



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2024 – 03:02 PM EST

PDB ID : 4M2X  
Title : Mycobacterium tuberculosis dihydrofolate reductase complexed with trimethoprim (TMQ)  
Authors : Jung, H.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2013-08-05  
Resolution : 2.26 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

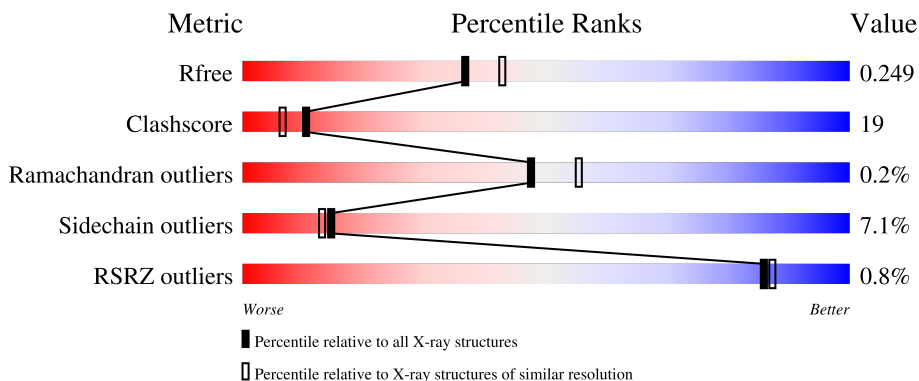
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\geq 3$ , 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	162	
1	C	162	
1	E	162	
1	G	162	

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

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
3	TMQ	A	202	-	-	X	-
3	TMQ	E	202	-	-	X	-
4	ACT	E	203	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 5467 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.

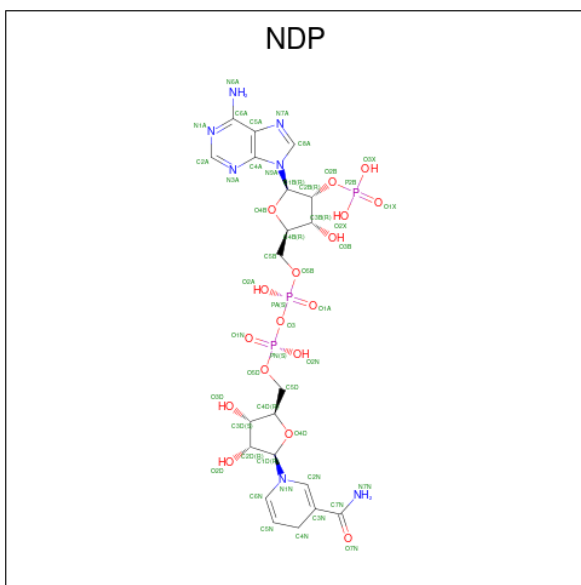
- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1244	783	228	228	5	0	0	0
1	C	159	1244	783	228	228	5	0	0	0
1	E	159	1244	783	228	228	5	0	0	0
1	G	159	1244	783	228	228	5	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

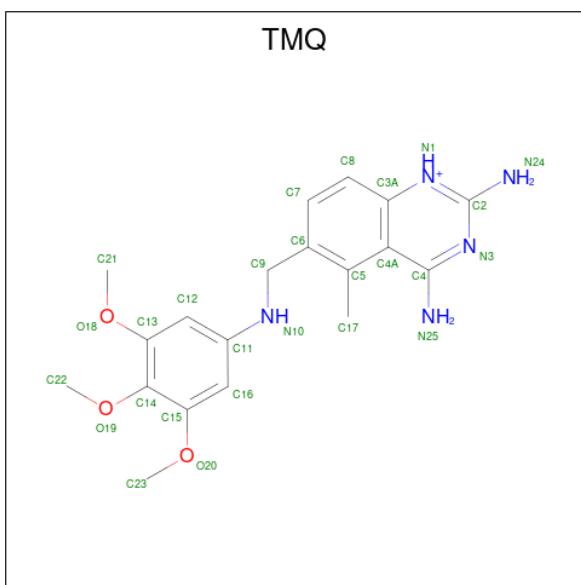
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P0A546
A	-1	SER	-	expression tag	UNP P0A546
A	0	HIS	-	expression tag	UNP P0A546
C	-2	GLY	-	expression tag	UNP P0A546
C	-1	SER	-	expression tag	UNP P0A546
C	0	HIS	-	expression tag	UNP P0A546
E	-2	GLY	-	expression tag	UNP P0A546
E	-1	SER	-	expression tag	UNP P0A546
E	0	HIS	-	expression tag	UNP P0A546
G	-2	GLY	-	expression tag	UNP P0A546
G	-1	SER	-	expression tag	UNP P0A546
G	0	HIS	-	expression tag	UNP P0A546

- 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>).



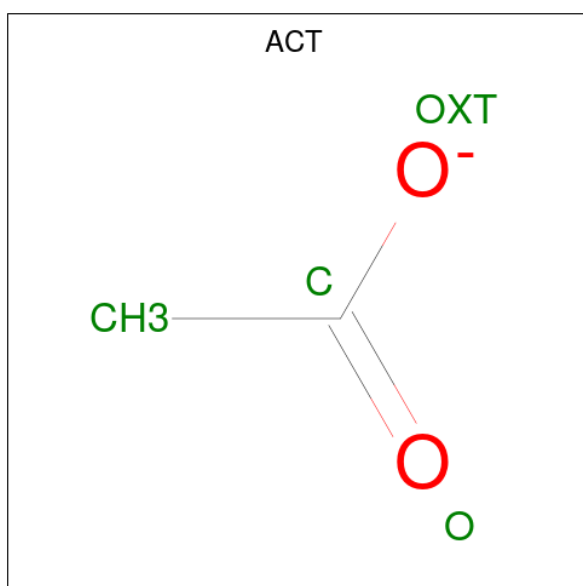
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
2	C	1	48	21	7	17	3	0	0
2	E	1	48	21	7	17	3	0	0
2	G	1	48	21	7	17	3	0	0

- Molecule 3 is TRIMETREXATE (three-letter code: TMQ) (formula:  $C_{19}H_{24}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	19	5	3		
3	C	1	Total	C	N	O	0	0
			27	19	5	3		
3	E	1	Total	C	N	O	0	0
			27	19	5	3		
3	G	1	Total	C	N	O	0	0
			27	19	5	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



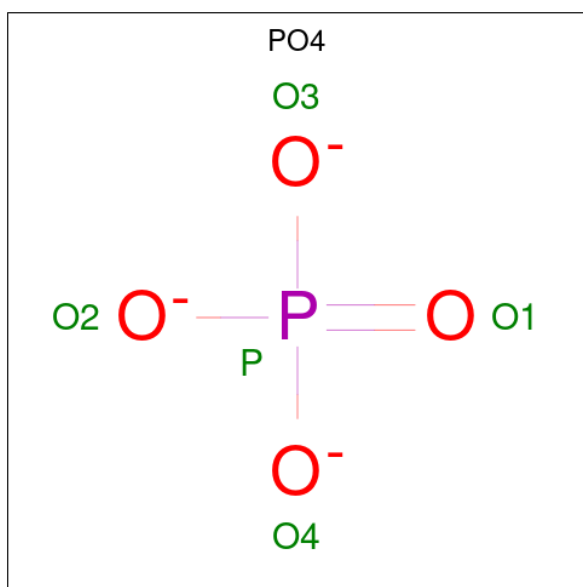
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	G	1	Total 4	C 2	O 2	0	0
4	G	1	Total 4	C 2	O 2	0	0
4	G	1	Total 4	C 2	O 2	0	0
4	G	1	Total 4	C 2	O 2	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 6 is water.

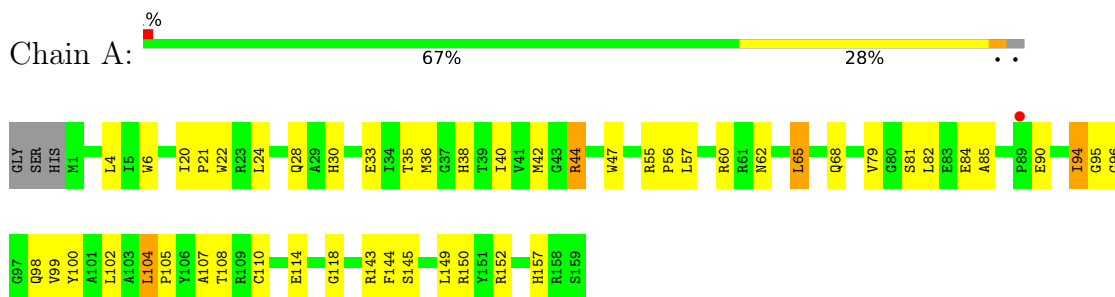
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	C	26	Total	O	0	0
			26	26		
6	E	29	Total	O	0	0
			29	29		
6	G	15	Total	O	0	0
			15	15		



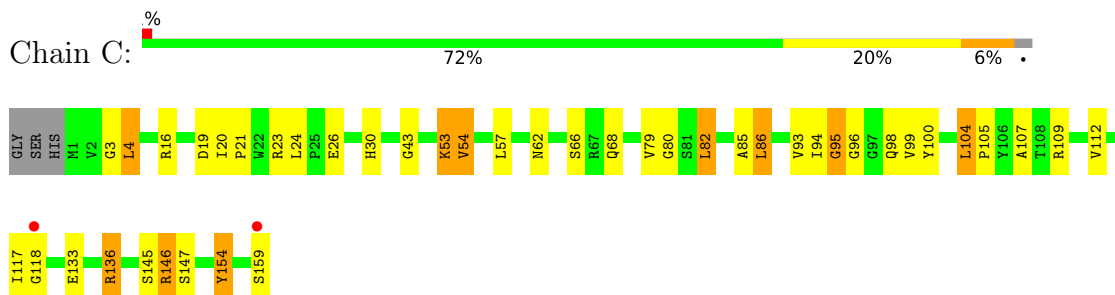
### 3 Residue-property plots [i](#)

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.

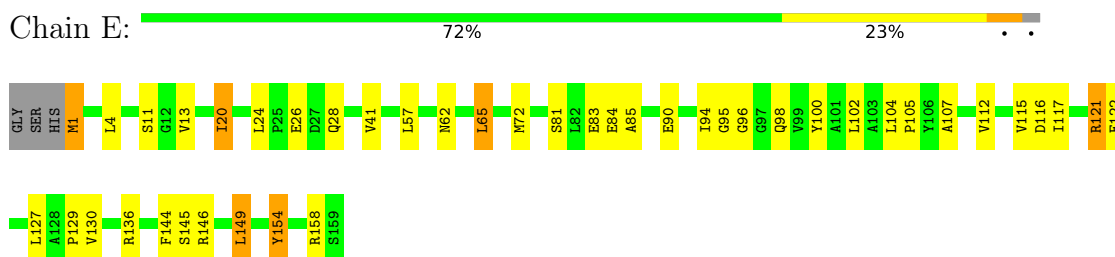
- Molecule 1: Dihydrofolate reductase



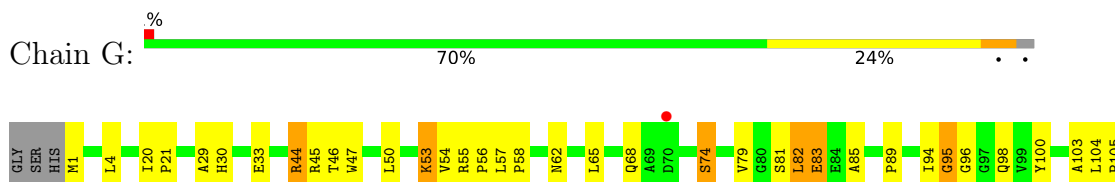
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.09Å 64.84Å 68.06Å 93.48° 94.10° 100.25°	Depositor
Resolution (Å)	30.86 – 2.26 67.70 – 2.26	Depositor EDS
% Data completeness (in resolution range)	95.6 (30.86-2.26) 95.6 (67.70-2.26)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.27Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.197 , 0.261 0.186 , 0.249	Depositor DCC
$R_{free}$ test set	1375 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtrriage
Anisotropy	0.006	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NDP, TMQ, ACT

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	0.49	0/1275	0.66	0/1732
1	C	0.50	0/1275	0.68	0/1732
1	E	0.49	0/1275	0.70	0/1732
1	G	0.51	0/1275	0.66	0/1732
All	All	0.50	0/5100	0.68	0/6928

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ILE	Peptide
1	C	95	GLY	Peptide
1	G	95	GLY	Peptide

## 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	1244	0	1223	42	0
1	C	1244	0	1223	40	0
1	E	1244	0	1223	39	0
1	G	1244	0	1223	47	0
2	A	48	0	26	8	0
2	C	48	0	26	9	0
2	E	48	0	26	7	0
2	G	48	0	26	17	0
3	A	27	0	24	9	0
3	C	27	0	24	8	0
3	E	27	0	24	11	0
3	G	27	0	24	7	0
4	A	24	0	18	2	0
4	C	24	0	18	2	0
4	E	24	0	18	6	0
4	G	16	0	12	1	0
5	A	5	0	0	0	0
6	A	28	0	0	2	0
6	C	26	0	0	2	0
6	E	29	0	0	1	0
6	G	15	0	0	2	0
All	All	5467	0	5158	196	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 19.

