



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:07 AM UTC

PDB ID : 8PML / pdb_00008pml
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

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:

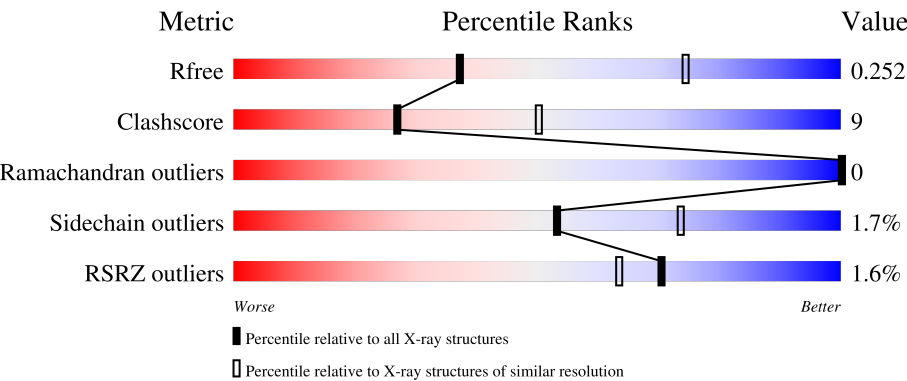
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 $\leq 5\%$. 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	0% 80%17%.
1	B	413	0% 76%20%..
1	C	413	2% 76%20%... .
1	D	413	2% 82%15%. .
1	E	413	2% 77%19%..

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Mol	Chain	Length	Quality of chain
1	F	413	% 77% 19% ..

2 Entry composition [i](#)

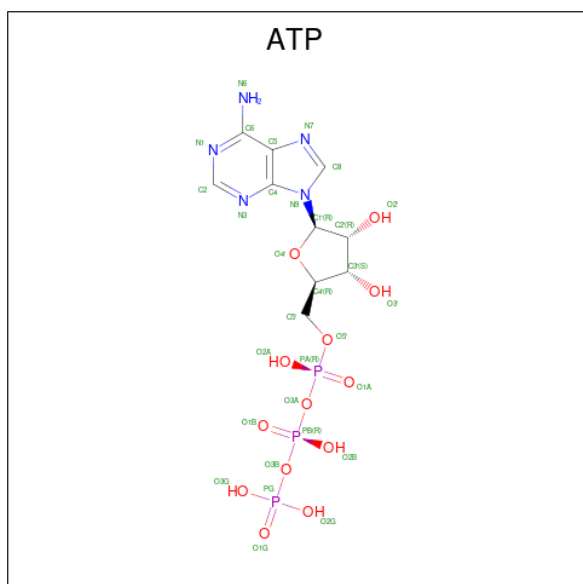
There are 3 unique types of molecules in this entry. The entry contains 18777 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	401	Total	C	N	O	S	0	0	0
			3090	1958	542	578	12			
1	B	402	Total	C	N	O	S	0	0	0
			3099	1963	543	581	12			
1	C	402	Total	C	N	O	S	0	0	0
			3099	1963	543	581	12			
1	D	402	Total	C	N	O	S	0	0	0
			3099	1963	543	581	12			
1	E	402	Total	C	N	O	S	0	0	0
			3099	1963	543	581	12			
1	F	402	Total	C	N	O	S	0	0	0
			3099	1963	543	581	12			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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		

