



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:25 AM BST

PDB ID : 6RXC  
Title : Leishmania major pteridine reductase 1 (LmPTR1) in complex with inhibitor 4 (NMT-C0026)  
Authors : Di Pisa, F.; Dello Iacono, L.; Pozzi, C.; Mangani, S.  
Deposited on : 2019-06-07  
Resolution : 2.10 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 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 : 2.13.1  
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) : 2.13.1

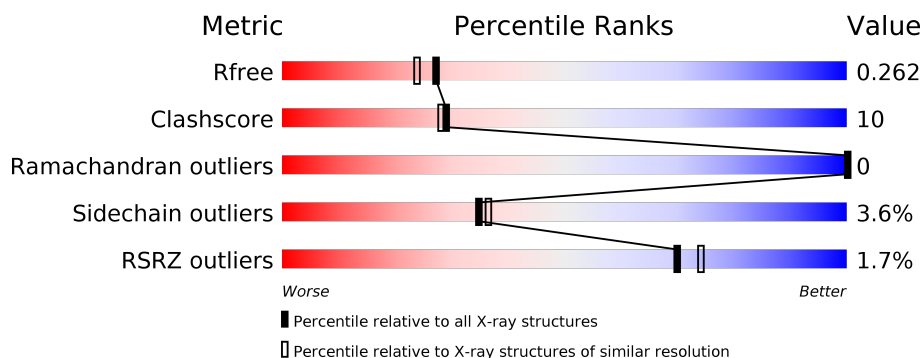
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	291	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>10%</div> </div> </div>
1	C	291	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>10%</div> </div> </div>
2	B	291	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>10%</div> </div> </div>
2	D	291	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>12%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8684 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 Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	1	0
			1942	1229	347	355	11			
1	C	261	Total	C	N	O	S	0	1	0
			1932	1223	345	353	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q01782
A	-1	SER	-	expression tag	UNP Q01782
A	0	HIS	-	expression tag	UNP Q01782
A	162	VAL	PHE	conflict	UNP Q01782
C	-2	GLY	-	expression tag	UNP Q01782
C	-1	SER	-	expression tag	UNP Q01782
C	0	HIS	-	expression tag	UNP Q01782
C	162	VAL	PHE	conflict	UNP Q01782

- Molecule 2 is a protein called Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	1	0
			1932	1220	343	358	11			
2	D	256	Total	C	N	O	S	0	0	0
			1891	1197	335	349	10			

There are 8 discrepancies between the modelled and reference sequences:

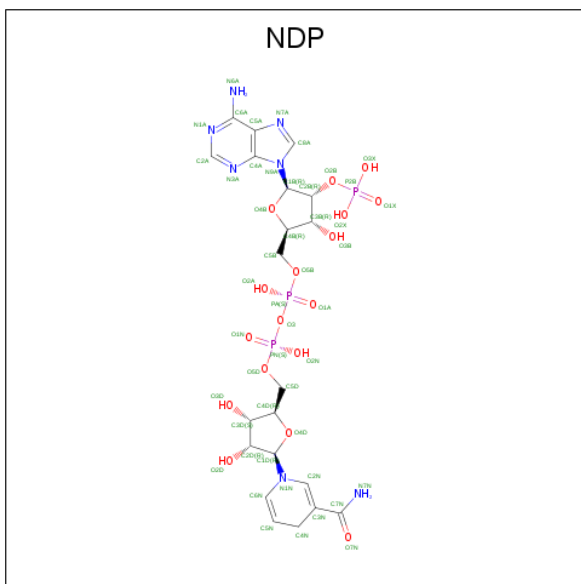
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q01782
B	-1	SER	-	expression tag	UNP Q01782
B	0	HIS	-	expression tag	UNP Q01782
B	162	VAL	PHE	conflict	UNP Q01782

*Continued on next page...*

Continued from previous page...

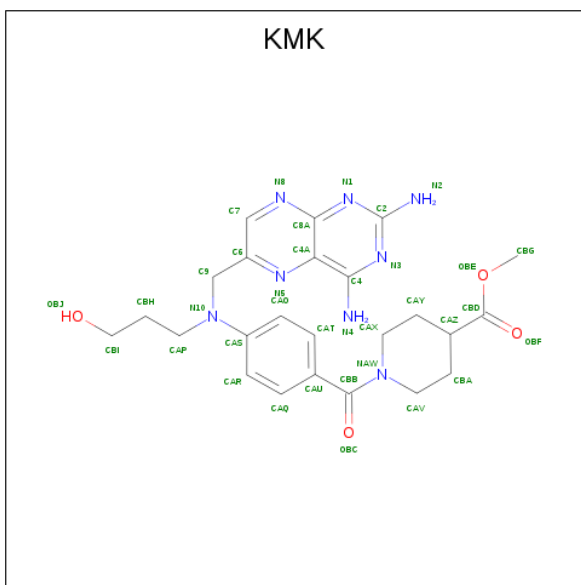
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP Q01782
D	-1	SER	-	expression tag	UNP Q01782
D	0	HIS	-	expression tag	UNP Q01782
D	162	VAL	PHE	conflict	UNP Q01782

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



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

- Molecule 4 is methyl 1-[4-[[2,4-bis(azanyl)pteridin-6-yl]methyl-(3-oxidanylpropyl)amino]phenyl]carbonylpiperidine-4-carboxylate (three-letter code: KMK) (formula: C<sub>24</sub>H<sub>30</sub>N<sub>8</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 36	C 24	N 8	O 4	0	0
4	B	1	Total 36	C 24	N 8	O 4	0	0
4	C	1	Total 36	C 24	N 8	O 4	0	0
4	D	1	Total 36	C 24	N 8	O 4	0	0

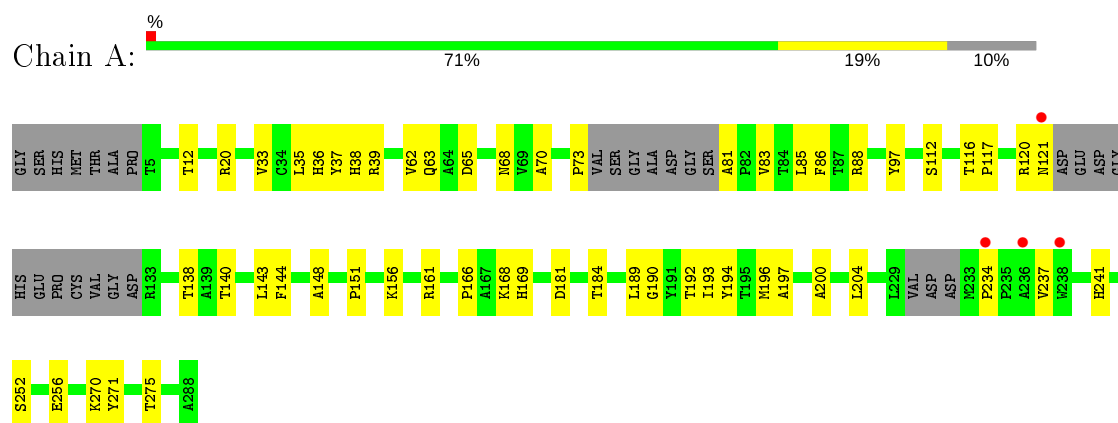
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	186	Total O 186 186	0	0
5	B	156	Total O 156 156	0	0
5	C	171	Total O 171 171	0	0
5	D	138	Total O 138 138	0	0

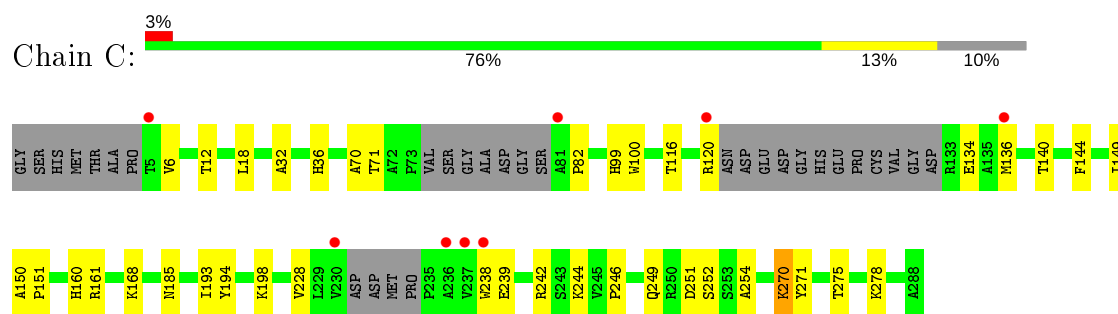
### 3 Residue-property plots

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

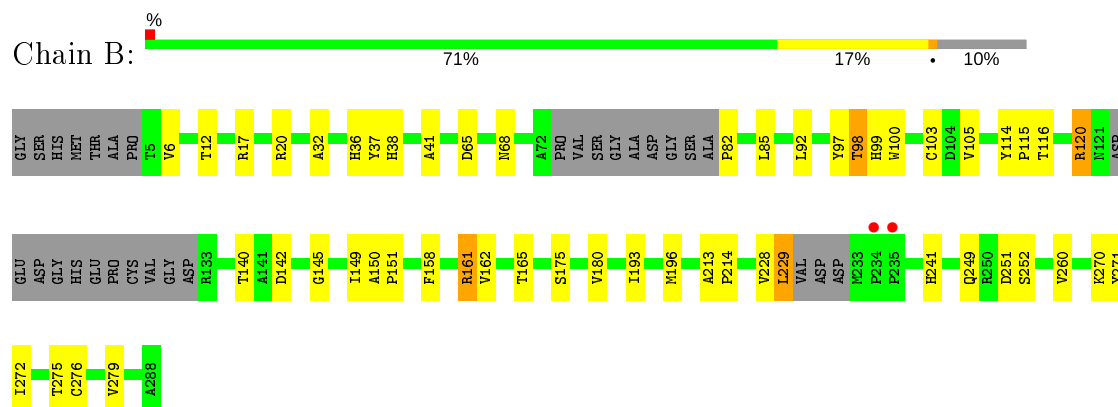
#### • Molecule 1: Pteridine reductase 1



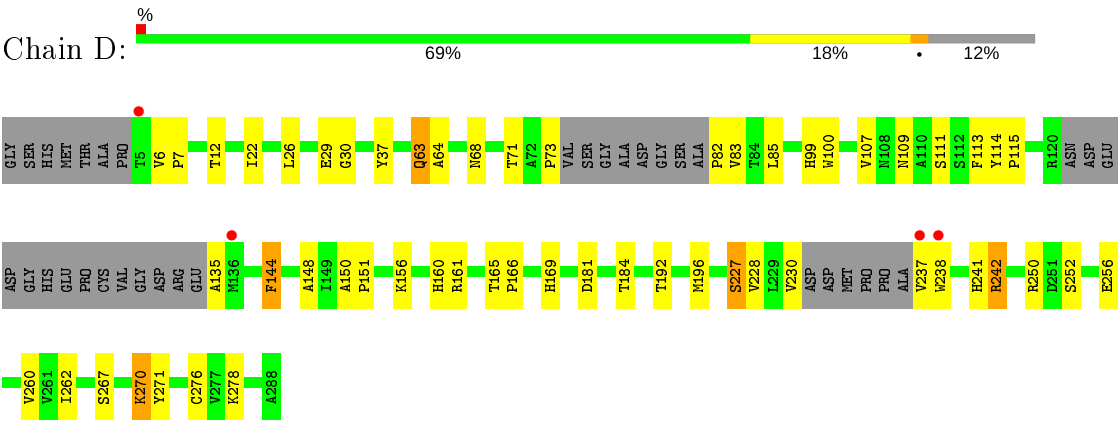
#### • Molecule 1: Pteridine reductase 1



