



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 8, 2024 – 10:58 am BST

PDB ID : 8PML  
Title : Structure of Nall protein , SPIKE allele from japonica rice, construct 46-458  
Authors : Huang, L.Y.; Rety, S.; Xi, X.G.  
Deposited on : 2023-06-29  
Resolution : 2.95 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 : 1.8.4, 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

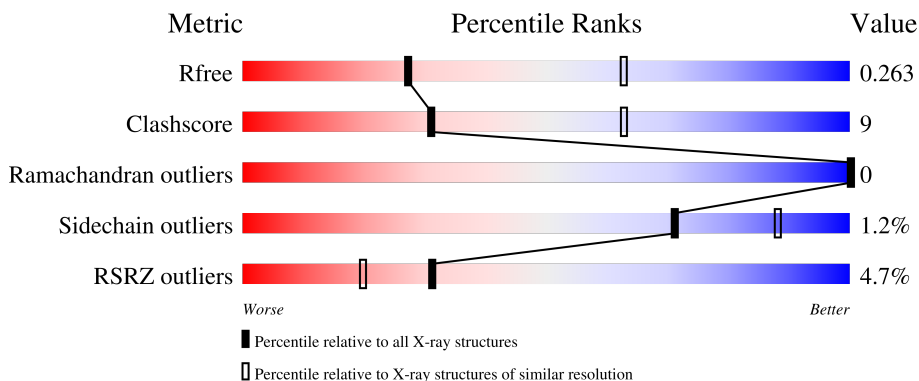
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	413	 4% 79% 17% ..
1	B	413	 5% 77% 19% ..
1	C	413	 5% 77% 19% ..
1	D	413	 4% 83% 14% .
1	E	413	 6% 77% 19% ..

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Mol	Chain	Length	Quality of chain
1	F	413	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '4%', a large green segment in the middle labeled '78%', and a yellow segment on the right labeled '19%'. The bar ends with a grey segment and two dots '••'.</p>

## 2 Entry composition [i](#)

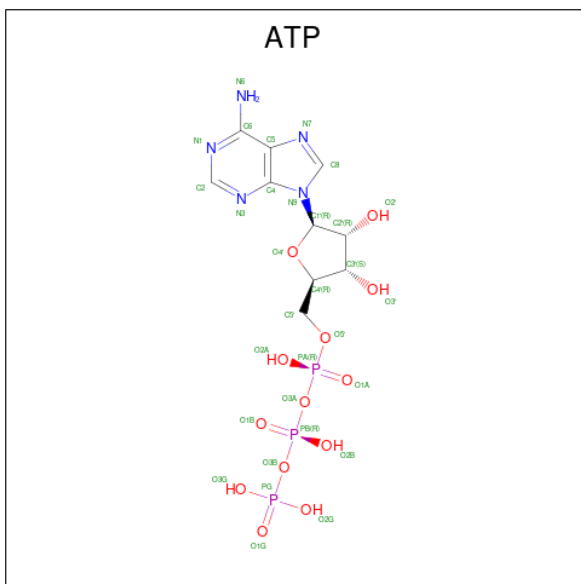
There are 3 unique types of molecules in this entry. The entry contains 18777 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein NARROW LEAF 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	Total 3090	C 1958	N 542	O 578	S 12	0	0	0
1	B	402	Total 3099	C 1963	N 543	O 581	S 12	0	0	0
1	C	402	Total 3099	C 1963	N 543	O 581	S 12	0	0	0
1	D	402	Total 3099	C 1963	N 543	O 581	S 12	0	0	0
1	E	402	Total 3099	C 1963	N 543	O 581	S 12	0	0	0
1	F	402	Total 3099	C 1963	N 543	O 581	S 12	0	0	0

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

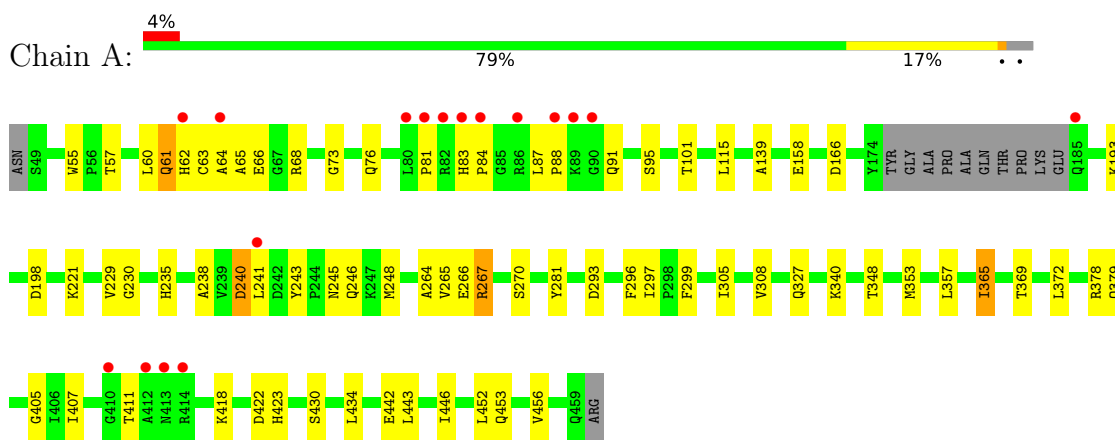
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

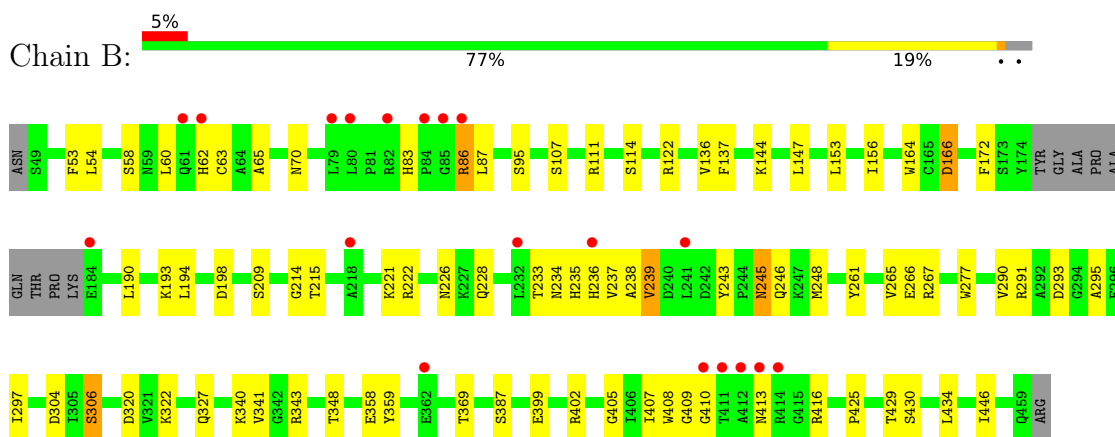
### 3 Residue-property plots [i](#)

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.

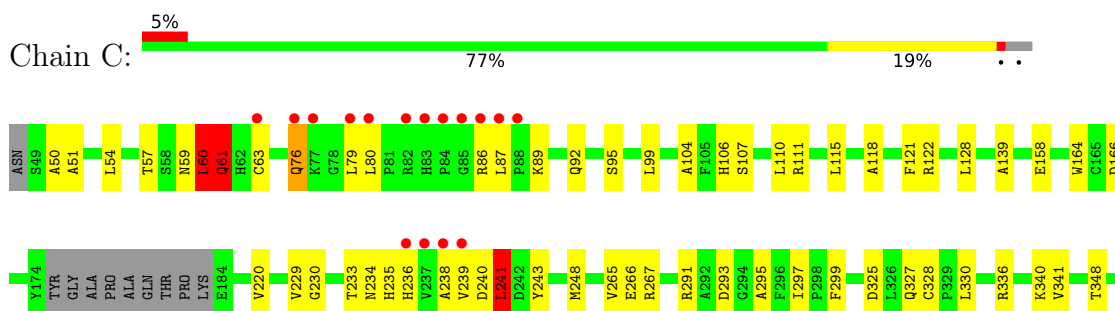
#### • Molecule 1: Protein NARROW LEAF 1

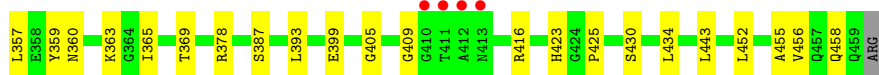


#### • Molecule 1: Protein NARROW LEAF 1

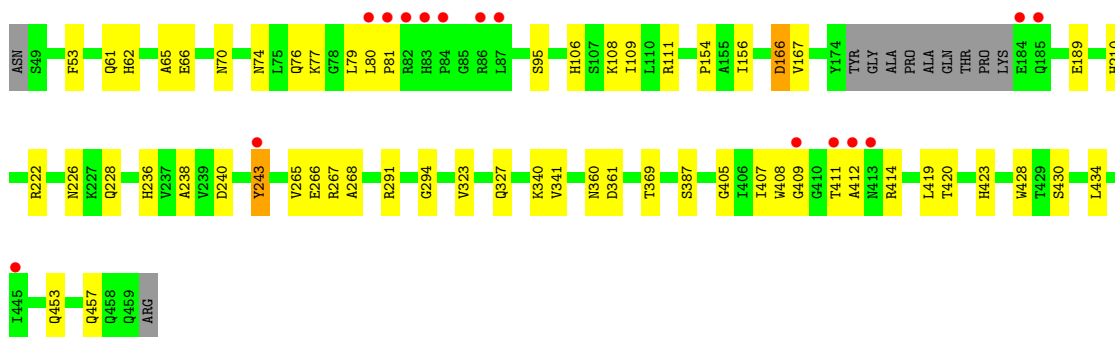
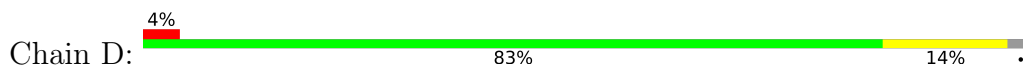


#### • Molecule 1: Protein NARROW LEAF 1

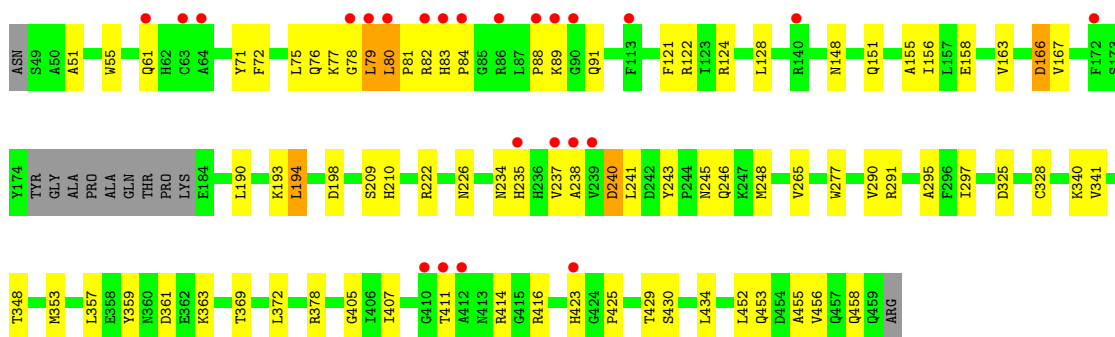
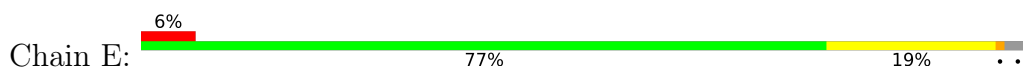




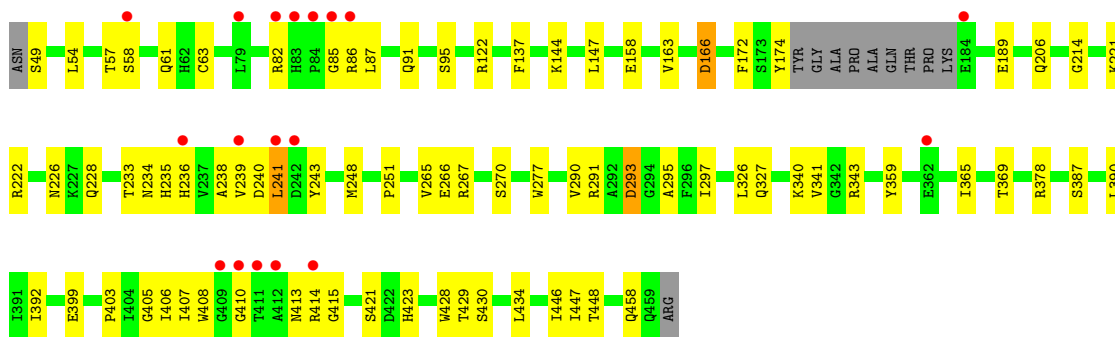
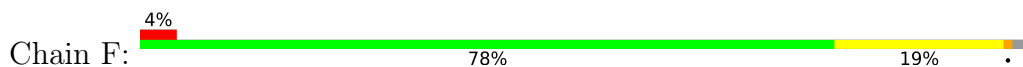
● Molecule 1: Protein NARROW LEAF 1



● Molecule 1: Protein NARROW LEAF 1



● Molecule 1: Protein NARROW LEAF 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.43Å 193.36Å 84.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.95 129.92 – 2.95	Depositor EDS
% Data completeness (in resolution range)	77.4 (87.71-2.95) 77.5 (129.92-2.95)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.96Å)	Xtrriage
Refinement program	PHENIX 1.21rc1_4903	Depositor
R, $R_{free}$	0.205 , 0.252 0.212 , 0.263	Depositor DCC
$R_{free}$ test set	2269 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.9	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	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 46.81 % 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 1.0850e-04. 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: ATP, 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	0.31	0/3157	0.58	1/4285 (0.0%)
1	B	0.34	1/3166 (0.0%)	0.59	2/4297 (0.0%)
1	C	0.31	0/3166	0.64	5/4297 (0.1%)
1	D	0.31	0/3166	0.58	2/4297 (0.0%)
1	E	0.33	0/3166	0.63	6/4297 (0.1%)
1	F	0.32	0/3166	0.60	3/4297 (0.1%)
All	All	0.32	1/18987 (0.0%)	0.60	19/25770 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	4
1	E	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	86	ARG	CB-CG	6.04	1.68	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	LEU	CB-CG-CD1	-11.51	91.43	111.00
1	F	241	LEU	CB-CG-CD2	-9.61	94.67	111.00
1	E	77	LYS	C-N-CA	7.08	137.16	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	E	80	LEU	CA-CB-CG	-6.49	100.37	115.30
1	A	240	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	E	79	LEU	CA-CB-CG	6.26	129.70	115.30
1	E	240	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	F	86	ARG	C-N-CA	5.72	136.00	121.70
1	C	241	LEU	CB-CG-CD2	5.70	120.68	111.00
1	C	76	GLN	CA-CB-CG	5.64	125.81	113.40
1	D	243	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	F	85	GLY	N-CA-C	5.42	126.65	113.10
1	C	61	GLN	N-CA-C	5.26	125.21	111.00
1	E	240	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	80	LEU	N-CA-C	5.08	124.72	111.00
1	C	60	LEU	C-N-CA	5.07	134.37	121.70
1	B	86	ARG	CB-CG-CD	5.05	124.73	111.60
1	D	77	LYS	C-N-CA	-5.05	111.70	122.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	LEU	Peptide
1	A	61	GLN	Peptide
1	A	81	PRO	Peptide
1	C	241	LEU	Peptide
1	C	60	LEU	Peptide
1	C	61	GLN	Peptide
1	C	86	ARG	Peptide
1	E	79	LEU	Peptide

## 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	3090	0	3056	47	0
1	B	3099	0	3062	75	0
1	C	3099	0	3062	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3099	0	3062	44	0
1	E	3099	0	3062	64	0
1	F	3099	0	3062	67	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	2	0
2	F	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	18777	0	18438	338	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 9.

