Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 02:54 am GMT

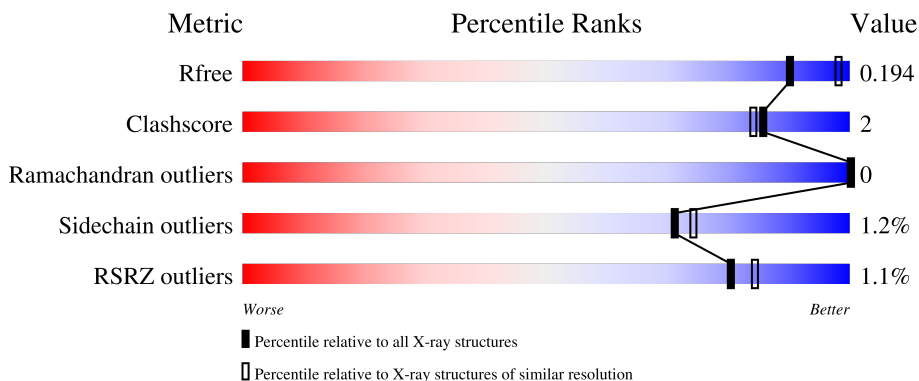|		
PDB ID	:	6T2B
Title	:	Glycoside hydrolase family 109 from Akkermansia muciniphila in complex with GalNAc and NAD+.
Authors	:	Chaberski, E.K.; Fredslund, F.; Teze, D.; Shuoker, B.; Kunstmann, S.; Karlsson, E.N.; Hachem, M.A.; Welner, D.H.
Deposited on	:	2019-10-08
Resolution	:	2.13 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
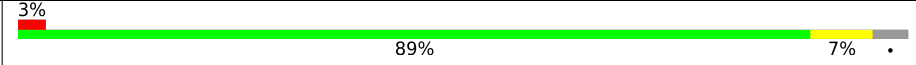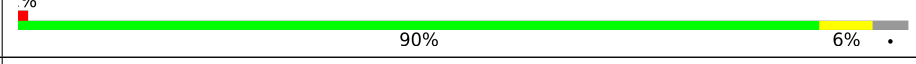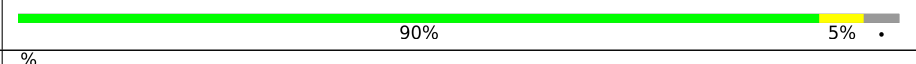*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	Percentile Ranks	Value
Rfree		0.194
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		1.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	456	3% — 89% 7% ·
1	B	456	.% — 90% 6% ·
1	C	456	90% 5% ·
1	D	456	.% — 89% 7% ·

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 15130 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 Glycosyl hydrolase family 109 protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total 3413	C 2149	N 612	O 622	S 30	0	3	0
1	B	439	Total 3413	C 2148	N 613	O 623	S 29	0	2	0
1	C	436	Total 3394	C 2137	N 610	O 618	S 29	0	2	0
1	D	437	Total 3402	C 2141	N 612	O 620	S 29	0	2	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP A0A2N8I799
A	474	LEU	-	expression tag	UNP A0A2N8I799
A	475	GLU	-	expression tag	UNP A0A2N8I799
A	476	HIS	-	expression tag	UNP A0A2N8I799
A	477	HIS	-	expression tag	UNP A0A2N8I799
A	478	HIS	-	expression tag	UNP A0A2N8I799
A	479	HIS	-	expression tag	UNP A0A2N8I799
A	480	HIS	-	expression tag	UNP A0A2N8I799
A	481	HIS	-	expression tag	UNP A0A2N8I799
B	26	MET	-	initiating methionine	UNP A0A2N8I799
B	474	LEU	-	expression tag	UNP A0A2N8I799
B	475	GLU	-	expression tag	UNP A0A2N8I799
B	476	HIS	-	expression tag	UNP A0A2N8I799
B	477	HIS	-	expression tag	UNP A0A2N8I799
B	478	HIS	-	expression tag	UNP A0A2N8I799
B	479	HIS	-	expression tag	UNP A0A2N8I799
B	480	HIS	-	expression tag	UNP A0A2N8I799
B	481	HIS	-	expression tag	UNP A0A2N8I799
C	26	MET	-	initiating methionine	UNP A0A2N8I799
C	474	LEU	-	expression tag	UNP A0A2N8I799
C	475	GLU	-	expression tag	UNP A0A2N8I799

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Chain	Residue	Modelled	Actual	Comment	Reference
C	476	HIS	-	expression tag	UNP A0A2N8I799
C	477	HIS	-	expression tag	UNP A0A2N8I799
C	478	HIS	-	expression tag	UNP A0A2N8I799
C	479	HIS	-	expression tag	UNP A0A2N8I799
C	480	HIS	-	expression tag	UNP A0A2N8I799
C	481	HIS	-	expression tag	UNP A0A2N8I799
D	26	MET	-	initiating methionine	UNP A0A2N8I799
D	474	LEU	-	expression tag	UNP A0A2N8I799
D	475	GLU	-	expression tag	UNP A0A2N8I799
D	476	HIS	-	expression tag	UNP A0A2N8I799
D	477	HIS	-	expression tag	UNP A0A2N8I799
D	478	HIS	-	expression tag	UNP A0A2N8I799
D	479	HIS	-	expression tag	UNP A0A2N8I799
D	480	HIS	-	expression tag	UNP A0A2N8I799
D	481	HIS	-	expression tag	UNP A0A2N8I799

- Molecule 2 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).
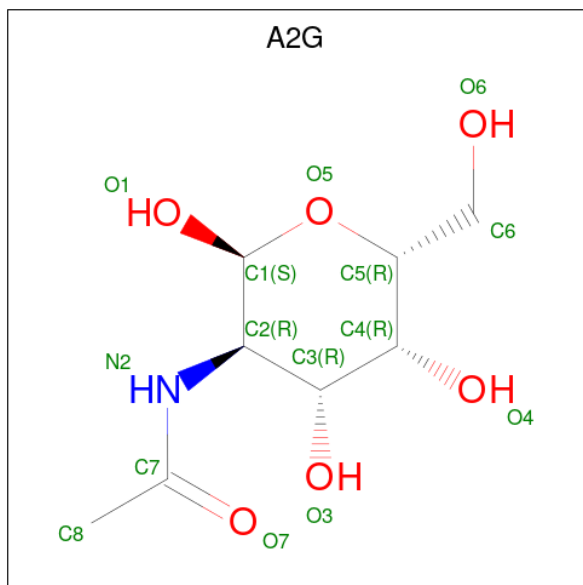
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 15	C 8	N 1	O 6	0	0
2	B	1	Total 15	C 8	N 1	O 6	0	0
2	C	1	Total 15	C 8	N 1	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total 15	C 8	N 1	O 6	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).
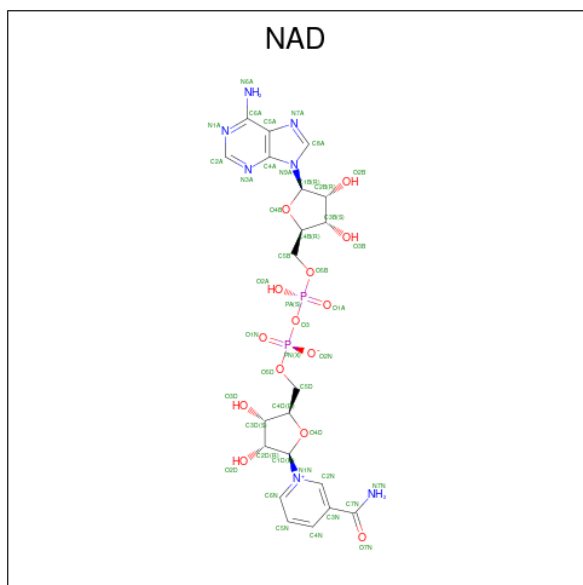
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