#### • Molecule 2: Pteridine reductase 1



● Molecule 2: Pteridine reductase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.27Å 103.44Å 136.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.50 – 2.10 82.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (82.50-2.10) 98.4 (82.50-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.213 , 0.261 0.214 , 0.262	Depositor DCC
$R_{free}$ test set	3890 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8684	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4661e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, KMK, CSX

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	0.62	0/1983	0.98	0/2702
1	C	0.53	0/1972	0.93	0/2685
2	B	0.58	0/1957	0.97	0/2664
2	D	0.52	0/1919	0.89	0/2613
All	All	0.57	0/7831	0.94	0/10664

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	1942	0	1946	39	0
1	C	1932	0	1945	27	0
2	B	1932	0	1924	45	0
2	D	1891	0	1889	48	0
3	A	48	0	26	0	0
3	B	48	0	26	2	0
3	C	48	0	26	1	0
3	D	48	0	26	0	0
4	A	36	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	36	0	0	1	0
4	C	36	0	0	1	0
4	D	36	0	0	3	0
5	A	186	0	0	6	0
5	B	156	0	0	4	0
5	C	171	0	0	5	0
5	D	138	0	0	6	0
All	All	8684	0	7808	152	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 10.

All (152) 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:C:71:THR:HG22	5:C:476:HOH:O	1.43	1.17
2:B:116:THR:HG21	2:B:193:ILE:HG13	1.48	0.96
1:A:181:ASP:HB3	1:A:184:THR:HG23	1.44	0.95
2:B:180:VAL:HG21	2:B:276[B]:CSX:HG	1.39	0.86
2:D:278:LYS:HE3	5:D:496:HOH:O	1.81	0.80
2:D:276:CSX:HB2	5:D:491:HOH:O	1.80	0.80
2:B:120:ARG:HH11	2:B:120:ARG:HG2	1.47	0.80
2:B:116:THR:CG2	2:B:193:ILE:HG13	2.13	0.78
2:B:140:THR:HG22	5:B:468:HOH:O	1.85	0.76
2:D:237:VAL:HG11	4:D:302:KMK:CBG	2.16	0.75
2:D:166:PRO:HB2	2:D:169:HIS:HD2	1.51	0.74
2:B:116:THR:CB	2:B:193:ILE:HG13	2.19	0.71
1:C:168:LYS:HG2	5:C:489:HOH:O	1.92	0.69
2:D:6:VAL:HG22	2:D:30:GLY:O	1.92	0.69
1:A:120:ARG:HG2	1:A:121:ASN:H	1.60	0.67
2:D:6:VAL:CG2	2:D:30:GLY:O	2.42	0.67
1:A:62:VAL:HG13	5:A:404:HOH:O	1.95	0.67
1:C:160:HIS:HB2	5:C:510:HOH:O	1.95	0.66
2:B:98:THR:HG22	2:B:99:HIS:N	2.10	0.66
1:A:168:LYS:HE2	1:A:169:HIS:NE2	2.10	0.66
1:C:228:VAL:HG23	1:C:228:VAL:O	1.96	0.66
2:D:276:CSX:CB	5:D:491:HOH:O	2.40	0.66
1:A:181:ASP:HB3	1:A:184:THR:CG2	2.23	0.65
2:D:238:TRP:CE2	2:D:242:ARG:HD3	2.32	0.64
2:D:71:THR:N	2:D:83:VAL:O	2.29	0.64
1:A:120:ARG:CG	1:A:121:ASN:H	2.12	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:181:ASP:HB3	2:D:184:THR:HG23	1.82	0.62
2:D:230:VAL:HG12	5:D:484:HOH:O	2.01	0.61
2:B:98:THR:CG2	2:B:99:HIS:N	2.63	0.61
2:D:242:ARG:HB2	2:D:250:ARG:HA	1.81	0.61
2:B:114:TYR:HB2	2:B:115:PRO:HD2	1.82	0.60
2:B:98:THR:HG22	2:B:99:HIS:H	1.64	0.60
2:D:6:VAL:HG22	2:D:7:PRO:HD2	1.83	0.60
1:A:97:TYR:CZ	1:A:161:ARG:HB3	2.38	0.59
2:D:238:TRP:CZ2	2:D:242:ARG:NH1	2.71	0.58
1:C:140:THR:O	1:C:144:PHE:HB2	2.03	0.57
2:B:12:THR:HA	2:B:36:HIS:HB3	1.88	0.55
2:D:148:ALA:C	2:D:151:PRO:HD2	2.27	0.55
2:D:238:TRP:HZ2	2:D:242:ARG:NH1	2.05	0.54
2:B:36:HIS:CD2	2:B:92:LEU:HD11	2.42	0.54
2:D:135:ALA:HB3	5:D:486:HOH:O	2.07	0.54
1:C:12:THR:HA	1:C:36:HIS:HB3	1.90	0.54
1:A:38:HIS:CE1	1:A:39:ARG:NH1	2.76	0.53
1:C:149:ILE:HG12	2:D:144:PHE:HE2	1.73	0.53
1:A:156:LYS:NZ	5:A:405:HOH:O	2.42	0.52
2:B:252:SER:HB3	2:D:271:TYR:CE2	2.44	0.52
1:A:256:GLU:OE2	1:C:270:LYS:HE3	2.09	0.52
2:B:6:VAL:HA	5:B:404:HOH:O	2.08	0.52
2:B:272:ILE:HD11	2:D:260:VAL:CG2	2.40	0.52
2:D:267:SER:O	2:D:270:LYS:HB3	2.10	0.52
2:B:120:ARG:HH11	2:B:120:ARG:CG	2.21	0.52
5:A:477:HOH:O	1:C:278:LYS:HD2	2.09	0.52
5:B:447:HOH:O	1:C:244:LYS:HE3	2.10	0.51
2:B:142:ASP:OD1	3:B:301:NDP:N6A	2.42	0.51
2:B:82:PRO:HA	5:B:441:HOH:O	2.10	0.51
1:C:99:HIS:HD2	1:C:100:TRP:CE2	2.28	0.51
2:B:105:VAL:HA	2:B:175:SER:O	2.10	0.51
2:B:272:ILE:HD11	2:D:260:VAL:HG21	1.92	0.51
2:B:213:ALA:N	2:B:214:PRO:CD	2.74	0.50
2:B:99:HIS:HD2	2:B:100:TRP:CE2	2.28	0.50
2:D:37:TYR:CZ	2:D:63:GLN:HB2	2.47	0.50
2:B:145:GLY:HA2	2:B:149:ILE:HB	1.94	0.50
2:D:12:THR:O	2:D:109:ASN:HB3	2.11	0.50
2:D:160:HIS:HB3	5:D:497:HOH:O	2.11	0.50
1:C:239:GLU:HA	1:C:242:ARG:NH1	2.27	0.49
1:C:116:THR:HG21	1:C:193:ILE:HD12	1.94	0.49
1:A:117:PRO:HG2	1:A:120:ARG:NH2	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:ASN:HA	2:D:85:LEU:HD22	1.94	0.49
2:B:271:TYR:CE2	2:D:252:SER:HB3	2.48	0.49
1:A:120:ARG:CG	1:A:121:ASN:N	2.76	0.48
2:B:260:VAL:HG21	2:B:279:VAL:HG21	1.94	0.48
1:C:144:PHE:CE2	1:C:193:ILE:HG23	2.48	0.48
2:B:97:TYR:CE1	2:B:103:CYS:HB2	2.48	0.48
1:A:148:ALA:C	1:A:151:PRO:HD2	2.34	0.48
2:D:73:PRO:HD3	2:D:82:PRO:HA	1.95	0.48
2:B:32:ALA:HB1	2:B:100:TRP:CE2	2.49	0.48
1:C:238:TRP:NE1	1:C:242:ARG:HD3	2.29	0.48
1:A:252:SER:HB3	1:C:271:TYR:CE2	2.48	0.48
2:D:238:TRP:CZ2	2:D:242:ARG:CZ	2.97	0.48
1:A:62:VAL:CG1	5:A:404:HOH:O	2.58	0.48
2:B:32:ALA:HB1	2:B:100:TRP:CZ2	2.49	0.47
2:B:270:LYS:HE3	2:D:256:GLU:OE2	2.14	0.47
1:A:166:PRO:HG2	5:A:426:HOH:O	2.14	0.47
2:B:68:ASN:HA	2:B:85:LEU:HD22	1.97	0.47
1:A:116:THR:N	1:A:190:GLY:O	2.48	0.46
2:D:114:TYR:HB2	2:D:115:PRO:HD2	1.97	0.46
2:B:120:ARG:HA	2:B:120:ARG:NH1	2.30	0.46
1:A:140:THR:O	1:A:144:PHE:HB2	2.15	0.46
1:A:271:TYR:CE2	1:C:252:SER:HB3	2.51	0.46
2:D:192:THR:O	2:D:196:MET:HG3	2.16	0.46
2:D:238:TRP:O	2:D:242:ARG:HG2	2.16	0.46
2:D:111:SER:OG	4:D:302:KMK:N2	2.50	0.45
1:C:134:GLU:HA	5:C:460:HOH:O	2.15	0.45
1:C:18:LEU:CD2	1:C:254:ALA:HA	2.45	0.45
2:D:26:LEU:O	2:D:29:GLU:HB2	2.16	0.45
1:A:33:VAL:HG12	1:A:35:LEU:CD2	2.47	0.45
2:B:37:TYR:CE2	2:B:41:ALA:HB2	2.52	0.45
2:D:237:VAL:HG12	2:D:237:VAL:O	2.17	0.45
2:B:17:ARG:NH1	2:B:228:VAL:HG23	2.32	0.45
2:D:227:SER:O	2:D:228:VAL:HG22	2.16	0.45
1:A:37:TYR:O	1:A:63:GLN:HA	2.17	0.45
1:A:83:VAL:HG12	1:A:88:ARG:HG3	1.99	0.44
2:B:180:VAL:HG21	2:B:276[B]:CSX:SG	2.49	0.44
1:A:120:ARG:HB3	5:A:538:HOH:O	2.17	0.44
1:C:194:TYR:CE1	1:C:198:LYS:HE2	2.53	0.44
2:B:213:ALA:HB3	2:B:214:PRO:HD3	2.00	0.44
1:A:197:ALA:O	1:A:200:ALA:HB3	2.18	0.44
1:A:36:HIS:HA	1:A:62:VAL:O	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:HIS:CD2	2:D:100:TRP:CE2	3.05	0.44
2:B:158:PHE:O	2:B:162:VAL:HG23	2.18	0.43
2:B:161:ARG:HA	2:B:161:ARG:HD2	1.56	0.43
1:A:33:VAL:CG1	1:A:35:LEU:HD23	2.49	0.43
1:A:234:PRO:HB2	1:A:237:VAL:HG23	2.01	0.43
3:C:301:NDP:H2D	4:C:302:KMK:N3	2.33	0.43
1:A:12:THR:HA	1:A:36:HIS:HB3	2.01	0.42
2:D:22:ILE:HD13	2:D:107:VAL:HG11	2.00	0.42
2:D:113:PHE:HB2	4:D:302:KMK:C2	2.49	0.42
1:A:38:HIS:CE1	1:A:65:ASP:HB2	2.54	0.42
1:A:73:PRO:HB3	1:A:81:ALA:N	2.34	0.42
2:D:227:SER:O	2:D:228:VAL:CG2	2.67	0.42
2:B:116:THR:HG21	2:B:193:ILE:CG1	2.32	0.42
2:D:161:ARG:HD2	2:D:161:ARG:HA	1.87	0.42
2:B:38:HIS:CD2	2:B:65:ASP:HB2	2.55	0.42
1:A:193:ILE:HD12	1:A:193:ILE:HG23	1.75	0.42
4:A:302:KMK:CAT	4:A:302:KMK:CAX	2.97	0.42
1:A:68:ASN:HA	1:A:85:LEU:HD22	2.01	0.42
1:C:70:ALA:HB1	1:C:82:PRO:HB2	2.01	0.42
2:B:229:LEU:HD22	2:B:251:ASP:HB3	2.00	0.42
1:A:33:VAL:CG1	1:A:35:LEU:CD2	2.98	0.41
2:B:150:ALA:HB3	2:B:151:PRO:HD3	2.02	0.41
2:B:38:HIS:CD2	2:B:65:ASP:HA	2.55	0.41
1:C:185:ASN:HB2	5:C:471:HOH:O	2.19	0.41
2:B:229:LEU:HD12	2:B:229:LEU:HA	1.90	0.41
1:C:246:PRO:O	1:C:249:GLN:NE2	2.53	0.41
2:D:150:ALA:HB3	2:D:151:PRO:HD3	2.01	0.41
1:C:32:ALA:HB1	1:C:100:TRP:CZ2	2.55	0.41
1:A:192:THR:O	1:A:196:MET:HG3	2.19	0.41
1:A:38:HIS:NE2	1:A:39:ARG:CZ	2.84	0.41
3:B:301:NDP:H2D	4:B:302:KMK:N3	2.35	0.41
1:C:251:ASP:OD1	1:C:251:ASP:N	2.53	0.41
2:D:99:HIS:HD2	2:D:100:TRP:CE2	2.39	0.41
2:B:114:TYR:HB2	2:B:115:PRO:CD	2.48	0.41
2:D:6:VAL:HG21	2:D:30:GLY:O	2.19	0.41
1:A:112:SER:HB2	1:A:143:LEU:HD23	2.03	0.41
1:A:194:TYR:CD1	1:A:194:TYR:C	2.94	0.41
1:A:70:ALA:HA	1:A:83:VAL:O	2.20	0.41
1:C:150:ALA:HB3	1:C:151:PRO:HD3	2.03	0.41
2:D:165:THR:HA	2:D:166:PRO:HD2	1.85	0.41
1:A:204:LEU:HB2	2:B:196:MET:SD	2.60	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:GLN:HE21	2:D:64:ALA:HA	1.86	0.40
2:D:156:LYS:HE2	2:D:160:HIS:HE1	1.87	0.40
1:C:161:ARG:HA	1:C:161:ARG:HD2	1.91	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	256/291 (88%)	243 (95%)	13 (5%)	0	100	100
1	C	254/291 (87%)	242 (95%)	12 (5%)	0	100	100
2	B	252/291 (87%)	235 (93%)	17 (7%)	0	100	100
2	D	247/291 (85%)	235 (95%)	12 (5%)	0	100	100
All	All	1009/1164 (87%)	955 (95%)	54 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/225 (88%)	191 (96%)	7 (4%)	36	38
1	C	198/225 (88%)	193 (98%)	5 (2%)	47	52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	195/224 (87%)	186 (95%)	9 (5%)	27	26
2	D	192/224 (86%)	185 (96%)	7 (4%)	35	36
All	All	783/898 (87%)	755 (96%)	28 (4%)	35	36

