



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:04 AM UTC

PDB ID : 7Q93 / pdb_00007q93
Title : Crystal Structure of Agrobacterium tumefaciens NADQ, NAD complex.
Authors : Cianci, M.; Minazzato, G.; Heroux, A.; Raffaelli, N.; Sorci, L.; Gasparrini, M.
Deposited on : 2021-11-11
Resolution : 2.19 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

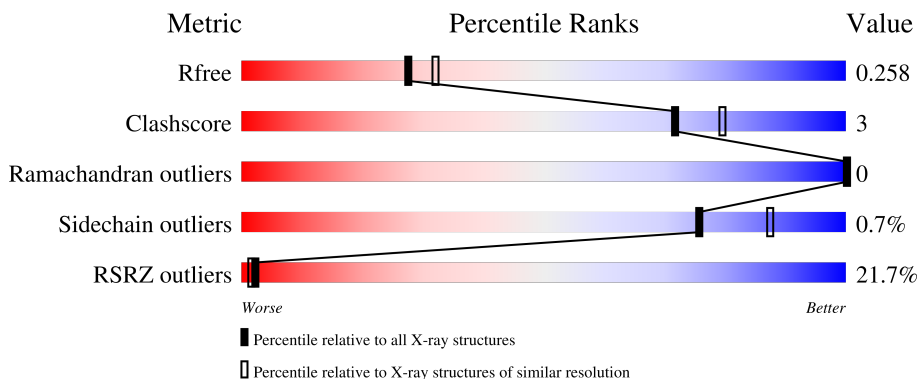
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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	336	7% 76% 19%
1	B	336	17% 72% 6% 22%
1	C	336	16% 71% 9% 20%
1	D	336	29% 69% 11% 19%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9097 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 NADQ transcription factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	Se	0	0	0
			2210	1406	402	398	4			
1	B	263	Total	C	N	O	Se	0	0	0
			2141	1365	388	384	4			
1	C	269	Total	C	N	O	Se	0	0	0
			2184	1393	395	392	4			
1	D	273	Total	C	N	O	Se	0	0	0
			2221	1413	407	398	3			

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MSE	-	initiating methionine	UNP A9CG24
A	-34	ARG	-	expression tag	UNP A9CG24
A	-33	GLY	-	expression tag	UNP A9CG24
A	-32	SER	-	expression tag	UNP A9CG24
A	-31	HIS	-	expression tag	UNP A9CG24
A	-30	HIS	-	expression tag	UNP A9CG24
A	-29	HIS	-	expression tag	UNP A9CG24
A	-28	HIS	-	expression tag	UNP A9CG24
A	-27	HIS	-	expression tag	UNP A9CG24
A	-26	HIS	-	expression tag	UNP A9CG24
A	-25	GLY	-	expression tag	UNP A9CG24
A	-24	MSE	-	expression tag	UNP A9CG24
A	-23	ALA	-	expression tag	UNP A9CG24
A	-22	SER	-	expression tag	UNP A9CG24
A	-21	MSE	-	expression tag	UNP A9CG24
A	-20	THR	-	expression tag	UNP A9CG24
A	-19	GLY	-	expression tag	UNP A9CG24
A	-18	GLY	-	expression tag	UNP A9CG24
A	-17	GLN	-	expression tag	UNP A9CG24
A	-16	GLN	-	expression tag	UNP A9CG24
A	-15	MSE	-	expression tag	UNP A9CG24

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	GLY	-	expression tag	UNP A9CG24
A	-13	ARG	-	expression tag	UNP A9CG24
A	-12	ASP	-	expression tag	UNP A9CG24
A	-11	LEU	-	expression tag	UNP A9CG24
A	-10	TYR	-	expression tag	UNP A9CG24
A	-9	ASP	-	expression tag	UNP A9CG24
A	-8	ASP	-	expression tag	UNP A9CG24
A	-7	ASP	-	expression tag	UNP A9CG24
A	-6	ASP	-	expression tag	UNP A9CG24
A	-5	LYS	-	expression tag	UNP A9CG24
A	-4	ASP	-	expression tag	UNP A9CG24
A	-3	HIS	-	expression tag	UNP A9CG24
A	-2	PRO	-	expression tag	UNP A9CG24
A	-1	PHE	-	expression tag	UNP A9CG24
A	0	THR	-	expression tag	UNP A9CG24
A	1	VAL	-	expression tag	UNP A9CG24
B	-35	MSE	-	initiating methionine	UNP A9CG24
B	-34	ARG	-	expression tag	UNP A9CG24
B	-33	GLY	-	expression tag	UNP A9CG24
B	-32	SER	-	expression tag	UNP A9CG24
B	-31	HIS	-	expression tag	UNP A9CG24
B	-30	HIS	-	expression tag	UNP A9CG24
B	-29	HIS	-	expression tag	UNP A9CG24
B	-28	HIS	-	expression tag	UNP A9CG24
B	-27	HIS	-	expression tag	UNP A9CG24
B	-26	HIS	-	expression tag	UNP A9CG24
B	-25	GLY	-	expression tag	UNP A9CG24
B	-24	MSE	-	expression tag	UNP A9CG24
B	-23	ALA	-	expression tag	UNP A9CG24
B	-22	SER	-	expression tag	UNP A9CG24
B	-21	MSE	-	expression tag	UNP A9CG24
B	-20	THR	-	expression tag	UNP A9CG24
B	-19	GLY	-	expression tag	UNP A9CG24
B	-18	GLY	-	expression tag	UNP A9CG24
B	-17	GLN	-	expression tag	UNP A9CG24
B	-16	GLN	-	expression tag	UNP A9CG24
B	-15	MSE	-	expression tag	UNP A9CG24
B	-14	GLY	-	expression tag	UNP A9CG24
B	-13	ARG	-	expression tag	UNP A9CG24
B	-12	ASP	-	expression tag	UNP A9CG24
B	-11	LEU	-	expression tag	UNP A9CG24
B	-10	TYR	-	expression tag	UNP A9CG24

