



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:14 am BST

PDB ID : 6VG0  
Title : CRYSTAL STRUCTURE OF HUMAN CYTOSOLIC ISOCITRATE DEHYDROGENASE (IDH1) R132H MUTANT IN COMPLEX WITH NADPH and AGI-15056  
Authors : Padyana, A.; Jin, L.  
Deposited on : 2020-01-07  
Resolution : 2.66 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

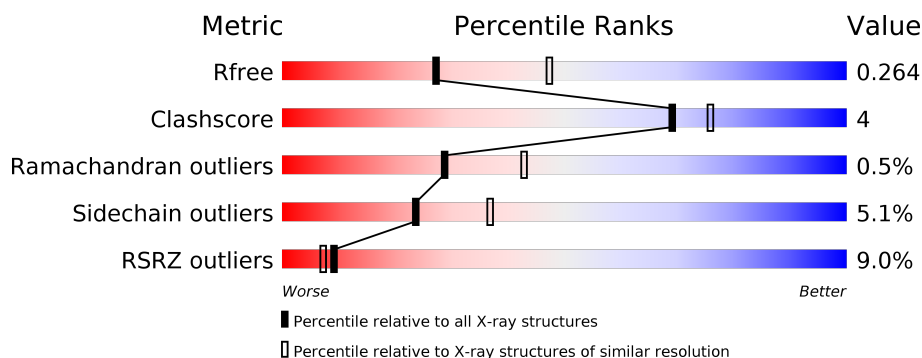
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	425	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>
1	B	425	<div> <div></div> <div> <div>84%</div> <div>13%</div> <div>•</div> </div> </div>
1	C	425	<div> <div>24%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10132 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	3	0
			3302	2097	564	623	18			
1	B	415	Total	C	N	O	S	0	1	0
			3294	2094	558	624	18			
1	C	404	Total	C	N	O	S	0	1	0
			3210	2041	544	607	18			

There are 36 discrepancies between the modelled and reference sequences:

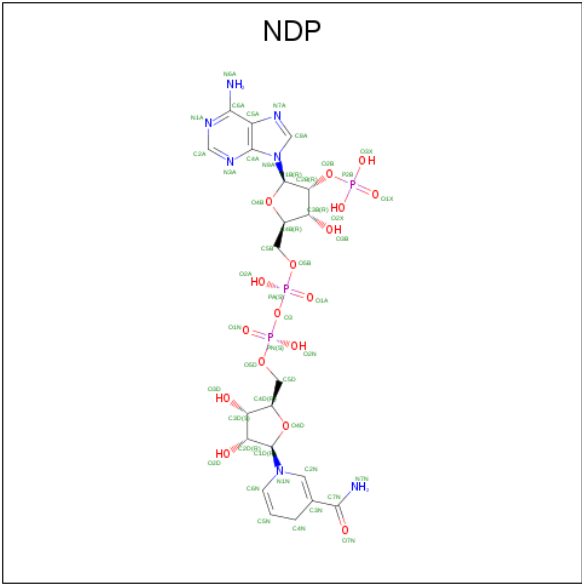
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	HIS	ARG	engineered mutation	UNP O75874
A	415	SER	-	expression tag	UNP O75874
A	416	LEU	-	expression tag	UNP O75874
A	417	GLU	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
A	423	HIS	-	expression tag	UNP O75874
A	424	HIS	-	expression tag	UNP O75874
A	425	HIS	-	expression tag	UNP O75874
B	132	HIS	ARG	engineered mutation	UNP O75874
B	415	SER	-	expression tag	UNP O75874
B	416	LEU	-	expression tag	UNP O75874
B	417	GLU	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874
B	423	HIS	-	expression tag	UNP O75874
B	424	HIS	-	expression tag	UNP O75874

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Chain	Residue	Modelled	Actual	Comment	Reference
B	425	HIS	-	expression tag	UNP O75874
C	132	HIS	ARG	engineered mutation	UNP O75874
C	415	SER	-	expression tag	UNP O75874
C	416	LEU	-	expression tag	UNP O75874
C	417	GLU	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874
C	423	HIS	-	expression tag	UNP O75874
C	424	HIS	-	expression tag	UNP O75874
C	425	HIS	-	expression tag	UNP O75874

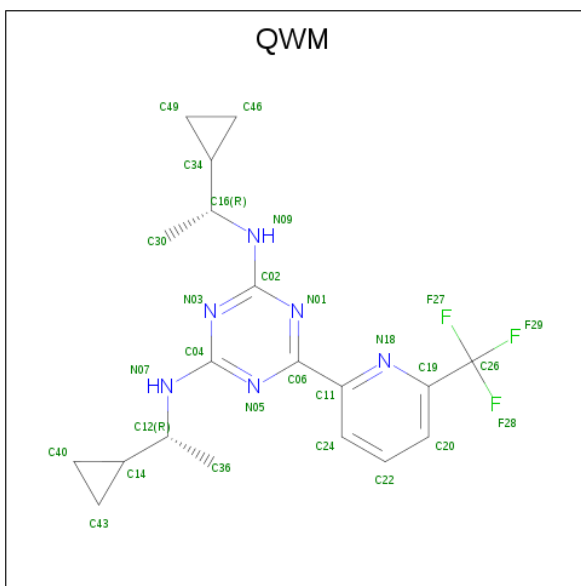
- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is N 2 ,N 4 -bis[(1R)-1-cyclopropylethyl]-6-[6-(trifluoromethyl)pyridin-2-yl]-1,3,5 -triazine-2,4-diamine (three-letter code: QWM) (formula: C<sub>19</sub>H<sub>23</sub>F<sub>3</sub>N<sub>6</sub>) (labeled as "Ligand

of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	F	N	0	1
			56	38	6	12		
3	C	1	Total	C	F	N	0	0
			28	19	3	6		

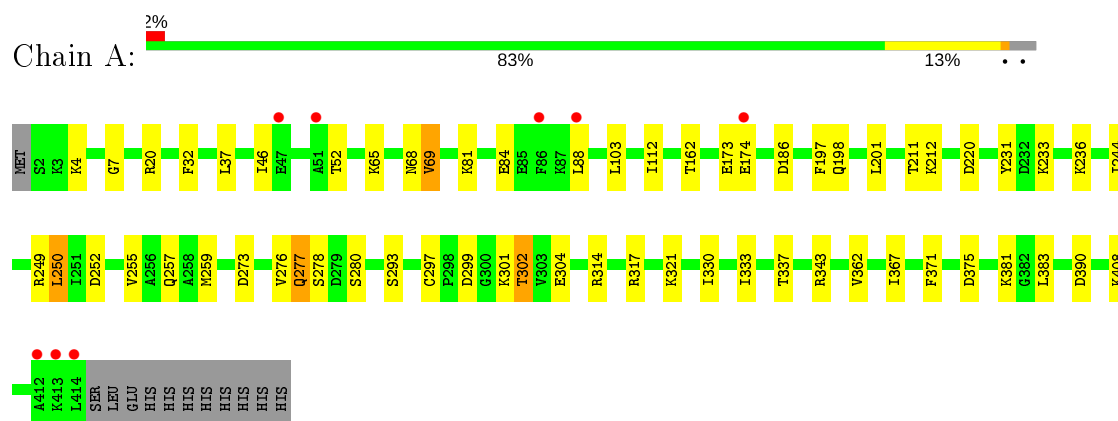
- Molecule 4 is water.