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	86	PHE
1	A	138	THR
1	A	189	LEU
1	A	241	HIS
1	A	270	LYS
1	A	275	THR
2	B	20	ARG
2	B	98	THR
2	B	120	ARG
2	B	161	ARG
2	B	165	THR
2	B	229	LEU
2	B	241	HIS
2	B	249	GLN
2	B	275	THR
1	C	6	VAL
1	C	120	ARG
1	C	136	MET
1	C	270	LYS
1	C	275	THR
2	D	63	GLN
2	D	144	PHE
2	D	227	SER
2	D	241	HIS
2	D	242	ARG
2	D	262	ILE
2	D	270	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	68	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	169	HIS
2	B	249	GLN
2	D	63	GLN
2	D	169	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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	CSX	D	276	2	3,6,7	0.50	0	1,6,8	1.38	0
2	CSX	B	276[A]	-	3,6,7	0.73	0	1,6,8	0.71	0
2	CSX	B	276[B]	-	3,6,7	0.75	0	1,6,8	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSX	D	276	2	-	1/1/5/7	-
2	CSX	B	276[A]	-	-	0/1/5/7	-
2	CSX	B	276[B]	-	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	D	276	CSX	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	276	CSX	2	0
2	B	276[B]	CSX	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	KMK	D	302	-	39,39,39	1.99	7 (17%)	52,54,54	2.35	21 (40%)
3	NDP	D	301	-	45,52,52	0.78	1 (2%)	53,80,80	0.99	5 (9%)
3	NDP	C	301	-	45,52,52	0.70	0	53,80,80	0.86	2 (3%)
4	KMK	A	302	-	39,39,39	2.21	10 (25%)	52,54,54	1.95	11 (21%)
3	NDP	B	301	-	45,52,52	0.88	1 (2%)	53,80,80	1.02	2 (3%)
3	NDP	A	301	-	45,52,52	0.93	2 (4%)	53,80,80	1.21	5 (9%)
4	KMK	B	302	-	39,39,39	1.86	11 (28%)	52,54,54	2.47	25 (48%)
4	KMK	C	302	-	39,39,39	2.31	13 (33%)	52,54,54	2.41	23 (44%)

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
4	KMK	D	302	-	-	2/26/36/36	0/4/4/4
3	NDP	D	301	-	-	1/30/77/77	0/5/5/5
3	NDP	C	301	-	-	3/30/77/77	0/5/5/5
4	KMK	A	302	-	-	6/26/36/36	1/4/4/4
3	NDP	B	301	-	-	2/30/77/77	0/5/5/5
3	NDP	A	301	-	-	1/30/77/77	0/5/5/5
4	KMK	B	302	-	-	10/26/36/36	0/4/4/4
4	KMK	C	302	-	-	5/26/36/36	1/4/4/4

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	302	KMK	C9-C6	-7.06	1.39	1.51
4	A	302	KMK	CAU-CBB	-6.35	1.39	1.50
4	A	302	KMK	C7-N8	6.20	1.41	1.31
4	A	302	KMK	C9-C6	-6.16	1.41	1.51
4	C	302	KMK	CAU-CBB	-6.06	1.40	1.50
4	D	302	KMK	C7-N8	6.04	1.41	1.31
4	D	302	KMK	CAU-CBB	-5.42	1.41	1.50
4	B	302	KMK	C7-N8	5.09	1.40	1.31
4	C	302	KMK	C7-N8	5.02	1.39	1.31
4	D	302	KMK	C9-C6	-4.38	1.44	1.51
4	B	302	KMK	CAZ-CBD	3.65	1.60	1.51
3	A	301	NDP	P2B-O2B	3.60	1.66	1.59
4	C	302	KMK	C9-N10	3.59	1.51	1.46
4	D	302	KMK	CAV-NAW	3.44	1.53	1.47
4	B	302	KMK	CAU-CBB	-3.32	1.44	1.50
4	A	302	KMK	CAX-NAW	3.27	1.52	1.47
4	B	302	KMK	CAY-CAZ	3.22	1.61	1.53
4	A	302	KMK	CBA-CAZ	3.08	1.61	1.53
4	B	302	KMK	C9-C6	-3.07	1.46	1.51
4	C	302	KMK	CAZ-CBD	3.02	1.59	1.51
4	D	302	KMK	C9-N10	2.99	1.50	1.46
3	B	301	NDP	P2B-O2B	2.87	1.64	1.59
4	D	302	KMK	CBA-CAZ	2.65	1.59	1.53
4	C	302	KMK	C6-N5	2.65	1.37	1.32
4	B	302	KMK	CAY-CAX	2.57	1.59	1.52
4	A	302	KMK	OBE-CBD	2.56	1.39	1.33
4	A	302	KMK	C9-N10	2.55	1.49	1.46
4	B	302	KMK	OBE-CBD	2.55	1.39	1.33
4	C	302	KMK	CAV-NAW	2.51	1.51	1.47
3	A	301	NDP	C8A-N7A	-2.47	1.30	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	KMK	CAZ-CBD	2.39	1.57	1.51
4	B	302	KMK	CBA-CAZ	2.35	1.59	1.53
4	C	302	KMK	CAR-CAQ	2.34	1.43	1.38
4	A	302	KMK	CAV-NAW	2.34	1.51	1.47
4	C	302	KMK	CAX-NAW	2.29	1.51	1.47
4	D	302	KMK	C6-N5	2.23	1.36	1.32
4	C	302	KMK	OBE-CBD	2.20	1.38	1.33
4	C	302	KMK	C4-N3	2.20	1.37	1.33
4	B	302	KMK	CAV-NAW	2.18	1.50	1.47
4	C	302	KMK	CAY-CAZ	2.15	1.58	1.53
4	B	302	KMK	CAX-NAW	2.13	1.50	1.47
4	C	302	KMK	CBA-CAZ	2.12	1.58	1.53
4	B	302	KMK	C4A-C8A	2.11	1.44	1.40
3	D	301	NDP	P2B-O2B	2.11	1.63	1.59
4	A	302	KMK	CAS-N10	-2.00	1.33	1.38

