



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:30 am BST

PDB ID : 4K42  
Title : Crystal structure of actin in complex with synthetic AplC tail analogue SF01 [(3R,4S,5R,6S,10R,11R,12R)-11-(acetyloxy)-1-(benzyloxy)-14-[formyl(methyl)amino]-5-hydroxy-4,6,10,12-tetramethyl-9-oxotetradecan-3-yl propanoate]  
Authors : Pereira, J.H.; Petchprayoon, C.; Moriarty, N.W.; Fink, S.J.; Cecere, G.; Paterson, I.; Adams, P.D.; Marriott, G.  
Deposited on : 2013-04-11  
Resolution : 2.90 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	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

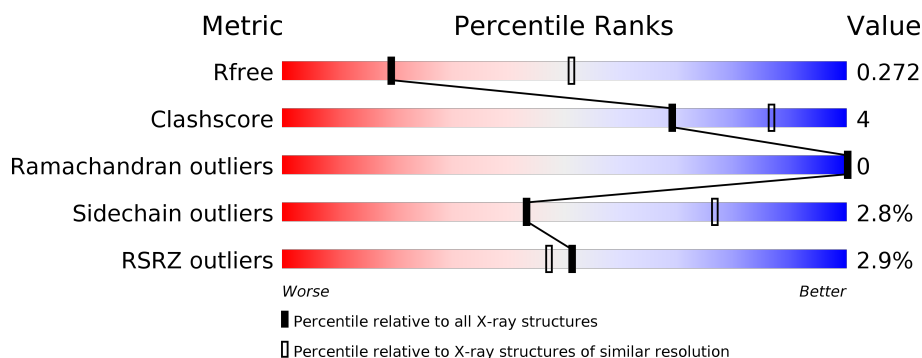
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	375	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>
1	B	375	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>• •</div> </div> </div>
1	C	375	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>• •</div> </div> </div>
1	D	375	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23113 atoms, of which 11450 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	360	Total	C	H	N	O	S	0	0	0
			5611	1784	2796	472	540	19			
1	B	361	Total	C	H	N	O	S	0	0	0
			5635	1790	2809	476	541	19			
1	C	361	Total	C	H	N	O	S	0	0	0
			5635	1790	2809	476	541	19			
1	D	360	Total	C	H	N	O	S	0	0	0
			5611	1784	2796	472	540	19			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

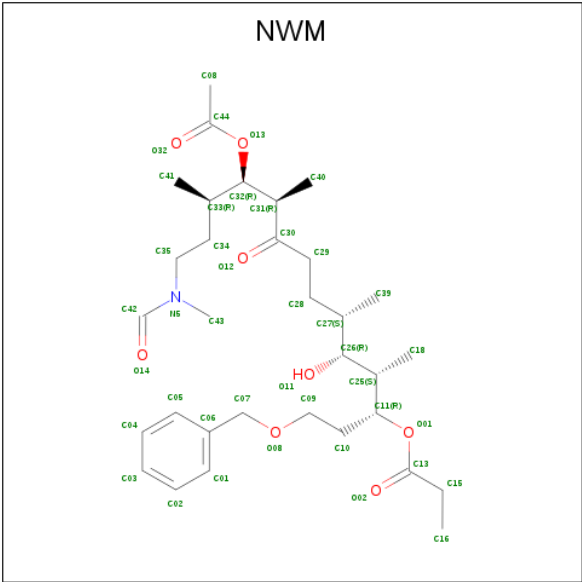
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
3	B	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
3	C	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
3	D	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0

- Molecule 4 is (3R,4S,5R,6S,10R,11R,12R)-11-(acetyloxy)-1-(benzyloxy)-14-[formyl(methyl) amino]-5-hydroxy-4,6,10,12-tetramethyl-9-oxotetradecan-3-yl propanoate (three-letter code: NWM) (formula: C<sub>32</sub>H<sub>51</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			90	32	49	1	8		
4	B	1	Total	C	H	N	O	0	0
			90	32	49	1	8		
4	C	1	Total	C	H	N	O	0	0
			90	32	49	1	8		
4	D	1	Total	C	H	N	O	0	0
			90	32	49	1	8		

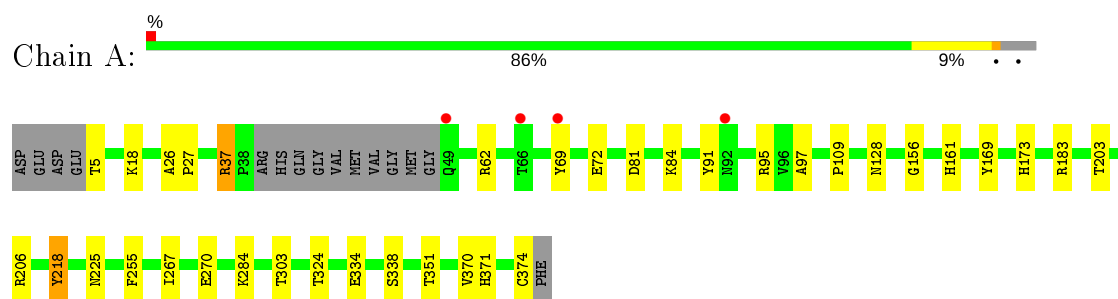
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	42	Total	O	0	0
			42	42		
5	B	15	Total	O	0	0
			15	15		
5	C	35	Total	O	0	0
			35	35		
5	D	13	Total	O	0	0
			13	13		

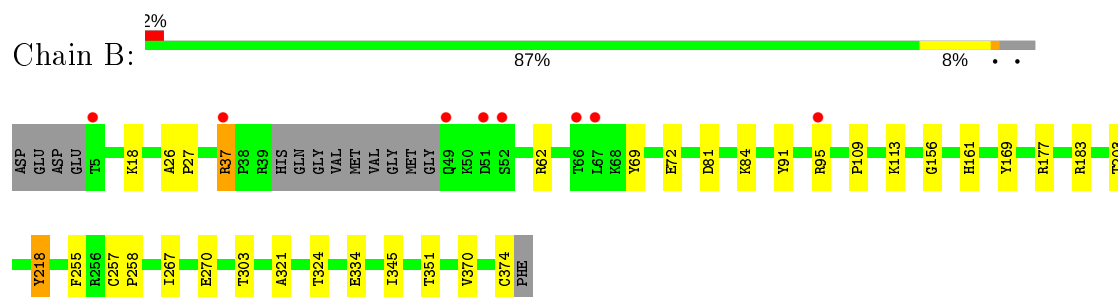
### 3 Residue-property plots [i](#)

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

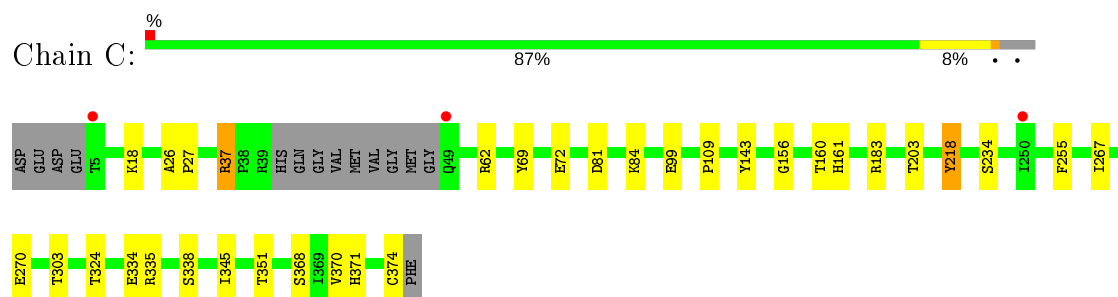
- Molecule 1: Actin, alpha skeletal muscle



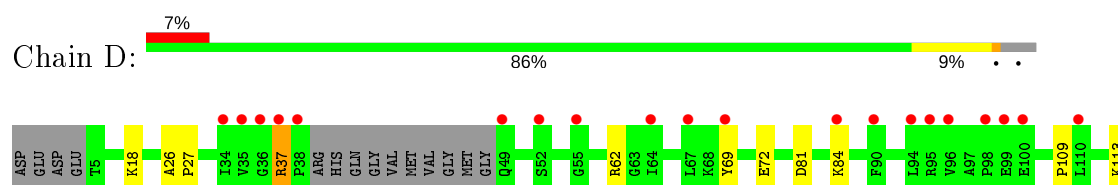
- Molecule 1: Actin, alpha skeletal muscle

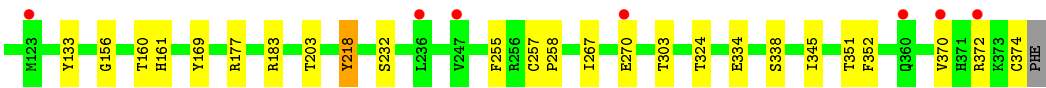


- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.65Å 67.34Å 207.85Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	49.19 – 2.90 49.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	84.0 (49.19-2.90) 74.9 (49.19-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.228 , 0.271 0.231 , 0.272	Depositor DCC
$R_{free}$ test set	1443 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	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 69.93 % 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 3.4033e-06. 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: NWM, CA, ADP

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	0.35	2/2875 (0.1%)	0.44	0/3897
1	B	0.33	0/2886	0.45	0/3911
1	C	0.29	0/2886	0.44	0/3911
1	D	0.27	0/2875	0.44	0/3897
All	All	0.31	2/11522 (0.0%)	0.44	0/15616

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	ASN	CG-ND2	-7.74	1.13	1.32
1	A	225	ASN	CG-OD1	-6.09	1.10	1.24