PGE

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

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

1PE
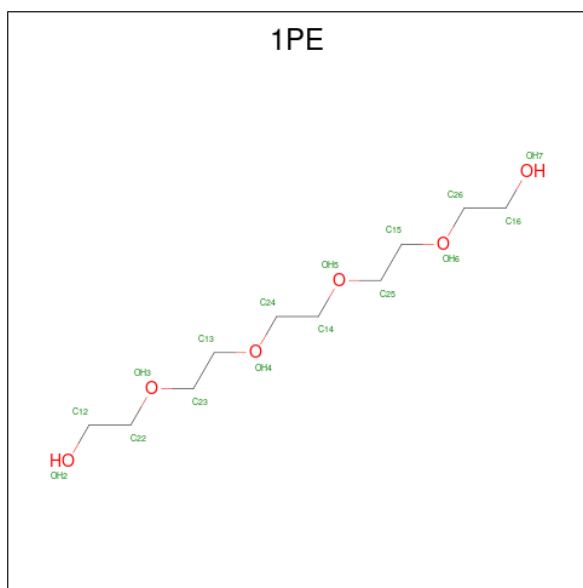
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 16	C 10	O 6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	276	Total 276	O 276	0	0
6	B	327	Total 327	O 327	0	0
6	C	330	Total 330	O 330	0	0
6	D	313	Total 313	O 313	0	0

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: Glycosyl hydrolase family 109 protein 2
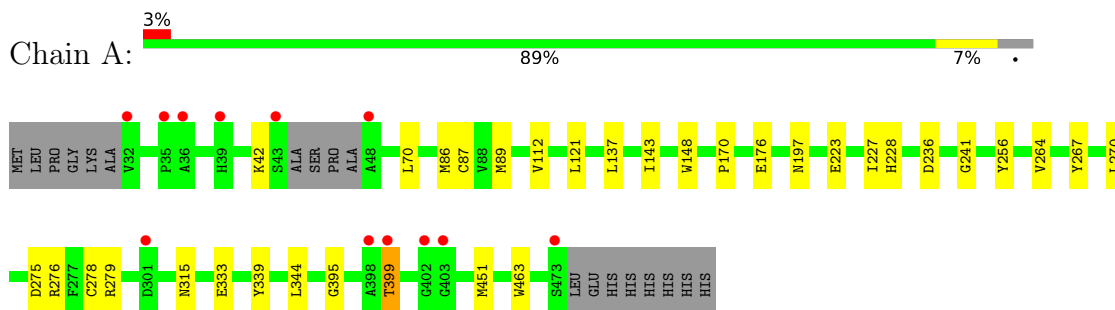
- Molecule 1: Glycosyl hydrolase family 109 protein 2
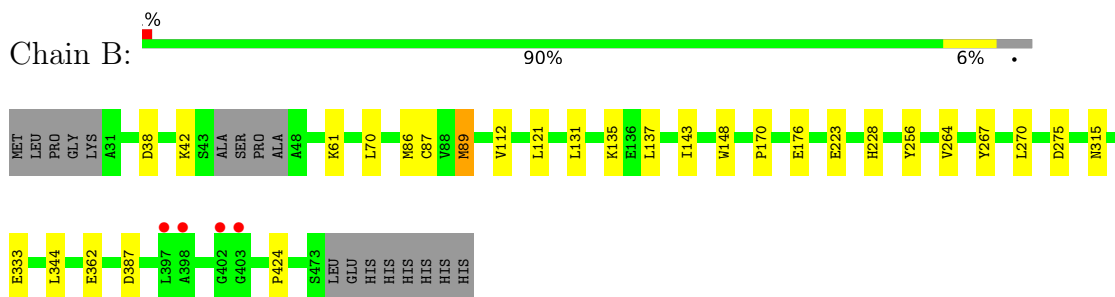
- Molecule 1: Glycosyl hydrolase family 109 protein 2

- Molecule 1: Glycosyl hydrolase family 109 protein 2

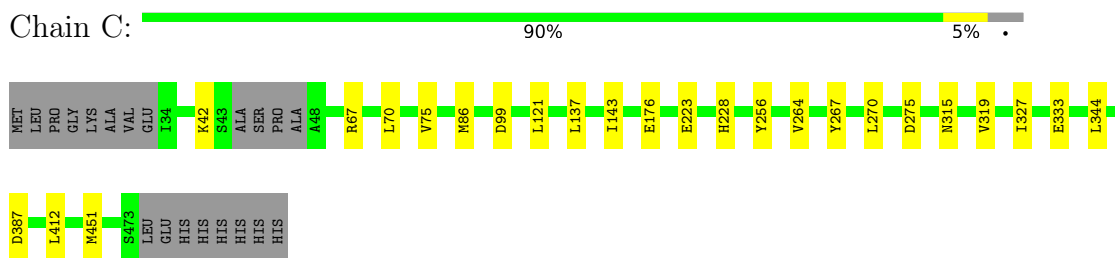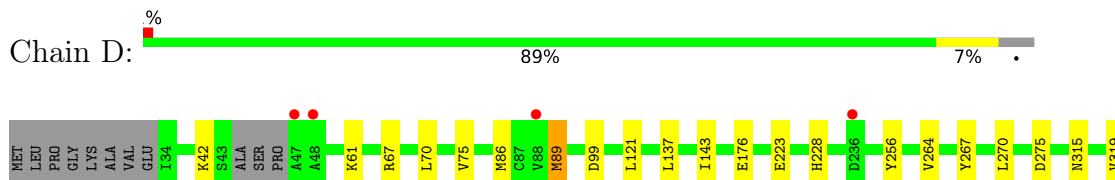I327 E333 L344 Y369 D387 H388 P389 K400 L412 P424 S473 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.11Å 182.64Å 70.87Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	70.87 – 2.13 91.32 – 2.13	Depositor EDS
% Data completeness (in resolution range)	93.6 (70.87-2.13) 93.5 (91.32-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.158 , 0.194 0.158 , 0.194	Depositor DCC
R_{free} test set	1896 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.4	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15130	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 1PE, NAD, PGE, A2G

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	0.28	0/3501	0.49	0/4733
1	B	0.29	0/3498	0.50	0/4729
1	C	0.29	0/3479	0.49	0/4703
1	D	0.28	0/3484	0.49	0/4709
All	All	0.28	0/13962	0.49	0/18874

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3413	0	3374	18	0
1	B	3413	0	3370	13	0
1	C	3394	0	3354	12	0
1	D	3402	0	3358	15	0
2	A	15	0	12	1	0
2	B	15	0	12	1	0
2	C	15	0	12	1	0
2	D	15	0	12	1	0
3	A	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	1	0
3	C	44	0	26	1	0
3	D	44	0	26	1	0
4	A	10	0	14	0	0
5	C	16	0	22	0	0
6	A	276	0	0	0	0
6	B	327	0	0	0	0
6	C	330	0	0	0	0
6	D	313	0	0	1	0
All	All	15130	0	13644	60	0

