



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2022 – 07:54 pm BST

PDB ID : 6S4A
Title : Structure of human MTHFD2 in complex with TH9028
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Deposited on : 2019-06-27
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)

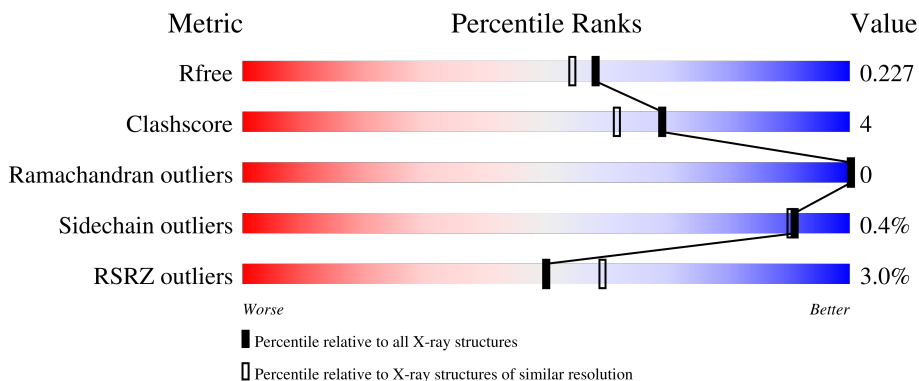
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	 3% 88% 6% 6%
1	B	316	 3% 88% 6% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.28.1

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KUK	A	401	X	-	-	-
2	KUK	B	401	X	-	-	-
3	PO4	A	404	-	-	-	X
5	MPD	B	406	-	-	X	-
5	MPD	B	407	-	-	X	-
5	MPD	B	409	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5005 atoms, of which 14 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.

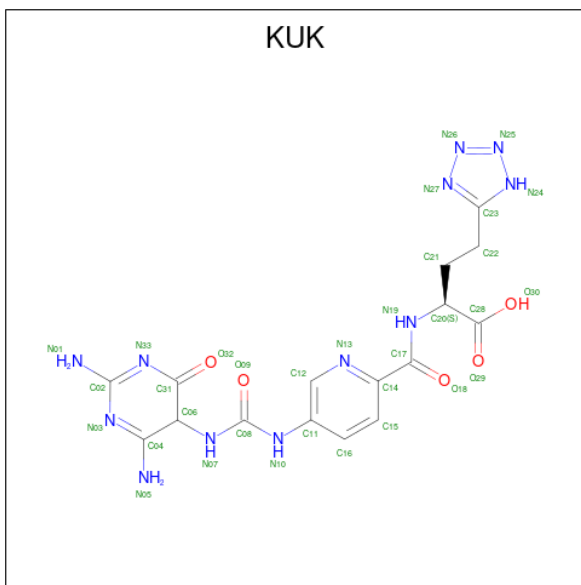
- Molecule 1 is a protein called Bifunctional methylenetetrahydrofolate dehydrogenase/cyclohydrolase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	Total 2266	C 1426	N 408	O 420	S 12	0	2	0
1	B	295	Total 2256	C 1421	N 402	O 421	S 12	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

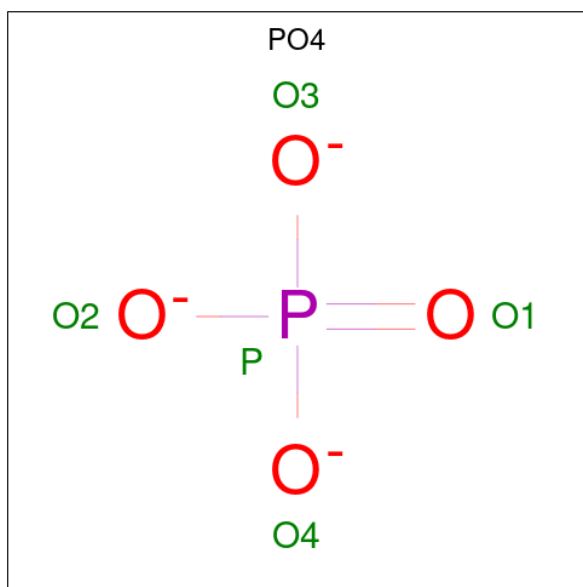
Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	initiating methionine	UNP P13995
B	35	MET	-	initiating methionine	UNP P13995

- Molecule 2 is (2 {S})-2-[[5-[[2,4-bis(azanyl)-6-oxidanylidene-5 {H}-pyrimidin-5-yl]carbamoyl amino]pyridin-2-yl]carbonylamino]-4-(1 {H}-1,2,3,4-tetrazol-5-yl)butanoic acid (three-letter code: KUK) (formula: C₁₆H₁₈N₁₂O₅) (labeled as "Ligand of Interest" by depositor).