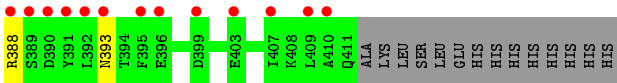
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	30	Total	O	0	0
			30	30		
4	C	20	Total	O	0	0
			20	20		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Isocitrate dehydrogenase [NADP] cytoplasmic





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	196.77Å 89.16Å 90.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.20 – 2.66 41.20 – 2.66	Depositor EDS
% Data completeness (in resolution range)	97.8 (41.20-2.66) 97.8 (41.20-2.66)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.206 , 0.264 0.206 , 0.264	Depositor DCC
$R_{free}$ test set	2305 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.9	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.021 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NDP, QWM

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	0.25	0/3371	0.43	0/4544
1	B	0.25	0/3363	0.43	0/4535
1	C	0.25	0/3277	0.42	0/4419
All	All	0.25	0/10011	0.43	0/13498

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	3302	0	3269	25	0
1	B	3294	0	3261	27	0
1	C	3210	0	3167	23	0
2	A	48	0	26	0	0
2	B	48	0	26	2	0
2	C	48	0	26	1	0
3	B	56	0	0	0	0
3	C	28	0	0	0	0
4	A	48	0	0	0	0
4	B	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	20	0	0	0	0
All	All	10132	0	9775	73	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 (73) 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:46:ILE:HD11	1:A:88:LEU:HD11	1.76	0.66
1:B:46:ILE:HD11	1:B:88:LEU:HD11	1.81	0.62
1:A:211:THR:HB	1:A:220:ASP:HB3	1.82	0.62
1:C:7:GLY:HA3	1:C:37:LEU:HD23	1.81	0.61
1:C:17:GLU:HB2	1:C:311:THR:HB	1.85	0.57
1:C:102:ILE:HG22	1:C:103:LEU:HD12	1.86	0.57
1:C:344:ALA:HB2	1:C:352:LEU:HB3	1.89	0.54
1:A:249:ARG:NH2	1:A:257:GLN:OE1	2.41	0.54
1:A:255:VAL:HG23	1:B:280:SER:HB2	1.90	0.54
1:B:415:SER:O	1:B:416:LEU:HB2	2.08	0.54
1:A:212:LYS:NZ	1:A:252:ASP:OD1	2.41	0.53
1:C:347:ASP:O	1:C:349:ASN:N	2.40	0.53
1:C:68:ASN:HA	1:C:302:THR:HG22	1.91	0.53
1:C:375:ASP:OD1	1:C:375:ASP:N	2.41	0.52
1:A:277[B]:GLN:O	1:A:280:SER:N	2.39	0.52
1:B:69:VAL:HG11	1:B:343:ARG:HD2	1.92	0.51
1:B:7:GLY:HA3	1:B:37:LEU:HD23	1.90	0.51
1:C:77:THR:N	2:C:502:NDP:O2D	2.40	0.51
1:A:112:ILE:HD13	1:A:330:ILE:HG22	1.94	0.50
1:C:197:PHE:CZ	1:C:231:TYR:HB2	2.47	0.50
1:A:201:LEU:HD23	1:A:244:ILE:HD11	1.94	0.50
1:A:277[A]:GLN:O	1:A:280:SER:N	2.40	0.49
1:C:282:ALA:HA	1:C:291:MET:HE3	1.95	0.48
1:C:83:VAL:HA	1:C:88:LEU:HD12	1.95	0.47
1:B:43:ASP:O	1:B:48:ASN:ND2	2.40	0.47
1:C:333:ILE:O	1:C:337:THR:HG23	2.14	0.47
1:A:297:CYS:SG	1:A:302:THR:OG1	2.68	0.47
1:C:209:LEU:HD22	1:C:227:PHE:CG	2.50	0.46
1:A:276:VAL:HA	1:B:252:ASP:OD1	2.16	0.46
1:B:198:GLN:HG2	1:B:300:GLY:HA3	1.99	0.45
1:B:192:PHE:CZ	1:B:268:ALA:HB1	2.51	0.45
1:A:362:VAL:HG23	1:A:408:LYS:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PHE:CZ	1:A:231:TYR:HB2	2.52	0.45
1:A:375:ASP:N	1:A:375:ASP:OD1	2.44	0.45
1:B:110:GLU:HB2	1:B:129:ILE:HG12	1.99	0.45
1:B:163:GLN:HG3	1:B:164:LYS:O	2.16	0.45
1:B:297:CYS:SG	1:B:302:THR:OG1	2.66	0.45
1:B:375:ASP:N	1:B:375:ASP:OD1	2.40	0.45
1:A:333:ILE:O	1:A:337:THR:HG23	2.17	0.45
1:B:136:GLY:HA2	1:B:140:ARG:HB2	1.99	0.44
1:B:261:SER:OG	1:B:262:GLU:N	2.50	0.44
1:C:382:GLY:O	1:C:386:VAL:HG23	2.18	0.44
1:A:250:LEU:HD22	1:A:250:LEU:HA	1.88	0.44
1:A:69:VAL:HG11	1:A:343:ARG:HD2	2.00	0.44
1:C:208:TYR:HA	1:C:247:GLU:O	2.18	0.44
1:C:90:GLN:HB2	1:C:92:TRP:CE2	2.52	0.44
1:C:233:LYS:HG2	1:C:234:GLN:HG3	2.00	0.43
1:B:2:SER:OG	1:B:3:LYS:N	2.50	0.43
1:A:68:ASN:O	1:A:302:THR:HA	2.18	0.43
1:B:372:MET:HB2	1:B:376:LEU:HD12	2.00	0.43
1:C:210:SER:HA	1:C:249:ARG:O	2.18	0.43
1:B:75:THR:O	2:B:502:NDP:H2N	2.19	0.43
1:A:381:LYS:NZ	1:A:390:ASP:OD2	2.52	0.42
1:B:144:PHE:CE1	1:B:179:ALA:HB3	2.54	0.42
1:C:32:PHE:N	1:C:33:PRO:HD2	2.34	0.42
1:A:7:GLY:HA3	1:A:37:LEU:HD23	2.02	0.42
1:B:249:ARG:NH2	4:B:602:HOH:O	2.49	0.42
1:A:273:ASP:O	1:A:277[A]:GLN:HG2	2.18	0.42
1:A:186:ASP:OD1	1:B:177:GLY:HA2	2.20	0.42
1:B:330:ILE:HD12	1:B:363:SER:HB3	2.02	0.42
1:B:362:VAL:HG23	1:B:408:LYS:HD2	2.00	0.42
1:B:151:LYS:HB2	1:B:151:LYS:HE3	1.79	0.42
1:B:381:LYS:HE2	1:B:381:LYS:HB3	1.89	0.41
1:A:81:LYS:HA	1:A:81:LYS:HD3	1.84	0.41
1:B:330:ILE:HG13	1:B:367:ILE:HD11	2.03	0.41
1:A:4:LYS:HE3	1:A:32:PHE:O	2.20	0.41
1:C:367:ILE:HG23	1:C:372:MET:HB3	2.03	0.41
1:C:388:ARG:NH2	1:C:393:ASN:HD22	2.18	0.41
1:C:60:ALA:O	1:C:64:ILE:HG13	2.20	0.41
1:A:367:ILE:HA	1:A:371:PHE:O	2.21	0.40
1:B:68:ASN:O	1:B:302:THR:HA	2.20	0.40
1:C:37:LEU:HB2	1:C:38:ASP:H	1.50	0.40
2:B:502:NDP:H2D	2:B:502:NDP:H6N	1.87	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	414/425 (97%)	391 (94%)	20 (5%)	3 (1%)	22	33
1	B	414/425 (97%)	395 (95%)	18 (4%)	1 (0%)	47	64
1	C	401/425 (94%)	374 (93%)	24 (6%)	3 (1%)	22	33
All	All	1229/1275 (96%)	1160 (94%)	62 (5%)	7 (1%)	29	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	SER
1	C	348	ASN
1	A	277[A]	GLN
1	A	277[B]	GLN
1	C	85	GLU
1	C	312	VAL
1	B	312	VAL

### 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	352/361 (98%)	329 (94%)	23 (6%)	17	26
1	B	352/361 (98%)	337 (96%)	15 (4%)	29	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	342/361 (95%)	327 (96%)	15 (4%)	28	43
All	All	1046/1083 (97%)	993 (95%)	53 (5%)	24	37

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	52	THR
1	A	65	LYS
1	A	69	VAL
1	A	84	GLU
1	A	103	LEU
1	A	162	THR
1	A	173	GLU
1	A	174	GLU
1	A	198	GLN
1	A	233	LYS
1	A	236	LYS
1	A	250	LEU
1	A	259	MET
1	A	293	SER
1	A	299	ASP
1	A	301	LYS
1	A	302	THR
1	A	304	GLU
1	A	314	ARG
1	A	317	ARG
1	A	321	LYS
1	A	383	LEU
1	B	47	GLU
1	B	142	THR
1	B	162	THR
1	B	174	GLU
1	B	184	ASN
1	B	233	LYS
1	B	250	LEU
1	B	259	MET
1	B	288	LEU
1	B	295	LEU
1	B	301	LYS
1	B	302	THR
1	B	383	LEU