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

All (60) 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:86:MET:HA	1:A:89:MET:HG3	1.67	0.75
1:B:121:LEU:HD22	1:B:137:LEU:HD21	1.72	0.71
1:A:42:LYS:NZ	1:A:176:GLU:OE2	2.28	0.63
1:D:86:MET:HE2	1:D:412:LEU:HD22	1.78	0.63
1:A:121:LEU:HD12	1:A:137:LEU:HD21	1.79	0.63
1:A:451[A]:MET:HE1	1:C:451[A]:MET:HG2	1.83	0.59
1:C:86:MET:HE2	1:C:412:LEU:HD22	1.84	0.59
2:A:501:A2G:H3	3:A:502:NAD:C4N	2.33	0.59
2:D:501:A2G:H3	3:D:502:NAD:C4N	2.34	0.58
2:B:501:A2G:H3	3:B:502:NAD:C4N	2.34	0.57
1:B:86:MET:HA	1:B:89:MET:HG3	1.86	0.57
1:C:121:LEU:HD12	1:C:137:LEU:HD21	1.86	0.57
1:D:86:MET:HA	1:D:89:MET:HG3	1.87	0.56
1:B:70:LEU:HD11	1:B:143:ILE:HG13	1.88	0.55
2:C:501:A2G:H3	3:C:502:NAD:C4N	2.37	0.54
1:C:223:GLU:HB2	1:C:344:LEU:HB3	1.92	0.52
1:D:223:GLU:HB2	1:D:344:LEU:HB3	1.93	0.51
1:D:121:LEU:HD12	1:D:137:LEU:HD21	1.93	0.51
1:D:61:LYS:HG2	1:D:424:PRO:HD3	1.92	0.51
1:D:228:HIS:O	1:D:333:GLU:HA	2.11	0.51
1:A:70:LEU:HD11	1:A:143:ILE:HG13	1.92	0.50
1:B:223:GLU:HB2	1:B:344:LEU:HB3	1.94	0.50
1:C:70:LEU:HD11	1:C:143:ILE:HG13	1.93	0.49
1:A:223:GLU:HB2	1:A:344:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LYS:NZ	1:B:176:GLU:OE2	2.35	0.48
1:C:228:HIS:O	1:C:333:GLU:HA	2.13	0.48
1:C:75:VAL:HG22	1:C:99:ASP:HB2	1.96	0.47
1:A:270:LEU:HD23	1:A:275:ASP:HB3	1.96	0.47
1:D:70:LEU:HD11	1:D:143:ILE:HG13	1.96	0.47
1:A:228:HIS:O	1:A:333:GLU:HA	2.15	0.47
1:B:61:LYS:HG2	1:B:424:PRO:HD3	1.96	0.46
1:C:42:LYS:NZ	1:C:176:GLU:OE2	2.42	0.46
1:B:148:TRP:CD1	1:B:170:PRO:HD2	2.50	0.45
1:C:264:VAL:HA	1:C:267:TYR:CD2	2.51	0.45
1:D:75:VAL:HG22	1:D:99:ASP:HB2	1.98	0.45
1:A:87[A]:CYS:SG	1:A:112:VAL:HG22	2.56	0.45
1:B:270:LEU:HD23	1:B:275:ASP:HB3	1.98	0.45
1:D:270:LEU:HD23	1:D:275:ASP:HB3	1.98	0.45
1:A:148:TRP:CD1	1:A:170:PRO:HD2	2.52	0.44
1:B:228:HIS:O	1:B:333:GLU:HA	2.17	0.44
1:D:389:PRO:HB2	1:D:473:SER:HA	1.99	0.44
1:C:319:VAL:HB	1:C:327:ILE:HB	2.00	0.43
1:B:131:LEU:O	1:B:135:LYS:HG3	2.18	0.43
1:D:264:VAL:HA	1:D:267:TYR:CD2	2.54	0.42
1:D:400:LYS:HE3	1:D:400:LYS:HB2	1.80	0.42
1:B:87[A]:CYS:SG	1:B:112:VAL:HG22	2.59	0.42
1:D:369:TYR:OH	6:D:601:HOH:O	2.19	0.42
1:A:278:CYS:SG	1:A:279:ARG:NH1	2.93	0.42
1:A:451[A]:MET:CE	1:C:451[A]:MET:HG2	2.49	0.42
1:A:236:ASP:HB2	1:A:241:GLY:HA3	2.02	0.41
1:C:270:LEU:HD23	1:C:275:ASP:HB3	2.02	0.41
1:A:264:VAL:HA	1:A:267:TYR:CD2	2.55	0.41
1:B:264:VAL:HA	1:B:267:TYR:CD2	2.55	0.41
1:A:395:GLY:O	1:A:399:THR:OG1	2.36	0.41
1:A:227:ILE:O	1:A:339:TYR:HA	2.21	0.41
1:A:276:ARG:HD2	1:A:463:TRP:CE2	2.55	0.41
1:B:362:GLU:H	1:B:362:GLU:HG3	1.65	0.41
1:D:319:VAL:HB	1:D:327:ILE:HB	2.03	0.40
1:D:42:LYS:NZ	1:D:176:GLU:OE2	2.46	0.40
1:A:197:ASN:OD1	1:A:197:ASN:N	2.50	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	437/456 (96%)	425 (97%)	12 (3%)	0	100	100
1	B	437/456 (96%)	425 (97%)	12 (3%)	0	100	100
1	C	434/456 (95%)	423 (98%)	11 (2%)	0	100	100
1	D	435/456 (95%)	423 (97%)	12 (3%)	0	100	100
All	All	1743/1824 (96%)	1696 (97%)	47 (3%)	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	359/370 (97%)	356 (99%)	3 (1%)	81	85
1	B	358/370 (97%)	353 (99%)	5 (1%)	67	70
1	C	356/370 (96%)	352 (99%)	4 (1%)	73	76
1	D	356/370 (96%)	351 (99%)	5 (1%)	67	70
All	All	1429/1480 (97%)	1412 (99%)	17 (1%)	71	74

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	TYR
1	A	315	ASN

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Mol	Chain	Res	Type
1	A	399	THR
1	B	38	ASP
1	B	89	MET
1	B	256	TYR
1	B	315	ASN
1	B	387	ASP
1	C	67	ARG
1	C	256	TYR
1	C	315	ASN
1	C	387	ASP
1	D	67	ARG
1	D	89	MET
1	D	256	TYR
1	D	315	ASN
1	D	387	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

10 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	#$|Z| > 2$
3	NAD	A	502	-	42,48,48	2.77	19 (45%)	50,73,73	1.51	8 (16%)
3	NAD	D	502	-	42,48,48	2.73	19 (45%)	50,73,73	1.51	7 (14%)
3	NAD	B	502	-	42,48,48	2.70	19 (45%)	50,73,73	1.44	8 (16%)
3	NAD	C	502	-	42,48,48	2.70	19 (45%)	50,73,73	1.51	8 (16%)
2	A2G	A	501	-	15,15,15	1.73	5 (33%)	21,21,21	1.26	2 (9%)
2	A2G	C	501	-	15,15,15	1.75	4 (26%)	21,21,21	1.18	3 (14%)
2	A2G	B	501	-	15,15,15	1.71	3 (20%)	21,21,21	1.19	2 (9%)
4	PGE	A	503	-	9,9,9	0.52	0	8,8,8	0.26	0
2	A2G	D	501	-	15,15,15	1.77	4 (26%)	21,21,21	1.28	2 (9%)
5	1PE	C	503	-	15,15,15	0.53	0	14,14,14	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	502	-	-	5/26/62/62	0/5/5/5
3	NAD	D	502	-	-	5/26/62/62	0/5/5/5
3	NAD	B	502	-	-	5/26/62/62	0/5/5/5
3	NAD	C	502	-	-	5/26/62/62	0/5/5/5
2	A2G	A	501	-	-	0/6/26/26	0/1/1/1
2	A2G	C	501	-	-	0/6/26/26	0/1/1/1
2	A2G	B	501	-	-	0/6/26/26	0/1/1/1
4	PGE	A	503	-	-	5/7/7/7	-
2	A2G	D	501	-	-	0/6/26/26	0/1/1/1
5	1PE	C	503	-	-	7/13/13/13	-