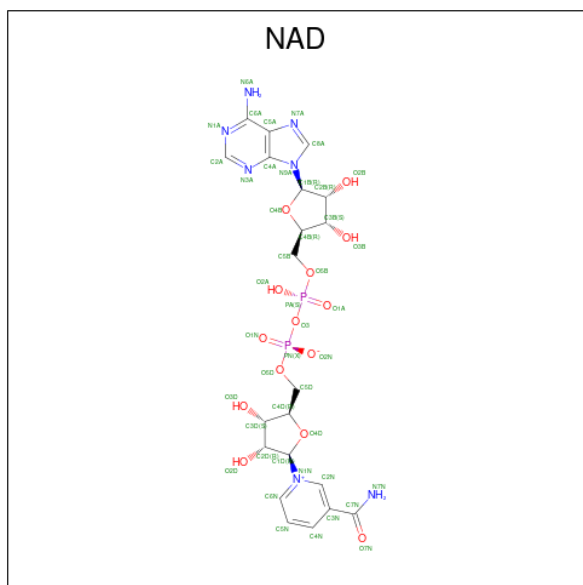
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	16	12	5	0	0
2	B	1	33	16	12	5	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



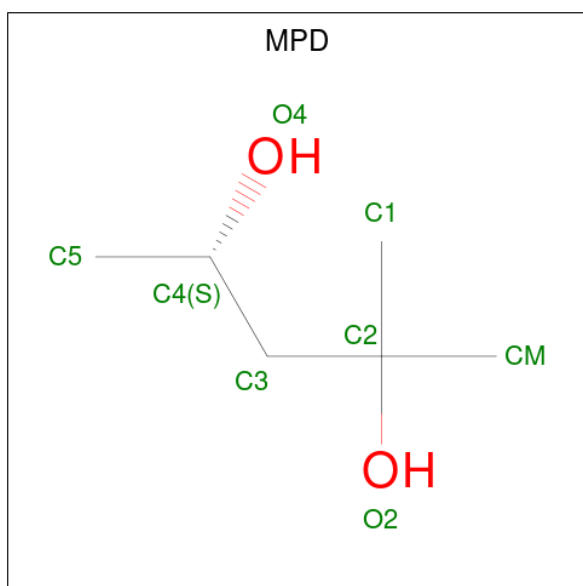
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	8	6	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C H O 22 6 14 2	0	0

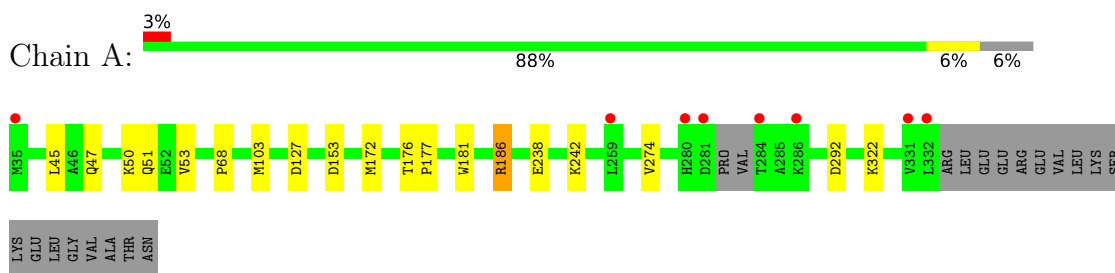
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	124	Total O 124 124	0	0
6	B	105	Total O 105 105	0	0

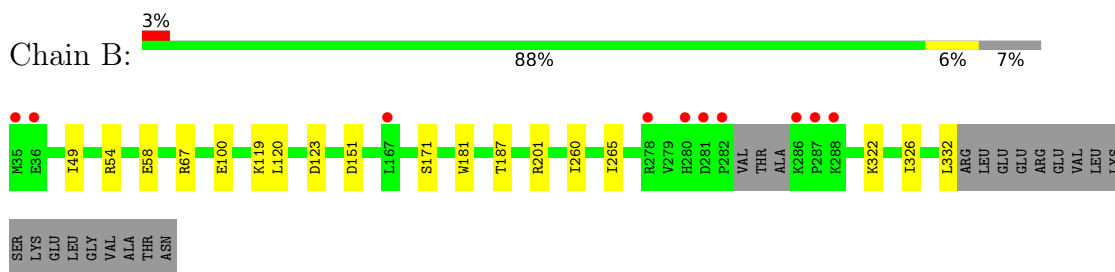
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Bifunctional methylenetetrahydrofolate dehydrogenase/cyclohydrolase, mitochondrial



- Molecule 1: Bifunctional methylenetetrahydrofolate dehydrogenase/cyclohydrolase, mitochondrial



4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	115.07Å 115.07Å 113.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	113.55 – 1.95 45.63 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (113.55-1.95) 99.9 (45.63-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.168 , 0.211 0.183 , 0.227	Depositor DCC
R_{free} test set	3073 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtrriage
Anisotropy	0.135	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5005	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: NAD, KUK, PO4, MPD

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	0.68	0/2302	0.79	2/3122 (0.1%)
1	B	0.67	0/2293	0.82	3/3112 (0.1%)
All	All	0.67	0/4595	0.81	5/6234 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	123	ASP	CB-CG-OD1	5.47	123.23	118.30
1	B	201	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	186	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	292	ASP	CB-CG-OD1	5.00	122.80	118.30

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	2266	0	2346	12	0
1	B	2256	0	2327	15	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	0	0	0
3	B	15	0	0	0	0
4	A	44	0	26	2	0
4	B	44	0	26	0	0
5	A	24	0	42	2	0
5	B	32	14	56	17	0
6	A	124	0	0	3	0
6	B	105	0	0	1	0
All	All	4991	14	4823	35	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 4.