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Mol	Chain	Res	Type
1	B	411	GLN
1	B	416	LEU
1	C	12	GLU
1	C	19	THR
1	C	37	LEU
1	C	52	THR
1	C	62	GLU
1	C	229	GLU
1	C	233	LYS
1	C	252	ASP
1	C	299	ASP
1	C	301	LYS
1	C	302	THR
1	C	317	ARG
1	C	338	ARG
1	C	347	ASP
1	C	354	PHE

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	QWM	B	501[B]	-	31,31,31	2.81	4 (12%)	46,46,46	2.78	18 (39%)
3	QWM	B	501[A]	-	31,31,31	2.79	4 (12%)	46,46,46	2.82	18 (39%)
2	NDP	C	502	-	45,52,52	0.54	0	53,80,80	0.53	1 (1%)
3	QWM	C	501	-	31,31,31	2.77	3 (9%)	46,46,46	2.84	20 (43%)
2	NDP	A	501	-	45,52,52	0.52	0	53,80,80	0.53	1 (1%)
2	NDP	B	502	-	45,52,52	0.50	0	53,80,80	0.54	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
3	QWM	B	501[B]	-	-	2/26/30/30	0/4/4/4
3	QWM	B	501[A]	-	-	10/26/30/30	0/4/4/4
2	NDP	C	502	-	-	9/30/77/77	0/5/5/5
3	QWM	C	501	-	-	9/26/30/30	0/4/4/4
2	NDP	A	501	-	-	11/30/77/77	0/5/5/5
2	NDP	B	502	-	-	11/30/77/77	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501[A]	QWM	C04-N07	10.35	1.48	1.34
3	B	501[B]	QWM	C04-N07	10.34	1.48	1.34
3	C	501	QWM	C04-N07	10.28	1.48	1.34
3	B	501[B]	QWM	C02-N09	10.22	1.47	1.34
3	B	501[A]	QWM	C02-N09	10.09	1.47	1.34
3	C	501	QWM	C02-N09	10.00	1.47	1.34
3	B	501[B]	QWM	C11-C06	-2.70	1.40	1.48
3	B	501[A]	QWM	C11-C06	-2.68	1.40	1.48
3	C	501	QWM	C11-C06	-2.67	1.40	1.48
3	B	501[A]	QWM	C26-C19	2.05	1.54	1.50
3	B	501[B]	QWM	C26-C19	2.05	1.54	1.50

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501[B]	QWM	C04-N05-C06	8.85	120.24	114.60
3	B	501[A]	QWM	C02-N01-C06	8.82	120.22	114.60
3	B	501[A]	QWM	C04-N05-C06	8.73	120.16	114.60
3	C	501	QWM	C04-N05-C06	8.45	119.99	114.60
3	C	501	QWM	C02-N01-C06	8.39	119.94	114.60
3	B	501[B]	QWM	C02-N01-C06	8.28	119.88	114.60
3	C	501	QWM	C02-N09-C16	-6.54	119.16	124.53
3	C	501	QWM	C04-N07-C12	-5.97	119.63	124.53
3	B	501[B]	QWM	C02-N09-C16	-5.41	120.09	124.53
3	B	501[A]	QWM	C04-N07-C12	-5.39	120.11	124.53
3	B	501[A]	QWM	C02-N09-C16	-5.26	120.21	124.53
3	B	501[B]	QWM	C26-C19-N18	4.63	119.81	114.56
3	B	501[A]	QWM	C26-C19-N18	4.59	119.77	114.56
3	B	501[B]	QWM	C04-N07-C12	-4.51	120.83	124.53
3	C	501	QWM	C26-C19-N18	4.05	119.15	114.56
3	B	501[B]	QWM	N05-C04-N03	-3.99	119.92	126.23
3	C	501	QWM	N05-C04-N03	-3.98	119.94	126.23
3	B	501[A]	QWM	N05-C04-N03	-3.97	119.96	126.23
3	B	501[B]	QWM	N03-C02-N01	-3.89	120.07	126.23
3	C	501	QWM	N03-C02-N01	-3.89	120.08	126.23
3	B	501[A]	QWM	N03-C02-N01	-3.89	120.09	126.23
3	C	501	QWM	C04-N03-C02	3.64	120.06	113.89
3	B	501[B]	QWM	C04-N03-C02	3.55	119.91	113.89
3	B	501[A]	QWM	C04-N03-C02	3.48	119.79	113.89
3	B	501[A]	QWM	N05-C06-N01	-3.37	119.79	125.23
3	B	501[B]	QWM	N05-C06-N01	-3.25	119.98	125.23
3	C	501	QWM	N05-C06-N01	-3.24	119.99	125.23
3	B	501[B]	QWM	C06-C11-N18	2.95	120.41	117.28
3	B	501[A]	QWM	C46-C34-C16	-2.56	114.89	119.16
3	B	501[B]	QWM	C11-C06-N01	2.45	120.80	117.48
3	B	501[B]	QWM	C40-C14-C12	-2.38	115.19	119.16
3	B	501[B]	QWM	C46-C34-C16	-2.38	115.19	119.16
3	B	501[A]	QWM	C11-C06-N05	2.36	120.68	117.48
3	B	501[A]	QWM	C43-C14-C12	-2.34	115.26	119.16
3	B	501[A]	QWM	C40-C14-C12	-2.34	115.26	119.16
3	B	501[B]	QWM	N07-C04-N03	2.34	120.69	117.18
2	C	502	NDP	C5A-C6A-N6A	2.34	123.90	120.35
3	C	501	QWM	C43-C14-C12	-2.33	115.27	119.16
3	C	501	QWM	C11-C06-N05	2.29	120.58	117.48
3	C	501	QWM	C46-C34-C16	-2.26	115.39	119.16
3	B	501[B]	QWM	C43-C14-C12	-2.26	115.39	119.16
2	B	502	NDP	C5A-C6A-N6A	2.26	123.78	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	QWM	N09-C02-N01	2.26	120.57	117.18
3	C	501	QWM	C49-C34-C16	-2.24	115.42	119.16
3	C	501	QWM	C36-C12-C14	-2.24	109.06	114.08
3	B	501[A]	QWM	C06-C11-N18	2.23	119.64	117.28
2	A	501	NDP	C5A-C6A-N6A	2.21	123.71	120.35
3	B	501[A]	QWM	N09-C02-N03	2.20	120.48	117.18
3	C	501	QWM	F28-C26-C19	-2.13	108.83	112.47
3	C	501	QWM	N07-C04-N05	2.13	120.37	117.18
3	C	501	QWM	C30-C16-C34	-2.12	109.32	114.08
3	B	501[B]	QWM	C36-C12-C14	-2.12	109.33	114.08
3	B	501[B]	QWM	C49-C34-C16	-2.09	115.67	119.16
3	B	501[A]	QWM	C36-C12-C14	-2.09	109.40	114.08
3	C	501	QWM	C40-C14-C12	-2.06	115.72	119.16
3	B	501[B]	QWM	C30-C16-C34	-2.06	109.47	114.08
3	C	501	QWM	F27-C26-C19	-2.03	109.00	112.47
3	B	501[A]	QWM	C49-C34-C16	-2.03	115.77	119.16
3	B	501[A]	QWM	C30-C16-C34	-2.02	109.56	114.08