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAD	O4D-C1D	8.18	1.52	1.41
3	C	502	NAD	O4D-C1D	8.05	1.52	1.41
3	B	502	NAD	O4D-C1D	7.94	1.52	1.41
3	D	502	NAD	O4D-C1D	7.63	1.51	1.41
3	A	502	NAD	O4B-C1B	6.28	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	NAD	O4B-C1B	5.86	1.49	1.41
3	D	502	NAD	O4B-C1B	5.86	1.49	1.41
3	C	502	NAD	C7N-N7N	5.62	1.43	1.33
3	C	502	NAD	O4B-C1B	5.58	1.48	1.41
3	A	502	NAD	C2D-C1D	-5.43	1.45	1.53
3	D	502	NAD	C7N-N7N	5.41	1.43	1.33
3	B	502	NAD	C2D-C1D	-5.39	1.45	1.53
3	B	502	NAD	C7N-N7N	5.37	1.43	1.33
3	A	502	NAD	C7N-N7N	5.30	1.43	1.33
3	D	502	NAD	C2D-C1D	-5.29	1.45	1.53
3	D	502	NAD	C4N-C3N	4.89	1.47	1.39
3	C	502	NAD	C2D-C1D	-4.82	1.46	1.53
3	A	502	NAD	C4N-C3N	4.81	1.47	1.39
3	B	502	NAD	C4N-C3N	4.79	1.47	1.39
3	C	502	NAD	C4N-C3N	4.78	1.47	1.39
3	A	502	NAD	C2B-C1B	-3.98	1.47	1.53
3	D	502	NAD	C2B-C1B	-3.88	1.47	1.53
3	C	502	NAD	C2B-C1B	-3.68	1.48	1.53
3	A	502	NAD	C2N-N1N	3.60	1.39	1.35
3	B	502	NAD	C2N-N1N	3.59	1.39	1.35
3	D	502	NAD	C2N-N1N	3.54	1.39	1.35
3	C	502	NAD	C2N-N1N	3.51	1.39	1.35
3	B	502	NAD	C2B-C1B	-3.35	1.48	1.53
2	D	501	A2G	C7-N2	3.31	1.45	1.34
2	C	501	A2G	C3-C2	-3.29	1.46	1.53
3	D	502	NAD	C3N-C7N	3.26	1.55	1.50
3	C	502	NAD	C5N-C4N	3.25	1.45	1.38
2	C	501	A2G	C7-N2	3.25	1.45	1.34
2	B	501	A2G	C7-N2	3.25	1.45	1.34
2	A	501	A2G	C7-N2	3.24	1.45	1.34
3	D	502	NAD	C5N-C4N	3.23	1.45	1.38
3	A	502	NAD	C5N-C4N	3.15	1.45	1.38
3	D	502	NAD	O7N-C7N	-3.04	1.18	1.24
3	B	502	NAD	O7N-C7N	-2.96	1.18	1.24
2	D	501	A2G	C2-N2	2.95	1.50	1.45
3	C	502	NAD	C3N-C7N	2.93	1.55	1.50
3	B	502	NAD	C5N-C4N	2.93	1.45	1.38
2	A	501	A2G	C3-C2	-2.91	1.47	1.53
3	A	502	NAD	O7N-C7N	-2.84	1.18	1.24
3	A	502	NAD	C6A-N6A	2.83	1.44	1.34
3	A	502	NAD	O2D-C2D	2.82	1.49	1.43
3	B	502	NAD	C6A-N6A	2.81	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NAD	C6A-N6A	2.79	1.44	1.34
3	D	502	NAD	C4A-N3A	-2.79	1.31	1.35
3	B	502	NAD	C4A-N3A	-2.78	1.31	1.35
3	C	502	NAD	C6A-N6A	2.78	1.44	1.34
2	B	501	A2G	C3-C2	-2.73	1.48	1.53
3	B	502	NAD	C2D-C3D	-2.71	1.45	1.53
3	D	502	NAD	C2D-C3D	-2.69	1.46	1.53
3	C	502	NAD	O7N-C7N	-2.69	1.19	1.24
3	C	502	NAD	O2D-C2D	2.68	1.49	1.43
3	A	502	NAD	C3N-C7N	2.64	1.54	1.50
3	B	502	NAD	O2D-C2D	2.62	1.49	1.43
3	A	502	NAD	C4A-N3A	-2.59	1.32	1.35
3	C	502	NAD	C4A-N3A	-2.57	1.32	1.35
3	A	502	NAD	C2D-C3D	-2.55	1.46	1.53
2	D	501	A2G	C3-C2	-2.54	1.48	1.53
3	D	502	NAD	O2D-C2D	2.51	1.48	1.43
3	C	502	NAD	C2D-C3D	-2.46	1.46	1.53
3	C	502	NAD	O4D-C4D	2.46	1.50	1.45
3	B	502	NAD	O2B-C2B	2.45	1.48	1.43
2	B	501	A2G	C2-N2	2.43	1.49	1.45
2	C	501	A2G	C2-N2	2.39	1.49	1.45
3	B	502	NAD	C3N-C7N	2.36	1.54	1.50
3	A	502	NAD	O4D-C4D	2.36	1.50	1.45
2	D	501	A2G	O3-C3	2.33	1.48	1.43
3	D	502	NAD	O2B-C2B	2.33	1.48	1.43
3	D	502	NAD	C3D-C4D	-2.33	1.47	1.53
3	D	502	NAD	O4D-C4D	2.30	1.50	1.45
3	B	502	NAD	C3D-C4D	-2.28	1.47	1.53
3	C	502	NAD	C2B-C3B	-2.28	1.47	1.53
3	C	502	NAD	C3D-C4D	-2.26	1.47	1.53
3	A	502	NAD	C3D-C4D	-2.25	1.47	1.53
3	B	502	NAD	C2B-C3B	-2.25	1.47	1.53
2	A	501	A2G	O3-C3	2.24	1.48	1.43
3	A	502	NAD	O2B-C2B	2.23	1.48	1.43
3	C	502	NAD	O2B-C2B	2.22	1.48	1.43
2	A	501	A2G	C2-N2	2.18	1.49	1.45
3	D	502	NAD	C2B-C3B	-2.16	1.47	1.53
3	D	502	NAD	C5A-N7A	2.16	1.47	1.39
3	B	502	NAD	O4D-C4D	2.15	1.49	1.45
3	B	502	NAD	C5A-N7A	2.06	1.47	1.39
3	A	502	NAD	C2B-C3B	-2.06	1.47	1.53
2	C	501	A2G	O3-C3	2.05	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAD	C5A-N7A	2.04	1.47	1.39
3	C	502	NAD	C5A-N7A	2.03	1.47	1.39
2	A	501	A2G	O5-C1	2.01	1.47	1.42

