Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2024 – 06:48 PM EDT

PDB ID	:	6NMM
Title	:	Ternary complex structure of the T130K mutant of ANT-4 with Neomycin, AMPCPP and Pyrophosphate
Authors	:	Cuneo, M.J.; Selvaraj, B.
Deposited on	:	2019-01-11
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

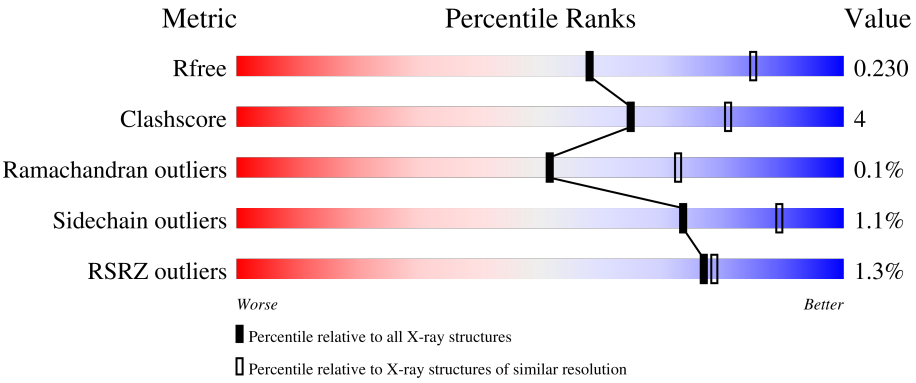
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	256	94%
1	B	256	86% 12%
1	C	256	88% 10%
1	D	256	3% 86% 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8755 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.

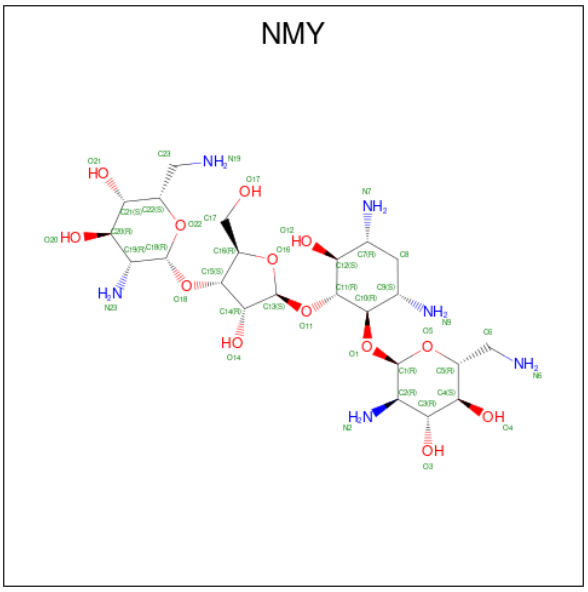
- Molecule 1 is a protein called Kanamycin nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	2	0
			2035	1295	333	394	13			
1	B	252	Total	C	N	O	S	0	1	0
			2025	1289	330	393	13			
1	C	252	Total	C	N	O	S	0	1	0
			2025	1289	330	393	13			
1	D	252	Total	C	N	O	S	0	1	0
			2025	1289	330	393	13			

There are 16 discrepancies between the modelled and reference sequences:

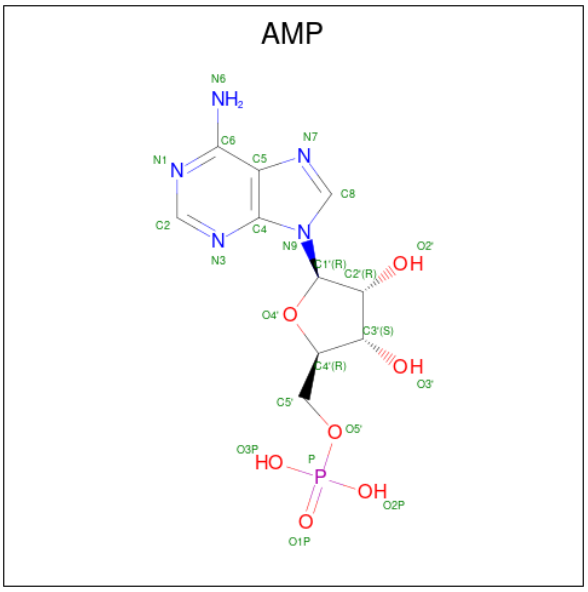
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q57514
A	-1	SER	-	expression tag	UNP Q57514
A	0	HIS	-	expression tag	UNP Q57514
A	80	ASP	TYR	conflict	UNP Q57514
B	-2	GLY	-	expression tag	UNP Q57514
B	-1	SER	-	expression tag	UNP Q57514
B	0	HIS	-	expression tag	UNP Q57514
B	80	ASP	TYR	conflict	UNP Q57514
C	-2	GLY	-	expression tag	UNP Q57514
C	-1	SER	-	expression tag	UNP Q57514
C	0	HIS	-	expression tag	UNP Q57514
C	80	ASP	TYR	conflict	UNP Q57514
D	-2	GLY	-	expression tag	UNP Q57514
D	-1	SER	-	expression tag	UNP Q57514
D	0	HIS	-	expression tag	UNP Q57514
D	80	ASP	TYR	conflict	UNP Q57514

- Molecule 2 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).



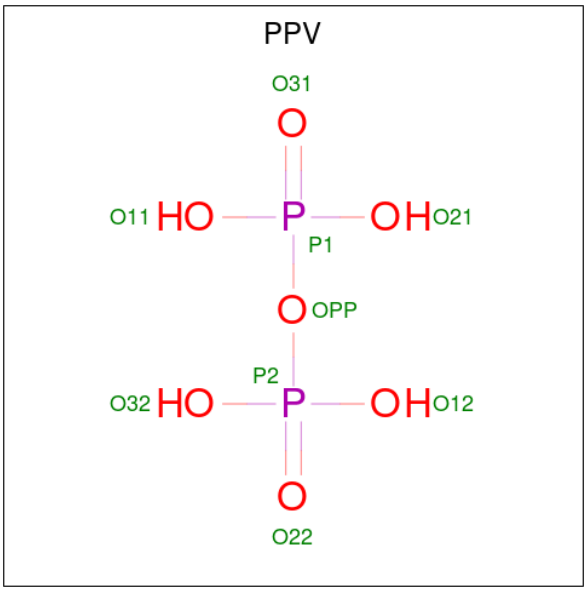
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 42 23 6 13	0	0
2	A	1	Total C N O 42 23 6 13	0	0
2	B	1	Total C N O 42 23 6 13	0	0
2	C	1	Total C N O 42 23 6 13	0	0
2	C	1	Total C N O 42 23 6 13	0	0
2	D	1	Total C N O 42 23 6 13	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 4 is PYROPHOSPHATE (three-letter code: PPV) (formula: $H_4O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 9 7 2	0	0
4	B	1	Total O P 9 7 2	0	0
4	C	1	Total O P 9 7 2	0	0
4	D	1	Total O P 9 7 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	B	2	Total Mg 2 2	0	0
5	C	2	Total Mg 2 2	0	0
5	D	2	Total Mg 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	58	Total O 58 58	0	0

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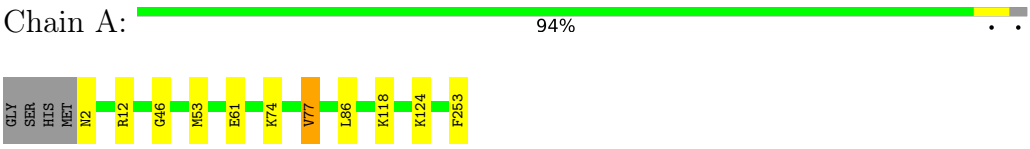
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	45	Total O 45 45	0	0
6	C	67	Total O 67 67	0	0
6	D	47	Total O 47 47	0	0

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.

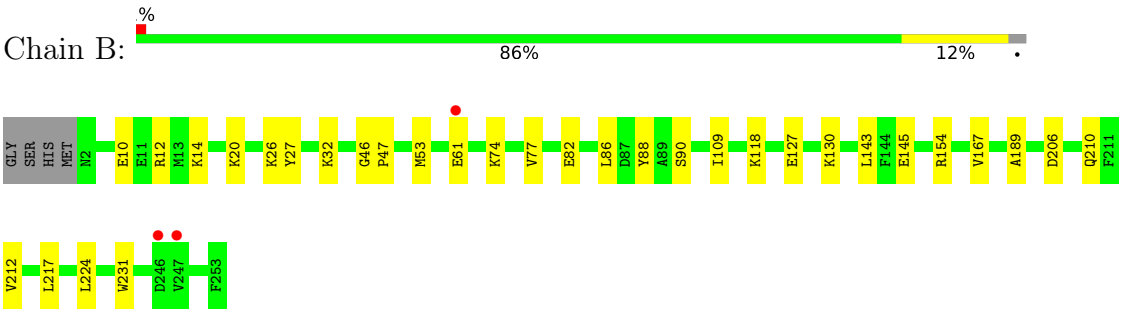
• Molecule 1: Kanamycin nucleotidyltransferase

Chain A:



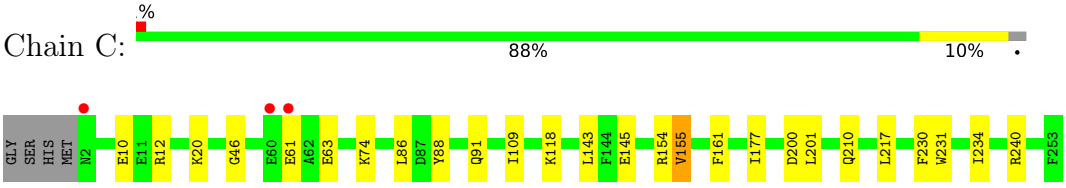
• Molecule 1: Kanamycin nucleotidyltransferase

Chain B:



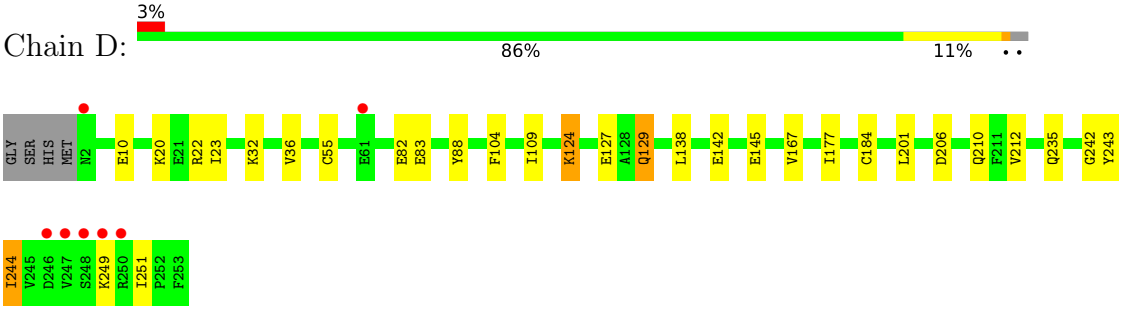
• Molecule 1: Kanamycin nucleotidyltransferase

Chain C:



• Molecule 1: Kanamycin nucleotidyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.51Å 59.25Å 102.04Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	38.58 – 2.50 38.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	86.6 (38.58-2.50) 86.6 (38.58-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.84 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.174 , 0.230 0.174 , 0.230	Depositor DCC
R_{free} test set	1499 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8755	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NMY, PPV, AMP, MG

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	0.24	0/2084	0.42	0/2822
1	B	0.25	0/2073	0.42	0/2807
1	C	0.25	0/2073	0.42	0/2807
1	D	0.25	0/2073	0.42	0/2807
All	All	0.25	0/8303	0.42	0/11243

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

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	2035	0	1956	7	0
1	B	2025	0	1950	21	0
1	C	2025	0	1950	18	0
1	D	2025	0	1950	18	0
2	A	84	0	88	4	0
2	B	42	0	45	2	0
2	C	84	0	90	7	0
2	D	42	0	45	3	0
3	A	44	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	12	0	0
3	C	44	0	24	0	0
3	D	22	0	12	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	58	0	0	1	0
6	B	45	0	0	0	0
6	C	67	0	0	2	0
6	D	47	0	0	0	0
All	All	8755	0	8146	68	0

