



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:52 PM UTC

PDB ID : 1M7A / pdb_00001m7a
Title : CANDIDA ALBICANS DIHYDROFOLATE REDUCTASE COMPLEXED
WITH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOS-
PHATE (NADPH) AND 7-[2-methoxy-1-(methoxymethyl)ethyl]-7H-pyrrolo[
3,2-f] quinazoline-1,3-diamine (GW557)
Authors : Whitlow, M.; Howard, A.J.; Kuyper, L.F.
Deposited on : 2002-07-19
Resolution : 1.76 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](#) ①) 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

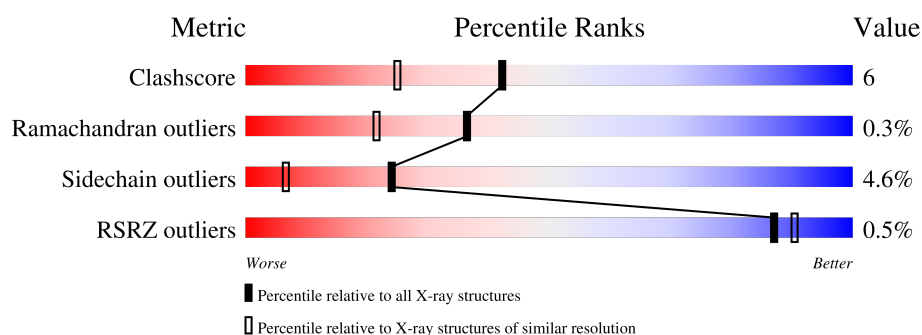
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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))
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	192	73% 20% 6%
1	B	192	74% 19% 6%

2 Entry composition [i](#)

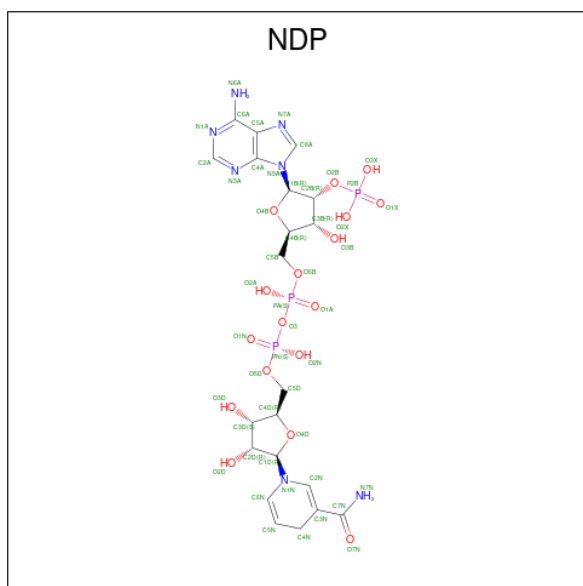
There are 4 unique types of molecules in this entry. The entry contains 3676 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDROFOLATE REDUCTASE.

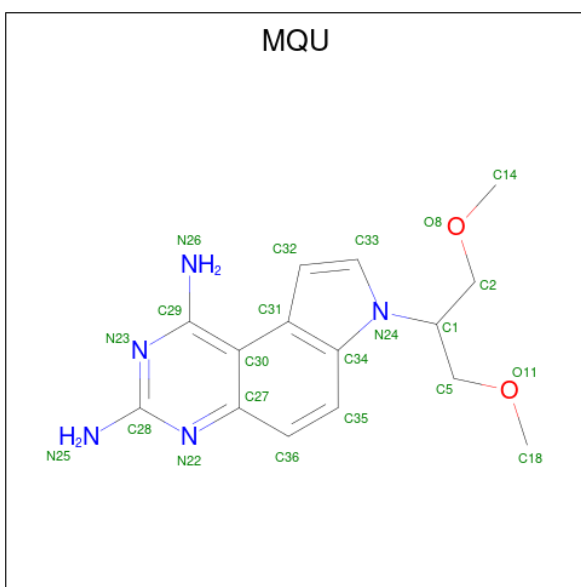
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	12	0
			1594	1023	271	296	4			
1	B	192	Total	C	N	O	S	0	11	0
			1589	1020	264	301	4			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 7-[2-METHOXY-1-(METHOXYMETHYL)ETHYL]-7H-PYRROLO[3,2-F] QUINAZOLINE-1,3-DIAMINE (CCD ID: MQU) (formula: $C_{15}H_{19}N_5O_2$).

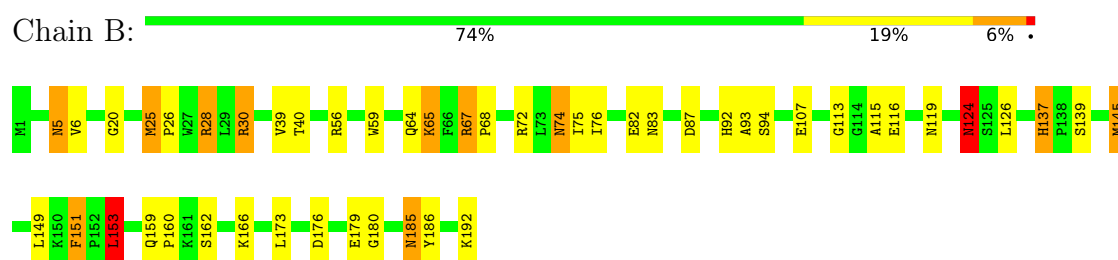


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	15	5	2		
3	B	1	Total	C	N	O	0	0
			22	15	5	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	168	Total	O	0	7
			175	175		
4	B	174	Total	O	0	4
			178	178		

● Molecule 1: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.91Å 67.28Å 38.49Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	10.00 – 1.76 10.00 – 1.77	Depositor EDS
% Data completeness (in resolution range)	94.9 (10.00-1.76) 90.7 (10.00-1.77)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.77Å)	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.151 , (Not available) 0.150 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3676	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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: NDP, MQU