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501[A]	QWM	C30-C16-C34-C46
3	B	501[A]	QWM	N09-C16-C34-C46
2	C	502	NDP	C5B-O5B-PA-O1A
2	C	502	NDP	C5D-O5D-PN-O3
2	C	502	NDP	C5D-O5D-PN-O1N
2	C	502	NDP	C5D-O5D-PN-O2N
3	C	501	QWM	C36-C12-C14-C40
3	C	501	QWM	N07-C12-C14-C43
3	C	501	QWM	N03-C04-N07-C12
3	C	501	QWM	N05-C04-N07-C12
3	C	501	QWM	C14-C12-N07-C04
2	A	501	NDP	C5B-O5B-PA-O3
2	A	501	NDP	C5D-O5D-PN-O1N
2	A	501	NDP	C5D-O5D-PN-O2N
2	B	502	NDP	C5B-O5B-PA-O3
2	B	502	NDP	C5D-O5D-PN-O1N
2	B	502	NDP	C5D-O5D-PN-O2N
2	C	502	NDP	C3B-C2B-O2B-P2B
2	B	502	NDP	C2D-C1D-N1N-C2N
2	B	502	NDP	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C2D-C1D-N1N-C2N
2	B	502	NDP	O4D-C1D-N1N-C2N
3	B	501[A]	QWM	C30-C16-C34-C49
2	A	501	NDP	C2D-C1D-N1N-C6N
2	A	501	NDP	O4D-C1D-N1N-C2N
2	B	502	NDP	O4D-C1D-N1N-C6N
2	A	501	NDP	C5D-O5D-PN-O3
2	A	501	NDP	C5B-O5B-PA-O1A
2	A	501	NDP	C5B-O5B-PA-O2A
2	B	502	NDP	C5B-O5B-PA-O1A
2	B	502	NDP	C5B-O5B-PA-O2A
3	B	501[A]	QWM	N07-C12-C14-C43
3	B	501[A]	QWM	N09-C16-C34-C49
2	C	502	NDP	O4D-C1D-N1N-C2N
3	C	501	QWM	N01-C06-C11-N18
2	A	501	NDP	O4D-C1D-N1N-C6N
3	C	501	QWM	N05-C06-C11-N18
3	C	501	QWM	N05-C06-C11-C24
3	C	501	QWM	N01-C06-C11-C24
3	B	501[A]	QWM	N01-C06-C11-N18
3	B	501[A]	QWM	N05-C06-C11-N18
3	B	501[B]	QWM	C14-C12-N07-C04
3	B	501[A]	QWM	C14-C12-N07-C04
3	B	501[A]	QWM	N01-C06-C11-C24
3	B	501[A]	QWM	N05-C06-C11-C24
2	C	502	NDP	C2B-O2B-P2B-O1X
2	C	502	NDP	C5B-O5B-PA-O3
2	A	501	NDP	C2B-O2B-P2B-O2X
2	B	502	NDP	C5D-O5D-PN-O3
2	B	502	NDP	C2N-C3N-C7N-N7N
2	C	502	NDP	C3D-C4D-C5D-O5D
3	B	501[B]	QWM	N01-C06-C11-N18

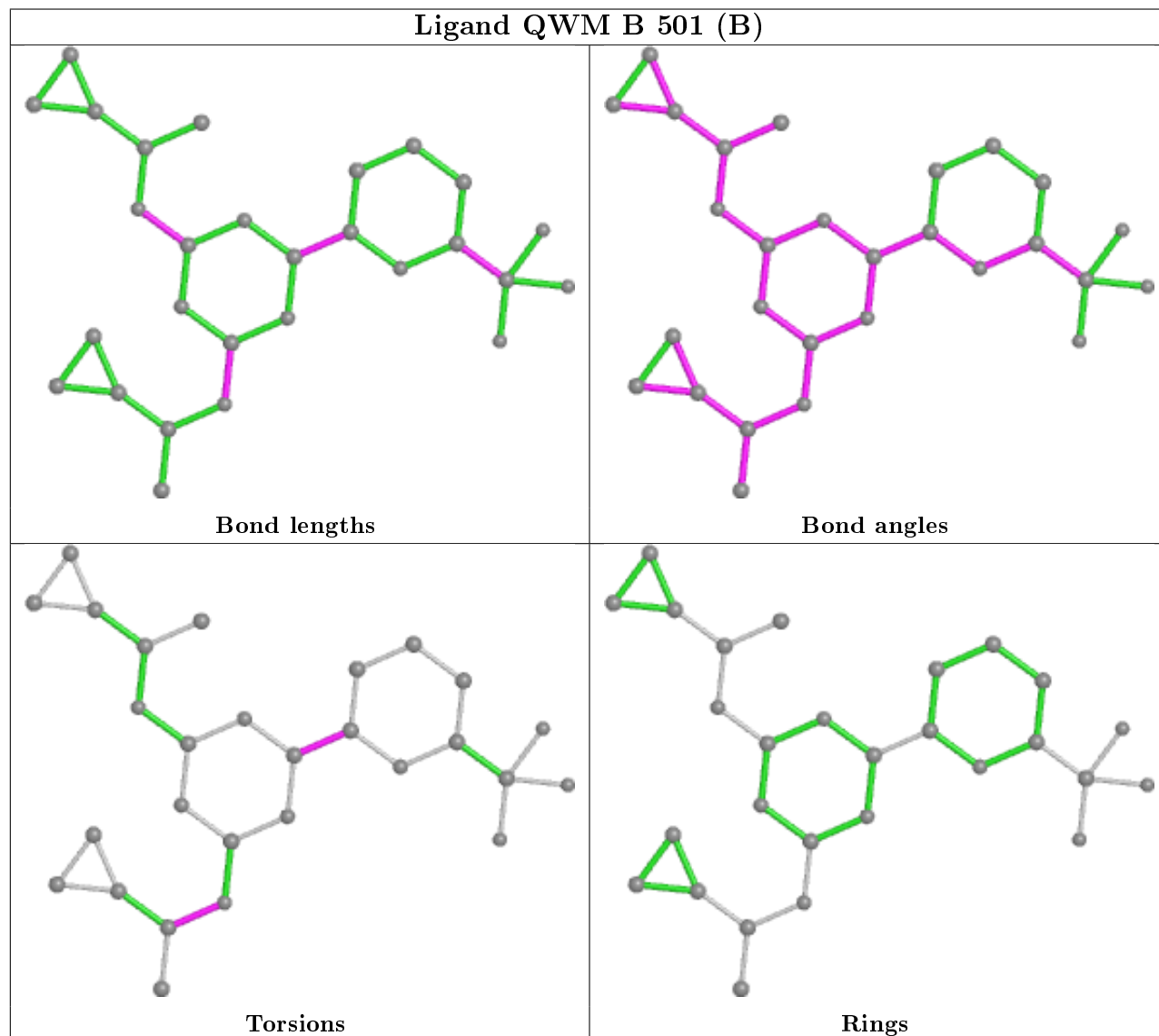
There are no ring outliers.

2 monomers are involved in 3 short contacts:

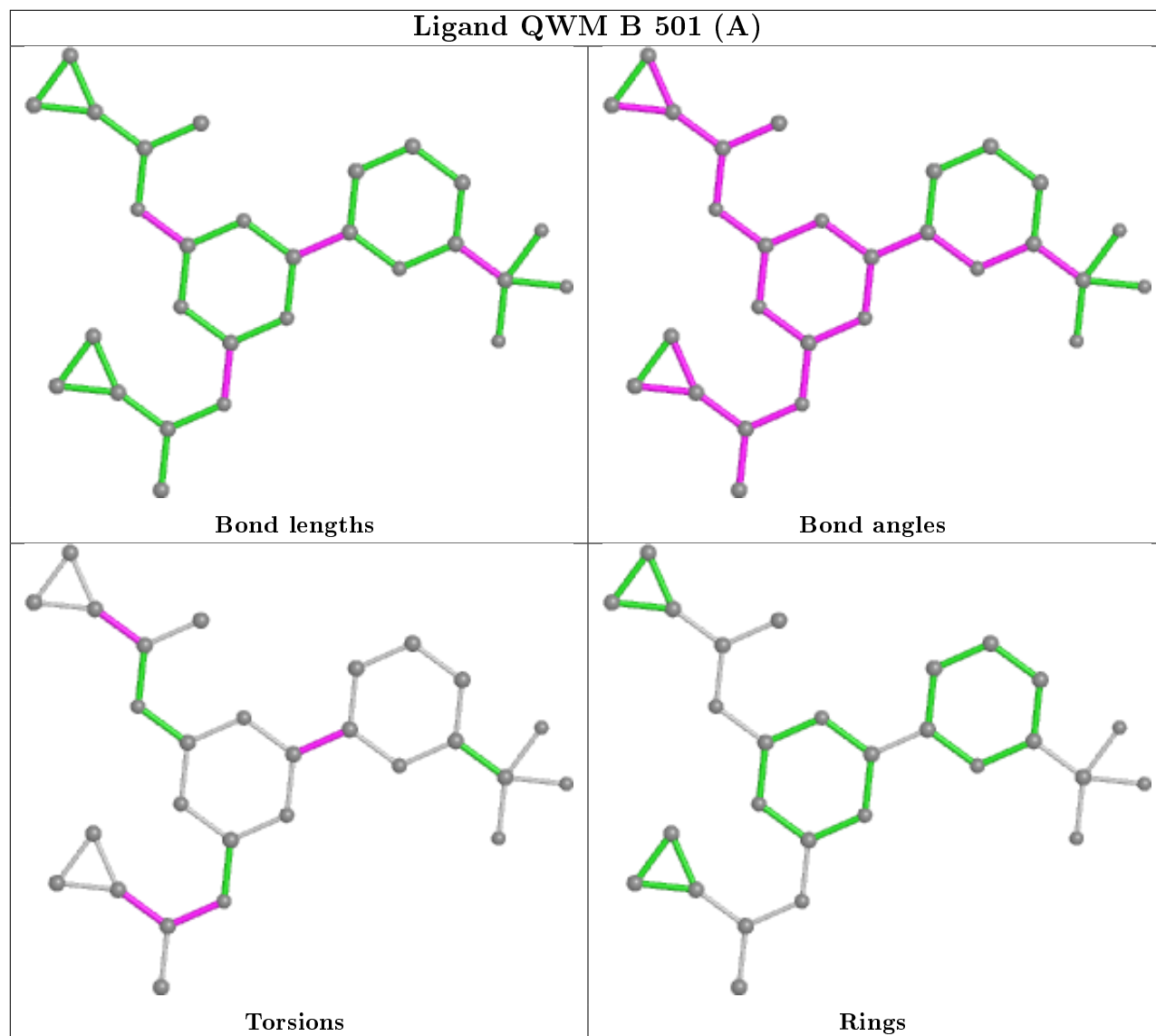
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	NDP	1	0
2	B	502	NDP	2	0