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

All (68) 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)
2:C:800:NMY:O16	2:C:800:NMY:C13	1.65	1.28
2:C:805:NMY:O16	2:C:805:NMY:C13	1.65	1.25
2:B:800:NMY:O16	2:B:800:NMY:C13	1.65	1.25
2:A:800:NMY:O16	2:A:800:NMY:C13	1.65	1.16
2:D:800:NMY:O16	2:D:800:NMY:C13	1.65	1.14
2:A:805:NMY:O16	2:A:805:NMY:C13	1.65	1.13
1:D:20:LYS:HD3	1:D:109:ILE:HG22	1.75	0.69
1:C:86:LEU:HD11	1:C:118:LYS:HD3	1.76	0.67
1:B:53:MET:HB2	1:B:77:VAL:HG12	1.77	0.66
1:B:74:LYS:NZ	1:C:145:GLU:OE1	2.32	0.63
1:A:74:LYS:NZ	1:D:145:GLU:OE1	2.32	0.61
1:A:86:LEU:HD11	1:A:118:LYS:HD3	1.83	0.61
1:B:10:GLU:HG2	1:B:14:LYS:HE3	1.85	0.59
1:D:127:GLU:OE1	1:D:129:GLN:HB2	2.03	0.59
1:B:86:LEU:HD11	1:B:118:LYS:HD3	1.83	0.58
1:D:138:LEU:HD12	1:D:142:GLU:HG3	1.86	0.58
1:C:200:ASP:OD1	1:C:240:ARG:NH2	2.37	0.57
2:D:800:NMY:H91	2:D:800:NMY:H5	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ARG:NH2	1:C:46:GLY:O	2.39	0.55
1:C:20:LYS:HD3	1:C:109:ILE:HG22	1.87	0.55
1:C:88:TYR:CG	2:C:800:NMY:H22	2.42	0.55
2:C:800:NMY:N9	6:C:901:HOH:O	2.33	0.54
1:D:167:VAL:HG22	1:D:212:VAL:HG13	1.91	0.53
1:B:12:ARG:NH2	1:B:46:GLY:O	2.43	0.52
1:B:145:GLU:OE2	1:C:74:LYS:NZ	2.40	0.51
1:A:253:PHE:OXT	1:D:22:ARG:NH2	2.43	0.51
1:A:53:MET:HB2	1:A:77:VAL:HG13	1.93	0.51
1:C:88:TYR:HA	1:C:91:GLN:OE1	2.11	0.51
1:B:10:GLU:O	1:B:14:LYS:HG3	2.11	0.51
1:D:249:LYS:HE2	1:D:251:ILE:H	1.76	0.50
1:D:104:PHE:HE1	1:D:184:CYS:HG	1.59	0.50
1:C:154:ARG:NH2	6:C:905:HOH:O	2.45	0.49
1:C:177:ILE:HD13	1:C:201:LEU:HD22	1.95	0.49
1:D:10:GLU:OE1	1:D:10:GLU:N	2.47	0.48
1:C:63:GLU:O	2:C:805:NMY:N9	2.47	0.48
1:B:32:LYS:NZ	1:B:82:GLU:OE2	2.47	0.47
2:A:800:NMY:H91	2:A:800:NMY:H5	1.78	0.47
1:C:20:LYS:HD3	1:C:109:ILE:CG2	2.45	0.46
1:D:32:LYS:NZ	1:D:82:GLU:OE2	2.48	0.46
1:A:12:ARG:NH2	1:A:46:GLY:O	2.50	0.45
1:B:88:TYR:CG	2:B:800:NMY:H22	2.52	0.45
3:A:801:AMP:O2P	6:A:901:HOH:O	2.21	0.45
1:B:206:ASP:O	1:B:210:GLN:HG2	2.17	0.45
1:B:47:PRO:HG2	1:C:155:VAL:HG21	1.98	0.45
1:D:177:ILE:HD13	1:D:201:LEU:HD22	1.99	0.45
1:A:61:GLU:HG2	2:A:805:NMY:H7	1.99	0.45
1:A:124:LYS:O	1:A:124:LYS:HG2	2.17	0.45
1:C:230:PHE:O	1:C:234:ILE:HG12	2.17	0.44
1:C:143:LEU:HB3	1:C:231:TRP:HZ3	1.81	0.44
1:B:127:GLU:OE2	1:B:127:GLU:N	2.38	0.44
1:C:61:GLU:HG2	2:C:805:NMY:H7	1.99	0.43
1:B:61:GLU:HG2	1:B:61:GLU:O	2.18	0.43
1:D:36:VAL:HG23	1:D:109:ILE:HG13	2.01	0.43
1:D:20:LYS:HD3	1:D:109:ILE:CG2	2.47	0.42
1:D:88:TYR:CG	2:D:800:NMY:H22	2.54	0.42
1:B:90:SER:O	1:B:130:LYS:HE2	2.18	0.42
2:C:800:NMY:H5	2:C:800:NMY:H91	1.84	0.42
1:B:20:LYS:HD3	1:B:109:ILE:HG22	2.02	0.41
1:B:189:ALA:HA	1:C:161:PHE:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:LYS:O	1:D:124:LYS:HG2	2.20	0.41
1:B:217:LEU:HD12	1:C:217:LEU:HD12	2.03	0.41
1:D:206:ASP:O	1:D:210:GLN:HG2	2.21	0.41
1:B:26:LYS:HD3	1:B:27:TYR:CE2	2.56	0.41
1:B:143:LEU:HB3	1:B:231:TRP:HZ3	1.86	0.40
1:B:154:ARG:HD3	1:B:224:LEU:HD13	2.02	0.40
1:B:167:VAL:HG22	1:B:212:VAL:HG13	2.03	0.40
1:D:23:ILE:HD13	1:D:55[B]:CYS:SG	2.62	0.40
1:D:242:GLY:O	1:D:244:ILE:N	2.55	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	252/256 (98%)	243 (96%)	9 (4%)	0	100	100
1	B	251/256 (98%)	241 (96%)	10 (4%)	0	100	100
1	C	251/256 (98%)	243 (97%)	8 (3%)	0	100	100
1	D	251/256 (98%)	242 (96%)	8 (3%)	1 (0%)	34	54
All	All	1005/1024 (98%)	969 (96%)	35 (4%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	243	TYR

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	223/224 (100%)	221 (99%)	2 (1%)	78 92
1	B	222/224 (99%)	222 (100%)	0	100 100
1	C	222/224 (99%)	219 (99%)	3 (1%)	67 86
1	D	222/224 (99%)	217 (98%)	5 (2%)	50 76
All	All	889/896 (99%)	879 (99%)	10 (1%)	73 89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	77	VAL
1	C	10	GLU
1	C	155	VAL
1	C	210	GLN
1	D	83	GLU
1	D	124	LYS
1	D	129	GLN
1	D	235	GLN
1	D	244	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	B	102	GLN
1	C	2	ASN
1	C	43	GLN
1	D	2	ASN
1	D	91	GLN
1	D	121	GLN
1	D	216	GLN
1	D	241	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	AMP	B	801	5,2	18,24,25	1.05	1 (5%)	18,35,38	1.40	3 (16%)
3	AMP	D	801	5,2	18,24,25	1.05	1 (5%)	18,35,38	1.34	3 (16%)
2	NMY	C	805	3	45,45,45	4.07	18 (40%)	63,67,67	1.54	13 (20%)
3	AMP	C	806	2	18,24,25	1.04	1 (5%)	18,35,38	1.42	3 (16%)
3	AMP	A	801	5,2	18,24,25	1.04	1 (5%)	18,35,38	1.38	3 (16%)
2	NMY	C	800	3	45,45,45	4.03	17 (37%)	63,67,67	1.14	4 (6%)
3	AMP	C	801	5,2	18,24,25	1.04	1 (5%)	18,35,38	1.40	3 (16%)
4	PPV	B	802	5	6,8,8	0.75	0	13,13,13	1.10	1 (7%)
2	NMY	A	805	3,1	45,45,45	4.10	17 (37%)	63,67,67	1.32	7 (11%)
3	AMP	A	806	2	18,24,25	1.03	1 (5%)	18,35,38	1.46	3 (16%)
4	PPV	A	802	5	6,8,8	0.74	0	13,13,13	1.10	1 (7%)
4	PPV	C	802	5	6,8,8	0.73	0	13,13,13	1.12	1 (7%)
2	NMY	B	800	3	45,45,45	4.02	17 (37%)	63,67,67	1.16	6 (9%)
2	NMY	D	800	3	45,45,45	4.03	17 (37%)	63,67,67	1.16	4 (6%)
4	PPV	D	802	5	6,8,8	0.74	0	13,13,13	1.02	1 (7%)
2	NMY	A	800	3	45,45,45	4.05	17 (37%)	63,67,67	1.09	3 (4%)

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	AMP	B	801	5,2	-	0/3/25/26	0/3/3/3
3	AMP	D	801	5,2	-	0/3/25/26	0/3/3/3
2	NMY	C	805	3	-	9/18/94/94	0/4/4/4
3	AMP	C	806	2	-	0/3/25/26	0/3/3/3
3	AMP	A	801	5,2	-	0/3/25/26	0/3/3/3
2	NMY	C	800	3	-	3/18/94/94	0/4/4/4
3	AMP	C	801	5,2	-	0/3/25/26	0/3/3/3
4	PPV	B	802	5	-	2/6/6/6	-
2	NMY	A	805	3,1	-	6/18/94/94	0/4/4/4
3	AMP	A	806	2	-	0/3/25/26	0/3/3/3
4	PPV	A	802	5	-	2/6/6/6	-
4	PPV	C	802	5	-	2/6/6/6	-
2	NMY	B	800	3	-	4/18/94/94	0/4/4/4
2	NMY	D	800	3	-	3/18/94/94	0/4/4/4
4	PPV	D	802	5	-	1/6/6/6	-
2	NMY	A	800	3	-	3/18/94/94	0/4/4/4

