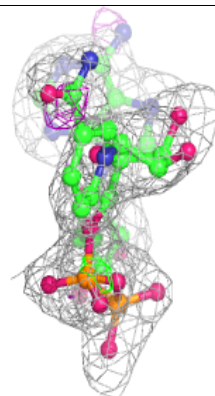
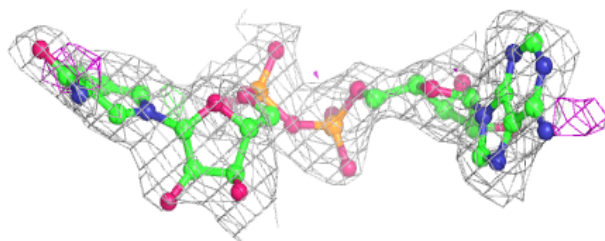
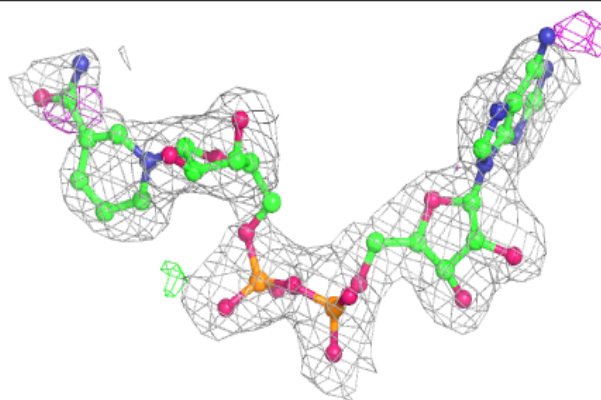


Electron density around OAA C 401:

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

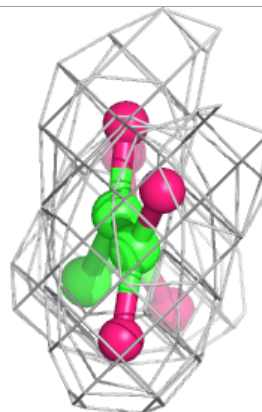
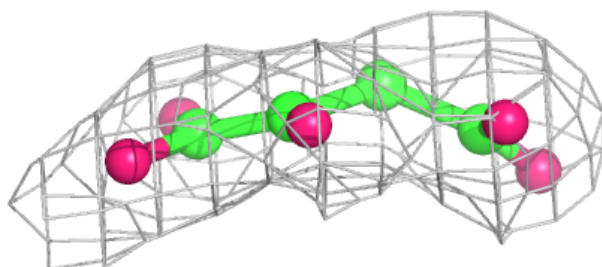
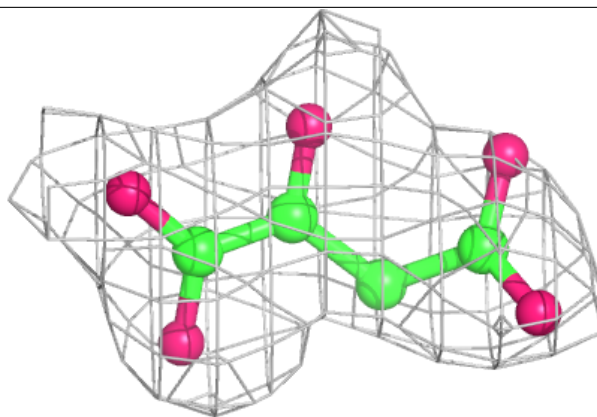
**Electron density around NAD A 400:**