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAD	N3A-C2A-N1A	-4.59	121.50	128.68
3	C	502	NAD	N3A-C2A-N1A	-4.45	121.72	128.68
3	B	502	NAD	N3A-C2A-N1A	-4.25	122.03	128.68
3	D	502	NAD	N3A-C2A-N1A	-4.23	122.07	128.68
3	B	502	NAD	C4A-C5A-N7A	-3.99	105.25	109.40
3	D	502	NAD	C4A-C5A-N7A	-3.96	105.28	109.40
3	C	502	NAD	C1B-N9A-C4A	-3.95	119.71	126.64
3	C	502	NAD	C4A-C5A-N7A	-3.94	105.30	109.40
3	D	502	NAD	C1B-N9A-C4A	-3.78	120.01	126.64
3	A	502	NAD	C1B-N9A-C4A	-3.76	120.04	126.64
3	A	502	NAD	C4A-C5A-N7A	-3.58	105.66	109.40
3	D	502	NAD	PN-O3-PA	-3.38	121.24	132.83
2	D	501	A2G	C4-C3-C2	3.28	115.14	110.34
3	C	502	NAD	PN-O3-PA	-3.15	122.01	132.83
3	B	502	NAD	C1B-N9A-C4A	-3.15	121.11	126.64
3	A	502	NAD	PN-O3-PA	-3.12	122.13	132.83
3	B	502	NAD	PN-O3-PA	-3.08	122.25	132.83
3	A	502	NAD	C3B-C2B-C1B	3.04	105.55	100.98
3	B	502	NAD	C3B-C2B-C1B	2.89	105.33	100.98
3	D	502	NAD	C3B-C2B-C1B	2.86	105.28	100.98
2	B	501	A2G	C4-C3-C2	2.71	114.31	110.34
3	C	502	NAD	C5N-C4N-C3N	-2.50	117.39	120.34
3	A	502	NAD	C2D-C3D-C4D	2.44	107.39	102.64
2	A	501	A2G	O5-C1-C2	2.44	111.97	109.52
3	A	502	NAD	C2B-C3B-C4B	2.42	107.35	102.64
2	C	501	A2G	C4-C3-C2	2.35	113.78	110.34
3	C	502	NAD	C3B-C2B-C1B	2.29	104.43	100.98
3	C	502	NAD	C2D-C3D-C4D	2.28	107.06	102.64
2	D	501	A2G	O5-C1-C2	2.27	111.80	109.52
2	C	501	A2G	O5-C1-C2	2.27	111.79	109.52
3	C	502	NAD	O3D-C3D-C4D	-2.26	104.52	111.05
3	D	502	NAD	C2B-C3B-C4B	2.23	106.97	102.64
3	D	502	NAD	C2D-C3D-C4D	2.22	106.97	102.64
2	A	501	A2G	C4-C3-C2	2.17	113.52	110.34
3	B	502	NAD	C2B-C3B-C4B	2.17	106.86	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	NAD	O3D-C3D-C4D	-2.15	104.83	111.05
3	B	502	NAD	C5N-C4N-C3N	-2.13	117.82	120.34
2	B	501	A2G	C8-C7-N2	2.04	119.56	116.10
2	C	501	A2G	C8-C7-N2	2.01	119.50	116.10
3	B	502	NAD	C2D-C3D-C4D	2.01	106.54	102.64

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NAD	O4D-C1D-N1N-C2N
3	A	502	NAD	O4D-C1D-N1N-C6N
3	A	502	NAD	C2D-C1D-N1N-C2N
3	B	502	NAD	O4D-C1D-N1N-C2N
3	B	502	NAD	O4D-C1D-N1N-C6N
3	C	502	NAD	O4D-C1D-N1N-C2N
3	C	502	NAD	O4D-C1D-N1N-C6N
3	C	502	NAD	C2D-C1D-N1N-C2N
3	D	502	NAD	O4D-C1D-N1N-C2N
3	D	502	NAD	O4D-C1D-N1N-C6N
3	D	502	NAD	C2D-C1D-N1N-C2N
4	A	503	PGE	O1-C1-C2-O2
5	C	503	1PE	OH4-C13-C23-OH3
3	A	502	NAD	O4B-C4B-C5B-O5B
5	C	503	1PE	OH5-C14-C24-OH4
3	A	502	NAD	C3B-C4B-C5B-O5B
4	A	503	PGE	O2-C3-C4-O3
5	C	503	1PE	OH7-C16-C26-OH6
3	D	502	NAD	O4B-C4B-C5B-O5B
5	C	503	1PE	OH6-C15-C25-OH5
4	A	503	PGE	O3-C5-C6-O4
3	D	502	NAD	C3B-C4B-C5B-O5B
3	B	502	NAD	O4B-C4B-C5B-O5B
3	C	502	NAD	O4B-C4B-C5B-O5B
5	C	503	1PE	C24-C14-OH5-C25
5	C	503	1PE	C13-C23-OH3-C22
4	A	503	PGE	C1-C2-O2-C3
4	A	503	PGE	C3-C4-O3-C5
3	B	502	NAD	C3B-C4B-C5B-O5B
3	C	502	NAD	C3B-C4B-C5B-O5B
5	C	503	1PE	C25-C15-OH6-C26
3	B	502	NAD	C2D-C1D-N1N-C2N

There are no ring outliers.
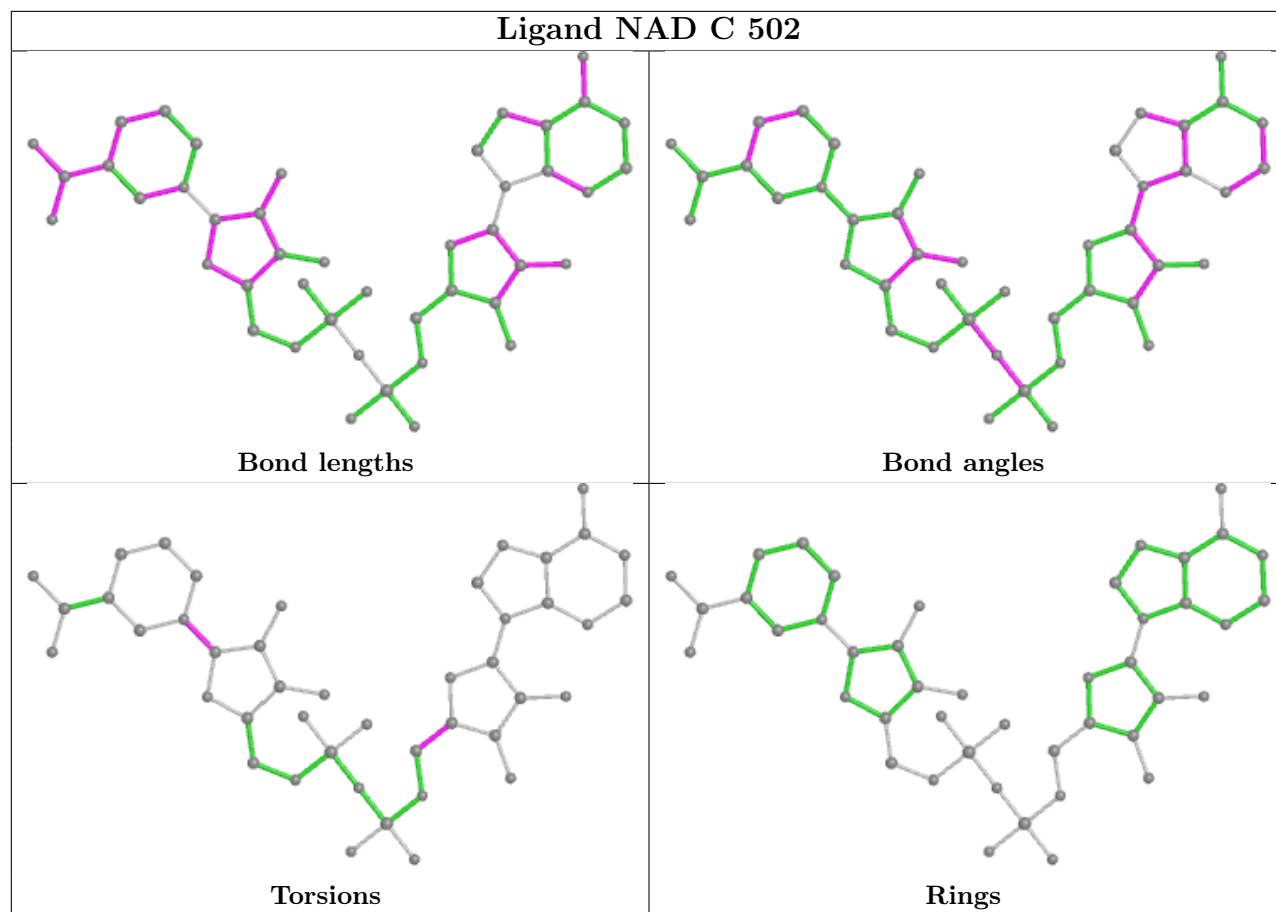
8 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAD	1	0
3	D	502	NAD	1	0
3	B	502	NAD	1	0
3	C	502	NAD	1	0
2	A	501	A2G	1	0
2	C	501	A2G	1	0
2	B	501	A2G	1	0
2	D	501	A2G	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 A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD C 502