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	805	NMY	C13-C14	-15.08	1.33	1.52
2	C	805	NMY	C13-C14	-14.98	1.33	1.52
2	A	800	NMY	C13-C14	-14.86	1.33	1.52
2	C	800	NMY	C13-C14	-14.76	1.34	1.52
2	D	800	NMY	C13-C14	-14.75	1.34	1.52
2	B	800	NMY	C13-C14	-14.61	1.34	1.52
2	C	805	NMY	O16-C13	13.49	1.65	1.41
2	C	800	NMY	O16-C13	13.26	1.65	1.41
2	A	800	NMY	O16-C13	13.25	1.65	1.41
2	A	805	NMY	O16-C13	13.16	1.65	1.41
2	D	800	NMY	O16-C13	13.11	1.65	1.41
2	B	800	NMY	O16-C13	13.01	1.65	1.41
2	B	800	NMY	C23-C22	-8.12	1.41	1.52
2	D	800	NMY	C23-C22	-8.06	1.41	1.52
2	A	800	NMY	C23-C22	-8.03	1.41	1.52
2	C	800	NMY	C23-C22	-7.93	1.41	1.52
2	A	805	NMY	C23-C22	-7.84	1.41	1.52
2	C	805	NMY	C23-C22	-7.68	1.41	1.52
2	A	805	NMY	C3-C2	-6.82	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	805	NMY	C3-C2	-6.79	1.45	1.53
2	C	800	NMY	C3-C2	-6.41	1.45	1.53
2	A	800	NMY	C3-C2	-6.36	1.45	1.53
2	B	800	NMY	C3-C2	-6.32	1.45	1.53
2	B	800	NMY	O16-C16	-6.32	1.30	1.45
2	D	800	NMY	C3-C2	-6.28	1.45	1.53
2	D	800	NMY	O16-C16	-6.24	1.31	1.45
2	A	800	NMY	O16-C16	-6.23	1.31	1.45
2	C	800	NMY	O16-C16	-6.20	1.31	1.45
2	A	805	NMY	O16-C16	-6.18	1.31	1.45
2	C	805	NMY	O16-C16	-6.08	1.31	1.45
2	A	800	NMY	C6-C5	-5.96	1.43	1.52
2	B	800	NMY	C6-C5	-5.94	1.44	1.52
2	C	800	NMY	C6-C5	-5.92	1.44	1.52
2	D	800	NMY	C6-C5	-5.91	1.44	1.52
2	C	805	NMY	C6-C5	-5.82	1.44	1.52
2	A	805	NMY	C6-C5	-5.75	1.44	1.52
2	A	805	NMY	O22-C22	4.95	1.56	1.44
2	C	800	NMY	C2-N2	4.73	1.54	1.47
2	C	805	NMY	C2-N2	4.73	1.54	1.47
2	B	800	NMY	C2-N2	4.72	1.54	1.47
2	D	800	NMY	C2-N2	4.72	1.54	1.47
2	A	800	NMY	C2-N2	4.71	1.54	1.47
2	A	805	NMY	C2-N2	4.70	1.54	1.47
2	C	805	NMY	O22-C22	4.69	1.55	1.44
2	A	805	NMY	C20-C19	-4.58	1.47	1.53
2	D	800	NMY	O22-C22	4.58	1.55	1.44
2	B	800	NMY	O22-C22	4.56	1.55	1.44
2	A	800	NMY	O22-C22	4.55	1.55	1.44
2	C	800	NMY	O22-C22	4.54	1.55	1.44
2	A	805	NMY	O5-C5	4.29	1.54	1.44
2	C	805	NMY	O5-C5	4.27	1.54	1.44
2	A	800	NMY	C20-C19	-4.27	1.48	1.53
2	A	800	NMY	C19-N23	4.27	1.53	1.47
2	C	805	NMY	C19-N23	4.26	1.53	1.47
2	A	805	NMY	C19-N23	4.25	1.53	1.47
2	B	800	NMY	C19-N23	4.25	1.53	1.47
2	C	800	NMY	C19-N23	4.25	1.53	1.47
2	D	800	NMY	C19-N23	4.20	1.53	1.47
2	D	800	NMY	C20-C19	-4.15	1.48	1.53
2	B	800	NMY	C20-C19	-4.13	1.48	1.53
2	B	800	NMY	O5-C5	4.11	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	NMY	C20-C19	-4.10	1.48	1.53
2	D	800	NMY	O5-C5	4.09	1.54	1.44
2	C	800	NMY	O5-C5	4.07	1.54	1.44
2	A	800	NMY	O5-C5	4.02	1.54	1.44
2	C	805	NMY	C20-C19	-3.90	1.48	1.53
2	C	805	NMY	O18-C15	-3.69	1.34	1.43
2	A	800	NMY	O18-C15	-3.68	1.34	1.43
2	C	800	NMY	O18-C15	-3.65	1.34	1.43
2	D	800	NMY	O18-C15	-3.60	1.34	1.43
2	A	805	NMY	O18-C15	-3.59	1.34	1.43
2	B	800	NMY	O18-C15	-3.51	1.34	1.43
2	B	800	NMY	O5-C1	2.94	1.49	1.41
2	D	800	NMY	O5-C1	2.92	1.49	1.41
2	C	805	NMY	O5-C1	2.88	1.49	1.41
2	A	805	NMY	O5-C1	2.86	1.49	1.41
2	A	800	NMY	O5-C1	2.82	1.49	1.41
2	A	805	NMY	C15-C16	2.82	1.60	1.52
2	C	800	NMY	O5-C1	2.81	1.49	1.41
2	B	800	NMY	C15-C16	2.78	1.60	1.52
2	D	800	NMY	C15-C16	2.74	1.60	1.52
2	C	805	NMY	O22-C18	2.73	1.48	1.41
2	A	805	NMY	O22-C18	2.71	1.48	1.41
2	C	800	NMY	C15-C16	2.66	1.60	1.52
2	A	800	NMY	C15-C16	2.65	1.60	1.52
2	D	800	NMY	O22-C18	2.59	1.48	1.41
2	C	805	NMY	C15-C16	2.56	1.59	1.52
2	A	800	NMY	O22-C18	2.54	1.48	1.41
3	D	801	AMP	C5-C4	2.51	1.47	1.40
3	C	801	AMP	C5-C4	2.51	1.47	1.40
2	C	800	NMY	O22-C18	2.51	1.48	1.41
2	B	800	NMY	O22-C18	2.50	1.48	1.41
3	A	806	AMP	C5-C4	2.48	1.47	1.40
3	A	801	AMP	C5-C4	2.48	1.47	1.40
3	B	801	AMP	C5-C4	2.48	1.47	1.40
3	C	806	AMP	C5-C4	2.46	1.47	1.40
2	B	800	NMY	O14-C14	2.46	1.48	1.43
2	A	805	NMY	O14-C14	2.45	1.48	1.43
2	D	800	NMY	O14-C14	2.44	1.48	1.43
2	C	800	NMY	O3-C3	2.43	1.48	1.43
2	D	800	NMY	O3-C3	2.42	1.48	1.43
2	A	805	NMY	O3-C3	2.42	1.48	1.43
2	A	800	NMY	O3-C3	2.42	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	805	NMY	O3-C3	2.42	1.48	1.43
2	C	800	NMY	O14-C14	2.41	1.48	1.43
2	B	800	NMY	O3-C3	2.40	1.48	1.43
2	C	805	NMY	O14-C14	2.39	1.48	1.43
2	A	800	NMY	O14-C14	2.38	1.48	1.43
2	C	805	NMY	O20-C20	2.00	1.47	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	805	NMY	C18-O18-C15	-4.01	108.05	117.96
2	B	800	NMY	C13-O11-C11	-3.80	108.56	117.96
2	D	800	NMY	C13-O11-C11	-3.68	108.85	117.96
2	C	805	NMY	C1-O1-C10	-3.62	109.00	117.96
2	C	805	NMY	O22-C18-C19	3.58	118.12	110.06
2	A	800	NMY	C13-O11-C11	-3.47	109.38	117.96
2	C	805	NMY	C21-C20-C19	3.42	116.95	111.07
2	A	805	NMY	C1-O1-C10	-3.41	109.51	117.96
2	A	805	NMY	C18-O18-C15	-3.32	109.74	117.96
2	C	800	NMY	C13-O11-C11	-3.32	109.75	117.96
3	C	801	AMP	N3-C2-N1	-3.25	123.59	128.68
3	A	806	AMP	N3-C2-N1	-3.24	123.62	128.68
2	C	805	NMY	C18-C19-C20	3.17	118.51	110.21
3	B	801	AMP	N3-C2-N1	-3.17	123.72	128.68
3	C	806	AMP	N3-C2-N1	-3.15	123.75	128.68
3	A	801	AMP	N3-C2-N1	-3.14	123.76	128.68
3	D	801	AMP	N3-C2-N1	-3.14	123.77	128.68
2	A	805	NMY	C1-O5-C5	3.13	119.82	113.69
2	C	805	NMY	O22-C22-C23	3.03	111.66	106.01
2	C	805	NMY	C1-O5-C5	2.99	119.55	113.69
2	A	805	NMY	O22-C22-C23	2.93	111.46	106.01
3	B	801	AMP	C3'-C2'-C1'	2.86	105.28	100.98
4	C	802	PPV	P2-OPP-P1	-2.72	123.48	132.83
3	A	806	AMP	C4-C5-N7	-2.71	106.57	109.40
3	A	801	AMP	C3'-C2'-C1'	2.70	105.04	100.98
3	A	806	AMP	C3'-C2'-C1'	2.69	105.03	100.98
3	C	801	AMP	C4-C5-N7	-2.67	106.62	109.40
3	C	806	AMP	C4-C5-N7	-2.60	106.69	109.40
3	B	801	AMP	C4-C5-N7	-2.60	106.69	109.40
3	A	801	AMP	C4-C5-N7	-2.60	106.69	109.40
3	D	801	AMP	C3'-C2'-C1'	2.58	104.87	100.98
3	C	806	AMP	C3'-C2'-C1'	2.57	104.85	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	805	NMY	O5-C1-C2	2.55	115.80	110.06
2	C	800	NMY	C18-O18-C15	-2.55	111.65	117.96
3	D	801	AMP	C4-C5-N7	-2.53	106.76	109.40
2	C	800	NMY	O22-C22-C23	2.51	110.67	106.01
2	A	800	NMY	C1-O1-C10	-2.49	111.81	117.96
3	C	801	AMP	C3'-C2'-C1'	2.48	104.71	100.98
2	A	800	NMY	C18-O18-C15	-2.38	112.07	117.96
2	C	805	NMY	C8-C7-C12	2.37	113.61	110.04
4	A	802	PPV	P2-OPP-P1	-2.36	124.74	132.83
2	B	800	NMY	O11-C13-C14	2.34	112.81	107.96
2	A	805	NMY	C3-C4-C5	2.33	114.40	110.24
2	C	805	NMY	O5-C1-C2	2.30	115.23	110.06
2	B	800	NMY	O5-C1-C2	2.26	115.15	110.06
2	C	800	NMY	O22-C22-C21	-2.26	105.60	109.69
2	A	805	NMY	O5-C5-C6	2.24	110.18	106.01
4	D	802	PPV	P2-OPP-P1	-2.23	125.18	132.83
2	B	800	NMY	C1-O1-C10	-2.23	112.45	117.96
2	D	800	NMY	C1-O1-C10	-2.21	112.48	117.96
2	C	805	NMY	O5-C5-C6	2.21	110.13	106.01
4	B	802	PPV	P2-OPP-P1	-2.18	125.34	132.83
2	B	800	NMY	O5-C5-C6	2.12	109.96	106.01
2	C	805	NMY	C13-O11-C11	-2.12	112.73	117.96
2	D	800	NMY	O5-C1-C2	2.11	114.81	110.06
2	D	800	NMY	C18-O18-C15	-2.09	112.79	117.96
2	B	800	NMY	C18-O18-C15	-2.04	112.92	117.96
2	C	805	NMY	C20-C21-C22	2.02	113.84	110.24
2	C	805	NMY	C20-C19-N23	-2.01	106.94	111.05

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	NMY	C21-C22-C23-N19
2	A	800	NMY	O22-C22-C23-N19
2	A	805	NMY	C4-C5-C6-N6
2	A	805	NMY	O5-C5-C6-N6
2	A	805	NMY	C14-C13-O11-C11
2	A	805	NMY	O16-C13-O11-C11
2	B	800	NMY	C21-C22-C23-N19
2	C	800	NMY	C21-C22-C23-N19
2	C	800	NMY	O22-C22-C23-N19
2	C	805	NMY	C4-C5-C6-N6

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Mol	Chain	Res	Type	Atoms
2	C	805	NMY	O5-C5-C6-N6
2	C	805	NMY	C14-C13-O11-C11
4	A	802	PPV	P1-OPP-P2-O32
4	B	802	PPV	P1-OPP-P2-O12
4	B	802	PPV	P1-OPP-P2-O32
4	C	802	PPV	P1-OPP-P2-O12
4	C	802	PPV	P1-OPP-P2-O32
4	D	802	PPV	P1-OPP-P2-O32
2	D	800	NMY	O5-C1-O1-C10
2	B	800	NMY	O5-C1-O1-C10
2	A	800	NMY	O5-C1-O1-C10
2	C	800	NMY	O5-C1-O1-C10
2	C	805	NMY	O16-C13-O11-C11
2	C	805	NMY	C15-C16-C17-O17
2	D	800	NMY	C21-C22-C23-N19
4	A	802	PPV	P1-OPP-P2-O22
2	B	800	NMY	O22-C22-C23-N19
2	D	800	NMY	O22-C22-C23-N19
2	C	805	NMY	O5-C1-O1-C10
2	A	805	NMY	C12-C11-O11-C13
2	C	805	NMY	C14-C15-O18-C18
2	A	805	NMY	C10-C11-O11-C13
2	C	805	NMY	O16-C16-C17-O17
2	B	800	NMY	C14-C13-O11-C11
2	C	805	NMY	C16-C15-O18-C18

There are no ring outliers.

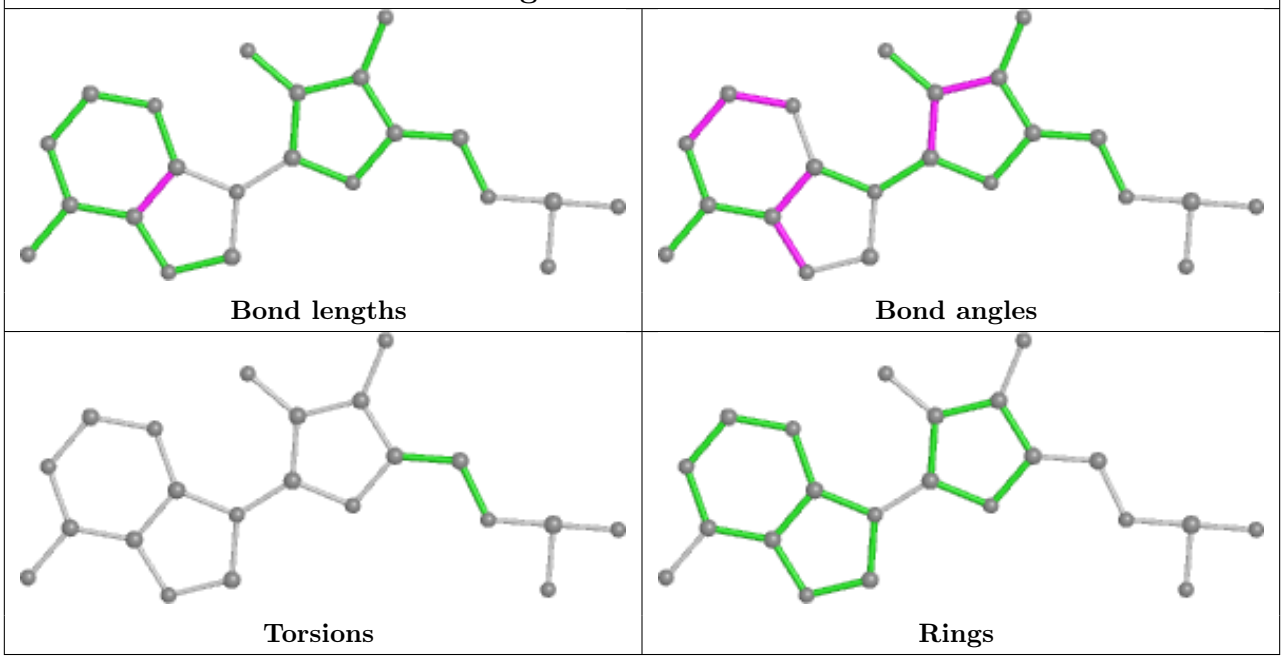
7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	805	NMY	3	0
3	A	801	AMP	1	0
2	C	800	NMY	4	0
2	A	805	NMY	2	0
2	B	800	NMY	2	0
2	D	800	NMY	3	0
2	A	800	NMY	2	0