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	2815	2796	2788	24	0
1	B	2826	2809	2801	20	3
1	C	2826	2809	2801	18	2
1	D	2815	2796	2788	25	1
2	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	11	12	1	0
3	B	27	11	12	1	0
3	C	27	11	12	1	0
3	D	27	11	12	1	0
4	A	41	49	51	4	0
4	B	41	49	51	4	0
4	C	41	49	51	6	0
4	D	41	49	51	3	0
5	A	42	0	0	1	1
5	B	15	0	0	0	0
5	C	35	0	0	1	1
5	D	13	0	0	0	0
All	All	11663	11450	11430	84	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:HIS:HE1	1:A:284:LYS:O	1.64	0.81
1:C:18:LYS:NZ	3:C:402:ADP:O2B	2.14	0.80
1:B:18:LYS:NZ	3:B:402:ADP:O2B	2.25	0.69
1:D:18:LYS:NZ	3:D:402:ADP:O2B	2.26	0.68
1:A:97:ALA:HB2	1:D:113:LYS:NZ	2.12	0.63
1:A:128:ASN:ND2	1:D:372:ARG:CD	2.65	0.59
1:A:351:THR:HG23	4:A:403:NWM:H332	1.85	0.57
1:C:351:THR:HG23	4:C:403:NWM:H332	1.88	0.56
1:A:169:TYR:CE1	4:A:403:NWM:H2	2.43	0.54
1:B:109:PRO:HG2	1:B:161:HIS:ND1	2.24	0.53
1:D:345:ILE:HD13	4:D:403:NWM:H161	1.90	0.53
1:A:334:GLU:N	1:A:334:GLU:OE1	2.41	0.53
1:B:345:ILE:HD13	4:B:403:NWM:H161	1.91	0.53
1:A:173:HIS:CE1	1:A:284:LYS:O	2.55	0.52
1:A:97:ALA:HB2	1:D:113:LYS:HZ2	1.74	0.52
4:C:403:NWM:H183	4:C:403:NWM:H282	1.91	0.52
1:A:128:ASN:ND2	1:D:372:ARG:HD3	2.24	0.51
1:D:334:GLU:OE1	1:D:334:GLU:N	2.39	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:GLY:O	1:D:303:THR:OG1	2.28	0.51
1:D:109:PRO:HG2	1:D:161:HIS:ND1	2.26	0.51
1:D:169:TYR:CE1	4:D:403:NWM:H2	2.46	0.50
1:B:370:VAL:HG23	1:B:374:CYS:SG	2.51	0.50
1:B:37:ARG:NH1	1:B:81:ASP:OD1	2.45	0.49
1:B:334:GLU:N	1:B:334:GLU:OE1	2.40	0.49
1:A:218:TYR:CE1	1:A:255:PHE:HB3	2.48	0.49
1:B:161:HIS:HE2	1:B:177:ARG:HG3	1.78	0.49
1:C:156:GLY:O	1:C:303:THR:OG1	2.29	0.49
1:C:334:GLU:OE1	1:C:334:GLU:N	2.42	0.49
1:A:37:ARG:NH1	1:A:81:ASP:OD1	2.46	0.48
1:D:37:ARG:NH1	1:D:81:ASP:OD1	2.46	0.48
1:C:37:ARG:NH1	1:C:81:ASP:OD1	2.46	0.48
1:D:72:GLU:HB2	1:D:183:ARG:HH12	1.79	0.48
1:C:72:GLU:HB2	1:C:183:ARG:HH12	1.79	0.48
1:B:351:THR:HG23	4:B:403:NWM:H332	1.96	0.48
1:C:218:TYR:CE1	1:C:255:PHE:HB3	2.49	0.47
1:D:218:TYR:CE1	1:D:255:PHE:HB3	2.49	0.47
1:B:156:GLY:O	1:B:303:THR:OG1	2.29	0.47
1:A:206:ARG:NH1	5:A:515:HOH:O	2.48	0.47
1:C:109:PRO:HG2	1:C:161:HIS:ND1	2.30	0.47
4:B:403:NWM:H282	4:B:403:NWM:H183	1.96	0.47
1:B:218:TYR:CE1	1:B:255:PHE:HB3	2.49	0.47
1:C:234:SER:N	5:C:505:HOH:O	2.45	0.47
1:D:351:THR:HG23	4:D:403:NWM:H332	1.97	0.46
1:A:72:GLU:HB2	1:A:183:ARG:HH12	1.80	0.46
1:B:72:GLU:HB2	1:B:183:ARG:HH12	1.80	0.46
1:A:95:ARG:NH1	1:B:91:TYR:O	2.49	0.45
1:C:370:VAL:HG23	1:C:374:CYS:SG	2.56	0.45
1:B:109:PRO:HD2	1:B:161:HIS:ND1	2.31	0.45
1:C:143:TYR:HE2	4:C:403:NWM:H433	1.82	0.45
1:D:370:VAL:HG23	1:D:374:CYS:SG	2.57	0.45
1:D:161:HIS:HE2	1:D:177:ARG:HG3	1.79	0.45
4:A:403:NWM:H183	4:A:403:NWM:H282	1.98	0.45
1:B:62:ARG:NH1	1:B:203:THR:OG1	2.50	0.45
1:A:156:GLY:O	1:A:303:THR:OG1	2.29	0.44
1:C:62:ARG:NH1	1:C:203:THR:OG1	2.50	0.44
1:A:62:ARG:NH1	1:A:203:THR:OG1	2.51	0.44
1:C:109:PRO:HB2	1:C:161:HIS:ND1	2.33	0.44
1:A:370:VAL:HG23	1:A:374:CYS:SG	2.58	0.44
1:A:109:PRO:HG2	1:A:161:HIS:ND1	2.33	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TYR:CE2	4:C:403:NWM:H433	2.53	0.43
1:D:257:CYS:HB3	1:D:258:PRO:HD3	2.01	0.43
1:A:18:LYS:NZ	3:A:402:ADP:O2B	2.51	0.43
1:A:97:ALA:CB	1:D:113:LYS:NZ	2.81	0.43
4:A:403:NWM:H403	4:A:403:NWM:H351	2.01	0.43
1:A:91:TYR:O	1:B:95:ARG:NH1	2.51	0.43
1:D:62:ARG:NH1	1:D:203:THR:OG1	2.52	0.43
1:D:26:ALA:HB1	1:D:27:PRO:HD2	2.01	0.42
1:A:109:PRO:HB2	1:A:161:HIS:ND1	2.34	0.42
1:D:109:PRO:HD2	1:D:161:HIS:ND1	2.35	0.42
1:B:26:ALA:HB1	1:B:27:PRO:HD2	2.02	0.42
1:C:26:ALA:HB1	1:C:27:PRO:HD2	2.01	0.42
1:A:26:ALA:HB1	1:A:27:PRO:HD2	2.01	0.42
1:A:97:ALA:CB	1:D:113:LYS:HZ1	2.33	0.42
1:C:345:ILE:HG21	4:C:403:NWM:H151	2.02	0.42
1:B:169:TYR:CE1	4:B:403:NWM:H2	2.56	0.41
1:D:109:PRO:CG	1:D:161:HIS:ND1	2.83	0.41
1:D:160:THR:O	1:D:161:HIS:HD2	2.04	0.41
1:B:109:PRO:CG	1:B:161:HIS:ND1	2.83	0.41
1:B:161:HIS:HD2	1:B:177:ARG:HA	1.84	0.41
1:C:160:THR:O	1:C:161:HIS:HD2	2.03	0.41
1:C:335:ARG:HA	1:C:338:SER:HB2	2.02	0.41
1:D:133:TYR:CD2	1:D:352:PHE:HZ	2.40	0.40
1:B:257:CYS:HB3	1:B:258:PRO:HD3	2.04	0.40
4:C:403:NWM:H351	4:C:403:NWM:H403	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ALA:O	5:A:527:HOH:O[1_445]	2.01	0.19
1:B:113:LYS:HZ2	1:C:99:GLU:OE1[1_455]	1.51	0.09
1:B:113:LYS:NZ	1:C:99:GLU:OE1[1_455]	2.13	0.07
1:D:232:SER:OG	5:C:515:HOH:O[2_555]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	356/375 (95%)	349 (98%)	7 (2%)	0	100	100
1	B	357/375 (95%)	349 (98%)	8 (2%)	0	100	100
1	C	357/375 (95%)	349 (98%)	8 (2%)	0	100	100
1	D	356/375 (95%)	348 (98%)	8 (2%)	0	100	100
All	All	1426/1500 (95%)	1395 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	306/318 (96%)	296 (97%)	10 (3%)	38	72
1	B	307/318 (96%)	300 (98%)	7 (2%)	50	80
1	C	307/318 (96%)	298 (97%)	9 (3%)	42	76
1	D	306/318 (96%)	298 (97%)	8 (3%)	46	77
All	All	1226/1272 (96%)	1192 (97%)	34 (3%)	43	76

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	37	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	69	TYR
1	A	84	LYS
1	A	218	TYR
1	A	267	ILE
1	A	270	GLU
1	A	324	THR
1	A	338	SER
1	A	371	HIS
1	B	37	ARG
1	B	69	TYR
1	B	84	LYS
1	B	218	TYR
1	B	267	ILE
1	B	270	GLU
1	B	324	THR
1	C	37	ARG
1	C	69	TYR
1	C	84	LYS
1	C	218	TYR
1	C	267	ILE
1	C	270	GLU
1	C	324	THR
1	C	368	SER
1	C	371	HIS
1	D	37	ARG
1	D	69	TYR
1	D	84	LYS
1	D	218	TYR
1	D	267	ILE
1	D	270	GLU
1	D	324	THR
1	D	338	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	NWM	A	403	-	40,41,41	1.67	5 (12%)	49,53,53	1.94	16 (32%)
4	NWM	C	403	-	40,41,41	1.71	5 (12%)	49,53,53	1.70	14 (28%)
3	ADP	A	402	2	24,29,29	0.87	1 (4%)	29,45,45	1.44	5 (17%)
3	ADP	B	402	-	24,29,29	0.98	2 (8%)	29,45,45	1.40	3 (10%)
4	NWM	B	403	-	40,41,41	1.68	5 (12%)	49,53,53	1.96	15 (30%)
3	ADP	D	402	2	24,29,29	0.88	1 (4%)	29,45,45	1.38	4 (13%)
4	NWM	D	403	-	40,41,41	1.63	6 (15%)	49,53,53	2.11	14 (28%)
3	ADP	C	402	2	24,29,29	0.91	1 (4%)	29,45,45	1.29	4 (13%)

