



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 04:19 AM EST

PDB ID : 1YXU  
Title : Crystal Structure of Kinase Pim1 in Complex with AMP  
Authors : Kumar, A.; Mandiyan, V.; Suzuki, Y.; Zhang, C.; Rice, J.; Tsai, J.; Artis, D.R.; Ibrahim, P.; Bremer, R.  
Deposited on : 2005-02-22  
Resolution : 2.24 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

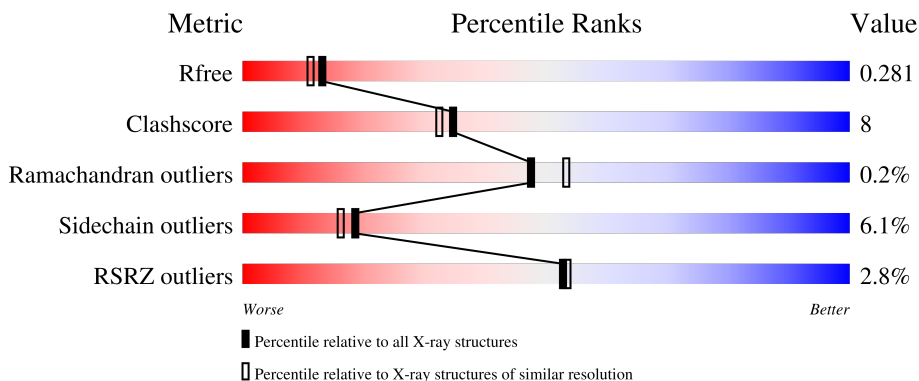
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	293	 4% 71% 20% • 7%
1	B	293	 3% 76% 16% • 7%
1	C	293	 2% 74% 18% • 7%
1	D	293	 2% 75% 15% • 7%

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

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	AMP	D	850	X	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9385 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 Proto-oncogene serine/threonine-protein kinase Pim-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	2224	1423	389	404	8	0	0	0
1	B	273	2224	1423	389	404	8	0	0	0
1	C	272	2217	1418	388	403	8	0	0	0
1	D	273	2224	1423	389	404	8	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

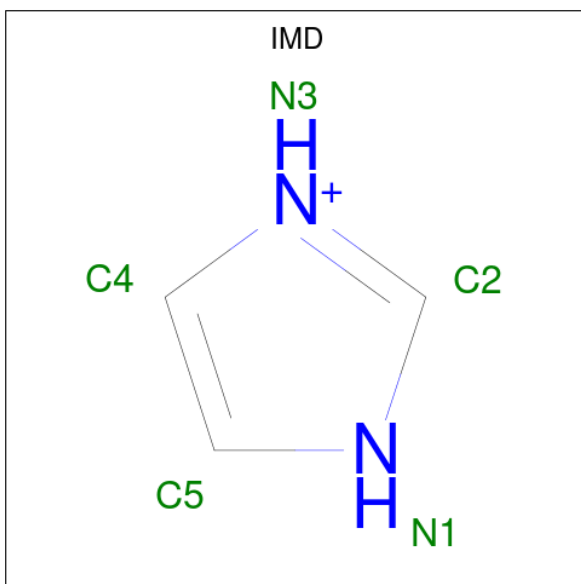
Chain	Residue	Modelled	Actual	Comment	Reference
A	314	VAL	-	expression tag	UNP P11309
A	315	ASP	-	expression tag	UNP P11309
A	316	HIS	-	expression tag	UNP P11309
A	317	HIS	-	expression tag	UNP P11309
A	318	HIS	-	expression tag	UNP P11309
A	319	HIS	-	expression tag	UNP P11309
A	320	HIS	-	expression tag	UNP P11309
A	321	HIS	-	expression tag	UNP P11309
B	314	VAL	-	expression tag	UNP P11309
B	315	ASP	-	expression tag	UNP P11309
B	316	HIS	-	expression tag	UNP P11309
B	317	HIS	-	expression tag	UNP P11309
B	318	HIS	-	expression tag	UNP P11309
B	319	HIS	-	expression tag	UNP P11309
B	320	HIS	-	expression tag	UNP P11309
B	321	HIS	-	expression tag	UNP P11309
C	314	VAL	-	expression tag	UNP P11309
C	315	ASP	-	expression tag	UNP P11309
C	316	HIS	-	expression tag	UNP P11309
C	317	HIS	-	expression tag	UNP P11309
C	318	HIS	-	expression tag	UNP P11309

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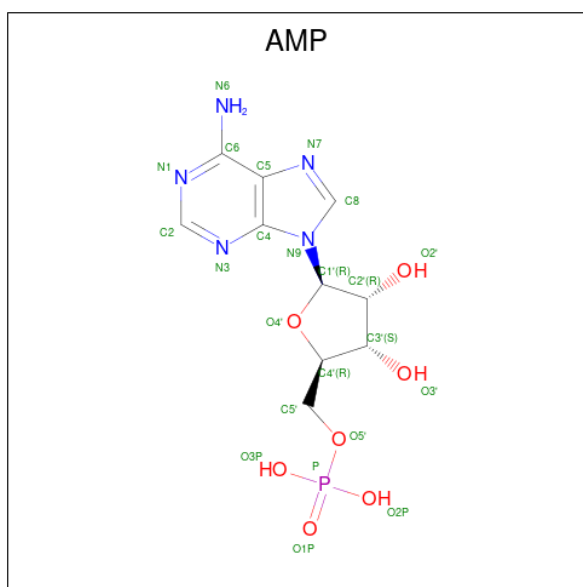
Chain	Residue	Modelled	Actual	Comment	Reference
C	319	HIS	-	expression tag	UNP P11309
C	320	HIS	-	expression tag	UNP P11309
C	321	HIS	-	expression tag	UNP P11309
D	314	VAL	-	expression tag	UNP P11309
D	315	ASP	-	expression tag	UNP P11309
D	316	HIS	-	expression tag	UNP P11309
D	317	HIS	-	expression tag	UNP P11309
D	318	HIS	-	expression tag	UNP P11309
D	319	HIS	-	expression tag	UNP P11309
D	320	HIS	-	expression tag	UNP P11309
D	321	HIS	-	expression tag	UNP P11309

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 5 3 2	0	0
2	B	1	Total C N 5 3 2	0	0
2	C	1	Total C N 5 3 2	0	0
2	D	1	Total C N 5 3 2	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
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

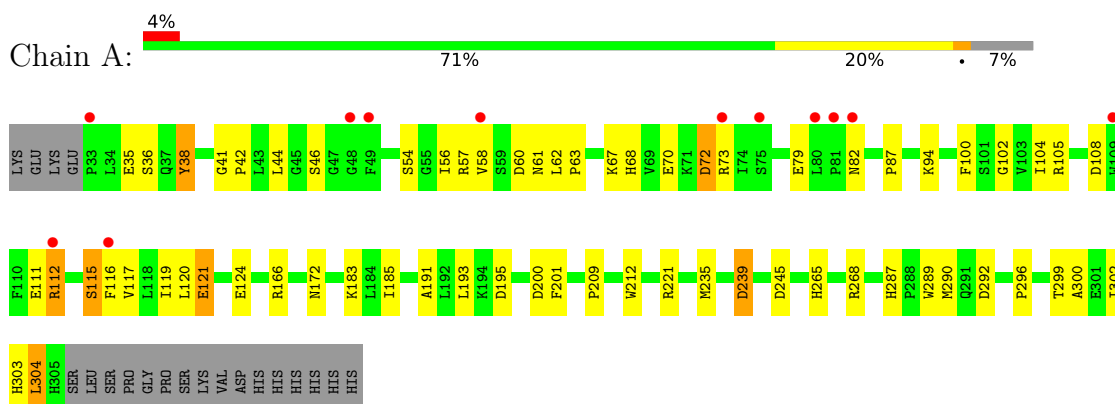
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	81	Total	O	0	0
			81	81		
4	C	80	Total	O	0	0
			80	80		
4	D	93	Total	O	0	0
			93	93		