All (196) 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:E:100:TYR:HB3	1:E:129:PRO:HG3	1.33	1.10
1:E:121:ARG:HH11	1:E:121:ARG:HG2	1.30	0.97
1:A:57:LEU:H	1:A:62:ASN:HD21	1.05	0.94
1:A:44:ARG:HH12	1:A:68:GLN:HE21	1.21	0.87
1:A:44:ARG:HH12	1:A:68:GLN:NE2	1.76	0.83
1:C:95:GLY:HA2	1:C:100:TYR:CZ	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LEU:H	1:C:62:ASN:HD21	1.30	0.80
3:E:202:TMQ:C11	3:E:202:TMQ:H7	2.09	0.80
1:G:44:ARG:HH12	1:G:68:GLN:HE21	1.31	0.79
1:C:96:GLY:HA3	2:C:201:NDP:O1A	1.82	0.79
1:G:44:ARG:HH12	1:G:68:GLN:NE2	1.82	0.77
1:A:57:LEU:H	1:A:62:ASN:ND2	1.83	0.76
1:C:54:VAL:HG22	1:C:57:LEU:HD23	1.65	0.76
1:G:57:LEU:H	1:G:62:ASN:HD21	1.33	0.75
1:E:121:ARG:HH11	1:E:121:ARG:CG	1.99	0.74
1:A:98:GLN:NE2	2:A:201:NDP:H8A	2.03	0.73
1:A:57:LEU:N	1:A:62:ASN:HD21	1.84	0.73
1:E:100:TYR:CB	1:E:129:PRO:HG3	2.18	0.72
1:E:24:LEU:H	4:E:203:ACT:H2	1.56	0.71
1:E:95:GLY:HA2	1:E:100:TYR:CZ	2.26	0.71
1:E:57:LEU:H	1:E:62:ASN:HD21	1.38	0.71
1:E:65:LEU:HD22	2:E:201:NDP:N3A	2.06	0.70
1:E:20:ILE:HD13	2:E:201:NDP:H2N	1.72	0.70
1:E:115:VAL:HG12	1:E:117:ILE:HG12	1.75	0.69
1:E:158:ARG:HH12	4:E:204:ACT:H1	1.58	0.68
1:E:96:GLY:HA3	2:E:201:NDP:O1A	1.95	0.66
1:A:55:ARG:O	1:A:55:ARG:HG3	1.95	0.65
1:A:20:ILE:HG12	2:A:201:NDP:H2N	1.78	0.65
1:C:30:HIS:HE1	6:C:308:HOH:O	1.80	0.65
1:A:42:MET:HA	1:A:95:GLY:HA3	1.79	0.65
3:G:202:TMQ:HN52	3:G:202:TMQ:C17	2.11	0.63
1:A:44:ARG:HH22	1:A:68:GLN:HE22	1.47	0.63
1:C:80:GLY:O	2:C:201:NDP:H2A	1.98	0.63
1:G:98:GLN:NE2	2:G:201:NDP:H8A	2.14	0.63
3:E:202:TMQ:C17	3:E:202:TMQ:HN52	2.12	0.63
1:G:20:ILE:CG1	2:G:201:NDP:H2N	2.29	0.62
1:G:20:ILE:HD11	2:G:201:NDP:H2N	1.82	0.61
3:E:202:TMQ:C11	3:E:202:TMQ:C7	2.77	0.61
1:A:79:VAL:HG21	1:A:85:ALA:HB2	1.83	0.61
1:C:20:ILE:HG12	2:C:201:NDP:H2N	1.81	0.61
3:A:202:TMQ:C17	3:A:202:TMQ:HN52	2.14	0.60
3:A:202:TMQ:H8	4:A:203:ACT:H2	1.83	0.60
1:G:45:ARG:HG3	2:G:201:NDP:H51A	1.84	0.60
1:E:121:ARG:NH1	1:E:127:LEU:HD11	2.16	0.60
1:C:96:GLY:HA3	2:C:201:NDP:PA	2.42	0.59
1:E:24:LEU:H	4:E:203:ACT:CH3	2.15	0.59
1:A:30:HIS:HD2	6:A:313:HOH:O	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:SER:OG	1:E:13:VAL:HG23	2.03	0.58
1:E:94:ILE:O	3:E:202:TMQ:H172	2.02	0.58
1:C:95:GLY:HA2	1:C:100:TYR:CE1	2.38	0.58
1:E:96:GLY:HA3	2:E:201:NDP:PA	2.44	0.58
1:G:20:ILE:HG12	2:G:201:NDP:H2N	1.84	0.58
2:G:201:NDP:O1N	4:G:203:ACT:H3	2.04	0.57
1:G:20:ILE:HD11	2:G:201:NDP:C2N	2.34	0.57
3:G:202:TMQ:HN52	3:G:202:TMQ:H172	1.69	0.57
1:E:121:ARG:HG2	1:E:127:LEU:HD21	1.86	0.57
1:E:26:GLU:OE2	1:E:146:ARG:HG2	2.05	0.56
1:G:104:LEU:HB3	1:G:105:PRO:HD3	1.87	0.56
1:A:114:GLU:OE2	4:A:204:ACT:O	2.24	0.56
1:A:4:LEU:O	1:A:110:CYS:HA	2.06	0.56
3:A:202:TMQ:O20	3:A:202:TMQ:H222	2.06	0.56
3:C:202:TMQ:H7	3:C:202:TMQ:C11	2.36	0.56
1:G:20:ILE:CD1	2:G:201:NDP:H2N	2.37	0.55
1:G:44:ARG:HH22	1:G:68:GLN:HE22	1.54	0.55
1:A:94:ILE:O	3:A:202:TMQ:H172	2.07	0.55
1:C:3:GLY:HA2	1:C:109:ARG:O	2.07	0.55
2:C:201:NDP:H42N	3:C:202:TMQ:C5	2.36	0.55
1:E:24:LEU:N	4:E:203:ACT:H2	2.20	0.55
3:A:202:TMQ:C11	3:A:202:TMQ:H7	2.36	0.54
1:A:144:PHE:CE2	1:A:150:ARG:HD3	2.42	0.54
3:C:202:TMQ:HN52	3:C:202:TMQ:C17	2.21	0.54
1:G:1:MET:HG3	1:G:89:PRO:O	2.08	0.54
1:G:96:GLY:HA3	2:G:201:NDP:PA	2.46	0.54
1:C:145:SER:O	1:C:146:ARG:C	2.47	0.53
1:A:4:LEU:HD13	1:A:107:ALA:HB2	1.90	0.53
1:E:81:SER:OG	1:E:84:GLU:HG3	2.08	0.53
1:G:30:HIS:HE1	6:G:313:HOH:O	1.92	0.53
1:A:21:PRO:HD2	1:A:22:TRP:CZ3	2.44	0.53
1:G:81:SER:OG	1:G:83:GLU:HG3	2.09	0.53
1:A:40:ILE:HD12	1:A:57:LEU:HD12	1.89	0.53
1:C:57:LEU:HD21	3:C:202:TMQ:H212	1.91	0.53
1:G:96:GLY:HA3	2:G:201:NDP:O1A	2.08	0.53
3:E:202:TMQ:HN52	3:E:202:TMQ:H172	1.72	0.52
1:E:100:TYR:HB3	1:E:129:PRO:CG	2.23	0.52
1:C:96:GLY:HA2	2:C:201:NDP:O5D	2.10	0.52
1:E:24:LEU:O	4:E:203:ACT:H3	2.10	0.52
1:G:57:LEU:H	1:G:62:ASN:ND2	2.05	0.52
1:G:29:ALA:O	1:G:33:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:TRP:CE2	1:G:55:ARG:HD3	2.45	0.51
1:A:55:ARG:HA	1:A:56:PRO:C	2.30	0.51
1:E:4:LEU:HD13	1:E:107:ALA:HB2	1.92	0.51
1:C:26:GLU:OE1	1:C:145:SER:HB2	2.10	0.51
1:C:24:LEU:H	4:C:203:ACT:H2	1.76	0.51
3:A:202:TMQ:HN52	3:A:202:TMQ:H172	1.76	0.50
1:A:28:GLN:OE1	3:A:202:TMQ:H223	2.11	0.50
1:E:145:SER:HB3	1:E:149:LEU:O	2.12	0.50
1:G:95:GLY:CA	1:G:100:TYR:CZ	2.95	0.50
1:A:98:GLN:HE21	2:A:201:NDP:H8A	1.73	0.49
2:G:201:NDP:H42N	3:G:202:TMQ:C5	2.43	0.49
3:E:202:TMQ:C7	3:E:202:TMQ:C16	2.90	0.49
1:C:117:ILE:O	1:C:118:GLY:C	2.50	0.49
1:E:122:GLU:OE2	4:E:207:ACT:O	2.30	0.49
1:G:96:GLY:HA2	2:G:201:NDP:O5D	2.12	0.49
1:C:117:ILE:O	1:C:117:ILE:HG13	2.14	0.48
1:C:112:VAL:HB	1:C:154:TYR:HB2	1.94	0.48
1:C:4:LEU:HD12	1:C:93:VAL:HB	1.95	0.48
1:E:96:GLY:HA2	2:E:201:NDP:O5D	2.14	0.48
1:A:118:GLY:O	1:G:133:GLU:HB3	2.12	0.48
1:E:57:LEU:H	1:E:62:ASN:ND2	2.09	0.47
1:G:112:VAL:HB	1:G:154:TYR:HB2	1.95	0.47
1:C:53:LYS:H	1:C:53:LYS:HD3	1.79	0.47
2:A:201:NDP:O1X	2:A:201:NDP:O3B	2.29	0.47
1:C:98:GLN:HE22	2:C:201:NDP:H3B	1.78	0.47
3:A:202:TMQ:O20	3:A:202:TMQ:C22	2.63	0.47
1:G:95:GLY:HA2	1:G:100:TYR:CZ	2.49	0.47
1:E:28:GLN:NE2	3:E:202:TMQ:O20	2.47	0.47
3:E:202:TMQ:H12	6:E:325:HOH:O	2.15	0.46
1:E:121:ARG:CG	1:E:121:ARG:NH1	2.68	0.46
1:C:79:VAL:HG21	1:C:85:ALA:HB2	1.98	0.46
1:C:94:ILE:O	3:C:202:TMQ:H172	2.16	0.46
1:C:66:SER:O	1:C:80:GLY:HA2	2.15	0.46
1:E:57:LEU:HD21	3:E:202:TMQ:H232	1.97	0.46
1:A:94:ILE:O	1:A:94:ILE:HG13	2.13	0.46
1:C:4:LEU:HD13	1:C:107:ALA:HB2	1.97	0.46
1:G:1:MET:CG	1:G:89:PRO:O	2.63	0.46
1:A:6:TRP:HB3	1:A:100:TYR:CZ	2.51	0.46
1:G:96:GLY:HA3	2:G:201:NDP:O2A	2.16	0.46
1:A:47:TRP:CZ2	1:A:55:ARG:HD3	2.51	0.45
3:C:202:TMQ:HN52	3:C:202:TMQ:H172	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:TMQ:C11	3:C:202:TMQ:C7	2.95	0.45
1:A:104:LEU:HB3	1:A:105:PRO:HD3	1.98	0.45
1:G:46:THR:O	1:G:50:LEU:HG	2.17	0.45
1:G:4:LEU:CD1	1:G:107:ALA:HB2	2.47	0.44
1:C:145:SER:O	1:C:147:SER:N	2.50	0.44
1:G:20:ILE:HA	1:G:21:PRO:HD3	1.56	0.44
2:A:201:NDP:H6N	2:A:201:NDP:H2D	1.75	0.44
1:A:35:THR:O	1:A:60:ARG:HG2	2.17	0.44
1:E:1:MET:HE2	1:E:90:GLU:HG3	2.00	0.44
1:E:104:LEU:HB3	1:E:105:PRO:HD3	1.98	0.44
1:A:81:SER:OG	1:A:84:GLU:HG3	2.18	0.44
1:G:56:PRO:HD3	1:G:74:SER:O	2.17	0.44
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.84	0.43
1:C:20:ILE:CG1	2:C:201:NDP:H2N	2.46	0.43
3:G:202:TMQ:H7	3:G:202:TMQ:C11	2.48	0.43
1:C:54:VAL:O	1:C:54:VAL:HG13	2.19	0.43
1:C:104:LEU:HB3	1:C:105:PRO:HD3	1.99	0.43
1:E:112:VAL:HB	1:E:154:TYR:HB2	2.01	0.43
1:G:45:ARG:CG	2:G:201:NDP:H51A	2.48	0.43
1:G:47:TRP:CE2	1:G:55:ARG:CD	3.01	0.43
1:G:95:GLY:HA2	1:G:100:TYR:CE2	2.53	0.43
1:G:104:LEU:HD22	1:G:129:PRO:HB2	2.00	0.43
1:A:82:LEU:CD1	1:A:102:LEU:HB3	2.49	0.43
1:E:28:GLN:HE22	3:E:202:TMQ:C23	2.31	0.43
1:E:96:GLY:CA	2:E:201:NDP:PA	3.07	0.43
1:A:4:LEU:HD13	1:A:107:ALA:CB	2.49	0.43
1:G:65:LEU:HD22	2:G:201:NDP:C2A	2.49	0.43
1:A:30:HIS:HE1	6:A:320:HOH:O	2.01	0.43
1:C:20:ILE:HA	1:C:21:PRO:HD3	1.69	0.43
3:E:202:TMQ:H7	3:E:202:TMQ:C16	2.49	0.43
1:G:45:ARG:HB2	2:G:201:NDP:O3	2.18	0.42
1:G:53:LYS:HG2	1:G:54:VAL:HG23	2.00	0.42
1:G:30:HIS:CE1	6:G:313:HOH:O	2.71	0.42
1:C:82:LEU:HD22	1:C:86:LEU:HD13	2.01	0.42
1:G:82:LEU:HD11	1:G:103:ALA:HB2	2.01	0.42
1:G:54:VAL:HG12	1:G:54:VAL:O	2.19	0.42
1:A:44:ARG:NH1	1:A:68:GLN:NE2	2.57	0.42
1:A:108:THR:O	1:A:157:HIS:HA	2.20	0.42
1:E:116:ASP:O	1:E:117:ILE:HD13	2.19	0.42
1:C:43:GLY:CA	1:C:99:VAL:HG21	2.49	0.42
1:A:95:GLY:O	1:A:99:VAL:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ARG:HB3	1:C:21:PRO:HG3	2.02	0.42
1:A:102:LEU:O	1:A:105:PRO:HD2	2.19	0.42
1:C:68:GLN:OE1	4:C:208:ACT:H1	2.20	0.41
1:C:19:ASP:OD1	1:C:20:ILE:N	2.49	0.41
1:C:20:ILE:HD11	2:C:201:NDP:C2N	2.50	0.41
1:G:115:VAL:CG1	1:G:149:LEU:HD13	2.49	0.41
1:E:98:GLN:HB2	2:E:201:NDP:O1A	2.19	0.41
3:G:202:TMQ:C17	3:G:202:TMQ:N25	2.81	0.41
3:C:202:TMQ:H211	6:C:305:HOH:O	2.19	0.41
1:A:38:HIS:CE1	1:A:90:GLU:CD	2.94	0.41
1:C:145:SER:C	1:C:147:SER:N	2.74	0.41
1:A:65:LEU:HD13	2:A:201:NDP:C4A	2.50	0.41
1:A:96:GLY:HA3	2:A:201:NDP:PA	2.60	0.41
1:C:154:TYR:N	1:C:154:TYR:CD1	2.89	0.41
1:E:41:VAL:HG21	1:E:85:ALA:HB1	2.03	0.41
1:G:57:LEU:N	1:G:62:ASN:HD21	2.11	0.41
1:G:94:ILE:O	3:G:202:TMQ:H172	2.21	0.41
1:G:54:VAL:HG12	1:G:57:LEU:HD23	2.02	0.41
1:A:24:LEU:HD11	1:A:145:SER:HB2	2.03	0.40
1:G:57:LEU:HA	1:G:58:PRO:HD3	1.77	0.40
1:A:143:ARG:O	1:A:150:ARG:HA	2.21	0.40
1:C:57:LEU:H	1:C:62:ASN:ND2	2.08	0.40
1:C:136:ARG:HE	1:C:136:ARG:HB2	1.73	0.40
2:G:201:NDP:H42N	3:G:202:TMQ:H172	2.02	0.40
1:G:79:VAL:HG21	1:G:85:ALA:HB2	2.03	0.40
2:A:201:NDP:H42N	3:A:202:TMQ:C5	2.51	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	157/162 (97%)	154 (98%)	3 (2%)	0	100	100
1	C	157/162 (97%)	152 (97%)	4 (2%)	1 (1%)	25	25
1	E	157/162 (97%)	153 (98%)	4 (2%)	0	100	100
1	G	157/162 (97%)	154 (98%)	3 (2%)	0	100	100
All	All	628/648 (97%)	613 (98%)	14 (2%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	146	ARG