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	302	KMK	N1-C2-N3	-6.71	118.27	127.22
4	A	302	KMK	N1-C2-N3	-5.95	119.28	127.22
4	B	302	KMK	CAU-CBB-NAW	5.81	126.10	118.72
4	A	302	KMK	C2-N1-C8A	5.71	121.87	115.36
4	D	302	KMK	C2-N1-C8A	5.67	121.84	115.36
4	D	302	KMK	N1-C2-N3	-5.39	120.03	127.22
4	C	302	KMK	CAO-CAS-N10	-4.83	114.72	121.38
4	D	302	KMK	CAU-CBB-NAW	4.81	124.82	118.72
4	B	302	KMK	C9-C6-N5	4.75	124.58	116.96
4	D	302	KMK	C6-C7-N8	-4.58	118.64	123.13
4	A	302	KMK	C6-C7-N8	-4.57	118.65	123.13
4	B	302	KMK	CAP-N10-CAS	4.41	127.94	121.18
4	B	302	KMK	CAX-CAY-CAZ	4.36	117.67	110.41
4	B	302	KMK	C7-C6-N5	-4.23	118.09	120.85
4	A	302	KMK	N8-C8A-N1	4.15	120.56	115.82
4	B	302	KMK	CAR-CAS-N10	4.09	127.02	121.38
4	C	302	KMK	OBE-CBD-CAZ	4.03	117.93	111.76
4	D	302	KMK	C6-C9-N10	3.95	119.41	114.27
4	B	302	KMK	N1-C2-N3	-3.90	122.03	127.22
4	C	302	KMK	C9-C6-N5	3.85	123.13	116.96
4	A	302	KMK	OBE-CBD-CAZ	3.84	117.63	111.76
4	D	302	KMK	C9-C6-N5	3.72	122.93	116.96
4	C	302	KMK	C7-N8-C8A	3.70	120.41	116.69

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	NDP	O2B-P2B-O1X	-3.65	95.31	109.39
4	C	302	KMK	C2-N1-C8A	3.62	119.49	115.36
4	B	302	KMK	C4-C4A-N5	3.59	123.09	120.33
4	C	302	KMK	CAO-CAT-CAU	-3.57	116.63	120.78
4	C	302	KMK	CAT-CAU-CBB	-3.55	111.28	120.29
4	B	302	KMK	C6-C9-N10	3.40	118.69	114.27
4	C	302	KMK	CAQ-CAR-CAS	-3.39	115.86	120.32
4	D	302	KMK	OBC-CBB-CAU	-3.37	113.68	120.23
4	B	302	KMK	OBE-CBD-CAZ	3.36	116.91	111.76
4	C	302	KMK	C6-C7-N8	-3.30	119.89	123.13
4	C	302	KMK	OBC-CBB-CAU	-3.21	113.97	120.23
4	C	302	KMK	N2-C2-N1	3.17	122.96	117.79
4	D	302	KMK	C4-C4A-N5	3.17	122.77	120.33
4	C	302	KMK	C4A-C4-N4	-3.16	115.55	120.35
4	D	302	KMK	CAX-NAW-CAV	3.15	118.69	112.62
4	C	302	KMK	N8-C8A-N1	3.14	119.41	115.82
4	B	302	KMK	N8-C8A-N1	3.10	119.36	115.82
4	D	302	KMK	CAX-CAY-CAZ	-3.10	105.25	110.41
4	C	302	KMK	C9-C6-C7	-3.09	116.22	121.60
4	D	302	KMK	N8-C8A-N1	2.97	119.21	115.82
4	B	302	KMK	CAY-CAZ-CBA	2.95	116.21	109.97
4	D	302	KMK	CAO-CAS-N10	-2.93	117.34	121.38
4	B	302	KMK	C7-N8-C8A	2.92	119.62	116.69
4	A	302	KMK	C7-N8-C8A	2.91	119.62	116.69
4	A	302	KMK	N2-C2-N3	2.88	121.73	117.25
3	B	301	NDP	C5A-C6A-N6A	2.88	124.72	120.35
4	B	302	KMK	CAQ-CAR-CAS	2.87	124.10	120.32
3	B	301	NDP	O2B-P2B-O1X	-2.87	98.30	109.39
4	C	302	KMK	N4-C4-N3	2.87	124.87	117.07
4	B	302	KMK	CAQ-CAU-CBB	2.84	127.49	120.29
4	C	302	KMK	CAT-CAO-CAS	2.80	124.01	120.32
4	B	302	KMK	OBC-CBB-NAW	-2.76	117.78	122.34
4	D	302	KMK	CAR-CAS-N10	2.76	125.18	121.38
4	D	302	KMK	OBE-CBD-CAZ	2.75	115.97	111.76
4	A	302	KMK	C4A-C4-N4	-2.75	116.18	120.35
4	C	302	KMK	CAR-CAS-N10	2.74	125.15	121.38
4	C	302	KMK	CAQ-CAU-CBB	2.70	127.13	120.29
4	D	302	KMK	N2-C2-N3	2.70	121.45	117.25
4	B	302	KMK	N2-C2-N1	2.66	122.13	117.79
3	A	301	NDP	O3B-C3B-C2B	2.62	118.60	111.17
4	D	302	KMK	C7-N8-C8A	2.60	119.31	116.69
4	D	302	KMK	CAT-CAO-CAS	2.60	123.75	120.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	KMK	C2-N1-C8A	2.59	118.32	115.36
4	D	302	KMK	C9-C6-C7	-2.56	117.14	121.60
3	A	301	NDP	O4B-C4B-C3B	-2.55	100.06	105.11
3	A	301	NDP	C5A-C6A-N6A	2.47	124.10	120.35
4	B	302	KMK	C9-C6-C7	-2.45	117.32	121.60
4	C	302	KMK	C6-C9-N10	2.37	117.35	114.27
4	B	302	KMK	C9-N10-CAP	-2.36	110.71	116.07
4	B	302	KMK	C6-N5-C4A	2.36	121.86	118.04
4	B	302	KMK	CAO-CAT-CAU	2.34	123.50	120.78
4	B	302	KMK	CAO-CAS-N10	-2.34	118.16	121.38
3	D	301	NDP	O4B-C4B-C3B	-2.33	100.50	105.11
3	C	301	NDP	O3D-C3D-C4D	-2.27	104.48	111.05
3	D	301	NDP	C3N-C7N-N7N	2.21	121.60	117.67
4	C	302	KMK	C4A-C4-N3	-2.20	119.56	121.01
4	A	302	KMK	OBC-CBB-CAU	-2.18	115.98	120.23
4	C	302	KMK	CAU-CBB-NAW	2.18	121.48	118.72
4	A	302	KMK	N4-C4-N3	2.17	122.97	117.07
3	D	301	NDP	O7N-C7N-C3N	-2.16	116.83	120.90
4	D	302	KMK	CAQ-CAU-CBB	2.15	125.72	120.29
4	D	302	KMK	C8A-C4A-N5	-2.13	119.83	122.41
4	B	302	KMK	CAR-CAS-CAO	-2.13	114.82	119.16
4	A	302	KMK	C9-C6-N5	2.13	120.37	116.96
4	B	302	KMK	OBC-CBB-CAU	-2.12	116.10	120.23
3	A	301	NDP	C3N-C2N-N1N	-2.10	120.09	123.10
4	C	302	KMK	CAQ-CAU-CAT	2.10	121.58	118.59
3	C	301	NDP	C5A-C6A-N6A	2.10	123.54	120.35
3	D	301	NDP	O2B-C2B-C3B	2.06	119.16	111.68
4	D	302	KMK	CAT-CAU-CBB	-2.04	115.11	120.29
3	D	301	NDP	O3X-P2B-O2X	2.01	115.32	107.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	NDP	C5B-O5B-PA-O3
4	B	302	KMK	N10-CAP-CBH-CBI
4	B	302	KMK	CAP-CBH-CBI-OBJ
4	C	302	KMK	CAZ-CBD-OBE-CBG
4	D	302	KMK	CAZ-CBD-OBE-CBG
4	B	302	KMK	CAZ-CBD-OBE-CBG
4	C	302	KMK	OBF-CBD-OBE-CBG
4	A	302	KMK	CAZ-CBD-OBE-CBG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	D	302	KMK	OBF-CBD-OBE-CBG
4	B	302	KMK	OBF-CBD-OBE-CBG
3	B	301	NDP	O4D-C1D-N1N-C6N
3	A	301	NDP	O4D-C1D-N1N-C6N
4	B	302	KMK	CBH-CAP-N10-CAS
4	A	302	KMK	OBF-CBD-OBE-CBG
3	D	301	NDP	O4D-C1D-N1N-C6N
3	C	301	NDP	O4D-C1D-N1N-C6N
4	A	302	KMK	N10-CAP-CBH-CBI
4	B	302	KMK	CAQ-CAU-CBB-OBC
4	B	302	KMK	CAQ-CAU-CBB-NAW
4	B	302	KMK	CBH-CAP-N10-C9
4	C	302	KMK	CAP-CBH-CBI-OBJ
4	B	302	KMK	CAT-CAU-CBB-OBC
4	B	302	KMK	CAT-CAU-CBB-NAW
4	A	302	KMK	CAY-CAZ-CBD-OBE
4	A	302	KMK	CBH-CAP-N10-CAS
4	C	302	KMK	N10-CAP-CBH-CBI
4	A	302	KMK	CAY-CAZ-CBD-OBF
3	B	301	NDP	PN-O3-PA-O2A
4	C	302	KMK	CBH-CAP-N10-CAS
3	C	301	NDP	C5B-O5B-PA-O1A

All (2) ring outliers are listed below:

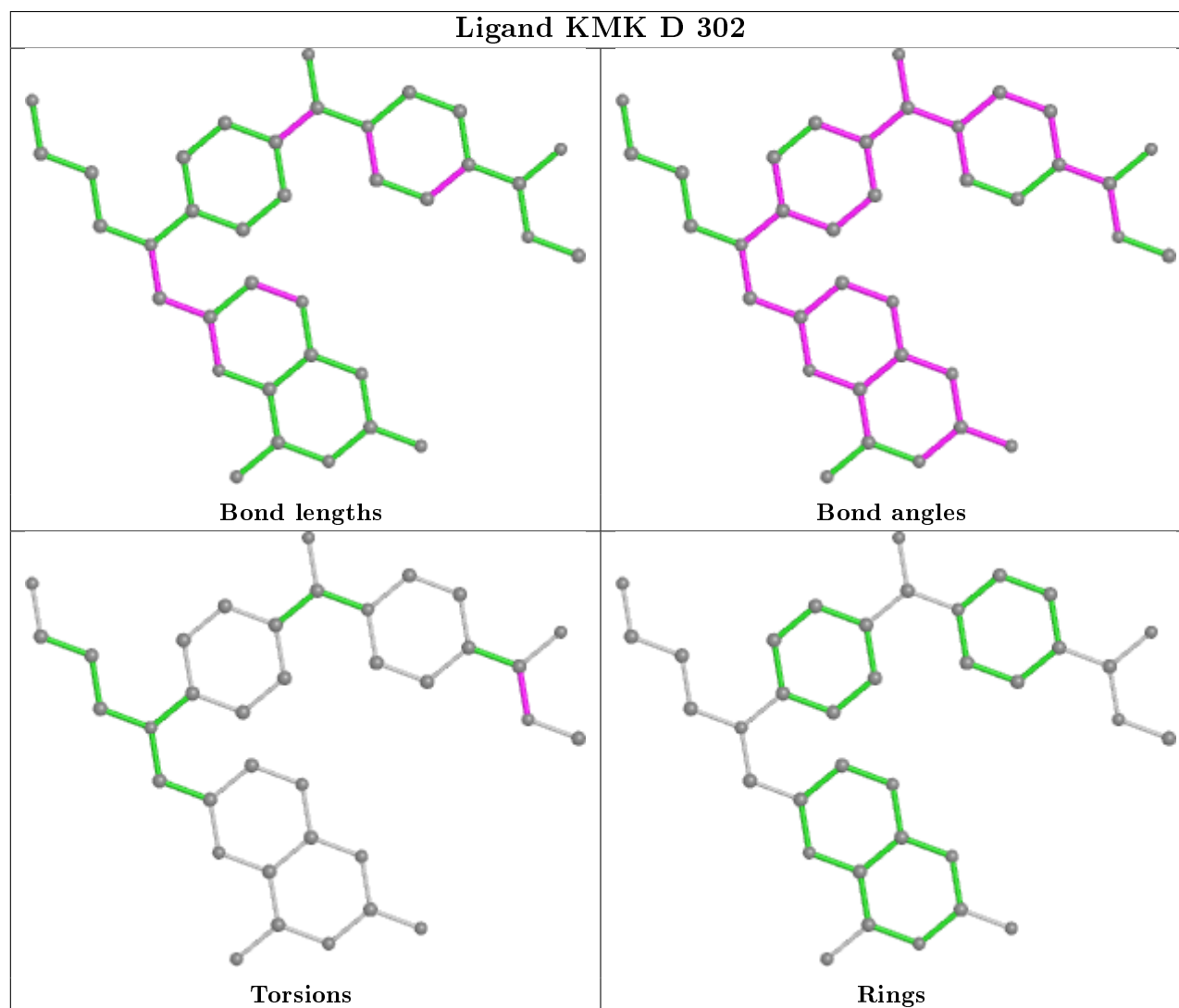
Mol	Chain	Res	Type	Atoms
4	C	302	KMK	CAV-CAX-CAY-CAZ-CBA-NAW
4	A	302	KMK	CAV-CAX-CAY-CAZ-CBA-NAW

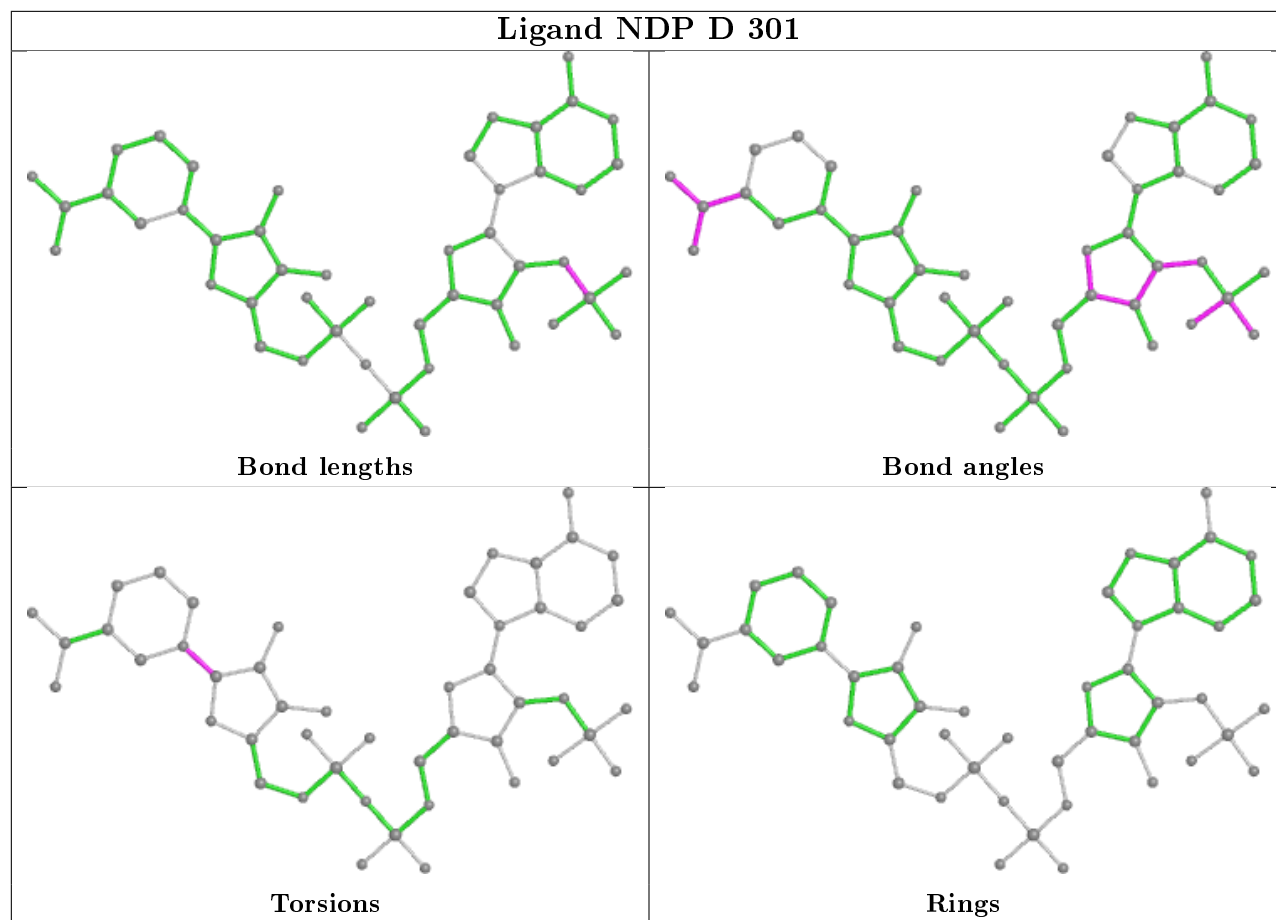
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	KMK	3	0
3	C	301	NDP	1	0
4	A	302	KMK	1	0
3	B	301	NDP	2	0
4	B	302	KMK	1	0
4	C	302	KMK	1	0

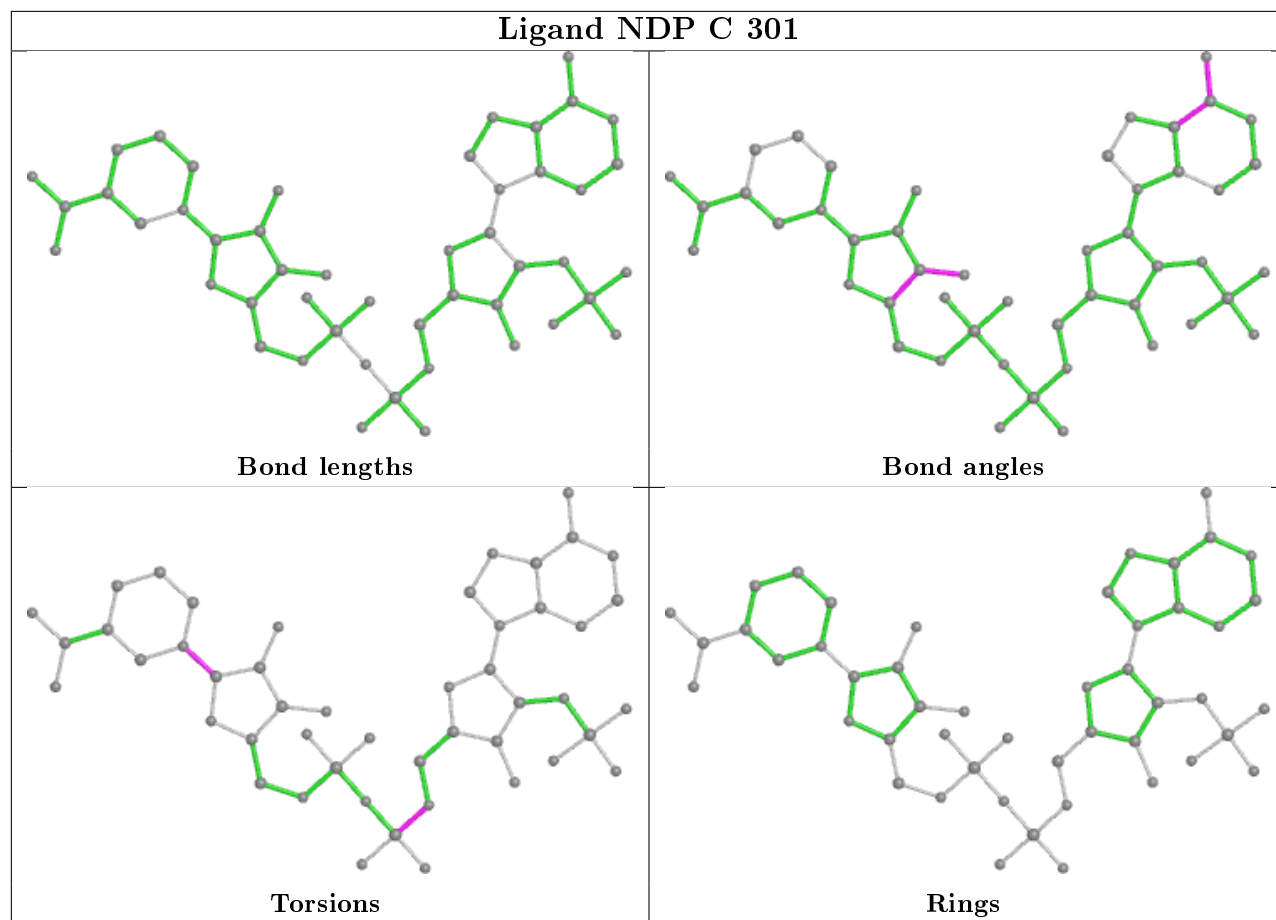
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