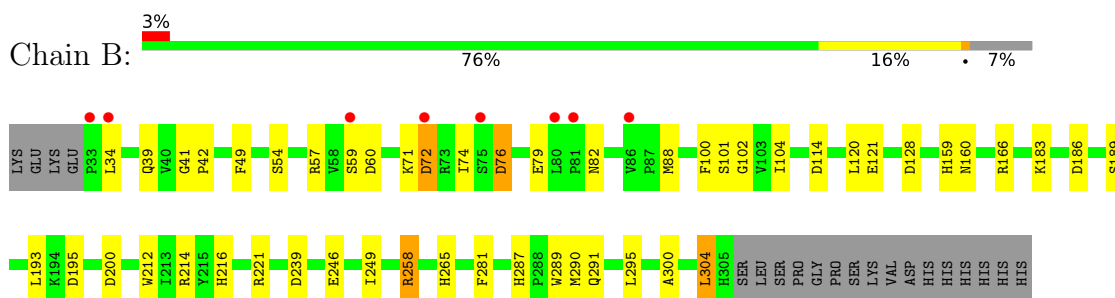
### 3 Residue-property plots [i](#)

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.

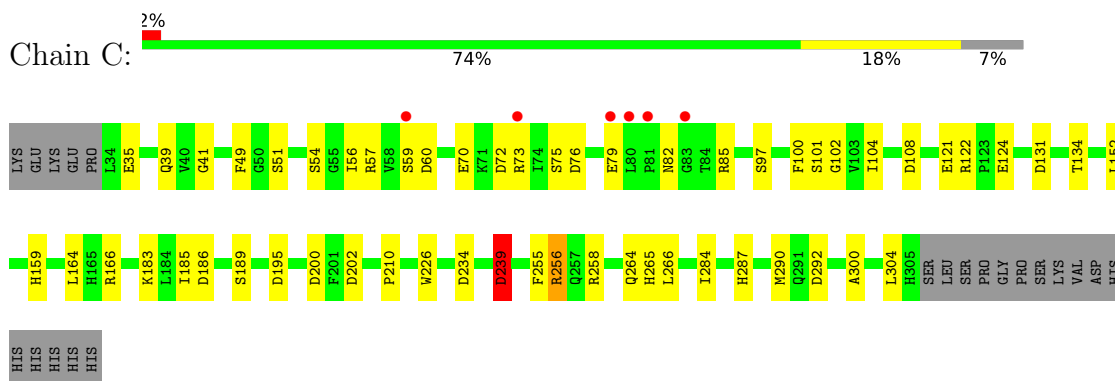
- Molecule 1: Proto-oncogene serine/threonine-protein kinase Pim-1



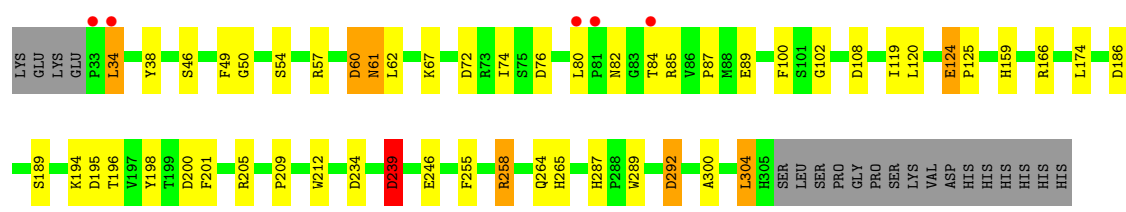
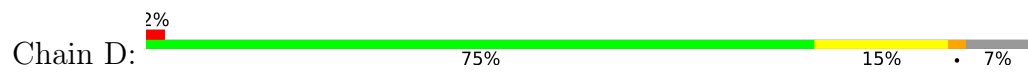
- Molecule 1: Proto-oncogene serine/threonine-protein kinase Pim-1



- Molecule 1: Proto-oncogene serine/threonine-protein kinase Pim-1



- Molecule 1: Proto-oncogene serine/threonine-protein kinase Pim-1





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.75Å 195.75Å 80.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.55 – 2.24 72.76 – 2.24	Depositor EDS
% Data completeness (in resolution range)	97.3 (72.55-2.24) 97.3 (72.76-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.25Å)	Xtrriage
Refinement program	REFMAC 5.1.25	Depositor
R, $R_{free}$	0.228 , 0.276 0.236 , 0.281	Depositor DCC
$R_{free}$ test set	4111 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtrriage
Anisotropy	0.366	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 27.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.077 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.65 % 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 1.9827e-05. 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: IMD, AMP

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	0.92	4/2284 (0.2%)	0.89	6/3100 (0.2%)
1	B	0.55	0/2284	0.82	8/3100 (0.3%)
1	C	0.58	0/2276	0.84	9/3089 (0.3%)
1	D	0.56	0/2284	0.82	7/3100 (0.2%)
All	All	0.67	4/9128 (0.0%)	0.85	30/12389 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	SER	CB-OG	25.71	1.75	1.42
1	A	111	GLU	CD-OE1	7.43	1.33	1.25
1	A	235	MET	SD-CE	-5.35	1.47	1.77
1	A	38	TYR	C-O	5.18	1.33	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ASP	CB-CG-OD2	7.99	125.49	118.30
1	C	195	ASP	CB-CG-OD2	7.30	124.87	118.30
1	A	200	ASP	CB-CG-OD2	6.91	124.52	118.30
1	C	76	ASP	CB-CG-OD2	6.86	124.47	118.30
1	B	200	ASP	CB-CG-OD2	6.70	124.33	118.30
1	D	200	ASP	CB-CG-OD2	6.65	124.29	118.30
1	B	128	ASP	CB-CG-OD2	6.34	124.01	118.30
1	D	108	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	195	ASP	CB-CG-OD2	6.16	123.85	118.30
1	D	72	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	195	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	60	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	239	ASP	CB-CG-OD2	5.87	123.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	ASP	CB-CG-OD2	5.83	123.55	118.30
1	D	292	ASP	CB-CG-OD2	5.79	123.52	118.30
1	D	195	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	239	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	60	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	200	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	292	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	60	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	202	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	72	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	72	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	60	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	245	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	76	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	114	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	108	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	108	ASP	CB-CG-OD2	5.01	122.81	118.30

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	2224	0	2170	49	0
1	B	2224	0	2170	32	0
1	C	2217	0	2162	28	0
1	D	2224	0	2170	40	0
2	A	5	0	5	1	0
2	B	5	0	5	0	0
2	C	5	0	5	0	0
2	D	5	0	5	0	0
3	A	23	0	12	4	0
3	B	23	0	12	5	0
3	C	23	0	12	3	0
3	D	23	0	11	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	130	0	0	3	0
4	B	81	0	0	2	0
4	C	80	0	0	3	0
4	D	93	0	0	2	0
All	All	9385	0	8739	148	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 8.