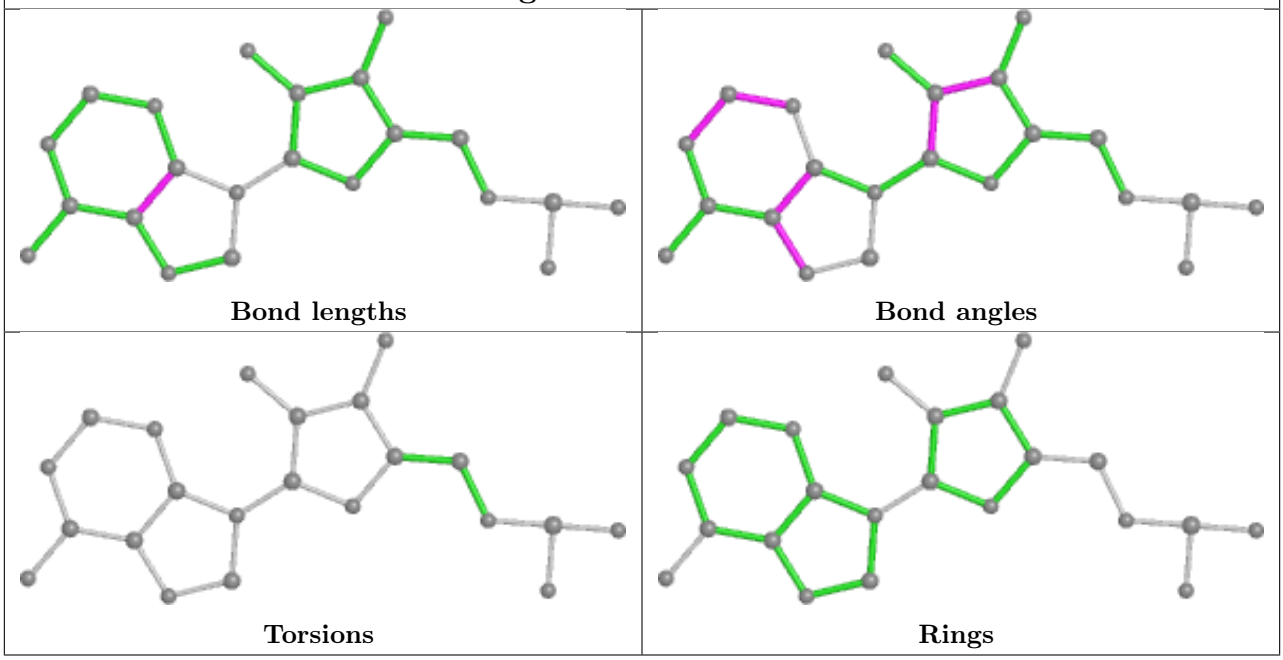
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