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	1.51	3/1690 (0.2%)	1.88	35/2290 (1.5%)
1	B	1.56	9/1681 (0.5%)	1.83	29/2275 (1.3%)
All	All	1.54	12/3371 (0.4%)	1.85	64/4565 (1.4%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	LEU	C-O	6.36	1.31	1.24
1	B	107	GLU	C-O	6.18	1.30	1.23
1	B	59	TRP	N-CA	6.10	1.53	1.46
1	B	180	GLY	N-CA	6.08	1.54	1.45
1	B	76	ILE	N-CA	5.80	1.52	1.46
1	B	25	MET	N-CA	5.68	1.54	1.45
1	B	186	TYR	N-CA	5.51	1.53	1.46
1	A	9	ILE	N-CA	5.44	1.52	1.46
1	B	40	THR	N-CA	5.42	1.53	1.46
1	B	145	MET	CA-CB	-5.33	1.45	1.53
1	B	92	HIS	N-CA	5.28	1.52	1.46
1	A	31	LYS	C-N	-5.07	1.27	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	PHE	CA-CB-CG	13.87	127.67	113.80
1	B	56	ARG	CD-NE-CZ	13.24	142.94	124.40
1	A	28	ARG	CD-NE-CZ	9.58	137.81	124.40
1	A	154	GLU	CB-CG-CD	8.91	127.75	112.60
1	A	137	HIS	CA-CB-CG	8.15	121.95	113.80
1	A	154	GLU	CA-CB-CG	7.63	129.36	114.10
1	B	74	ASN	CA-CB-CG	7.58	120.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	CD-NE-CZ	7.25	134.55	124.40
1	A	108	ARG	NE-CZ-NH1	-7.11	114.39	121.50
1	B	72	ARG	O-C-N	6.99	131.37	123.27
1	B	145	MET	N-CA-C	6.94	119.73	108.76
1	A	146	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	151	PHE	CA-CB-CG	6.91	120.71	113.80
1	B	119	ASN	CB-CA-C	6.84	123.28	110.63
1	B	124	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	A	90	ILE	O-C-N	6.74	130.35	123.07
1	B	67	ARG	CD-NE-CZ	6.71	133.79	124.40
1	B	30	ARG	CD-NE-CZ	6.49	133.49	124.40
1	A	46	PRO	N-CA-C	6.46	125.79	112.47
1	A	139	SER	N-CA-CB	-6.42	102.44	110.79
1	A	169	GLY	CA-C-N	6.41	130.06	120.31
1	A	169	GLY	C-N-CA	6.41	130.06	120.31
1	A	144	GLU	CB-CG-CD	6.39	123.46	112.60
1	A	87	ASP	CA-CB-CG	6.38	118.98	112.60
1	B	67	ARG	CB-CA-C	6.27	118.31	108.84
1	A	64	GLN	CA-C-N	6.19	129.20	120.28
1	A	64	GLN	C-N-CA	6.19	129.20	120.28
1	B	39	VAL	CA-C-O	-6.14	114.34	120.85
1	A	170	ASP	N-CA-C	6.11	118.90	111.82
1	B	87	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	145	MET	CB-CG-SD	-5.94	94.87	112.70
1	A	24	LYS	CG-CD-CE	5.92	124.91	111.30
1	B	124	ASN	CB-CG-ND2	5.90	125.25	116.40
1	A	115	ALA	N-CA-C	5.80	118.07	111.11
1	A	150	LYS	CA-CB-CG	5.79	125.67	114.10
1	B	113	GLY	O-C-N	-5.78	117.70	123.48
1	A	185	ASN	O-C-N	5.72	129.90	123.27
1	B	64	GLN	N-CA-C	5.60	118.92	111.75
1	A	24	LYS	CA-CB-CG	5.54	125.18	114.10
1	A	112	ILE	N-CA-C	5.53	117.43	112.17
1	B	185	ASN	O-C-N	5.49	129.64	123.27
1	B	179	GLU	N-CA-CB	5.49	119.46	110.90
1	B	153	LEU	CB-CA-C	5.48	121.88	110.32
1	B	39	VAL	O-C-N	5.48	127.47	121.83
1	B	56	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	A	31	LYS	CA-C-O	-5.44	113.71	119.97
1	B	75	ILE	O-C-N	5.36	129.05	123.26
1	B	82	GLU	CA-C-O	-5.31	114.90	120.80
1	B	162	SER	O-C-N	5.30	127.74	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	HIS	O-C-N	5.28	125.55	121.85
1	A	190	THR	CA-CB-OG1	-5.24	101.75	109.60
1	A	47	ASN	CA-C-N	-5.23	113.68	123.03
1	A	47	ASN	C-N-CA	-5.23	113.68	123.03
1	A	148	PHE	O-C-N	5.19	129.29	123.27
1	A	192	LYS	N-CA-CB	5.19	119.32	110.50
1	B	115	ALA	N-CA-C	5.17	117.31	111.11
1	B	6	VAL	O-C-N	5.14	128.73	123.18
1	B	116	GLU	CB-CG-CD	5.13	121.31	112.60
1	A	132	ILE	CA-C-N	-5.12	115.60	122.42
1	A	132	ILE	C-N-CA	-5.12	115.60	122.42
1	A	102	LEU	CA-CB-CG	5.06	134.02	116.30
1	A	132	ILE	O-C-N	5.02	128.97	123.10
1	B	192	LYS	N-CA-CB	5.01	119.02	110.50
1	A	192	LYS	CA-CB-CG	5.00	124.10	114.10

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	1594	0	1620	24	0
1	B	1589	0	1614	17	0
2	A	48	0	26	2	0
2	B	48	0	26	0	0
3	A	22	0	19	1	0
3	B	22	0	19	0	0
4	A	175	0	0	4	0
4	B	178	0	0	1	0
All	All	3676	0	3324	42	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 6.