### 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	127/129 (98%)	121 (95%)	6 (5%)	26	29
1	C	127/129 (98%)	116 (91%)	11 (9%)	10	8
1	E	127/129 (98%)	115 (91%)	12 (9%)	8	6
1	G	127/129 (98%)	120 (94%)	7 (6%)	21	21
All	All	508/516 (98%)	472 (93%)	36 (7%)	14	13

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	36	MET
1	A	44	ARG
1	A	65	LEU
1	A	104	LEU
1	A	152	ARG
1	C	4	LEU
1	C	23	ARG
1	C	53	LYS
1	C	54	VAL

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Mol	Chain	Res	Type
1	C	82	LEU
1	C	86	LEU
1	C	104	LEU
1	C	133	GLU
1	C	136	ARG
1	C	154	TYR
1	C	159	SER
1	E	1	MET
1	E	20	ILE
1	E	65	LEU
1	E	72	MET
1	E	83	GLU
1	E	102	LEU
1	E	121	ARG
1	E	130	VAL
1	E	136	ARG
1	E	144	PHE
1	E	149	LEU
1	E	154	TYR
1	G	44	ARG
1	G	53	LYS
1	G	74	SER
1	G	82	LEU
1	G	83	GLU
1	G	136	ARG
1	G	144	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	38	HIS
1	A	62	ASN
1	A	68	GLN
1	C	30	HIS
1	C	62	ASN
1	E	28	GLN
1	E	30	HIS
1	E	62	ASN
1	E	98	GLN
1	G	30	HIS
1	G	62	ASN

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Mol	Chain	Res	Type
1	G	68	GLN
1	G	98	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

31 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$
4	ACT	G	203	-	3,3,3	1.56	1 (33%)	3,3,3	1.20	0
4	ACT	E	204	-	3,3,3	2.76	2 (66%)	3,3,3	1.04	0
2	NDP	A	201	-	45,52,52	3.76	20 (44%)	53,80,80	2.11	8 (15%)
4	ACT	A	207	-	3,3,3	1.29	0	3,3,3	0.66	0
4	ACT	A	204	-	3,3,3	2.66	2 (66%)	3,3,3	1.25	0
4	ACT	C	205	-	3,3,3	2.84	2 (66%)	3,3,3	1.00	0
3	TMQ	E	202	-	29,29,29	5.55	19 (65%)	39,41,41	1.99	11 (28%)
4	ACT	A	203	-	3,3,3	2.86	2 (66%)	3,3,3	0.94	0
4	ACT	E	205	-	3,3,3	2.97	2 (66%)	3,3,3	0.58	0
4	ACT	G	206	-	3,3,3	2.78	1 (33%)	3,3,3	1.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACT	G	204	-	3,3,3	2.56	1 (33%)	3,3,3	1.53	0
4	ACT	A	206	-	3,3,3	2.86	2 (66%)	3,3,3	0.92	0
4	ACT	C	208	-	3,3,3	2.99	2 (66%)	3,3,3	0.65	0
4	ACT	E	207	-	3,3,3	2.77	2 (66%)	3,3,3	1.29	0
4	ACT	E	208	-	3,3,3	1.54	1 (33%)	3,3,3	1.22	0
3	TMQ	A	202	-	29,29,29	5.51	19 (65%)	39,41,41	2.05	7 (17%)
2	NDP	G	201	-	45,52,52	3.87	19 (42%)	53,80,80	1.89	11 (20%)
4	ACT	G	205	-	3,3,3	2.70	2 (66%)	3,3,3	0.97	0
4	ACT	C	207	-	3,3,3	1.49	1 (33%)	3,3,3	1.31	0
4	ACT	C	204	-	3,3,3	2.88	2 (66%)	3,3,3	0.91	0
4	ACT	E	203	-	3,3,3	1.45	1 (33%)	3,3,3	0.43	0
4	ACT	A	208	-	3,3,3	1.57	1 (33%)	3,3,3	0.93	0
4	ACT	C	203	-	3,3,3	1.65	1 (33%)	3,3,3	1.30	0
4	ACT	E	206	-	3,3,3	1.28	0	3,3,3	0.38	0
4	ACT	C	206	-	3,3,3	1.51	1 (33%)	3,3,3	0.40	0
3	TMQ	C	202	-	29,29,29	5.54	19 (65%)	39,41,41	2.10	10 (25%)
3	TMQ	G	202	-	29,29,29	5.54	20 (68%)	39,41,41	2.01	9 (23%)
4	ACT	A	205	-	3,3,3	2.57	1 (33%)	3,3,3	1.60	0
2	NDP	C	201	-	45,52,52	3.87	21 (46%)	53,80,80	1.78	10 (18%)
2	NDP	E	201	-	45,52,52	3.85	20 (44%)	53,80,80	1.94	7 (13%)
5	PO4	A	209	-	4,4,4	0.82	0	6,6,6	0.90	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
3	TMQ	C	202	-	-	2/11/11/11	0/3/3/3
3	TMQ	G	202	-	-	2/11/11/11	0/3/3/3
2	NDP	A	201	-	-	6/30/77/77	0/5/5/5
3	TMQ	A	202	-	-	2/11/11/11	0/3/3/3
2	NDP	G	201	-	-	4/30/77/77	0/5/5/5
2	NDP	C	201	-	-	5/30/77/77	0/5/5/5
3	TMQ	E	202	-	-	1/11/11/11	0/3/3/3
2	NDP	E	201	-	-	2/30/77/77	0/5/5/5