All (148) 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:115:SER:OG	1:A:115:SER:CB	1.75	1.34
1:D:67:LYS:HZ2	3:D:850:AMP:N6	1.67	0.92
1:D:120:LEU:HD13	3:D:850:AMP:C8	2.11	0.85
1:D:67:LYS:NZ	3:D:850:AMP:N6	2.27	0.81
1:C:121:GLU:OE2	1:C:183:LYS:NZ	2.16	0.78
1:A:87:PRO:HD3	1:A:116:PHE:CZ	2.21	0.76
1:B:265:HIS:HD2	1:B:287:HIS:CE1	2.04	0.76
1:B:101:SER:O	1:B:183:LYS:NZ	2.21	0.73
1:D:80:LEU:HD13	1:D:82:ASN:HD21	1.54	0.73
1:B:265:HIS:HD2	1:B:287:HIS:HE1	1.35	0.72
1:D:186:ASP:HA	3:D:850:AMP:N6	2.05	0.72
1:D:100:PHE:CE2	1:D:102:GLY:HA3	2.25	0.71
1:C:166:ARG:HD3	1:C:189:SER:O	1.89	0.71
1:A:287:HIS:HD2	1:A:289:TRP:H	1.40	0.69
1:B:265:HIS:CD2	1:B:287:HIS:HE1	2.11	0.68
1:A:46:SER:OG	4:A:628:HOH:O	2.11	0.68
1:B:49:PHE:CD2	3:B:650:AMP:O1P	2.49	0.66
1:D:166:ARG:HD3	1:D:189:SER:O	1.96	0.65
1:A:112:ARG:CD	1:A:117:VAL:HG21	2.26	0.65
1:C:265:HIS:HD2	1:C:287:HIS:CE1	2.13	0.65
1:A:112:ARG:CD	1:A:117:VAL:CG2	2.76	0.64
1:A:292:ASP:OD2	4:A:625:HOH:O	2.15	0.63
1:A:100:PHE:CE2	1:A:102:GLY:HA3	2.34	0.62
1:B:166:ARG:HD3	1:B:189:SER:O	1.99	0.62
1:A:87:PRO:HD3	1:A:116:PHE:CE1	2.34	0.62
1:C:265:HIS:HD2	1:C:287:HIS:HE1	1.45	0.62
1:D:246:GLU:H	1:D:246:GLU:CD	2.03	0.62
1:A:87:PRO:CG	1:A:116:PHE:CD1	2.83	0.61
1:B:100:PHE:CE2	1:B:102:GLY:HA3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:SER:O	1:C:183:LYS:HG2	2.01	0.61
1:A:87:PRO:HG3	1:A:116:PHE:CD1	2.36	0.61
1:A:42:PRO:HD2	1:A:54:SER:CB	2.30	0.60
1:C:300:ALA:HA	1:C:304:LEU:HB2	1.83	0.60
1:C:122:ARG:HG3	3:C:750:AMP:HN61	1.66	0.59
1:D:67:LYS:NZ	3:D:850:AMP:HN62	1.99	0.59
1:B:41:GLY:N	1:B:54:SER:O	2.36	0.59
1:D:287:HIS:CD2	1:D:289:TRP:H	2.21	0.58
1:A:268:ARG:NH1	4:A:675:HOH:O	2.35	0.58
1:A:112:ARG:HD2	1:A:117:VAL:CG2	2.34	0.58
1:B:295:LEU:HD21	1:C:256:ARG:NH1	2.18	0.58
1:A:62:LEU:HD12	1:A:63:PRO:HD2	1.85	0.57
1:B:120:LEU:HD13	3:B:650:AMP:H2'	1.87	0.57
1:A:120:LEU:CD1	3:A:550:AMP:O2'	2.52	0.57
1:A:112:ARG:HD3	1:A:117:VAL:CG2	2.35	0.57
1:C:97:SER:HB2	4:C:755:HOH:O	2.04	0.57
1:D:194:LYS:HE2	1:D:198:TYR:CE2	2.39	0.56
1:D:201:PHE:HB3	1:D:212:TRP:CZ2	2.40	0.56
1:C:265:HIS:CD2	1:C:287:HIS:HE1	2.23	0.56
1:C:266:LEU:HD11	1:C:284:ILE:HG23	1.88	0.56
1:D:287:HIS:HD2	1:D:289:TRP:H	1.53	0.56
1:B:101:SER:HB2	1:B:183:LYS:HZ1	1.70	0.56
1:D:239:ASP:OD1	4:D:939:HOH:O	2.18	0.56
1:A:42:PRO:HD2	1:A:54:SER:HB3	1.87	0.56
1:A:287:HIS:CD2	1:A:289:TRP:H	2.22	0.55
1:D:100:PHE:CZ	1:D:102:GLY:HA3	2.41	0.55
1:A:302:ILE:HG22	1:A:303:HIS:CD2	2.42	0.54
1:B:287:HIS:HD2	1:B:289:TRP:H	1.55	0.54
1:C:51:SER:OG	4:C:795:HOH:O	2.18	0.54
1:D:265:HIS:CD2	1:D:287:HIS:HE1	2.26	0.54
1:A:166:ARG:NH1	1:A:191:ALA:HB2	2.23	0.53
1:D:265:HIS:HD2	1:D:287:HIS:HE1	1.57	0.53
1:B:41:GLY:CA	1:B:54:SER:O	2.56	0.53
1:A:172:ASN:OD1	3:A:550:AMP:O3P	2.27	0.53
1:B:42:PRO:HD2	1:B:54:SER:HB3	1.91	0.52
1:A:57:ARG:NH1	1:A:62:LEU:HD22	2.24	0.52
1:D:60:ASP:O	1:D:61:ASN:C	2.48	0.52
1:A:42:PRO:HD2	1:A:54:SER:HB2	1.92	0.51
1:A:296:PRO:O	1:A:299:THR:HB	2.10	0.51
1:A:193:LEU:HD11	1:A:221:ARG:NH1	2.26	0.51
1:C:41:GLY:N	1:C:54:SER:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HD2	1:A:117:VAL:HG21	1.92	0.50
1:B:120:LEU:HD13	3:B:650:AMP:C2'	2.41	0.50
1:B:300:ALA:HA	1:B:304:LEU:HB2	1.93	0.50
1:B:71:LYS:HA	1:B:74:ILE:HD12	1.94	0.50
1:C:100:PHE:CE2	1:C:102:GLY:HA3	2.46	0.50
1:A:104:ILE:HD11	1:A:121:GLU:O	2.12	0.50
1:A:265:HIS:ND1	1:A:287:HIS:HE1	2.10	0.50
1:C:49:PHE:CD2	3:C:750:AMP:O1P	2.65	0.50
1:B:193:LEU:HD21	1:B:221:ARG:HH21	1.77	0.49
1:D:80:LEU:HD12	1:D:84:THR:HB	1.94	0.49
1:D:67:LYS:HZ1	3:D:850:AMP:HN62	1.58	0.49
1:B:246:GLU:H	1:B:246:GLU:CD	2.16	0.49
1:C:131:ASP:HA	4:C:775:HOH:O	2.12	0.49
1:D:60:ASP:O	1:D:62:LEU:N	2.46	0.49
1:A:104:ILE:HB	1:A:185:ILE:HG22	1.95	0.49
1:D:120:LEU:HD13	3:D:850:AMP:N7	2.28	0.48
1:A:87:PRO:HD3	1:A:116:PHE:CE2	2.48	0.48
1:A:57:ARG:NH1	1:A:62:LEU:CD2	2.77	0.48
1:C:159:HIS:HE2	1:C:164:LEU:HD12	1.78	0.48
1:D:67:LYS:NZ	1:D:89:GLU:OE2	2.47	0.48
1:D:265:HIS:HD2	1:D:287:HIS:CE1	2.32	0.48
1:B:49:PHE:CG	3:B:650:AMP:O1P	2.66	0.47
1:C:255:PHE:CZ	1:C:264:GLN:HG2	2.50	0.47
1:A:38:TYR:CZ	1:A:119:ILE:HG21	2.49	0.47
1:A:41:GLY:HA3	1:A:54:SER:HB3	1.96	0.47
1:A:209:PRO:HD2	1:A:212:TRP:HB3	1.95	0.47
1:D:209:PRO:HD3	4:D:882:HOH:O	2.15	0.47
1:C:234:ASP:HA	1:C:239:ASP:O	2.14	0.47
1:C:57:ARG:HD3	1:C:59:SER:OG	2.15	0.47
1:C:159:HIS:NE2	1:C:164:LEU:HD12	2.31	0.46
1:A:68:HIS:HE1	1:A:112:ARG:NH1	2.14	0.46
1:A:112:ARG:HD2	1:A:117:VAL:HG23	1.97	0.46
1:C:186:ASP:HB2	3:C:750:AMP:O5'	2.16	0.46
1:B:258:ARG:NH2	4:B:704:HOH:O	2.48	0.45
1:B:214:ARG:HD2	1:B:249:ILE:HG23	1.98	0.45
1:B:100:PHE:CZ	1:B:102:GLY:HA3	2.51	0.45
1:D:174:LEU:HD11	3:D:850:AMP:H2'	1.99	0.45
1:A:239:ASP:HA	2:A:500:IMD:H5	1.99	0.45
1:B:159:HIS:HD1	1:B:281:PHE:HE2	1.64	0.44
1:D:300:ALA:HA	1:D:304:LEU:HB2	1.99	0.44
1:A:104:ILE:HG23	1:A:104:ILE:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:PRO:HD3	1:C:226:TRP:CZ2	2.53	0.44
1:C:255:PHE:CE2	1:C:264:GLN:HG2	2.53	0.44
1:D:46:SER:HA	1:D:50:GLY:O	2.17	0.44
1:A:300:ALA:HA	1:A:304:LEU:HB2	2.00	0.44
1:D:186:ASP:CA	3:D:850:AMP:N6	2.79	0.44
1:D:74:ILE:HD13	1:D:87:PRO:HG3	1.99	0.44
1:B:212:TRP:CE3	1:B:216:HIS:HA	2.54	0.43
1:A:44:LEU:HD21	1:A:54:SER:HB2	2.01	0.43
1:A:68:HIS:CE1	1:A:112:ARG:NH1	2.87	0.43
1:C:210:PRO:HD3	1:C:226:TRP:CH2	2.54	0.43
1:B:265:HIS:CD2	1:B:287:HIS:CE1	2.91	0.43
1:A:121:GLU:OE2	1:A:183:LYS:NZ	2.43	0.43
1:B:57:ARG:HD3	1:B:59:SER:OG	2.18	0.43
1:C:104:ILE:HD13	1:C:185:ILE:HG22	2.01	0.43
1:D:38:TYR:CE1	1:D:119:ILE:HG21	2.54	0.43
1:D:258:ARG:HD3	1:D:258:ARG:C	2.39	0.43
1:A:120:LEU:HD13	3:A:550:AMP:O2'	2.19	0.42
1:C:266:LEU:HB2	1:C:287:HIS:CD2	2.54	0.42
1:A:67:LYS:HZ2	3:A:550:AMP:C3'	2.32	0.42
1:A:112:ARG:CD	1:A:117:VAL:HG23	2.49	0.41
1:D:246:GLU:CD	1:D:246:GLU:N	2.72	0.41
1:D:194:LYS:HE2	1:D:198:TYR:CD2	2.55	0.41
1:B:186:ASP:HB2	3:B:650:AMP:O5'	2.19	0.41
1:D:124:GLU:HA	1:D:125:PRO:HA	1.92	0.41
1:B:41:GLY:HA3	1:B:54:SER:O	2.18	0.41
1:B:101:SER:HA	4:B:657:HOH:O	2.20	0.41
1:B:104:ILE:O	1:B:104:ILE:CG2	2.68	0.41
1:A:62:LEU:HA	1:A:63:PRO:HD3	1.95	0.41
1:A:104:ILE:O	1:A:104:ILE:CG2	2.68	0.41
1:C:41:GLY:CA	1:C:54:SER:O	2.69	0.41
1:D:57:ARG:NH1	1:D:62:LEU:HD22	2.36	0.40
1:D:100:PHE:CE2	1:D:102:GLY:CA	3.01	0.40
1:D:255:PHE:CE2	1:D:264:GLN:HG2	2.56	0.40
1:D:49:PHE:HB3	1:D:186:ASP:OD2	2.21	0.40
1:B:258:ARG:C	1:B:258:ARG:HD3	2.42	0.40
1:D:234:ASP:HA	1:D:239:ASP:O	2.21	0.40
1:A:201:PHE:HB3	1:A:212:TRP:CZ2	2.57	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	271/293 (92%)	258 (95%)	13 (5%)	0	100	100
1	B	271/293 (92%)	259 (96%)	12 (4%)	0	100	100
1	C	270/293 (92%)	258 (96%)	12 (4%)	0	100	100
1	D	271/293 (92%)	260 (96%)	9 (3%)	2 (1%)	22	20
All	All	1083/1172 (92%)	1035 (96%)	46 (4%)	2 (0%)	47	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	61	ASN
1	D	34	LEU