All (338) 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:B:107:SER:HB2	1:B:111:ARG:HH12	1.29	0.94
1:E:240:ASP:OD2	1:E:245:ASN:HB2	1.72	0.88
1:F:234:ASN:HD21	1:F:387:SER:HB2	1.37	0.87
1:B:107:SER:HB2	1:B:111:ARG:NH1	1.92	0.85
1:A:240:ASP:OD1	1:A:245:ASN:N	2.08	0.84
1:A:238:ALA:HB1	1:A:265:VAL:HG21	1.61	0.83
1:B:83:HIS:CE1	1:B:86:ARG:HA	2.14	0.82
1:A:63:CYS:HA	1:A:66:GLU:HB3	1.61	0.82
1:A:62:HIS:O	1:A:66:GLU:N	2.11	0.81
1:B:234:ASN:HD21	1:B:387:SER:HB2	1.49	0.78
1:C:236:HIS:NE2	1:C:293:ASP:OD2	2.17	0.77
1:B:83:HIS:O	1:B:83:HIS:ND1	2.17	0.77
1:D:266:GLU:HG2	1:D:267:ARG:HG3	1.65	0.76
1:F:234:ASN:HB2	1:F:293:ASP:HB3	1.66	0.75
1:F:226:ASN:HD21	1:F:228:GLN:HG2	1.50	0.74
1:C:107:SER:O	1:C:111:ARG:HG2	1.88	0.74
1:E:210:HIS:HB2	1:E:245:ASN:OD1	1.87	0.74
1:B:410:GLY:O	1:B:413:ASN:ND2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:LEU:HD12	1:E:372:LEU:HD12	1.67	0.74
1:D:226:ASN:HD21	1:D:228:GLN:HG2	1.51	0.74
1:C:239:VAL:HG21	1:F:241:LEU:HD22	1.70	0.74
1:B:226:ASN:HD21	1:B:228:GLN:HG2	1.51	0.74
1:A:266:GLU:HG2	1:A:267:ARG:HG3	1.71	0.71
1:E:209:SER:HB2	1:E:245:ASN:HB3	1.71	0.71
1:B:209:SER:HB2	1:B:245:ASN:HB2	1.72	0.71
1:E:72:PHE:HA	1:E:75:LEU:HD12	1.71	0.71
1:A:83:HIS:CG	1:A:84:PRO:HD2	2.26	0.70
1:D:222:ARG:NH2	1:D:226:ASN:OD1	2.25	0.70
1:B:234:ASN:O	1:B:237:VAL:HG12	1.91	0.70
1:B:261:TYR:OH	1:E:61:GLN:NE2	2.25	0.69
1:F:61:GLN:OE1	1:F:63:CYS:N	2.25	0.69
1:F:414:ARG:HB2	1:F:428:TRP:O	1.91	0.69
1:E:155:ALA:HA	1:E:167:VAL:HB	1.74	0.69
1:B:322:LYS:HD2	1:B:402:ARG:HH21	1.56	0.69
1:A:357:LEU:HD12	1:A:372:LEU:HD12	1.73	0.69
1:A:61:GLN:O	1:A:63:CYS:N	2.26	0.68
1:C:378:ARG:HD2	1:C:423:HIS:CD2	2.29	0.68
1:B:243:TYR:OH	1:E:361:ASP:OD2	2.07	0.68
1:B:266:GLU:HG2	1:B:267:ARG:HG3	1.76	0.68
1:B:62:HIS:HA	1:B:65:ALA:HB3	1.76	0.67
1:A:308:VAL:HG23	1:A:452:LEU:HD21	1.75	0.67
1:C:266:GLU:HG2	1:C:267:ARG:HG3	1.75	0.67
1:B:111:ARG:NH1	1:B:358:GLU:OE2	2.28	0.67
1:A:240:ASP:CG	1:A:245:ASN:H	1.99	0.66
1:F:266:GLU:HG2	1:F:267:ARG:HG3	1.76	0.66
1:D:420:THR:H	1:D:423:HIS:CE1	2.14	0.66
1:E:369:THR:HG21	1:E:430:SER:HB3	1.78	0.66
1:D:369:THR:HG21	1:D:430:SER:HB3	1.79	0.65
1:A:88:PRO:HD2	1:A:91:GLN:NE2	2.12	0.65
1:F:369:THR:HG21	1:F:430:SER:HB3	1.80	0.64
1:F:234:ASN:ND2	1:F:387:SER:HB2	2.09	0.64
1:C:235:HIS:HB3	1:C:295:ALA:HB2	1.80	0.64
1:C:235:HIS:O	1:C:239:VAL:HG23	1.98	0.64
1:B:83:HIS:CE1	1:B:86:ARG:HD3	2.33	0.63
1:B:234:ASN:HB2	1:B:293:ASP:HB3	1.80	0.63
1:D:419:LEU:H	1:D:423:HIS:HE1	1.46	0.63
1:A:422:ASP:OD1	1:A:423:HIS:N	2.31	0.63
1:C:235:HIS:CE1	1:F:241:LEU:HD13	2.33	0.63
1:A:378:ARG:HD2	1:A:423:HIS:CE1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASN:HB2	1:C:61:GLN:HG3	1.79	0.63
1:D:414:ARG:NH1	1:D:428:TRP:O	2.32	0.63
1:C:235:HIS:HE1	1:F:241:LEU:HD13	1.63	0.62
1:E:411:THR:O	1:E:414:ARG:NH1	2.32	0.62
1:B:122:ARG:HH21	1:B:166:ASP:HB3	1.63	0.62
1:F:410:GLY:N	1:F:413:ASN:OD1	2.24	0.62
1:F:82:ARG:NE	1:F:158:GLU:OE1	2.30	0.61
1:F:226:ASN:ND2	1:F:228:GLN:HG2	2.15	0.61
1:B:410:GLY:N	1:B:413:ASN:OD1	2.27	0.61
1:E:71:TYR:O	1:E:75:LEU:HG	1.99	0.61
1:C:416:ARG:HB3	1:C:425:PRO:HB2	1.81	0.61
1:F:214:GLY:HA2	1:F:343:ARG:HH21	1.66	0.61
1:E:88:PRO:HD2	1:E:91:GLN:NE2	2.16	0.61
1:B:239:VAL:HG21	1:E:241:LEU:HG	1.82	0.60
1:A:243:TYR:OH	1:D:361:ASP:OD2	2.20	0.60
1:D:62:HIS:CD2	1:D:66:GLU:HB2	2.37	0.60
1:A:83:HIS:CD2	1:A:84:PRO:HD2	2.36	0.60
1:C:236:HIS:NE2	1:C:409:GLY:O	2.35	0.60
1:B:291:ARG:HH22	1:B:359:TYR:HD2	1.48	0.59
1:A:235:HIS:ND1	1:A:293:ASP:OD1	2.35	0.59
1:B:369:THR:HG21	1:B:430:SER:HB3	1.84	0.59
1:C:239:VAL:HG21	1:F:241:LEU:CD2	2.32	0.59
1:C:122:ARG:HH21	1:C:166:ASP:HB3	1.67	0.59
1:C:248:MET:HG3	1:C:297:ILE:HG12	1.85	0.59
1:F:82:ARG:HE	1:F:158:GLU:CD	2.05	0.59
1:B:226:ASN:ND2	1:B:228:GLN:HG2	2.16	0.59
1:F:248:MET:HG3	1:F:297:ILE:HG12	1.85	0.59
1:D:405:GLY:HA2	1:D:434:LEU:HB2	1.85	0.58
1:E:124:ARG:NH1	2:E:1001:ATP:O1B	2.36	0.58
1:B:87:LEU:HD12	1:B:164:TRP:CD1	2.39	0.58
1:D:291:ARG:HD3	1:D:408:TRP:CZ2	2.39	0.58
1:E:240:ASP:OD2	1:E:245:ASN:CB	2.48	0.57
1:D:226:ASN:ND2	1:D:228:GLN:HG2	2.18	0.57
1:F:405:GLY:HA2	1:F:434:LEU:HB2	1.86	0.57
1:F:206:GLN:NE2	1:F:251:PRO:O	2.30	0.56
1:C:236:HIS:CD2	1:C:409:GLY:O	2.58	0.56
1:C:365:ILE:HD12	1:F:243:TYR:CE2	2.39	0.56
1:F:122:ARG:HH21	1:F:166:ASP:HB3	1.69	0.56
1:C:240:ASP:HB3	1:C:241:LEU:HD22	1.87	0.56
1:D:210:HIS:CG	1:D:243:TYR:HE2	2.23	0.56
1:B:214:GLY:HA2	1:B:343:ARG:HH21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:GLY:HA2	1:A:434:LEU:HB2	1.87	0.56
1:E:405:GLY:HA2	1:E:434:LEU:HB2	1.87	0.56
1:B:243:TYR:CE2	1:E:363:LYS:HD2	2.41	0.56
1:B:405:GLY:HA2	1:B:434:LEU:HB2	1.87	0.56
1:E:291:ARG:NH1	1:E:369:THR:OG1	2.36	0.55
1:A:55:TRP:O	1:A:57:THR:HG23	2.06	0.55
1:A:305:ILE:O	1:A:308:VAL:HG22	2.07	0.55
1:D:210:HIS:CG	1:D:243:TYR:CE2	2.94	0.55
1:B:83:HIS:NE2	1:B:87:LEU:HD22	2.22	0.54
1:C:121:PHE:HB2	1:C:128:LEU:HD22	1.88	0.54
1:E:411:THR:HG22	1:E:414:ARG:HH12	1.72	0.54
1:E:209:SER:CB	1:E:245:ASN:HB3	2.36	0.54
1:F:214:GLY:HA2	1:F:343:ARG:NH2	2.23	0.54
1:A:365:ILE:HG13	1:D:243:TYR:OH	2.07	0.54
1:C:54:LEU:HB2	1:F:54:LEU:HB2	1.90	0.54
1:E:291:ARG:HH22	1:E:359:TYR:HD2	1.56	0.54
1:C:111:ARG:HH12	1:C:360:ASN:HD22	1.55	0.54
1:D:210:HIS:CD2	1:D:243:TYR:HE2	2.26	0.53
1:C:111:ARG:NH1	1:C:360:ASN:HD22	2.06	0.53
1:E:340:LYS:HE3	1:E:348:THR:OG1	2.08	0.53
1:F:95:SER:HB2	1:F:327:GLN:HA	1.90	0.53
1:C:363:LYS:HB2	1:F:243:TYR:OH	2.09	0.53
1:E:452:LEU:O	1:E:456:VAL:HG13	2.09	0.53
1:B:238:ALA:HB1	1:B:265:VAL:HG21	1.91	0.52
1:B:243:TYR:CZ	1:E:363:LYS:HD2	2.45	0.52
1:B:304:ASP:OD1	1:B:306:SER:OG	2.21	0.52
1:E:121:PHE:HB2	1:E:128:LEU:HD22	1.91	0.52
1:F:87:LEU:HD12	1:F:91:GLN:NE2	2.24	0.52
1:E:416:ARG:HB3	1:E:425:PRO:HB2	1.91	0.52
1:A:193:LYS:HB3	1:A:198:ASP:HB2	1.92	0.52
1:E:193:LYS:HB3	1:E:198:ASP:HB2	1.91	0.52
1:B:83:HIS:HE1	1:B:86:ARG:CG	2.23	0.52
1:D:95:SER:HB2	1:D:327:GLN:HA	1.91	0.52
1:E:122:ARG:HH21	1:E:166:ASP:HB3	1.74	0.52
1:C:115:LEU:HD11	1:C:139:ALA:HB2	1.92	0.52
1:F:410:GLY:O	1:F:413:ASN:ND2	2.43	0.52
1:A:87:LEU:HD12	1:A:91:GLN:NE2	2.25	0.51
1:C:59:ASN:HB2	1:C:61:GLN:CG	2.39	0.51
1:D:387:SER:HB3	1:D:409:GLY:HA2	1.92	0.51
1:E:155:ALA:O	1:E:156:ILE:HG12	2.10	0.51
1:A:369:THR:HG21	1:A:430:SER:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:TYR:HA	1:F:415:GLY:HA3	1.92	0.51
1:F:291:ARG:HD3	1:F:408:TRP:CZ2	2.45	0.51
1:C:99:LEU:HD21	1:C:330:LEU:HD11	1.92	0.51
1:D:189:GLU:HG2	1:F:421:SER:OG	2.10	0.51
1:D:291:ARG:NH1	1:D:369:THR:OG1	2.41	0.51
1:E:240:ASP:C	1:E:241:LEU:HD22	2.31	0.51
1:C:238:ALA:HB1	1:C:265:VAL:HG21	1.91	0.51
1:C:235:HIS:CE1	1:F:241:LEU:CD1	2.95	0.50
1:D:291:ARG:HH11	1:D:369:THR:HG1	1.60	0.50
1:D:453:GLN:O	1:D:457:GLN:HG2	2.11	0.50
1:A:270:SER:OG	1:D:240:ASP:OD2	2.08	0.50
1:C:336:ARG:HG2	1:C:393:LEU:HD22	1.93	0.50
1:D:238:ALA:HB2	1:D:265:VAL:HG21	1.93	0.50
1:A:241:LEU:HD11	1:D:236:HIS:CD2	2.47	0.50
1:F:233:THR:O	1:F:295:ALA:N	2.45	0.50
1:B:87:LEU:HD12	1:B:164:TRP:CG	2.47	0.49
1:C:240:ASP:O	1:C:241:LEU:HB2	2.11	0.49
1:D:70:ASN:OD1	1:D:74:ASN:ND2	2.45	0.49
1:B:53:PHE:HE2	1:E:55:TRP:CD2	2.30	0.49
1:B:233:THR:O	1:B:295:ALA:N	2.45	0.49
1:F:240:ASP:HB2	1:F:243:TYR:O	2.12	0.49
1:B:222:ARG:HH22	1:B:228:GLN:HG3	1.77	0.49
1:F:340:LYS:HD3	1:F:407:ILE:HD11	1.95	0.49
1:B:156:ILE:HD12	1:B:166:ASP:HA	1.93	0.49
1:B:58:SER:HB3	1:E:51:ALA:HA	1.95	0.49
1:D:419:LEU:HB2	1:D:423:HIS:CE1	2.48	0.49
1:F:235:HIS:O	1:F:239:VAL:HG23	2.12	0.49
1:B:235:HIS:CD2	1:E:241:LEU:HD12	2.48	0.49
1:B:407:ILE:HD13	1:B:429:THR:HG21	1.95	0.49
1:C:95:SER:HB2	1:C:327:GLN:HA	1.95	0.49
1:F:235:HIS:CE1	1:F:293:ASP:HA	2.48	0.49
1:F:277:TRP:CD1	1:F:290:VAL:HG11	2.48	0.49
1:C:243:TYR:CE2	1:F:365:ILE:HD12	2.48	0.49
1:B:277:TRP:CD1	1:B:290:VAL:HG11	2.48	0.48