Bond lengths

Bond angles

Torsions

Rings
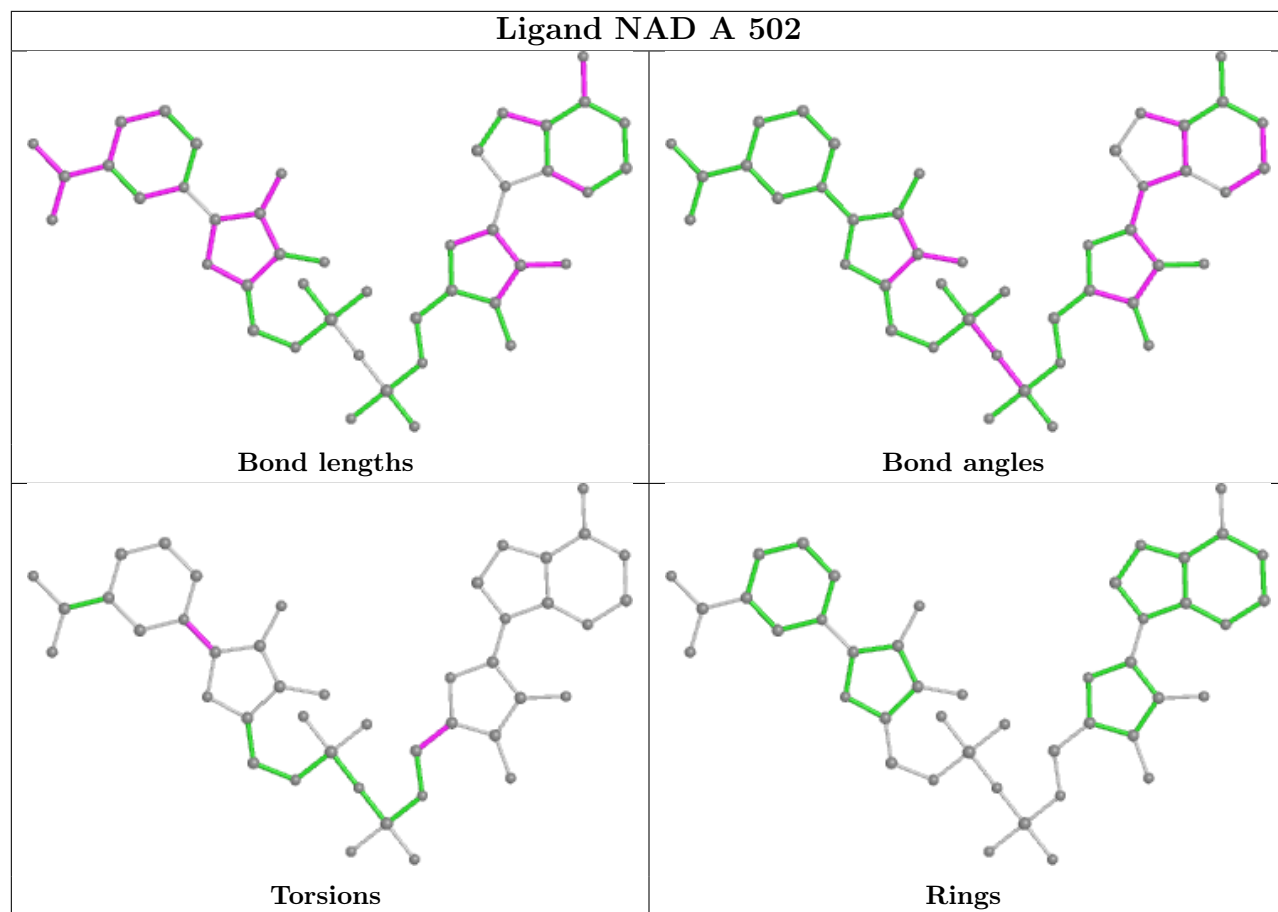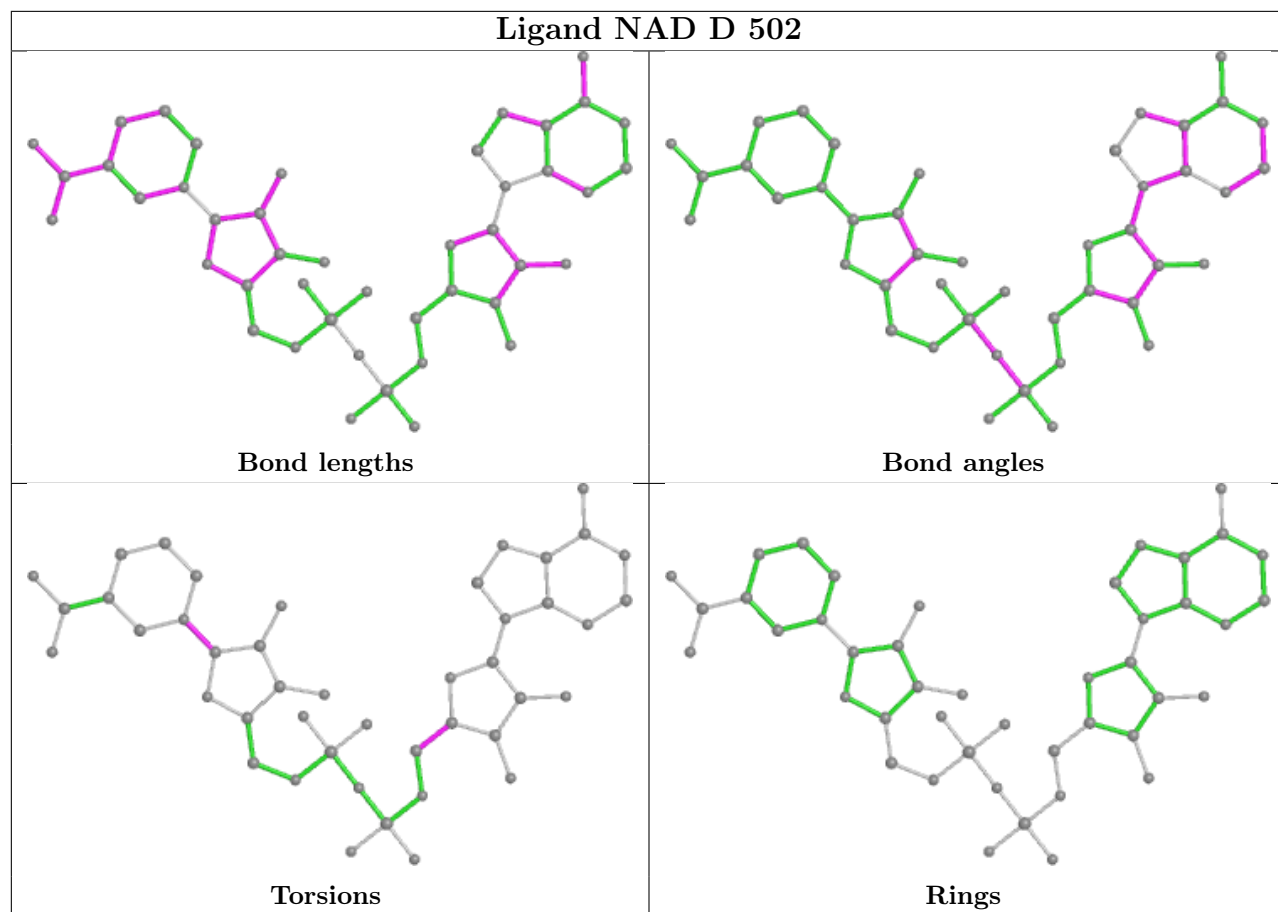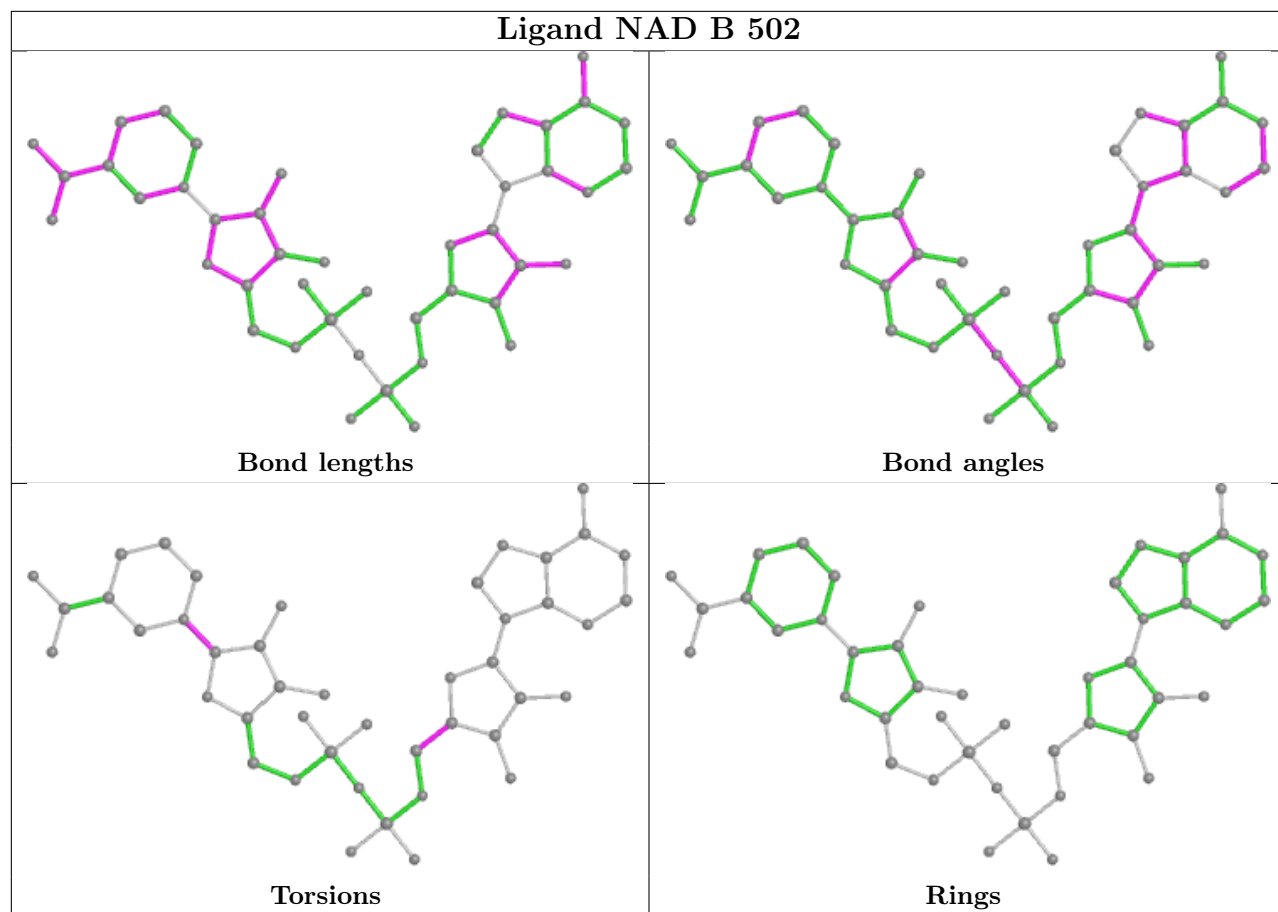
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	438/456 (96%)	-0.46	12 (2%)	54	61	22, 32, 69, 93	0
1	B	439/456 (96%)	-0.57	4 (0%)	84	87	19, 28, 54, 82	0
1	C	436/456 (95%)	-0.60	0	100	100	20, 28, 52, 71	0
1	D	437/456 (95%)	-0.60	4 (0%)	84	87	18, 29, 53, 82	0
All	All	1750/1824 (95%)	-0.56	20 (1%)	80	84	18, 30, 55, 93	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	LEU	3.6
1	A	473	SER	3.6
1	A	48	ALA	3.4
1	B	398	ALA	3.3
1	A	35	PRO	3.0
1	A	39	HIS	3.0
1	B	403	GLY	2.9
1	A	36	ALA	2.7
1	D	47	ALA	2.7
1	A	301	ASP	2.6
1	D	48	ALA	2.6
1	A	398	ALA	2.5
1	A	403	GLY	2.3
1	A	32	VAL	2.2
1	A	399	THR	2.1