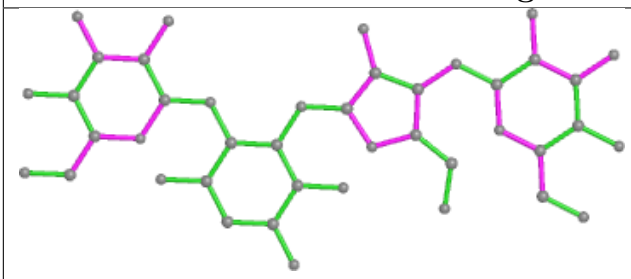
Ligand AMP B 801



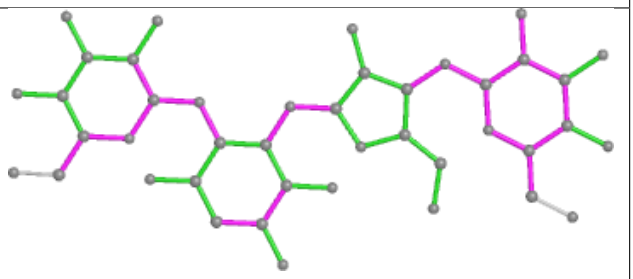
Ligand AMP D 801



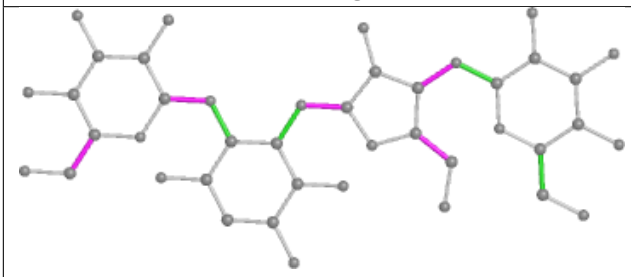
Ligand NMY C 805



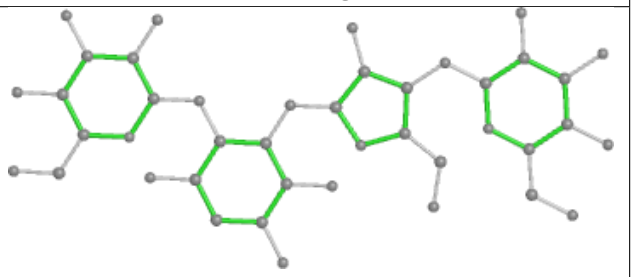
Bond lengths



Bond angles

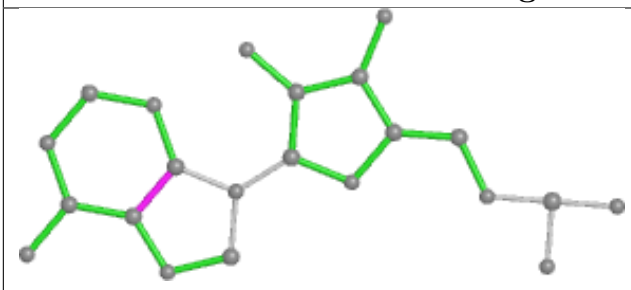


Torsions

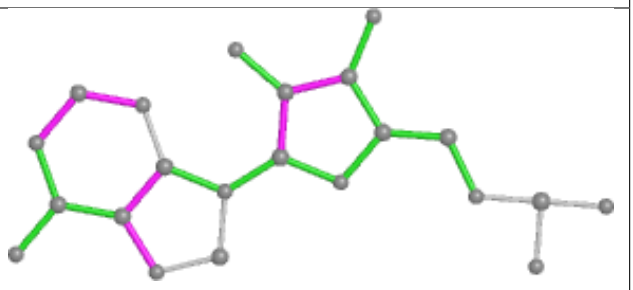


Rings

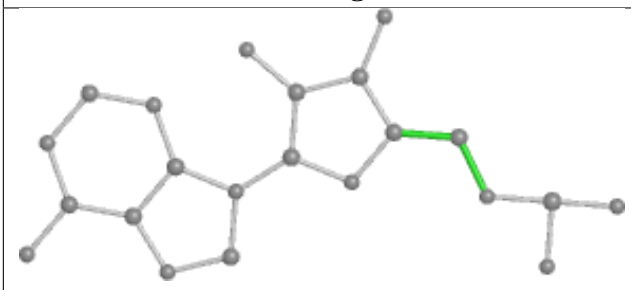
Ligand AMP C 806



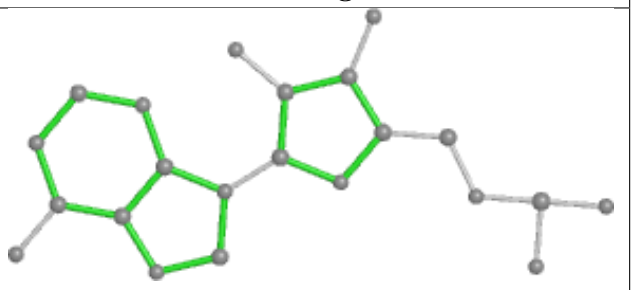
Bond lengths



Bond angles

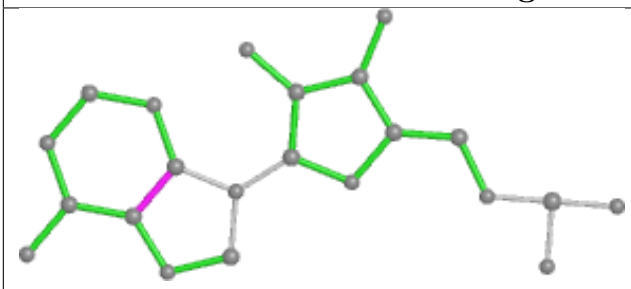


Torsions

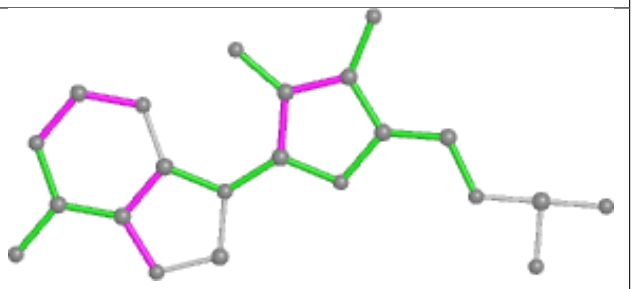


Rings

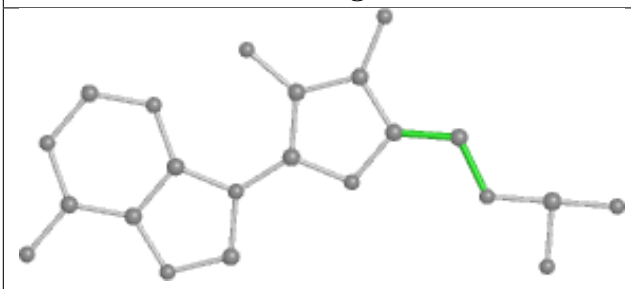
Ligand AMP A 801



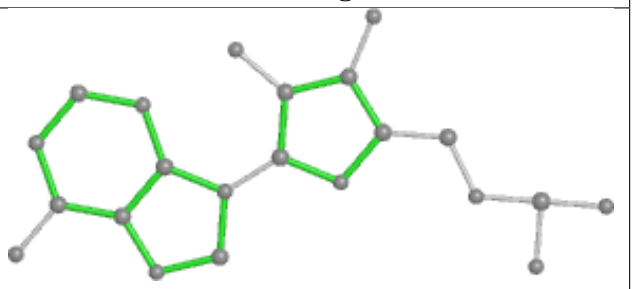
Bond lengths



Bond angles

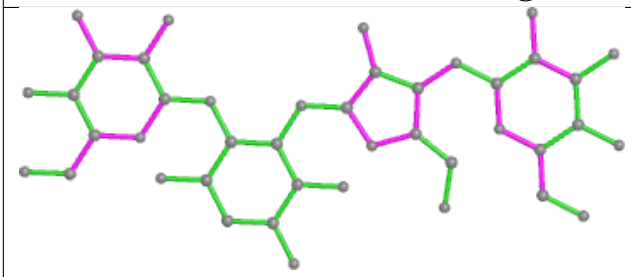


Torsions

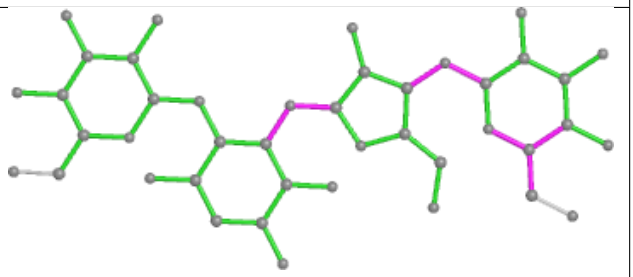


Rings

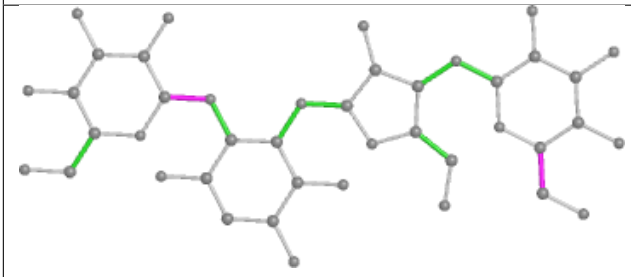
Ligand NMY C 800



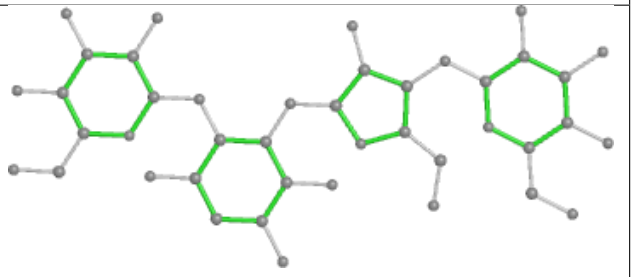
Bond lengths



Bond angles

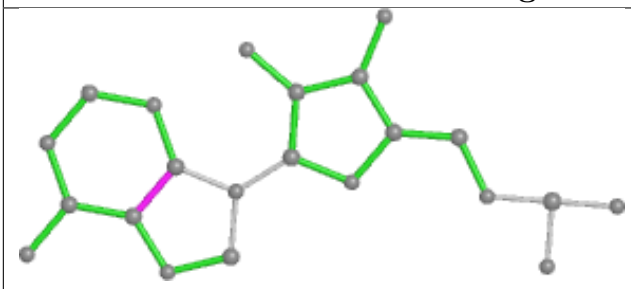


Torsions

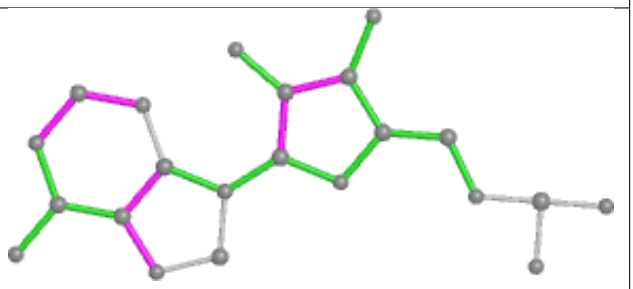


Rings

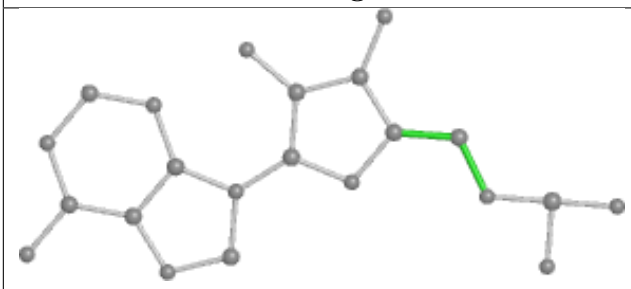
Ligand AMP C 801



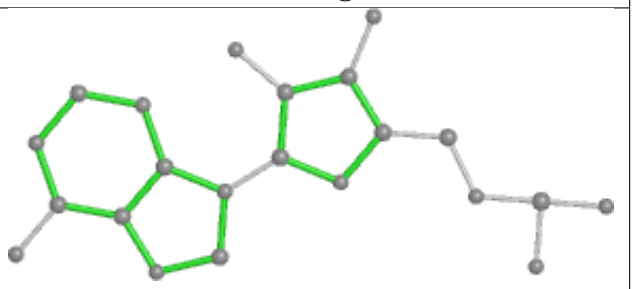
Bond lengths



Bond angles

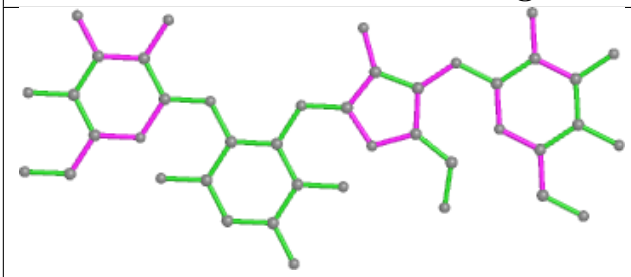


Torsions

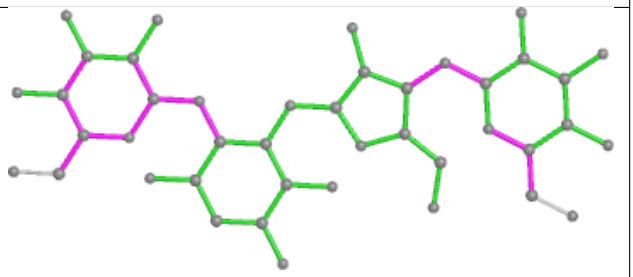


Rings

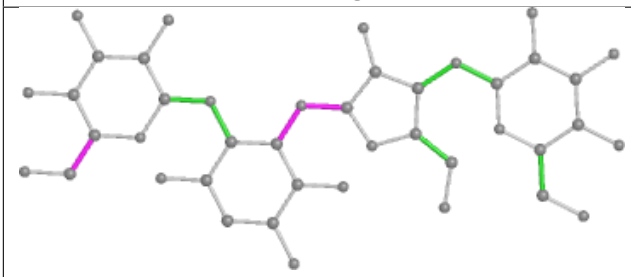
Ligand NMY A 805



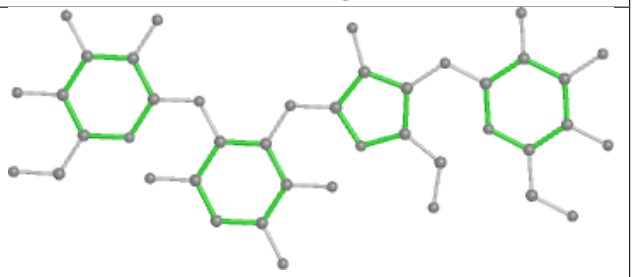
Bond lengths



Bond angles

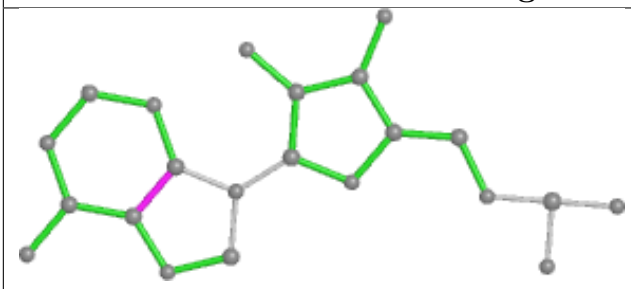


Torsions

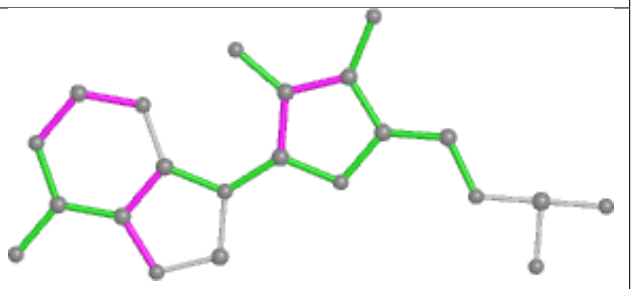


Rings

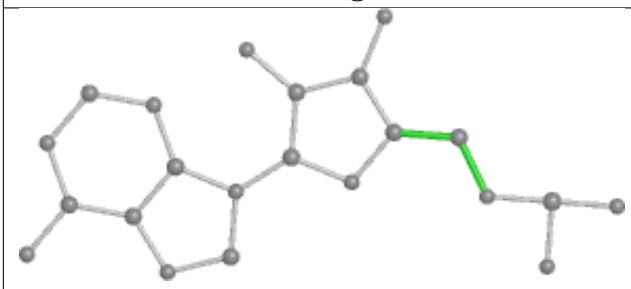
Ligand AMP A 806



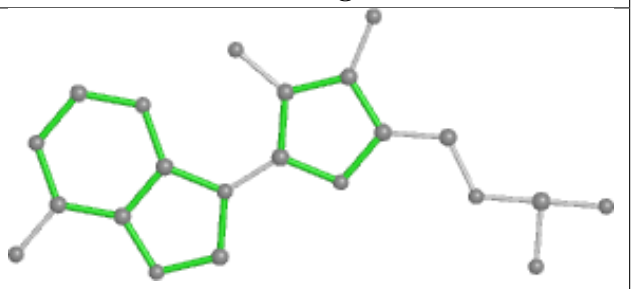
Bond lengths



Bond angles

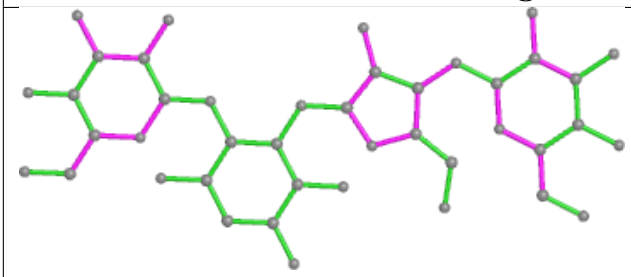


Torsions

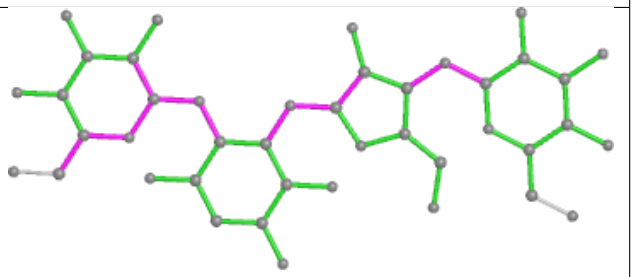


Rings

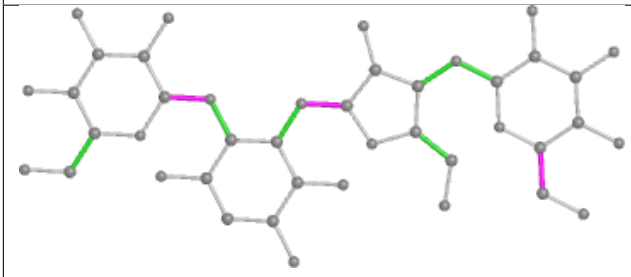
Ligand NMY B 800



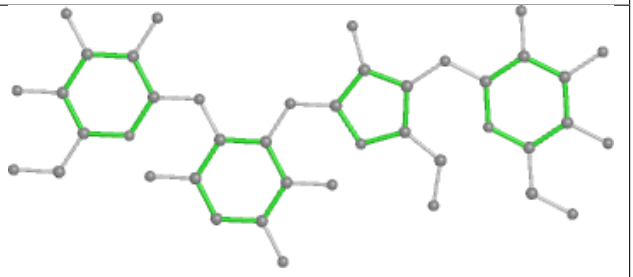
Bond lengths



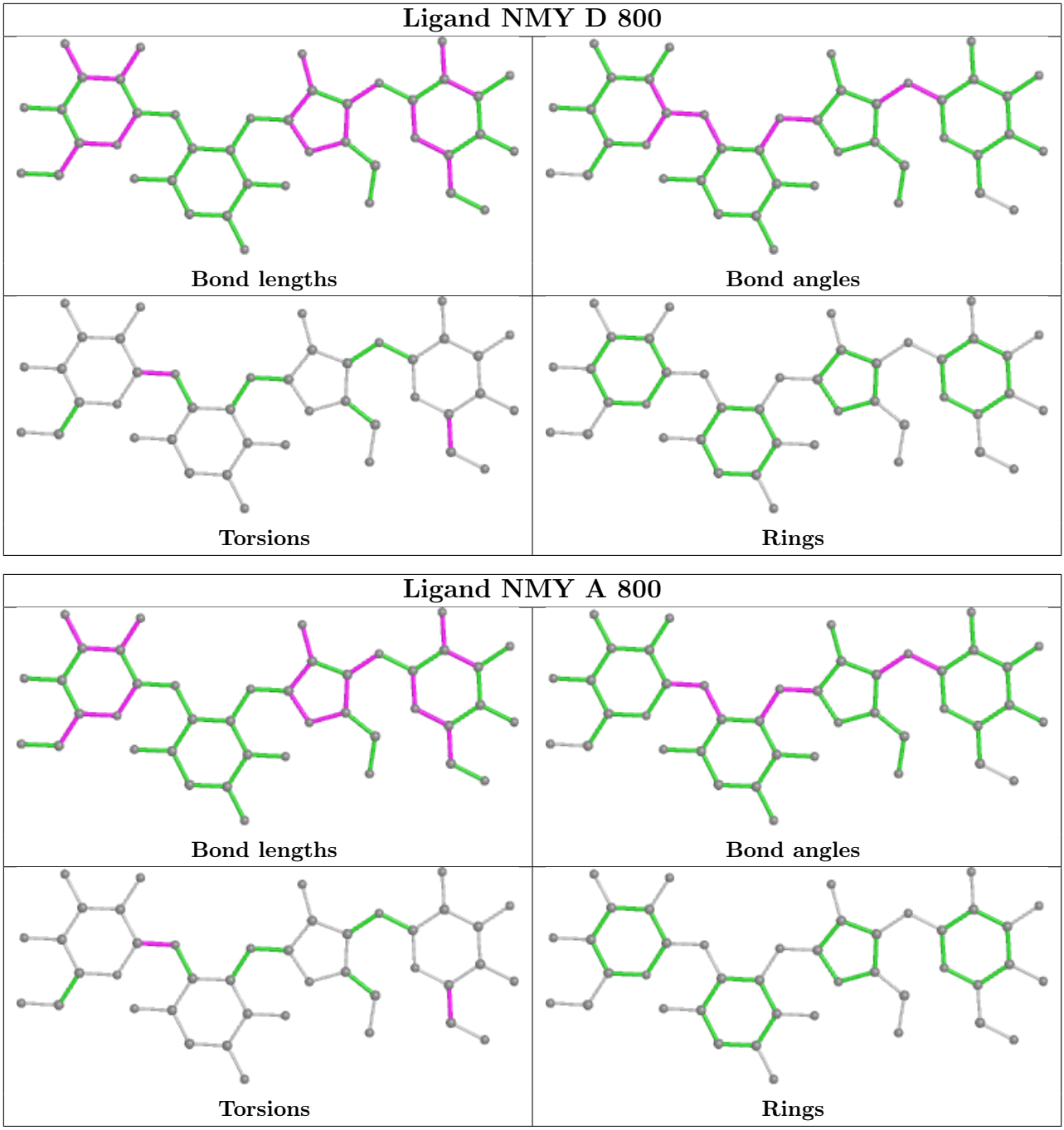
Bond angles



Torsions



Rings



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	252/256 (98%)	-0.37	0 100 100	12, 25, 48, 64	0