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	ASP	-	expression tag	UNP A9CG24
B	-8	ASP	-	expression tag	UNP A9CG24
B	-7	ASP	-	expression tag	UNP A9CG24
B	-6	ASP	-	expression tag	UNP A9CG24
B	-5	LYS	-	expression tag	UNP A9CG24
B	-4	ASP	-	expression tag	UNP A9CG24
B	-3	HIS	-	expression tag	UNP A9CG24
B	-2	PRO	-	expression tag	UNP A9CG24
B	-1	PHE	-	expression tag	UNP A9CG24
B	0	THR	-	expression tag	UNP A9CG24
B	1	VAL	-	expression tag	UNP A9CG24
C	-35	MSE	-	initiating methionine	UNP A9CG24
C	-34	ARG	-	expression tag	UNP A9CG24
C	-33	GLY	-	expression tag	UNP A9CG24
C	-32	SER	-	expression tag	UNP A9CG24
C	-31	HIS	-	expression tag	UNP A9CG24
C	-30	HIS	-	expression tag	UNP A9CG24
C	-29	HIS	-	expression tag	UNP A9CG24
C	-28	HIS	-	expression tag	UNP A9CG24
C	-27	HIS	-	expression tag	UNP A9CG24
C	-26	HIS	-	expression tag	UNP A9CG24
C	-25	GLY	-	expression tag	UNP A9CG24
C	-24	MSE	-	expression tag	UNP A9CG24
C	-23	ALA	-	expression tag	UNP A9CG24
C	-22	SER	-	expression tag	UNP A9CG24
C	-21	MSE	-	expression tag	UNP A9CG24
C	-20	THR	-	expression tag	UNP A9CG24
C	-19	GLY	-	expression tag	UNP A9CG24
C	-18	GLY	-	expression tag	UNP A9CG24
C	-17	GLN	-	expression tag	UNP A9CG24
C	-16	GLN	-	expression tag	UNP A9CG24
C	-15	MSE	-	expression tag	UNP A9CG24
C	-14	GLY	-	expression tag	UNP A9CG24
C	-13	ARG	-	expression tag	UNP A9CG24
C	-12	ASP	-	expression tag	UNP A9CG24
C	-11	LEU	-	expression tag	UNP A9CG24
C	-10	TYR	-	expression tag	UNP A9CG24
C	-9	ASP	-	expression tag	UNP A9CG24
C	-8	ASP	-	expression tag	UNP A9CG24
C	-7	ASP	-	expression tag	UNP A9CG24
C	-6	ASP	-	expression tag	UNP A9CG24
C	-5	LYS	-	expression tag	UNP A9CG24