All (35) 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)
5:B:406:MPD:HM1	5:B:409:MPD:H11	1.42	0.97
1:B:326:ILE:HD13	5:B:406:MPD:H53	1.51	0.93
5:B:406:MPD:CM	5:B:409:MPD:H11	2.18	0.70
1:A:274:VAL:O	4:A:405:NAD:H2N	1.92	0.70
1:A:51:GLN:NE2	6:A:502:HOH:O	2.26	0.68
5:B:406:MPD:H12	5:B:406:MPD:H52	1.79	0.64
5:B:406:MPD:HM1	5:B:409:MPD:C1	2.22	0.63
1:A:181:TRP:CE2	5:A:407:MPD:H53	2.34	0.63
1:B:181:TRP:CE2	5:B:409:MPD:H53	2.34	0.61
5:B:406:MPD:CM	5:B:409:MPD:C1	2.78	0.61
1:B:100:GLU:OE1	5:B:407:MPD:C5	2.49	0.60
1:B:119:LYS:NZ	5:B:407:MPD:H13	2.17	0.60
5:B:409:MPD:O4	5:B:409:MPD:H12	2.04	0.57
1:B:54:ARG:HH21	5:B:408:MPD:HM3	1.73	0.53
5:A:407:MPD:O4	5:A:407:MPD:HM1	2.09	0.53
1:B:171:SER:O	5:B:406:MPD:H4	2.09	0.53
1:A:103:MET:HB3	6:A:621:HOH:O	2.10	0.51
1:A:47:GLN:HA	1:A:50:LYS:HE3	1.94	0.50
1:B:100:GLU:OE1	5:B:407:MPD:H51	2.12	0.49
1:B:119:LYS:HZ1	5:B:407:MPD:H13	1.77	0.48
1:B:119:LYS:HE2	5:B:407:MPD:HM3	1.95	0.47
1:A:238:GLU:O	1:A:242:LYS:HG3	2.14	0.47
1:A:176:THR:HB	1:A:177:PRO:HD3	1.96	0.47
1:B:49:ILE:HG23	1:B:322:LYS:HE2	1.97	0.46
1:A:68:PRO:HA	1:A:127:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:HG22	1:A:322:LYS:HD2	2.00	0.43
1:B:260:ILE:CG2	1:B:265:ILE:HD11	2.48	0.43
1:B:187:THR:HG22	1:B:187:THR:O	2.19	0.42
1:B:120:LEU:HD21	5:B:407:MPD:HM1	2.01	0.42
1:A:153:ASP:O	1:A:172:MET:HG2	2.20	0.42
1:B:151:ASP:HB2	6:B:547:HOH:O	2.19	0.42
1:A:45:LEU:HD11	1:A:186:ARG:CD	2.50	0.41
1:A:45:LEU:HD11	1:A:186:ARG:HD3	2.02	0.41
1:B:181:TRP:CZ2	5:B:409:MPD:H53	2.56	0.41
4:A:405:NAD:H5N	6:A:537:HOH:O	2.20	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	294/316 (93%)	289 (98%)	5 (2%)	0	100	100
1	B	293/316 (93%)	286 (98%)	7 (2%)	0	100	100
All	All	587/632 (93%)	575 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	249/265 (94%)	249 (100%)	0	100	100
1	B	249/265 (94%)	247 (99%)	2 (1%)	81	80
All	All	498/530 (94%)	496 (100%)	2 (0%)	91	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	58	GLU
1	B	332	LEU

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	KUK	A	401	-	29,35,35	1.86	8 (27%)	31,48,48	2.30	12 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	402	-	4,4,4	1.36	0	6,6,6	1.08	0
5	MPD	A	408	-	7,7,7	0.49	0	9,10,10	1.15	0
3	PO4	B	403	-	4,4,4	1.03	0	6,6,6	0.51	0
5	MPD	B	407	-	7,7,7	0.64	0	9,10,10	1.09	1 (11%)
3	PO4	A	404	-	4,4,4	0.81	0	6,6,6	0.56	0
5	MPD	B	406	-	7,7,7	0.86	0	9,10,10	1.46	2 (22%)
3	PO4	B	404	-	4,4,4	0.87	0	6,6,6	0.49	0
4	NAD	B	405	-	42,48,48	1.10	5 (11%)	50,73,73	1.48	11 (22%)
5	MPD	B	409	-	7,7,7	0.58	0	9,10,10	0.39	0
3	PO4	A	403	-	4,4,4	0.78	0	6,6,6	0.66	0
2	KUK	B	401	-	29,35,35	2.27	11 (37%)	31,48,48	1.85	9 (29%)
3	PO4	B	402	-	4,4,4	1.32	1 (25%)	6,6,6	0.96	0
5	MPD	A	406	-	7,7,7	0.58	0	9,10,10	0.76	0
5	MPD	B	408	-	7,7,7	0.50	0	9,10,10	0.39	0
5	MPD	A	407	-	7,7,7	0.40	0	9,10,10	0.90	0
4	NAD	A	405	-	42,48,48	1.63	7 (16%)	50,73,73	2.04	13 (26%)