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

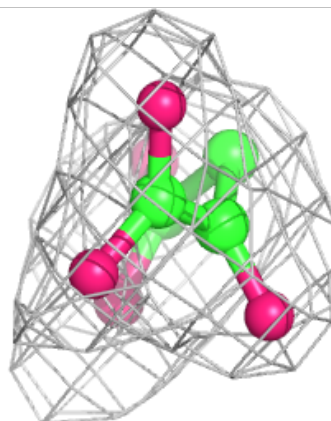
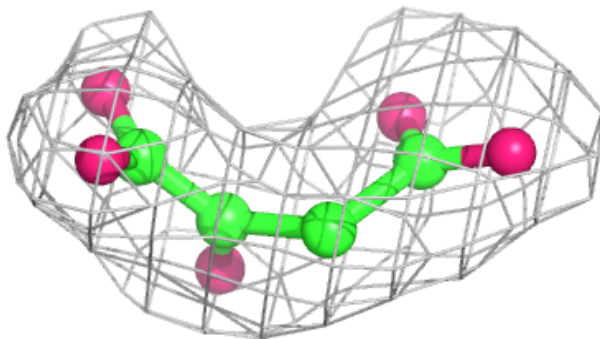
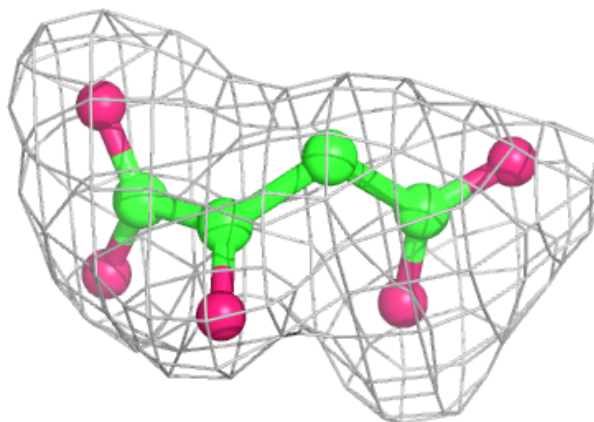


Electron density around OAA A 401:

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

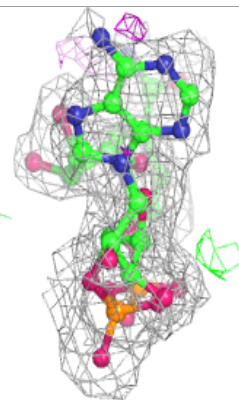
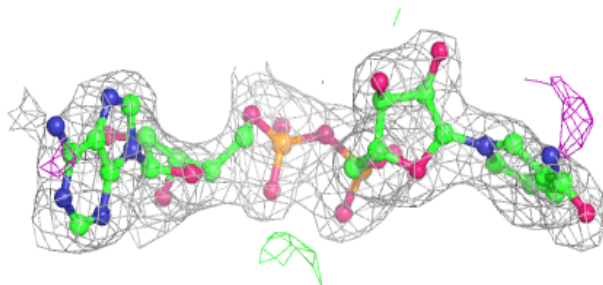
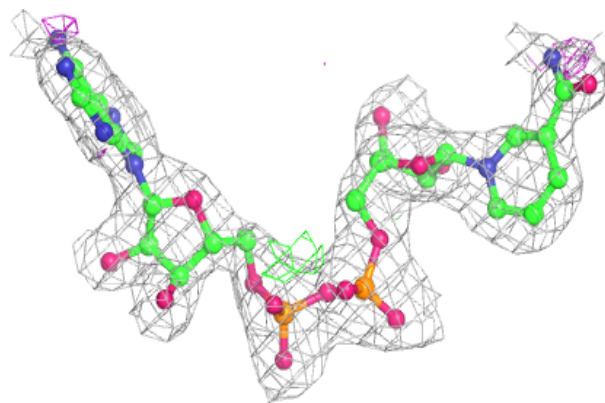
**Electron density around OAA D 401:**

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

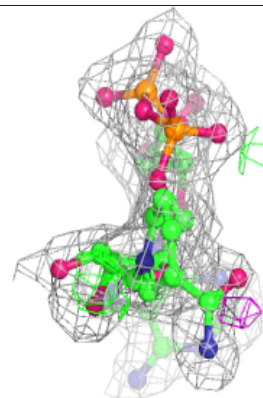
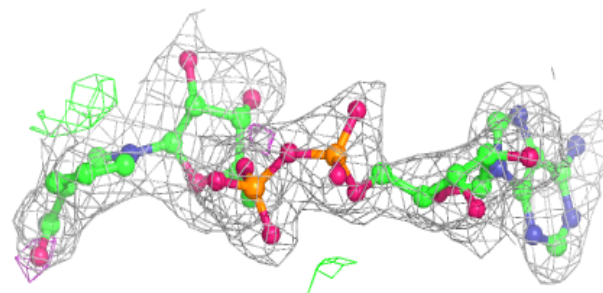
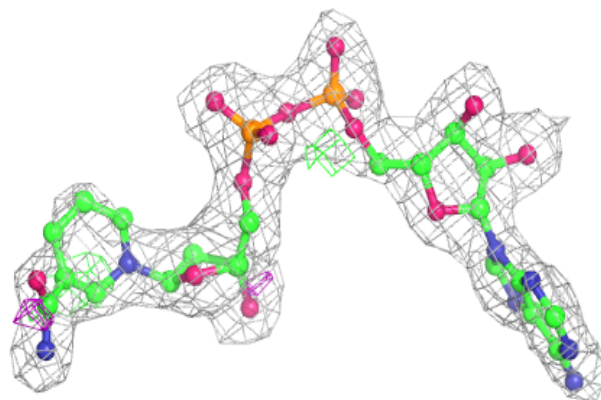