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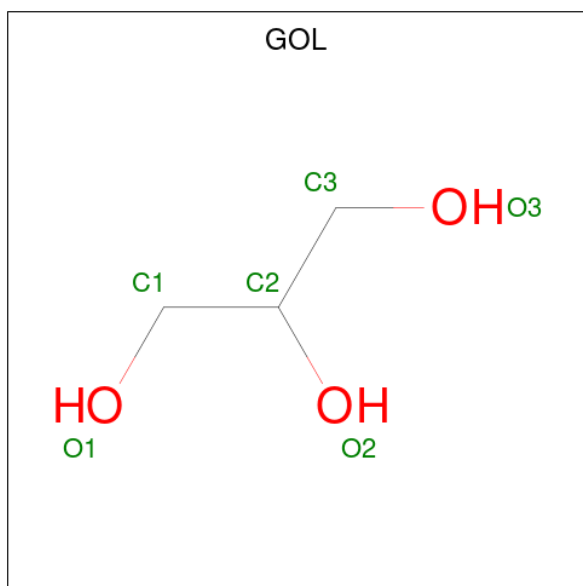
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	ASP	-	expression tag	UNP A9CG24
C	-3	HIS	-	expression tag	UNP A9CG24
C	-2	PRO	-	expression tag	UNP A9CG24
C	-1	PHE	-	expression tag	UNP A9CG24
C	0	THR	-	expression tag	UNP A9CG24
C	1	VAL	-	expression tag	UNP A9CG24
D	-35	MSE	-	initiating methionine	UNP A9CG24
D	-34	ARG	-	expression tag	UNP A9CG24
D	-33	GLY	-	expression tag	UNP A9CG24
D	-32	SER	-	expression tag	UNP A9CG24
D	-31	HIS	-	expression tag	UNP A9CG24
D	-30	HIS	-	expression tag	UNP A9CG24
D	-29	HIS	-	expression tag	UNP A9CG24
D	-28	HIS	-	expression tag	UNP A9CG24
D	-27	HIS	-	expression tag	UNP A9CG24
D	-26	HIS	-	expression tag	UNP A9CG24
D	-25	GLY	-	expression tag	UNP A9CG24
D	-24	MSE	-	expression tag	UNP A9CG24
D	-23	ALA	-	expression tag	UNP A9CG24
D	-22	SER	-	expression tag	UNP A9CG24
D	-21	MSE	-	expression tag	UNP A9CG24
D	-20	THR	-	expression tag	UNP A9CG24
D	-19	GLY	-	expression tag	UNP A9CG24
D	-18	GLY	-	expression tag	UNP A9CG24
D	-17	GLN	-	expression tag	UNP A9CG24
D	-16	GLN	-	expression tag	UNP A9CG24
D	-15	MSE	-	expression tag	UNP A9CG24
D	-14	GLY	-	expression tag	UNP A9CG24
D	-13	ARG	-	expression tag	UNP A9CG24
D	-12	ASP	-	expression tag	UNP A9CG24
D	-11	LEU	-	expression tag	UNP A9CG24
D	-10	TYR	-	expression tag	UNP A9CG24
D	-9	ASP	-	expression tag	UNP A9CG24
D	-8	ASP	-	expression tag	UNP A9CG24
D	-7	ASP	-	expression tag	UNP A9CG24
D	-6	ASP	-	expression tag	UNP A9CG24
D	-5	LYS	-	expression tag	UNP A9CG24
D	-4	ASP	-	expression tag	UNP A9CG24
D	-3	HIS	-	expression tag	UNP A9CG24
D	-2	PRO	-	expression tag	UNP A9CG24
D	-1	PHE	-	expression tag	UNP A9CG24
D	0	THR	-	expression tag	UNP A9CG24

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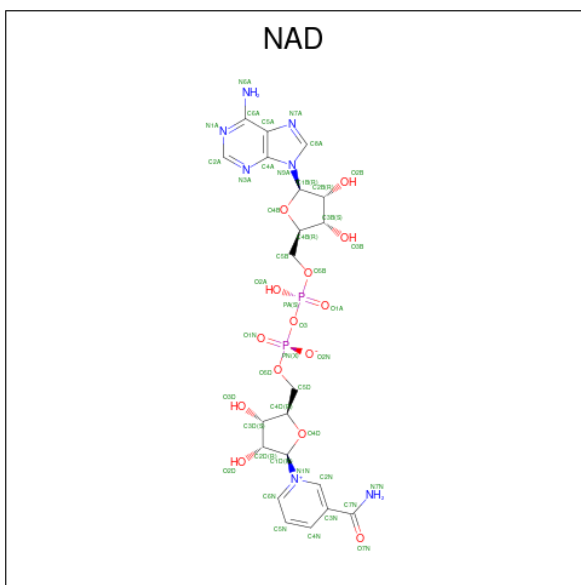
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP A9CG24

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



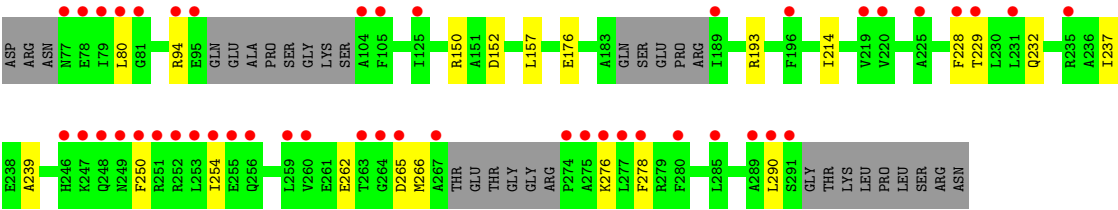
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