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	NWM	A	403	-	-	16/53/53/53	0/1/1/1
4	NWM	C	403	-	-	12/53/53/53	0/1/1/1
3	ADP	A	402	2	-	2/12/32/32	0/3/3/3
3	ADP	B	402	-	-	4/12/32/32	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NWM	B	403	-	-	14/53/53/53	0/1/1/1
3	ADP	D	402	2	-	2/12/32/32	0/3/3/3
4	NWM	D	403	-	-	16/53/53/53	0/1/1/1
3	ADP	C	402	2	-	2/12/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	NWM	O01-C11	-5.55	1.36	1.46
4	B	403	NWM	O01-C11	-5.43	1.36	1.46
4	A	403	NWM	O01-C11	-5.12	1.37	1.46
4	C	403	NWM	C34-C35	-5.05	1.41	1.52
4	A	403	NWM	C34-C35	-4.99	1.41	1.52
4	D	403	NWM	C34-C35	-4.98	1.41	1.52
4	B	403	NWM	C34-C35	-4.97	1.41	1.52
4	D	403	NWM	O01-C11	-4.89	1.37	1.46
4	A	403	NWM	C18-C25	-3.57	1.46	1.53
4	B	403	NWM	C29-C30	3.56	1.56	1.51
4	C	403	NWM	C18-C25	-3.42	1.46	1.53
4	A	403	NWM	C29-C30	3.39	1.55	1.51
4	D	403	NWM	C29-C30	3.29	1.55	1.51
4	C	403	NWM	C29-C30	3.28	1.55	1.51
4	B	403	NWM	C18-C25	-3.26	1.46	1.53
4	D	403	NWM	C18-C25	-3.16	1.46	1.53
4	D	403	NWM	O13-C44	2.66	1.41	1.35
4	B	403	NWM	O13-C44	2.65	1.41	1.35
4	C	403	NWM	O13-C44	2.62	1.41	1.35
3	B	402	ADP	C5-C4	2.62	1.47	1.40
3	C	402	ADP	C5-C4	2.47	1.47	1.40
3	D	402	ADP	C5-C4	2.31	1.47	1.40
3	A	402	ADP	C5-C4	2.28	1.47	1.40
4	A	403	NWM	O13-C44	2.22	1.40	1.35
3	B	402	ADP	C2-N3	2.10	1.35	1.32
4	D	403	NWM	O01-C13	2.02	1.40	1.34

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	NWM	C34-C35-N5	6.85	123.17	112.15
4	B	403	NWM	C34-C35-N5	6.01	121.83	112.15
4	A	403	NWM	C34-C35-N5	5.55	121.08	112.15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	NWM	C34-C35-N5	4.88	120.01	112.15
4	B	403	NWM	O13-C44-C08	4.45	119.28	111.09
4	D	403	NWM	O01-C11-C10	4.39	116.73	107.78
4	D	403	NWM	O13-C44-C08	4.34	119.07	111.09
4	D	403	NWM	C09-C10-C11	4.29	120.12	113.24
3	A	402	ADP	N3-C2-N1	-4.06	122.33	128.68
4	D	403	NWM	O01-C13-C15	3.87	121.58	110.80
4	A	403	NWM	O13-C44-C08	3.80	118.08	111.09
4	A	403	NWM	O01-C13-C15	3.63	120.91	110.80
3	D	402	ADP	N3-C2-N1	-3.62	123.02	128.68
4	C	403	NWM	O13-C44-C08	3.54	117.60	111.09
3	B	402	ADP	C4-C5-N7	-3.44	105.81	109.40
4	B	403	NWM	C09-C10-C11	3.38	118.67	113.24
3	C	402	ADP	N3-C2-N1	-3.34	123.46	128.68
4	A	403	NWM	O08-C07-C06	3.34	121.49	110.80
3	D	402	ADP	PA-O3A-PB	-3.21	121.83	132.83
4	C	403	NWM	O01-C13-C15	3.20	119.73	110.80
4	D	403	NWM	C18-C25-C11	3.13	116.01	111.43
3	B	402	ADP	N3-C2-N1	-3.10	123.83	128.68
3	B	402	ADP	PA-O3A-PB	-3.10	122.19	132.83
3	A	402	ADP	PA-O3A-PB	-3.01	122.51	132.83
4	A	403	NWM	C07-O08-C09	2.97	122.16	112.86
4	B	403	NWM	O01-C13-C15	2.93	118.97	110.80
4	B	403	NWM	O08-C07-C06	2.88	120.03	110.80
4	B	403	NWM	C18-C25-C11	2.87	115.63	111.43
4	A	403	NWM	O08-C09-C10	2.83	120.51	109.78
4	C	403	NWM	O08-C09-C10	2.82	120.49	109.78
3	A	402	ADP	C2-N1-C6	2.81	123.56	118.75
4	A	403	NWM	O11-C26-C27	2.77	115.03	109.83
4	A	403	NWM	C09-C10-C11	2.76	117.68	113.24
4	B	403	NWM	C40-C31-C32	2.74	119.12	112.92
4	B	403	NWM	C32-O13-C44	2.73	121.94	117.72
4	B	403	NWM	C18-C25-C26	2.71	116.87	111.39
4	D	403	NWM	O13-C32-C33	2.71	111.96	108.22
4	C	403	NWM	O08-C07-C06	2.69	119.41	110.80
3	C	402	ADP	C4-C5-N7	-2.66	106.63	109.40
3	C	402	ADP	PA-O3A-PB	-2.65	123.73	132.83
4	C	403	NWM	C40-C31-C32	2.65	118.91	112.92
4	D	403	NWM	O01-C11-C25	2.64	112.48	107.78
4	B	403	NWM	O01-C11-C10	2.63	113.14	107.78
4	D	403	NWM	C07-O08-C09	2.63	121.10	112.86
4	D	403	NWM	C39-C27-C28	2.58	114.40	110.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	NWM	O08-C09-C10	2.57	119.52	109.78
4	A	403	NWM	O01-C11-C10	2.55	112.97	107.78
4	A	403	NWM	C18-C25-C26	2.53	116.51	111.39
4	A	403	NWM	C39-C27-C28	2.50	114.28	110.36
4	D	403	NWM	C40-C31-C32	2.45	118.47	112.92
4	A	403	NWM	O13-C32-C33	2.44	111.59	108.22
4	C	403	NWM	C41-C33-C34	2.42	114.15	110.36
4	A	403	NWM	C28-C27-C26	2.35	115.21	111.39
4	C	403	NWM	C18-C25-C26	2.35	116.14	111.39
4	D	403	NWM	C18-C25-C26	2.35	116.14	111.39
4	B	403	NWM	C39-C27-C28	2.33	114.02	110.36
4	C	403	NWM	C32-O13-C44	2.33	121.33	117.72
4	B	403	NWM	C28-C27-C26	2.31	115.14	111.39
4	C	403	NWM	O11-C26-C25	2.30	114.61	109.49
4	A	403	NWM	O01-C11-C25	2.26	111.80	107.78
4	C	403	NWM	C07-O08-C09	2.24	119.87	112.86
4	C	403	NWM	O11-C26-C27	2.20	113.95	109.83
3	A	402	ADP	C4-C5-N7	-2.20	107.11	109.40
4	C	403	NWM	C09-C10-C11	2.19	116.76	113.24
4	B	403	NWM	C41-C33-C32	2.18	114.71	111.15
4	B	403	NWM	O11-C26-C27	2.17	113.90	109.83
3	A	402	ADP	O3B-PB-O2B	2.16	115.89	107.64
4	D	403	NWM	O11-C26-C27	2.14	113.85	109.83
3	D	402	ADP	C2-N1-C6	2.13	122.40	118.75
4	A	403	NWM	O11-C26-C25	2.13	114.23	109.49
4	A	403	NWM	C28-C29-C30	2.13	118.60	114.34
3	D	402	ADP	C4-C5-N7	-2.07	107.24	109.40
3	C	402	ADP	C2-N1-C6	2.02	122.20	118.75
4	C	403	NWM	C39-C27-C28	2.01	113.51	110.36
4	D	403	NWM	C41-C33-C34	2.01	113.51	110.36