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	201	NDP	C2A-N3A	11.51	1.50	1.32
2	C	201	NDP	C6N-C5N	11.47	1.53	1.33
2	E	201	NDP	C2A-N3A	11.14	1.50	1.32
2	A	201	NDP	C2A-N3A	11.13	1.50	1.32
2	E	201	NDP	C6N-C5N	11.03	1.53	1.33
2	G	201	NDP	C6N-C5N	10.89	1.52	1.33
2	C	201	NDP	C2A-N3A	10.88	1.49	1.32
2	A	201	NDP	C6N-C5N	10.67	1.52	1.33
2	E	201	NDP	C2A-N1A	9.99	1.52	1.33
2	C	201	NDP	C2A-N1A	9.93	1.52	1.33
2	A	201	NDP	C2A-N1A	9.68	1.51	1.33
2	G	201	NDP	C2A-N1A	9.64	1.51	1.33
3	G	202	TMQ	C2-N3	9.62	1.52	1.35
3	C	202	TMQ	C2-N3	9.59	1.52	1.35
3	E	202	TMQ	C16-C11	9.52	1.55	1.39
3	A	202	TMQ	C2-N3	9.36	1.52	1.35
3	E	202	TMQ	C2-N3	9.34	1.52	1.35
3	E	202	TMQ	C12-C11	9.23	1.54	1.39
3	G	202	TMQ	C16-C11	9.13	1.54	1.39
3	C	202	TMQ	C16-C11	9.08	1.54	1.39
3	C	202	TMQ	C12-C11	8.95	1.54	1.39
3	A	202	TMQ	C16-C11	8.88	1.54	1.39
3	A	202	TMQ	C12-C11	8.82	1.53	1.39
3	G	202	TMQ	C8-C3A	8.82	1.57	1.41
3	C	202	TMQ	C12-C13	8.80	1.54	1.38
3	G	202	TMQ	C12-C11	8.74	1.53	1.39
3	G	202	TMQ	C8-C7	8.71	1.55	1.36
3	A	202	TMQ	C8-C3A	8.71	1.57	1.41
3	C	202	TMQ	C8-C7	8.67	1.54	1.36
3	A	202	TMQ	C8-C7	8.66	1.54	1.36
3	E	202	TMQ	C8-C7	8.56	1.54	1.36
3	E	202	TMQ	C8-C3A	8.52	1.56	1.41
3	E	202	TMQ	C12-C13	8.38	1.54	1.38
3	G	202	TMQ	C7-C6	8.34	1.53	1.39
3	G	202	TMQ	C16-C15	8.33	1.54	1.38
3	G	202	TMQ	C12-C13	8.32	1.54	1.38
3	E	202	TMQ	C16-C15	8.32	1.54	1.38
3	C	202	TMQ	C16-C15	8.23	1.53	1.38
3	C	202	TMQ	C8-C3A	8.18	1.56	1.41
2	G	201	NDP	C4A-N3A	8.16	1.46	1.35
3	A	202	TMQ	C12-C13	8.13	1.53	1.38
3	A	202	TMQ	C7-C6	8.11	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	TMQ	C16-C15	8.07	1.53	1.38
3	E	202	TMQ	C7-C6	7.88	1.52	1.39
2	C	201	NDP	C4A-N3A	7.86	1.46	1.35
3	C	202	TMQ	C7-C6	7.76	1.52	1.39
2	A	201	NDP	C4A-N3A	7.45	1.45	1.35
2	E	201	NDP	C4A-N3A	7.36	1.45	1.35
3	E	202	TMQ	C13-C14	6.98	1.55	1.41
3	A	202	TMQ	C13-C14	6.84	1.55	1.41
3	G	202	TMQ	C15-C14	6.72	1.55	1.41
3	C	202	TMQ	C13-C14	6.68	1.55	1.41
3	G	202	TMQ	C13-C14	6.46	1.54	1.41
2	C	201	NDP	C2N-C3N	6.41	1.52	1.34
2	E	201	NDP	C2N-C3N	6.37	1.52	1.34
3	E	202	TMQ	C15-C14	6.27	1.54	1.41
3	C	202	TMQ	C3A-N1	6.26	1.47	1.37
3	C	202	TMQ	C15-C14	6.25	1.54	1.41
2	G	201	NDP	C2N-C3N	6.12	1.52	1.34
3	A	202	TMQ	C4-N3	6.05	1.44	1.33
3	C	202	TMQ	C2-N24	6.05	1.46	1.33
3	A	202	TMQ	C15-C14	6.04	1.53	1.41
3	A	202	TMQ	C3A-N1	5.95	1.47	1.37
2	G	201	NDP	C8A-N7A	5.92	1.45	1.34
3	E	202	TMQ	C5-C4A	5.90	1.59	1.44
3	A	202	TMQ	C2-N24	5.80	1.45	1.33
3	C	202	TMQ	C4-N3	5.74	1.44	1.33
3	E	202	TMQ	C4-N3	5.72	1.44	1.33
2	A	201	NDP	C2N-C3N	5.71	1.50	1.34
3	G	202	TMQ	C4-N3	5.67	1.44	1.33
3	E	202	TMQ	C3A-N1	5.67	1.46	1.37
3	C	202	TMQ	C5-C4A	5.58	1.58	1.44
3	G	202	TMQ	C5-C4A	5.58	1.58	1.44
2	E	201	NDP	C8A-N7A	5.57	1.44	1.34
2	A	201	NDP	C8A-N7A	5.54	1.44	1.34
2	E	201	NDP	C7N-N7N	5.52	1.48	1.33
3	A	202	TMQ	C5-C4A	5.41	1.57	1.44
3	G	202	TMQ	C3A-N1	5.30	1.46	1.37
2	C	201	NDP	C8A-N7A	5.26	1.44	1.34
3	G	202	TMQ	C2-N24	5.18	1.44	1.33
3	E	202	TMQ	C2-N24	5.14	1.44	1.33
2	G	201	NDP	C7N-N7N	4.88	1.46	1.33
2	A	201	NDP	C7N-N7N	4.77	1.46	1.33
2	C	201	NDP	C7N-N7N	4.75	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	NDP	P2B-O1X	4.75	1.65	1.50
2	G	201	NDP	P2B-O1X	4.71	1.65	1.50
3	A	202	TMQ	C4A-C3A	4.65	1.50	1.42
4	E	205	ACT	O-C	4.50	1.42	1.22
4	C	208	ACT	O-C	4.47	1.42	1.22
3	E	202	TMQ	C4A-C3A	4.42	1.50	1.42
2	C	201	NDP	P2B-O1X	4.37	1.64	1.50
4	C	204	ACT	O-C	4.33	1.42	1.22
2	E	201	NDP	PN-O1N	4.32	1.66	1.50
4	A	206	ACT	O-C	4.32	1.42	1.22
2	C	201	NDP	O4B-C1B	4.28	1.47	1.41
4	G	206	ACT	O-C	4.26	1.41	1.22
3	C	202	TMQ	C4A-C3A	4.25	1.49	1.42
3	G	202	TMQ	C4A-C3A	4.25	1.49	1.42
2	A	201	NDP	P2B-O1X	4.20	1.64	1.50
2	G	201	NDP	PA-O1A	4.19	1.65	1.50
4	A	203	ACT	O-C	4.13	1.41	1.22
4	C	205	ACT	O-C	4.12	1.41	1.22
2	A	201	NDP	PN-O1N	4.02	1.65	1.50
4	E	204	ACT	O-C	3.98	1.40	1.22
4	G	205	ACT	O-C	3.92	1.40	1.22
2	E	201	NDP	PA-O1A	3.92	1.64	1.50
2	E	201	NDP	C5A-C4A	3.90	1.51	1.40
4	E	207	ACT	O-C	3.89	1.40	1.22
2	C	201	NDP	C5A-C4A	3.88	1.51	1.40
2	G	201	NDP	PN-O1N	3.87	1.64	1.50
4	G	204	ACT	O-C	3.83	1.39	1.22
2	C	201	NDP	PA-O1A	3.81	1.64	1.50
4	A	204	ACT	O-C	3.79	1.39	1.22
4	A	205	ACT	O-C	3.79	1.39	1.22
2	G	201	NDP	C5A-C4A	3.72	1.50	1.40
2	A	201	NDP	PA-O1A	3.61	1.63	1.50
2	A	201	NDP	C5A-C4A	3.54	1.50	1.40
2	E	201	NDP	C6N-N1N	3.53	1.46	1.37
3	C	202	TMQ	C2-N1	3.51	1.51	1.34
3	G	202	TMQ	C2-N1	3.46	1.50	1.34
2	C	201	NDP	PN-O1N	3.45	1.63	1.50
2	A	201	NDP	C6N-N1N	3.45	1.45	1.37
2	G	201	NDP	C6N-N1N	3.43	1.45	1.37
3	A	202	TMQ	C6-C5	3.42	1.54	1.40
3	E	202	TMQ	C2-N1	3.41	1.50	1.34
2	C	201	NDP	C6N-N1N	3.32	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	202	TMQ	C6-C5	3.31	1.53	1.40
3	A	202	TMQ	C2-N1	3.30	1.50	1.34
2	G	201	NDP	O4B-C1B	3.29	1.45	1.41
2	E	201	NDP	C6A-N6A	3.21	1.45	1.34
2	C	201	NDP	C6A-N6A	3.11	1.45	1.34
2	A	201	NDP	P2B-O2B	3.09	1.65	1.59
3	E	202	TMQ	C6-C5	3.09	1.53	1.40
2	A	201	NDP	C6A-N6A	3.05	1.45	1.34
2	G	201	NDP	C6A-N6A	2.97	1.44	1.34
2	A	201	NDP	O4B-C1B	2.97	1.45	1.41
3	E	202	TMQ	O20-C15	2.97	1.41	1.37
3	C	202	TMQ	C6-C5	2.96	1.52	1.40
3	G	202	TMQ	O20-C15	2.93	1.41	1.37
3	E	202	TMQ	C4-N25	2.85	1.44	1.34
2	C	201	NDP	P2B-O2B	2.85	1.64	1.59
3	A	202	TMQ	C4-N25	2.79	1.44	1.34
2	A	201	NDP	P2B-O2X	2.73	1.65	1.54
3	C	202	TMQ	C4-N25	2.73	1.44	1.34
2	A	201	NDP	O7N-C7N	-2.73	1.18	1.24
3	G	202	TMQ	C4-N25	2.69	1.43	1.34
2	C	201	NDP	C7N-C3N	2.68	1.54	1.48
2	E	201	NDP	P2B-O2X	2.65	1.65	1.54
2	G	201	NDP	P2B-O2X	2.61	1.64	1.54
4	C	203	ACT	OXT-C	2.56	1.43	1.30
2	G	201	NDP	P2B-O2B	2.56	1.64	1.59
2	C	201	NDP	O7N-C7N	-2.53	1.18	1.24
2	C	201	NDP	P2B-O3X	-2.53	1.45	1.54
2	E	201	NDP	P2B-O2B	2.46	1.64	1.59
4	E	207	ACT	OXT-C	-2.45	1.19	1.30
4	A	203	ACT	OXT-C	-2.42	1.19	1.30
2	G	201	NDP	C7N-C3N	2.40	1.53	1.48
4	E	204	ACT	OXT-C	-2.36	1.19	1.30
2	C	201	NDP	P2B-O2X	2.35	1.63	1.54
4	G	205	ACT	OXT-C	-2.34	1.19	1.30
4	A	208	ACT	OXT-C	2.33	1.42	1.30
4	A	204	ACT	OXT-C	-2.31	1.19	1.30
4	C	205	ACT	OXT-C	-2.26	1.19	1.30
4	G	203	ACT	OXT-C	2.24	1.41	1.30
4	C	206	ACT	OXT-C	2.24	1.41	1.30
2	A	201	NDP	P2B-O3X	-2.24	1.46	1.54
3	C	202	TMQ	O18-C13	2.23	1.40	1.37
2	E	201	NDP	P2B-O3X	-2.23	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	208	ACT	OXT-C	-2.22	1.20	1.30
4	E	208	ACT	OXT-C	2.19	1.41	1.30
4	E	205	ACT	OXT-C	-2.18	1.20	1.30
2	E	201	NDP	O4B-C1B	2.15	1.44	1.41
4	E	203	ACT	OXT-C	2.14	1.41	1.30
2	E	201	NDP	O7N-C7N	-2.14	1.19	1.24
2	G	201	NDP	O7N-C7N	-2.12	1.19	1.24
4	A	206	ACT	OXT-C	-2.12	1.20	1.30
2	E	201	NDP	C7N-C3N	2.10	1.53	1.48
2	A	201	NDP	C5A-N7A	2.09	1.47	1.39
4	C	204	ACT	OXT-C	-2.08	1.20	1.30
2	C	201	NDP	C6A-N1A	2.06	1.46	1.37
3	A	202	TMQ	O18-C13	2.06	1.40	1.37
3	G	202	TMQ	O18-C13	2.04	1.40	1.37
4	C	207	ACT	OXT-C	2.04	1.40	1.30
2	G	201	NDP	PA-O2A	-2.03	1.45	1.55
2	E	201	NDP	C6A-N1A	2.01	1.46	1.37
2	C	201	NDP	C5A-N7A	2.01	1.47	1.39
2	A	201	NDP	C7N-C3N	2.01	1.53	1.48