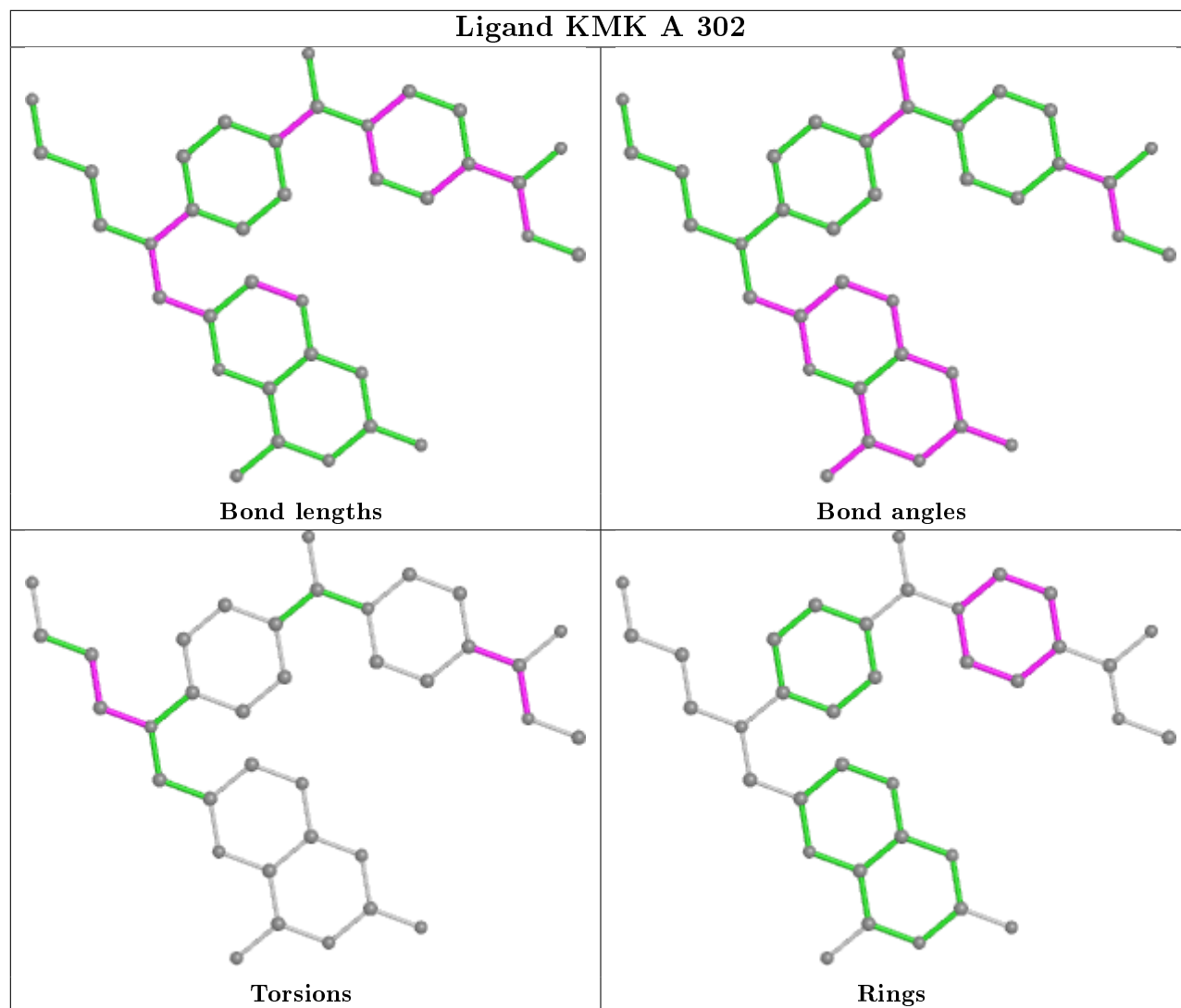
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