All (42) 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:13:LEU:HD23	1:A:145:MET:HE1	1.59	0.83
1:B:124:ASN:HD22	1:B:126:LEU:H	1.31	0.77
1:B:28:ARG:HH11	1:B:30:ARG:HG2	1.50	0.75
1:A:64:GLN:HG2	1:A:65:LYS:HE3	1.69	0.74
1:A:28:ARG:HH21	1:A:28:ARG:HB3	1.57	0.70
1:A:176:ASP:H	1:A:185:ASN:HD21	1.40	0.67
1:B:176:ASP:H	1:B:185:ASN:HD21	1.45	0.62
1:B:176:ASP:H	1:B:185:ASN:ND2	1.99	0.59
1:A:18:GLY:HA3	1:A:145:MET:HE3	1.86	0.57
1:B:137:HIS:HD2	1:B:139:SER:H	1.51	0.57
1:B:83:ASN:ND2	1:B:94:SER:H	2.03	0.56
1:A:176:ASP:H	1:A:185:ASN:ND2	2.03	0.56
1:A:119:ASN:HB3	1:A:150:LYS:HE2	1.89	0.55
1:B:83:ASN:HD21	1:B:94:SER:H	1.58	0.52
1:B:67:ARG:HA	1:B:68:PRO:C	2.35	0.51
1:A:65:LYS:H	1:A:65:LYS:CD	2.24	0.51
1:A:137:HIS:CD2	1:A:143:ILE:HD11	2.46	0.51
2:A:193:NDP:H2D	4:A:367:HOH:O	2.11	0.51
1:B:159:GLN:HB3	1:B:160:PRO:HD2	1.92	0.51
1:B:137:HIS:CD2	1:B:139:SER:H	2.30	0.50
1:B:151:PHE:HB2	1:B:153:LEU:HD13	1.93	0.49
1:B:5:ASN:ND2	4:B:297:HOH:O	2.46	0.49
1:A:65:LYS:H	1:A:65:LYS:HD2	1.77	0.48
1:A:117:ILE:HG23	1:A:121[A]:LEU:HD12	1.94	0.48
1:A:41[B]:THR:HG21	4:A:446:HOH:O	2.13	0.47
1:A:57:LYS:NZ	2:A:193:NDP:O3B	2.48	0.47
1:B:83:ASN:HD22	1:B:93:ALA:HA	1.80	0.45
1:A:29:LEU:O	1:A:33[A]:ILE:HG12	2.17	0.44
1:A:42[A]:ARG:HH11	1:A:170:ASP:HB2	1.81	0.44
1:B:149:LEU:HD22	1:B:151:PHE:CZ	2.53	0.44
1:A:4:PRO:HG3	1:A:100:LEU:HD13	2.01	0.43
1:A:4:PRO:CG	1:A:100:LEU:HD13	2.50	0.42
1:A:33[A]:ILE:HD13	3:A:194:MQU:H36	2.02	0.42
1:A:125:SER:HB2	4:A:399:HOH:O	2.19	0.42
1:A:137:HIS:CG	1:A:138:PRO:HD2	2.54	0.41
1:A:42[A]:ARG:NH1	1:A:170:ASP:HB2	2.35	0.41
1:A:150:LYS:HG3	4:A:233:HOH:O	2.20	0.41
1:B:20:GLY:O	1:B:145:MET:HB2	2.21	0.41
1:A:28:ARG:HB3	1:A:28:ARG:NH2	2.32	0.41
1:A:168:VAL:HG21	1:A:173:LEU:HD21	2.03	0.40
1:B:25:MET:HA	1:B:26:PRO:HD3	1.78	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	202/192 (105%)	198 (98%)	3 (2%)	1 (0%)	24	11
1	B	201/192 (105%)	197 (98%)	4 (2%)	0	100	100
All	All	403/384 (105%)	395 (98%)	7 (2%)	1 (0%)	36	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PRO

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	186/177 (105%)	178 (96%)	8 (4%)	26	8
1	B	186/177 (105%)	176 (95%)	10 (5%)	20	5
All	All	372/354 (105%)	354 (95%)	18 (5%)	24	6

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	28	ARG
1	A	65	LYS
1	A	74	ASN
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	120	GLU
1	A	145	MET
1	A	154	GLU
1	B	5	ASN
1	B	28	ARG
1	B	65[A]	LYS
1	B	65[B]	LYS
1	B	74	ASN
1	B	124	ASN
1	B	153	LEU
1	B	166	LYS
1	B	173[A]	LEU
1	B	173[B]	LEU

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	47	ASN
1	A	89	ASN
1	A	159	GLN
1	A	185	ASN
1	B	5	ASN
1	B	83	ASN
1	B	101	ASN
1	B	124	ASN
1	B	137	HIS
1	B	185	ASN

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

4 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	NDP	B	195	-	51,52,52	1.77	11 (21%)	71,80,80	1.37	8 (11%)
3	MQU	B	196	-	24,24,24	1.54	5 (20%)	30,34,34	1.95	10 (33%)
2	NDP	A	193	-	51,52,52	1.58	9 (17%)	71,80,80	1.50	12 (16%)
3	MQU	A	194	-	24,24,24	1.26	4 (16%)	30,34,34	1.90	5 (16%)

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	NDP	B	195	-	-	2/34/77/77	0/5/5/5
3	MQU	B	196	-	-	2/10/10/10	0/3/3/3
2	NDP	A	193	-	-	3/34/77/77	0/5/5/5
3	MQU	A	194	-	-	3/10/10/10	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	195	NDP	C4N-C3N	-5.53	1.39	1.50
2	B	195	NDP	PN-O3	5.26	1.65	1.59
2	A	193	NDP	P2B-O2B	4.49	1.67	1.59
2	A	193	NDP	C7N-C3N	4.49	1.58	1.48
2	B	195	NDP	C7N-C3N	4.27	1.57	1.48
3	B	196	MQU	C33-N24	-4.24	1.34	1.39
2	A	193	NDP	PA-O3	-3.64	1.55	1.59
3	B	196	MQU	C27-N22	3.28	1.42	1.37
2	B	195	NDP	P2B-O2X	-3.17	1.43	1.54
2	B	195	NDP	P2B-O2B	3.02	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	195	NDP	PA-O2A	-2.85	1.42	1.55
3	A	194	MQU	C33-N24	-2.83	1.36	1.39
3	A	194	MQU	C27-N22	2.82	1.42	1.37
2	A	193	NDP	C4N-C5N	-2.70	1.42	1.49
2	A	193	NDP	C2A-N1A	2.57	1.38	1.33
2	B	195	NDP	O4B-C1B	-2.55	1.36	1.42
3	B	196	MQU	C33-C32	2.51	1.42	1.35
3	A	194	MQU	C31-C34	2.50	1.43	1.41
2	A	193	NDP	P2B-O3X	-2.50	1.45	1.54
3	B	196	MQU	C35-C34	-2.46	1.35	1.39
2	A	193	NDP	PN-O3	2.45	1.62	1.59
2	A	193	NDP	C3B-C2B	2.39	1.58	1.53
2	B	195	NDP	PN-O2N	-2.38	1.44	1.55
2	A	193	NDP	C5D-C4D	2.37	1.58	1.51
2	B	195	NDP	C4N-C5N	-2.31	1.43	1.49
2	B	195	NDP	C6N-N1N	2.18	1.42	1.37
3	A	194	MQU	C33-C32	2.13	1.41	1.35
3	B	196	MQU	C29-N26	2.08	1.41	1.34
2	B	195	NDP	PA-O3	2.07	1.61	1.59