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	NDP	C3N-C2N-N1N	-9.96	108.88	123.10
3	G	202	TMQ	C4-C4A-C3A	7.35	119.86	114.86
2	E	201	NDP	C3N-C2N-N1N	-7.30	112.68	123.10
3	A	202	TMQ	C4-C4A-C3A	6.71	119.43	114.86
3	C	202	TMQ	C4-C4A-C3A	6.22	119.09	114.86
3	C	202	TMQ	N1-C2-N3	-6.20	118.95	127.22
3	E	202	TMQ	C4-C4A-C3A	6.19	119.08	114.86
2	G	201	NDP	C3N-C2N-N1N	-6.13	114.34	123.10
2	E	201	NDP	C1D-N1N-C6N	-5.62	108.72	120.83
2	C	201	NDP	N3A-C2A-N1A	-5.61	119.90	128.68
2	G	201	NDP	C1D-N1N-C6N	-5.57	108.83	120.83
2	C	201	NDP	C1D-N1N-C6N	-5.56	108.84	120.83
2	E	201	NDP	N3A-C2A-N1A	-5.45	120.16	128.68
3	A	202	TMQ	N1-C2-N3	-5.33	120.11	127.22
3	E	202	TMQ	N1-C2-N3	-5.27	120.20	127.22
2	A	201	NDP	N3A-C2A-N1A	-5.23	120.50	128.68
2	C	201	NDP	C3N-C2N-N1N	-5.22	115.65	123.10
2	G	201	NDP	N3A-C2A-N1A	-5.16	120.61	128.68
2	A	201	NDP	C1D-N1N-C6N	-5.12	109.81	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	202	TMQ	N1-C2-N3	-5.00	120.55	127.22
2	E	201	NDP	C1D-N1N-C2N	4.73	128.99	121.11
2	G	201	NDP	C1D-N1N-C2N	4.73	128.98	121.11
2	A	201	NDP	C1D-N1N-C2N	4.12	127.97	121.11
3	A	202	TMQ	O18-C13-C14	4.07	122.31	115.16
3	A	202	TMQ	O18-C13-C12	-3.81	117.57	124.12
2	A	201	NDP	PN-O3-PA	-3.75	119.96	132.83
2	G	201	NDP	C4A-C5A-N7A	-3.74	105.50	109.40
3	A	202	TMQ	O20-C15-C16	-3.51	118.09	124.12
3	A	202	TMQ	O20-C15-C14	3.39	121.12	115.16
2	C	201	NDP	C1D-N1N-C2N	3.36	126.71	121.11
3	C	202	TMQ	C17-C5-C6	-3.35	116.97	120.80
2	E	201	NDP	C4A-C5A-N7A	-3.35	105.91	109.40
3	C	202	TMQ	O18-C13-C14	3.32	120.99	115.16
3	E	202	TMQ	O18-C13-C12	-3.30	118.44	124.12
3	G	202	TMQ	O20-C15-C14	3.21	120.81	115.16
3	C	202	TMQ	O18-C13-C12	-3.08	118.81	124.12
3	E	202	TMQ	O18-C13-C14	3.08	120.57	115.16
3	G	202	TMQ	O18-C13-C12	-3.03	118.91	124.12
3	G	202	TMQ	C5-C4A-C4	-3.02	120.51	127.18
3	E	202	TMQ	C5-C4A-C4	-2.98	120.61	127.18
3	G	202	TMQ	O18-C13-C14	2.92	120.29	115.16
2	A	201	NDP	C4A-C5A-N7A	-2.88	106.40	109.40
2	C	201	NDP	C4A-C5A-N7A	-2.83	106.45	109.40
3	E	202	TMQ	O20-C15-C14	2.80	120.08	115.16
3	A	202	TMQ	C5-C4A-C4	-2.74	121.14	127.18
3	C	202	TMQ	O20-C15-C14	2.73	119.95	115.16
3	C	202	TMQ	C5-C4A-C4	-2.72	121.17	127.18
3	C	202	TMQ	O20-C15-C16	-2.72	119.44	124.12
3	C	202	TMQ	C22-O19-C14	2.61	121.93	114.78
2	G	201	NDP	O5B-C5B-C4B	-2.54	100.25	108.99
2	C	201	NDP	C1B-N9A-C4A	-2.50	122.26	126.64
2	E	201	NDP	PN-O3-PA	-2.46	124.38	132.83
2	C	201	NDP	O5B-C5B-C4B	-2.46	100.53	108.99
3	E	202	TMQ	N24-C2-N3	2.45	121.06	117.25
3	C	202	TMQ	N24-C2-N1	2.37	121.65	117.79
3	E	202	TMQ	C7-C8-C3A	-2.34	117.90	120.84
2	G	201	NDP	O2B-C2B-C1B	-2.31	101.78	110.10
3	E	202	TMQ	C23-O20-C15	2.31	121.01	117.53
3	E	202	TMQ	C6-C9-N10	-2.30	105.87	113.38
2	C	201	NDP	PN-O3-PA	-2.30	124.94	132.83
3	G	202	TMQ	C23-O20-C15	2.29	120.98	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	202	TMQ	O20-C15-C16	-2.28	120.19	124.12
2	G	201	NDP	O4D-C1D-C2D	-2.22	101.80	106.64
2	A	201	NDP	O2B-C2B-C1B	-2.20	102.17	110.10
3	G	202	TMQ	C22-O19-C14	2.18	120.75	114.78
2	A	201	NDP	O5B-C5B-C4B	-2.15	101.60	108.99
2	C	201	NDP	O4D-C1D-N1N	2.14	112.23	108.06
2	E	201	NDP	C4D-O4D-C1D	-2.13	104.78	109.47
2	C	201	NDP	O7N-C7N-N7N	-2.10	117.96	122.88
2	G	201	NDP	PN-O3-PA	-2.10	125.61	132.83
2	G	201	NDP	C1B-N9A-C4A	-2.06	123.02	126.64
3	E	202	TMQ	C17-C5-C6	-2.02	118.48	120.80
2	G	201	NDP	O4D-C4D-C5D	-2.00	102.78	109.37

There are no chirality outliers.

All (24) torsion outliers are listed below:

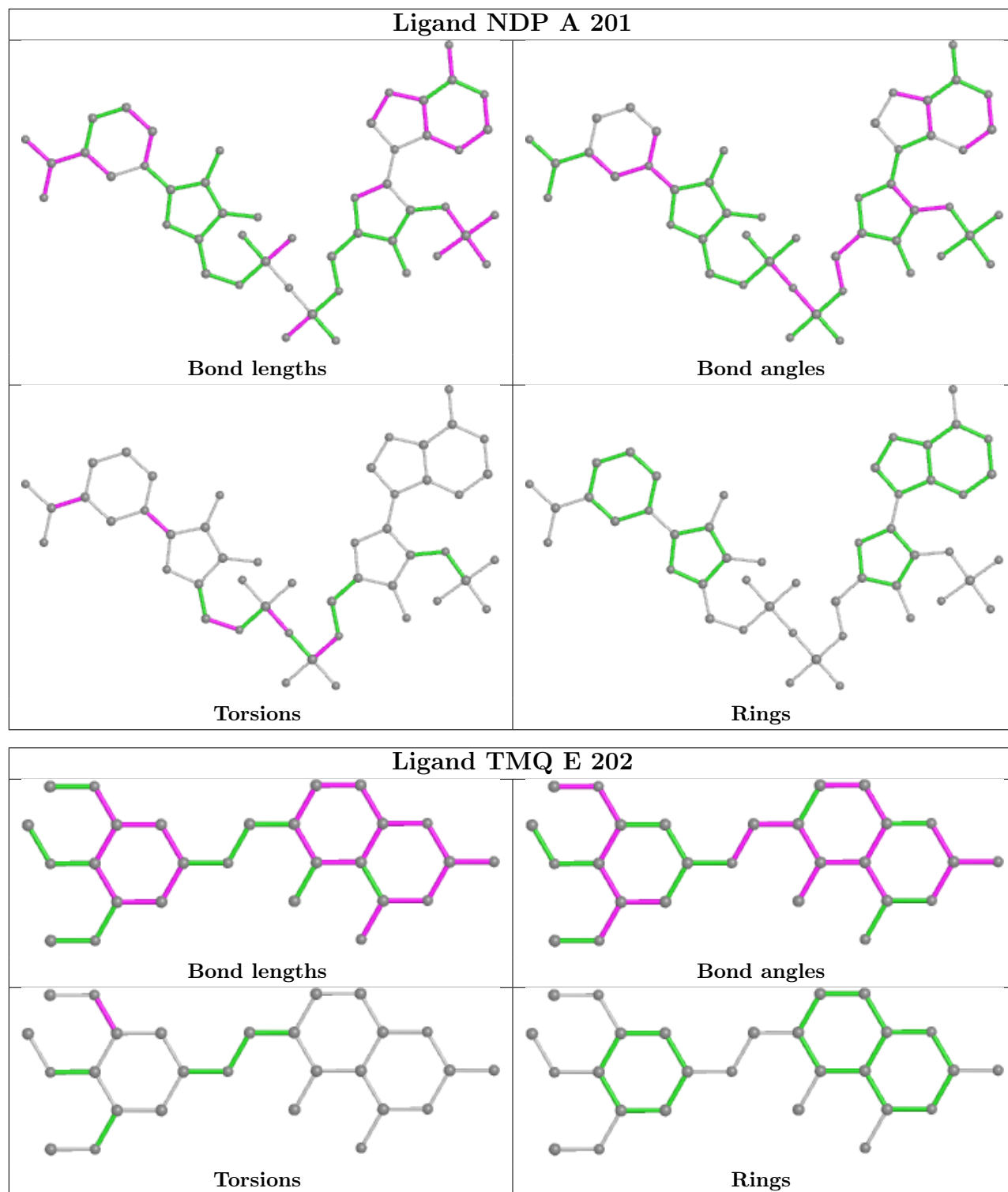
Mol	Chain	Res	Type	Atoms
2	A	201	NDP	C5B-O5B-PA-O1A
2	C	201	NDP	PA-O3-PN-O5D
2	G	201	NDP	C5B-O5B-PA-O1A
2	G	201	NDP	C5B-O5B-PA-O3
3	C	202	TMQ	C15-C14-O19-C22
3	A	202	TMQ	C13-C14-O19-C22
3	C	202	TMQ	C13-C14-O19-C22
3	A	202	TMQ	C15-C14-O19-C22
3	G	202	TMQ	C14-C15-O20-C23
2	G	201	NDP	O4D-C1D-N1N-C2N
2	A	201	NDP	PA-O3-PN-O5D
2	G	201	NDP	PA-O3-PN-O5D
3	G	202	TMQ	C16-C15-O20-C23
2	A	201	NDP	O4D-C1D-N1N-C2N
2	A	201	NDP	C5B-O5B-PA-O3
2	C	201	NDP	O4D-C1D-N1N-C2N
2	E	201	NDP	O4D-C1D-N1N-C2N
2	A	201	NDP	C4D-C5D-O5D-PN
2	C	201	NDP	C2D-C1D-N1N-C2N
2	E	201	NDP	C2D-C1D-N1N-C2N
3	E	202	TMQ	C14-C15-O20-C23
2	A	201	NDP	C2N-C3N-C7N-N7N
2	C	201	NDP	C5B-O5B-PA-O1A
2	C	201	NDP	C4D-C5D-O5D-PN