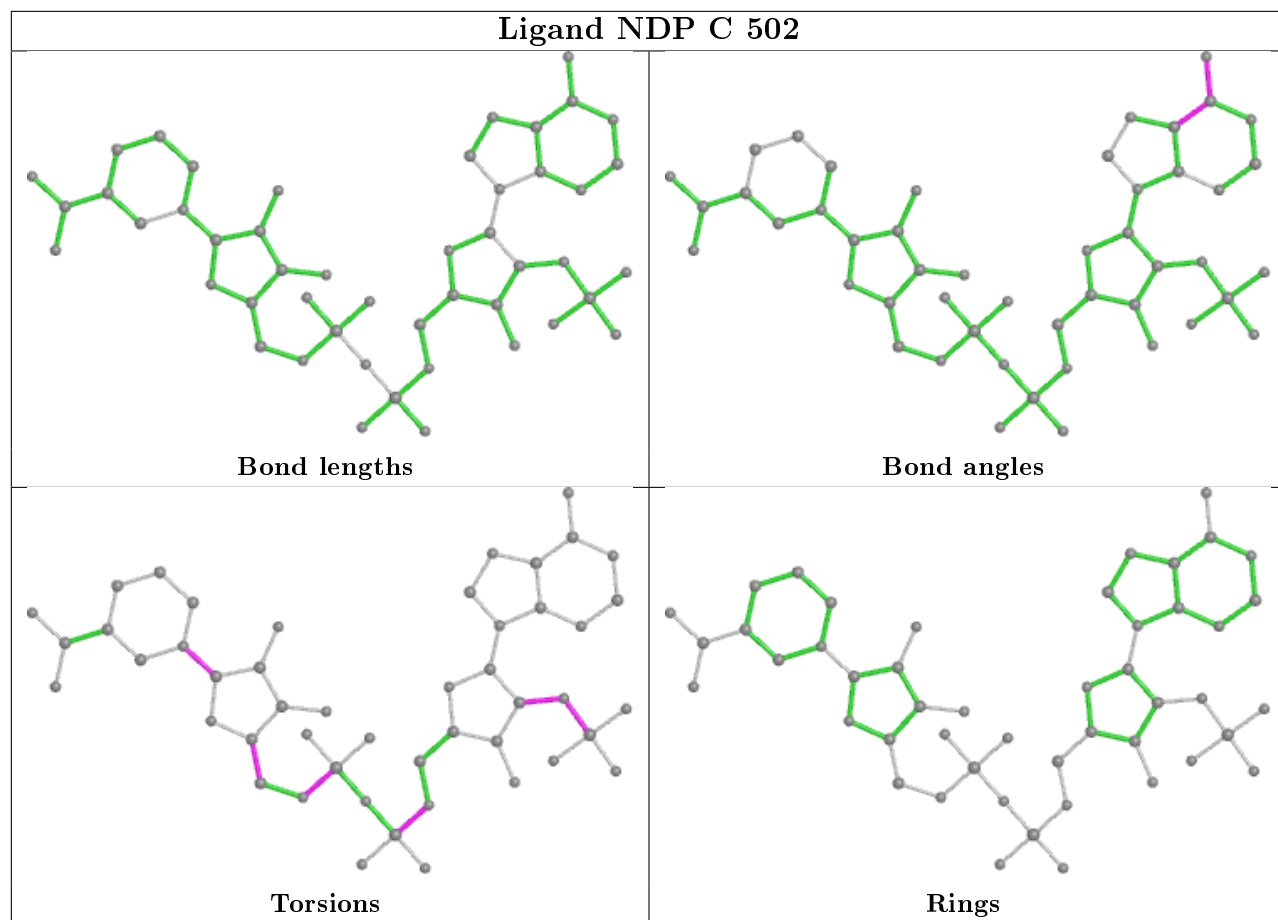
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