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	NWM	O08-C09-C10-C11
4	A	403	NWM	O01-C11-C25-C26
4	A	403	NWM	C34-C35-N5-C43
4	C	403	NWM	O08-C09-C10-C11
3	A	402	ADP	PA-O3A-PB-O2B
3	A	402	ADP	PA-O3A-PB-O3B
3	B	402	ADP	C5'-O5'-PA-O3A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	403	NWM	O08-C09-C10-C11
4	B	403	NWM	O01-C11-C25-C26
4	B	403	NWM	C34-C35-N5-C43
4	B	403	NWM	C34-C35-N5-C42
3	D	402	ADP	PA-O3A-PB-O3B
4	D	403	NWM	C09-C10-C11-O01
4	D	403	NWM	C09-C10-C11-C25
4	D	403	NWM	O01-C11-C25-C26
4	D	403	NWM	C34-C35-N5-C43
4	D	403	NWM	C34-C35-N5-C42
3	C	402	ADP	PA-O3A-PB-O2B
4	A	403	NWM	C06-C07-O08-C09
4	C	403	NWM	O02-C13-O01-C11
4	C	403	NWM	C15-C13-O01-C11
4	A	403	NWM	C41-C33-C34-C35
4	B	403	NWM	C41-C33-C34-C35
4	C	403	NWM	C41-C33-C34-C35
4	D	403	NWM	C41-C33-C34-C35
4	C	403	NWM	C27-C28-C29-C30
4	B	403	NWM	C18-C25-C26-O11
4	A	403	NWM	C15-C13-O01-C11
4	D	403	NWM	O02-C13-O01-C11
4	C	403	NWM	C40-C31-C32-C33
4	B	403	NWM	C40-C31-C32-C33
4	C	403	NWM	C34-C35-N5-C43
4	A	403	NWM	O02-C13-O01-C11
4	C	403	NWM	C32-C33-C34-C35
4	B	403	NWM	C32-C33-C34-C35
4	D	403	NWM	C06-C07-O08-C09
4	D	403	NWM	C18-C25-C26-O11
4	A	403	NWM	C27-C28-C29-C30
4	A	403	NWM	C32-C33-C34-C35
4	D	403	NWM	C32-C33-C34-C35
4	D	403	NWM	C15-C13-O01-C11
4	B	403	NWM	O01-C11-C25-C18
4	D	403	NWM	O01-C11-C25-C18
4	A	403	NWM	C18-C25-C26-O11
4	B	403	NWM	O02-C13-O01-C11
3	D	402	ADP	PA-O3A-PB-O2B
4	C	403	NWM	C10-C09-O08-C07
4	B	403	NWM	C10-C09-O08-C07
3	B	402	ADP	C5'-O5'-PA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	402	ADP	C5'-O5'-PA-O2A
4	B	403	NWM	C10-C11-C25-C26
4	D	403	NWM	C10-C11-C25-C26
4	A	403	NWM	C40-C31-C32-C33
3	B	402	ADP	C3'-C4'-C5'-O5'
4	C	403	NWM	C06-C07-O08-C09
4	D	403	NWM	C40-C31-C32-C33
4	A	403	NWM	C10-C09-O08-C07
3	C	402	ADP	PA-O3A-PB-O1B
4	A	403	NWM	C08-C44-O13-C32
4	C	403	NWM	C18-C25-C26-O11
4	A	403	NWM	O01-C11-C25-C18
4	D	403	NWM	O08-C09-C10-C11
4	A	403	NWM	C40-C31-C32-O13
4	C	403	NWM	C40-C31-C32-O13
4	B	403	NWM	C40-C31-C32-O13
4	D	403	NWM	C40-C31-C32-O13
4	A	403	NWM	C34-C35-N5-C42
4	B	403	NWM	C11-C25-C26-O11

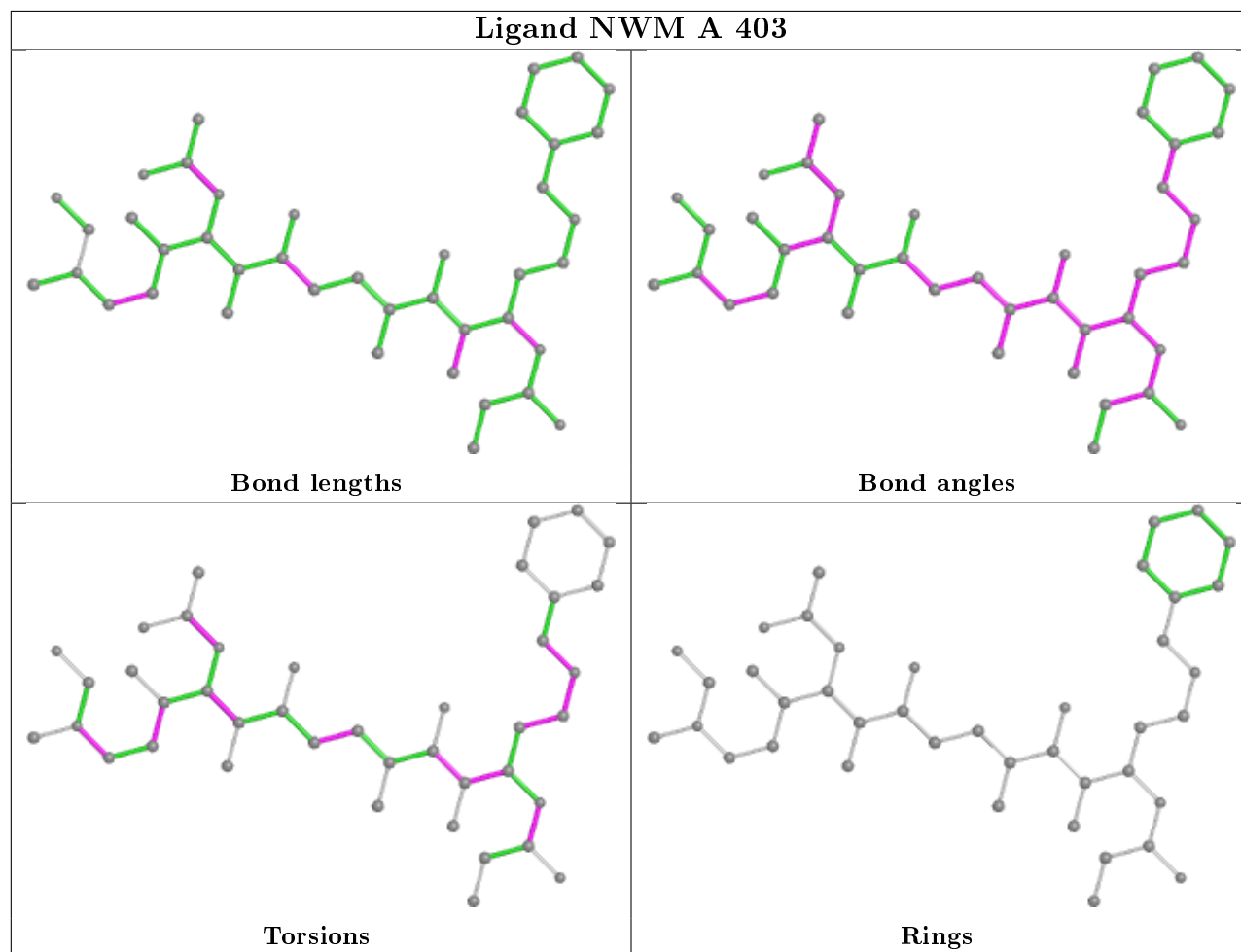
There are no ring outliers.

8 monomers are involved in 21 short contacts:

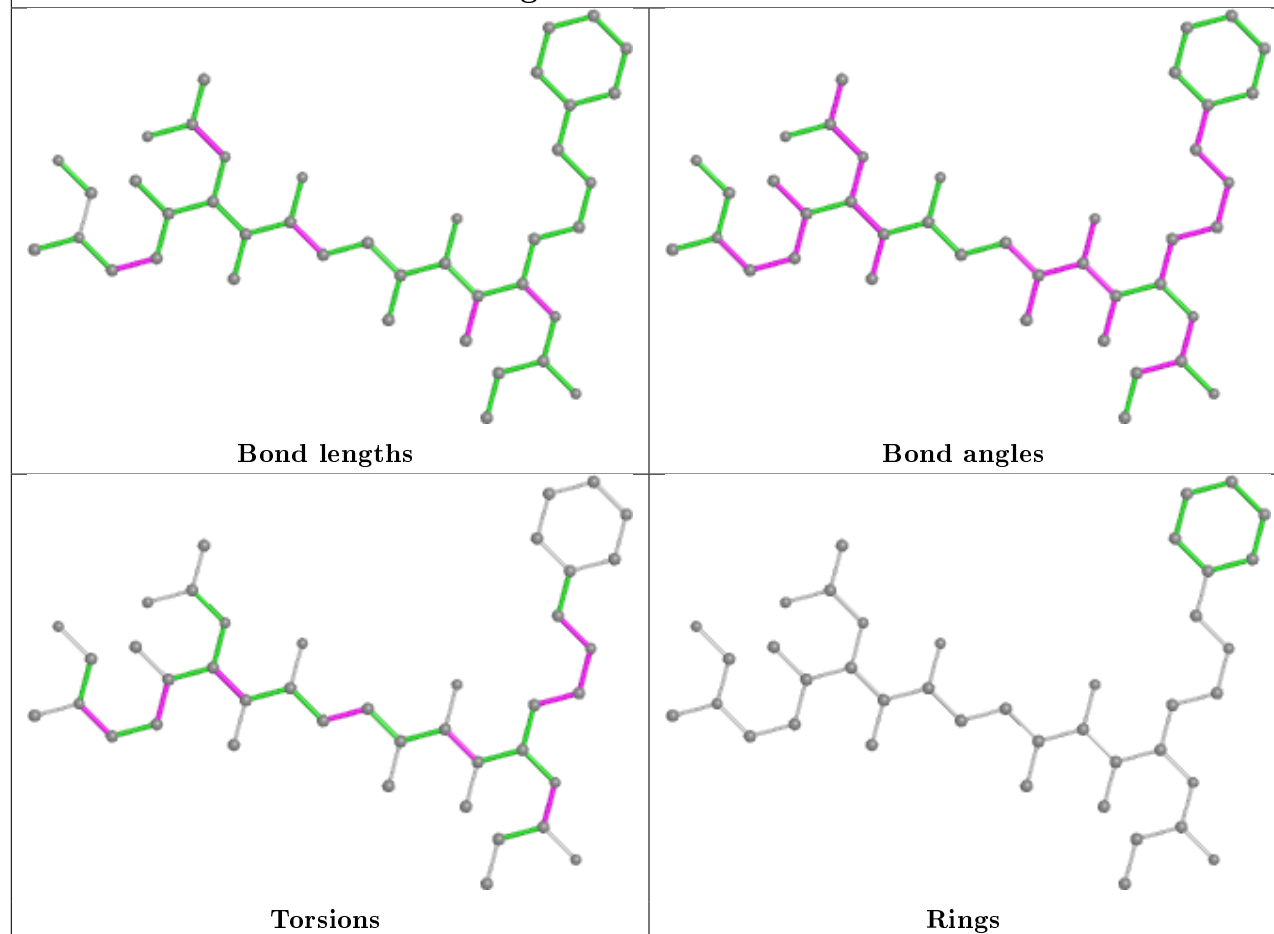
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	NWM	4	0
4	C	403	NWM	6	0
3	A	402	ADP	1	0
3	B	402	ADP	1	0
4	B	403	NWM	4	0
3	D	402	ADP	1	0
4	D	403	NWM	3	0
3	C	402	ADP	1	0

