



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:43 AM UTC

PDB ID : 6K96 / pdb_00006k96
Title : Crystal structure of Ari2
Authors : Miyanaga, A.; Tsunoda, T.; Kudo, F.; Eguchi, T.
Deposited on : 2019-06-14
Resolution : 2.50 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

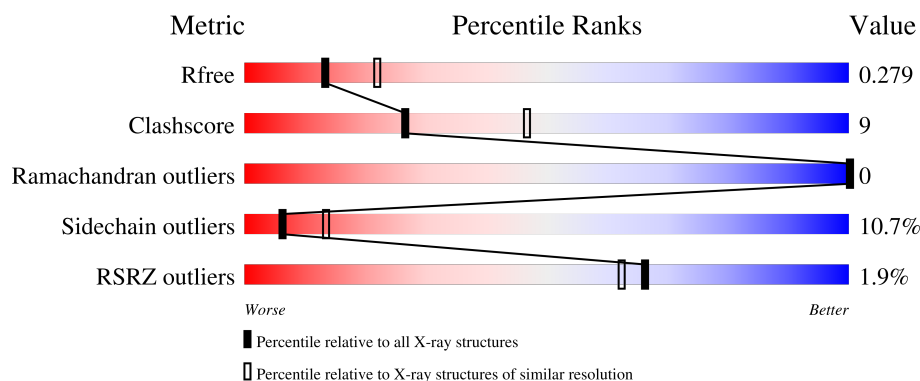
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	378	63% 21% • 12%
1	B	378	2% 66% 21% • 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5365 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 Five-membered-cyclitol-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2486	1577	431	474	4			
1	B	343	Total	C	N	O	S	0	0	0
			2562	1623	447	489	3			

There are 40 discrepancies between the modelled and reference sequences:

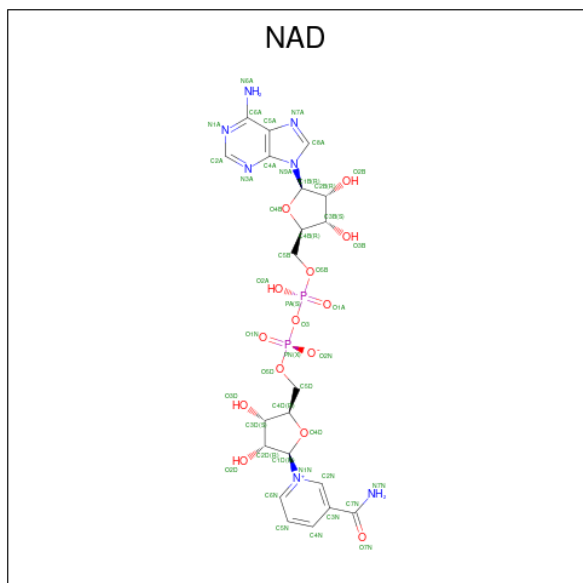
Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ASP	-	expression tag	UNP A0A1B4ZC85
A	360	PRO	-	expression tag	UNP A0A1B4ZC85
A	361	ASN	-	expression tag	UNP A0A1B4ZC85
A	362	SER	-	expression tag	UNP A0A1B4ZC85
A	363	SER	-	expression tag	UNP A0A1B4ZC85
A	364	SER	-	expression tag	UNP A0A1B4ZC85
A	365	VAL	-	expression tag	UNP A0A1B4ZC85
A	366	ASP	-	expression tag	UNP A0A1B4ZC85
A	367	LYS	-	expression tag	UNP A0A1B4ZC85
A	368	LEU	-	expression tag	UNP A0A1B4ZC85
A	369	ALA	-	expression tag	UNP A0A1B4ZC85
A	370	ALA	-	expression tag	UNP A0A1B4ZC85
A	371	LEU	-	expression tag	UNP A0A1B4ZC85
A	372	GLU	-	expression tag	UNP A0A1B4ZC85
A	373	HIS	-	expression tag	UNP A0A1B4ZC85
A	374	HIS	-	expression tag	UNP A0A1B4ZC85
A	375	HIS	-	expression tag	UNP A0A1B4ZC85
A	376	HIS	-	expression tag	UNP A0A1B4ZC85
A	377	HIS	-	expression tag	UNP A0A1B4ZC85
A	378	HIS	-	expression tag	UNP A0A1B4ZC85
B	359	ASP	-	expression tag	UNP A0A1B4ZC85
B	360	PRO	-	expression tag	UNP A0A1B4ZC85
B	361	ASN	-	expression tag	UNP A0A1B4ZC85
B	362	SER	-	expression tag	UNP A0A1B4ZC85
B	363	SER	-	expression tag	UNP A0A1B4ZC85

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	364	SER	-	expression tag	UNP A0A1B4ZC85
B	365	VAL	-	expression tag	UNP A0A1B4ZC85
B	366	ASP	-	expression tag	UNP A0A1B4ZC85
B	367	LYS	-	expression tag	UNP A0A1B4ZC85
B	368	LEU	-	expression tag	UNP A0A1B4ZC85
B	369	ALA	-	expression tag	UNP A0A1B4ZC85
B	370	ALA	-	expression tag	UNP A0A1B4ZC85
B	371	LEU	-	expression tag	UNP A0A1B4ZC85
B	372	GLU	-	expression tag	UNP A0A1B4ZC85
B	373	HIS	-	expression tag	UNP A0A1B4ZC85
B	374	HIS	-	expression tag	UNP A0A1B4ZC85
B	375	HIS	-	expression tag	UNP A0A1B4ZC85
B	376	HIS	-	expression tag	UNP A0A1B4ZC85
B	377	HIS	-	expression tag	UNP A0A1B4ZC85
B	378	HIS	-	expression tag	UNP A0A1B4ZC85