1:C:76:GLN:HA	1:C:79:LEU:CD1	2.43	0.48
1:C:340:LYS:HG2	1:C:341:VAL:N	2.28	0.48
1:E:80:LEU:C	1:E:82:ARG:H	2.15	0.48
1:E:190:LEU:O	1:E:194:LEU:HD13	2.13	0.48
1:E:241:LEU:HD22	1:E:241:LEU:N	2.28	0.48
1:F:239:VAL:HG12	1:F:240:ASP:H	1.78	0.48
1:B:399:GLU:OE1	1:B:399:GLU:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:HD23	1:C:63:CYS:SG	2.54	0.48
1:B:60:LEU:HG	1:B:63:CYS:HB3	1.96	0.48
1:B:265:VAL:HA	1:B:297:ILE:HG13	1.96	0.48
1:D:76:GLN:O	1:D:79:LEU:HG	2.14	0.48
1:D:108:LYS:HA	1:D:111:ARG:HG2	1.96	0.48
1:F:340:LYS:HG2	1:F:341:VAL:N	2.29	0.48
1:B:190:LEU:O	1:B:194:LEU:HD13	2.14	0.47
1:C:50:ALA:HB3	1:F:57:THR:OG1	2.14	0.47
1:C:106:HIS:O	1:C:110:LEU:HB2	2.13	0.47
1:E:340:LYS:HG2	1:E:341:VAL:N	2.29	0.47
1:B:248:MET:HG3	1:B:297:ILE:HG12	1.95	0.47
1:A:308:VAL:CG2	1:A:452:LEU:HD21	2.44	0.47
1:B:340:LYS:HD3	1:B:407:ILE:CD1	2.44	0.47
1:A:267:ARG:NH2	1:A:442:GLU:OE1	2.48	0.47
1:B:246:GLN:O	1:B:265:VAL:HG23	2.14	0.47
1:C:452:LEU:O	1:C:456:VAL:HG13	2.15	0.47
1:F:399:GLU:OE1	1:F:399:GLU:N	2.41	0.47
1:B:111:ARG:HA	1:B:114:SER:HG	1.80	0.47
1:E:81:PRO:HB3	1:E:158:GLU:OE2	2.15	0.47
1:C:291:ARG:HH22	1:C:359:TYR:HD2	1.63	0.47
1:F:235:HIS:CE1	1:F:270:SER:HA	2.50	0.46
1:F:291:ARG:HH22	1:F:359:TYR:HD2	1.61	0.46
1:B:87:LEU:HA	1:B:87:LEU:HD13	1.72	0.46
1:D:340:LYS:HD3	1:D:407:ILE:HD11	1.97	0.46
1:C:325:ASP:HB3	1:C:328:CYS:SG	2.55	0.46
1:E:455:ALA:HA	1:E:458:GLN:HE21	1.81	0.46
1:B:236:HIS:ND1	1:B:409:GLY:O	2.48	0.46
1:F:241:LEU:O	1:F:241:LEU:HG	2.16	0.46
1:A:248:MET:HG3	1:A:297:ILE:HG12	1.96	0.46
1:B:291:ARG:HD3	1:B:408:TRP:CZ2	2.51	0.46
1:C:378:ARG:HD2	1:C:423:HIS:CG	2.50	0.46
1:E:378:ARG:CZ	1:E:423:HIS:ND1	2.79	0.46
1:C:87:LEU:HB3	1:C:164:TRP:CD1	2.51	0.46
1:E:148:ASN:OD1	1:E:151:GLN:N	2.45	0.46
1:B:214:GLY:C	1:B:343:ARG:HE	2.19	0.46
1:B:340:LYS:HD3	1:B:407:ILE:HD11	1.96	0.46
1:C:220:VAL:HG21	1:C:443:LEU:HD13	1.98	0.46
1:C:234:ASN:HD21	1:C:387:SER:HB3	1.81	0.46
1:E:265:VAL:HA	1:E:297:ILE:HG13	1.97	0.46
1:E:453:GLN:O	1:E:456:VAL:HG22	2.16	0.46
1:F:458:GLN:O	1:F:458:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:ARG:HH22	1:F:228:GLN:HG3	1.79	0.46
1:C:399:GLU:OE1	1:C:399:GLU:N	2.40	0.45
1:E:88:PRO:HD2	1:E:91:GLN:HE21	1.81	0.45
1:A:73:GLY:O	1:A:76:GLN:HB3	2.15	0.45
1:E:277:TRP:CD1	1:E:290:VAL:HG11	2.51	0.45
1:F:235:HIS:CD2	1:F:236:HIS:HD2	2.35	0.45
1:F:407:ILE:HD13	1:F:429:THR:HG21	1.99	0.45
1:A:87:LEU:HD12	1:A:91:GLN:HE21	1.82	0.45
1:A:453:GLN:HA	1:A:456:VAL:HG12	1.99	0.45
1:E:91:GLN:O	1:E:163:VAL:HA	2.15	0.45
1:F:137:PHE:HB3	1:F:172:PHE:CB	2.47	0.45
1:A:221:LYS:HB3	1:A:446:ILE:HD11	1.99	0.45
1:D:154:PRO:O	1:D:167:VAL:HB	2.17	0.45
1:B:111:ARG:HA	1:B:114:SER:OG	2.16	0.45
1:D:76:GLN:OE1	1:D:79:LEU:HD11	2.17	0.45
1:F:144:LYS:HA	1:F:147:LEU:HD12	1.98	0.44
1:B:340:LYS:HE3	1:B:348:THR:OG1	2.17	0.44
1:B:416:ARG:HB3	1:B:425:PRO:HB2	1.99	0.44
1:C:89:LYS:HE2	1:C:92:GLN:OE1	2.17	0.44
1:B:144:LYS:HA	1:B:147:LEU:HD12	1.99	0.44
1:D:80:LEU:N	1:D:81:PRO:HD3	2.33	0.44
1:E:222:ARG:NH2	1:E:226:ASN:HB3	2.33	0.44
1:F:95:SER:HB2	1:F:326:LEU:O	2.17	0.44
1:A:246:GLN:HG2	1:A:264:ALA:HB1	1.98	0.44
1:B:137:PHE:HB3	1:B:172:PHE:CB	2.47	0.44
1:B:320:ASP:O	1:B:402:ARG:HD2	2.18	0.44
1:C:60:LEU:HB3	1:C:63:CYS:SG	2.58	0.44
1:F:447:ILE:HG13	1:F:448:THR:HG23	2.00	0.44
1:B:340:LYS:HG2	1:B:341:VAL:N	2.32	0.44
1:E:340:LYS:HD3	1:E:407:ILE:HD11	1.99	0.44
1:E:222:ARG:HH21	1:E:226:ASN:HB3	1.83	0.43
1:F:238:ALA:HB1	1:F:265:VAL:HG21	2.00	0.43
1:C:87:LEU:HD13	1:C:87:LEU:HA	1.84	0.43
1:E:407:ILE:HD13	1:E:429:THR:HG21	2.01	0.43
1:C:51:ALA:HA	1:F:58:SER:HB3	2.01	0.43
1:A:296:PHE:HB2	1:A:443:LEU:HD11	2.01	0.43
1:D:62:HIS:CE1	1:D:65:ALA:HB3	2.54	0.43
1:F:392:ILE:HA	1:F:403:PRO:HA	2.00	0.43
1:C:118:ALA:HB2	1:C:357:LEU:HD12	2.01	0.43
1:D:62:HIS:O	1:D:62:HIS:CG	2.71	0.43
1:F:221:LYS:HB3	1:F:446:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:HIS:CE1	1:B:86:ARG:CD	3.02	0.43
1:D:109:ILE:HD12	1:D:109:ILE:HA	1.92	0.43
1:E:124:ARG:CZ	2:E:1001:ATP:O1B	2.67	0.43
1:B:107:SER:HB2	1:B:111:ARG:CZ	2.48	0.42
1:D:411:THR:HG22	1:D:412:ALA:N	2.34	0.42
1:E:76:GLN:C	1:E:78:GLY:H	2.22	0.42
1:E:238:ALA:HB1	1:E:265:VAL:HG21	2.00	0.42
1:A:95:SER:HB2	1:A:327:GLN:HA	2.01	0.42
1:A:340:LYS:HD3	1:A:407:ILE:HD11	2.01	0.42
1:D:61:GLN:HA	1:D:62:HIS:HA	1.77	0.42
1:B:236:HIS:CE1	1:B:409:GLY:O	2.72	0.42
1:E:238:ALA:CB	1:E:265:VAL:HG21	2.49	0.42
1:A:65:ALA:O	1:A:68:ARG:HB3	2.19	0.42
1:C:455:ALA:HA	1:C:458:GLN:HE21	1.83	0.42
1:C:76:GLN:HA	1:C:79:LEU:HD11	2.01	0.42
1:E:353:MET:HB2	1:E:372:LEU:HD22	2.01	0.42
1:C:230:GLY:HA2	1:C:299:PHE:CD2	2.54	0.42
1:C:369:THR:HG21	1:C:430:SER:HB3	2.01	0.42
1:A:267:ARG:HA	1:D:53:PHE:O	2.19	0.42
1:D:156:ILE:HD13	1:D:166:ASP:HA	2.02	0.42
1:C:241:LEU:HA	1:C:241:LEU:HD13	1.76	0.42
1:C:340:LYS:HE3	1:C:348:THR:OG1	2.19	0.42
1:D:340:LYS:HE3	1:D:340:LYS:HB3	1.85	0.42
1:F:214:GLY:C	1:F:343:ARG:HE	2.22	0.42
1:C:57:THR:HG1	1:F:49:SER:N	2.18	0.42
1:E:158:GLU:O	1:E:158:GLU:HG3	2.20	0.42
1:E:246:GLN:O	1:E:265:VAL:HG23	2.20	0.42
1:F:408:TRP:CZ2	1:F:410:GLY:HA3	2.54	0.42
1:B:193:LYS:HB3	1:B:198:ASP:HB2	2.02	0.42
1:C:240:ASP:OD1	1:C:241:LEU:N	2.52	0.42
1:A:230:GLY:HA2	1:A:299:PHE:CD2	2.54	0.41
1:A:353:MET:HB2	1:A:372:LEU:HD22	2.02	0.41
1:B:95:SER:HB2	1:B:327:GLN:HA	2.02	0.41
1:B:209:SER:HB3	1:B:248:MET:HE1	2.01	0.41
1:A:115:LEU:HD11	1:A:139:ALA:HB2	2.01	0.41
1:A:453:GLN:O	1:A:456:VAL:HG12	2.20	0.41
1:B:54:LEU:HD23	1:B:54:LEU:HA	1.86	0.41
1:C:111:ARG:HH12	1:C:360:ASN:ND2	2.17	0.41
1:D:106:HIS:HB3	1:D:109:ILE:HG22	2.02	0.41
1:C:405:GLY:HA2	1:C:434:LEU:HB2	2.02	0.41
1:E:83:HIS:CD2	1:E:84:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:HIS:HA	1:E:295:ALA:HB2	2.02	0.41
1:C:363:LYS:HD2	1:F:243:TYR:CZ	2.55	0.41
1:E:369:THR:CG2	1:E:430:SER:HB3	2.47	0.41
1:F:340:LYS:HD3	1:F:407:ILE:CD1	2.50	0.41
1:F:390:LEU:HD23	1:F:406:ILE:HG22	2.01	0.41
1:B:234:ASN:ND2	1:B:387:SER:HB2	2.27	0.41
1:B:215:THR:OG1	1:B:343:ARG:HG2	2.20	0.41
1:C:54:LEU:HD23	1:C:54:LEU:HA	1.93	0.41
1:C:378:ARG:HD2	1:C:423:HIS:NE2	2.36	0.41
1:F:91:GLN:O	1:F:163:VAL:HA	2.21	0.41
1:A:241:LEU:HA	1:A:241:LEU:HD12	1.75	0.41
1:D:340:LYS:HG2	1:D:341:VAL:N	2.35	0.41
1:F:235:HIS:CE1	1:F:293:ASP:CG	2.94	0.41
1:E:248:MET:HG3	1:E:297:ILE:HG12	2.02	0.41
1:B:235:HIS:NE2	1:B:236:HIS:CD2	2.89	0.41
1:C:111:ARG:HH22	1:C:360:ASN:ND2	2.19	0.41
1:A:418:LYS:HE3	1:A:418:LYS:HB3	1.95	0.41
1:B:122:ARG:NH2	1:B:166:ASP:HB3	2.33	0.41
1:C:104:ALA:HA	1:C:107:SER:OG	2.21	0.41
1:C:233:THR:O	1:C:295:ALA:N	2.54	0.40
1:E:82:ARG:HA	1:E:83:HIS:HA	1.53	0.40
1:E:325:ASP:HB3	1:E:328:CYS:SG	2.61	0.40
1:B:221:LYS:HB3	1:B:446:ILE:HD11	2.03	0.40
1:C:158:GLU:O	1:C:158:GLU:HG3	2.21	0.40
1:C:235:HIS:O	1:C:239:VAL:N	2.54	0.40
1:E:89:LYS:HD3	1:E:89:LYS:O	2.21	0.40
1:F:378:ARG:HD2	1:F:423:HIS:CG	2.56	0.40
1:B:136:VAL:HG21	1:B:153:LEU:HD22	2.02	0.40
1:D:268:ALA:HA	1:D:294:GLY:O	2.22	0.40
1:A:64:ALA:O	1:A:281:TYR:HE1	2.04	0.40
1:A:158:GLU:HG3	1:A:158:GLU:O	2.22	0.40
1:A:340:LYS:HE3	1:A:348:THR:OG1	2.21	0.40
1:B:107:SER:CB	1:B:111:ARG:HH22	2.34	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	397/413 (96%)	391 (98%)	6 (2%)	0	100	100
1	B	398/413 (96%)	394 (99%)	4 (1%)	0	100	100
1	C	398/413 (96%)	393 (99%)	5 (1%)	0	100	100
1	D	398/413 (96%)	397 (100%)	1 (0%)	0	100	100
1	E	398/413 (96%)	391 (98%)	7 (2%)	0	100	100
1	F	398/413 (96%)	393 (99%)	5 (1%)	0	100	100
All	All	2387/2478 (96%)	2359 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	333/342 (97%)	326 (98%)	7 (2%)	53	80
1	B	334/342 (98%)	329 (98%)	5 (2%)	65	85
1	C	334/342 (98%)	332 (99%)	2 (1%)	86	94
1	D	334/342 (98%)	331 (99%)	3 (1%)	78	91
1	E	334/342 (98%)	329 (98%)	5 (2%)	65	85
1	F	334/342 (98%)	331 (99%)	3 (1%)	78	91
All	All	2003/2052 (98%)	1978 (99%)	25 (1%)	71	88