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

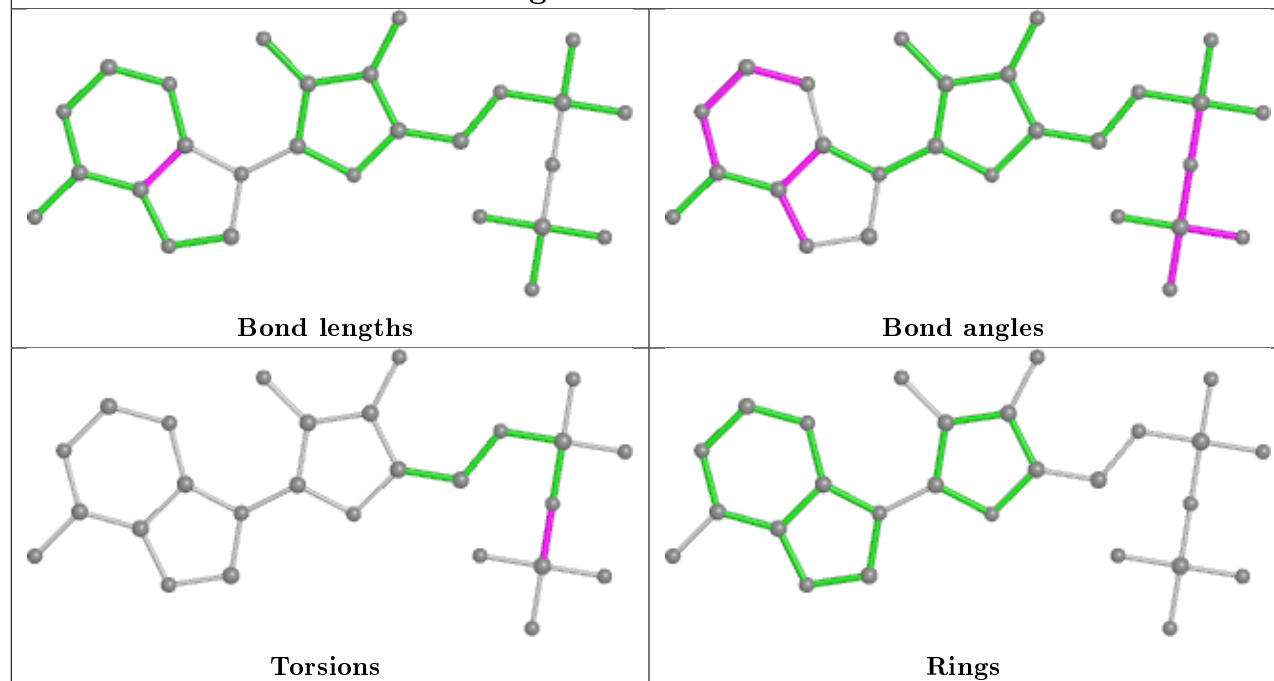
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

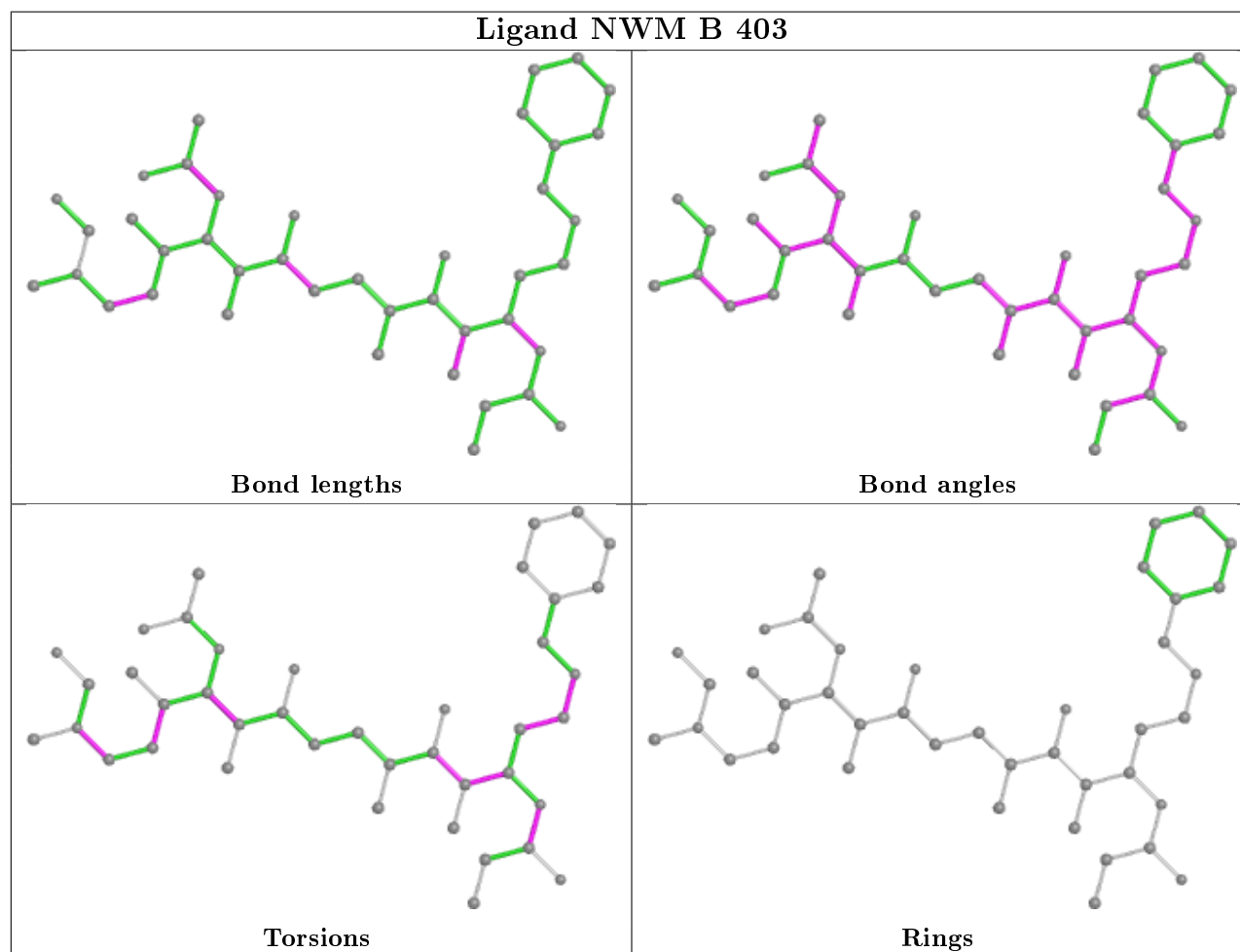
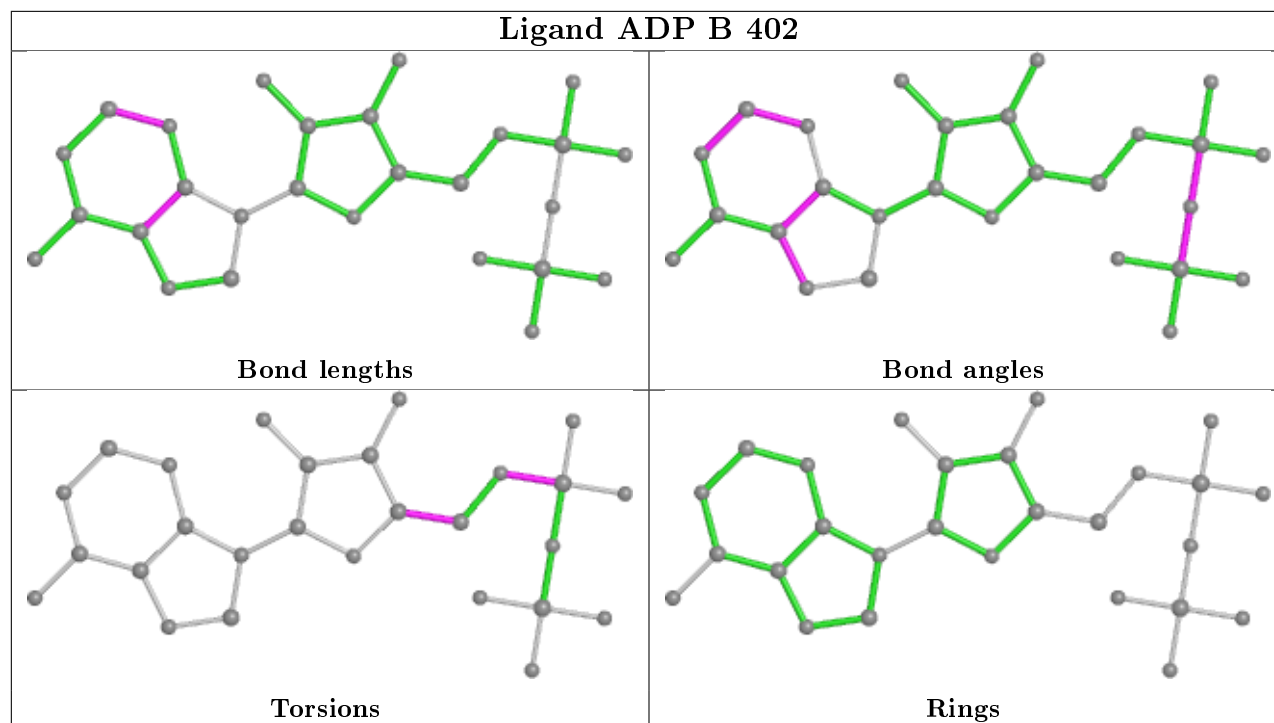