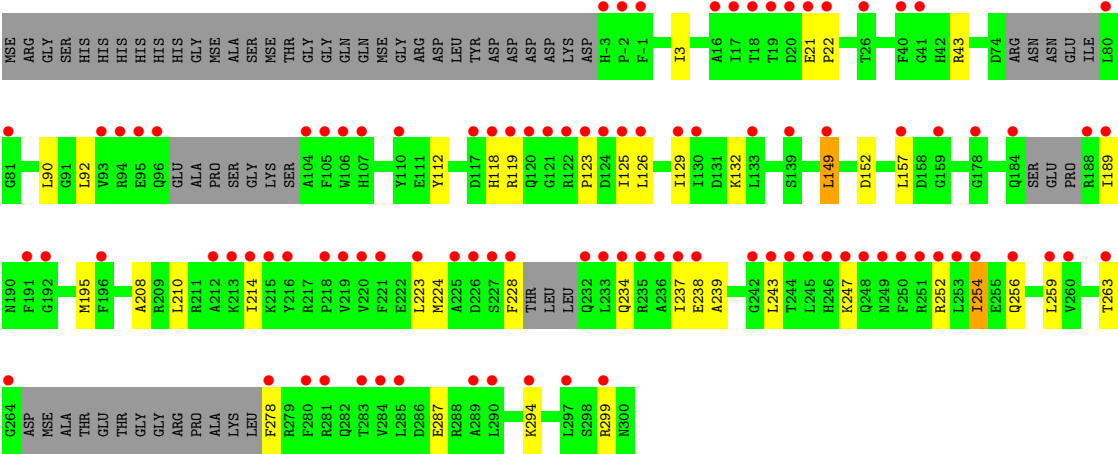
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total K 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	93	Total O 93 93	0	0
5	B	57	Total O 57 57	0	0
5	C	71	Total O 71 71	0	0
5	D	57	Total O 57 57	0	0



● Molecule 1: NADQ transcription factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.66Å 133.72Å 87.80Å 90.00° 101.05° 90.00°	Depositor
Resolution (Å)	86.17 – 2.19 86.17 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.7 (86.17-2.19) 98.7 (86.17-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.228 , 0.259 0.228 , 0.258	Depositor DCC
R_{free} test set	3403 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9097	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, GOL, 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	0.11	0/2255	0.27	0/3039
1	B	0.10	0/2185	0.25	0/2945
1	C	0.09	0/2229	0.25	0/3005
1	D	0.10	0/2268	0.26	0/3058
All	All	0.10	0/8937	0.26	0/12047

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2210	0	2165	9	0
1	B	2141	0	2103	11	0
1	C	2184	0	2148	19	0
1	D	2221	0	2174	24	0
2	A	12	0	16	0	0
2	C	6	0	8	0	0
3	D	44	0	26	1	0
4	D	1	0	0	0	0
5	A	93	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	57	0	0	0	0
5	C	71	0	0	1	0
5	D	57	0	0	0	0
All	All	9097	0	8640	58	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 3.