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	194	MQU	C31-C32-C33	-5.80	102.14	107.04
3	B	196	MQU	C31-C32-C33	-4.82	102.97	107.04
2	A	193	NDP	C1D-N1N-C2N	-4.77	113.28	121.14
3	A	194	MQU	C32-C33-N24	4.61	113.89	110.31
2	B	195	NDP	C3N-C2N-N1N	-4.31	116.87	123.20
3	A	194	MQU	N22-C28-N23	-4.11	121.99	127.21
2	B	195	NDP	C6N-N1N-C2N	3.81	123.40	119.32
2	A	193	NDP	O2N-PN-O3	3.71	117.30	107.27
3	B	196	MQU	N22-C28-N23	-3.56	122.68	127.21
3	B	196	MQU	C35-C36-C27	-3.10	117.09	120.80
2	A	193	NDP	C1D-N1N-C6N	3.10	127.32	120.77
2	B	195	NDP	C1D-N1N-C2N	-3.09	116.05	121.14
3	B	196	MQU	C35-C34-C31	2.93	124.72	122.35
2	A	193	NDP	O2B-P2B-O1X	-2.91	98.97	109.33
3	B	196	MQU	C34-N24-C33	2.90	110.04	107.77
2	A	193	NDP	C3N-C2N-N1N	-2.88	118.98	123.20
3	B	196	MQU	C29-C30-C27	2.69	116.79	114.90
3	A	194	MQU	C1-N24-C33	-2.68	121.29	125.07
2	A	193	NDP	O4B-C1B-C2B	2.56	111.00	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	196	MQU	C36-C27-C30	2.48	123.86	119.31
2	A	193	NDP	O5D-C5D-C4D	-2.36	100.96	108.99
2	A	193	NDP	N6A-C6A-N1A	2.35	123.60	118.38
2	B	195	NDP	C3B-C2B-C1B	-2.28	98.43	102.81
2	A	193	NDP	O3X-P2B-O1X	2.27	119.67	110.83
3	B	196	MQU	C34-C31-C32	2.23	108.72	106.93
3	B	196	MQU	C32-C33-N24	2.20	112.02	110.31
2	B	195	NDP	O2X-P2B-O1X	2.18	119.34	110.83
2	B	195	NDP	P2B-O2B-C2B	-2.18	117.62	123.43
2	A	193	NDP	C2D-C3D-C4D	-2.17	98.42	102.61
2	A	193	NDP	O2D-C2D-C1D	2.16	117.53	110.10
3	A	194	MQU	N25-C28-N23	2.14	120.43	117.22
2	B	195	NDP	O2B-P2B-O1X	-2.12	101.77	109.33
2	A	193	NDP	O4D-C1D-C2D	-2.07	102.18	106.62
3	B	196	MQU	N25-C28-N23	2.07	120.32	117.22
2	B	195	NDP	O2N-PN-O3	2.02	112.72	107.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	194	MQU	C2-C1-C5-O11
3	A	194	MQU	N24-C1-C5-O11
3	B	196	MQU	C5-C1-C2-O8
3	B	196	MQU	N24-C1-C2-O8
3	A	194	MQU	C1-C5-O11-C18
2	A	193	NDP	O4D-C1D-N1N-C2N
2	B	195	NDP	O4D-C1D-N1N-C2N
2	A	193	NDP	PN-O3-PA-O1A
2	A	193	NDP	PN-O3-PA-O2A
2	B	195	NDP	PN-O3-PA-O1A