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	KUK	A	401	-	1/1/8/11	0/21/41/41	0/2/3/3
5	MPD	A	408	-	-	2/5/5/5	-
5	MPD	B	407	-	-	1/5/5/5	-
5	MPD	B	406	-	-	2/5/5/5	-
4	NAD	B	405	-	-	7/26/62/62	0/5/5/5
5	MPD	B	409	-	-	2/5/5/5	-
2	KUK	B	401	-	1/1/8/11	1/21/41/41	0/2/3/3
5	MPD	A	406	-	-	1/5/5/5	-
5	MPD	B	408	-	-	0/5/5/5	-
5	MPD	A	407	-	-	4/5/5/5	-
4	NAD	A	405	-	-	14/26/62/62	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	NAD	C3N-C7N	5.21	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	NAD	O7N-C7N	5.08	1.33	1.24
2	B	401	KUK	C23-N27	5.01	1.37	1.33
2	A	401	KUK	C17-N19	4.89	1.44	1.34
2	B	401	KUK	C23-N24	3.96	1.36	1.33
2	B	401	KUK	C02-N03	3.93	1.44	1.36
2	A	401	KUK	C08-N07	3.88	1.43	1.35
2	B	401	KUK	C17-N19	3.83	1.42	1.34
2	A	401	KUK	C02-N33	3.81	1.43	1.35
2	B	401	KUK	C06-N07	-3.63	1.39	1.45
2	B	401	KUK	C02-N33	3.57	1.42	1.35
2	A	401	KUK	C02-N03	3.43	1.43	1.36
4	A	405	NAD	C2A-N3A	3.10	1.37	1.32
4	B	405	NAD	C3N-C7N	2.98	1.55	1.50
2	B	401	KUK	C08-N07	2.94	1.41	1.35
2	A	401	KUK	C08-N10	2.57	1.42	1.37
4	A	405	NAD	C7N-N7N	2.57	1.37	1.33
4	A	405	NAD	O4D-C1D	2.56	1.44	1.41
2	B	401	KUK	C08-N10	2.56	1.42	1.37
4	A	405	NAD	C5A-C4A	2.54	1.47	1.40
2	B	401	KUK	O32-C31	-2.47	1.18	1.23
4	B	405	NAD	C2A-N3A	2.43	1.36	1.32
4	A	405	NAD	O4B-C1B	2.33	1.44	1.41
2	A	401	KUK	C02-N01	2.31	1.41	1.34
2	A	401	KUK	C31-N33	2.25	1.44	1.39
2	B	401	KUK	C22-C23	2.18	1.53	1.50
4	B	405	NAD	C5A-C4A	2.17	1.46	1.40
3	B	402	PO4	P-O2	-2.16	1.48	1.54
2	B	401	KUK	C02-N01	2.13	1.40	1.34
2	A	401	KUK	C23-N24	2.13	1.35	1.33
4	B	405	NAD	O7N-C7N	2.07	1.28	1.24
4	B	405	NAD	O4D-C1D	2.06	1.44	1.41

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	NAD	C3N-C2N-N1N	6.93	127.20	120.43
2	A	401	KUK	C11-C12-N13	-6.60	118.19	124.13
2	B	401	KUK	C11-C12-N13	-5.02	119.62	124.13
4	A	405	NAD	C2N-C3N-C4N	-4.86	112.75	118.26
4	B	405	NAD	N3A-C2A-N1A	-4.69	121.34	128.68
4	A	405	NAD	C4A-C5A-N7A	-4.46	104.75	109.40
2	A	401	KUK	C16-C11-C12	4.30	122.08	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	NAD	C3N-C7N-N7N	-4.14	112.79	117.75
4	A	405	NAD	O7N-C7N-C3N	4.11	124.56	119.63
4	A	405	NAD	N3A-C2A-N1A	-3.83	122.70	128.68
2	A	401	KUK	N01-C02-N33	3.65	122.80	117.06
2	A	401	KUK	C23-N27-N26	3.55	107.92	104.33
2	A	401	KUK	C23-N24-N25	3.45	107.81	104.33
2	A	401	KUK	N03-C02-N33	-3.43	120.85	126.43
4	B	405	NAD	C3N-C2N-N1N	3.29	123.64	120.43
2	B	401	KUK	C23-N24-N25	3.19	107.55	104.33
2	B	401	KUK	C16-C11-C12	3.07	120.85	117.80
2	B	401	KUK	C23-N27-N26	3.02	107.38	104.33
2	A	401	KUK	C15-C16-C11	-2.86	116.99	120.30
4	B	405	NAD	C1B-N9A-C4A	-2.84	121.65	126.64
2	B	401	KUK	C15-C16-C11	-2.74	117.13	120.30
2	A	401	KUK	C12-N13-C14	2.69	121.54	117.36
2	A	401	KUK	C20-N19-C17	2.66	125.77	122.34
4	A	405	NAD	O4B-C1B-C2B	-2.64	103.06	106.93
2	B	401	KUK	C12-N13-C14	2.59	121.39	117.36
5	B	406	MPD	O4-C4-C3	2.54	121.63	111.36
4	A	405	NAD	C6N-C5N-C4N	2.53	123.12	119.44
2	B	401	KUK	N01-C02-N33	2.50	121.00	117.06
2	B	401	KUK	N03-C02-N33	-2.50	122.38	126.43
4	B	405	NAD	C4A-C5A-N7A	-2.49	106.81	109.40
4	A	405	NAD	C2N-N1N-C1D	-2.38	113.83	119.14
4	A	405	NAD	C4N-C3N-C7N	2.38	127.41	121.04
4	B	405	NAD	C3D-C2D-C1D	2.36	104.53	100.98
2	A	401	KUK	O32-C31-N33	2.35	122.43	119.91
4	A	405	NAD	C6N-N1N-C2N	-2.35	119.83	121.97
5	B	406	MPD	O2-C2-CM	-2.33	100.60	108.08
4	B	405	NAD	C4N-C3N-C7N	2.21	126.95	121.04
2	B	401	KUK	C20-N19-C17	-2.20	119.50	122.34
4	B	405	NAD	O4D-C1D-C2D	2.18	110.11	106.93
2	A	401	KUK	N10-C08-N07	-2.14	110.78	113.76
4	B	405	NAD	O7N-C7N-C3N	2.13	122.19	119.63
4	B	405	NAD	O4B-C4B-C3B	2.12	109.31	105.11
4	A	405	NAD	O3B-C3B-C4B	-2.11	104.94	111.05
2	A	401	KUK	C06-C04-N05	2.10	121.95	116.79
5	B	407	MPD	O4-C4-C3	2.09	119.81	111.36
4	B	405	NAD	O4D-C4D-C3D	2.08	109.23	105.11
4	B	405	NAD	C2N-N1N-C1D	-2.04	114.58	119.14
4	A	405	NAD	C5N-C6N-N1N	-2.04	117.48	120.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	KUK	C06
2	B	401	KUK	C06