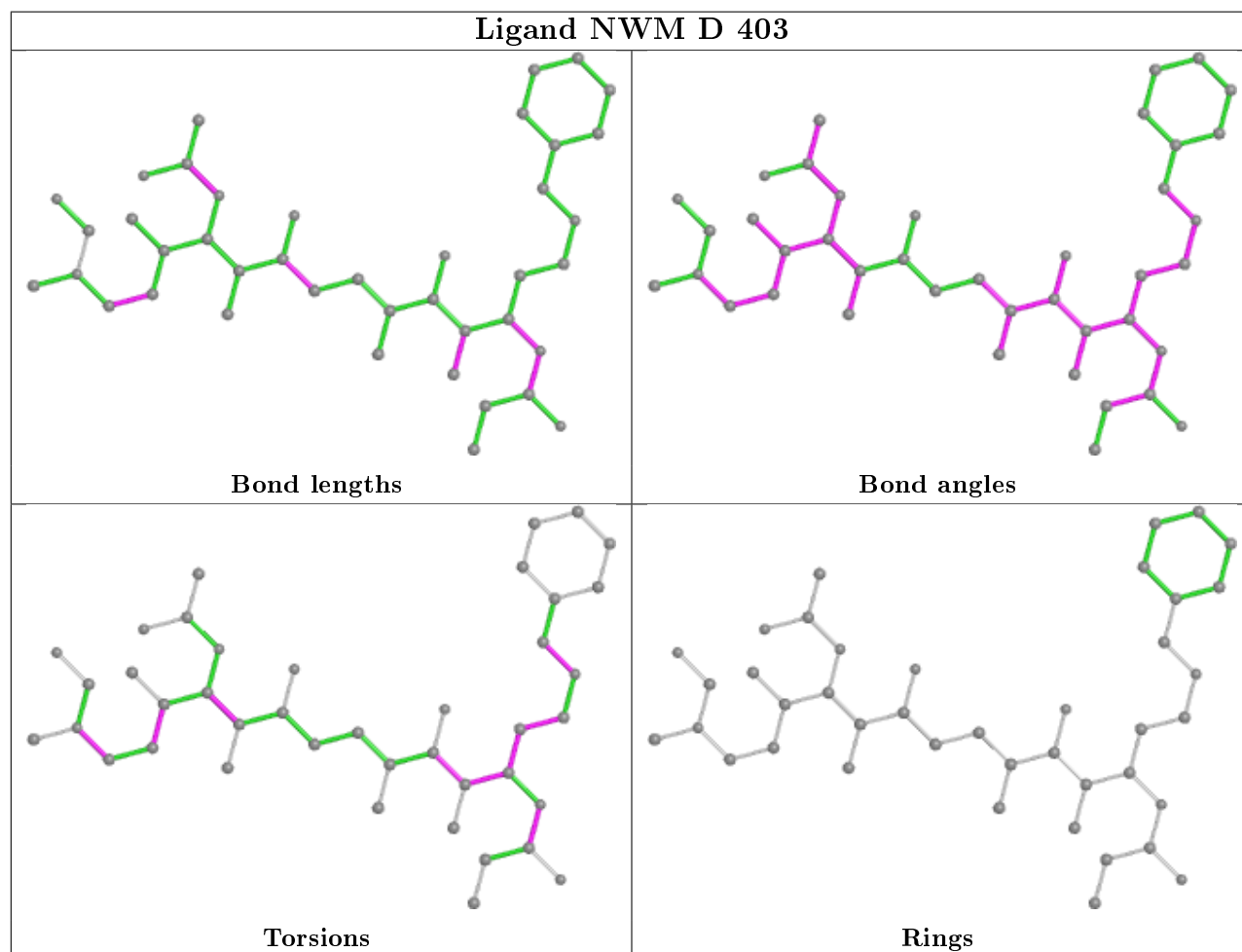
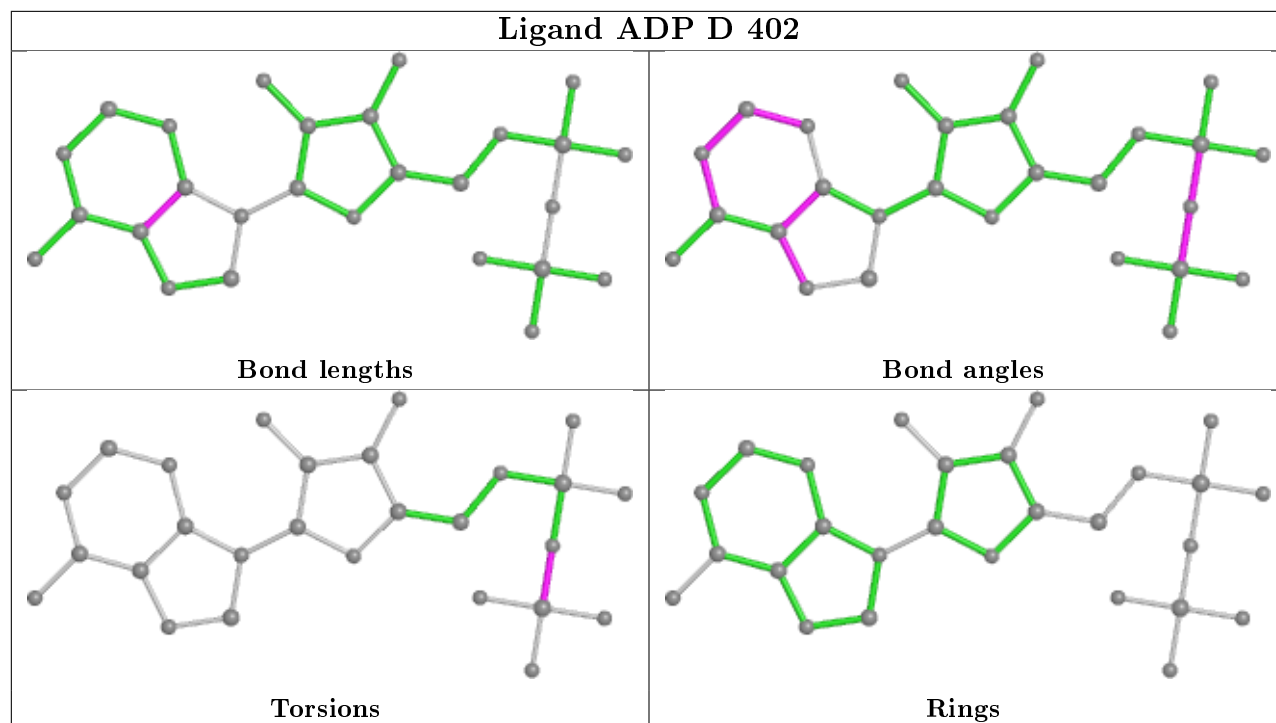
## Ligand NWM C 403