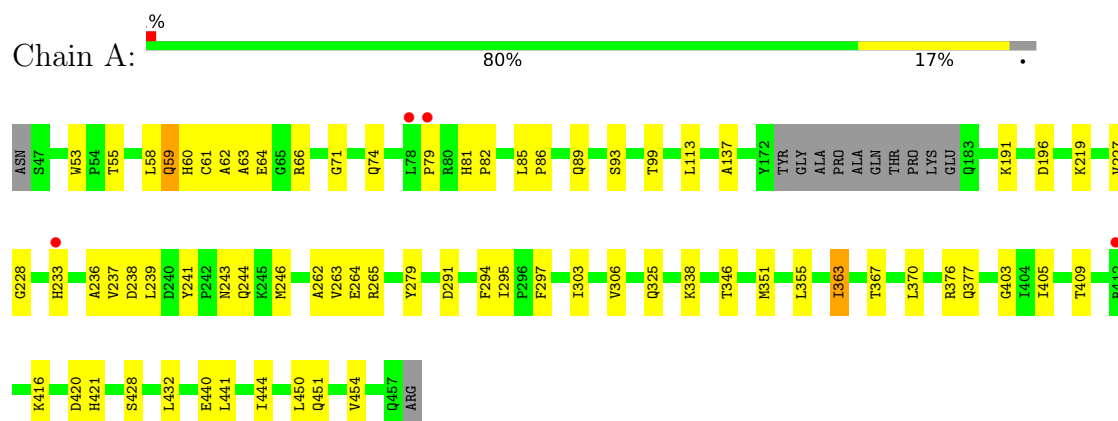
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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		

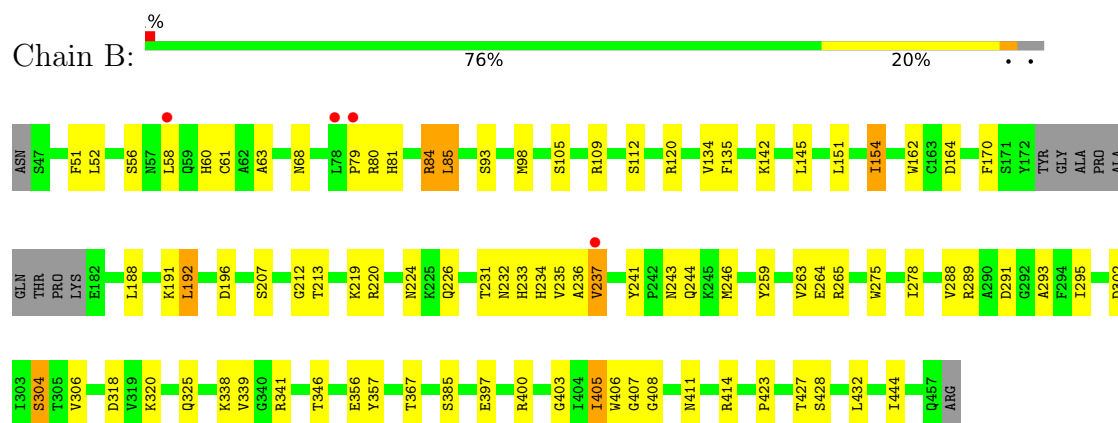
3 Residue-property plots

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.