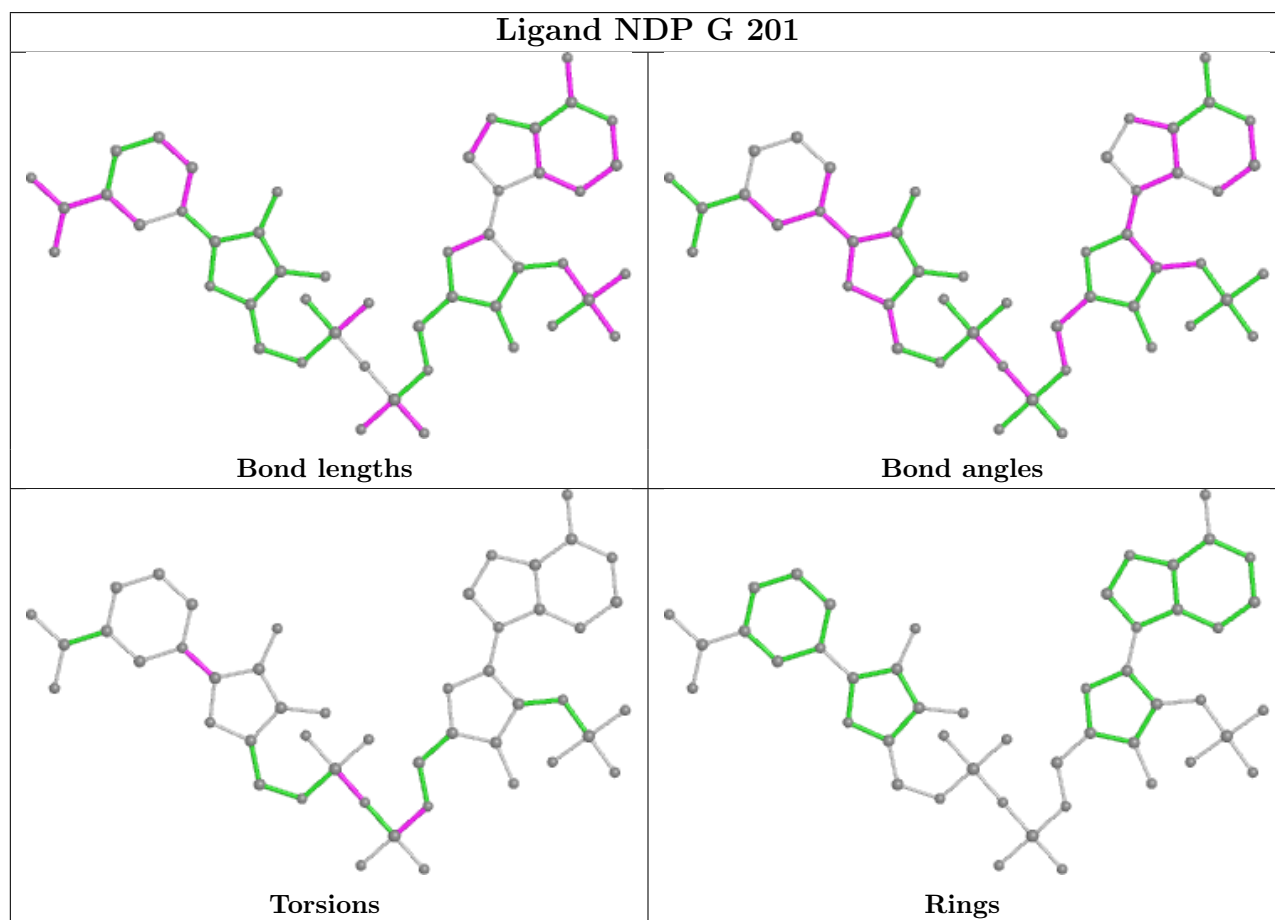
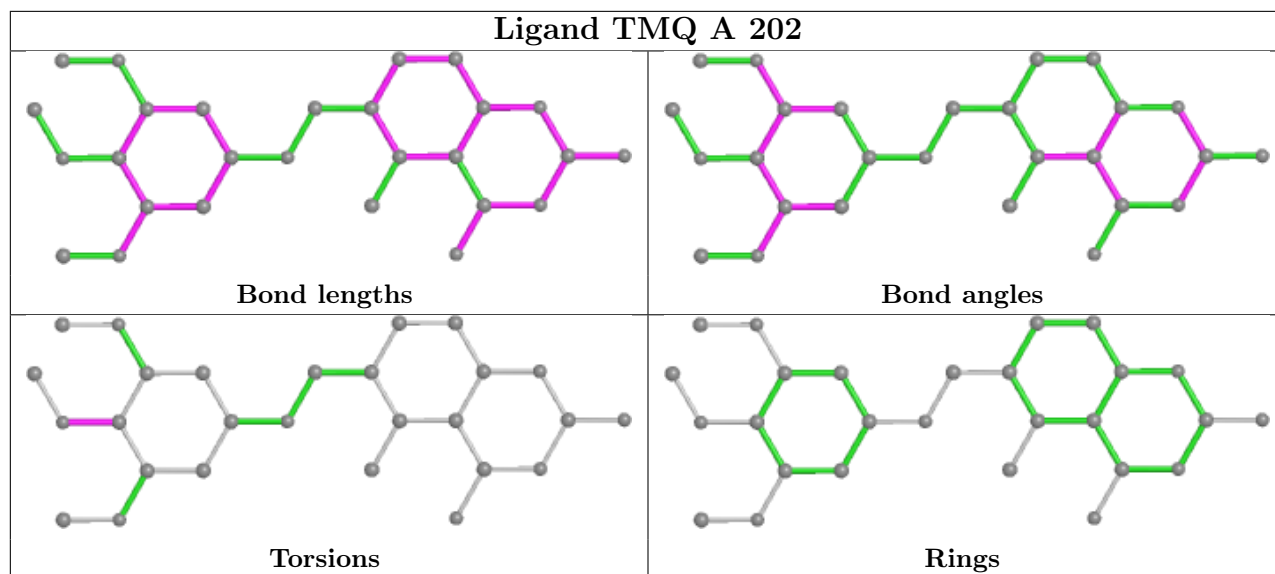
There are no ring outliers.

16 monomers are involved in 81 short contacts:

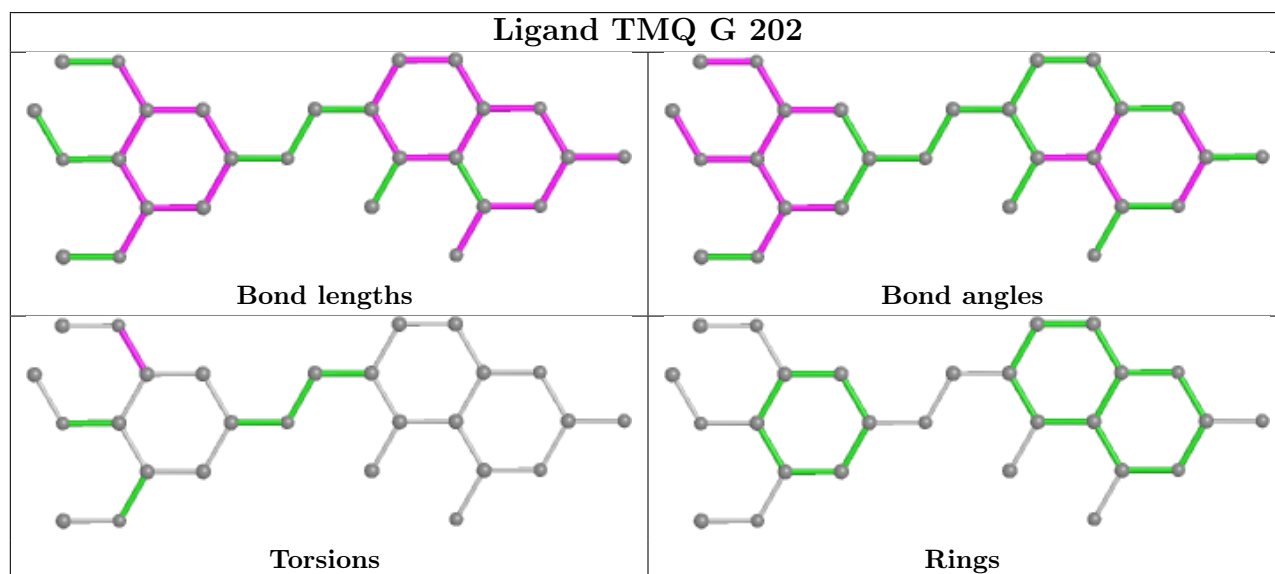
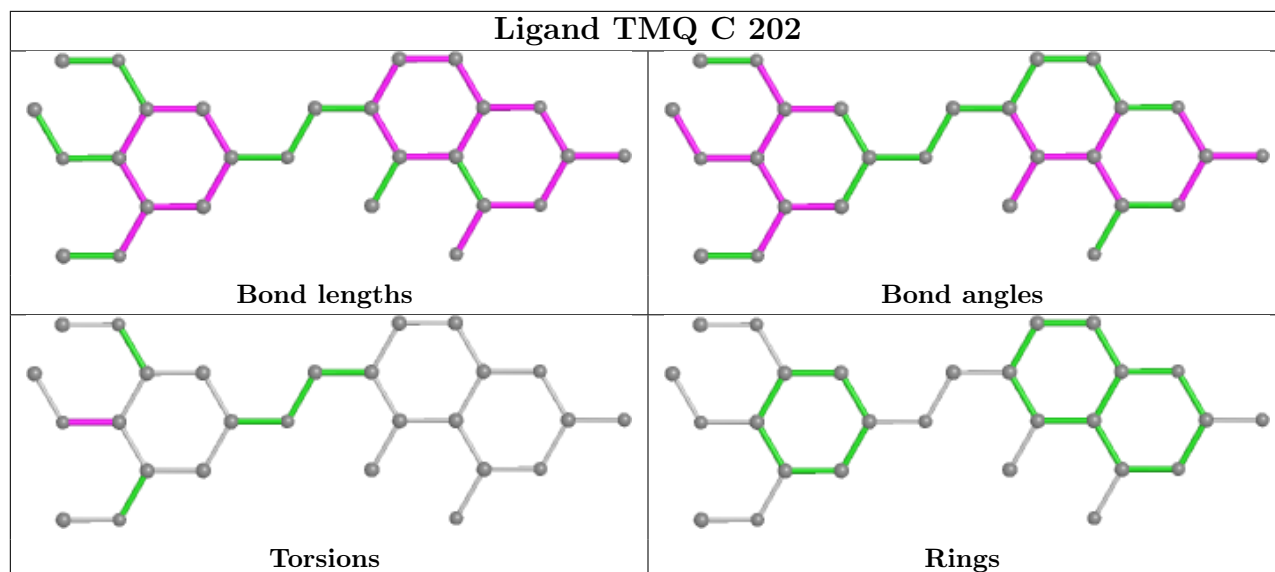
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	203	ACT	1	0
4	E	204	ACT	1	0
2	A	201	NDP	8	0
4	A	204	ACT	1	0
3	E	202	TMQ	11	0
4	A	203	ACT	1	0
4	C	208	ACT	1	0
4	E	207	ACT	1	0
3	A	202	TMQ	9	0
2	G	201	NDP	17	0
4	E	203	ACT	4	0
4	C	203	ACT	1	0
3	C	202	TMQ	8	0
3	G	202	TMQ	7	0
2	C	201	NDP	9	0
2	E	201	NDP	7	0