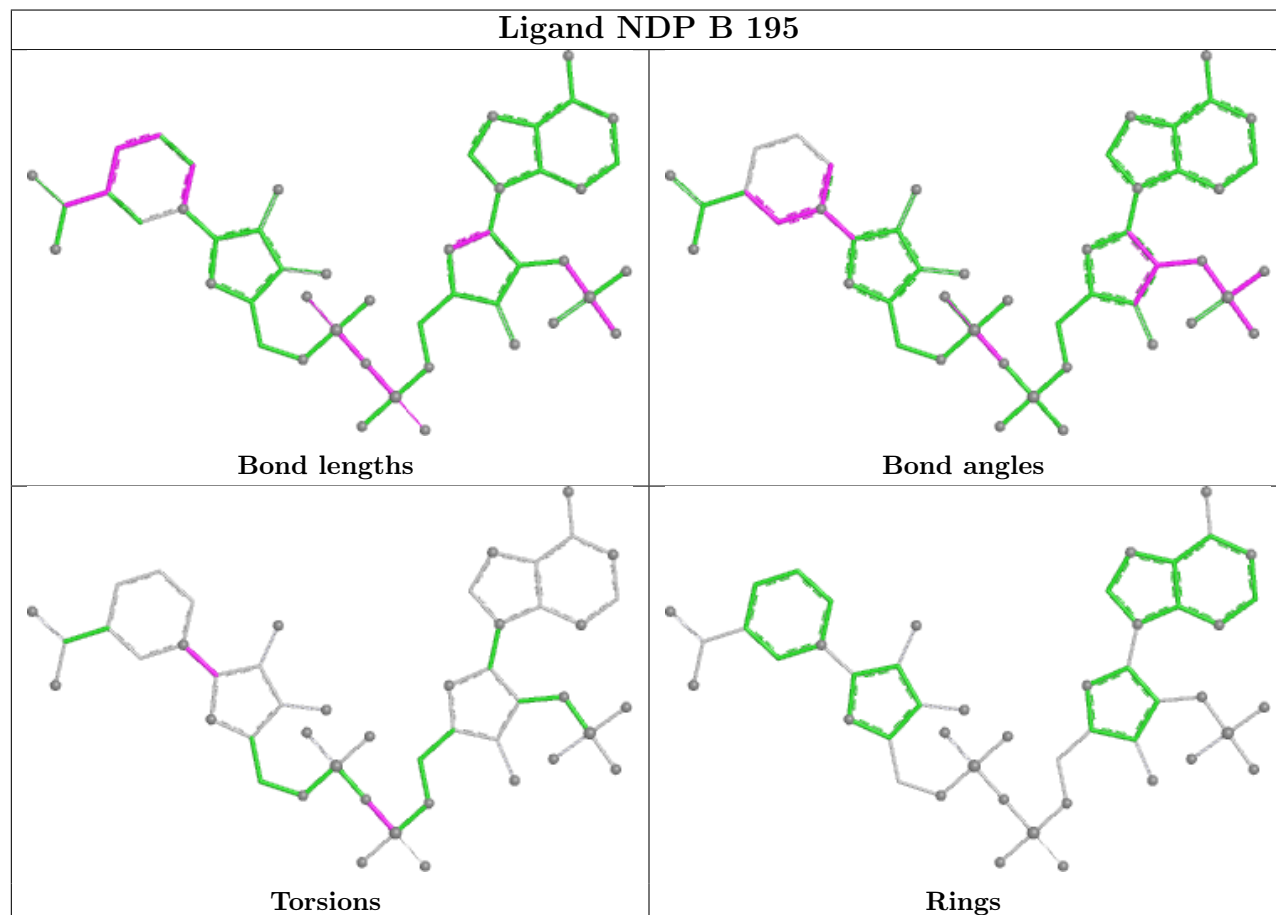
There are no ring outliers.

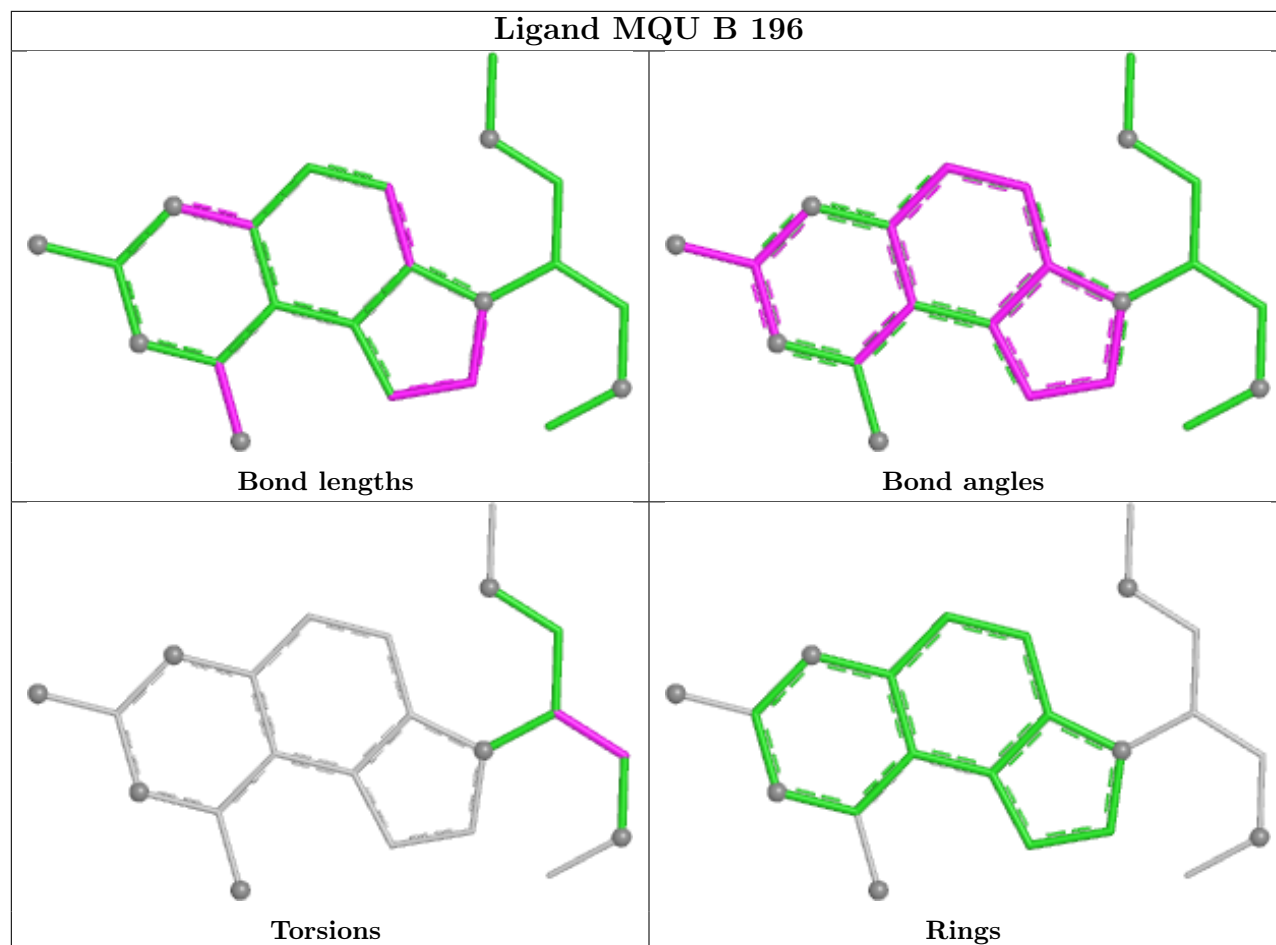
2 monomers are involved in 3 short contacts:

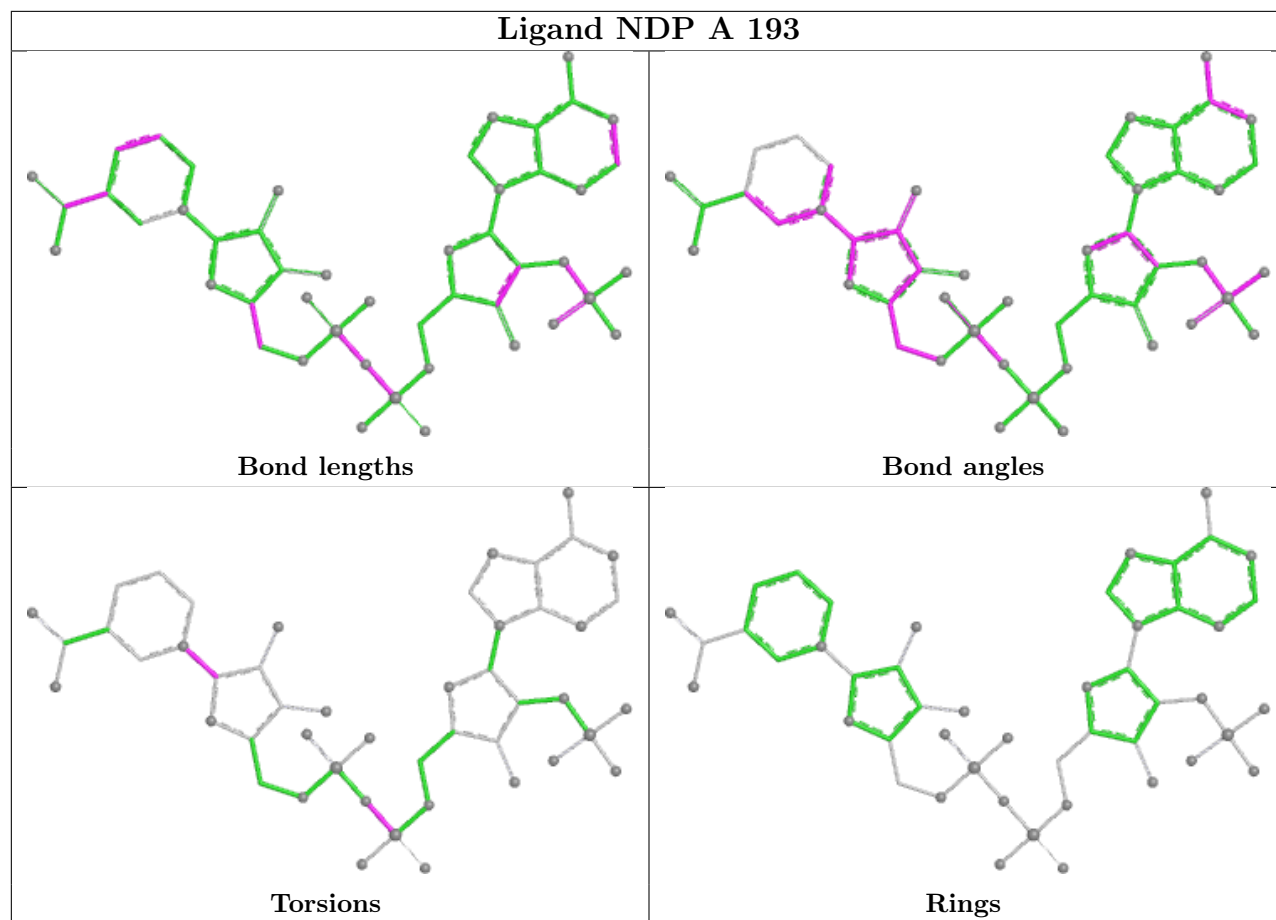
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	193	NDP	2	0
3	A	194	MQU	1	0

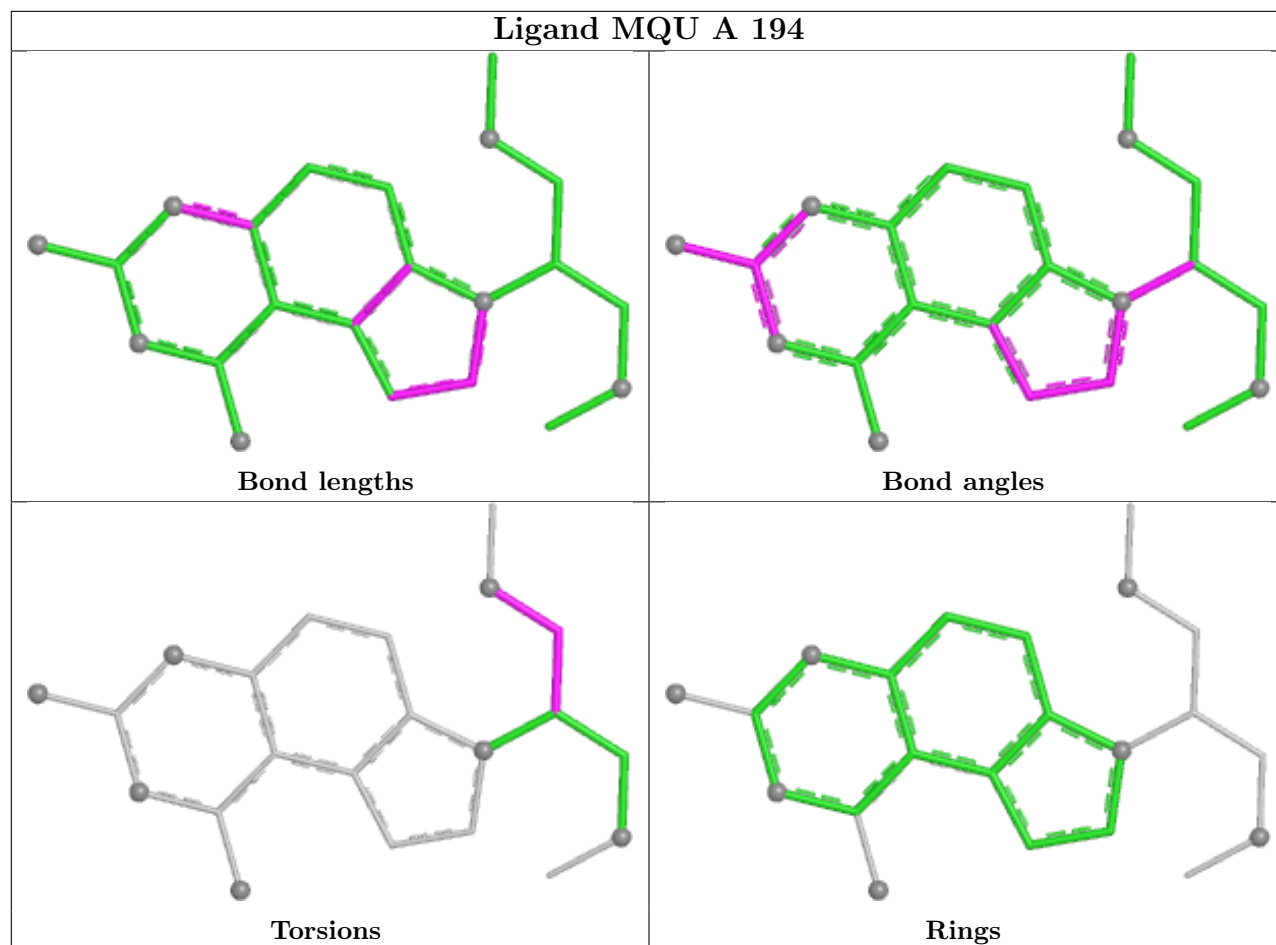
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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	192/192 (100%)	-0.61	2 (1%) 79 84	6, 15, 33, 50	17 (8%)
1	B	192/192 (100%)	-0.73	0 100 100	6, 13, 30, 45	20 (10%)
All	All	384/384 (100%)	-0.67	2 (0%) 87 90	6, 14, 32, 50	37 (9%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	PRO	2.5
1	A	47	ASN	2.2