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	THR
1	A	166	ASP
1	A	229	VAL
1	A	267	ARG
1	A	365	ILE
1	A	379	GLN
1	A	411	THR
1	B	70	ASN
1	B	166	ASP
1	B	239	VAL
1	B	245	ASN
1	B	306	SER
1	C	80	LEU
1	C	229	VAL
1	D	166	ASP
1	D	323	VAL
1	D	360	ASN
1	E	166	ASP
1	E	194	LEU
1	E	234	ASN
1	E	237	VAL
1	E	243	TYR
1	F	166	ASP
1	F	189	GLU
1	F	293	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	210	HIS
1	B	61	GLN
1	B	234	ASN
1	B	236	HIS
1	C	235	HIS
1	C	360	ASN
1	C	458	GLN
1	D	62	HIS
1	D	74	ASN
1	E	61	GLN
1	E	236	HIS

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Mol	Chain	Res	Type
1	E	458	GLN
1	F	91	GLN
1	F	234	ASN
1	F	236	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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$
2	ATP	C	1001	3	26,33,33	0.90	1 (3%)	31,52,52	1.44	5 (16%)
2	ATP	F	1001	3	26,33,33	0.96	1 (3%)	31,52,52	1.42	5 (16%)
2	ATP	A	1001	3	26,33,33	0.92	1 (3%)	31,52,52	1.40	5 (16%)
2	ATP	B	1001	3	26,33,33	0.93	1 (3%)	31,52,52	1.44	5 (16%)
2	ATP	E	1001	3	26,33,33	0.91	1 (3%)	31,52,52	1.52	8 (25%)
2	ATP	D	1001	3	26,33,33	0.95	1 (3%)	31,52,52	1.45	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	C	1001	3	-	2/18/38/38	0/3/3/3
2	ATP	F	1001	3	-	2/18/38/38	0/3/3/3
2	ATP	A	1001	3	-	2/18/38/38	0/3/3/3
2	ATP	B	1001	3	-	2/18/38/38	0/3/3/3
2	ATP	E	1001	3	-	2/18/38/38	0/3/3/3
2	ATP	D	1001	3	-	2/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	ATP	C5-C4	2.57	1.47	1.40
2	F	1001	ATP	C5-C4	2.54	1.47	1.40
2	A	1001	ATP	C5-C4	2.52	1.47	1.40
2	E	1001	ATP	C5-C4	2.44	1.47	1.40
2	B	1001	ATP	C5-C4	2.44	1.47	1.40
2	C	1001	ATP	C5-C4	2.42	1.47	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	ATP	PA-O3A-PB	-3.26	121.63	132.83
2	C	1001	ATP	PA-O3A-PB	-3.24	121.70	132.83
2	B	1001	ATP	C4-C5-N7	-3.23	106.04	109.40
2	A	1001	ATP	N3-C2-N1	-3.18	123.72	128.68
2	C	1001	ATP	N3-C2-N1	-3.16	123.73	128.68
2	F	1001	ATP	C4-C5-N7	-3.14	106.13	109.40
2	D	1001	ATP	N3-C2-N1	-3.05	123.92	128.68
2	E	1001	ATP	N3-C2-N1	-3.02	123.96	128.68
2	B	1001	ATP	N3-C2-N1	-3.01	123.98	128.68
2	D	1001	ATP	PB-O3B-PG	-2.93	122.79	132.83
2	D	1001	ATP	C3'-C2'-C1'	2.92	105.38	100.98
2	F	1001	ATP	PA-O3A-PB	-2.88	122.96	132.83
2	C	1001	ATP	C3'-C2'-C1'	2.87	105.30	100.98
2	F	1001	ATP	N3-C2-N1	-2.87	124.20	128.68
2	A	1001	ATP	PB-O3B-PG	-2.85	123.03	132.83
2	A	1001	ATP	C3'-C2'-C1'	2.83	105.23	100.98
2	C	1001	ATP	C4-C5-N7	-2.81	106.47	109.40
2	B	1001	ATP	PB-O3B-PG	-2.80	123.22	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1001	ATP	O2B-PB-O1B	2.80	126.06	112.24
2	B	1001	ATP	C3'-C2'-C1'	2.79	105.18	100.98
2	A	1001	ATP	PA-O3A-PB	-2.78	123.28	132.83
2	E	1001	ATP	C4-C5-N7	-2.77	106.51	109.40
2	F	1001	ATP	C3'-C2'-C1'	2.73	105.09	100.98
2	C	1001	ATP	PB-O3B-PG	-2.72	123.51	132.83
2	F	1001	ATP	PB-O3B-PG	-2.70	123.55	132.83
2	B	1001	ATP	PA-O3A-PB	-2.69	123.60	132.83
2	E	1001	ATP	C3'-C2'-C1'	2.64	104.95	100.98
2	E	1001	ATP	PA-O3A-PB	-2.53	124.15	132.83
2	A	1001	ATP	C4-C5-N7	-2.49	106.81	109.40
2	D	1001	ATP	C4-C5-N7	-2.42	106.88	109.40
2	E	1001	ATP	O3G-PG-O2G	2.30	116.42	107.64
2	E	1001	ATP	PB-O3B-PG	-2.22	125.21	132.83
2	E	1001	ATP	O3B-PG-O1G	-2.03	99.91	111.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	PA-O3A-PB-O2B
2	C	1001	ATP	PA-O3A-PB-O2B
2	D	1001	ATP	PA-O3A-PB-O2B
2	E	1001	ATP	PA-O3A-PB-O2B
2	B	1001	ATP	PA-O3A-PB-O2B
2	F	1001	ATP	PA-O3A-PB-O2B
2	A	1001	ATP	PA-O3A-PB-O1B
2	B	1001	ATP	PA-O3A-PB-O1B
2	C	1001	ATP	PA-O3A-PB-O1B
2	D	1001	ATP	PA-O3A-PB-O1B
2	E	1001	ATP	PA-O3A-PB-O1B
2	F	1001	ATP	PA-O3A-PB-O1B

There are no ring outliers.

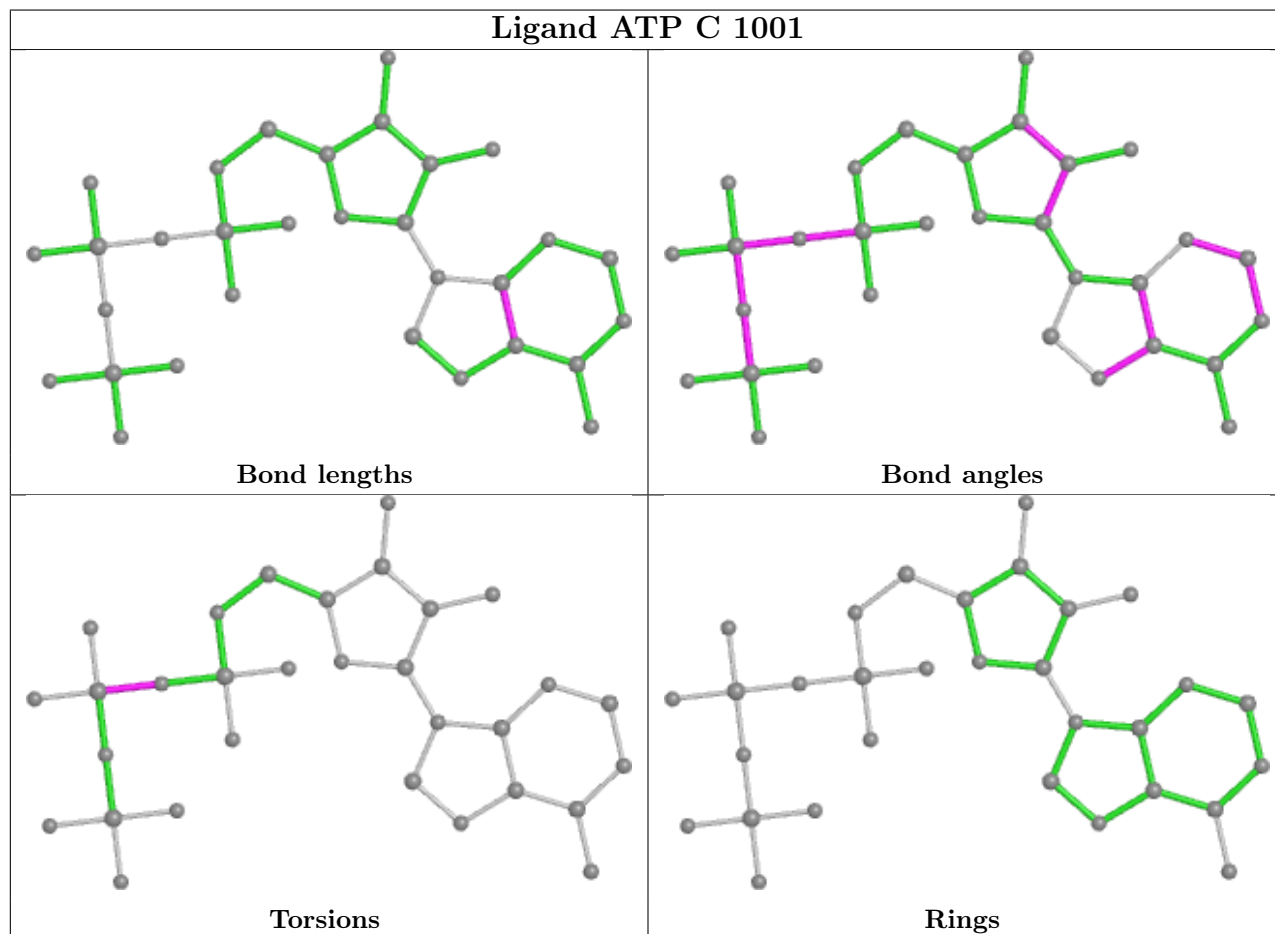
1 monomer is involved in 2 short contacts:

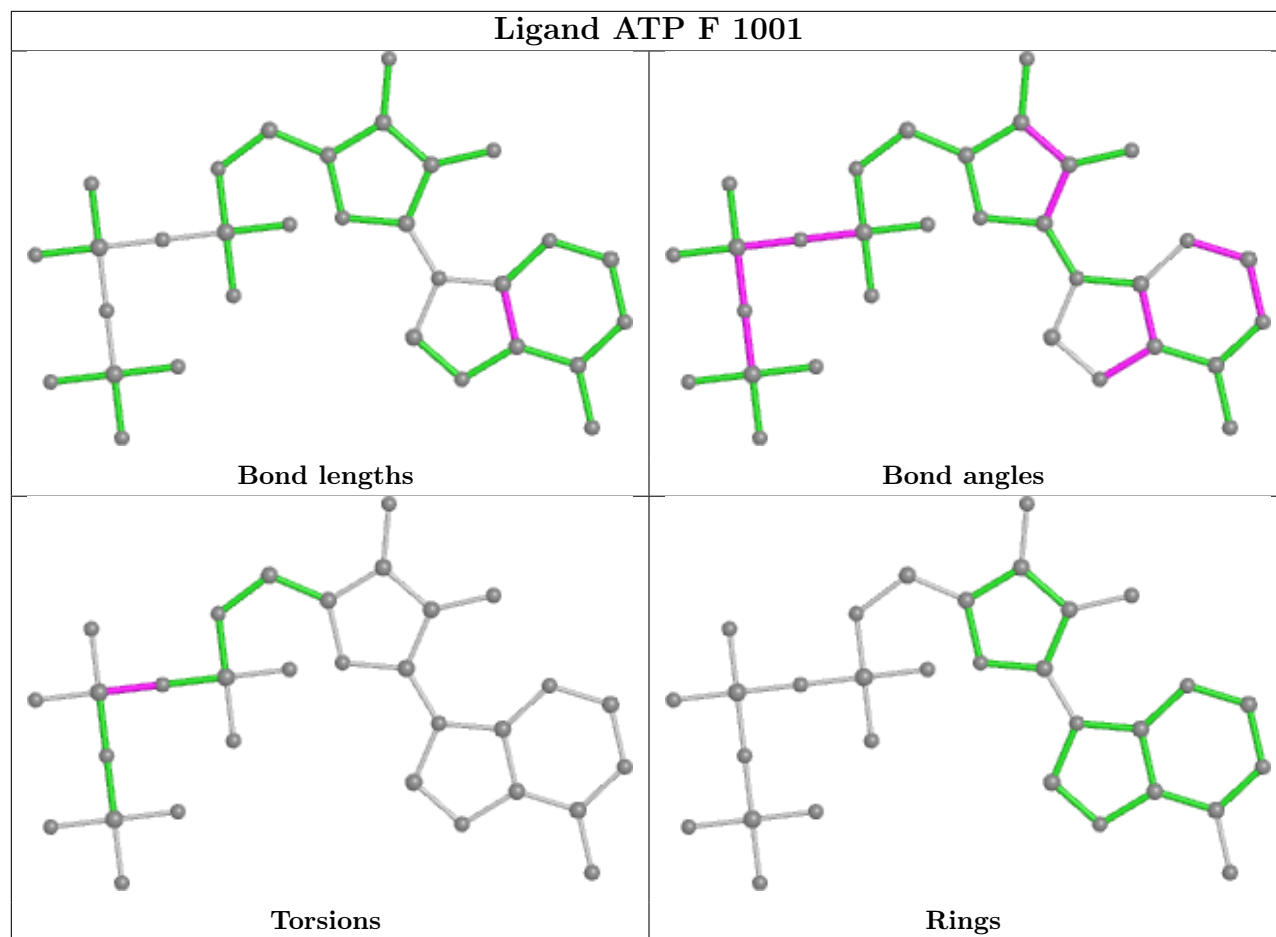
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1001	ATP	2	0