All (34) torsion outliers are listed below:

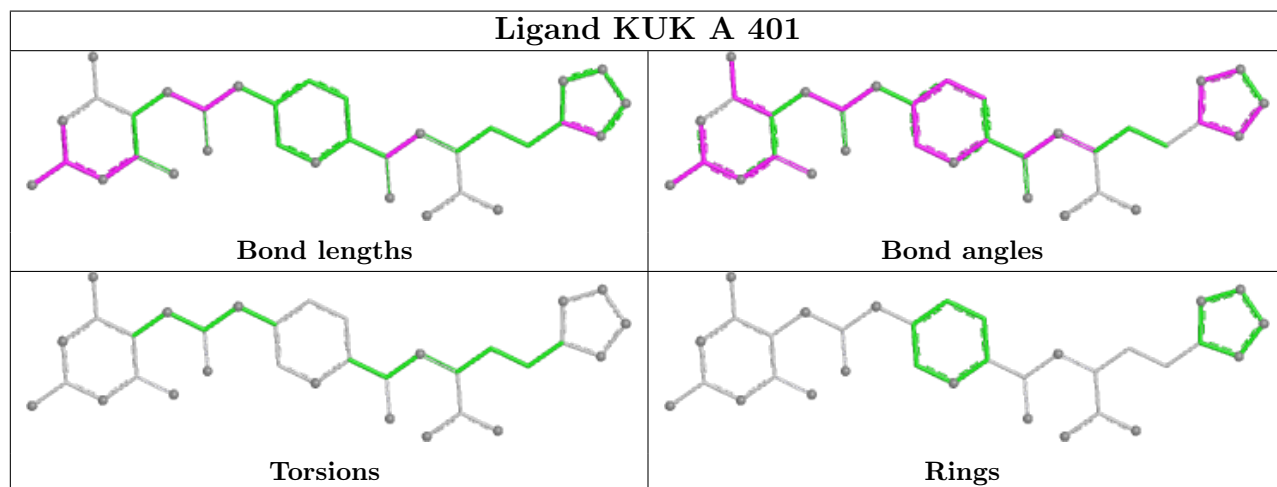
Mol	Chain	Res	Type	Atoms
2	B	401	KUK	C21-C22-C23-N24
4	A	405	NAD	C5B-O5B-PA-O1A
4	A	405	NAD	C5B-O5B-PA-O2A
4	A	405	NAD	C5B-O5B-PA-O3
4	A	405	NAD	C5D-O5D-PN-O3
4	A	405	NAD	C5D-O5D-PN-O1N
4	A	405	NAD	C5D-O5D-PN-O2N
4	A	405	NAD	O4D-C1D-N1N-C2N
4	A	405	NAD	O4D-C1D-N1N-C6N
4	A	405	NAD	C2D-C1D-N1N-C2N
4	A	405	NAD	C2D-C1D-N1N-C6N
4	B	405	NAD	O4D-C1D-N1N-C6N
5	A	408	MPD	C2-C3-C4-O4
4	A	405	NAD	C3B-C4B-C5B-O5B
4	A	405	NAD	O4B-C4B-C5B-O5B
4	B	405	NAD	O4D-C4D-C5D-O5D
4	B	405	NAD	PN-O3-PA-O1A
4	B	405	NAD	C3D-C4D-C5D-O5D
4	B	405	NAD	PN-O3-PA-O5B
5	A	407	MPD	O2-C2-C3-C4
5	A	408	MPD	C2-C3-C4-C5
5	B	406	MPD	C2-C3-C4-C5
5	B	406	MPD	C2-C3-C4-O4
5	A	407	MPD	C1-C2-C3-C4
5	A	407	MPD	CM-C2-C3-C4
5	B	409	MPD	C1-C2-C3-C4
4	A	405	NAD	C4D-C5D-O5D-PN
4	B	405	NAD	C5B-O5B-PA-O3
4	B	405	NAD	O4B-C4B-C5B-O5B
4	A	405	NAD	PN-O3-PA-O1A
5	A	406	MPD	C2-C3-C4-C5
5	A	407	MPD	C2-C3-C4-O4
5	B	407	MPD	C2-C3-C4-O4
5	B	409	MPD	C2-C3-C4-O4