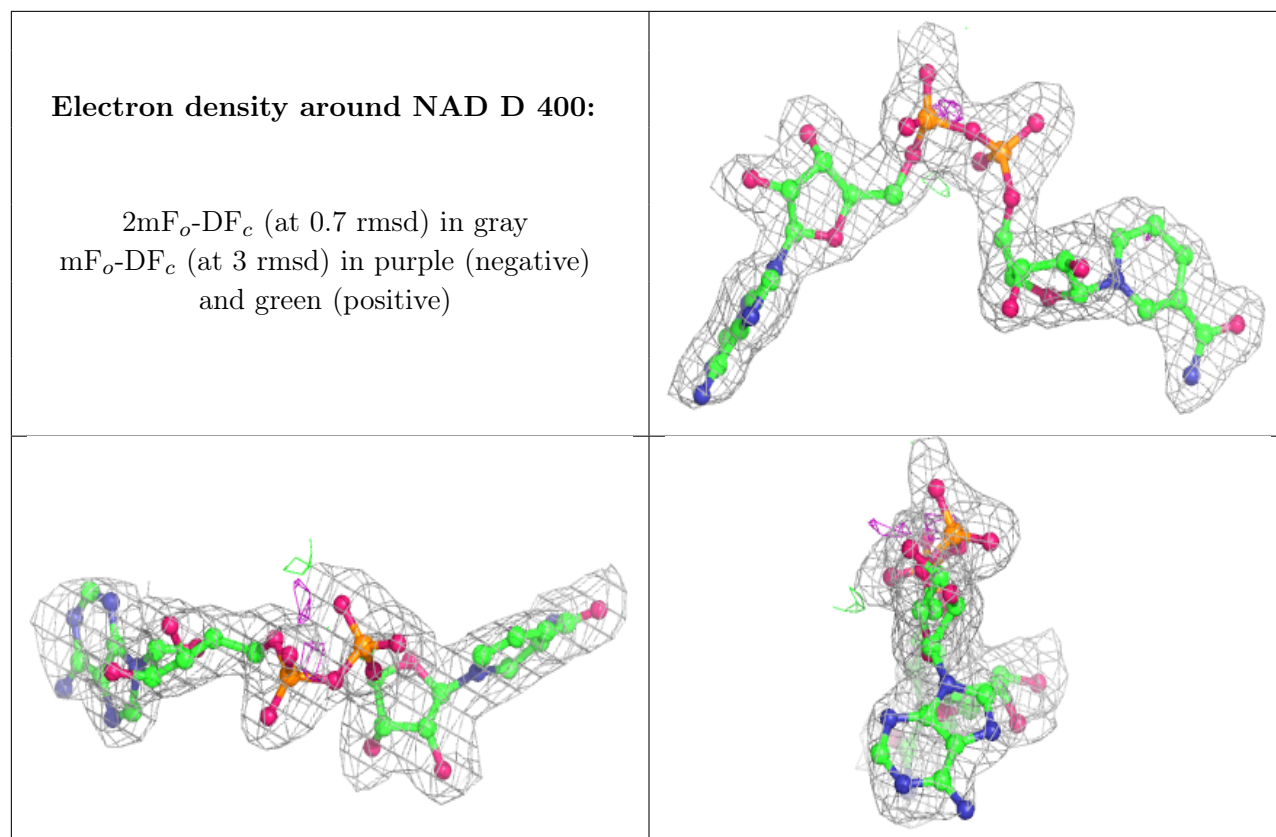
Electron density around NAD C 400:

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

**Electron density around NAD B 400:**

$2mF_o-DF_c$ (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.