All (58) 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:B:195:MSE:HE3	1:B:200:ARG:HG2	1.57	0.87
1:D:234:GLN:HE22	1:D:247:LYS:HA	1.46	0.80
1:D:132:LYS:HE2	1:D:189:ILE:HG12	1.73	0.70
1:A:22:PRO:HD3	1:A:239:ALA:HB1	1.74	0.69
1:A:28:ARG:HG3	1:A:31:ALA:HB3	1.77	0.66
1:B:23:ARG:HA	1:B:108:GLY:HA2	1.80	0.62
1:C:43:ARG:NH1	3:D:401:NAD:O1A	2.31	0.61
1:D:152:ASP:HA	1:D:157:LEU:H	1.65	0.60
1:D:123:PRO:HG2	1:D:126:LEU:HD23	1.85	0.59
1:D:90:LEU:HD21	1:D:210:LEU:HG	1.84	0.59
1:B:152:ASP:HA	1:B:157:LEU:H	1.68	0.59
1:C:228:PHE:O	1:C:278:PHE:N	2.35	0.58
1:C:290:LEU:HD21	1:D:149:LEU:HD23	1.85	0.57
1:B:22:PRO:HD3	1:B:239:ALA:HB1	1.86	0.57
1:D:214:ILE:HD12	1:D:237:ILE:HG23	1.86	0.57
1:D:208:ALA:HB1	1:D:299:ARG:HH22	1.70	0.55
1:C:229:THR:HG23	1:C:232:GLN:H	1.72	0.54
1:B:251:ARG:O	1:B:255:GLU:HG2	2.08	0.54
1:C:22:PRO:HD3	1:C:239:ALA:HB1	1.89	0.53
1:C:265:ASP:OD1	1:C:266:MSE:N	2.41	0.53
1:D:228:PHE:O	1:D:278:PHE:N	2.43	0.52
1:C:19:THR:OG1	1:C:20:ASP:N	2.39	0.52
1:D:112:TYR:CZ	1:D:195:MSE:HE3	2.45	0.52
1:A:246:HIS:ND1	1:A:249:ASN:OD1	2.42	0.49
1:D:252:ARG:HH12	1:D:256:GLN:HG2	1.77	0.49
1:D:22:PRO:HD3	1:D:239:ALA:HB1	1.94	0.48
1:B:90:LEU:HD21	1:B:210:LEU:HG	1.96	0.48
1:B:265:ASP:OD1	1:B:266:MSE:N	2.46	0.47
1:D:125:ILE:O	1:D:129:ILE:HG12	2.15	0.47
1:C:150:ARG:NH1	1:C:176:GLU:OE1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ASP:HA	1:D:157:LEU:N	2.30	0.46
1:C:29:GLU:O	1:C:193:ARG:NH2	2.47	0.45
1:B:92:LEU:HD21	1:B:210:LEU:HD11	1.99	0.45
1:C:214:ILE:HD12	1:C:237:ILE:HG23	1.98	0.45
1:C:73:ARG:CZ	1:D:43:ARG:HB2	2.46	0.45
1:B:94:ARG:HH12	1:B:225:ALA:HB2	1.82	0.45
1:A:23:ARG:HH21	1:A:95:GLU:CD	2.25	0.45
1:B:128:SER:O	1:B:132:LYS:HG2	2.17	0.44
1:B:247:LYS:O	1:B:251:ARG:HG3	2.17	0.44
1:C:68:TYR:CG	1:D:294:LYS:HG3	2.53	0.44
1:D:238:GLU:HB2	1:D:243:LEU:O	2.18	0.44
1:C:80:LEU:HD11	1:D:3:ILE:HG21	1.99	0.43
1:D:21:GLU:OE2	1:D:119:ARG:NH2	2.48	0.43
1:D:224:MSE:HA	1:D:224:MSE:HE2	2.01	0.43
1:A:105:PHE:CD1	1:A:105:PHE:N	2.85	0.43
1:A:217:ARG:HG2	1:A:219:VAL:HG23	2.00	0.43
1:D:92:LEU:HD21	1:D:210:LEU:HD21	2.00	0.42
1:D:118:HIS:HB2	1:D:243:LEU:HD23	2.01	0.42
1:C:94:ARG:HA	1:C:94:ARG:HD2	1.81	0.42
1:C:152:ASP:HA	1:C:157:LEU:H	1.84	0.42
1:C:250:PHE:CE2	1:C:254:ILE:HD11	2.54	0.42
1:A:266:MSE:CE	1:A:274:PRO:HB2	2.50	0.41
1:D:254:ILE:HG23	1:D:259:LEU:HB2	2.02	0.41
1:D:92:LEU:HB3	1:D:223:LEU:HG	2.02	0.41
1:C:46:GLN:HG3	5:C:505:HOH:O	2.20	0.41
1:A:252:ARG:HD2	1:C:40:PHE:HB3	2.03	0.41
1:C:262:GLU:CD	1:C:276:LYS:HD3	2.46	0.40
1:A:105:PHE:N	1:A:105:PHE:HD1	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/336 (78%)	256 (98%)	5 (2%)	0	100	100
1	B	253/336 (75%)	247 (98%)	6 (2%)	0	100	100
1	C	259/336 (77%)	251 (97%)	8 (3%)	0	100	100
1	D	261/336 (78%)	250 (96%)	11 (4%)	0	100	100
All	All	1034/1344 (77%)	1004 (97%)	30 (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	225/270 (83%)	224 (100%)	1 (0%)	84	92
1	B	218/270 (81%)	217 (100%)	1 (0%)	81	90
1	C	222/270 (82%)	222 (100%)	0	100	100
1	D	226/270 (84%)	222 (98%)	4 (2%)	51	68
All	All	891/1080 (82%)	885 (99%)	6 (1%)	76	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	PHE
1	B	94	ARG
1	D	149	LEU
1	D	254	ILE
1	D	263	THR
1	D	287	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN

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Mol	Chain	Res	Type
1	A	257	GLN
1	B	54	HIS
1	B	58	HIS
1	B	246	HIS
1	C	258	GLN
1	C	282	GLN
1	D	232	GLN
1	D	234	GLN
1	D	246	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	GOL	A	401	-	5,5,5	0.95	0	5,5,5	1.36	1 (20%)
2	GOL	A	402	-	5,5,5	0.89	0	5,5,5	1.21	1 (20%)
2	GOL	C	401	-	5,5,5	0.93	0	5,5,5	1.16	1 (20%)
3	NAD	D	401	-	46,48,48	0.63	1 (2%)	64,73,73	0.60	1 (1%)

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	GOL	A	401	-	-	0/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	C	401	-	-	0/4/4/4	-
3	NAD	D	401	-	-	2/30/62/62	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NAD	C2N-N1N	2.55	1.37	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	NAD	C6N-N1N-C2N	-2.63	119.64	121.88
2	A	401	GOL	C3-C2-C1	-2.30	103.36	111.80
2	A	402	GOL	C3-C2-C1	-2.21	103.67	111.80
2	C	401	GOL	C3-C2-C1	-2.21	103.69	111.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	NAD	PN-O3-PA-O5B
3	D	401	NAD	PA-O3-PN-O1N