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.

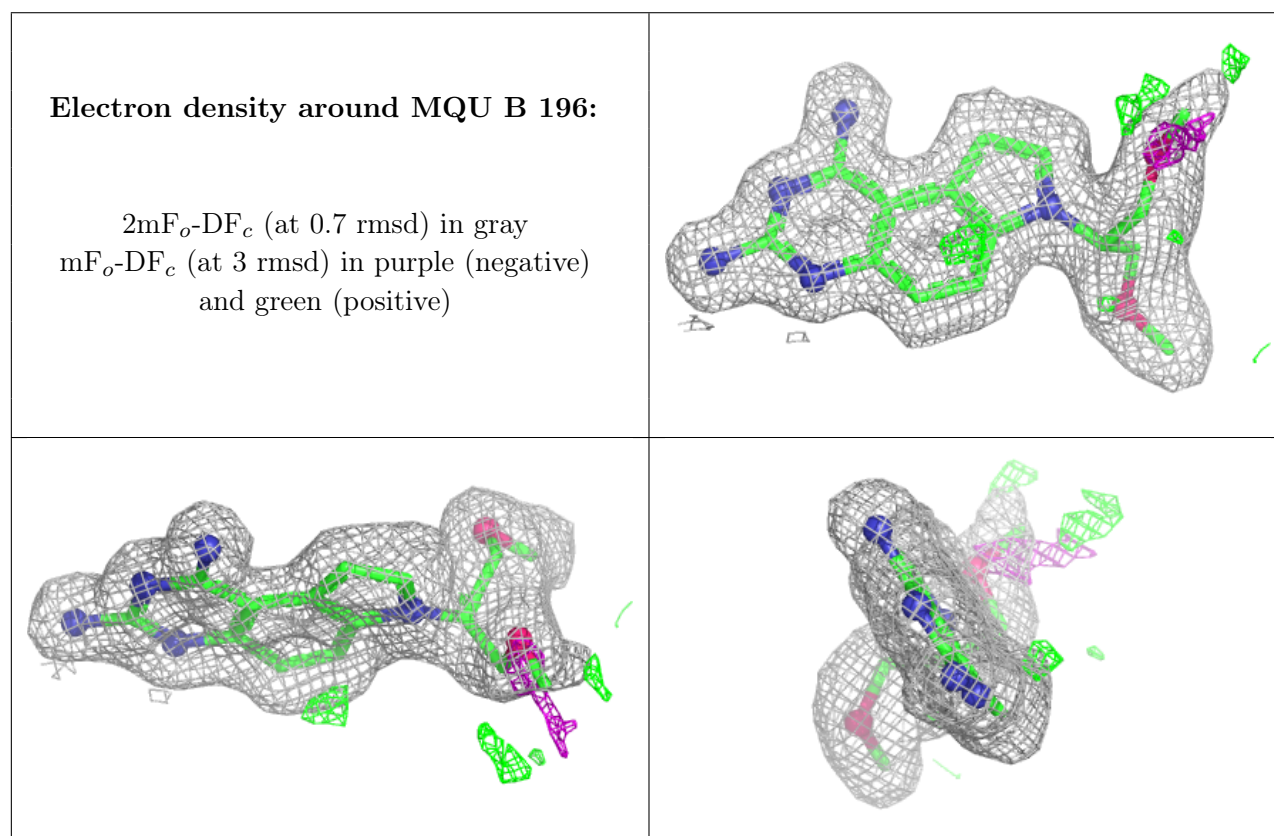
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MQU	B	196	22/22	0.95	0.06	6,13,31,35	0
3	MQU	A	194	22/22	0.96	0.06	7,14,40,47	0
2	NDP	A	193	48/48	0.98	0.04	4,13,20,27	0