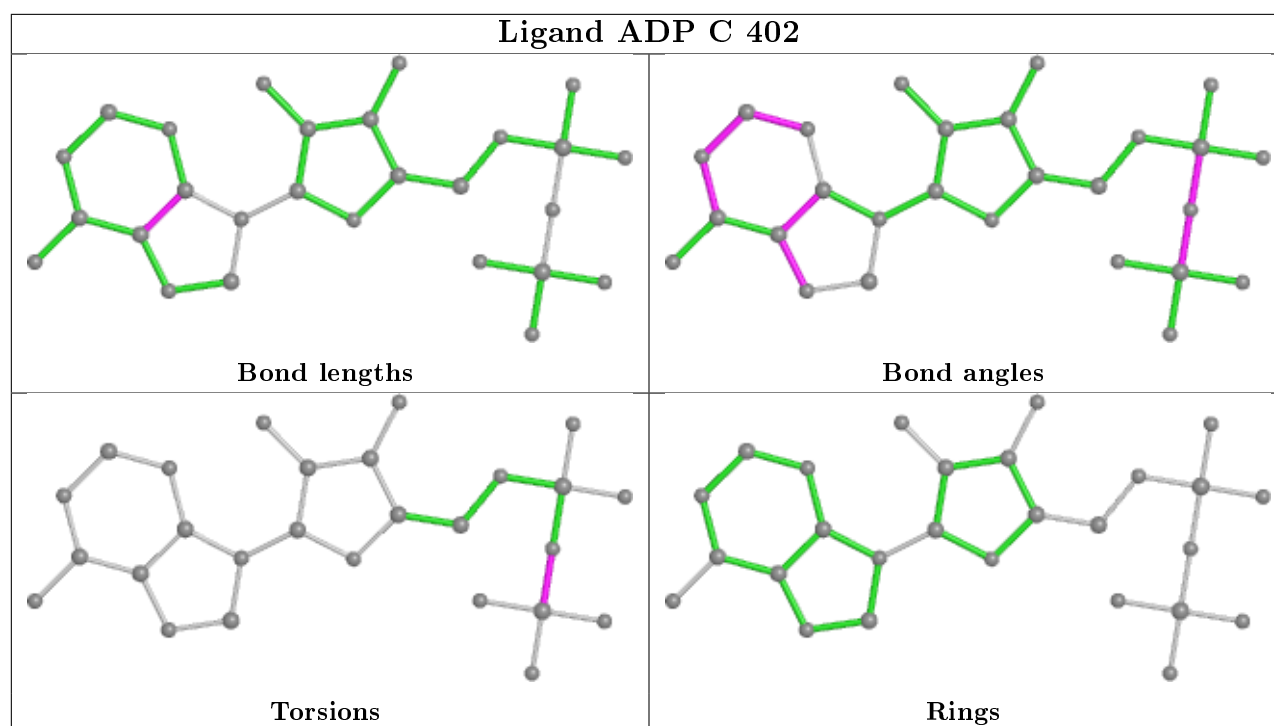
## Ligand ADP A 402











## 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	360/375 (96%)	-0.01	4 (1%) 80 80	23, 44, 77, 133	0
1	B	361/375 (96%)	0.19	8 (2%) 62 59	30, 54, 89, 136	0
1	C	361/375 (96%)	0.18	3 (0%) 86 86	35, 58, 94, 138	0
1	D	360/375 (96%)	0.59	27 (7%) 14 11	47, 76, 133, 169	0
All	All	1442/1500 (96%)	0.24	42 (2%) 51 47	23, 58, 108, 169	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	95	ARG	6.9
1	D	49	GLN	5.1
1	D	96	VAL	4.7
1	D	37	ARG	4.6
1	D	55	GLY	3.6
1	B	52	SER	3.6
1	D	38	PRO	3.4
1	B	37	ARG	3.4
1	D	67	LEU	3.3
1	A	49	GLN	3.2
1	B	49	GLN	3.1
1	D	99	GLU	3.1
1	D	52	SER	3.0
1	D	94	LEU	3.0
1	D	98	PRO	2.9
1	B	95	ARG	2.9
1	B	51	ASP	2.9
1	D	370	VAL	2.9
1	D	236	LEU	2.8
1	D	34	ILE	2.8
1	D	247	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	123	MET	2.7
1	D	35	VAL	2.7
1	A	69	TYR	2.6
1	C	49	GLN	2.5
1	D	360	GLN	2.4
1	A	66	THR	2.4
1	D	36	GLY	2.3
1	A	92	ASN	2.3
1	D	100	GLU	2.3
1	B	5	THR	2.2
1	D	69	TYR	2.2
1	D	372	ARG	2.2
1	D	110	LEU	2.2
1	D	270	GLU	2.2
1	D	64	ILE	2.1
1	C	5	THR	2.1
1	C	250	ILE	2.1
1	D	84	LYS	2.1
1	B	66	THR	2.1
1	D	90	PHE	2.1
1	B	67	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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.

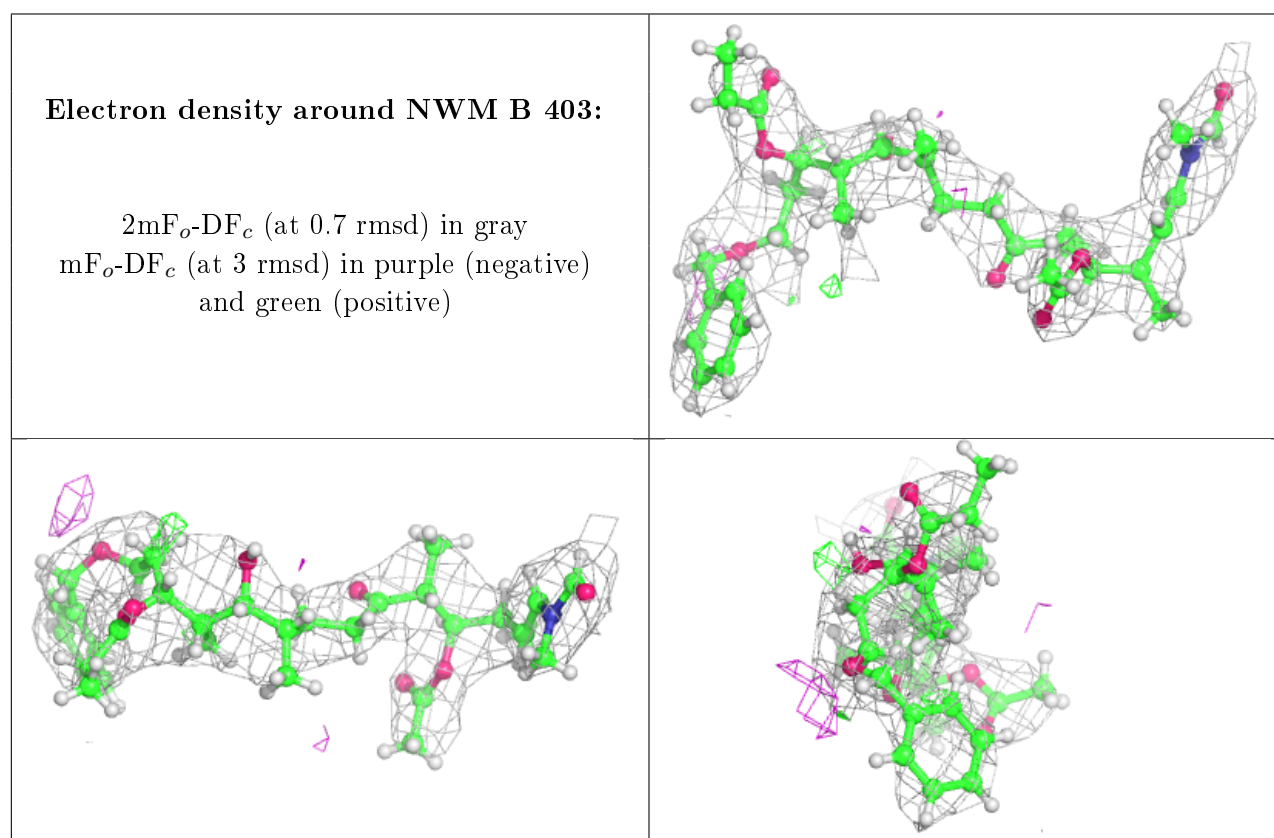
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NWM	B	403	41/41	0.91	0.28	27,51,71,74	0
4	NWM	D	403	41/41	0.91	0.25	24,66,85,86	0

*Continued on next page...*

*Continued from previous page...*

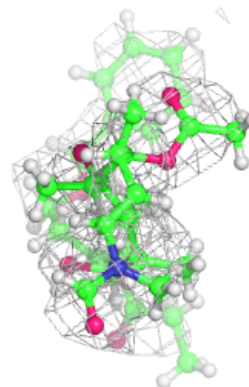
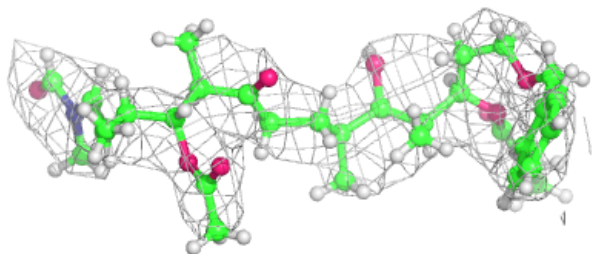
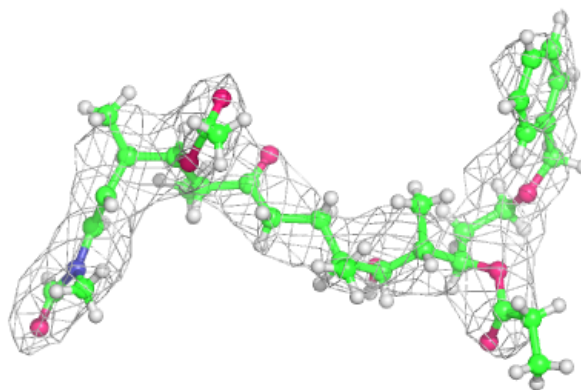
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NWM	C	403	41/41	0.92	0.26	39,52,65,70	0
4	NWM	A	403	41/41	0.93	0.24	20,44,55,65	0
2	CA	C	401	1/1	0.93	0.21	49,49,49,49	0
2	CA	D	401	1/1	0.96	0.17	56,56,56,56	0
3	ADP	A	402	27/27	0.96	0.15	15,24,47,50	0
3	ADP	C	402	27/27	0.97	0.16	24,37,50,54	0
2	CA	B	401	1/1	0.97	0.19	52,52,52,52	0
2	CA	A	401	1/1	0.97	0.13	33,33,33,33	0
3	ADP	D	402	27/27	0.97	0.14	28,40,52,107	0
3	ADP	B	402	27/27	0.97	0.15	22,36,53,54	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.

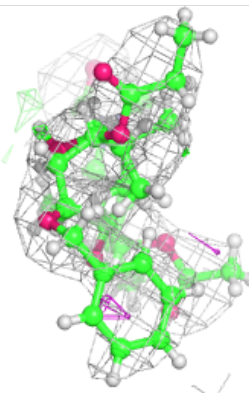
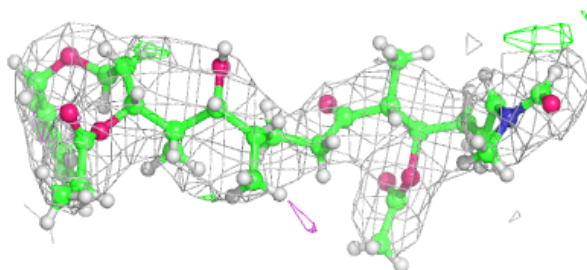
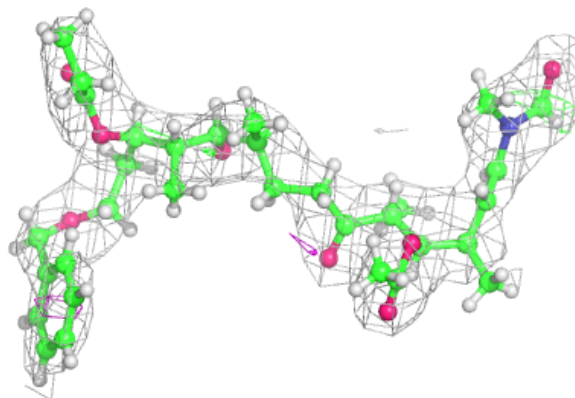