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



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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

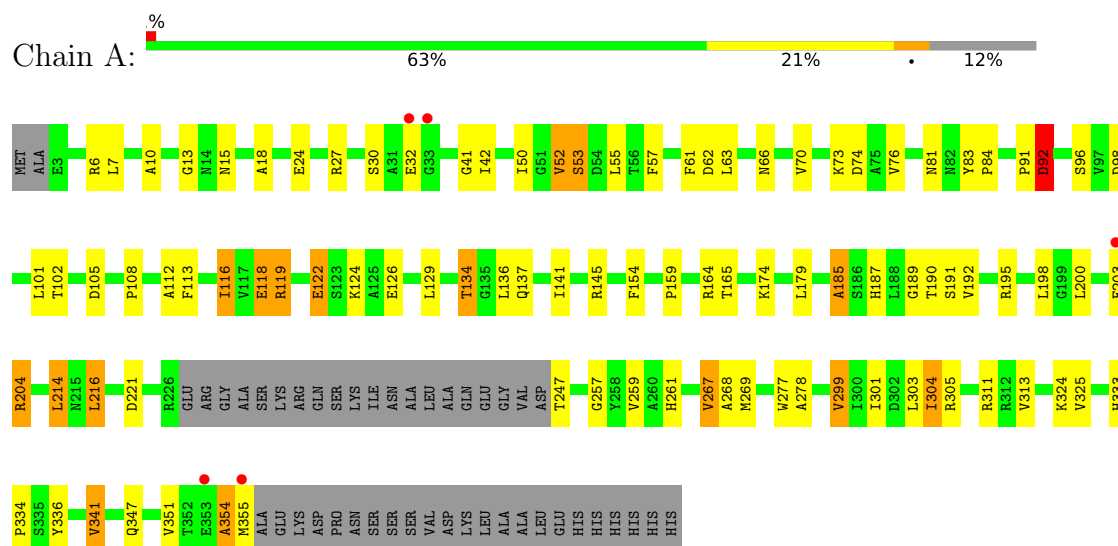
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	116	Total O 116 116	0	0
5	B	93	Total O 93 93	0	0

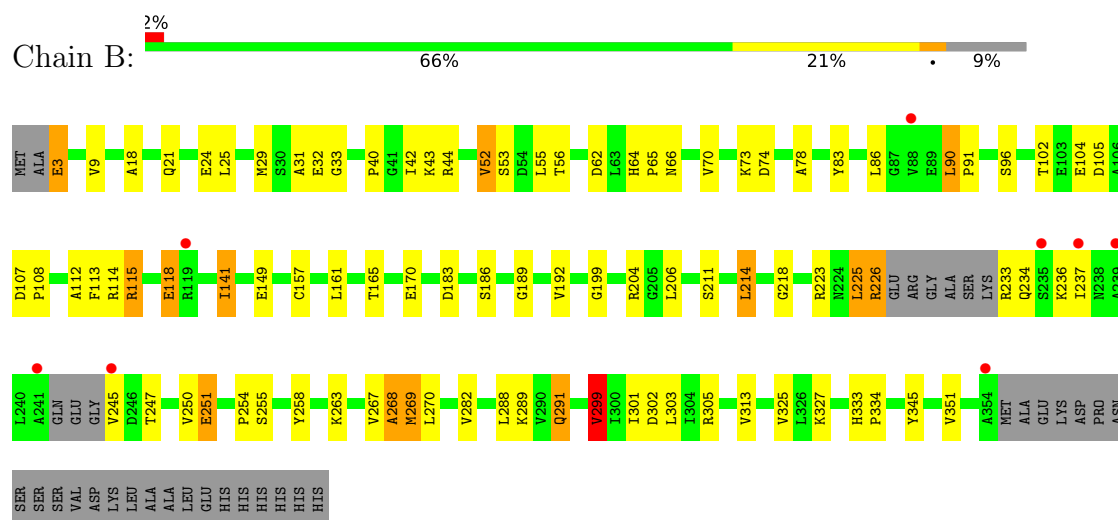
3 Residue-property plots

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: Five-membered-cyclitol-phosphate synthase



- Molecule 1: Five-membered-cyclitol-phosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.18Å 101.18Å 389.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.18 – 2.50 47.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.18-2.50) 97.0 (47.18-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.226 , 0.280 0.229 , 0.279	Depositor DCC
R_{free} test set	2061 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5365	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.50% 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: GOL, NAD, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.29	10/2532 (0.4%)	1.61	23/3440 (0.7%)
1	B	1.22	6/2607 (0.2%)	1.59	16/3540 (0.5%)
All	All	1.25	16/5139 (0.3%)	1.60	39/6980 (0.6%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	ASN	C-O	9.46	1.35	1.24
1	A	267	VAL	C-O	-7.28	1.16	1.24
1	B	267	VAL	C-O	-6.63	1.17	1.24
1	B	268	ALA	C-O	-6.57	1.15	1.24
1	A	336	TYR	C-O	5.91	1.30	1.23
1	A	185	ALA	C-O	-5.79	1.16	1.24
1	A	41	GLY	C-O	-5.77	1.16	1.24
1	A	10	ALA	C-O	-5.68	1.17	1.23
1	B	211	SER	C-O	-5.57	1.17	1.23
1	A	63	LEU	C-O	5.27	1.30	1.24
1	A	311	ARG	C-O	5.27	1.30	1.24
1	B	251	GLU	C-O	-5.27	1.17	1.24
1	A	187	HIS	C-O	5.23	1.30	1.24
1	B	90	LEU	C-N	5.11	1.39	1.33
1	B	157	CYS	C-O	5.11	1.30	1.24
1	A	257	GLY	C-O	5.00	1.30	1.23