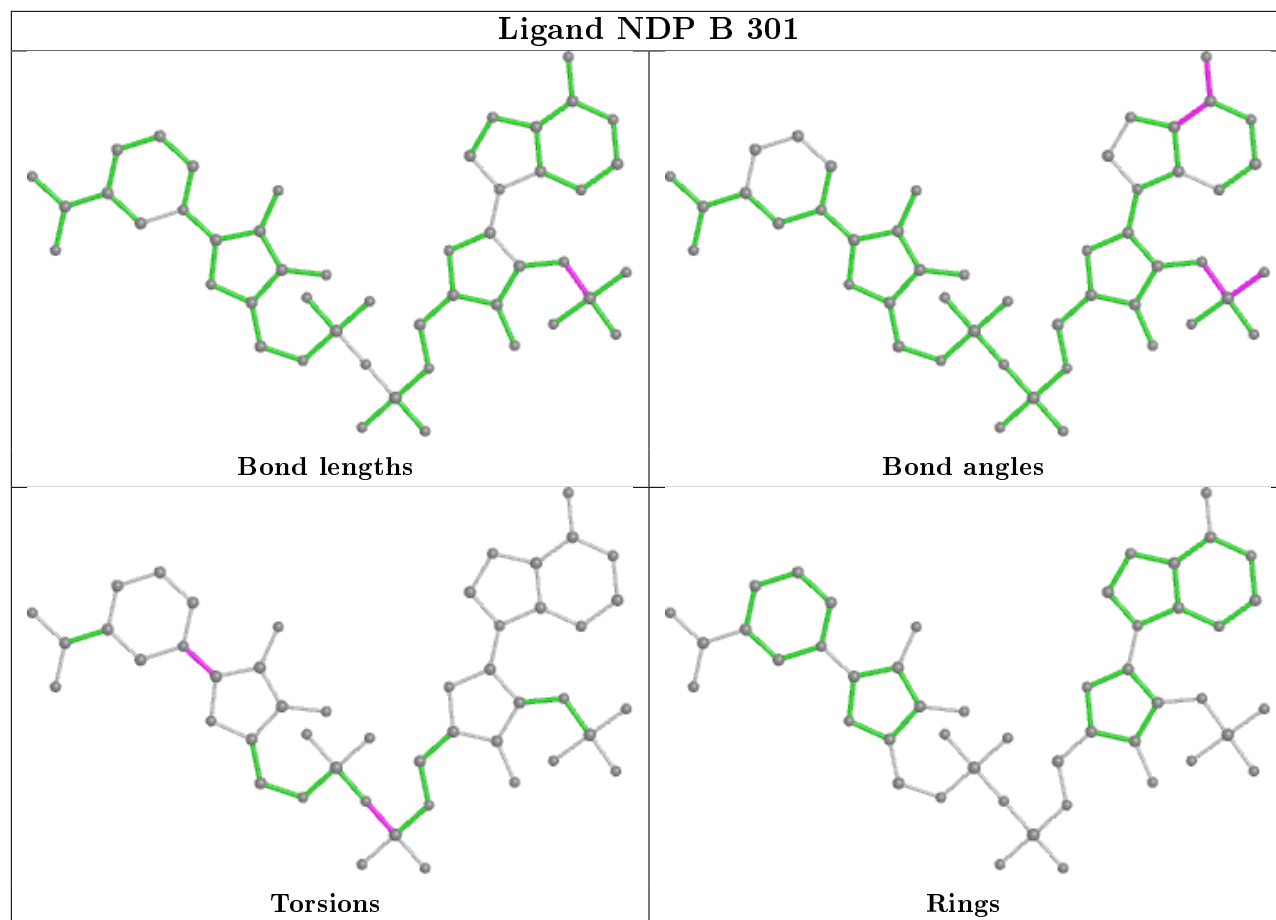


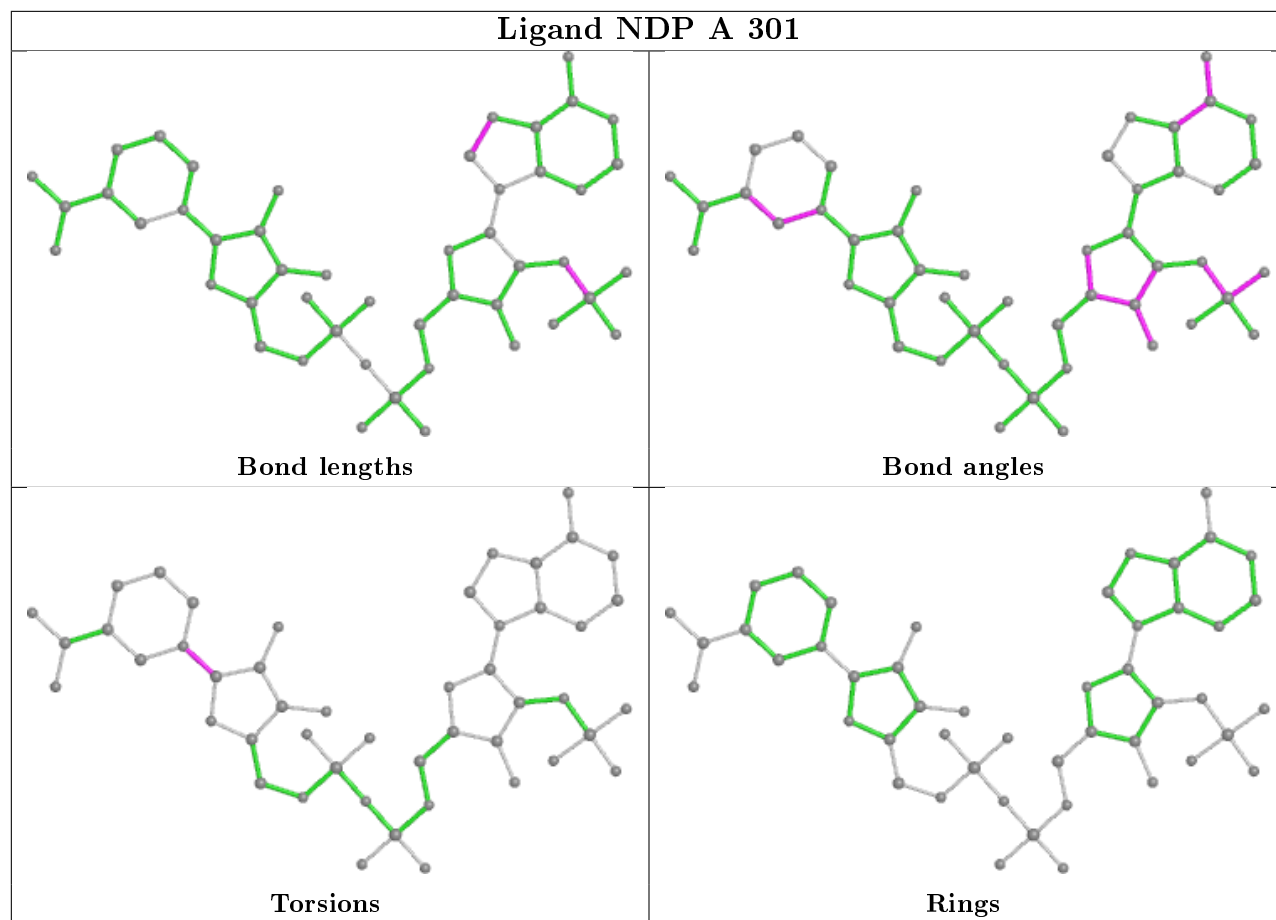


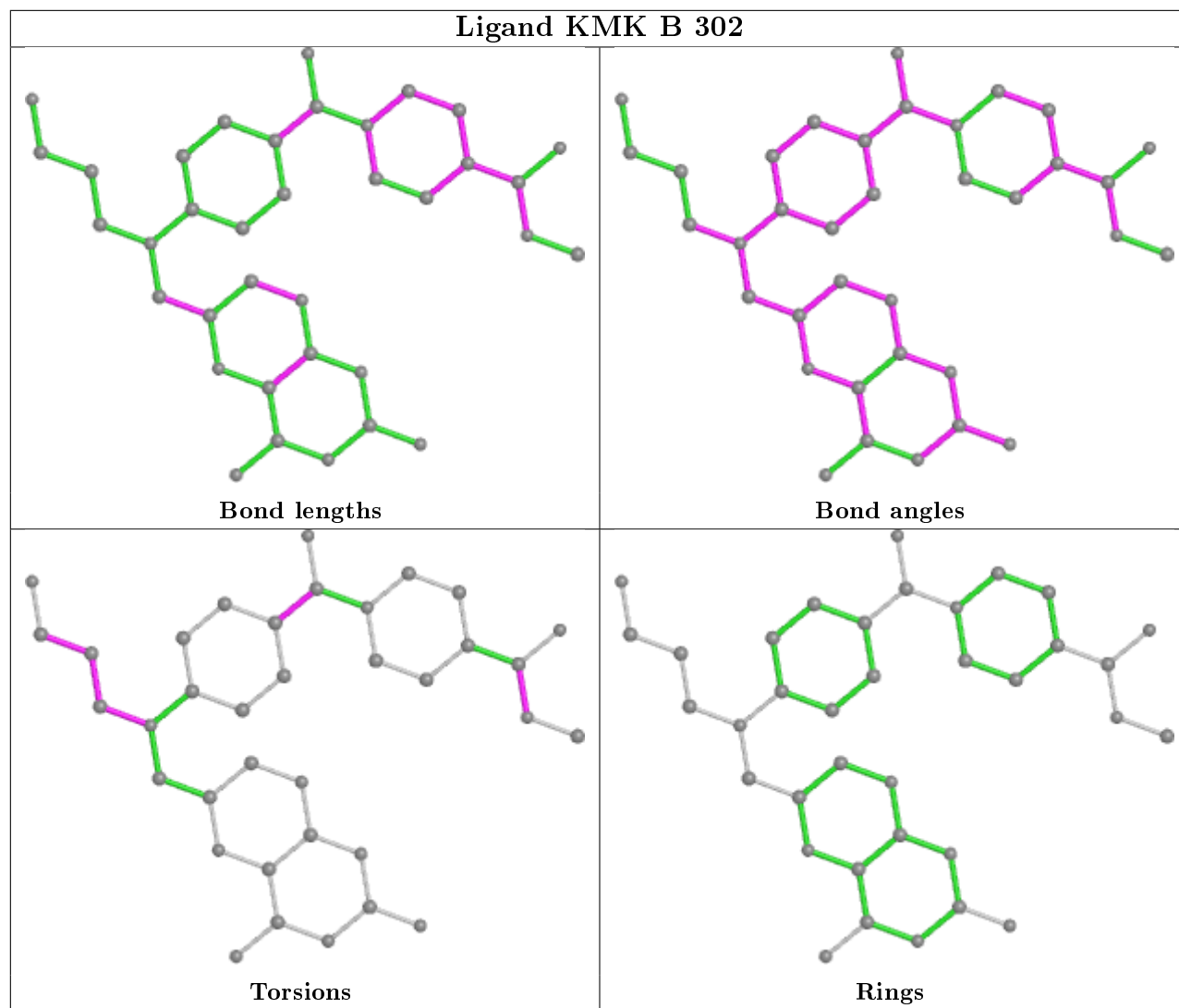


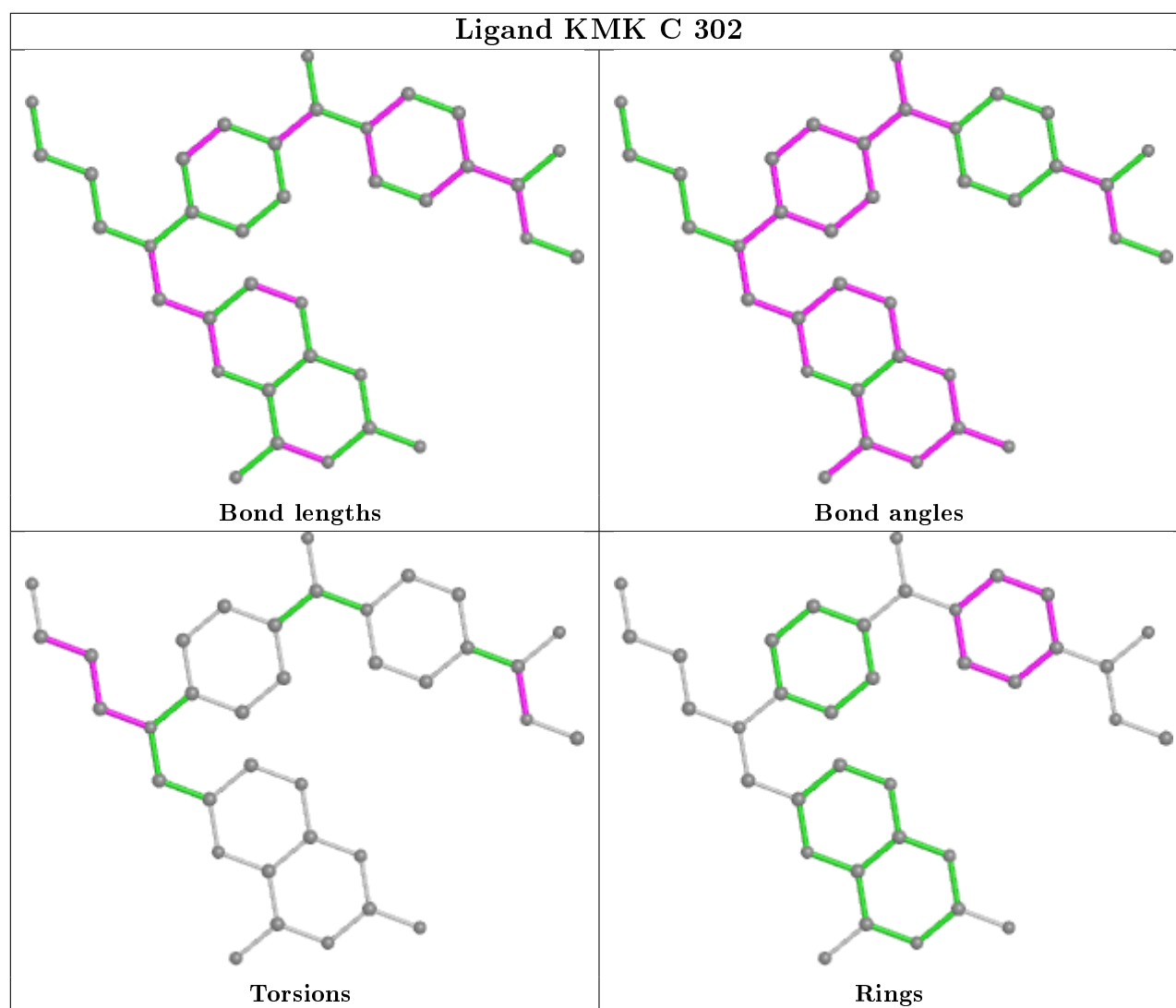












## 5.7 Other polymers [i](#)

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 ⓘ

### 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	263/291 (90%)	-0.02	4 (1%) 73 77	12, 22, 48, 79	0
1	C	261/291 (89%)	-0.11	8 (3%) 49 55	12, 22, 50, 75	0
2	B	260/291 (89%)	0.13	2 (0%) 86 88	14, 29, 52, 67	0
2	D	255/291 (87%)	-0.02	4 (1%) 72 75	16, 27, 50, 77	0
All	All	1039/1164 (89%)	-0.00	18 (1%) 70 74	12, 25, 51, 79	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	238	TRP	4.5
1	C	236	ALA	4.4
1	A	121	ASN	4.1
2	D	238	TRP	3.9
1	A	234	PRO	3.5
2	D	136	MET	3.3
2	D	5	THR	3.3
2	D	237	VAL	3.3
1	A	236	ALA	3.1
1	C	5	THR	2.8
1	C	81	ALA	2.7
2	B	234	PRO	2.5
1	C	136	MET	2.4
1	A	238	TRP	2.2
2	B	235	PRO	2.2
1	C	230	VAL	2.1
1	C	237	VAL	2.1
1	C	120	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CSX	B	276[A]	7/8	0.88	0.17	25,26,31,32	4
2	CSX	B	276[B]	7/8	0.88	0.17	26,30,36,40	4
2	CSX	D	276	7/8	0.91	0.12	25,31,49,50	0

## 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.

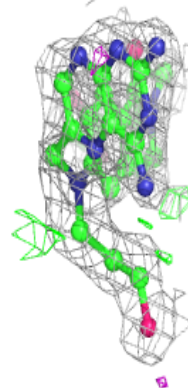
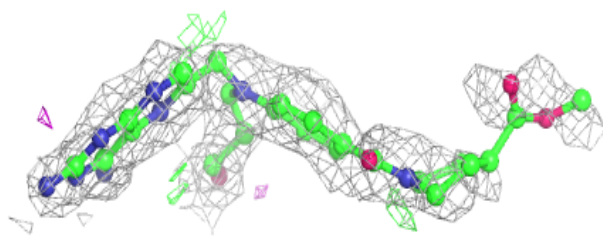
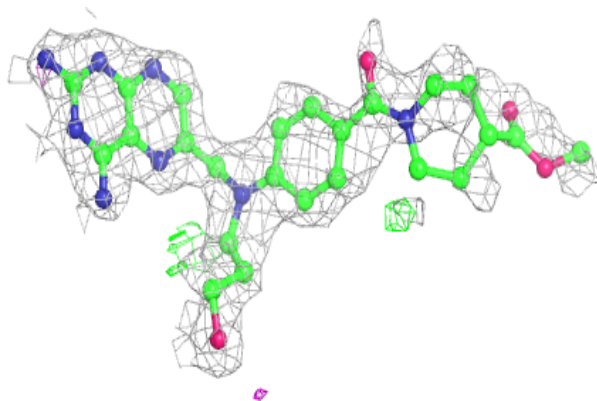
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	KMK	B	302	36/36	0.87	0.21	29,45,82,90	0
4	KMK	A	302	36/36	0.90	0.19	24,46,76,77	0
4	KMK	C	302	36/36	0.92	0.15	21,36,94,113	0
4	KMK	D	302	36/36	0.93	0.19	26,42,61,70	0
3	NDP	B	301	48/48	0.95	0.12	18,24,30,33	0
3	NDP	D	301	48/48	0.96	0.11	21,29,34,35	0
3	NDP	C	301	48/48	0.97	0.10	14,22,26,29	0
3	NDP	A	301	48/48	0.97	0.11	14,21,27,28	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.