1	B	402	GLY	2.1
1	A	43	SER	2.1
1	D	236	ASP	2.0
1	A	402	GLY	2.0
1	D	88	VAL	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
4	PGE	A	503	10/10	0.83	0.14	58,59,61,61	0
5	1PE	C	503	16/16	0.93	0.14	37,42,45,47	0
2	A2G	B	501	15/15	0.95	0.08	26,28,30,31	0
2	A2G	A	501	15/15	0.96	0.08	29,31,33,33	0
2	A2G	D	501	15/15	0.96	0.08	22,25,29,29	0
2	A2G	C	501	15/15	0.97	0.08	25,27,31,32	0
3	NAD	A	502	44/44	0.97	0.08	27,31,34,35	0
3	NAD	D	502	44/44	0.98	0.08	18,26,30,31	0
3	NAD	B	502	44/44	0.98	0.08	19,25,27,27	0
3	NAD	C	502	44/44	0.98	0.08	20,25,28,28	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 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
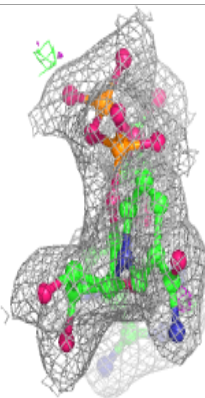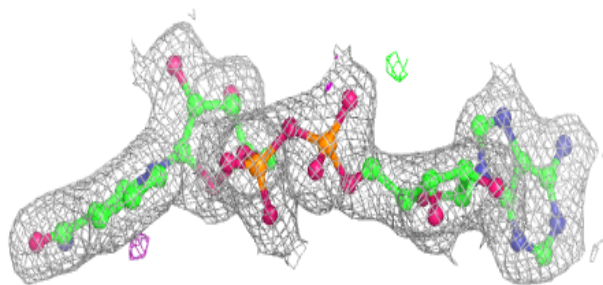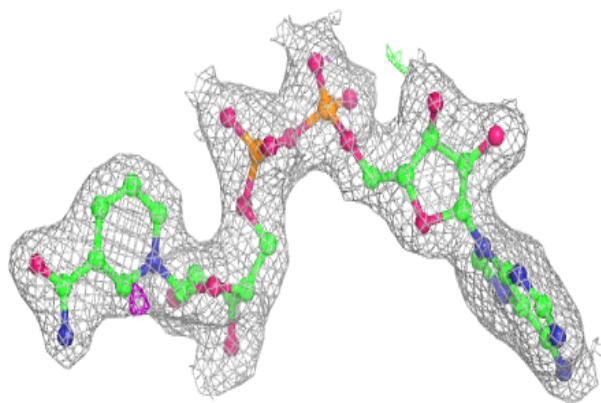and green (positive)