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	LEU	CA-C-N	7.12	127.08	120.03
1	B	90	LEU	C-N-CA	7.12	127.08	120.03
1	B	291	GLN	CB-CA-C	-6.72	100.32	111.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	THR	CA-CB-OG1	-6.67	99.59	109.60
1	A	92	ASP	CB-CA-C	6.30	117.33	110.08
1	A	221	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	354	ALA	CA-C-N	6.09	132.66	121.70
1	A	354	ALA	C-N-CA	6.09	132.66	121.70
1	B	351	VAL	N-CA-C	-6.08	104.92	110.82
1	A	118	GLU	N-CA-C	-5.79	105.05	111.36
1	B	291	GLN	CB-CG-CD	5.78	122.43	112.60
1	A	136	LEU	CA-C-N	5.62	127.82	120.28
1	A	136	LEU	C-N-CA	5.62	127.82	120.28
1	A	204	ARG	CB-CG-CD	5.61	124.19	111.30
1	B	289	LYS	CA-C-O	-5.48	114.44	120.36
1	A	203	GLU	CB-CG-CD	5.45	121.87	112.60
1	A	134	THR	CA-C-O	-5.44	114.84	121.05
1	A	214	LEU	CA-C-O	-5.39	114.81	121.06
1	A	198	LEU	CA-C-N	5.37	125.90	119.94
1	A	198	LEU	C-N-CA	5.37	125.90	119.94
1	B	74	ASP	CA-C-N	5.30	127.64	120.38
1	B	74	ASP	C-N-CA	5.30	127.64	120.38
1	A	126	GLU	N-CA-C	-5.29	107.38	113.88
1	B	199	GLY	CA-C-N	5.28	127.66	120.54
1	B	199	GLY	C-N-CA	5.28	127.66	120.54
1	A	216	LEU	CA-C-O	-5.27	114.59	120.66
1	A	74	ASP	CA-C-N	5.22	127.53	120.38
1	A	74	ASP	C-N-CA	5.22	127.53	120.38
1	B	225	LEU	CA-C-N	5.19	131.05	121.70
1	B	225	LEU	C-N-CA	5.19	131.05	121.70
1	B	234	GLN	CA-C-N	5.19	127.49	120.38
1	B	234	GLN	C-N-CA	5.19	127.49	120.38
1	B	299	VAL	CB-CA-C	5.17	115.61	111.06
1	A	134	THR	N-CA-C	-5.15	102.06	110.20
1	A	118	GLU	CB-CG-CD	5.13	121.33	112.60
1	A	341	VAL	CA-C-N	5.12	127.14	120.28
1	A	341	VAL	C-N-CA	5.12	127.14	120.28
1	A	119	ARG	CG-CD-NE	-5.11	100.77	112.00
1	A	13	GLY	O-C-N	5.04	128.21	122.86

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	2486	0	2498	47	0
1	B	2562	0	2578	53	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	16	0	0
4	B	6	0	8	1	0
5	A	116	0	0	3	0
5	B	93	0	0	4	0
All	All	5365	0	5152	96	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 9.