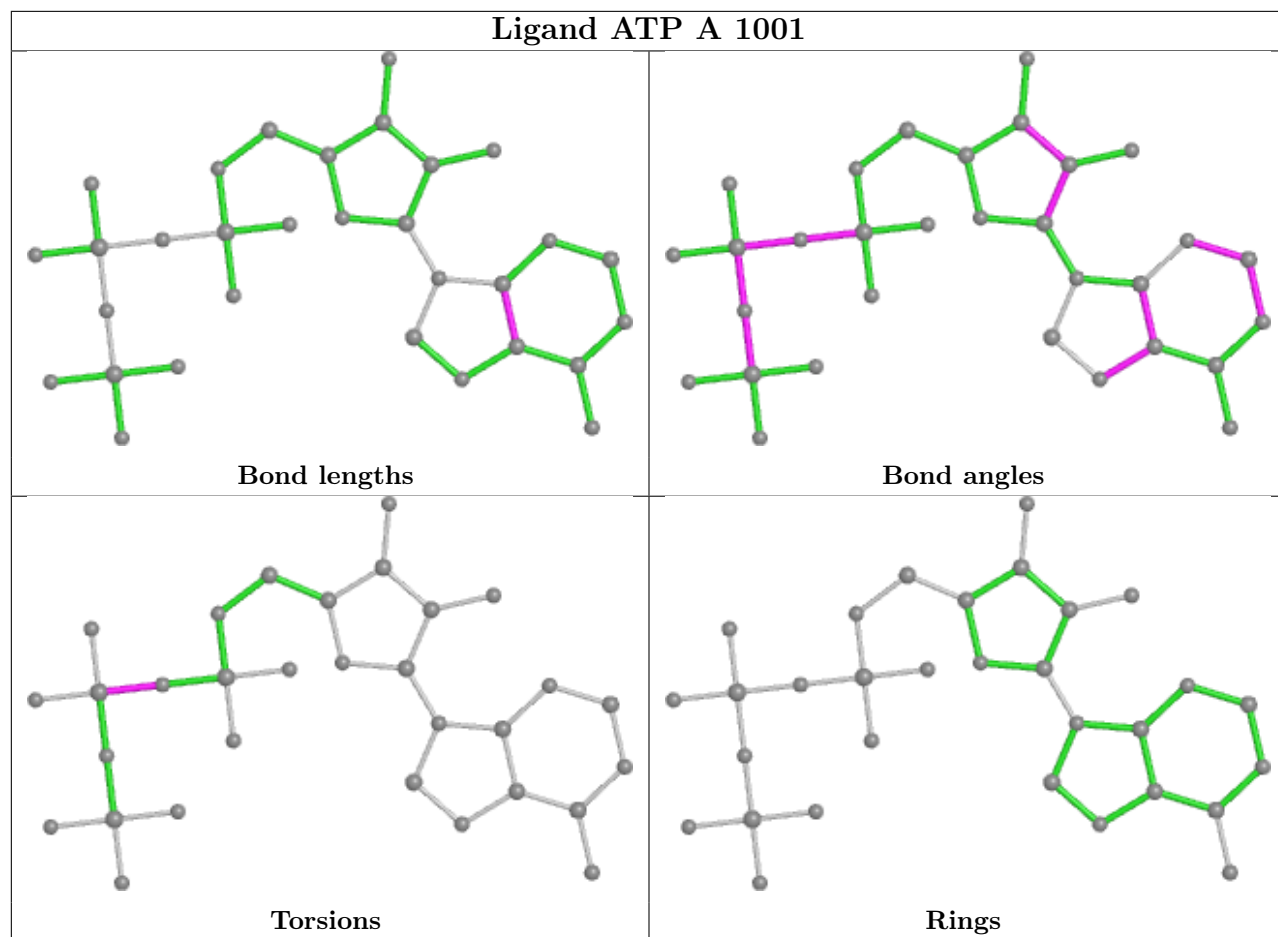
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

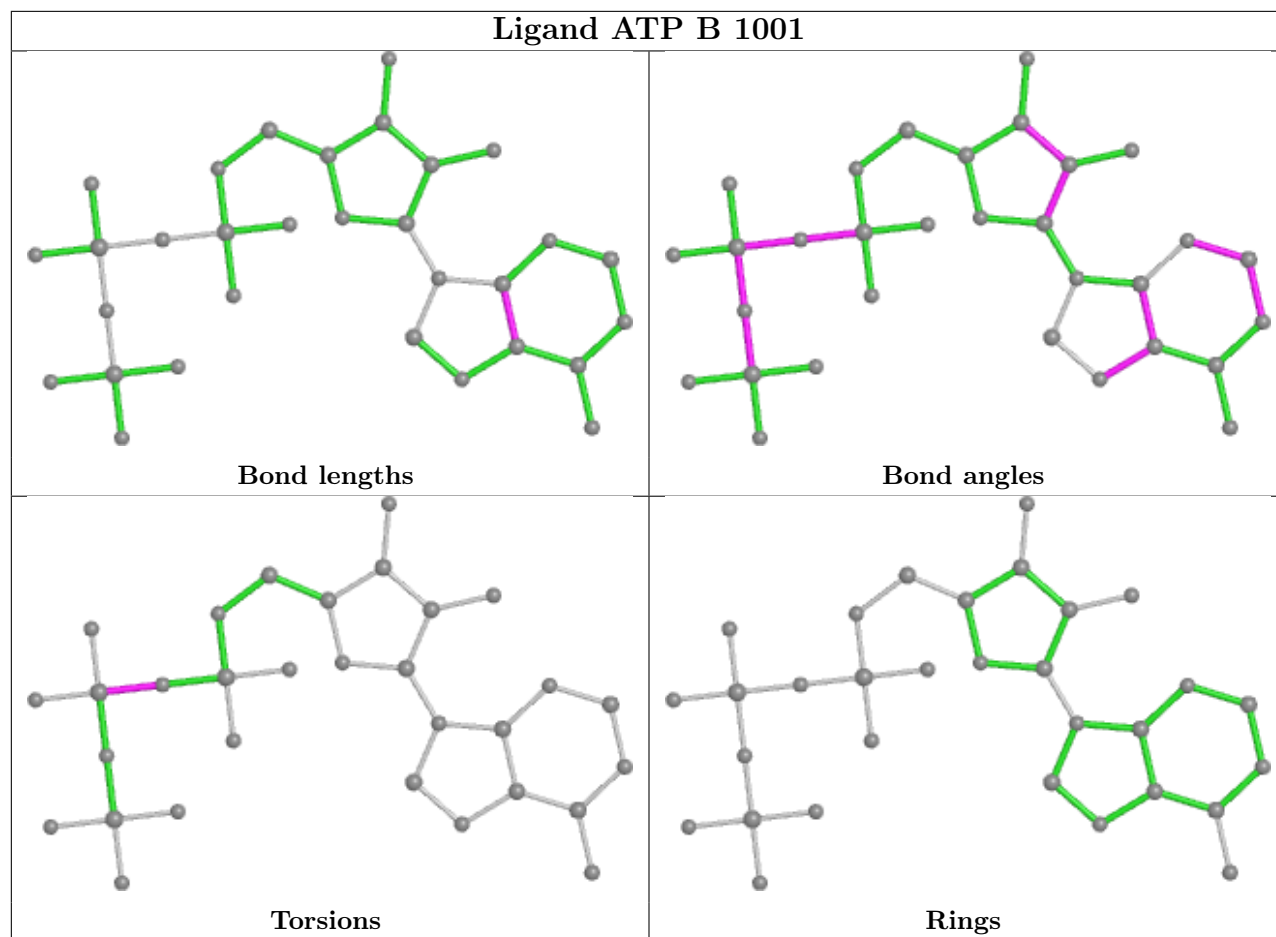


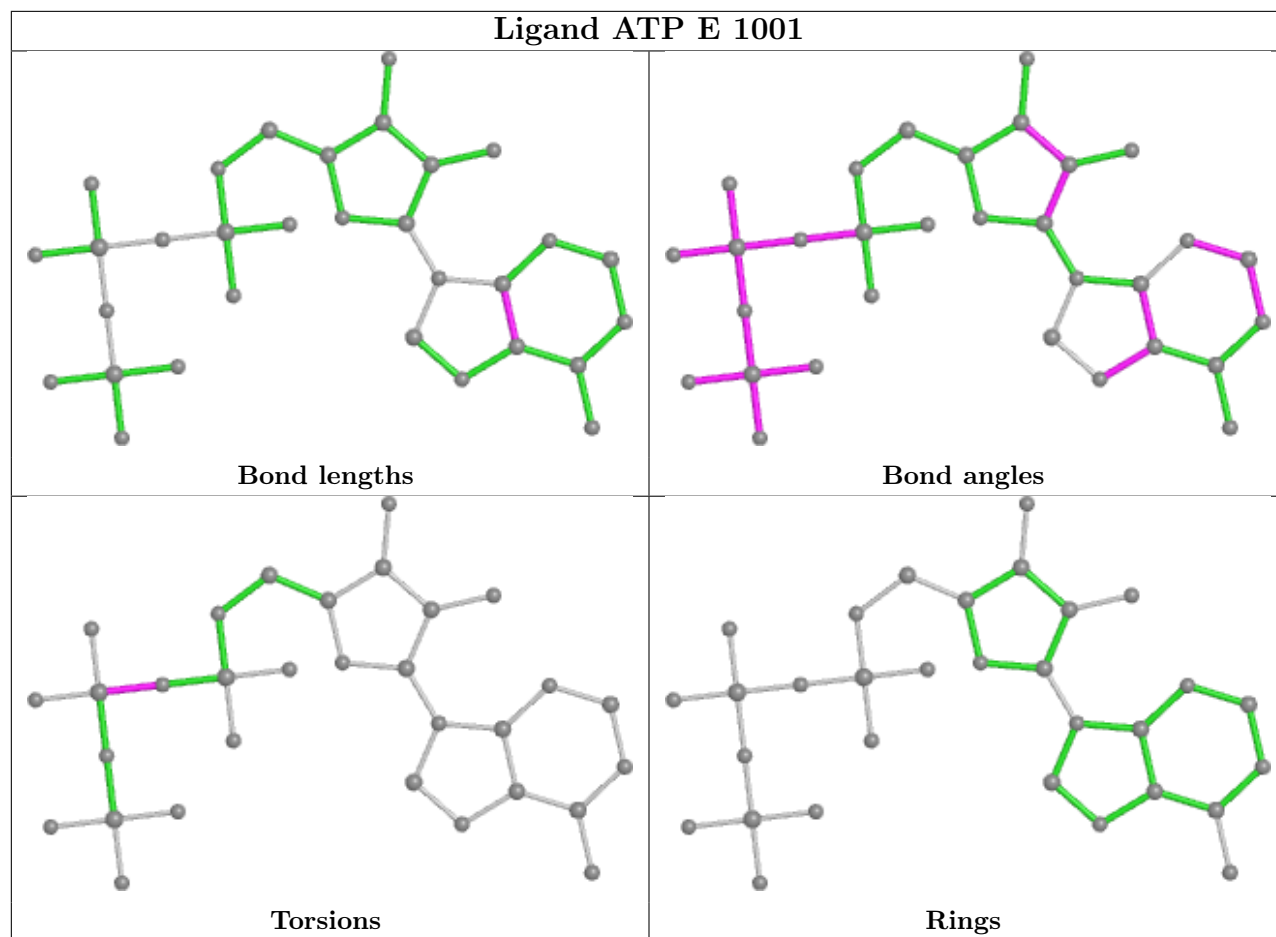
addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