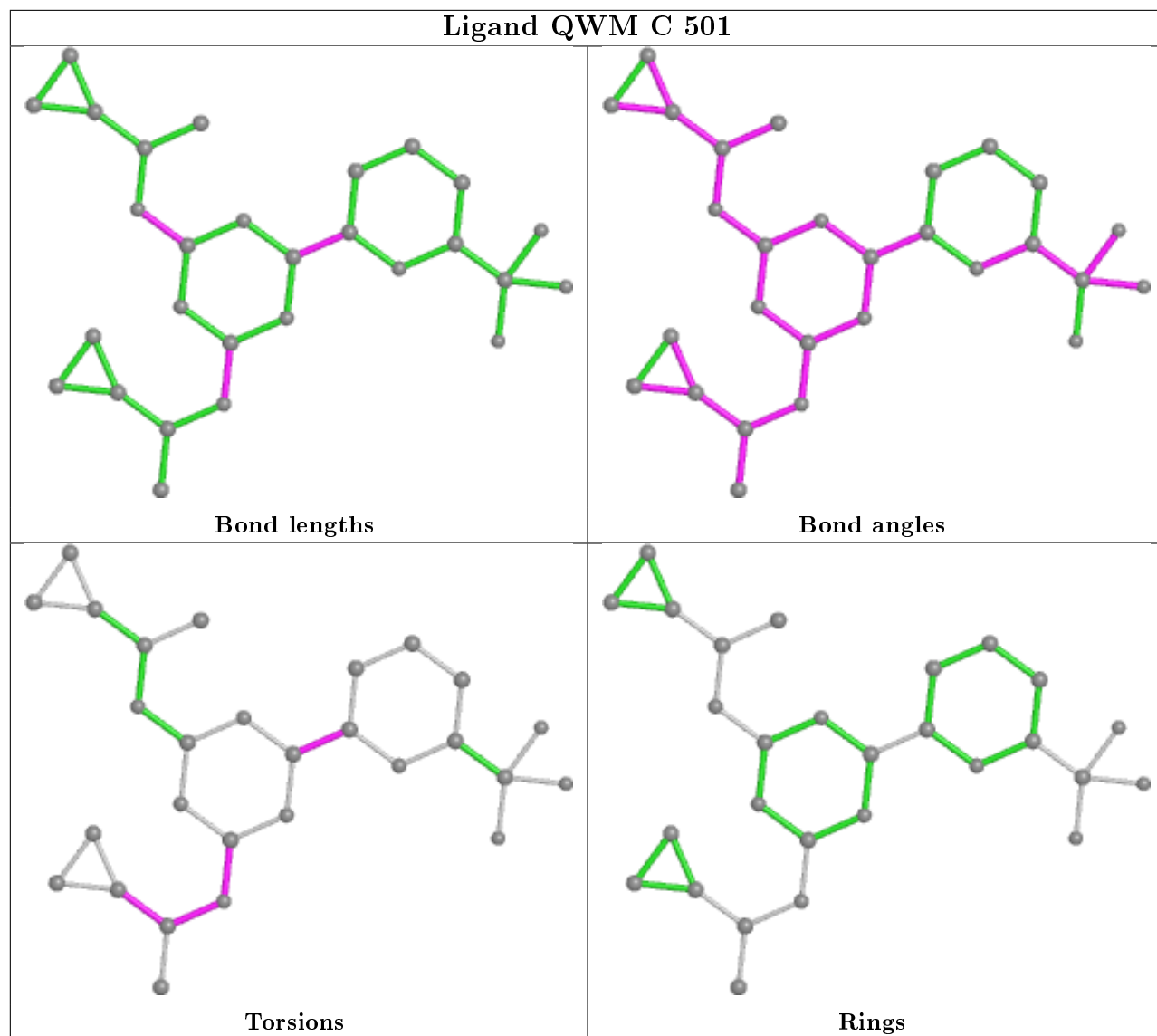


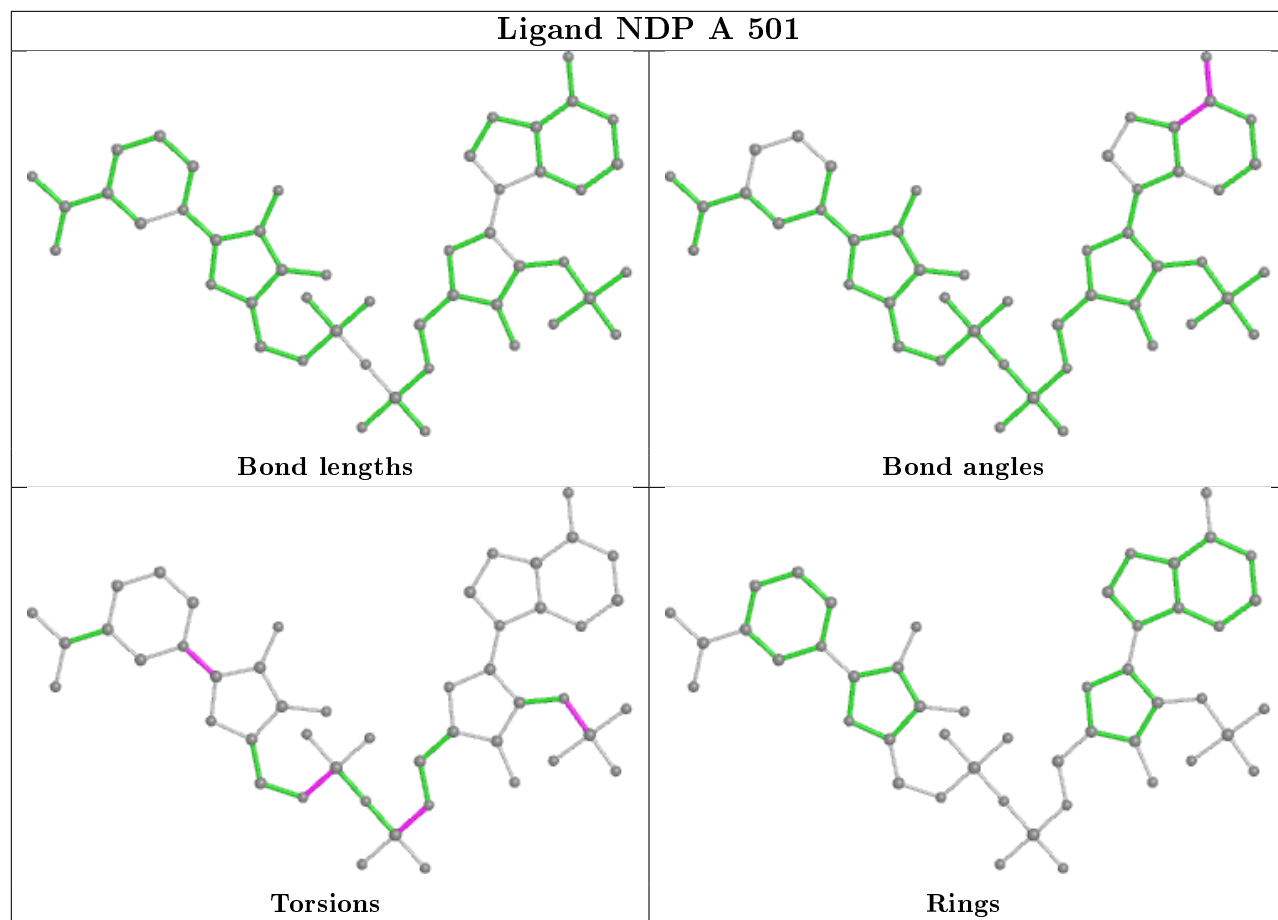
## Ligand QWM B 501 (A)