All (96) 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:269:MET:SD	1:B:269:MET:HE3	2.05	0.96
1:A:214:LEU:HD21	1:B:269:MET:HE1	1.53	0.91
1:B:214:LEU:HD11	1:B:269:MET:HE2	1.55	0.89
1:B:301:ILE:O	1:B:305:ARG:HD3	1.80	0.82
1:B:107:ASP:OD1	1:B:108:PRO:HD2	1.79	0.81
1:A:24:GLU:HG3	1:A:91:PRO:HD3	1.65	0.78
1:B:115:ARG:O	1:B:118:GLU:HB3	1.91	0.70
1:A:301:ILE:O	1:A:305:ARG:HD3	1.92	0.70
1:B:24:GLU:HG3	1:B:91:PRO:HD3	1.74	0.70
1:B:114:ARG:NH1	1:B:149:GLU:OE2	2.27	0.68
1:B:263:LYS:NZ	5:B:502:HOH:O	2.27	0.67
1:B:44:ARG:HD3	5:B:570:HOH:O	1.96	0.66
1:B:24:GLU:HG3	1:B:91:PRO:CD	2.27	0.64
1:B:29:MET:HE1	1:B:40:PRO:CD	2.30	0.62
1:B:107:ASP:OD1	1:B:108:PRO:CD	2.47	0.62
1:A:119:ARG:HD2	1:A:122:GLU:OE1	2.00	0.61
1:A:24:GLU:HG3	1:A:91:PRO:CD	2.30	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ALA:HB3	1:B:288:LEU:HB3	1.83	0.60
1:B:78:ALA:HA	4:B:402:GOL:H2	1.84	0.60
1:B:21:GLN:HA	1:B:90:LEU:HD21	1.85	0.59
1:A:299:VAL:HG13	1:A:325:VAL:HB	1.84	0.58
1:A:129:LEU:HD13	1:A:304:ILE:HD11	1.86	0.57
1:B:233:ARG:HG3	1:B:254:PRO:HG3	1.86	0.57
1:B:226:ARG:NH1	1:B:255:SER:OG	2.38	0.56
1:B:66:ASN:O	1:B:70:VAL:HG21	2.06	0.54
1:B:183:ASP:OD1	5:B:501:HOH:O	2.18	0.54
1:A:66:ASN:O	1:A:70:VAL:HG21	2.09	0.53
1:A:301:ILE:O	1:A:305:ARG:CD	2.56	0.53
1:A:204:ARG:NH1	5:A:503:HOH:O	2.41	0.53
1:A:216:LEU:HD11	1:B:214:LEU:HD21	1.91	0.53
1:B:105:ASP:HB3	1:B:112:ALA:HB3	1.91	0.52
1:B:214:LEU:CD1	1:B:269:MET:HE2	2.32	0.52
1:B:236:LYS:HD2	1:B:254:PRO:HB3	1.91	0.52
1:B:108:PRO:HA	1:B:113:PHE:CG	2.44	0.52
1:B:29:MET:HE1	1:B:40:PRO:HD2	1.90	0.51
1:B:303:LEU:HD21	1:B:325:VAL:HG23	1.91	0.51
1:B:42:ILE:HD12	1:B:52:VAL:HG21	1.91	0.51
1:A:42:ILE:HD12	1:A:52:VAL:HG21	1.91	0.51
1:A:354:ALA:C	1:A:355:MET:HG3	2.36	0.51
1:A:6:ARG:NE	1:A:124:LYS:O	2.34	0.50
1:A:108:PRO:HA	1:A:113:PHE:CG	2.47	0.50
1:B:299:VAL:HG13	1:B:325:VAL:HB	1.94	0.49
1:A:27:ARG:NH1	1:A:53:SER:O	2.45	0.49
1:A:92:ASP:OD1	1:A:92:ASP:C	2.56	0.49
1:A:105:ASP:HB3	1:A:112:ALA:HB3	1.95	0.49
1:B:3:GLU:O	1:B:3:GLU:HG3	2.14	0.48
1:A:102:THR:OG1	1:A:105:ASP:OD2	2.31	0.47
1:A:159:PRO:O	1:A:164:ARG:NH2	2.47	0.47
1:B:24:GLU:CG	1:B:91:PRO:HD3	2.42	0.47
1:A:189:GLY:O	1:A:192:VAL:HG12	2.16	0.46
1:A:137:GLN:O	1:A:141:ILE:HG12	2.16	0.46
1:A:98:ASP:OD2	1:A:119:ARG:HD3	2.15	0.46
1:A:277:TRP:O	1:A:278:ALA:HB3	2.15	0.46
1:B:189:GLY:O	1:B:192:VAL:HG12	2.16	0.46
1:A:7:LEU:HD23	1:A:57:PHE:CE2	2.52	0.45
1:A:303:LEU:HD21	1:A:325:VAL:HG23	1.98	0.45
1:A:52:VAL:HG22	1:A:301:ILE:HG12	1.98	0.45
1:B:21:GLN:HG2	1:B:90:LEU:HD21	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ARG:HB2	1:B:254:PRO:HG3	1.98	0.45
1:B:44:ARG:CZ	1:B:345:TYR:CE2	3.00	0.45
1:A:24:GLU:CD	1:A:27:ARG:HH21	2.25	0.45
1:A:267:VAL:HG21	5:B:505:HOH:O	2.16	0.45
1:B:270:LEU:C	1:B:270:LEU:HD12	2.42	0.45
1:B:333:HIS:N	1:B:334:PRO:CD	2.80	0.45
1:A:101:LEU:HG	1:A:116:ILE:HD13	1.98	0.44
1:B:141:ILE:HD13	1:B:141:ILE:HA	1.85	0.44
1:A:61:PHE:CD1	1:A:61:PHE:N	2.86	0.44
1:A:24:GLU:OE1	1:A:27:ARG:NE	2.36	0.43
1:A:324:LYS:HD2	1:A:341:VAL:HG11	2.01	0.43
1:B:233:ARG:HG3	1:B:254:PRO:HD3	2.01	0.43
1:B:247:THR:HA	1:B:250:VAL:HG23	2.01	0.42
1:B:301:ILE:HD12	1:B:301:ILE:HA	1.89	0.42
1:A:141:ILE:O	1:A:145:ARG:HG3	2.19	0.42
1:B:24:GLU:CD	1:B:91:PRO:HD3	2.43	0.42
1:B:25:LEU:HD13	1:B:86:LEU:HD13	2.02	0.42
1:A:216:LEU:HD21	1:B:214:LEU:HD22	2.00	0.42
1:B:303:LEU:HD21	1:B:325:VAL:CG2	2.50	0.42
1:A:154:PHE:HB3	1:A:179:LEU:HD12	2.02	0.42
1:B:218:GLY:HA2	1:B:258:TYR:CE1	2.54	0.42
1:A:259:VAL:CG1	1:A:261:HIS:CE1	3.03	0.42
1:A:83:TYR:CG	1:A:84:PRO:HD2	2.54	0.42
1:A:333:HIS:N	1:A:334:PRO:CD	2.83	0.42
1:B:31:ALA:O	1:B:33:GLY:N	2.53	0.41
1:A:351:VAL:O	1:A:355:MET:N	2.53	0.41
1:B:226:ARG:NH1	1:B:226:ARG:HG3	2.34	0.41
1:A:347:GLN:O	1:A:351:VAL:HG23	2.20	0.41
1:B:233:ARG:O	1:B:233:ARG:HG2	2.18	0.41
1:B:206:LEU:CD2	1:B:282:VAL:HG21	2.50	0.41
1:B:18:ALA:HA	1:B:83:TYR:CE2	2.56	0.41
1:A:76:VAL:O	1:A:81:ASN:ND2	2.40	0.41
1:A:190:THR:HG23	1:A:268:ALA:HB1	2.03	0.41
1:B:64:HIS:HA	1:B:65:PRO:HD3	1.98	0.41
1:A:18:ALA:HA	1:A:83:TYR:CE2	2.56	0.40
1:A:204:ARG:CZ	5:A:503:HOH:O	2.69	0.40
1:A:185:ALA:HB1	5:A:545:HOH:O	2.21	0.40
1:B:214:LEU:HD11	1:B:269:MET:CE	2.39	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	329/378 (87%)	312 (95%)	17 (5%)	0	100	100
1	B	337/378 (89%)	320 (95%)	17 (5%)	0	100	100
All	All	666/756 (88%)	632 (95%)	34 (5%)	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	257/293 (88%)	234 (91%)	23 (9%)	9	20
1	B	265/293 (90%)	232 (88%)	33 (12%)	4	9
All	All	522/586 (89%)	466 (89%)	56 (11%)	6	13