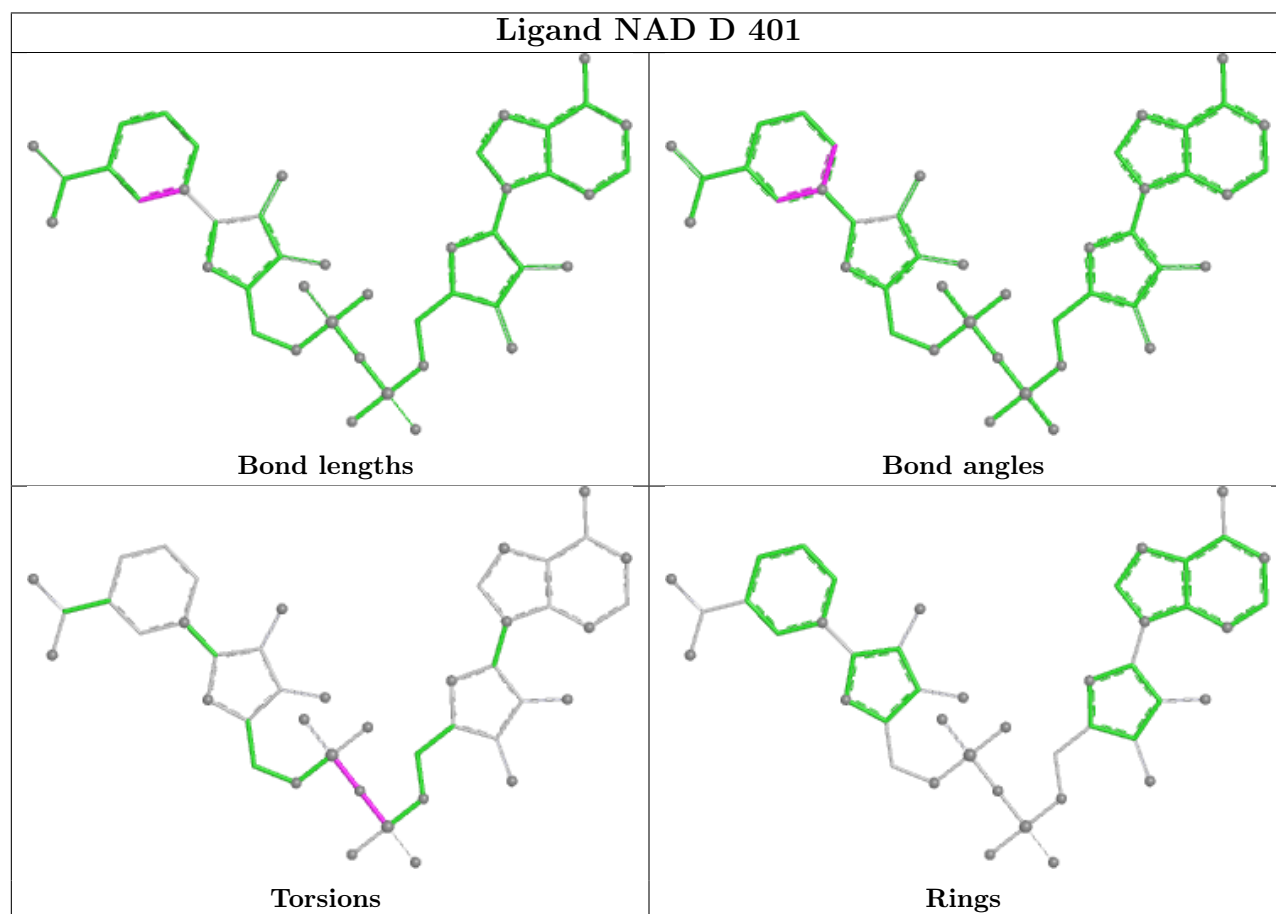
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	NAD	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