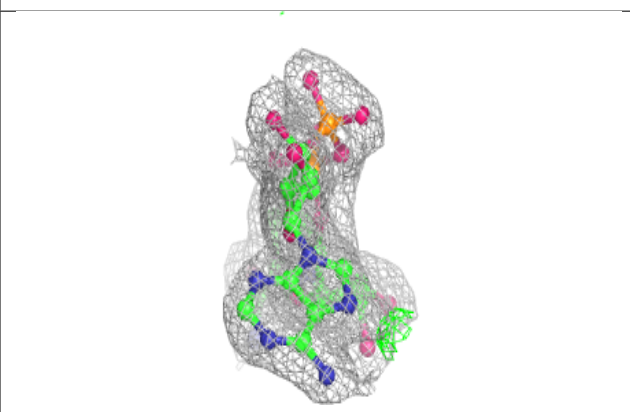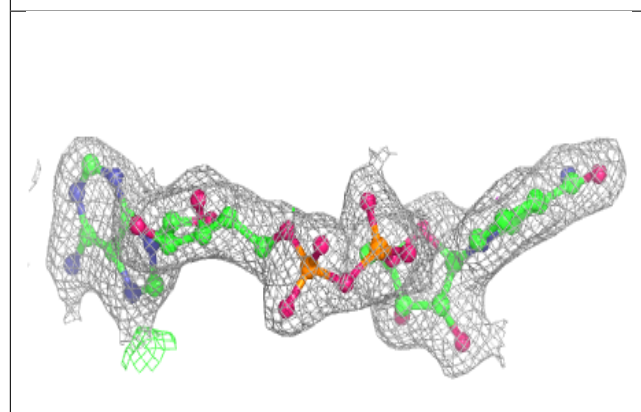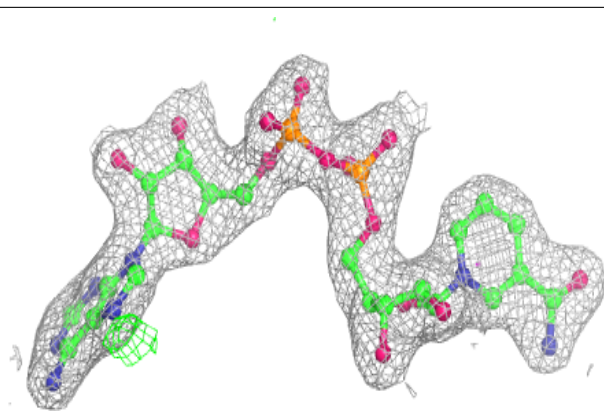
Electron density around NAD D 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
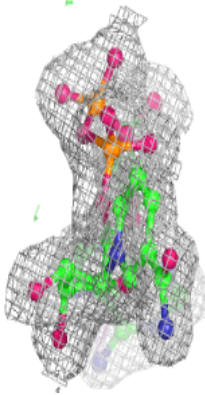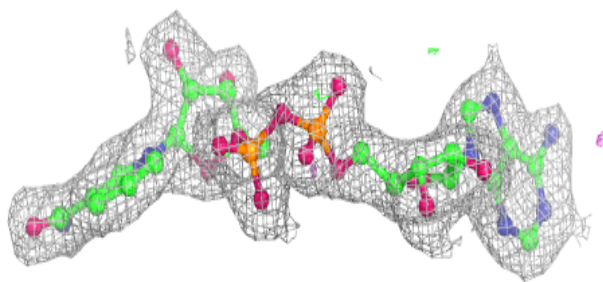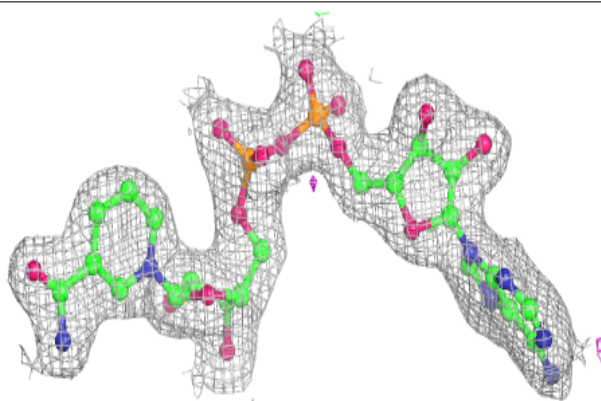$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
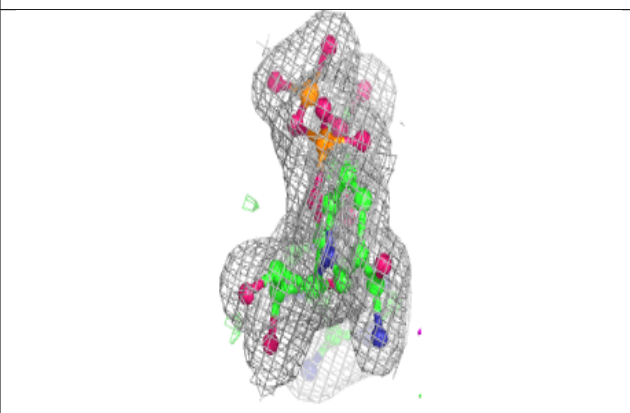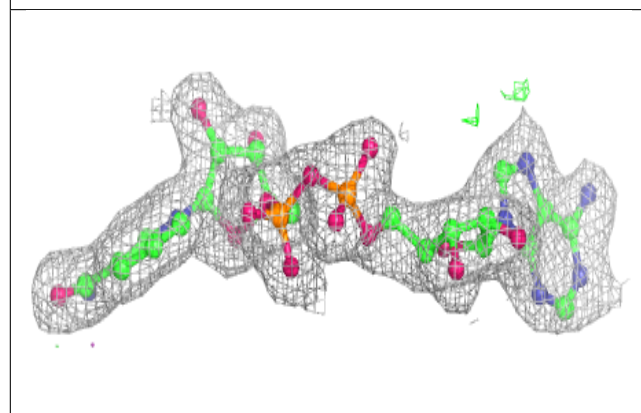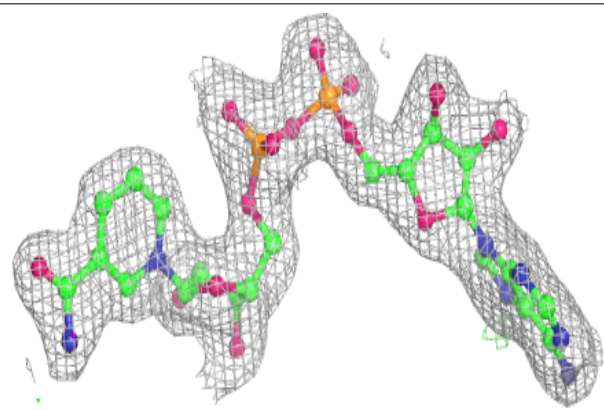
Electron density around NAD B 502:

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

Electron density around NAD C 502:

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

6.5 Other polymers (i)

There are no such residues in this entry.