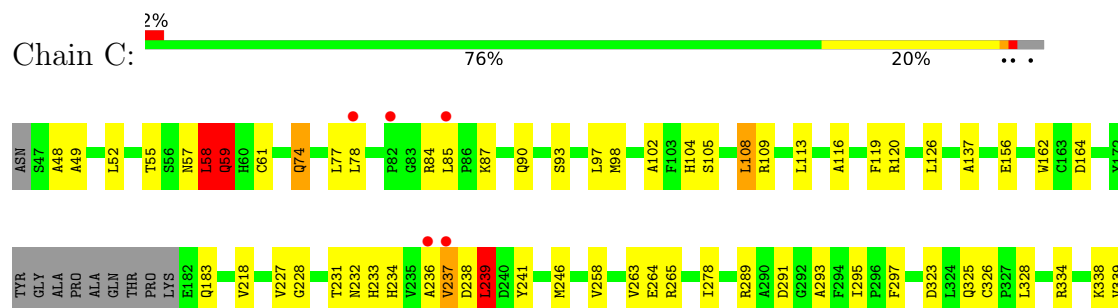
• Molecule 1: Protein NARROW LEAF 1



• Molecule 1: Protein NARROW LEAF 1

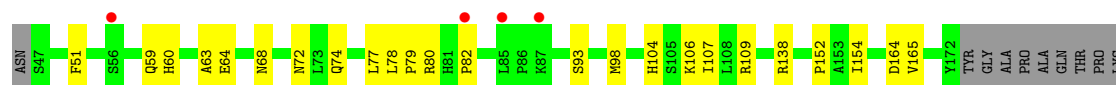
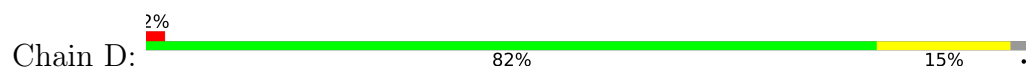


• Molecule 1: Protein NARROW LEAF 1

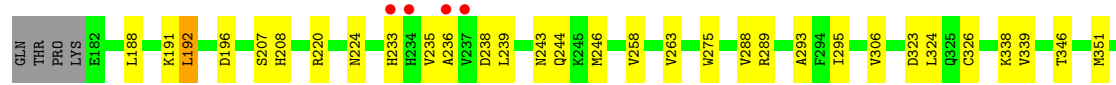
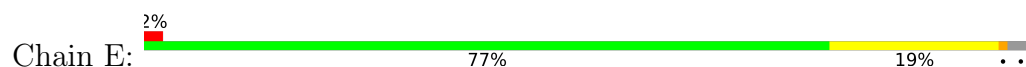




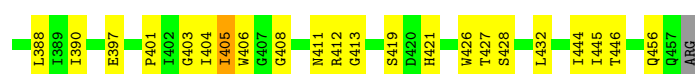
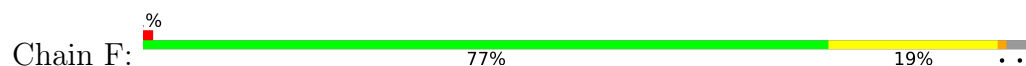
● Molecule 1: Protein NARROW LEAF 1



● 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, α , β , γ	175.43Å 193.36Å 84.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.95 87.71 – 2.95	Depositor EDS
% Data completeness (in resolution range)	77.4 (87.71-2.95) 77.6 (87.71-2.95)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.21rc1_4903	Depositor
R, R_{free}	0.205 , 0.252 0.205 , 0.252	Depositor DCC
R_{free} test set	2269 reflections (3.71%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18777	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	0/3157	0.57	0/4285
1	B	0.27	1/3166 (0.0%)	0.56	1/4297 (0.0%)
1	C	0.25	0/3166	0.64	7/4297 (0.2%)
1	D	0.24	0/3166	0.56	0/4297
1	E	0.25	0/3166	0.65	9/4297 (0.2%)
1	F	0.26	0/3166	0.56	2/4297 (0.0%)
All	All	0.25	1/18987 (0.0%)	0.59	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	84	ARG	CB-CG	5.46	1.68	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	75	LYS	CA-C-N	8.04	137.16	121.41
1	E	75	LYS	C-N-CA	8.04	137.16	121.41
1	C	59	GLN	N-CA-C	6.76	125.21	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	78	LEU	N-CA-C	6.75	124.72	109.81
1	C	58	LEU	CA-C-N	6.72	134.37	121.54
1	C	58	LEU	C-N-CA	6.72	134.37	121.54
1	E	79	PRO	CA-C-N	6.53	131.04	121.31
1	E	79	PRO	C-N-CA	6.53	131.04	121.31
1	C	239	LEU	CB-CG-CD1	-6.42	91.43	110.70
1	C	74	GLN	CA-CB-CG	5.85	125.81	114.10
1	B	84	ARG	CB-CG-CD	5.84	124.73	111.30
1	F	83	GLY	N-CA-C	5.68	126.65	113.18
1	C	237	VAL	CA-C-N	5.67	132.55	121.66
1	C	237	VAL	C-N-CA	5.67	132.55	121.66
1	E	76	GLY	CA-C-N	5.51	132.06	121.54
1	E	76	GLY	C-N-CA	5.51	132.06	121.54
1	F	239	LEU	CB-CG-CD2	-5.34	94.67	110.70
1	E	78	LEU	CA-C-N	5.01	126.11	119.84
1	E	78	LEU	C-N-CA	5.01	126.11	119.84