### 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	244/263 (93%)	226 (93%)	18 (7%)	13	10
1	B	244/263 (93%)	231 (95%)	13 (5%)	22	21
1	C	243/263 (92%)	227 (93%)	16 (7%)	16	14
1	D	244/263 (93%)	232 (95%)	12 (5%)	25	25
All	All	975/1052 (93%)	916 (94%)	59 (6%)	18	16

All (59) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	35	GLU
1	A	36	SER
1	A	56	ILE
1	A	58	VAL
1	A	61	ASN
1	A	70	GLU
1	A	72	ASP
1	A	73	ARG
1	A	79	GLU
1	A	82	ASN
1	A	94	LYS
1	A	105	ARG
1	A	112	ARG
1	A	121	GLU
1	A	124	GLU
1	A	239	ASP
1	A	290	MET
1	A	304	LEU
1	B	34	LEU
1	B	39	GLN
1	B	72	ASP
1	B	76	ASP
1	B	79	GLU
1	B	82	ASN
1	B	88	MET
1	B	121	GLU
1	B	160	ASN
1	B	258	ARG
1	B	290	MET
1	B	291	GLN
1	B	304	LEU
1	C	35	GLU
1	C	39	GLN
1	C	56	ILE
1	C	70	GLU
1	C	73	ARG
1	C	75	SER
1	C	79	GLU
1	C	82	ASN
1	C	85	ARG
1	C	124	GLU
1	C	134	THR
1	C	152	LEU