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	32	GLU
1	A	50	ILE
1	A	52	VAL
1	A	53	SER
1	A	55	LEU
1	A	62	ASP
1	A	73	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	92	ASP
1	A	96	SER
1	A	116	ILE
1	A	118	GLU
1	A	122	GLU
1	A	134	THR
1	A	165	THR
1	A	174	LYS
1	A	191	SER
1	A	195	ARG
1	A	200	LEU
1	A	247	THR
1	A	299	VAL
1	A	304	ILE
1	A	313	VAL
1	B	3	GLU
1	B	9	VAL
1	B	32	GLU
1	B	43	LYS
1	B	52	VAL
1	B	53	SER
1	B	55	LEU
1	B	56	THR
1	B	62	ASP
1	B	73	LYS
1	B	96	SER
1	B	104	GLU
1	B	115	ARG
1	B	118	GLU
1	B	141	ILE
1	B	161	LEU
1	B	165	THR
1	B	170	GLU
1	B	186	SER
1	B	204	ARG
1	B	214	LEU
1	B	223	ARG
1	B	225	LEU
1	B	226	ARG
1	B	237	ILE
1	B	245	VAL
1	B	251	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	269	MET
1	B	291	GLN
1	B	299	VAL
1	B	302	ASP
1	B	313	VAL
1	B	327	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	A	347	GLN
1	B	347	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	A	400	3	46,48,48	0.90	3 (6%)	64,73,73	1.48	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	402	-	5,5,5	0.23	0	5,5,5	0.46	0
4	GOL	A	402	-	5,5,5	0.25	0	5,5,5	0.47	0
2	NAD	B	400	3	46,48,48	1.38	2 (4%)	64,73,73	1.12	5 (7%)
4	GOL	A	403	-	5,5,5	0.18	0	5,5,5	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	400	3	-	5/30/62/62	0/5/5/5
4	GOL	B	402	-	-	4/4/4/4	-
4	GOL	A	402	-	-	2/4/4/4	-
2	NAD	B	400	3	-	10/30/62/62	0/5/5/5
4	GOL	A	403	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	NAD	C2N-N1N	8.22	1.44	1.35
2	A	400	NAD	C6N-N1N	3.23	1.42	1.35
2	A	400	NAD	O4D-C1D	2.40	1.44	1.40
2	B	400	NAD	O4D-C1D	2.31	1.43	1.40
2	A	400	NAD	PA-O3	-2.19	1.57	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	NAD	C6N-N1N-C2N	-5.14	117.50	121.88
2	A	400	NAD	C4D-O4D-C1D	-4.01	106.26	109.92
2	A	400	NAD	C2N-C3N-C7N	-3.93	108.13	119.46
2	B	400	NAD	C6N-N1N-C2N	-3.78	118.66	121.88
2	A	400	NAD	C4N-C3N-C7N	3.56	130.74	121.06
2	A	400	NAD	O2A-PA-O3	3.49	116.70	107.27
2	A	400	NAD	C6N-N1N-C1D	3.05	125.72	119.73
2	A	400	NAD	O3-PA-O1A	-2.69	102.62	110.70
2	B	400	NAD	O4B-C1B-C2B	-2.68	100.88	106.62
2	B	400	NAD	O2N-PN-O1N	2.50	124.08	112.44
2	B	400	NAD	O2B-C2B-C1B	2.39	118.33	110.10
2	B	400	NAD	O2B-C2B-C3B	-2.25	104.60	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	NAD	C2N-C3N-C4N	2.16	120.78	118.26

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	NAD	C5B-O5B-PA-O1A
2	B	400	NAD	C5B-O5B-PA-O1A
2	B	400	NAD	O4D-C1D-N1N-C2N
4	A	402	GOL	O1-C1-C2-C3
4	B	402	GOL	O1-C1-C2-C3
4	B	402	GOL	C1-C2-C3-O3
4	B	402	GOL	O2-C2-C3-O3
4	A	403	GOL	C1-C2-C3-O3
4	A	403	GOL	O2-C2-C3-O3
4	B	402	GOL	O1-C1-C2-O2
2	B	400	NAD	O4B-C4B-C5B-O5B
2	B	400	NAD	C3B-C4B-C5B-O5B
2	B	400	NAD	C2B-C1B-N9A-C8A
4	A	402	GOL	O1-C1-C2-O2
2	A	400	NAD	C5B-O5B-PA-O2A
2	B	400	NAD	C5B-O5B-PA-O2A
2	B	400	NAD	C5B-O5B-PA-O3
2	B	400	NAD	C2B-C1B-N9A-C4A
2	B	400	NAD	O4D-C1D-N1N-C6N
2	B	400	NAD	PN-O3-PA-O1A
2	A	400	NAD	C2B-C1B-N9A-C8A
2	A	400	NAD	C2B-C1B-N9A-C4A
2	A	400	NAD	O4B-C4B-C5B-O5B