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	267/336 (79%)	0.68	22 (8%) 17 15	26, 40, 59, 77	0
1	B	259/336 (77%)	1.22	57 (22%) 2 1	29, 47, 97, 119	0
1	C	265/336 (78%)	1.02	53 (20%) 3 2	25, 43, 83, 99	0
1	D	270/336 (80%)	1.64	98 (36%) 1 0	29, 52, 96, 110	0
All	All	1061/1344 (78%)	1.14	230 (21%) 2 1	25, 45, 90, 119	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	264	GLY	7.5
1	D	233	LEU	7.5
1	A	105	PHE	7.0
1	D	228	PHE	5.5
1	D	259	LEU	5.4
1	B	104	ALA	5.3
1	D	236	ALA	5.3
1	C	1	VAL	5.2
1	C	259	LEU	5.1
1	D	-2	PRO	4.9
1	C	275	ALA	4.9
1	B	285	LEU	4.9
1	C	289	ALA	4.8
1	B	277	LEU	4.8
1	D	245	LEU	4.8
1	B	253	LEU	4.7
1	D	278	PHE	4.6
1	D	294	LYS	4.5
1	A	80	LEU	4.4
1	D	17	ILE	4.4
1	C	274	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	291	SER	4.3
1	B	246	HIS	4.3
1	C	267	ALA	4.2
1	B	292	GLY	4.2
1	C	290	LEU	4.2
1	D	227	SER	4.2
1	B	230	LEU	4.2
1	D	21	GLU	4.1
1	D	280	PHE	4.1
1	D	19	THR	4.1
1	C	105	PHE	4.1
1	D	93	VAL	4.1
1	D	221	PHE	4.1
1	B	259	LEU	4.0
1	D	260	VAL	4.0
1	D	122	ARG	4.0
1	D	196	PHE	4.0
1	C	77	ASN	4.0
1	B	260	VAL	4.0
1	B	216	TYR	4.0
1	B	218	PRO	4.0
1	D	284	VAL	3.9
1	B	278	PHE	3.9
1	D	254	ILE	3.9
1	B	227	SER	3.9
1	D	16	ALA	3.9
1	D	123	PRO	3.9
1	A	157	LEU	3.8
1	B	254	ILE	3.8
1	B	276	LYS	3.8
1	D	220	VAL	3.8
1	D	232	GLN	3.7
1	B	106	TRP	3.7
1	D	225	ALA	3.7
1	D	242	GLY	3.6
1	D	106	TRP	3.6
1	B	264	GLY	3.6
1	B	225	ALA	3.6
1	D	20	ASP	3.6
1	D	250	PHE	3.6
1	B	293	THR	3.6
1	C	253	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	253	LEU	3.6
1	C	254	ILE	3.5
1	D	216	TYR	3.5
1	B	20	ASP	3.5
1	C	264	GLY	3.5
1	C	79	ILE	3.5
1	D	237	ILE	3.5
1	D	219	VAL	3.5
1	D	244	THR	3.5
1	A	216	TYR	3.4
1	D	218	PRO	3.4
1	C	228	PHE	3.4
1	D	247	LYS	3.4
1	C	285	LEU	3.4
1	C	278	PHE	3.4
1	D	191	PHE	3.4
1	B	94	ARG	3.3
1	D	105	PHE	3.3
1	B	247	LYS	3.3
1	D	80	LEU	3.3
1	D	285	LEU	3.3
1	C	250	PHE	3.3
1	D	95	GLU	3.3
1	B	158	ASP	3.3
1	A	68	TYR	3.2
1	D	125	ILE	3.2
1	A	77	ASN	3.2
1	A	196	PHE	3.2
1	A	291	SER	3.2
1	D	235	ARG	3.2
1	C	196	PHE	3.2
1	B	219	VAL	3.1
1	C	3	ILE	3.1
1	A	28	ARG	3.1
1	D	188	ARG	3.1
1	B	280	PHE	3.1
1	D	121	GLY	3.1
1	B	263	THR	3.1
1	B	251	ARG	3.1
1	C	219	VAL	3.1
1	C	59	HIS	3.0
1	C	246	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	246	HIS	3.0
1	D	126	LEU	3.0
1	D	263	THR	3.0
1	D	104	ALA	3.0
1	C	229	THR	3.0
1	B	250	PHE	3.0
1	A	79	ILE	3.0
1	D	22	PRO	3.0
1	B	228	PHE	3.0
1	C	78	GLU	2.9
1	C	277	LEU	2.9
1	C	189	ILE	2.9
1	D	251	ARG	2.9
1	B	196	PHE	2.9
1	D	223	LEU	2.9
1	B	226	ASP	2.9
1	D	107	HIS	2.9
1	D	159	GLY	2.9
1	B	231	LEU	2.8
1	D	130	ILE	2.8
1	D	238	GLU	2.8
1	A	73	ARG	2.8
1	B	149	LEU	2.8
1	B	220	VAL	2.8
1	D	119	ARG	2.8
1	D	-3	HIS	2.8
1	C	260	VAL	2.8
1	D	214	ILE	2.8
1	C	94	ARG	2.8
1	C	95	GLU	2.8
1	D	283	THR	2.8
1	B	1	VAL	2.8
1	B	40	PHE	2.7
1	D	215	LYS	2.7
1	D	297	LEU	2.7
1	B	257	GLN	2.7
1	C	81	GLY	2.7
1	D	41	GLY	2.7
1	D	40	PHE	2.7
1	B	233	LEU	2.7
1	C	73	ARG	2.7
1	D	243	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	234	GLN	2.7
1	B	284	VAL	2.7
1	B	290	LEU	2.7
1	B	265	ASP	2.7
1	D	129	ILE	2.7
1	C	263	THR	2.6
1	D	94	ARG	2.6
1	D	120	GLN	2.6
1	B	283	THR	2.6
1	D	-1	PHE	2.6
1	C	256	GLN	2.6
1	C	255	GLU	2.6
1	B	244	THR	2.6
1	C	104	ALA	2.6
1	D	18	THR	2.6
1	C	247	LYS	2.6
1	A	158	ASP	2.6
1	D	234	GLN	2.5
1	D	213	LYS	2.5
1	D	81	GLY	2.5
1	D	189	ILE	2.5
1	D	118	HIS	2.5
1	C	235	ARG	2.5
1	C	125	ILE	2.5
1	D	248	GLN	2.4
1	D	26	THR	2.4
1	D	124	ASP	2.4
1	B	68	TYR	2.4
1	D	96	GLN	2.4
1	C	280	PHE	2.4
1	C	18	THR	2.4
1	C	248	GLN	2.3
1	B	145	ALA	2.3
1	B	105	PHE	2.3
1	D	139	SER	2.3
1	A	3	ILE	2.3
1	D	256	GLN	2.3
1	B	124	ASP	2.3
1	C	276	LYS	2.3
1	B	262	GLU	2.3
1	C	19	THR	2.3
1	D	249	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	252	ARG	2.3
1	D	117	ASP	2.3
1	D	149	LEU	2.3
1	B	249	ASN	2.2
1	D	212	ALA	2.2
1	A	97	GLU	2.2
1	B	281	ARG	2.2
1	A	268	THR	2.2
1	D	178	GLY	2.2
1	D	252	ARG	2.2
1	D	184	GLN	2.2
1	D	299	ARG	2.2
1	B	229	THR	2.2
1	C	265	ASP	2.2
1	A	55	GLU	2.1
1	C	225	ALA	2.1
1	D	289	ALA	2.1
1	C	231	LEU	2.1
1	D	226	ASP	2.1
1	B	19	THR	2.1
1	D	192	GLY	2.1
1	B	261	GLU	2.1
1	C	249	ASN	2.1
1	A	123	PRO	2.1
1	C	251	ARG	2.1
1	D	281	ARG	2.1
1	A	64	LEU	2.1
1	D	133	LEU	2.1
1	D	290	LEU	2.1
1	A	96	GLN	2.1
1	B	279	ARG	2.1
1	D	110	TYR	2.1
1	C	17	ILE	2.1
1	B	221	PHE	2.1
1	A	106	TRP	2.1
1	A	289	ALA	2.1
1	C	80	LEU	2.0
1	C	220	VAL	2.0
1	A	184	GLN	2.0
1	B	157	LEU	2.0
1	D	157	LEU	2.0