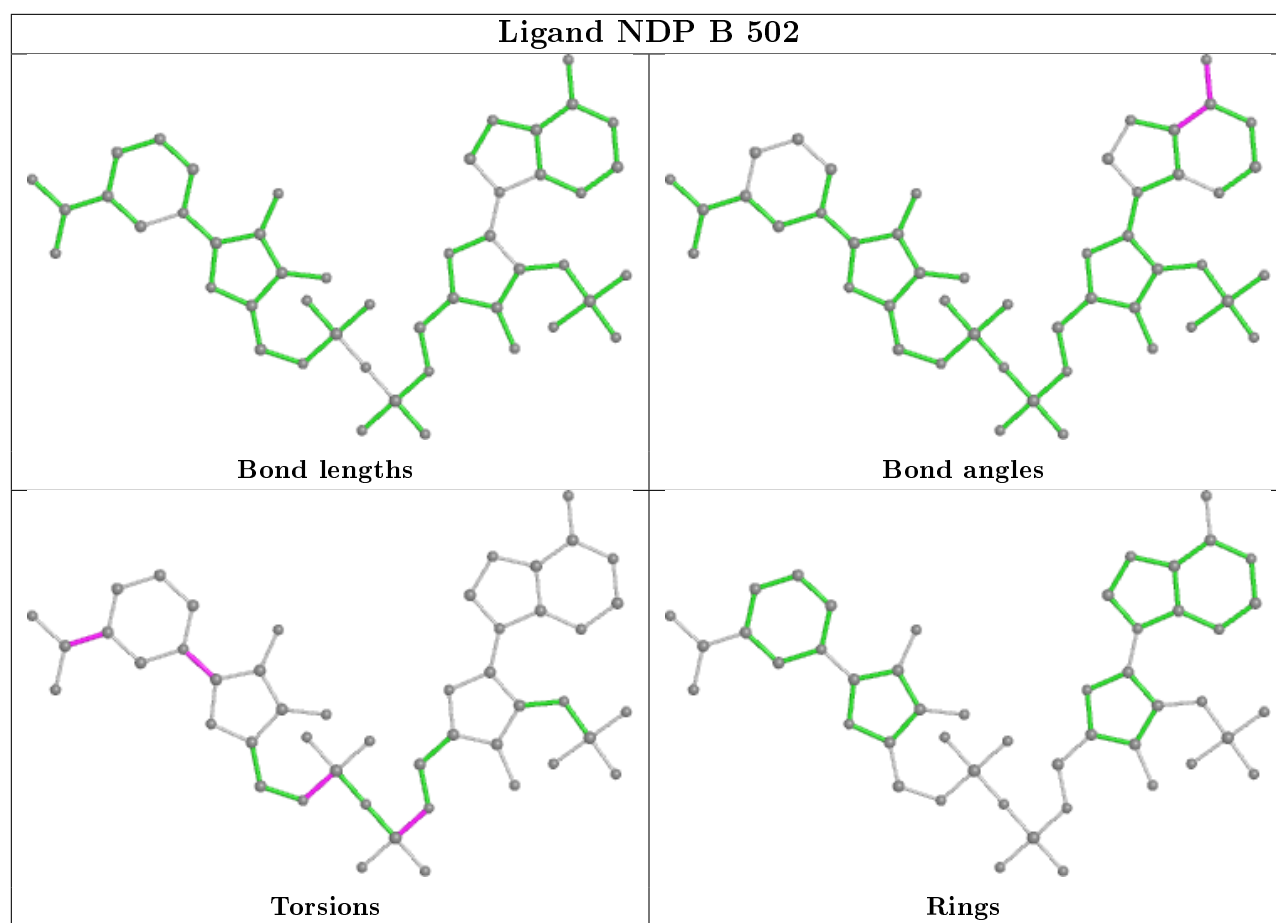




## Ligand QWM C 501







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	413/425 (97%)	-0.17	8 (1%) 66 63	22, 37, 67, 95	0
1	B	415/425 (97%)	-0.22	1 (0%) 95 96	21, 38, 63, 101	0
1	C	404/425 (95%)	1.12	102 (25%) 0 0	20, 76, 94, 111	163 (40%)
All	All	1232/1275 (96%)	0.23	111 (9%) 9 7	20, 40, 90, 111	163 (13%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	TRP	8.6
1	C	386	VAL	8.1
1	C	88	LEU	8.0
1	C	83	VAL	7.3
1	C	86	PHE	6.9
1	C	48	ASN	6.8
1	C	81	LYS	6.5
1	C	324	GLU	6.2
1	C	51	ALA	6.1
1	C	391	TYR	6.0
1	C	54	ASP	6.0
1	C	47	GLU	5.9
1	C	52	THR	5.8
1	C	49	ARG	5.7
1	A	413	LYS	5.3
1	C	84	GLU	5.3
1	C	317	ARG	5.3
1	C	390	ASP	5.2
1	C	318	MET	5.2
1	A	412	ALA	5.2
1	C	42	TYR	5.0
1	C	387	GLN	5.0
1	C	53	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	327	THR	4.9
1	C	89	LYS	4.8
1	C	85	GLU	4.6
1	C	90	GLN	4.5
1	C	316	TYR	4.4
1	A	414	LEU	4.3
1	C	313	THR	4.3
1	C	314	ARG	4.2
1	C	322	GLY	4.2
1	C	383	LEU	4.2
1	C	393	ASN	4.2
1	C	46	ILE	4.1
1	C	388	ARG	4.1
1	C	389	SER	4.1
1	C	25	LEU	4.0
1	C	374	LYS	4.0
1	C	323	GLN	4.0
1	C	392	LEU	3.9
1	C	312	VAL	3.9
1	C	14	GLN	3.9
1	C	410	ALA	3.8
1	C	5	ILE	3.8
1	C	91	MET	3.7
1	C	381	LYS	3.7
1	C	384	PRO	3.7
1	C	15	GLY	3.7
1	C	56	VAL	3.7
1	C	82	ARG	3.6
1	C	396	GLU	3.6
1	C	6	SER	3.5
1	C	350	LYS	3.5
1	C	403	GLU	3.4
1	C	321	LYS	3.4
1	C	59	ASP	3.4
1	C	325	THR	3.3
1	C	319	TYR	3.2
1	A	86	PHE	3.2
1	C	315	HIS	3.2
1	C	399	ASP	3.2
1	C	87	LYS	3.1
1	C	7	GLY	3.0
1	C	12	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	23	TRP	2.9
1	C	377	ALA	2.9
1	C	351	GLU	2.8
1	C	22	ILE	2.8
1	C	28	GLU	2.8
1	C	43	ASP	2.8
1	A	51	ALA	2.7
1	C	407	ILE	2.7
1	C	353	ALA	2.6
1	C	283	GLN	2.6
1	C	102	ILE	2.6
1	A	174	GLU	2.6
1	C	376	LEU	2.6
1	C	36	GLU	2.6
1	C	10	VAL	2.5
1	C	326	SER	2.5
1	C	37	LEU	2.5
1	C	32	PHE	2.5
1	C	379	CYS	2.4
1	C	95	PRO	2.4
1	C	382	GLY	2.4
1	C	100	ARG	2.4
1	A	88	LEU	2.4
1	C	44	LEU	2.4
1	C	395	PHE	2.4
1	C	385	ASN	2.3
1	B	86	PHE	2.3
1	C	21	ILE	2.3
1	C	372	MET	2.3
1	C	31	ILE	2.3
1	C	39	LEU	2.3
1	C	340	LEU	2.3
1	C	369	ALA	2.3
1	A	47	GLU	2.2
1	C	336	TRP	2.2
1	C	69	VAL	2.2
1	C	174	GLU	2.2
1	C	50	ASP	2.2
1	C	371	PHE	2.2
1	C	35	VAL	2.2
1	C	58	LYS	2.1
1	C	30	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	409	LEU	2.1
1	C	34	TYR	2.1
1	C	16	ASP	2.1
1	C	18	MET	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

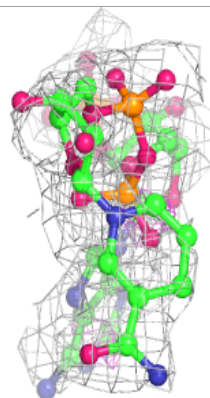
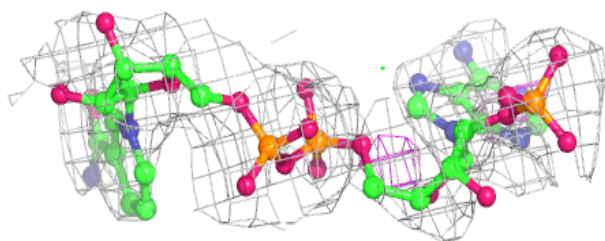
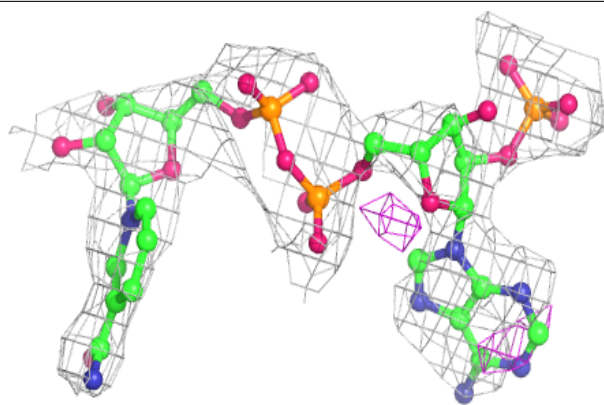
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	NDP	C	502	48/48	0.75	0.27	78,98,116,131	0
3	QWM	C	501	28/28	0.89	0.30	37,58,66,67	28
3	QWM	B	501[B]	28/28	0.95	0.25	25,37,42,44	28
3	QWM	B	501[A]	28/28	0.95	0.25	26,37,41,44	28
2	NDP	B	502	48/48	0.97	0.12	28,39,47,53	0
2	NDP	A	501	48/48	0.98	0.12	27,40,54,58	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.

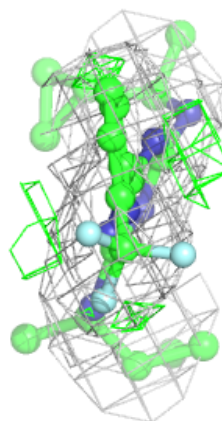
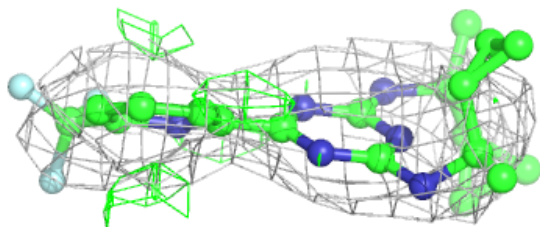
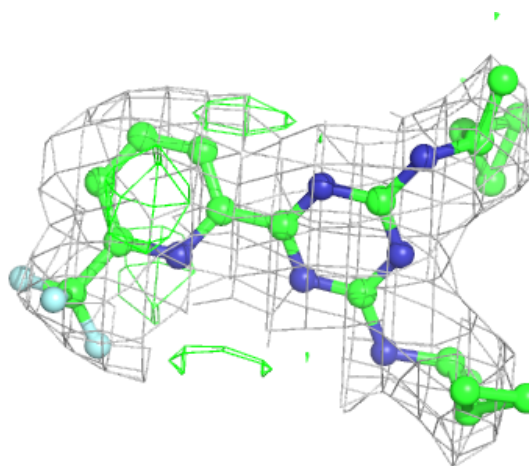
**Electron density around NDP C 502:**