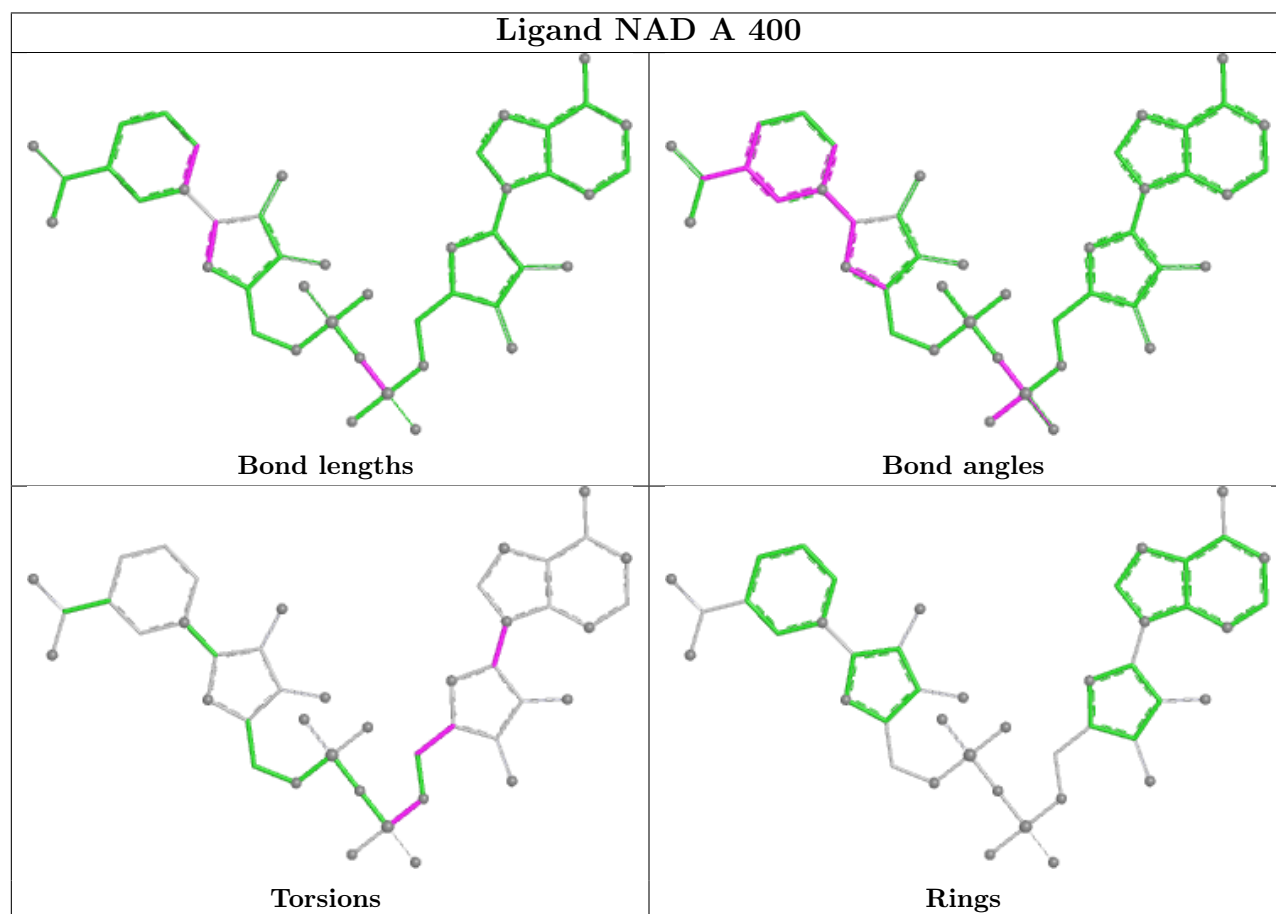
There are no ring outliers.