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](#)

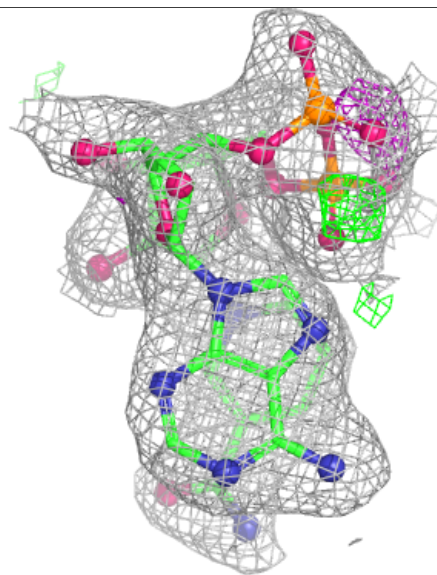
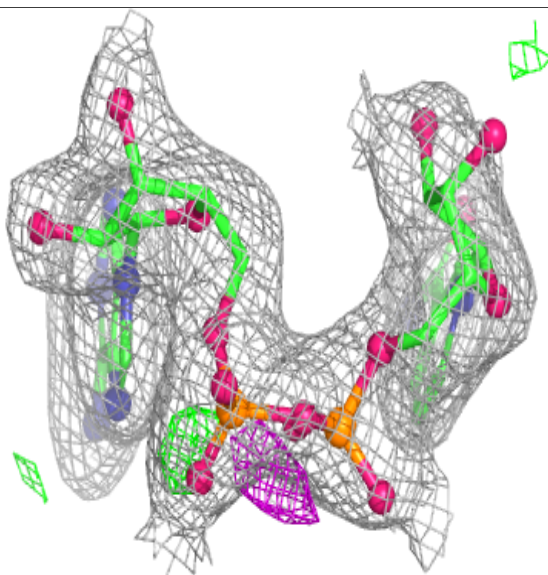
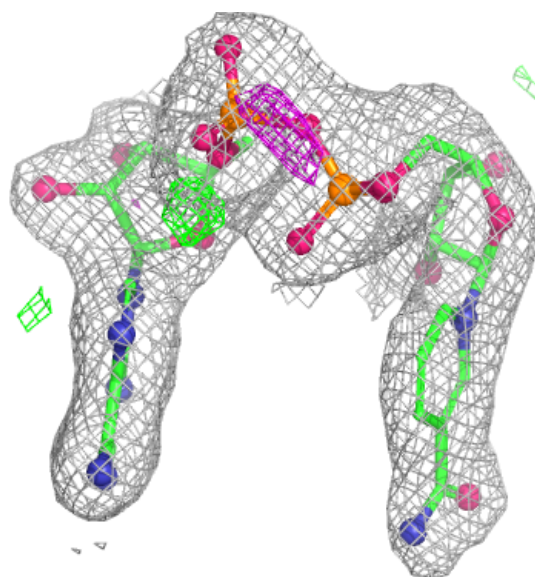
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	A	402	6/6	0.69	0.24	41,57,66,74	0
2	GOL	A	401	6/6	0.78	0.17	57,59,64,74	0
2	GOL	C	401	6/6	0.79	0.18	56,60,61,62	0
3	NAD	D	401	44/44	0.91	0.09	34,44,58,60	0
4	K	D	402	1/1	0.98	0.06	38,38,38,38	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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.