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Mol	Chain	Res	Type
1	C	239	ASP
1	C	256	ARG
1	C	258	ARG
1	C	290	MET
1	D	34	LEU
1	D	54	SER
1	D	76	ASP
1	D	85	ARG
1	D	124	GLU
1	D	159	HIS
1	D	196	THR
1	D	205	ARG
1	D	239	ASP
1	D	258	ARG
1	D	292	ASP
1	D	304	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	61	ASN
1	A	68	HIS
1	A	216	HIS
1	A	287	HIS
1	B	39	GLN
1	B	157	HIS
1	B	265	HIS
1	B	287	HIS
1	B	291	GLN
1	C	39	GLN
1	C	252	GLN
1	C	265	HIS
1	C	287	HIS
1	D	82	ASN
1	D	265	HIS
1	D	287	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](#)

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
3	AMP	A	550	-	22,25,25	1.46	3 (13%)	25,38,38	1.83	4 (16%)
3	AMP	C	750	-	22,25,25	1.45	2 (9%)	25,38,38	1.81	5 (20%)
3	AMP	B	650	-	22,25,25	1.44	3 (13%)	25,38,38	2.78	9 (36%)
3	AMP	D	850	-	22,25,25	1.38	2 (9%)	25,38,38	2.18	6 (24%)
2	IMD	A	500	-	3,5,5	0.45	0	4,5,5	0.75	0
2	IMD	B	600	-	3,5,5	0.41	0	4,5,5	0.53	0
2	IMD	D	800	-	3,5,5	0.45	0	4,5,5	0.58	0
2	IMD	C	700	-	3,5,5	0.35	0	4,5,5	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	A	550	-	-	2/6/26/26	0/3/3/3
3	AMP	C	750	-	-	6/6/26/26	0/3/3/3
3	AMP	B	650	-	-	6/6/26/26	0/3/3/3
3	AMP	D	850	-	1/1/5/5	4/6/26/26	0/3/3/3
2	IMD	A	500	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMD	B	600	-	-	-	0/1/1/1
2	IMD	D	800	-	-	-	0/1/1/1
2	IMD	C	700	-	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	850	AMP	C2-N3	4.77	1.39	1.32
3	A	550	AMP	C2-N3	4.55	1.39	1.32
3	C	750	AMP	C2-N3	4.54	1.39	1.32
3	B	650	AMP	C2-N3	4.18	1.38	1.32
3	B	650	AMP	C2-N1	3.35	1.40	1.33
3	A	550	AMP	C2-N1	3.22	1.39	1.33
3	C	750	AMP	C2-N1	3.21	1.39	1.33
3	D	850	AMP	C2-N1	2.61	1.38	1.33
3	A	550	AMP	C4-N3	2.10	1.38	1.35
3	B	650	AMP	C4-N3	2.09	1.38	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	650	AMP	O3'-C3'-C4'	9.15	137.51	111.05
3	A	550	AMP	N3-C2-N1	-6.64	118.31	128.68
3	B	650	AMP	N3-C2-N1	-6.58	118.40	128.68
3	D	850	AMP	N3-C2-N1	-6.42	118.65	128.68
3	C	750	AMP	N3-C2-N1	-6.09	119.15	128.68
3	D	850	AMP	O3'-C3'-C4'	4.60	124.36	111.05
3	D	850	AMP	C2'-C3'-C4'	3.83	110.08	102.64
3	D	850	AMP	O3'-C3'-C2'	3.63	123.57	111.82
3	B	650	AMP	O3P-P-O5'	3.59	116.29	106.73
3	C	750	AMP	P-O5'-C5'	3.46	127.81	118.30
3	A	550	AMP	O4'-C1'-C2'	-3.30	102.11	106.93
3	C	750	AMP	O3P-P-O5'	2.95	114.58	106.73
3	B	650	AMP	P-O5'-C5'	2.90	126.28	118.30
3	B	650	AMP	O4'-C1'-C2'	-2.88	102.72	106.93
3	A	550	AMP	C3'-C2'-C1'	2.49	104.72	100.98
3	D	850	AMP	P-O5'-C5'	2.43	124.99	118.30
3	C	750	AMP	O4'-C1'-C2'	-2.43	103.38	106.93
3	B	650	AMP	C1'-N9-C4	-2.41	122.41	126.64
3	B	650	AMP	O3P-P-O1P	-2.39	101.33	110.68
3	B	650	AMP	O4'-C4'-C5'	2.27	116.83	109.37
3	D	850	AMP	C5-C6-N6	-2.19	117.02	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	650	AMP	C3'-C2'-C1'	2.06	104.07	100.98
3	C	750	AMP	O3P-P-O1P	-2.04	102.68	110.68
3	A	550	AMP	O3'-C3'-C4'	-2.03	105.18	111.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	850	AMP	C3'

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	650	AMP	C5'-O5'-P-O1P
3	B	650	AMP	C5'-O5'-P-O2P
3	B	650	AMP	C5'-O5'-P-O3P
3	B	650	AMP	C3'-C4'-C5'-O5'
3	C	750	AMP	C5'-O5'-P-O1P
3	C	750	AMP	C5'-O5'-P-O2P
3	C	750	AMP	C5'-O5'-P-O3P
3	C	750	AMP	C3'-C4'-C5'-O5'
3	D	850	AMP	C5'-O5'-P-O3P
3	D	850	AMP	C3'-C4'-C5'-O5'
3	A	550	AMP	O4'-C4'-C5'-O5'
3	A	550	AMP	C3'-C4'-C5'-O5'
3	D	850	AMP	O4'-C4'-C5'-O5'
3	B	650	AMP	O4'-C4'-C5'-O5'
3	B	650	AMP	C4'-C5'-O5'-P
3	C	750	AMP	O4'-C4'-C5'-O5'
3	C	750	AMP	C4'-C5'-O5'-P
3	D	850	AMP	C5'-O5'-P-O2P