**Electron density around NWM D 403:**

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

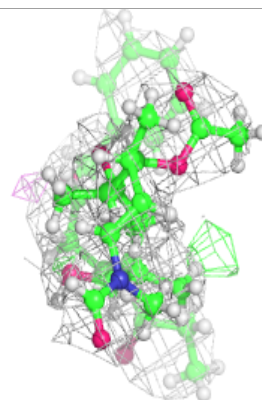
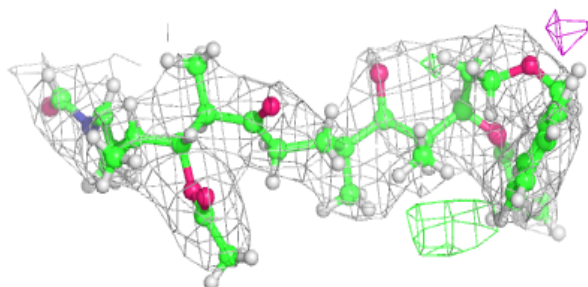
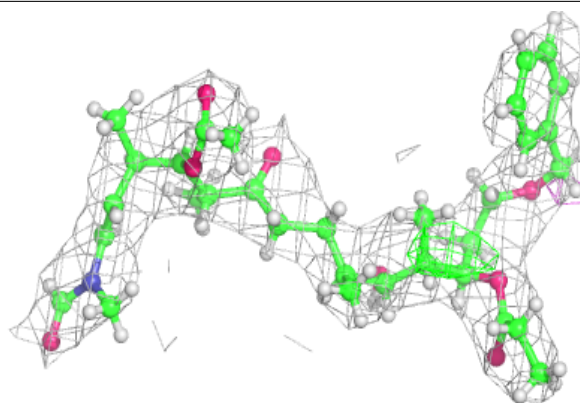
**Electron density around NWM C 403:**

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

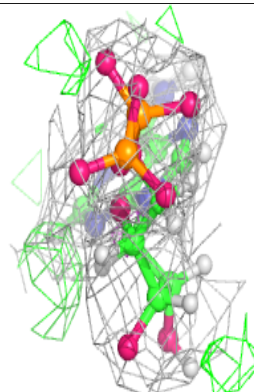
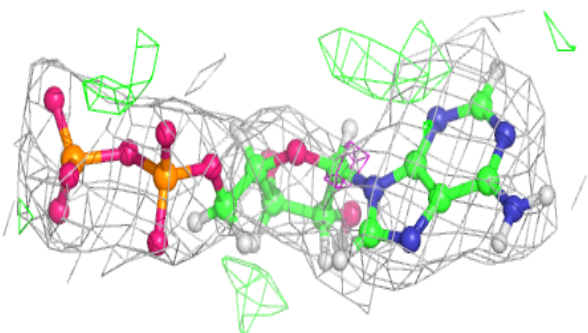
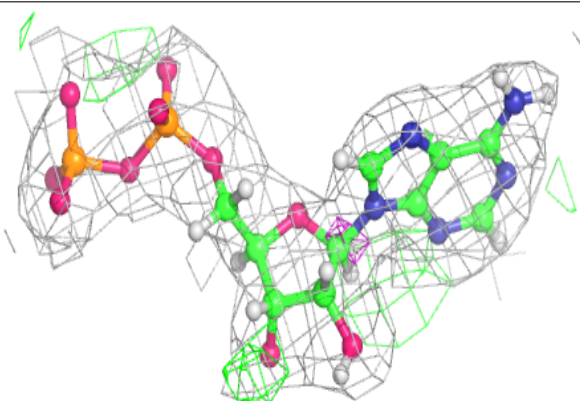


**Electron density around NWM A 403:**

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

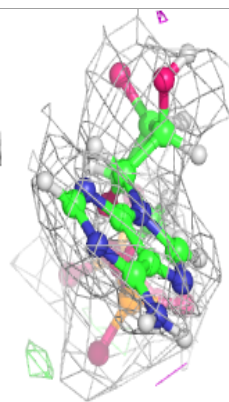
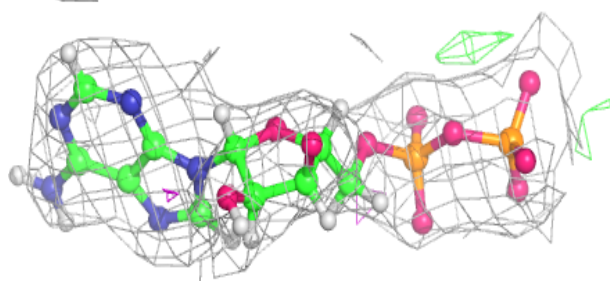
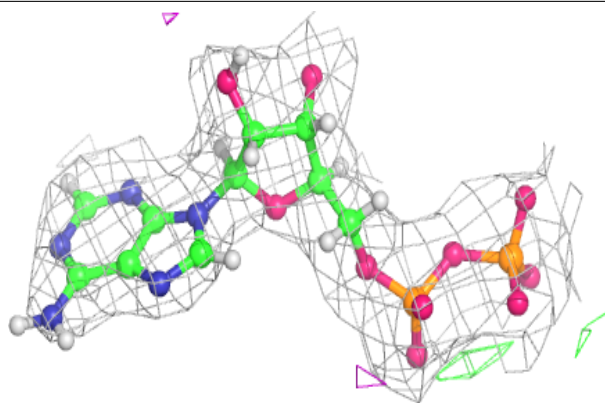
**Electron density around ADP A 402:**

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

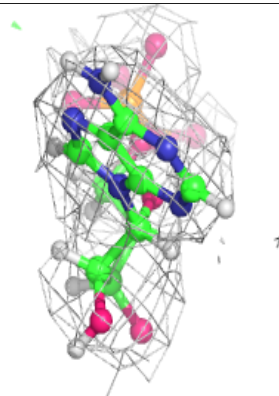
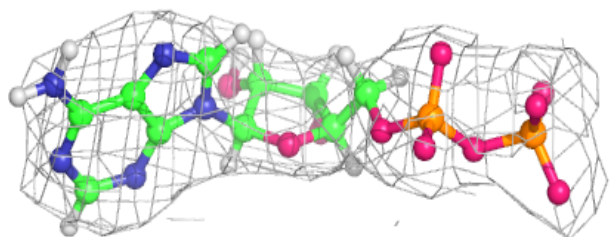
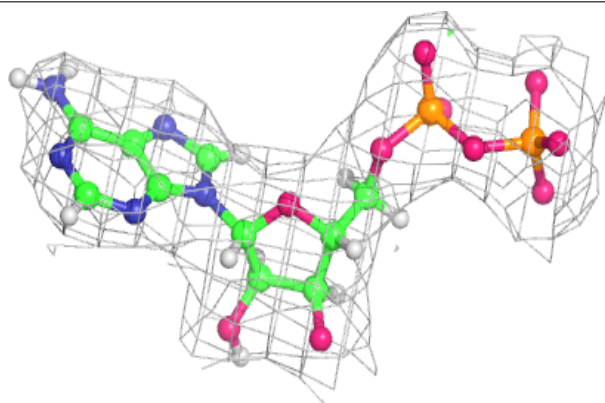


**Electron density around ADP C 402:**

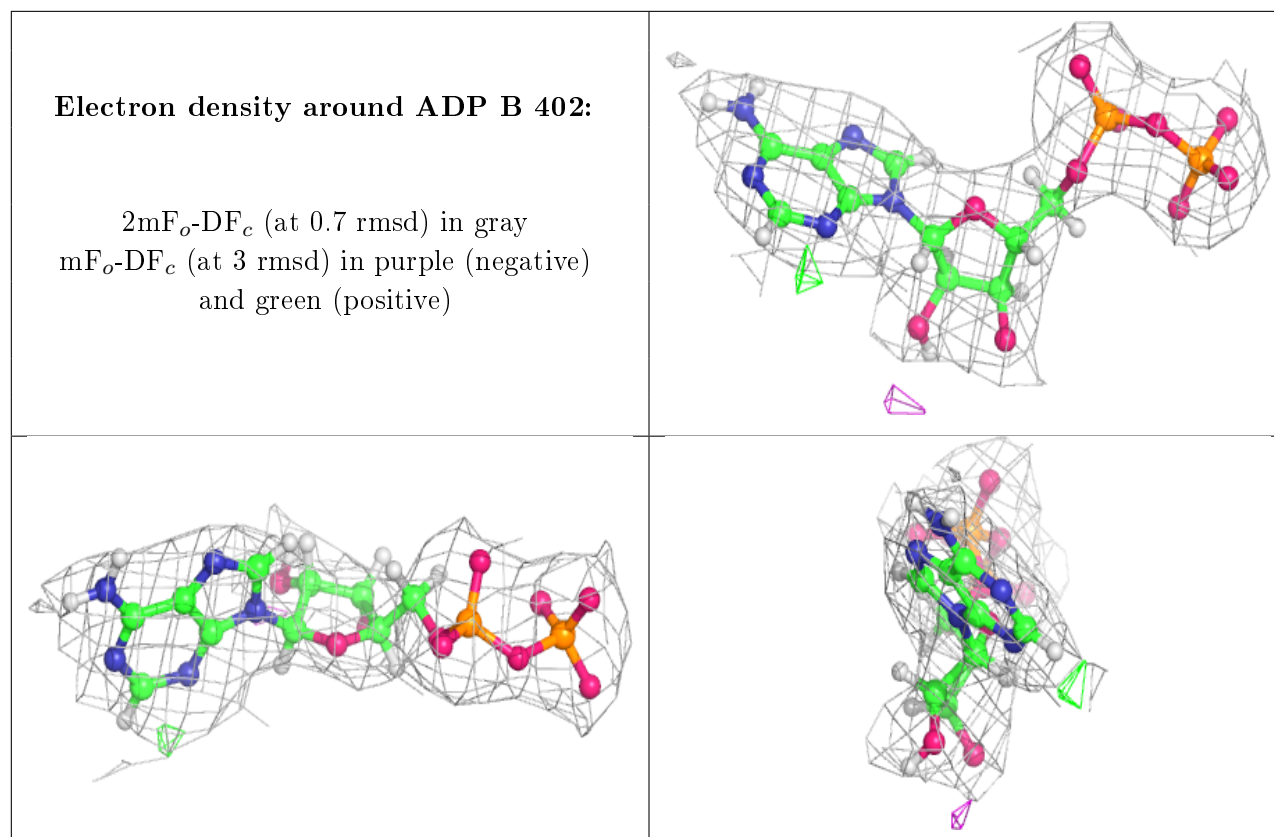
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP D 402:**

$2mF_o-DF_c$  (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.