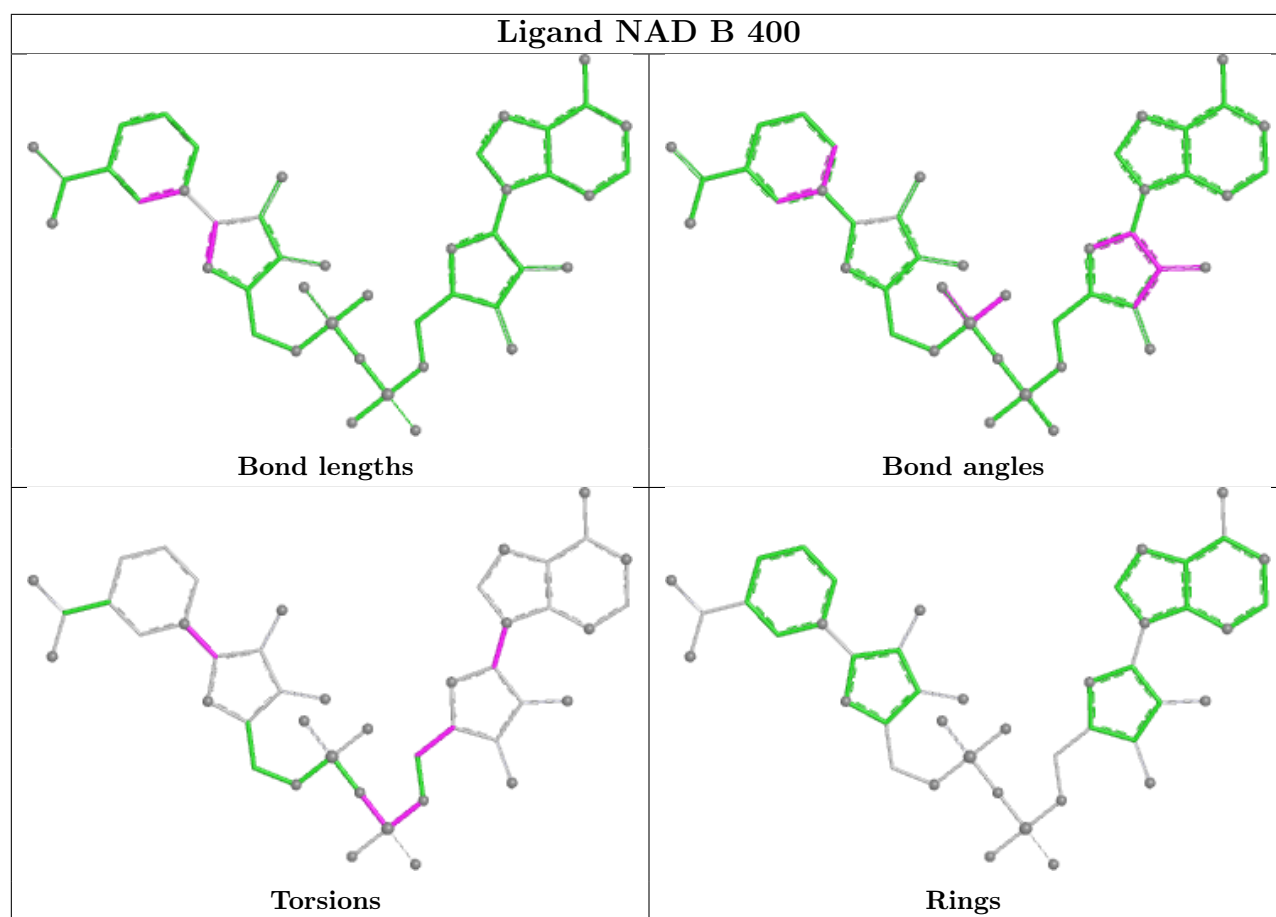
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/378 (88%)	0.04	5 (1%) 72 68	23, 38, 58, 77	0
1	B	343/378 (90%)	0.43	8 (2%) 61 57	24, 44, 70, 84	0
All	All	676/756 (89%)	0.24	13 (1%) 66 62	23, 41, 67, 84	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	ALA	4.3
1	B	237	ILE	3.9
1	B	241	ALA	2.7
1	B	235	SER	2.6
1	A	33	GLY	2.5
1	B	245	VAL	2.5
1	B	239	ALA	2.3
1	B	119	ARG	2.2
1	B	88	VAL	2.2
1	A	32	GLU	2.2
1	A	353	GLU	2.1
1	A	203	GLU	2.0
1	A	355	MET	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](#)

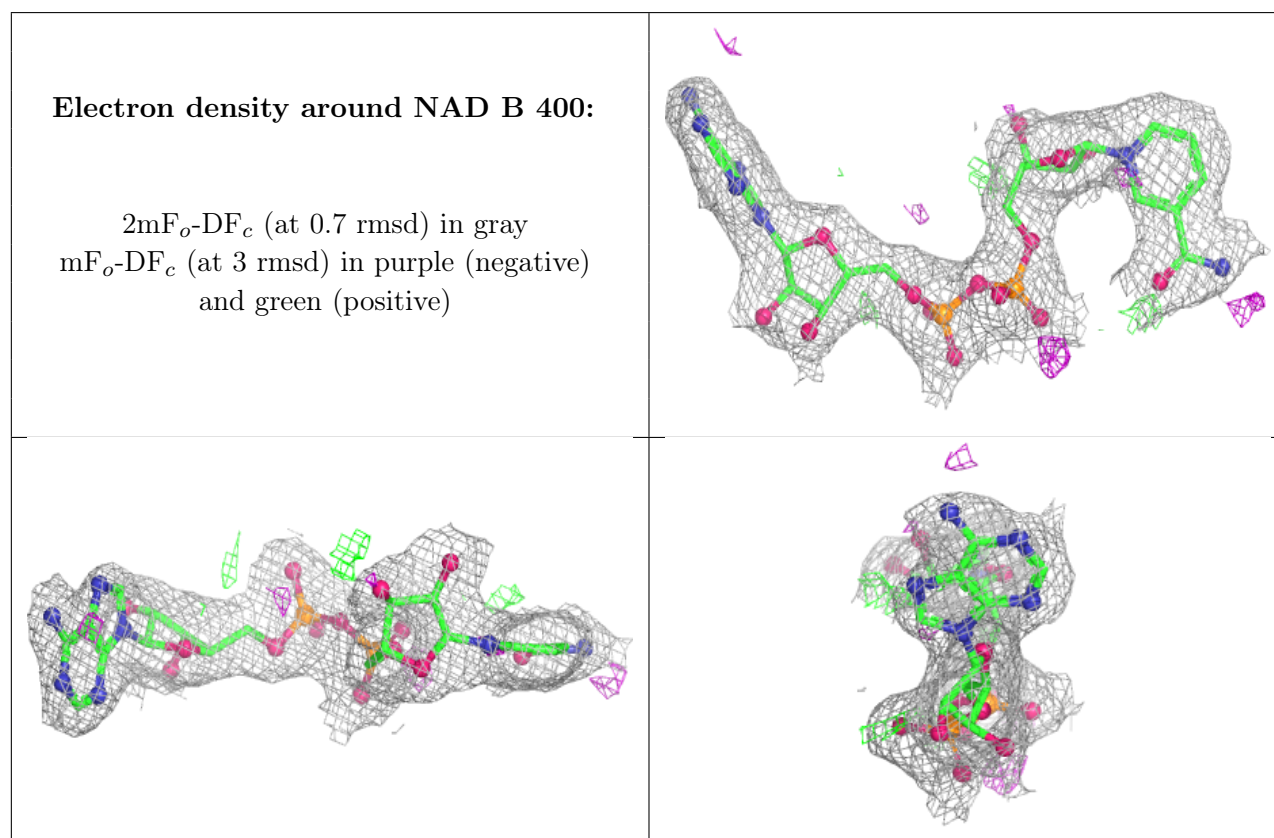
There are no oligosaccharides in this entry.