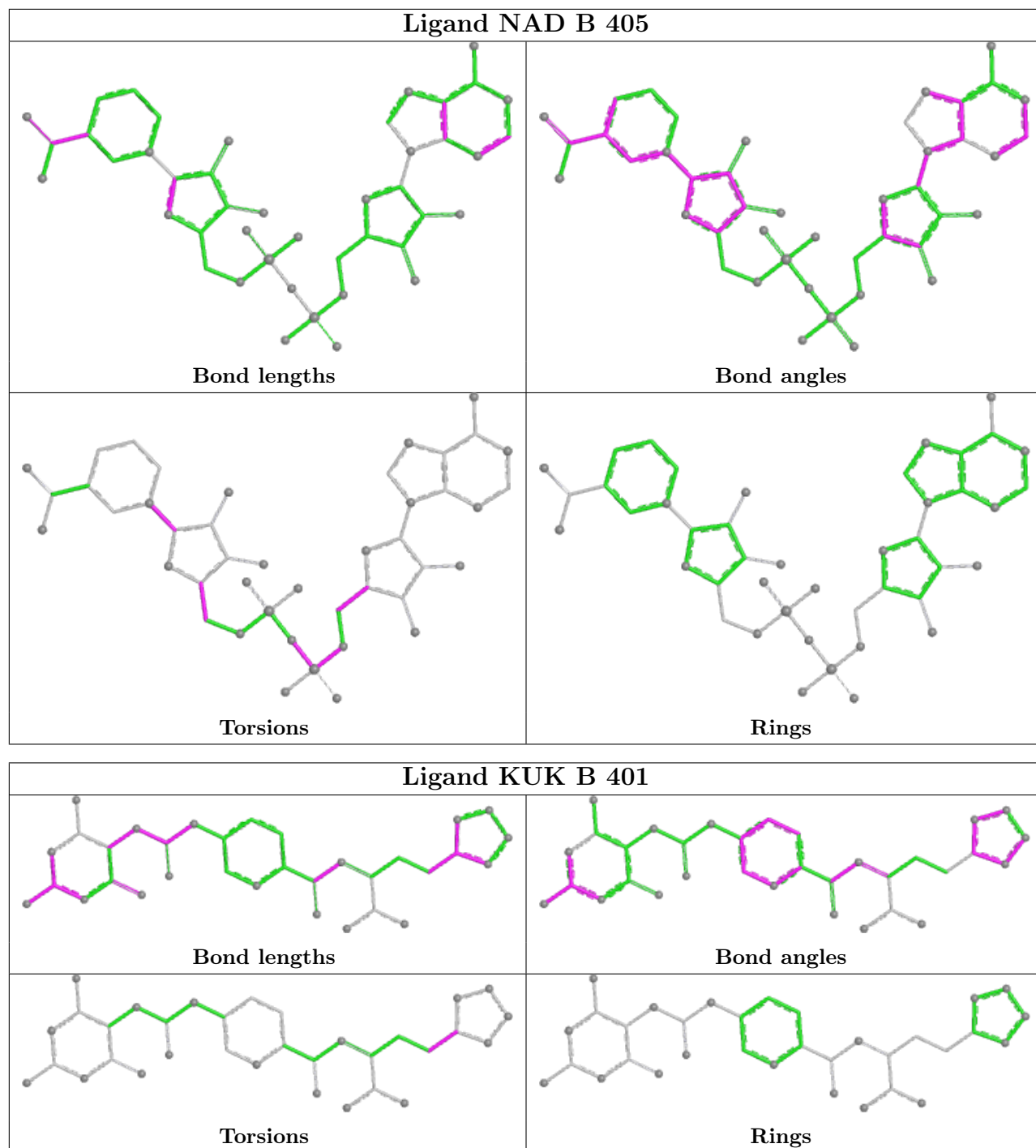
There are no ring outliers.