1	B	252/256 (98%)	-0.33	3 (1%) 79 80	13, 26, 47, 71	0
1	C	252/256 (98%)	-0.30	3 (1%) 79 80	11, 26, 48, 72	0
1	D	252/256 (98%)	-0.24	7 (2%) 53 56	15, 29, 51, 77	0
All	All	1008/1024 (98%)	-0.31	13 (1%) 77 79	11, 27, 49, 77	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	247	VAL	5.5
1	C	61	GLU	3.8
1	D	249	LYS	3.5
1	C	60	GLU	3.1
1	D	248	SER	2.8
1	D	246	ASP	2.6
1	C	2	ASN	2.5
1	D	61	GLU	2.4
1	D	250	ARG	2.3
1	B	246	ASP	2.2
1	D	2	ASN	2.1
1	B	247	VAL	2.1
1	B	61	GLU	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

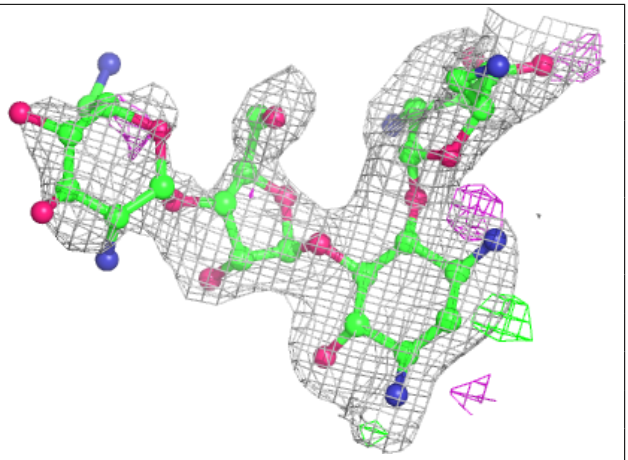
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

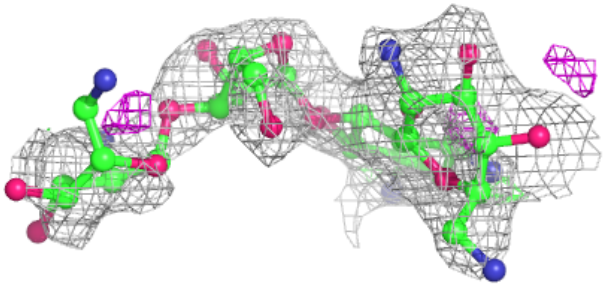
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NMY	C	805	42/42	0.84	0.26	33,54,83,88	0
2	NMY	A	805	42/42	0.91	0.18	21,41,75,78	0
2	NMY	D	800	42/42	0.93	0.15	32,40,50,54	0
3	AMP	C	806	22/23	0.93	0.16	26,37,52,56	0
2	NMY	B	800	42/42	0.94	0.16	22,30,40,43	0
3	AMP	D	801	22/23	0.95	0.11	28,37,45,59	0
3	AMP	A	806	22/23	0.96	0.12	20,26,32,38	0
3	AMP	B	801	22/23	0.96	0.15	19,26,34,38	0
2	NMY	A	800	42/42	0.96	0.14	11,26,33,41	0
2	NMY	C	800	42/42	0.96	0.15	16,24,30,35	0
4	PPV	B	802	9/9	0.96	0.14	25,34,46,60	0
4	PPV	D	802	9/9	0.96	0.11	31,36,51,63	0
3	AMP	A	801	22/23	0.97	0.15	21,29,38,45	0
5	MG	D	804	1/1	0.97	0.10	25,25,25,25	0
4	PPV	C	802	9/9	0.98	0.11	15,21,32,34	0
4	PPV	A	802	9/9	0.98	0.12	24,27,41,41	0
5	MG	B	804	1/1	0.98	0.18	13,13,13,13	0
5	MG	C	803	1/1	0.98	0.17	7,7,7,7	0
5	MG	C	804	1/1	0.98	0.16	13,13,13,13	0
3	AMP	C	801	22/23	0.98	0.14	12,18,26,27	0
5	MG	A	804	1/1	0.99	0.18	11,11,11,11	0
5	MG	B	803	1/1	0.99	0.08	10,10,10,10	0
5	MG	D	803	1/1	0.99	0.08	24,24,24,24	0
5	MG	A	803	1/1	0.99	0.13	15,15,15,15	0

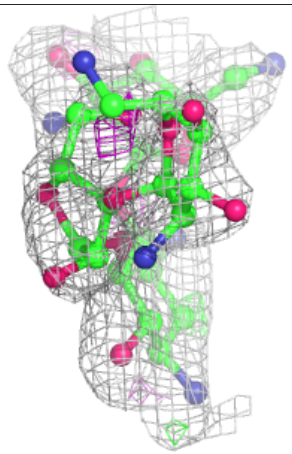
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NMY C 805:

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

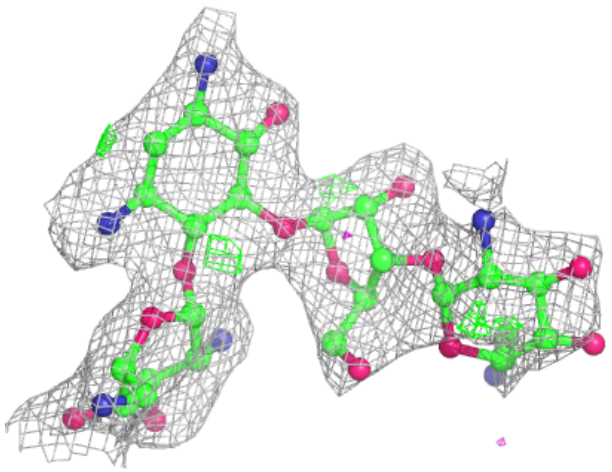


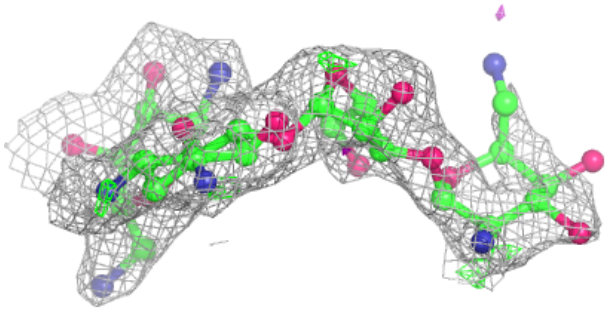




Electron density around NMY A 805:

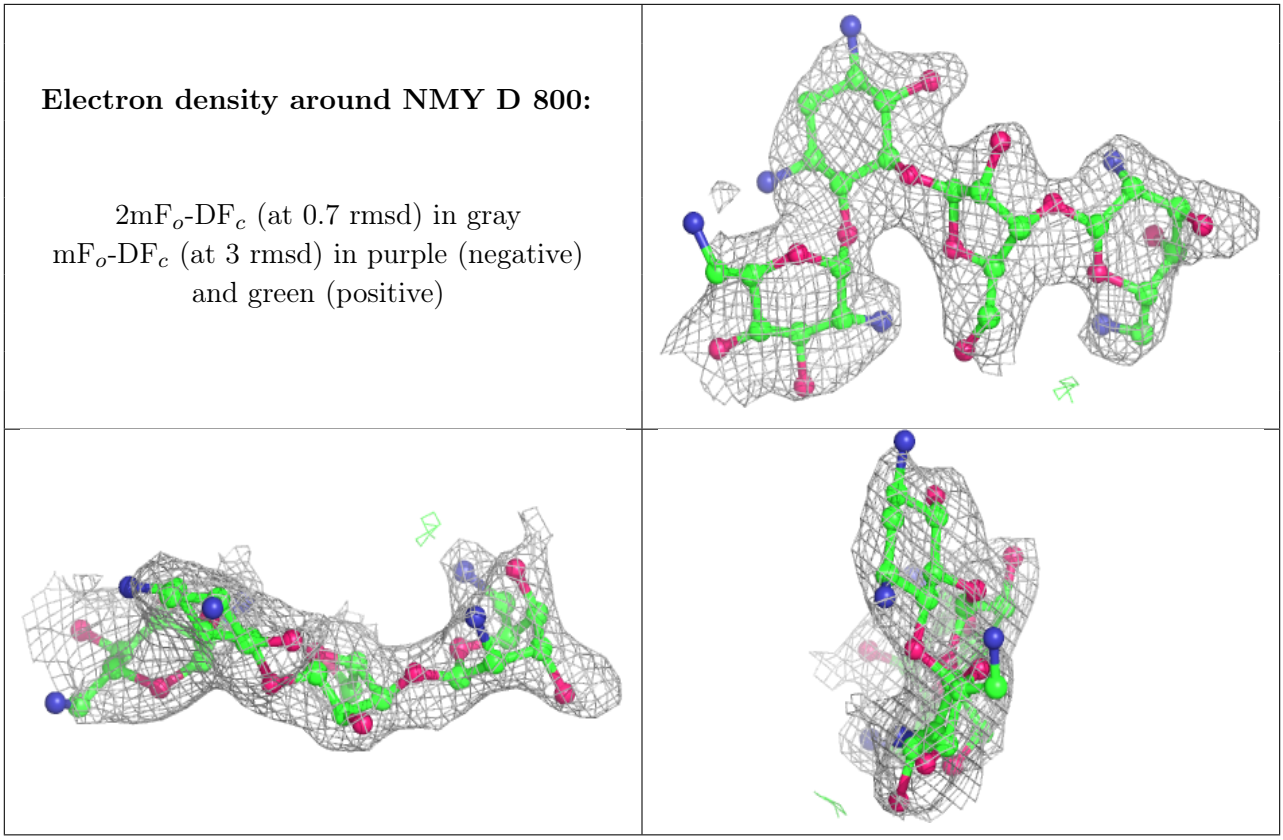
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