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



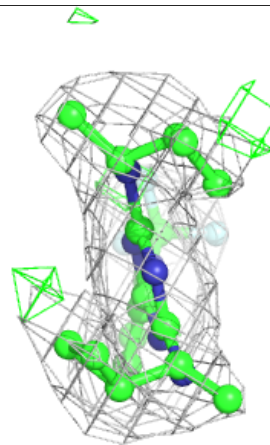
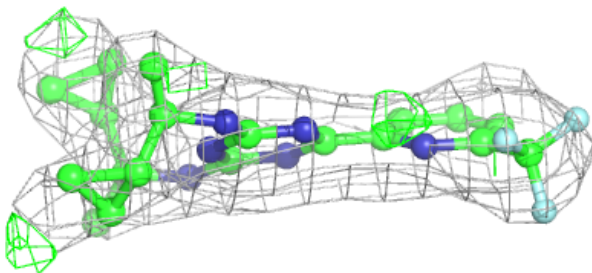
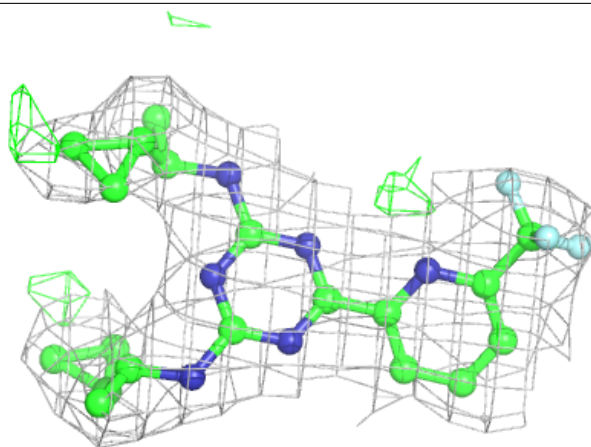
**Electron density around QWM C 501:**

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



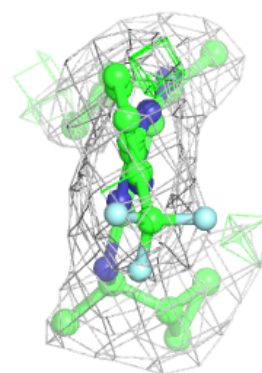
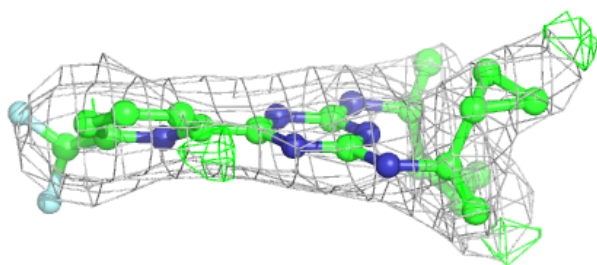
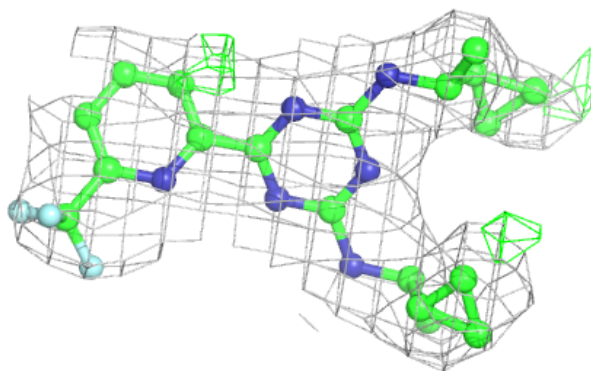
**Electron density around QWM B 501 (B):**

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

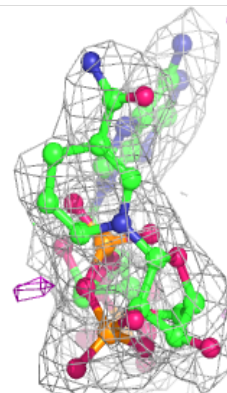
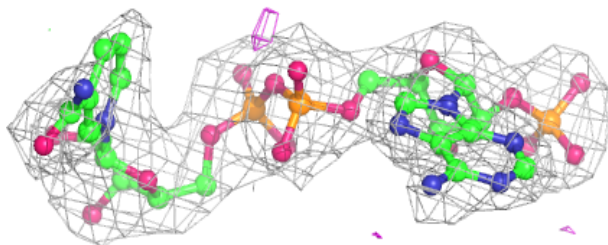
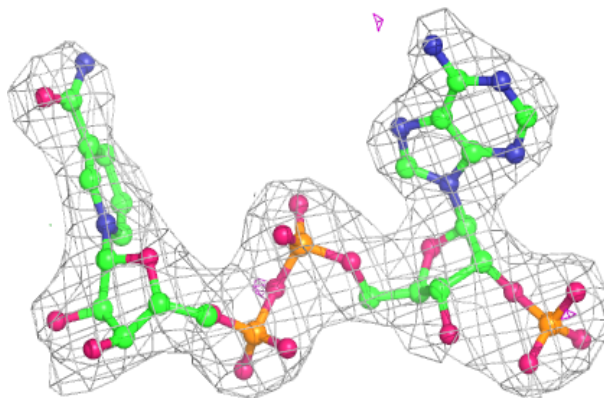


**Electron density around QWM B 501 (A):**

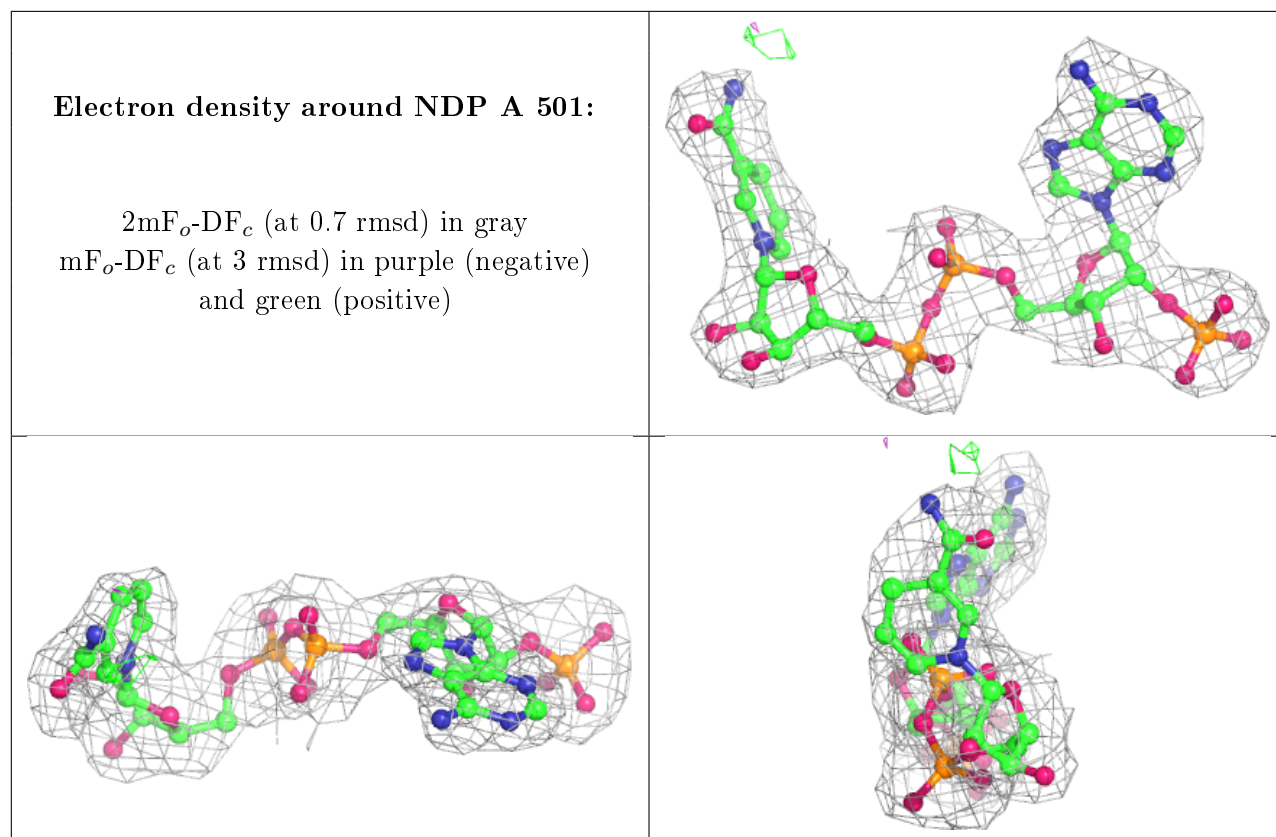
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NDP B 502:**

$2mF_o-DF_c$  (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.