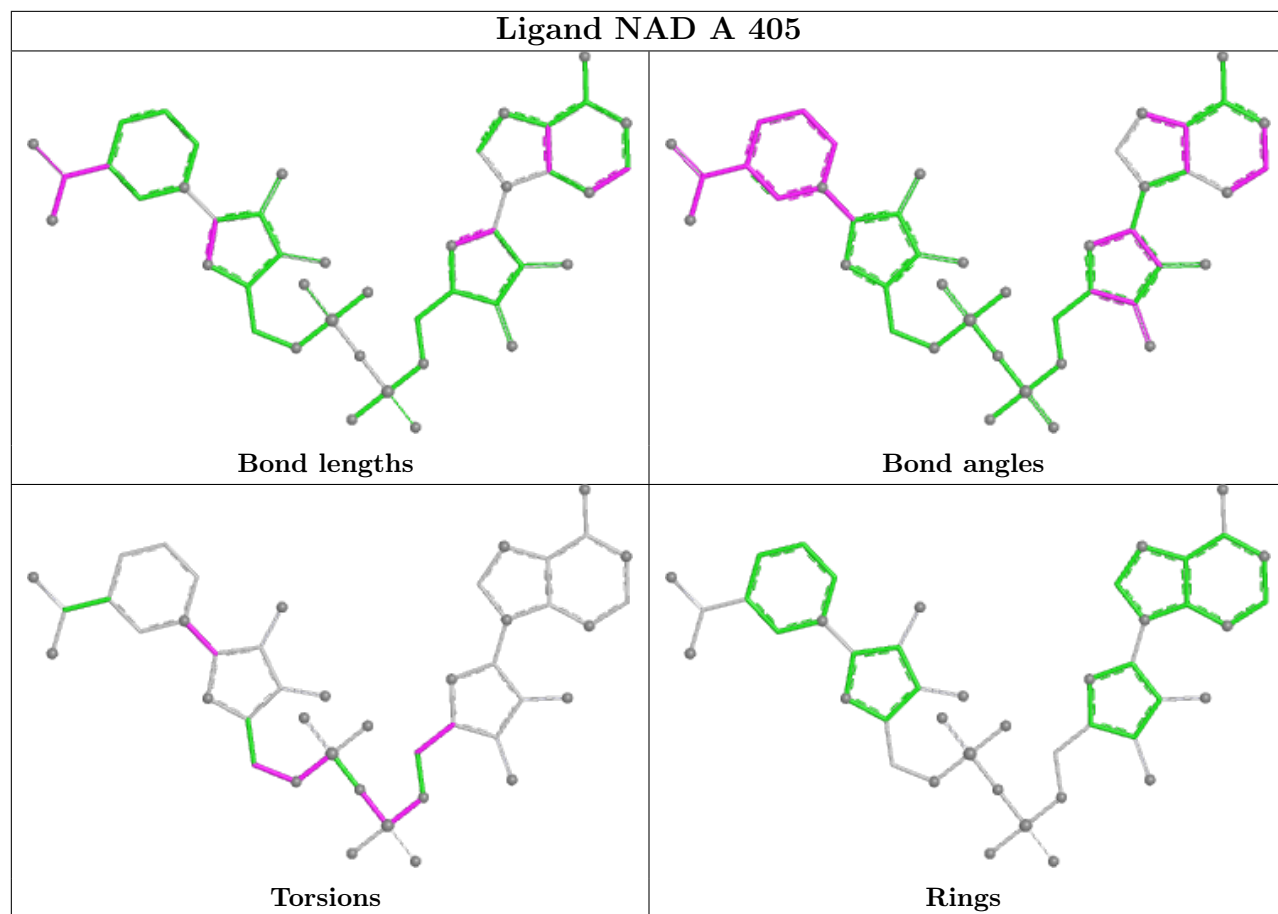
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	407	MPD	6	0
5	B	406	MPD	7	0
5	B	409	MPD	7	0
5	B	408	MPD	1	0
5	A	407	MPD	2	0
4	A	405	NAD	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	296/316 (93%)	-0.15	8 (2%) 54 63	41, 53, 78, 121	0
1	B	295/316 (93%)	-0.16	10 (3%) 45 55	43, 55, 84, 122	0
All	All	591/632 (93%)	-0.16	18 (3%) 50 59	41, 54, 83, 122	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	MET	5.0
1	A	332	LEU	4.6
1	B	287	PRO	4.5
1	A	331	VAL	4.3
1	A	286	LYS	3.6
1	B	280	HIS	3.6
1	B	281	ASP	3.4
1	A	280	HIS	3.2
1	B	35	MET	3.2
1	A	284	THR	3.1
1	B	36	GLU	2.7
1	B	288	LYS	2.7
1	A	281	ASP	2.5
1	A	259	LEU	2.5
1	B	286	LYS	2.3
1	B	282	PRO	2.3
1	B	167	LEU	2.2
1	B	278	ARG	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

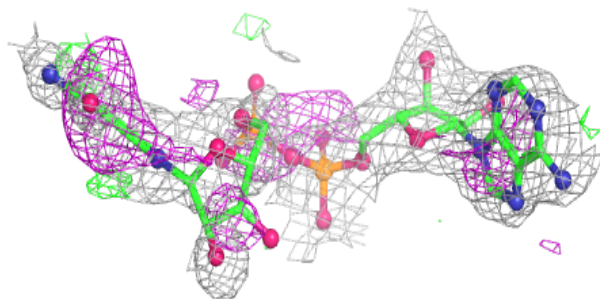
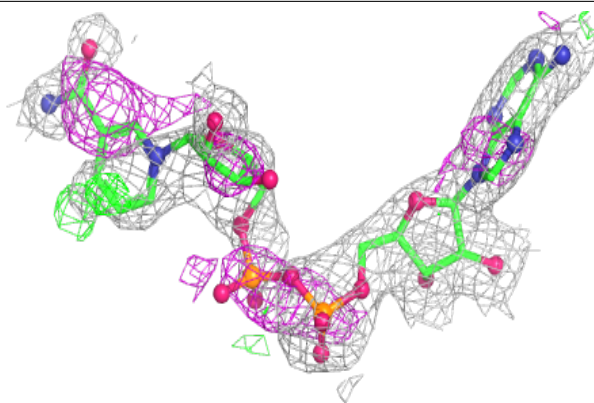
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	A	404	5/5	0.39	0.78	165,168,175,183	0
5	MPD	B	408	8/8	0.69	0.25	120,123,130,136	0
5	MPD	B	406	8/8	0.81	0.23	58,86,97,99	0
4	NAD	A	405	44/44	0.82	0.25	49,88,147,172	0
4	NAD	B	405	44/44	0.83	0.20	53,86,145,151	0
5	MPD	A	408	8/8	0.86	0.14	76,85,88,93	0
5	MPD	B	409	8/8	0.86	0.37	20,20,20,20	0
3	PO4	B	403	5/5	0.90	0.22	101,108,111,113	0
5	MPD	A	406	8/8	0.92	0.15	74,79,89,92	0
5	MPD	A	407	8/8	0.93	0.12	55,60,65,70	0
2	KUK	A	401	33/33	0.94	0.10	35,43,68,74	0
3	PO4	B	404	5/5	0.94	0.21	115,119,125,129	0
3	PO4	A	403	5/5	0.96	0.22	108,111,116,120	0
2	KUK	B	401	33/33	0.96	0.10	39,49,99,102	0
5	MPD	B	407	8/8	0.97	0.20	67,82,89,95	0
3	PO4	B	402	5/5	0.99	0.07	54,54,54,56	0
3	PO4	A	402	5/5	1.00	0.10	48,52,55,62	0