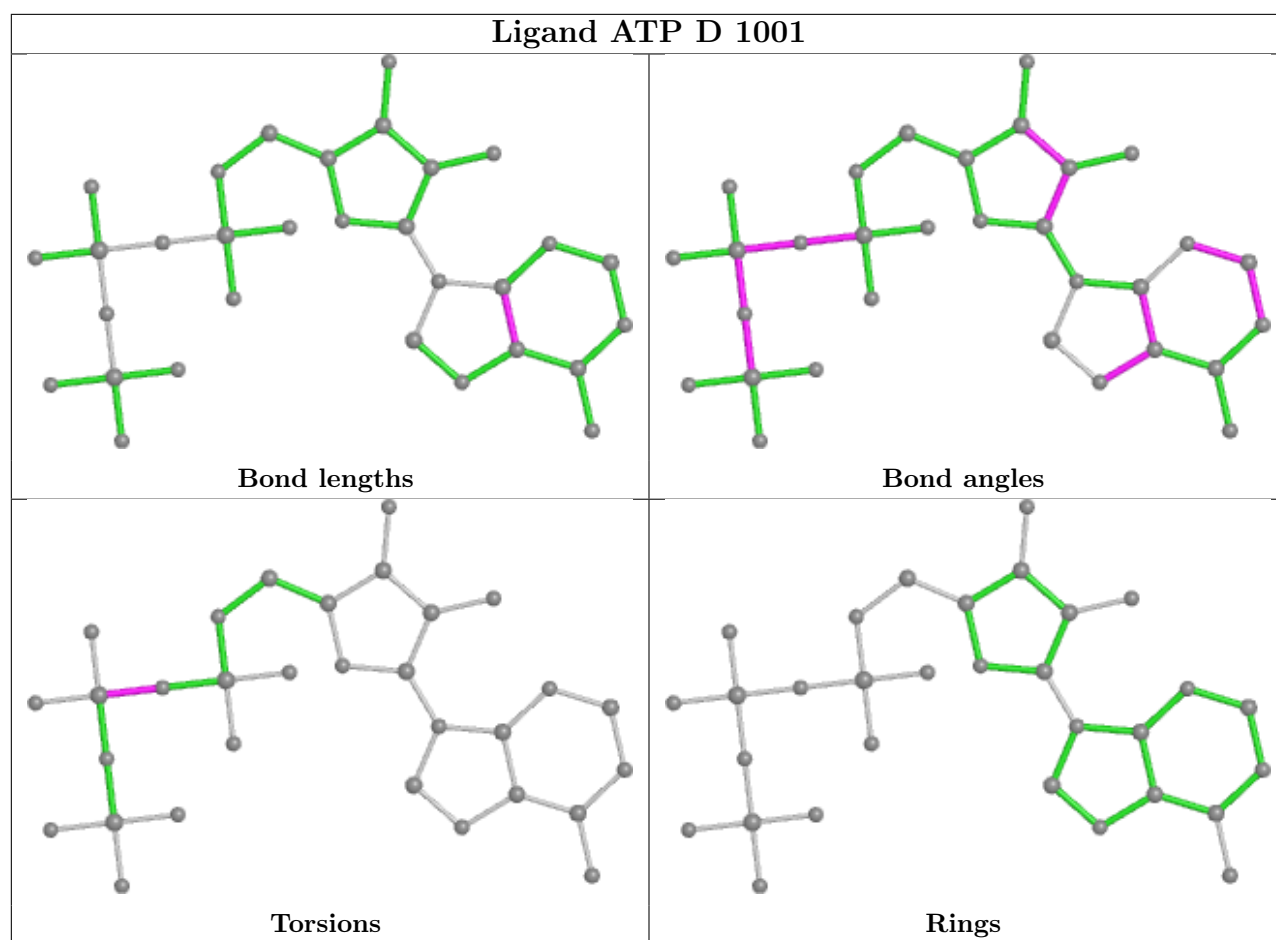












## 5.7 Other polymers [i](#)

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	401/413 (97%)	0.17	17 (4%) 36 23	38, 64, 116, 191	0
1	B	402/413 (97%)	0.11	19 (4%) 31 20	37, 60, 106, 160	0
1	C	402/413 (97%)	0.15	20 (4%) 28 18	38, 68, 116, 157	0
1	D	402/413 (97%)	0.13	15 (3%) 41 27	39, 63, 114, 188	0
1	E	402/413 (97%)	0.18	24 (5%) 21 13	43, 68, 120, 189	0
1	F	402/413 (97%)	0.05	18 (4%) 33 21	36, 59, 104, 150	0
All	All	2411/2478 (97%)	0.13	113 (4%) 31 20	36, 63, 115, 191	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	83	HIS	10.1
1	A	81	PRO	9.4
1	A	83	HIS	9.1
1	B	85	GLY	8.0
1	F	83	HIS	7.7
1	A	80	LEU	7.5
1	D	81	PRO	7.4
1	E	82	ARG	6.8
1	A	82	ARG	6.8
1	D	82	ARG	6.6
1	D	83	HIS	6.5
1	C	80	LEU	6.2
1	B	82	ARG	5.9
1	C	76	GLN	5.7
1	C	413	ASN	5.7
1	B	62	HIS	5.6
1	E	80	LEU	5.6
1	E	78	GLY	5.4
1	C	239	VAL	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	84	PRO	5.2
1	B	84	PRO	5.1
1	C	238	ALA	5.0
1	B	61	GLN	4.9
1	A	84	PRO	4.7
1	E	239	VAL	4.7
1	B	411	THR	4.6
1	C	85	GLY	4.5
1	C	79	LEU	4.5
1	C	87	LEU	4.4
1	E	238	ALA	4.4
1	D	86	ARG	4.2
1	A	413	ASN	4.1
1	D	80	LEU	4.1
1	C	84	PRO	4.1
1	F	411	THR	4.0
1	F	82	ARG	4.0
1	D	185	GLN	4.0
1	E	79	LEU	4.0
1	F	242	ASP	3.9
1	D	412	ALA	3.8
1	D	84	PRO	3.7
1	F	86	ARG	3.7
1	A	412	ALA	3.7
1	A	185	GLN	3.7
1	A	89	LYS	3.7
1	D	409	GLY	3.6
1	C	236	HIS	3.6
1	B	184	GLU	3.6
1	C	63	CYS	3.6
1	E	410	GLY	3.5
1	F	410	GLY	3.5
1	F	412	ALA	3.5
1	C	412	ALA	3.4
1	E	86	ARG	3.3
1	B	80	LEU	3.3
1	E	64	ALA	3.3
1	C	83	HIS	3.2
1	B	236	HIS	3.1
1	F	184	GLU	3.1
1	F	239	VAL	3.1
1	C	86	ARG	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	84	PRO	3.0
1	F	241	LEU	3.0
1	C	411	THR	2.9
1	A	414	ARG	2.9
1	D	87	LEU	2.9
1	D	243	TYR	2.8
1	A	241	LEU	2.8
1	E	89	LYS	2.8
1	F	58	SER	2.8
1	A	64	ALA	2.8
1	B	410	GLY	2.8
1	E	113	PHE	2.7
1	A	62	HIS	2.7
1	E	61	GLN	2.7
1	B	86	ARG	2.7
1	F	414	ARG	2.6
1	A	86	ARG	2.6
1	A	90	GLY	2.5
1	E	235	HIS	2.5
1	C	410	GLY	2.5
1	E	88	PRO	2.4
1	B	412	ALA	2.4
1	F	236	HIS	2.4
1	E	412	ALA	2.4
1	E	63	CYS	2.4
1	C	82	ARG	2.4
1	F	85	GLY	2.4
1	D	411	THR	2.4
1	B	241	LEU	2.3
1	B	362	GLU	2.3
1	E	411	THR	2.3
1	C	88	PRO	2.3
1	A	88	PRO	2.2
1	B	414	ARG	2.2
1	E	237	VAL	2.2
1	C	77	LYS	2.2
1	B	232	LEU	2.2
1	D	445	ILE	2.2
1	D	184	GLU	2.2
1	F	362	GLU	2.2
1	A	410	GLY	2.2
1	B	413	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	413	ASN	2.2
1	E	140	ARG	2.1
1	B	79	LEU	2.1
1	E	423	HIS	2.1
1	E	90	GLY	2.1
1	B	218	ALA	2.1
1	C	237	VAL	2.0
1	E	172	PHE	2.0
1	F	79	LEU	2.0
1	F	409	GLY	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](#)

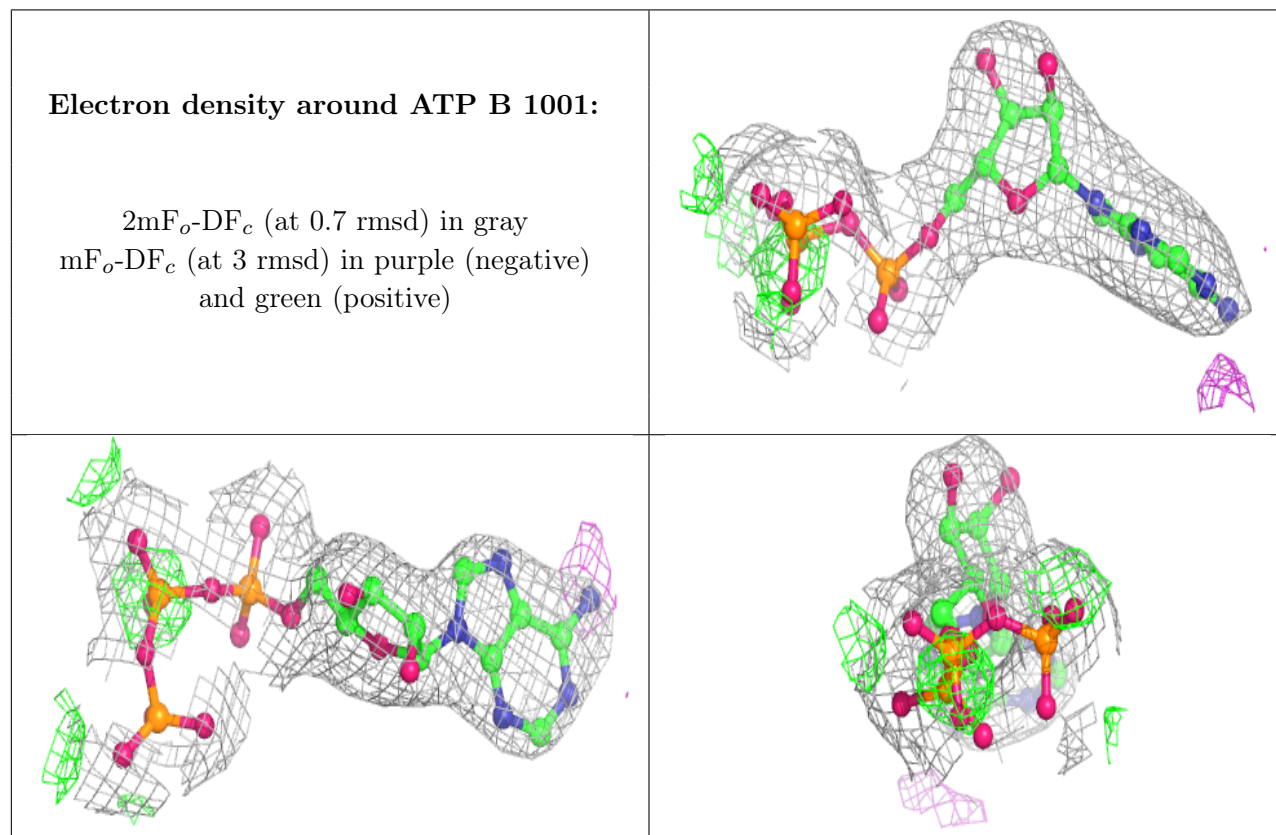
There are no monosaccharides in this entry.

## 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.

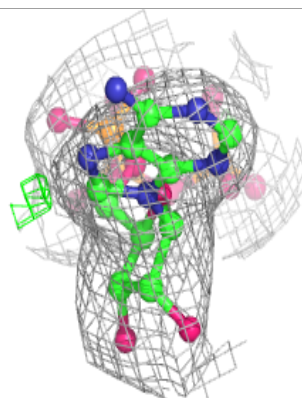
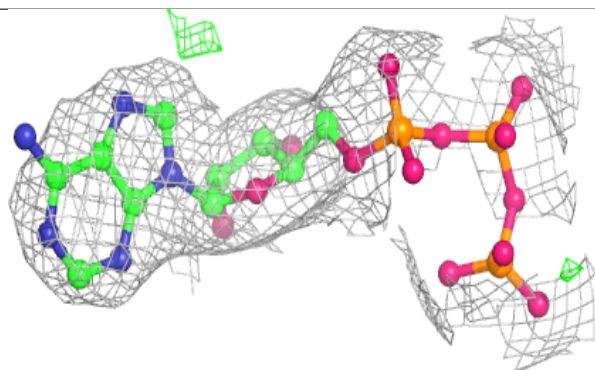
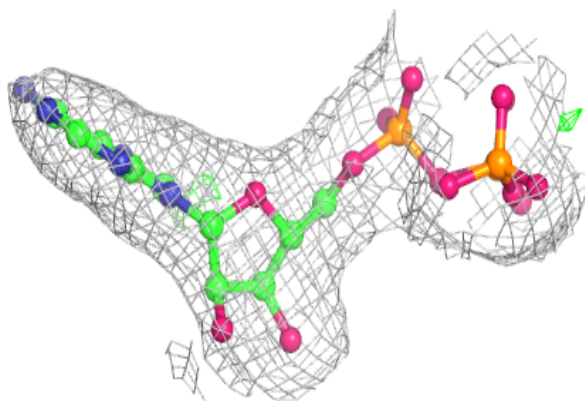
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ATP	B	1001	31/31	0.96	0.19	41,51,64,84	0
2	ATP	C	1001	31/31	0.96	0.17	51,65,77,87	0
2	ATP	E	1001	31/31	0.96	0.17	48,63,73,89	0
3	MG	E	1002	1/1	0.96	0.11	54,54,54,54	0
2	ATP	A	1001	31/31	0.97	0.16	39,50,67,75	0
2	ATP	F	1001	31/31	0.97	0.18	44,53,65,72	0
3	MG	A	1002	1/1	0.97	0.17	55,55,55,55	0
3	MG	B	1002	1/1	0.97	0.16	48,48,48,48	0
2	ATP	D	1001	31/31	0.97	0.16	40,51,64,69	0
3	MG	F	1002	1/1	0.97	0.16	49,49,49,49	0
3	MG	C	1002	1/1	0.98	0.15	49,49,49,49	0
3	MG	D	1002	1/1	0.98	0.17	48,48,48,48	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.

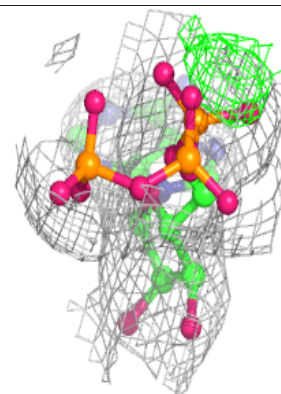
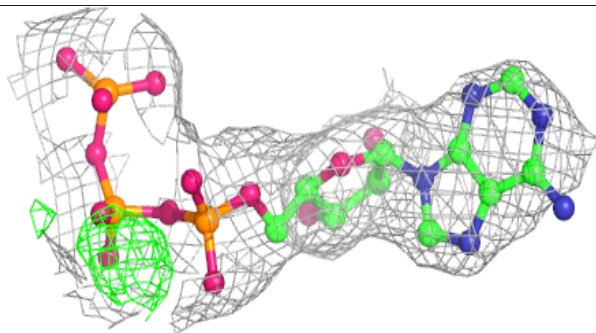
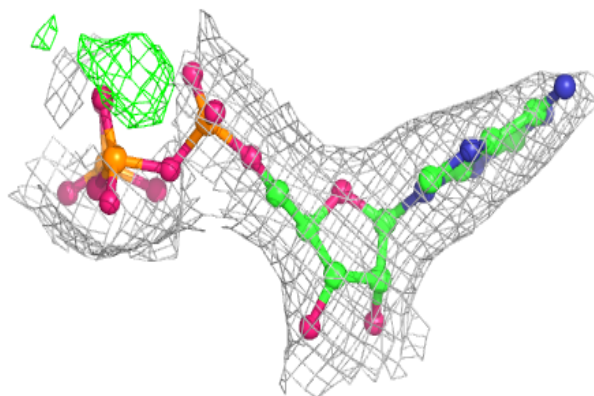