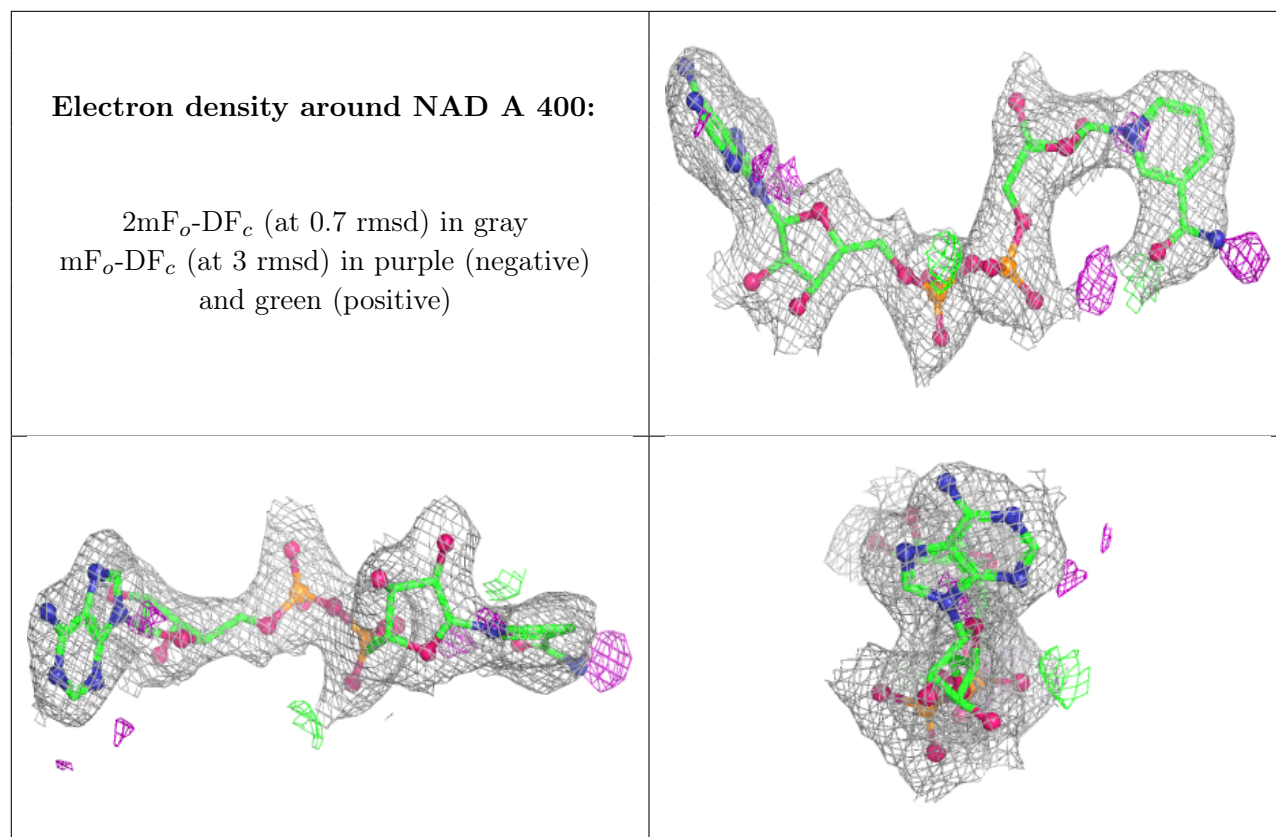
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
4	GOL	A	402	6/6	0.81	0.19	61,63,64,64	0
4	GOL	A	403	6/6	0.84	0.17	61,65,66,66	0
4	GOL	B	402	6/6	0.88	0.13	61,63,65,65	0
3	NA	A	401	1/1	0.93	0.17	25,25,25,25	0
3	NA	B	401	1/1	0.95	0.06	27,27,27,27	0
2	NAD	B	400	44/44	0.97	0.08	26,28,41,42	0
2	NAD	A	400	44/44	0.98	0.06	25,27,29,29	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.