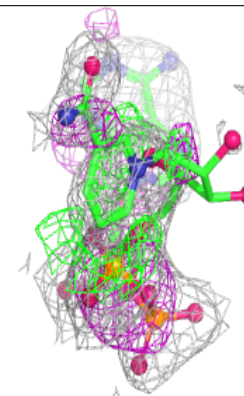
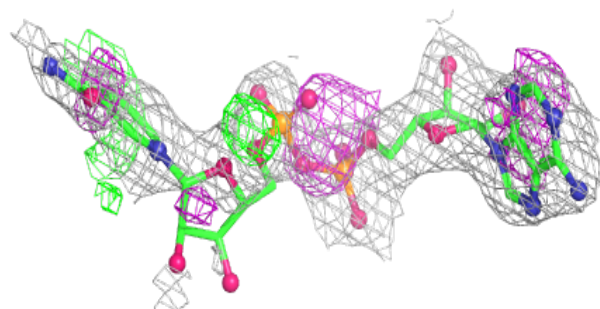
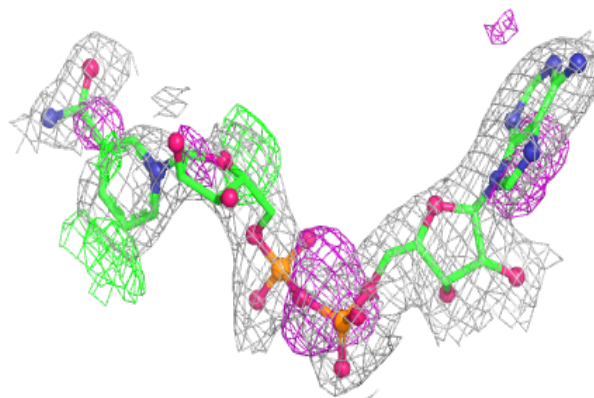
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD A 405:

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

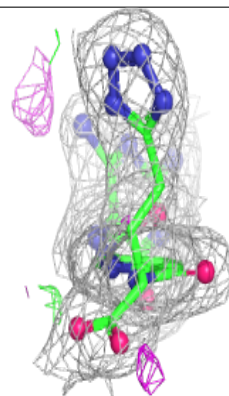
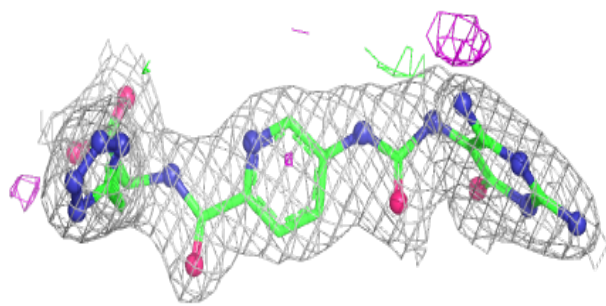
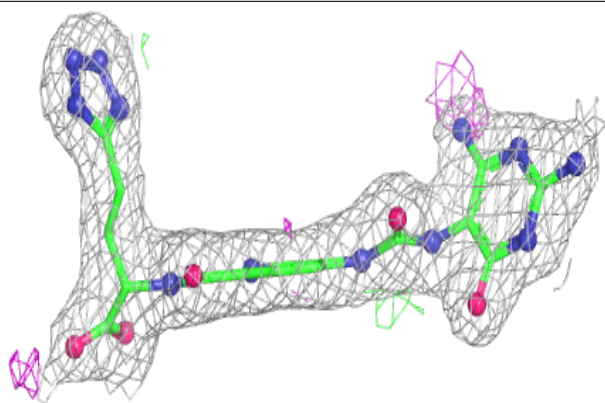
**Electron density around NAD B 405:**

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

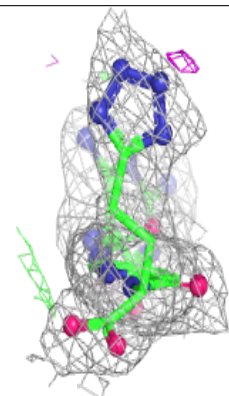
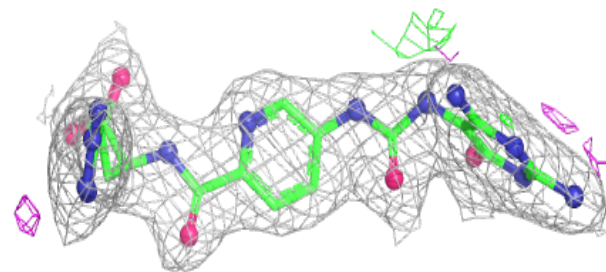
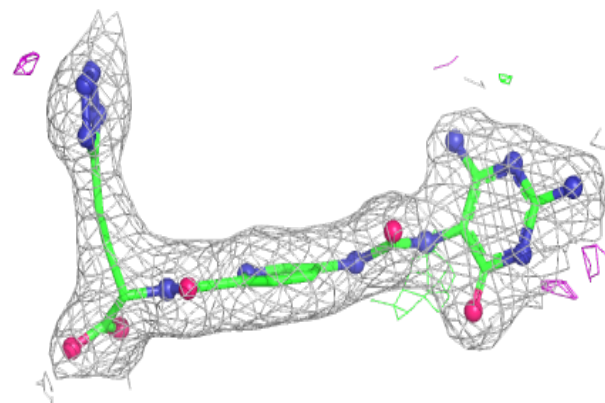


Electron density around KUK A 401:

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

**Electron density around KUK B 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.