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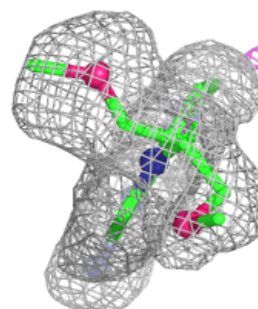
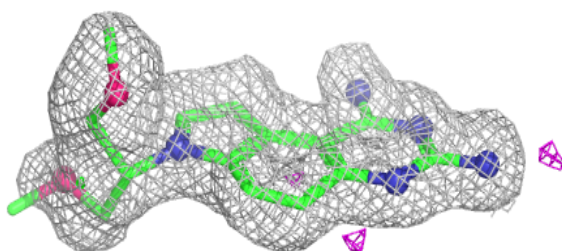
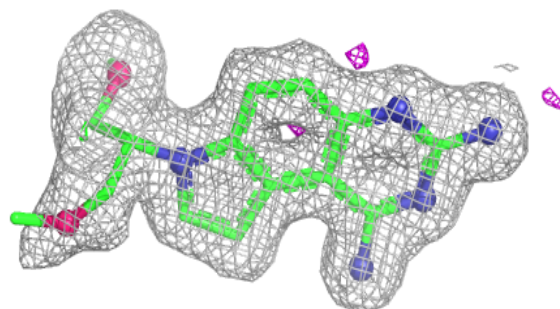
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	B	195	48/48	0.98	0.04	6,11,18,22	0

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.

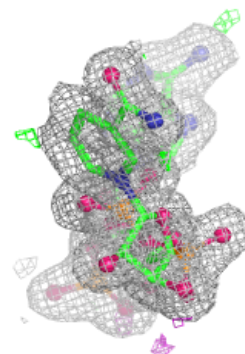
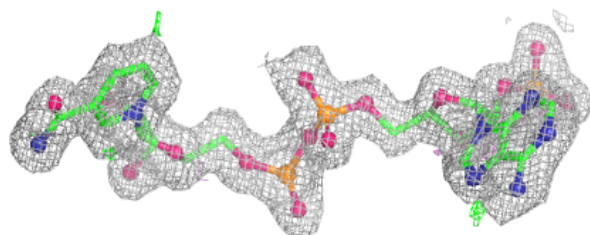
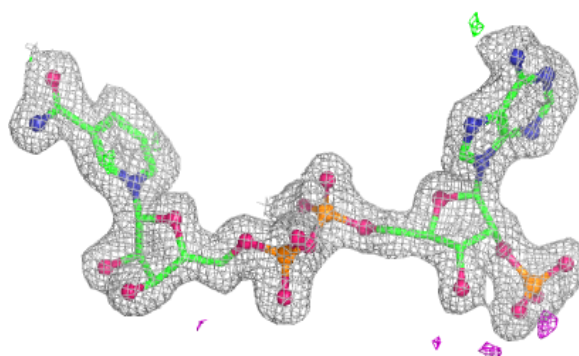


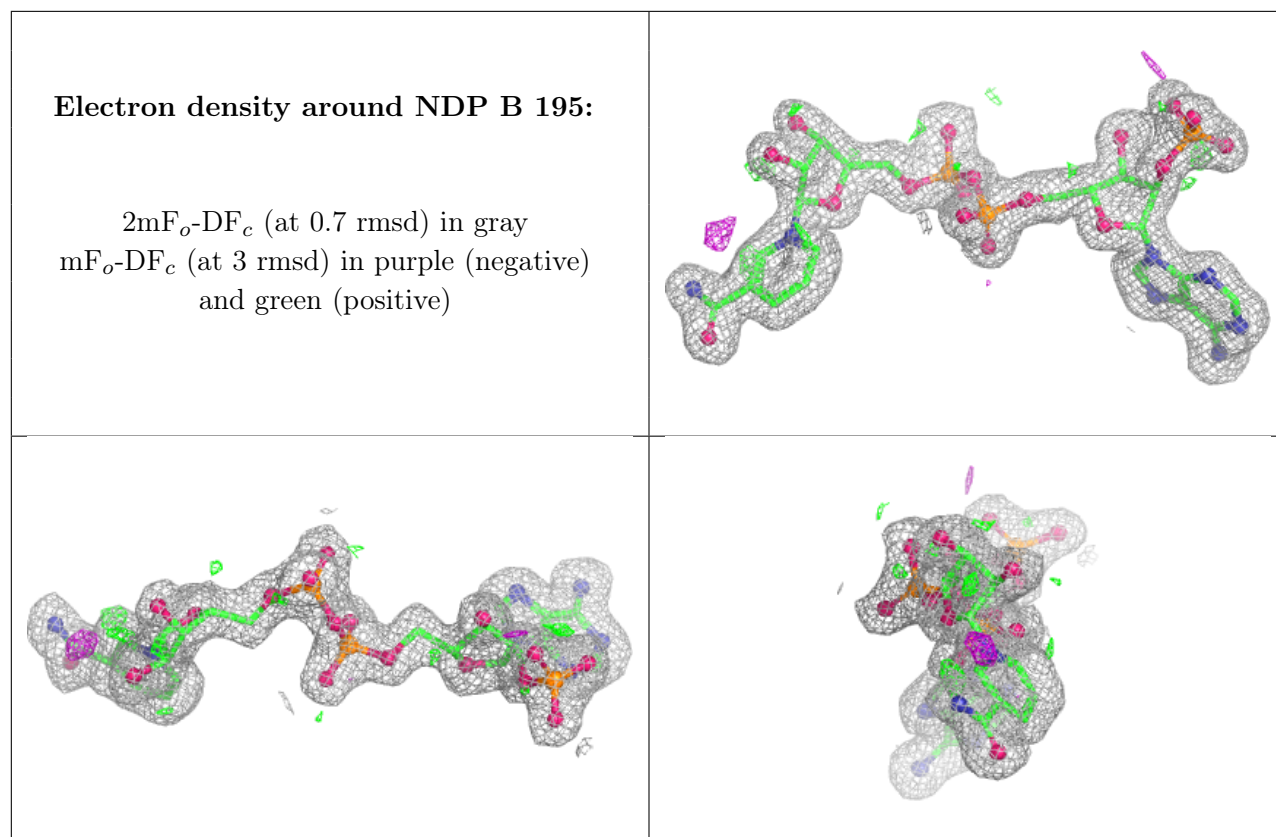
Electron density around MQU A 194:

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

**Electron density around NDP A 193:**

$2mF_o-DF_c$ (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.