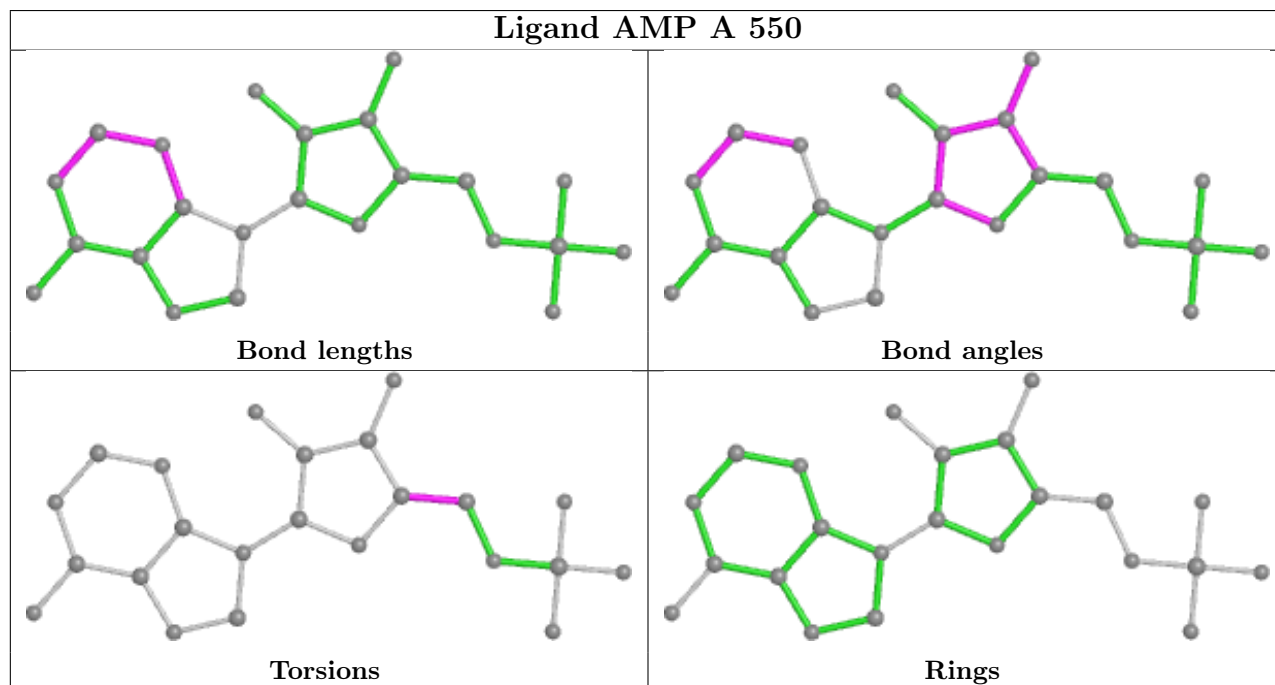
There are no ring outliers.

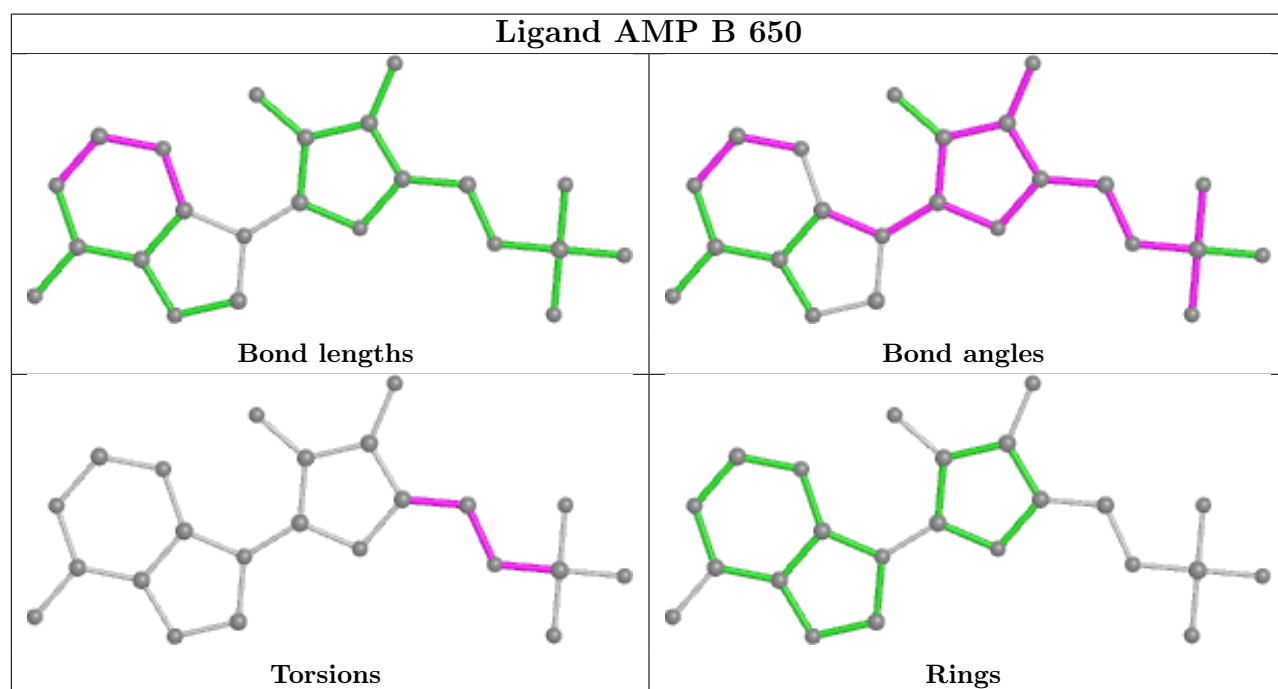
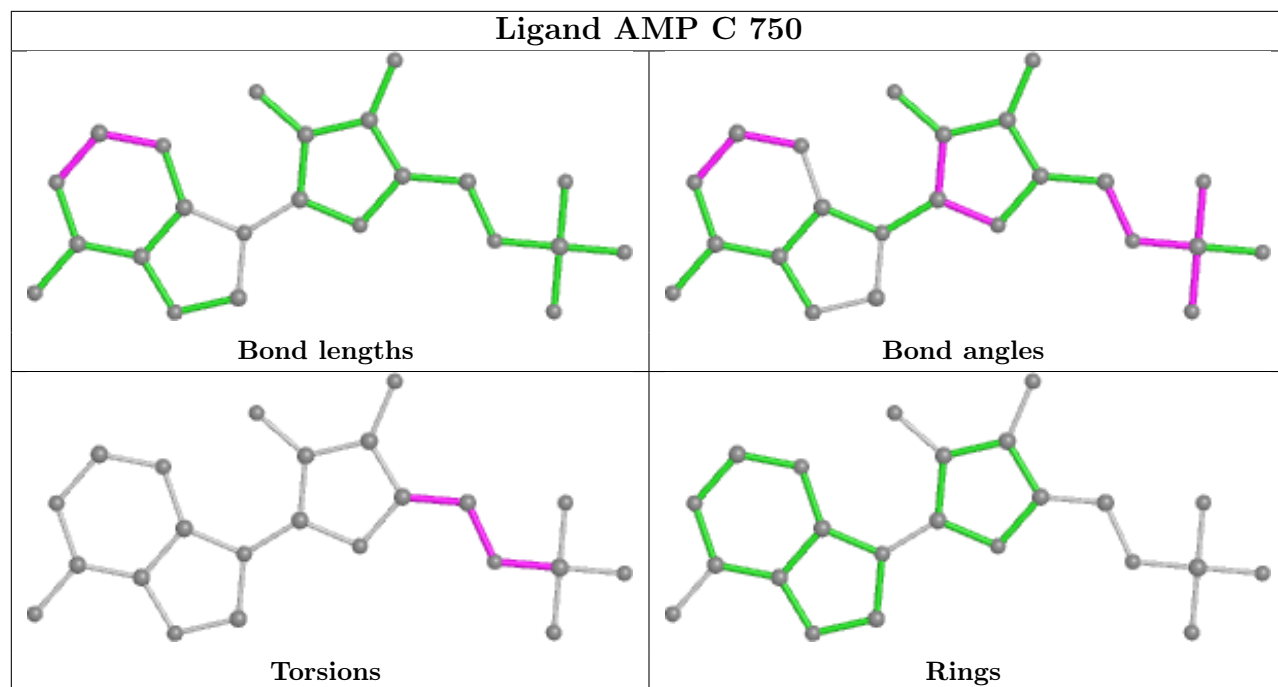
5 monomers are involved in 22 short contacts:

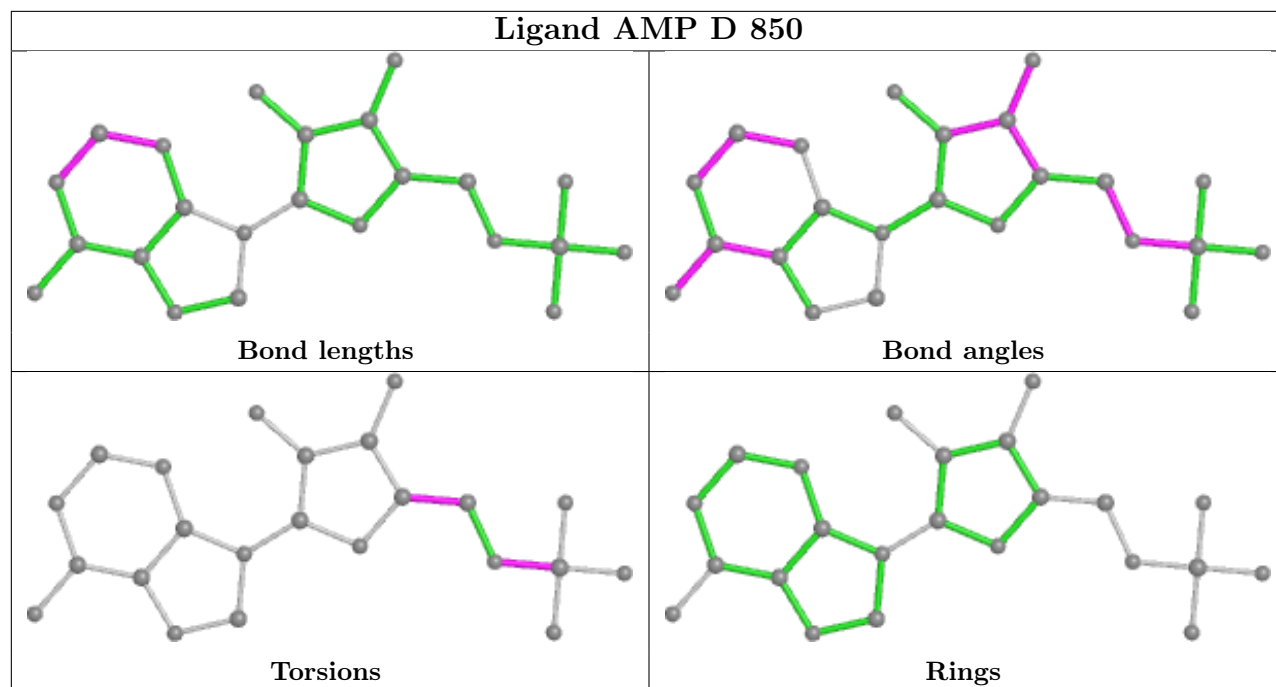
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	550	AMP	4	0
3	C	750	AMP	3	0
3	B	650	AMP	5	0
3	D	850	AMP	9	0
2	A	500	IMD	1	0

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	273/293 (93%)	0.06	12 (4%) 34 34	19, 26, 36, 38	0
1	B	273/293 (93%)	-0.05	8 (2%) 51 52	17, 26, 34, 39	0
1	C	272/293 (92%)	-0.15	6 (2%) 62 63	19, 26, 35, 36	0
1	D	273/293 (93%)	-0.10	5 (1%) 68 69	18, 26, 34, 40	0
All	All	1091/1172 (93%)	-0.06	31 (2%) 53 53	17, 26, 35, 40	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	33	PRO	7.9
1	D	80	LEU	6.1
1	B	80	LEU	6.0
1	B	75	SER	3.8
1	D	81	PRO	3.7
1	B	81	PRO	3.7
1	C	81	PRO	3.7
1	A	116	PHE	3.6
1	A	33	PRO	3.4
1	C	80	LEU	3.4
1	A	80	LEU	3.4
1	A	73	ARG	3.4
1	C	59	SER	3.3
1	D	34	LEU	3.3
1	C	79	GLU	3.0
1	C	83	GLY	2.9
1	A	112	ARG	2.8
1	A	49	PHE	2.6
1	C	73	ARG	2.5
1	A	58	VAL	2.5
1	A	82	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	84	THR	2.4
1	B	33	PRO	2.3
1	A	48	GLY	2.3
1	A	75	SER	2.3
1	A	109	TRP	2.2
1	B	59	SER	2.2
1	B	34	LEU	2.2
1	A	81	PRO	2.1
1	B	72	ASP	2.1
1	B	86	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

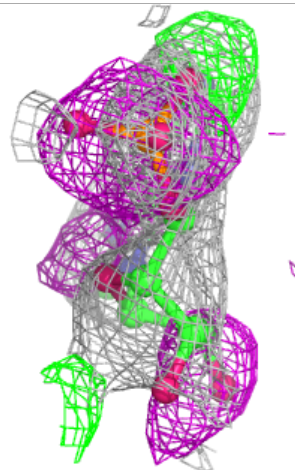
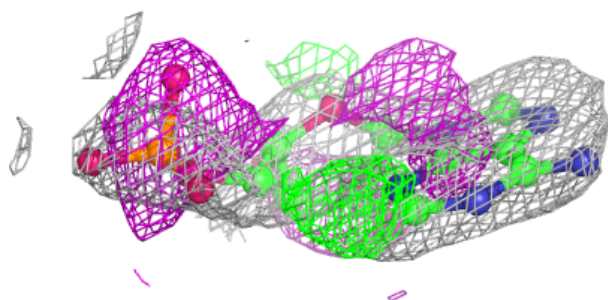
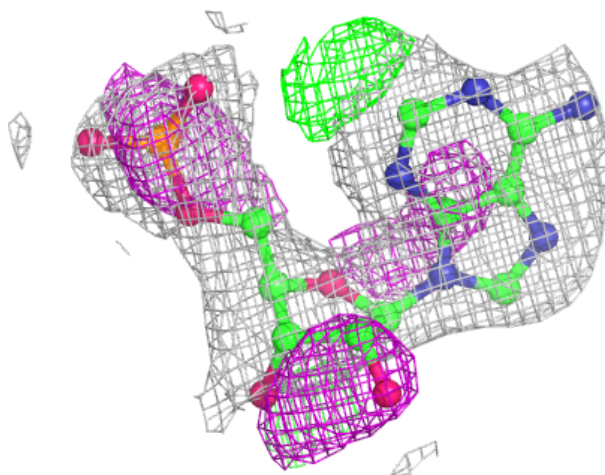
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	AMP	A	550	23/23	0.72	0.34	64,68,81,83	0
3	AMP	C	750	23/23	0.73	0.29	61,65,78,80	0
3	AMP	B	650	23/23	0.81	0.30	63,66,80,82	0
3	AMP	D	850	23/23	0.85	0.27	64,66,77,78	0
2	IMD	B	600	5/5	0.94	0.14	50,50,51,51	0
2	IMD	C	700	5/5	0.97	0.07	51,52,52,52	0
2	IMD	D	800	5/5	0.97	0.10	51,52,52,53	0
2	IMD	A	500	5/5	0.98	0.14	42,43,44,44	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.