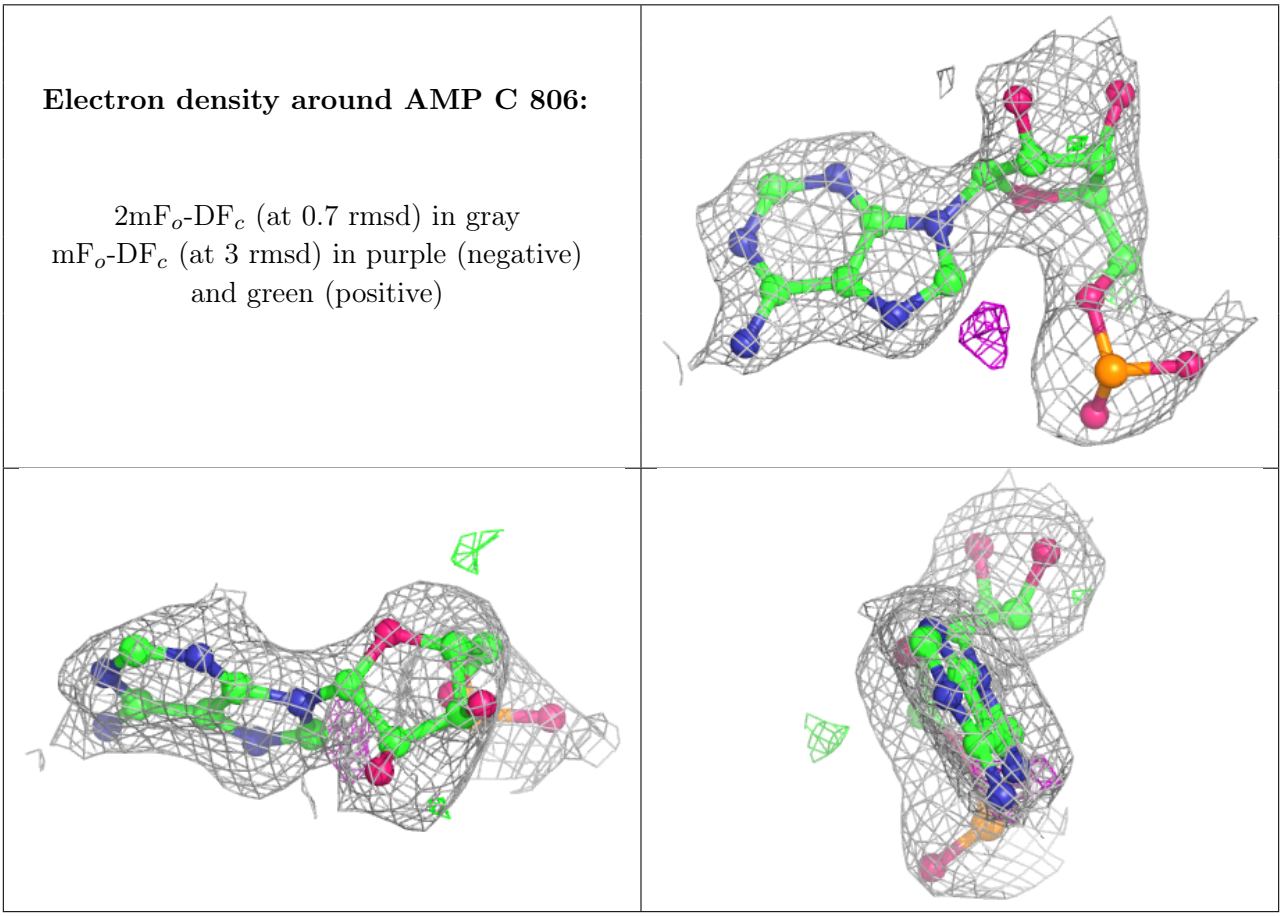
Electron density around NMY D 800:

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



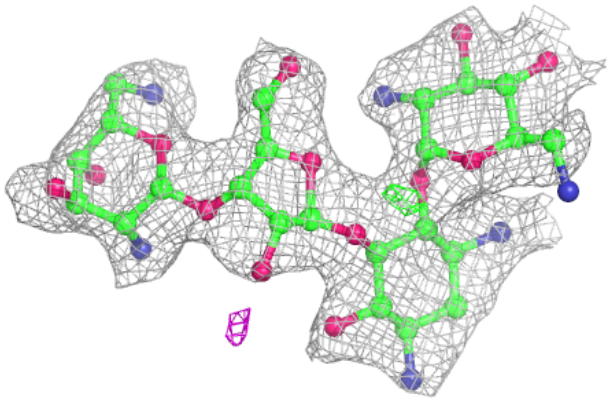
Electron density around AMP C 806:

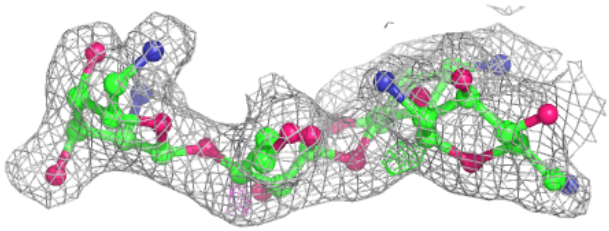
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

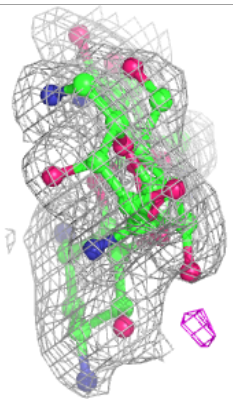


Electron density around NMY B 800:

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

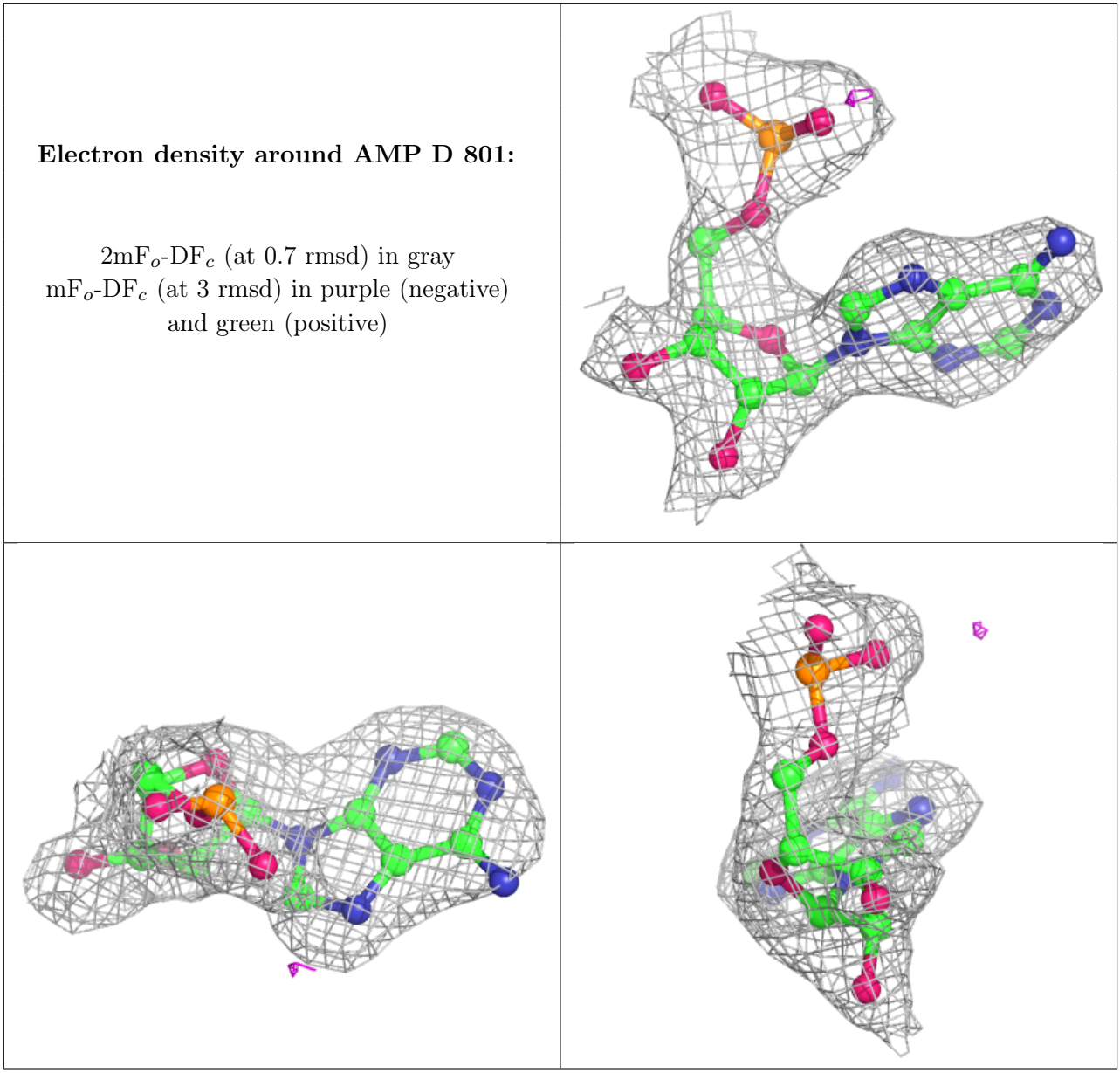






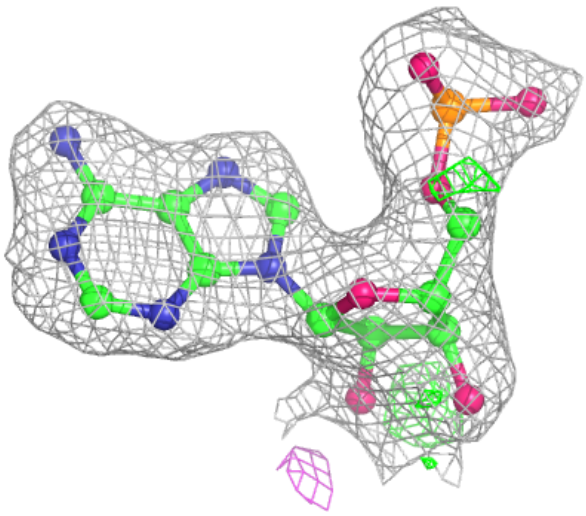
Electron density around AMP D 801:

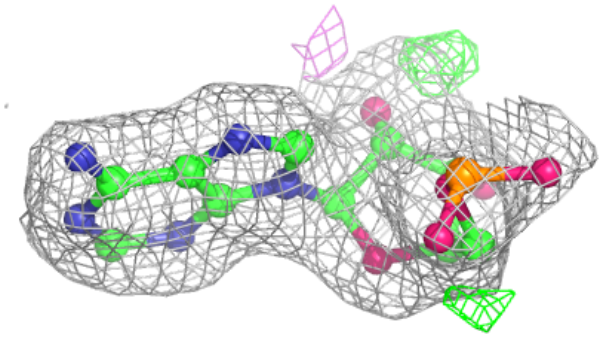
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

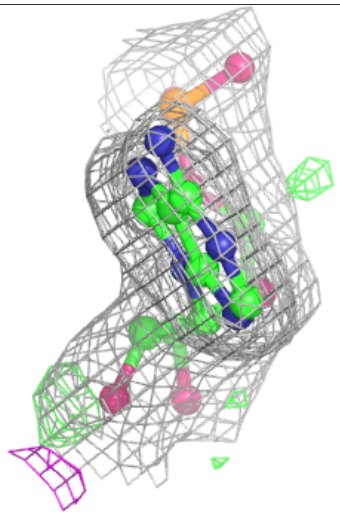


Electron density around AMP A 806:

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

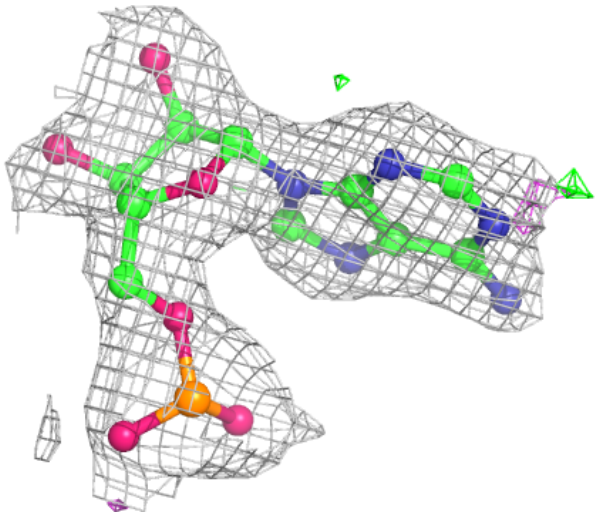


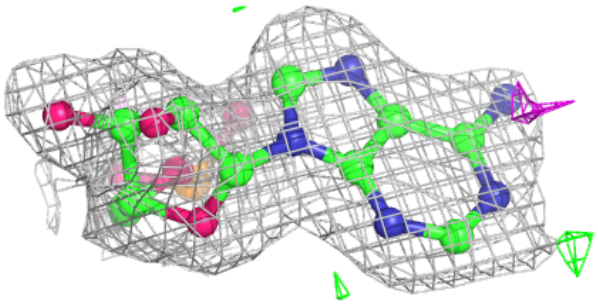


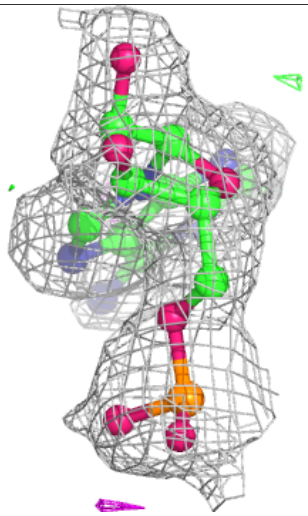


Electron density around AMP B 801:

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

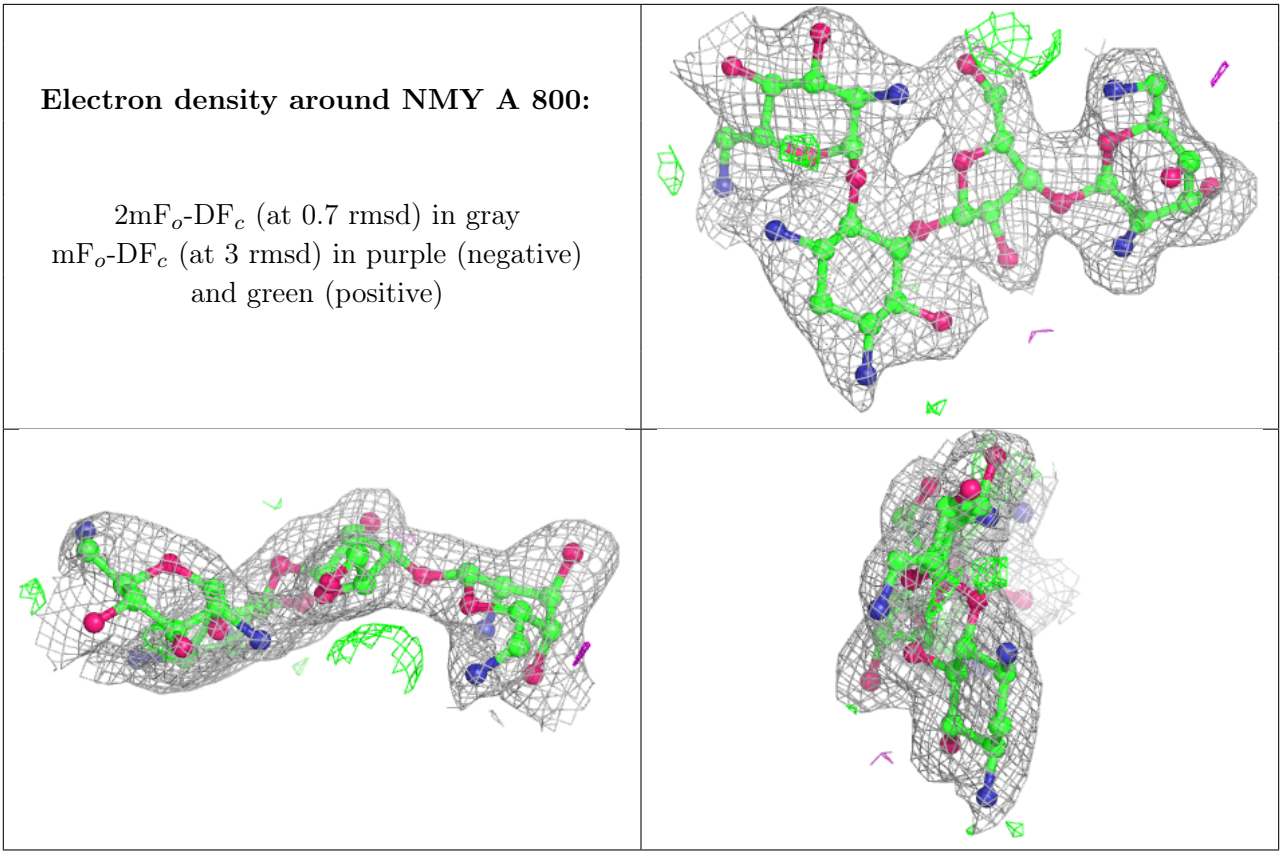






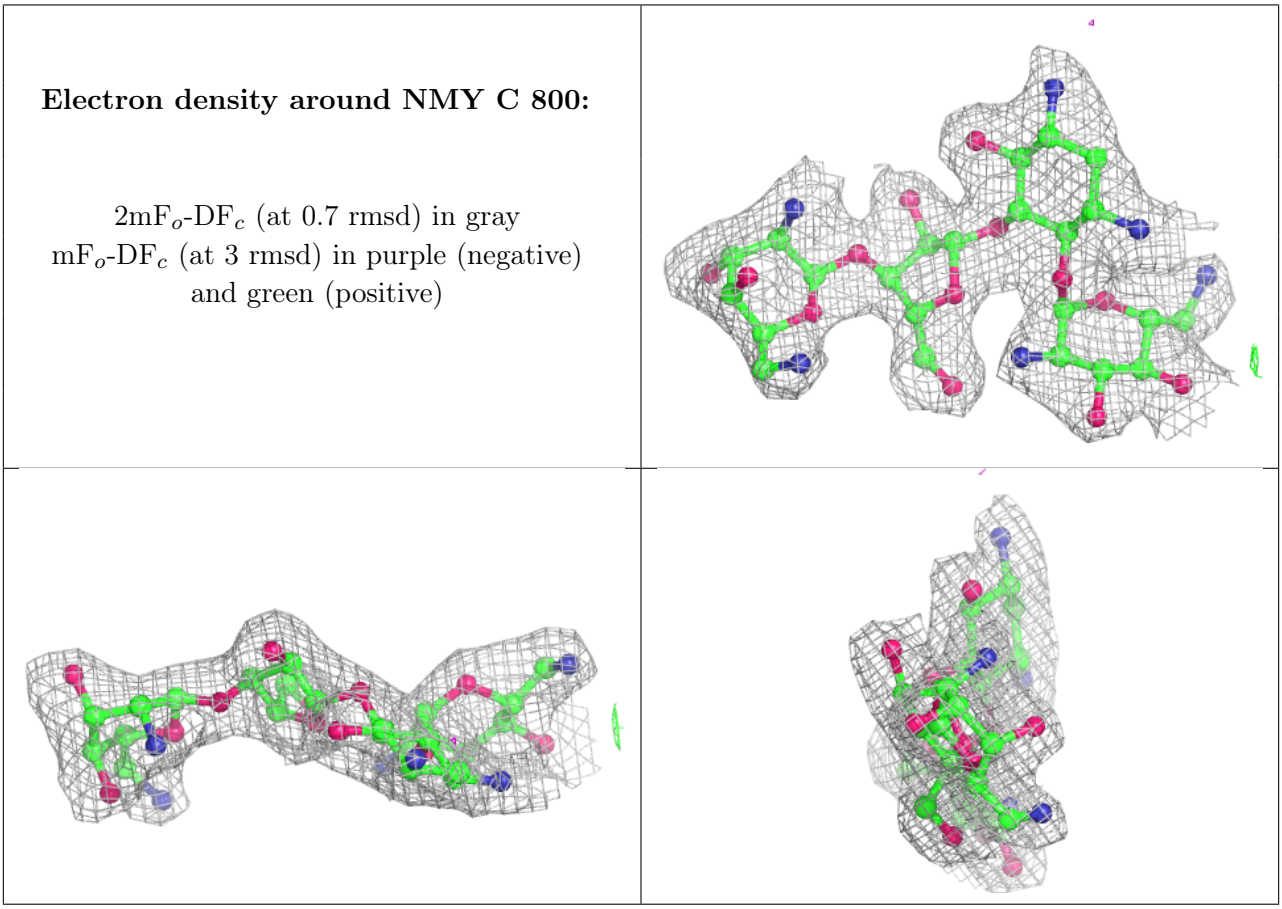
Electron density around NMY A 800:

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



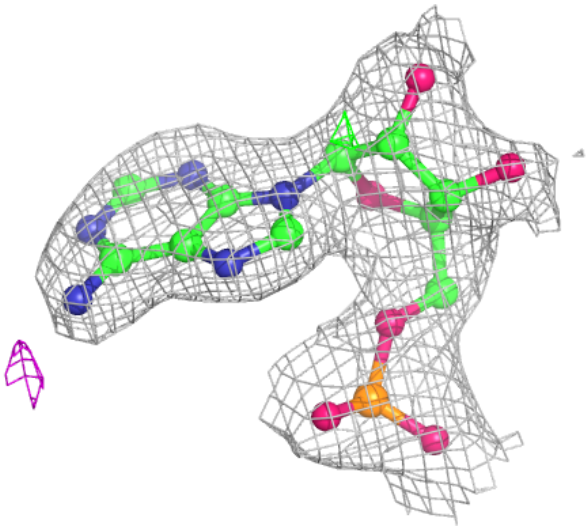
Electron density around NMY C 800:

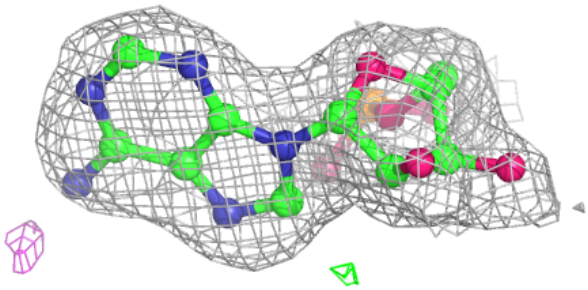
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

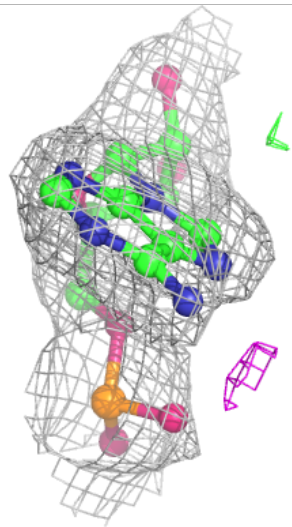


Electron density around AMP A 801:

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

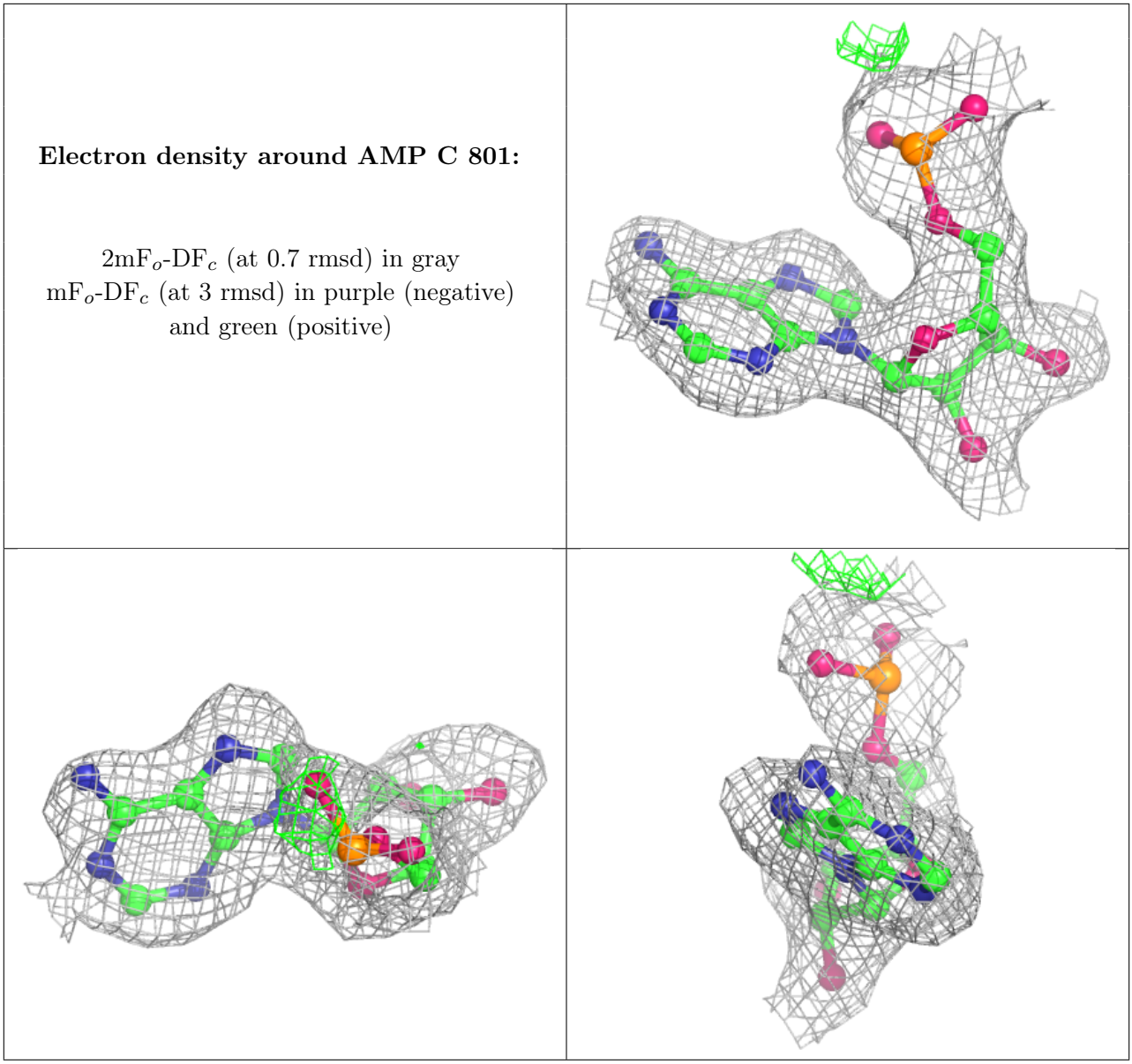






Electron density around AMP C 801:

$2mF_o$-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.