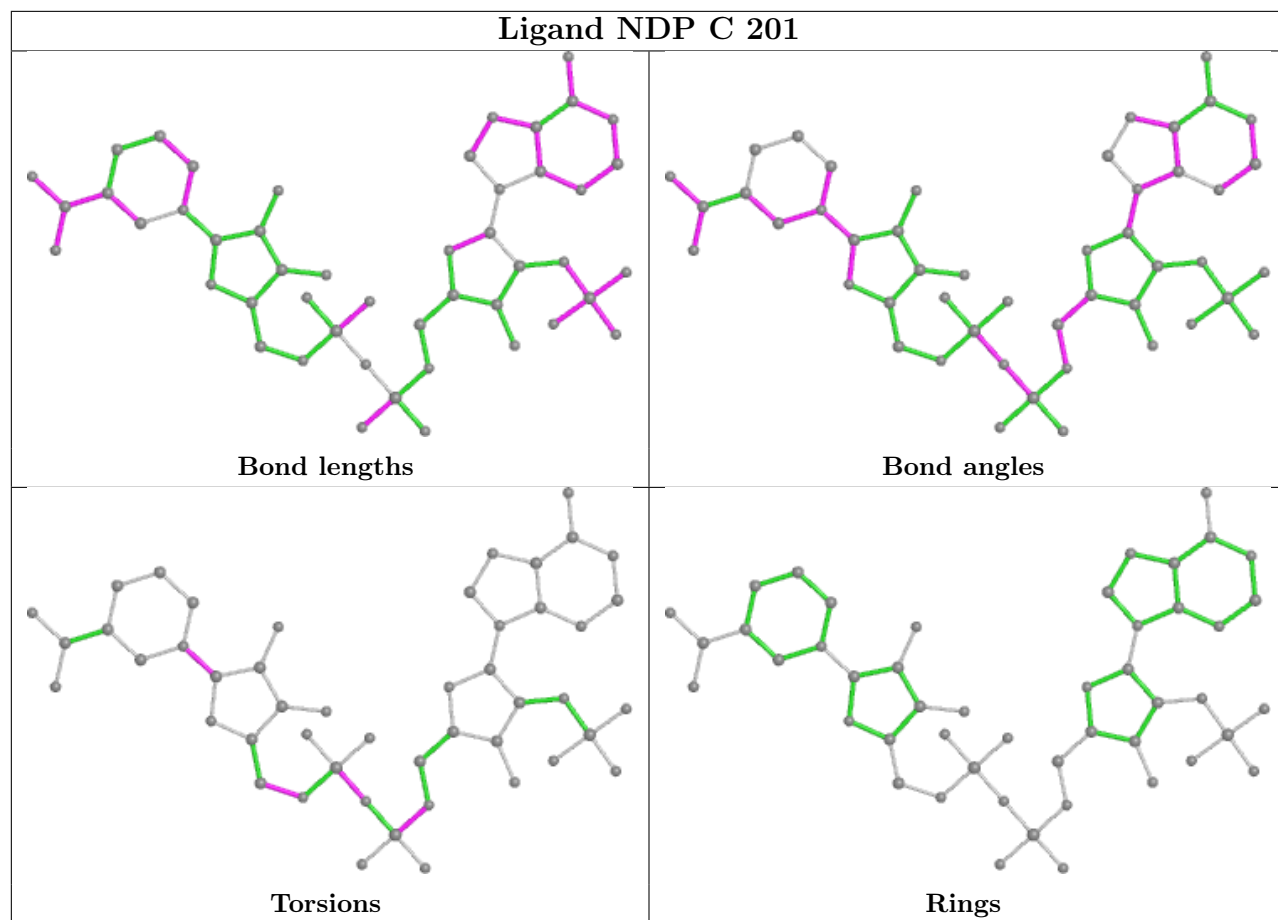
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

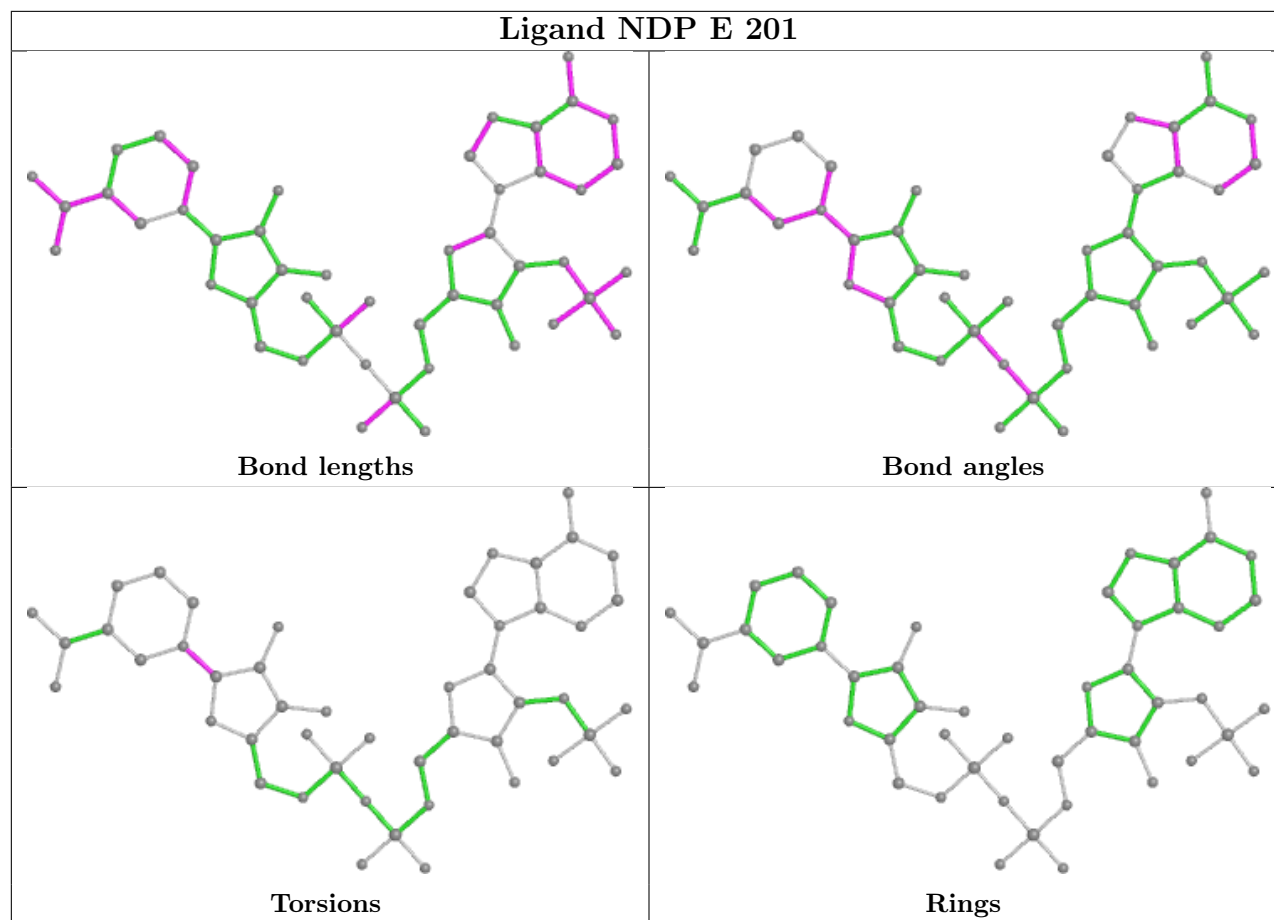












## 5.7 Other polymers [\(i\)](#)

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, 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	159/162 (98%)	-0.01	1 (0%) 89 89	22, 31, 48, 52	0
1	C	159/162 (98%)	-0.01	2 (1%) 77 79	22, 31, 43, 55	0
1	E	159/162 (98%)	-0.01	0 100 100	24, 32, 46, 52	0
1	G	159/162 (98%)	-0.00	2 (1%) 77 79	24, 31, 44, 54	0
All	All	636/648 (98%)	-0.01	5 (0%) 86 87	22, 31, 46, 55	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	70	ASP	3.9
1	C	118	GLY	2.4
1	A	89	PRO	2.3
1	C	159	SER	2.3
1	G	144	PHE	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,

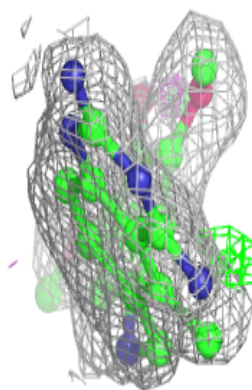
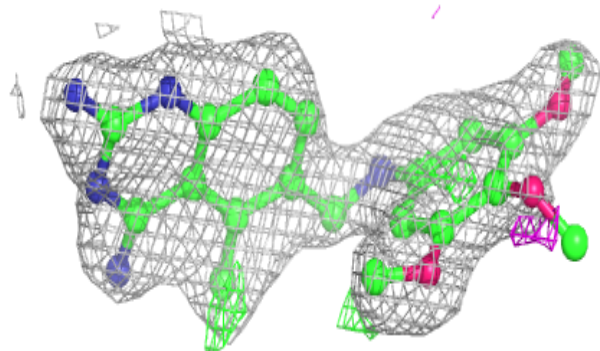
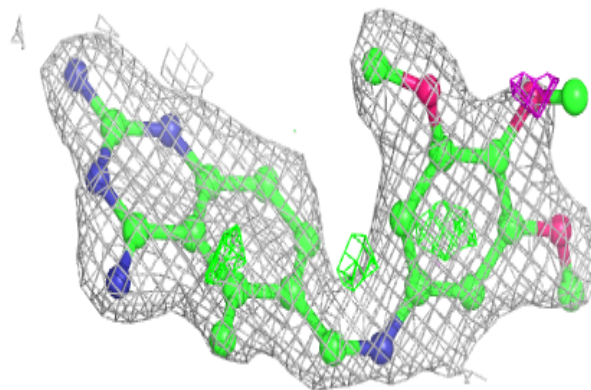
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	ACT	C	205	4/4	0.66	0.20	45,47,47,53	0
4	ACT	C	207	4/4	0.75	0.20	38,41,42,49	0
4	ACT	A	207	4/4	0.80	0.25	36,40,41,48	0
4	ACT	C	203	4/4	0.80	0.14	33,38,41,41	0
4	ACT	C	208	4/4	0.82	0.18	29,32,36,38	0
4	ACT	G	206	4/4	0.83	0.17	32,37,42,42	0
4	ACT	E	208	4/4	0.85	0.16	40,40,46,46	0
4	ACT	A	208	4/4	0.85	0.24	27,35,39,45	0
5	PO4	A	209	5/5	0.85	0.25	20,30,43,54	0
4	ACT	E	203	4/4	0.86	0.16	40,43,44,47	0
4	ACT	C	204	4/4	0.86	0.15	30,31,36,40	0
4	ACT	E	206	4/4	0.89	0.18	36,37,39,41	0
3	TMQ	G	202	27/27	0.89	0.19	23,35,46,50	0
4	ACT	A	206	4/4	0.89	0.17	34,35,39,47	0
4	ACT	E	204	4/4	0.89	0.17	30,33,34,44	0
4	ACT	E	207	4/4	0.90	0.17	32,36,38,44	0
4	ACT	C	206	4/4	0.90	0.15	30,33,40,42	0
4	ACT	E	205	4/4	0.90	0.14	29,34,36,39	0
4	ACT	A	205	4/4	0.90	0.17	26,39,39,40	0
4	ACT	A	204	4/4	0.91	0.14	33,34,38,53	0
4	ACT	G	205	4/4	0.91	0.18	26,38,43,43	0
4	ACT	G	204	4/4	0.92	0.14	27,29,38,42	0
4	ACT	A	203	4/4	0.92	0.22	30,36,37,40	0
3	TMQ	E	202	27/27	0.93	0.17	24,32,42,43	0
3	TMQ	A	202	27/27	0.93	0.18	26,33,44,48	0
3	TMQ	C	202	27/27	0.93	0.17	24,33,49,51	0
4	ACT	G	203	4/4	0.94	0.15	28,29,35,37	0
2	NDP	G	201	48/48	0.96	0.15	21,29,37,41	0
2	NDP	A	201	48/48	0.97	0.14	20,27,34,42	0
2	NDP	E	201	48/48	0.97	0.14	25,30,39,44	0
2	NDP	C	201	48/48	0.98	0.14	20,26,35,40	0