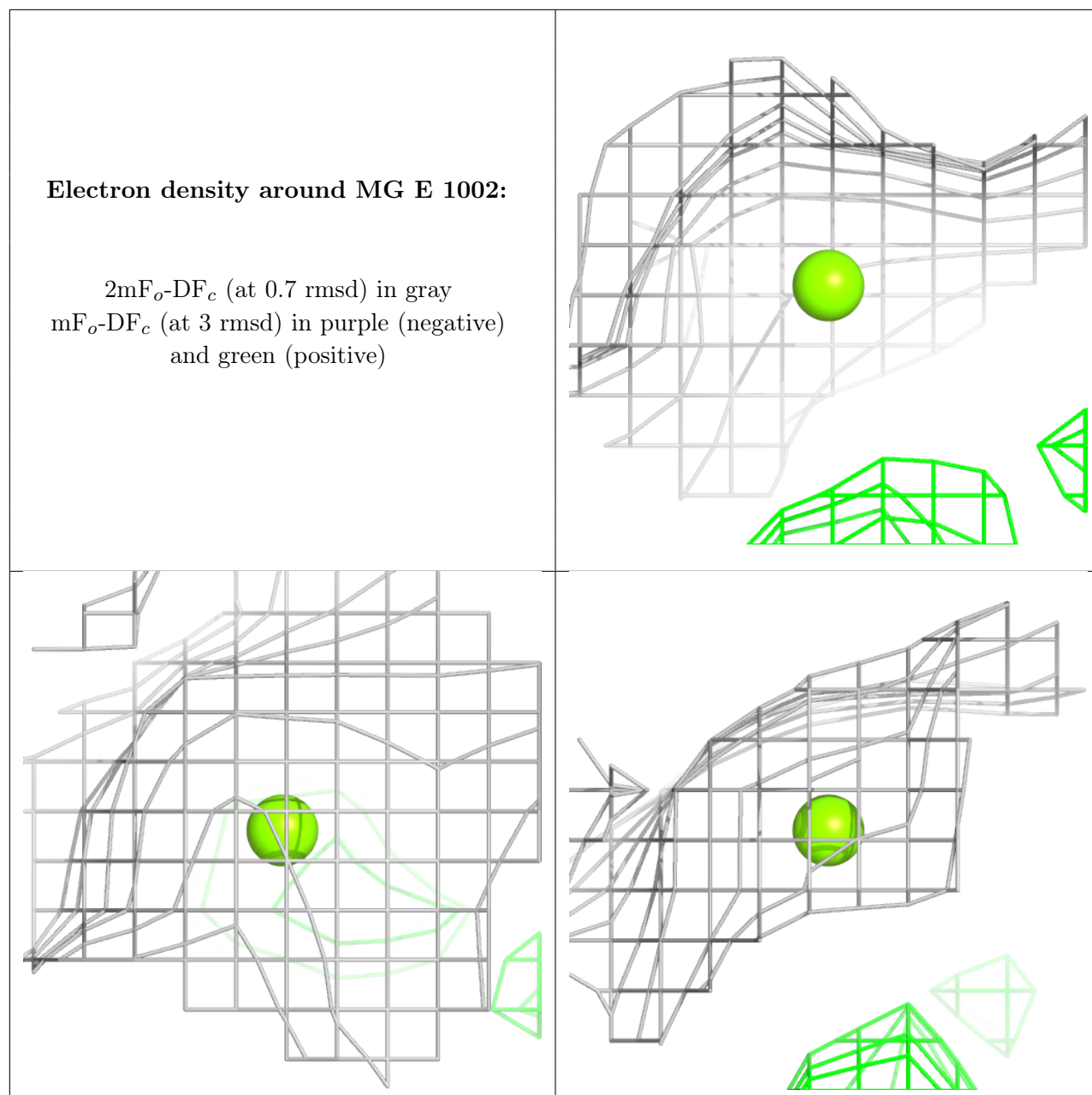
**Electron density around ATP C 1001:**

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

**Electron density around ATP E 1001:**

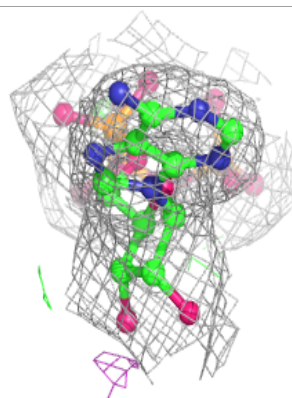
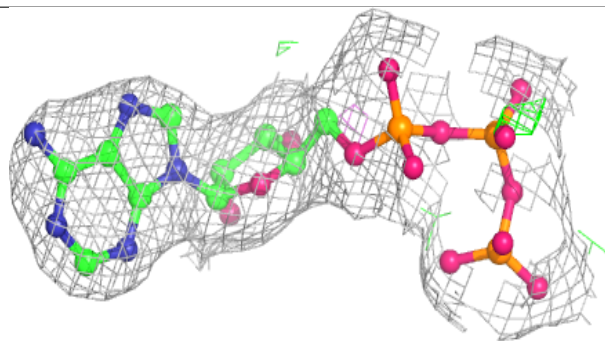
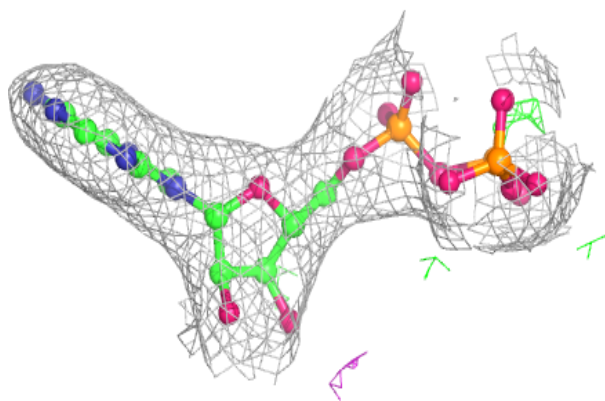
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



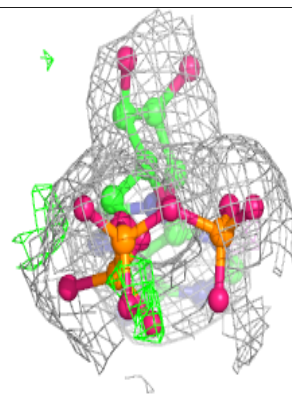
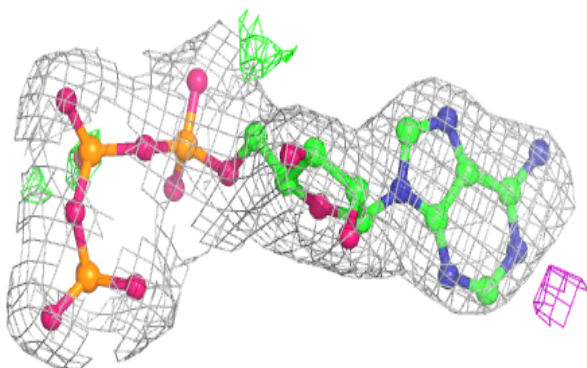
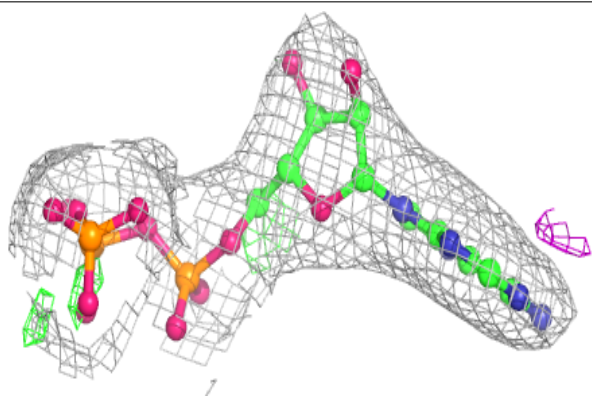


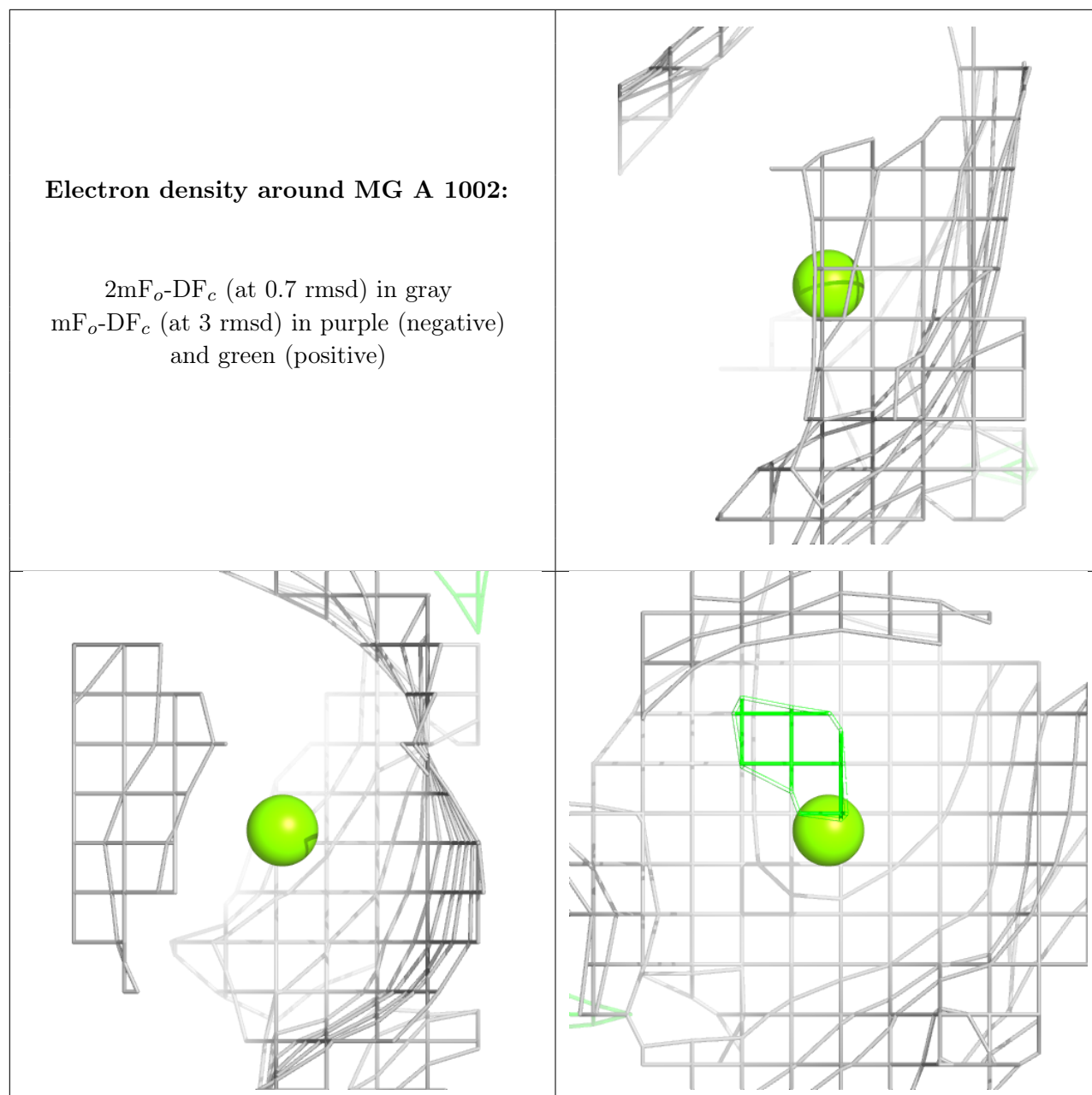
**Electron density around ATP A 1001:**

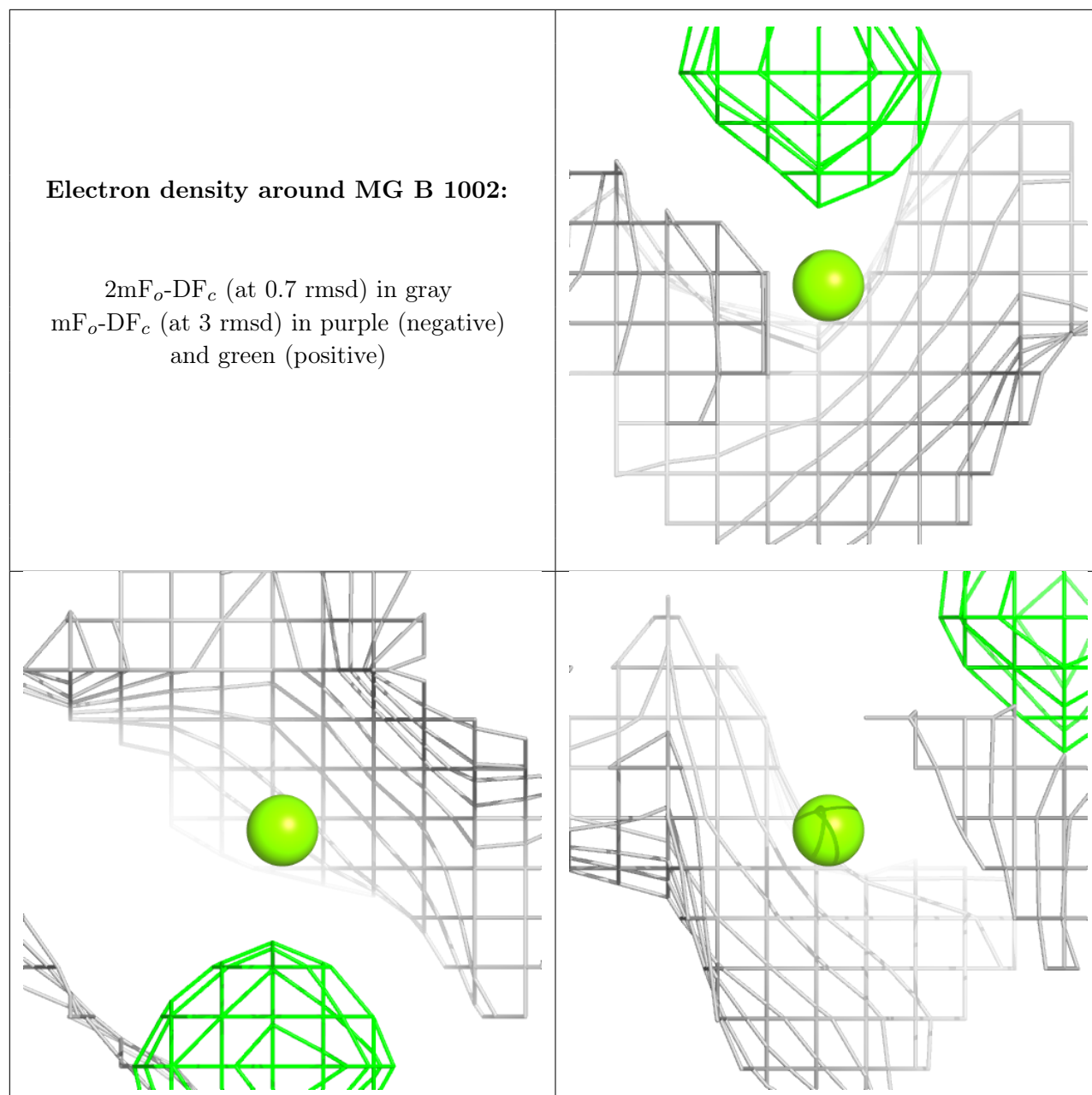
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ATP F 1001:**