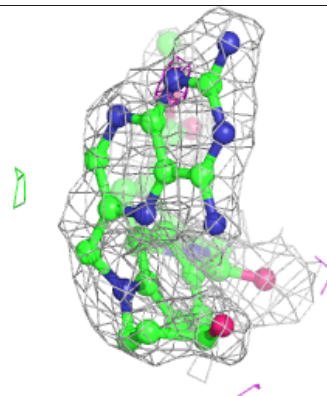
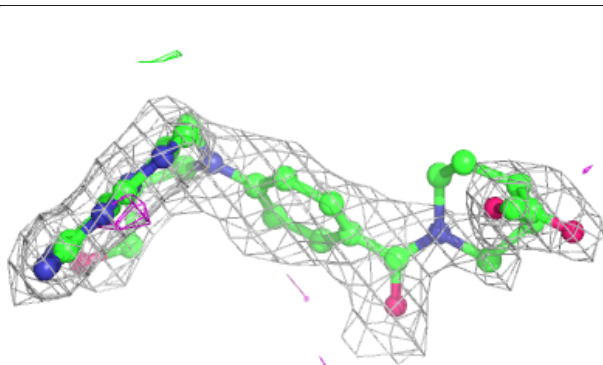
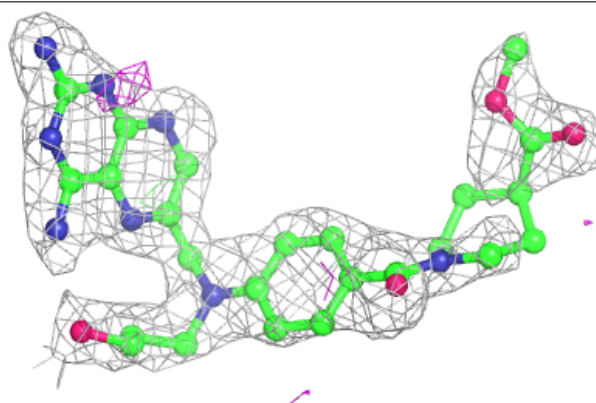


**Electron density around KMK B 302:**

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

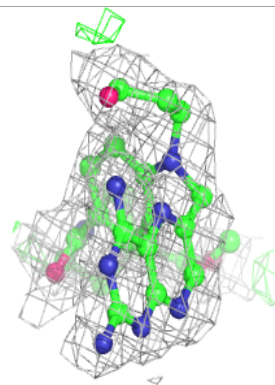
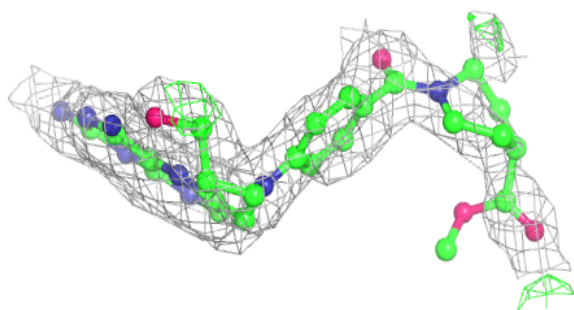
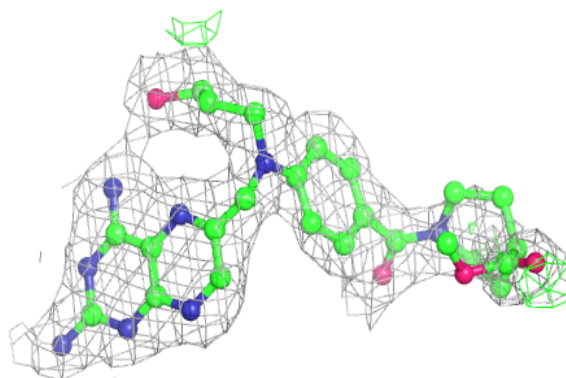
**Electron density around KMK A 302:**

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

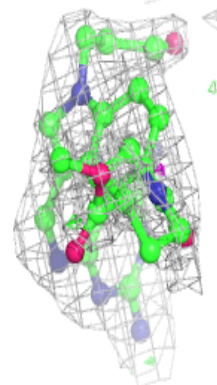
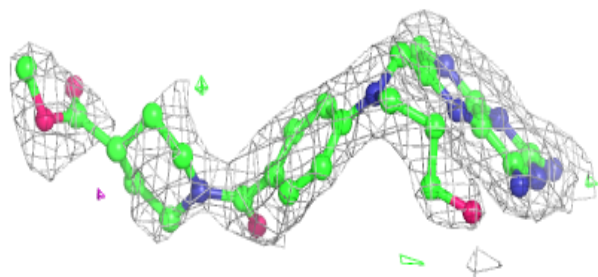
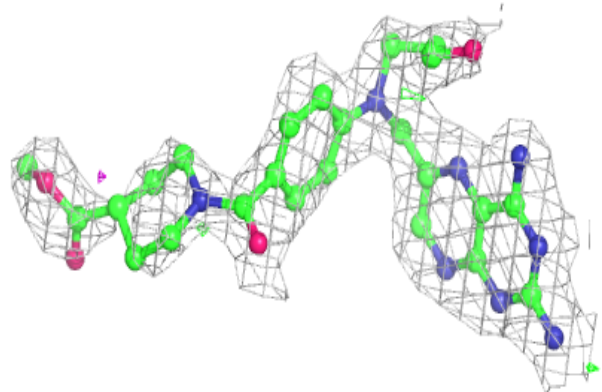


**Electron density around KMK C 302:**

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

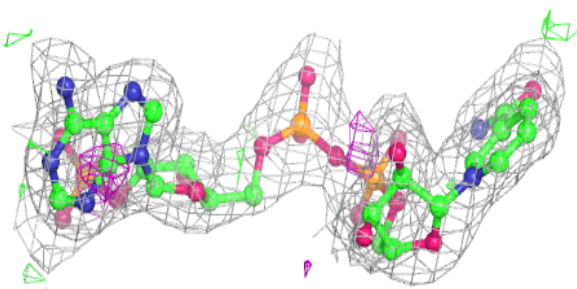
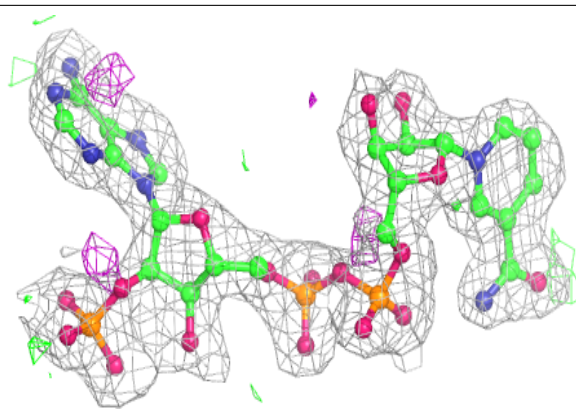
**Electron density around KMK D 302:**

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

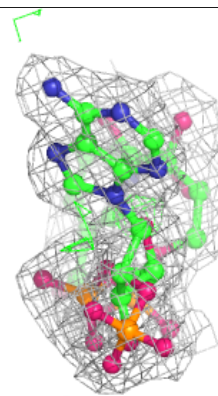
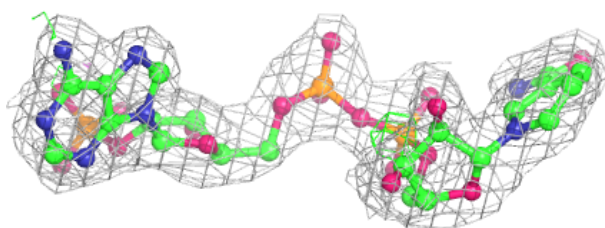
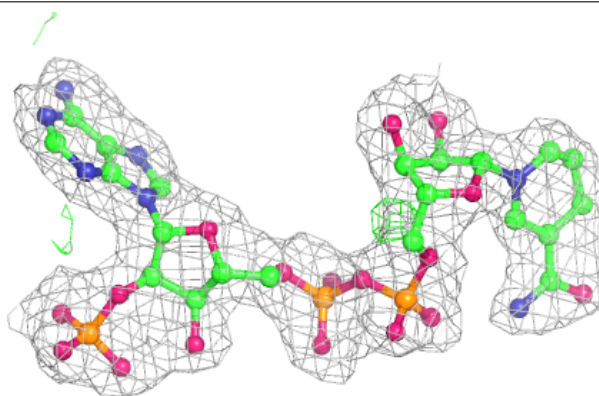


**Electron density around NDP B 301:**

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

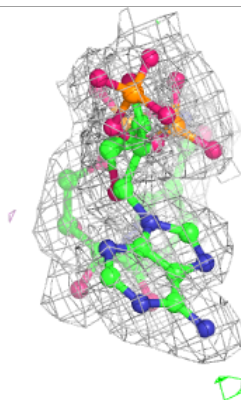
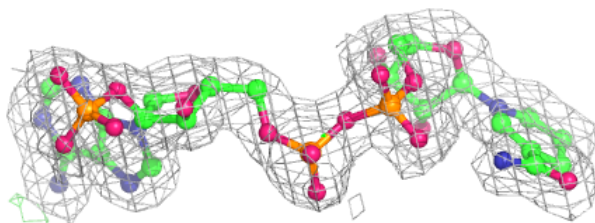
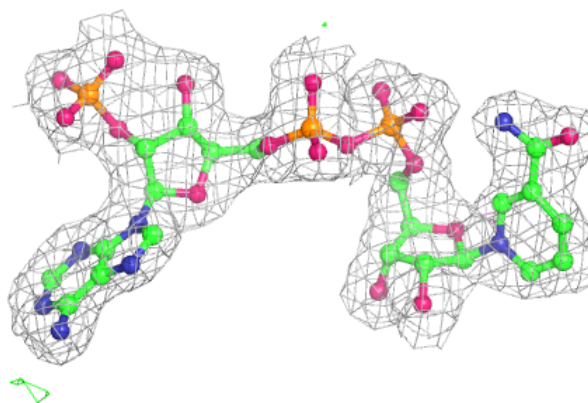
**Electron density around NDP D 301:**

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

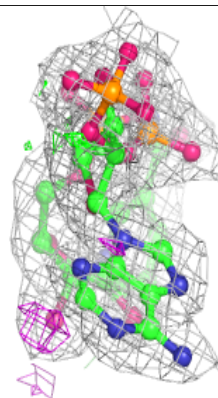
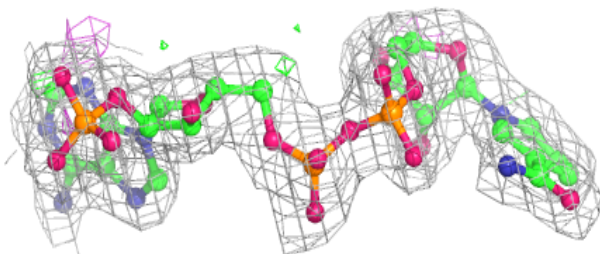
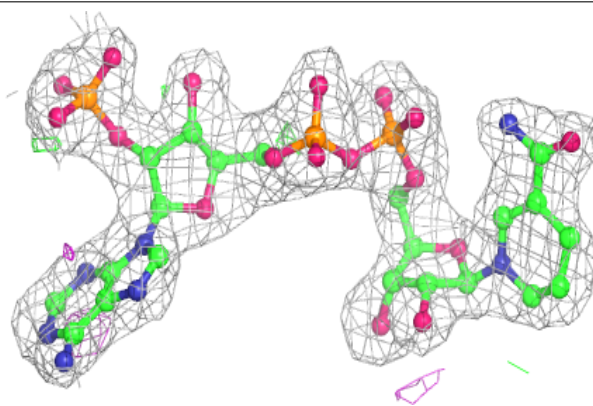


**Electron density around NDP C 301:**

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

**Electron density around NDP A 301:**

$2mF_o-DF_c$  (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.