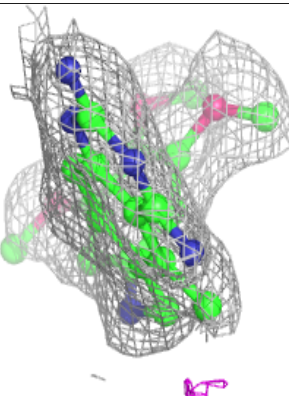
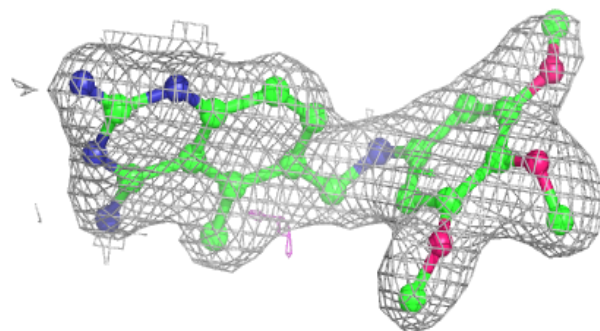
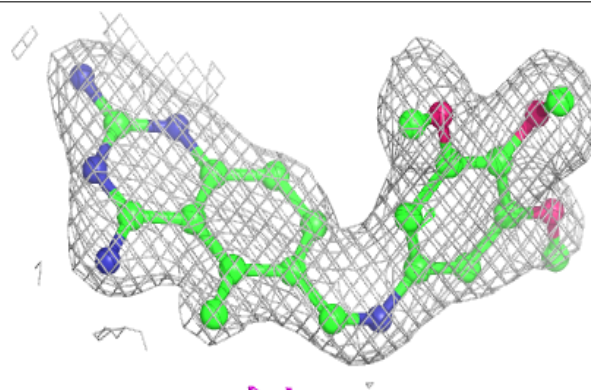
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TMQ G 202:**

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

**Electron density around TMQ E 202:**

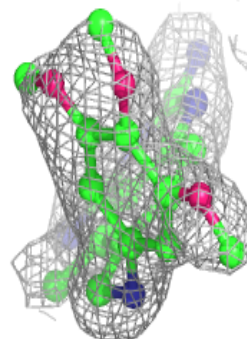
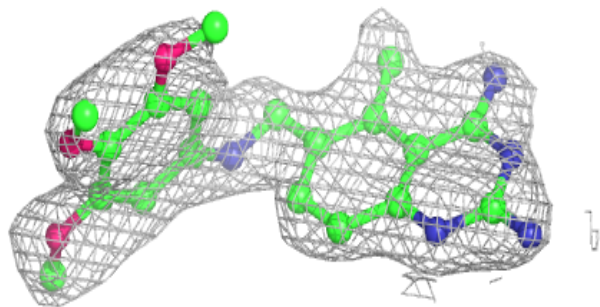
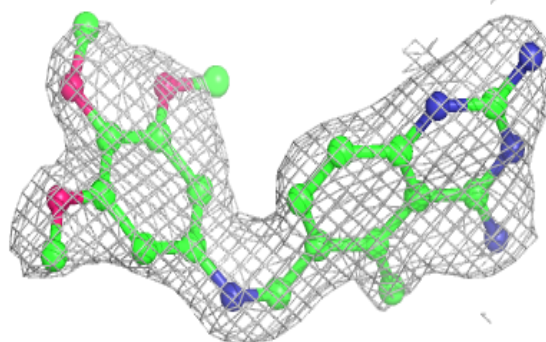
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



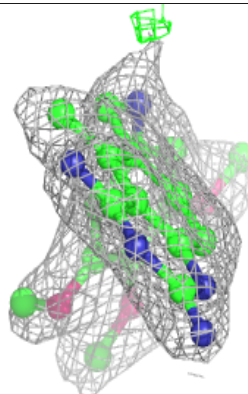
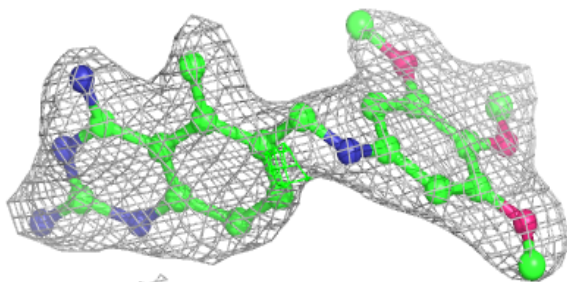
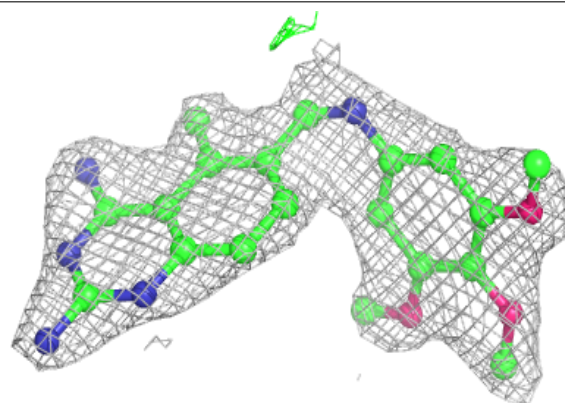


**Electron density around TMQ A 202:**

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

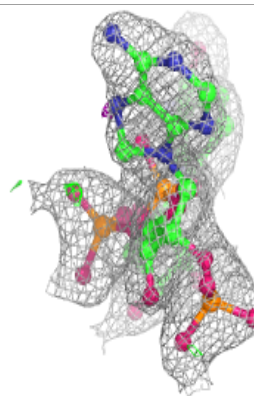
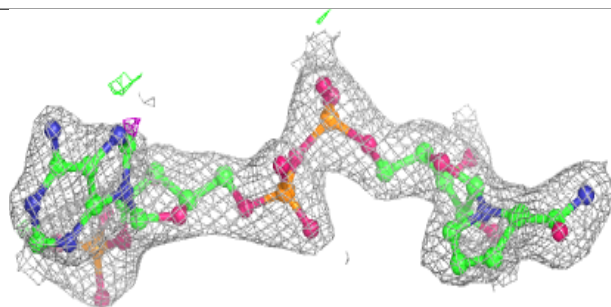
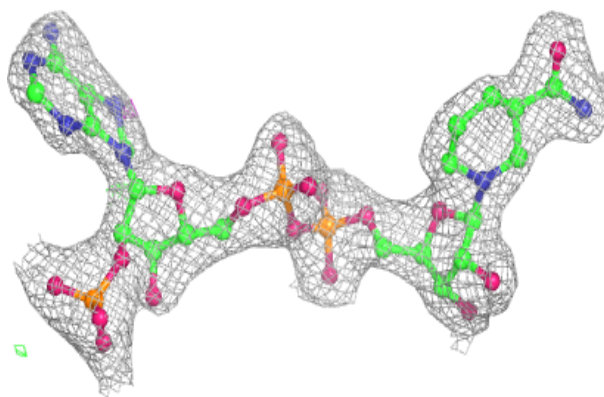
**Electron density around TMQ C 202:**

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

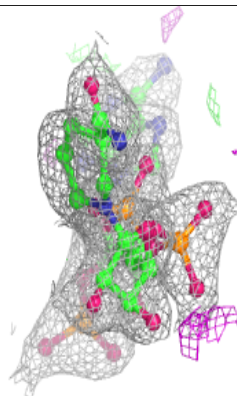
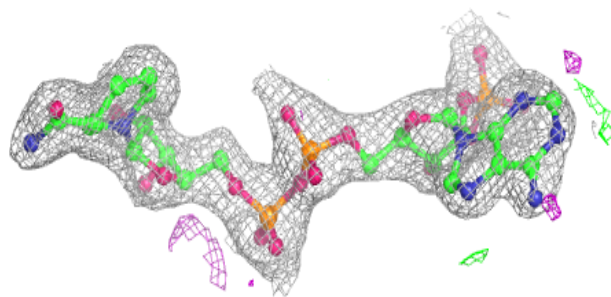
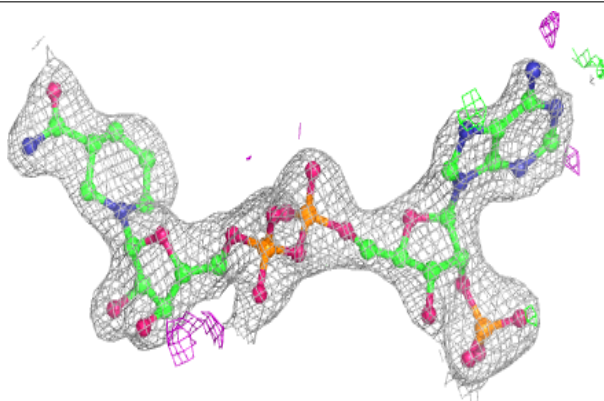


**Electron density around NDP G 201:**

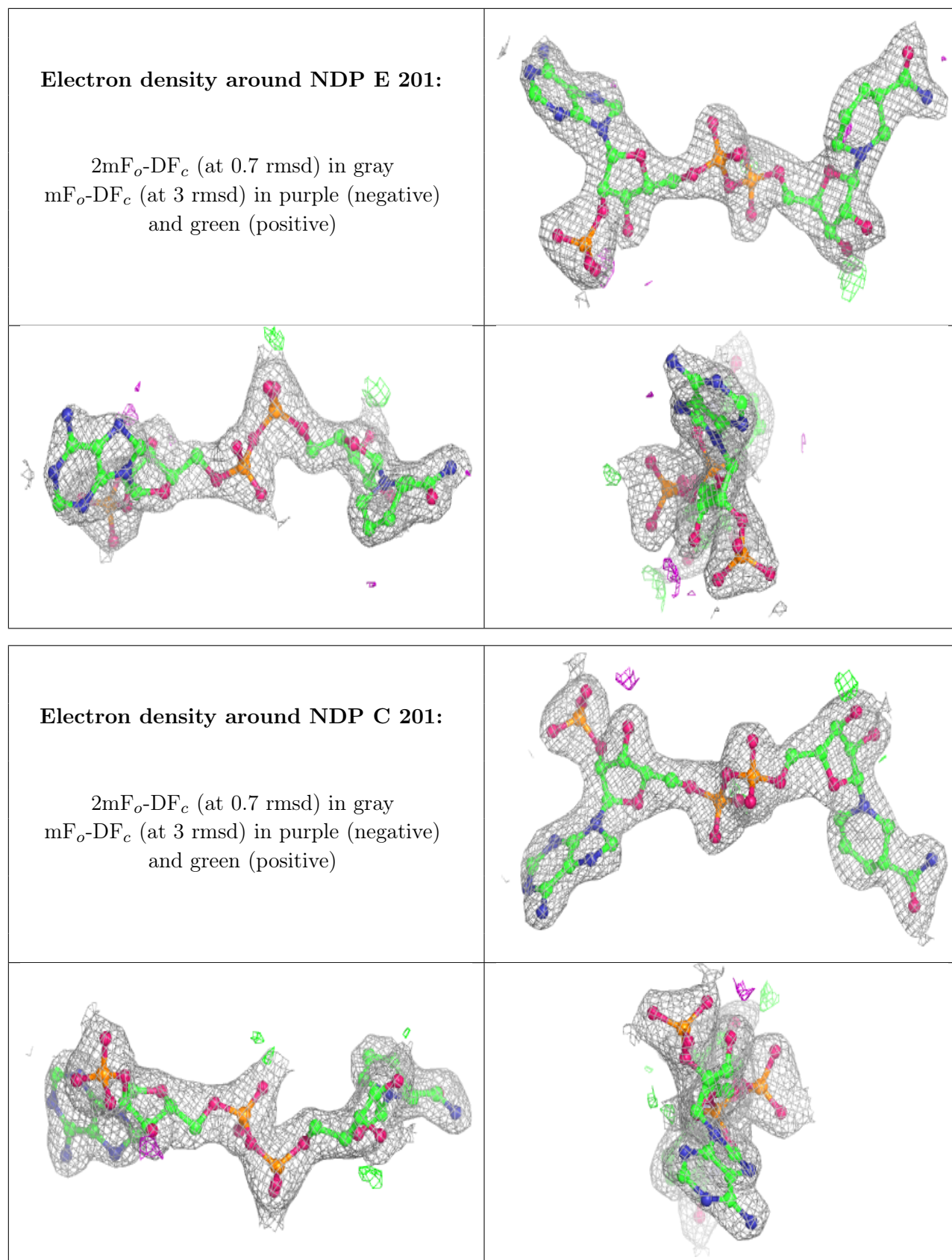
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NDP A 201:**

$2mF_o-DF_c$  (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.