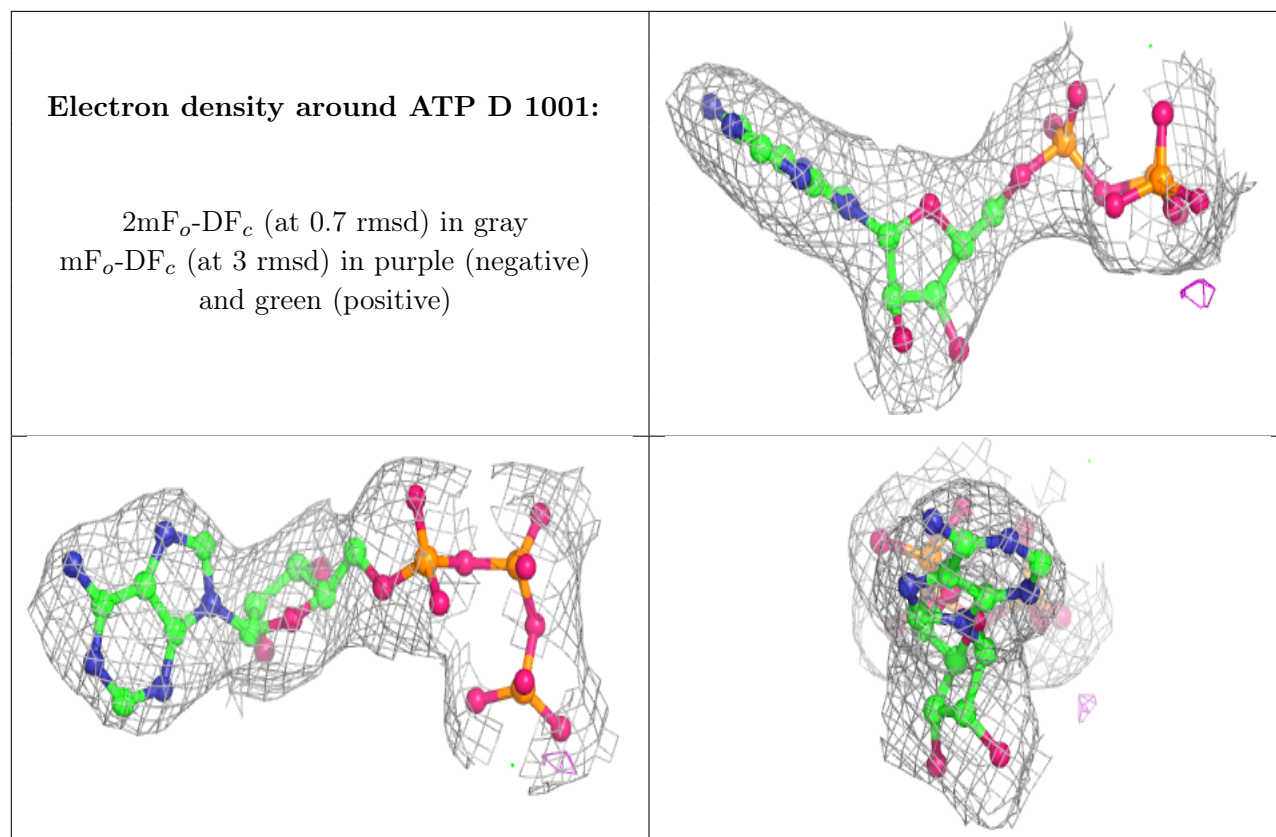
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

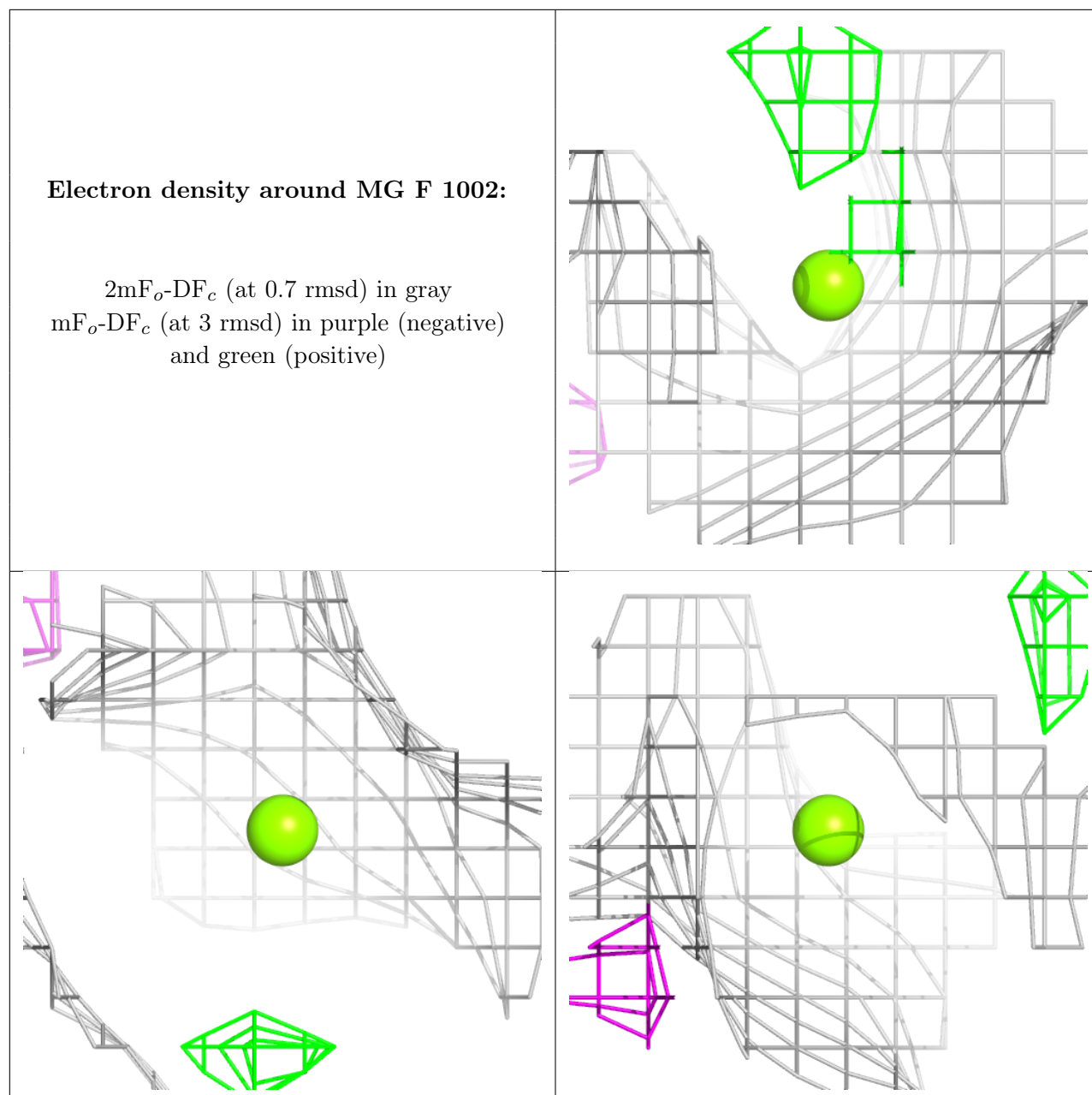


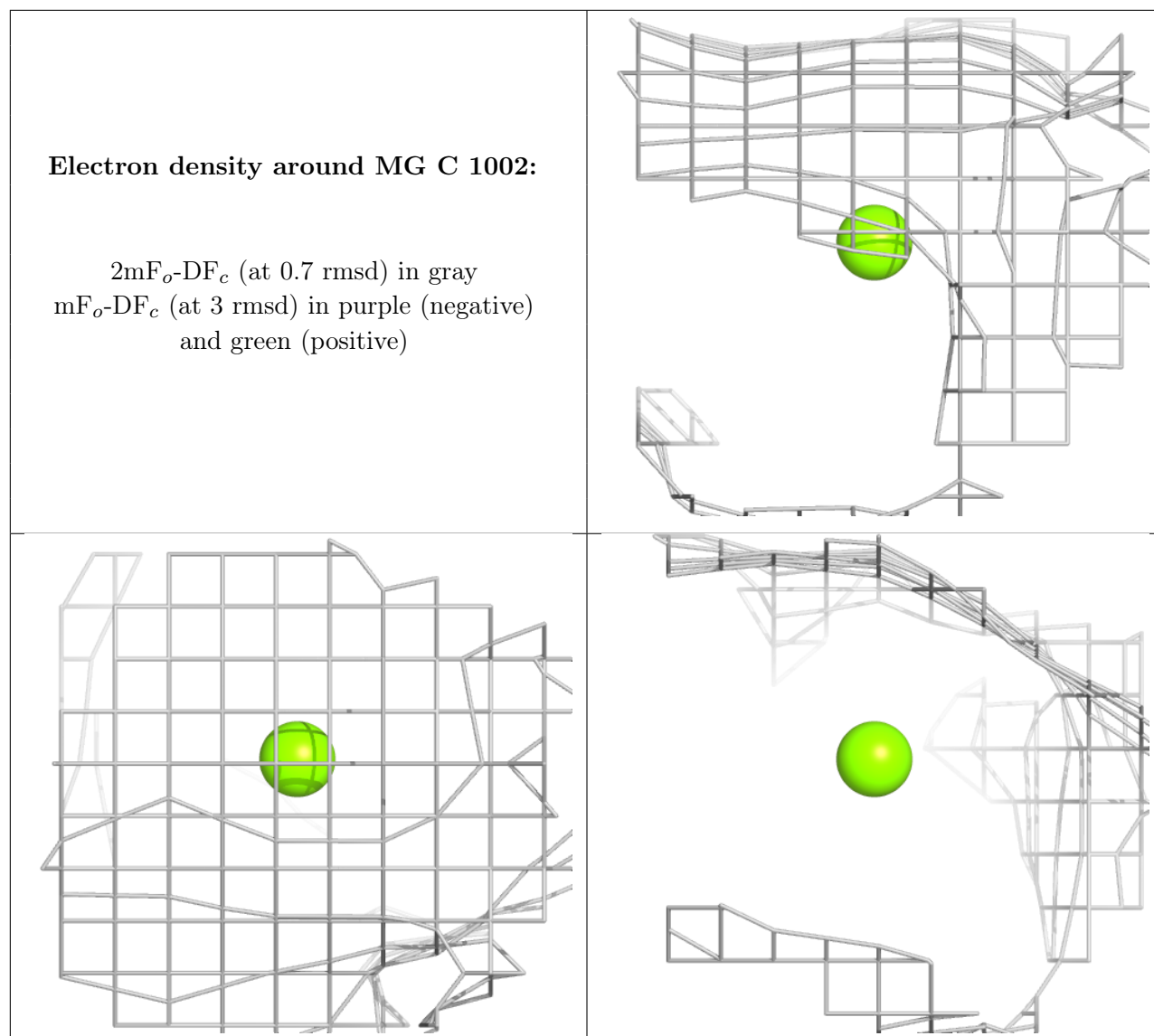


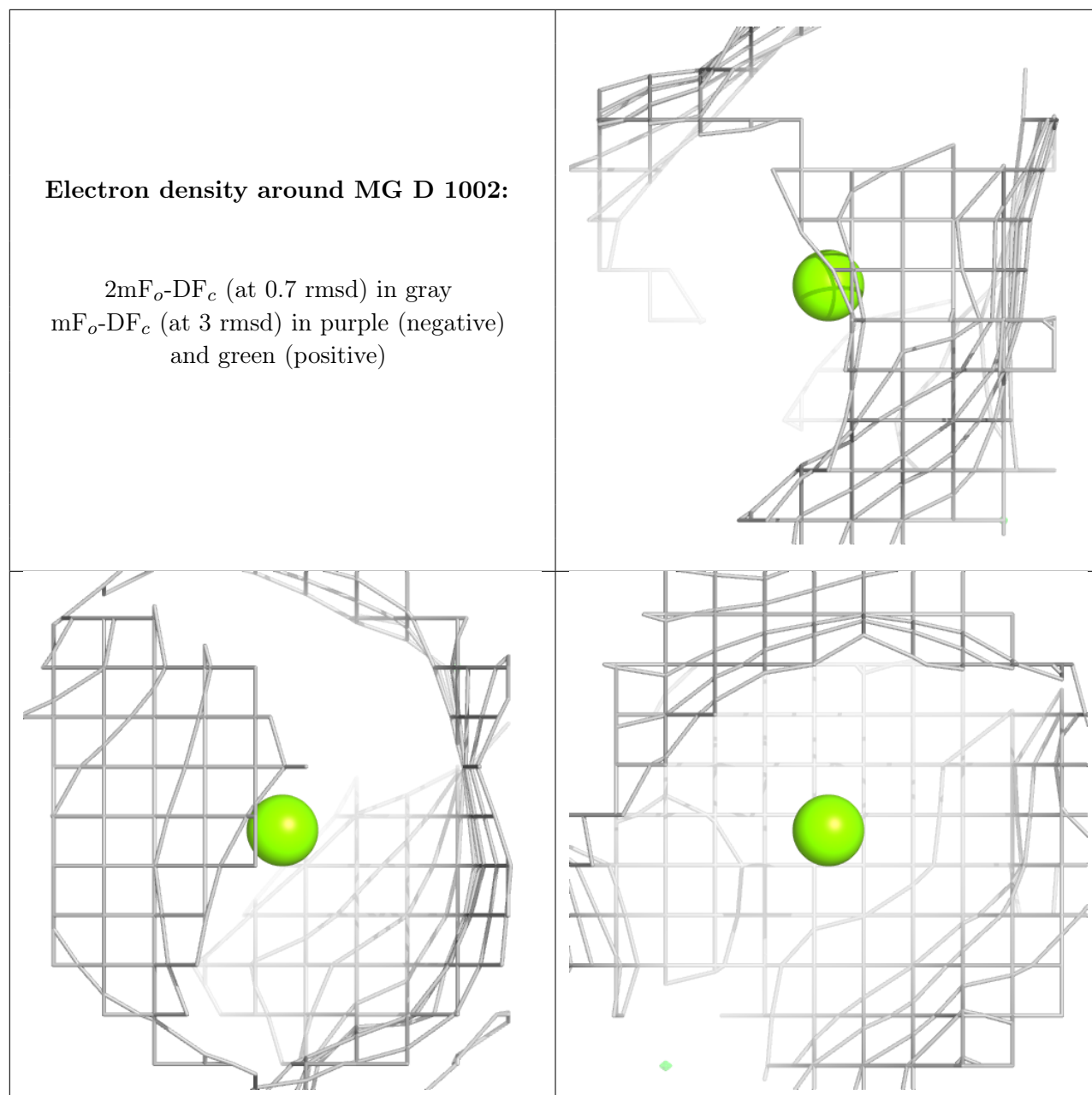












## 6.5 Other polymers [i](#)

There are no such residues in this entry.