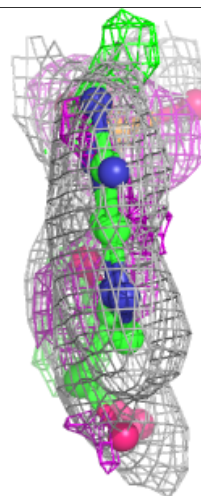
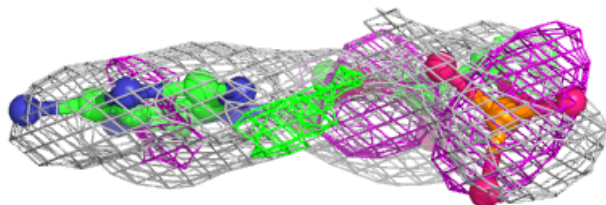
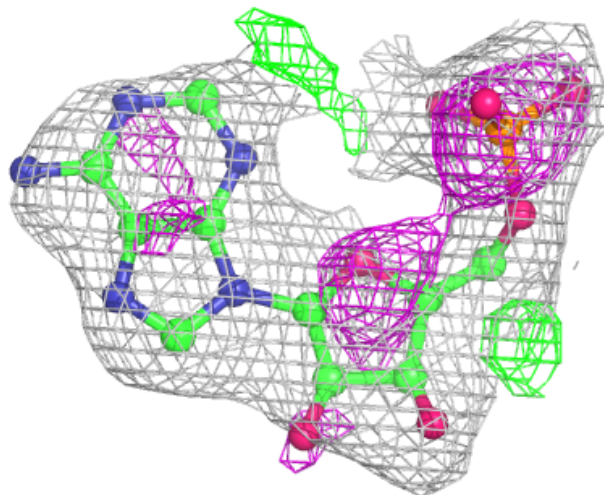
**Electron density around AMP A 550:**

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



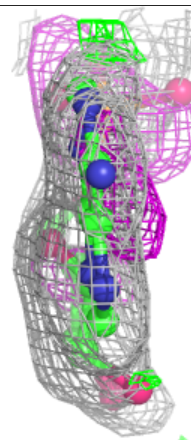
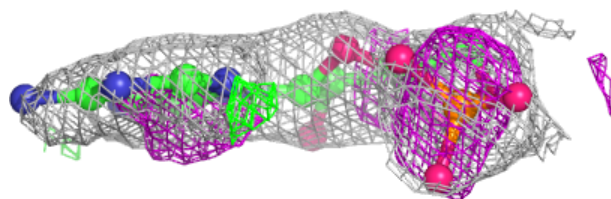
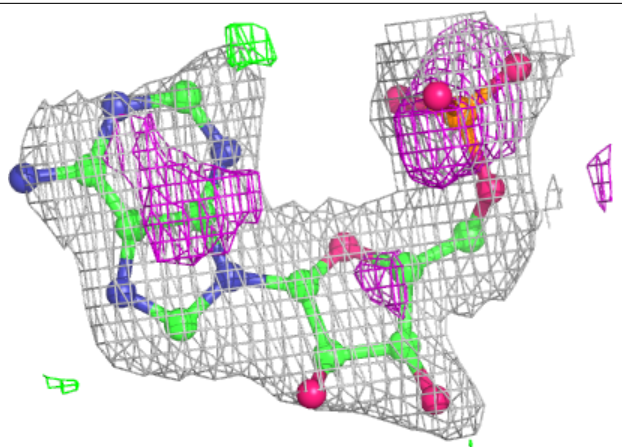
**Electron density around AMP C 750:**

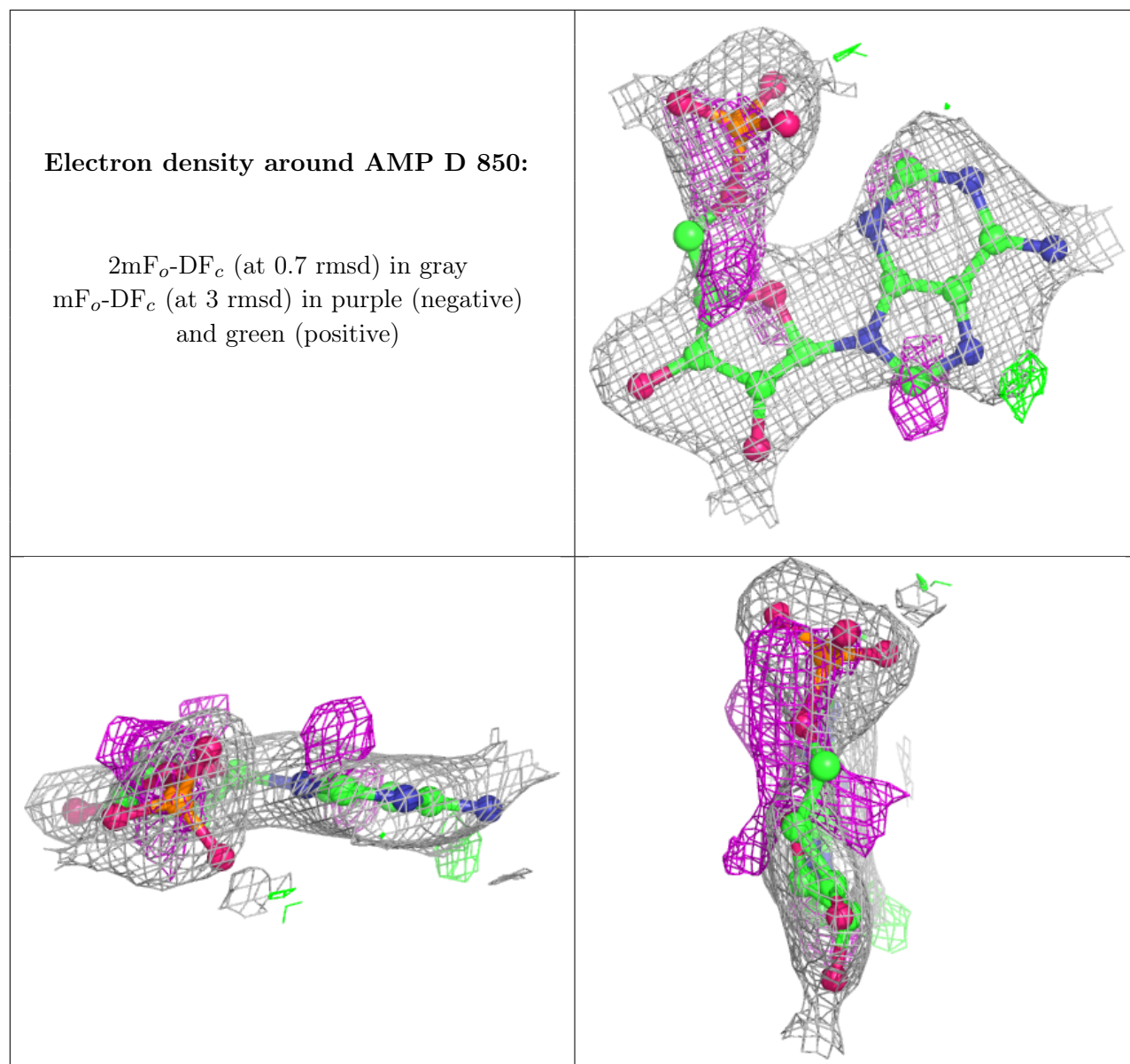
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AMP B 650:**

$2mF_o-DF_c$  (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.