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	LEU	Peptide
1	A	59	GLN	Peptide
1	A	79	PRO	Peptide
1	C	239	LEU	Peptide
1	C	58	LEU	Peptide
1	C	59	GLN	Peptide
1	C	84	ARG	Peptide
1	E	77	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	45	0
1	B	3099	0	3062	75	0
1	C	3099	0	3062	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3099	0	3062	46	0
1	E	3099	0	3062	65	0
1	F	3099	0	3062	68	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	344	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 (344) 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:105:SER:HB2	1:B:109:ARG:HH12	1.29	0.94
1:E:238:ASP:OD2	1:E:243:ASN:HB2	1.72	0.88
1:F:232:ASN:HD21	1:F:385:SER:HB2	1.37	0.87
1:B:105:SER:HB2	1:B:109:ARG:NH1	1.92	0.85
1:A:238:ASP:OD1	1:A:243:ASN:N	2.08	0.84
1:A:236:ALA:HB1	1:A:263:VAL:HG21	1.61	0.83
1:B:81:HIS:CE1	1:B:84:ARG:HA	2.14	0.82
1:A:61:CYS:HA	1:A:64:GLU:HB3	1.61	0.82
1:A:60:HIS:O	1:A:64:GLU:N	2.11	0.81
1:B:232:ASN:HD21	1:B:385:SER:HB2	1.49	0.78
1:C:234:HIS:NE2	1:C:291:ASP:OD2	2.17	0.77
1:B:81:HIS:ND1	1:B:81:HIS:O	2.17	0.77
1:D:264:GLU:HG2	1:D:265:ARG:HG3	1.65	0.76
1:F:232:ASN:HB2	1:F:291:ASP:HB3	1.66	0.75
1:F:224:ASN:HD21	1:F:226:GLN:HG2	1.50	0.74
1:C:105:SER:O	1:C:109:ARG:HG2	1.88	0.74
1:E:208:HIS:HB2	1:E:243:ASN:OD1	1.87	0.74
1:B:408:GLY:O	1:B:411:ASN:ND2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:LEU:HD12	1:E:370:LEU:HD12	1.67	0.74
1:D:224:ASN:HD21	1:D:226:GLN:HG2	1.51	0.74
1:C:237:VAL:HG21	1:F:239:LEU:HD22	1.70	0.74
1:B:224:ASN:HD21	1:B:226:GLN:HG2	1.51	0.74
1:A:264:GLU:HG2	1:A:265:ARG:HG3	1.71	0.71
1:E:207:SER:HB2	1:E:243:ASN:HB3	1.71	0.71
1:A:238:ASP:CG	1:A:243:ASN:H	1.99	0.71
1:B:207:SER:HB2	1:B:243:ASN:HB2	1.72	0.71
1:E:70:PHE:HA	1:E:73:LEU:HD12	1.71	0.71
1:A:81:HIS:CG	1:A:82:PRO:HD2	2.26	0.70
1:D:220:ARG:NH2	1:D:224:ASN:OD1	2.25	0.70
1:B:232:ASN:O	1:B:235:VAL:HG12	1.91	0.70
1:B:259:TYR:OH	1:E:59:GLN:NE2	2.25	0.69
1:F:59:GLN:OE1	1:F:61:CYS:N	2.25	0.69
1:F:412:ARG:HB2	1:F:426:TRP:O	1.91	0.69
1:E:153:ALA:HA	1:E:165:VAL:HB	1.74	0.69
1:B:320:LYS:HD2	1:B:400:ARG:HH21	1.56	0.69
1:A:355:LEU:HD12	1:A:370:LEU:HD12	1.73	0.69
1:A:59:GLN:O	1:A:61:CYS:N	2.26	0.68
1:C:376:ARG:HD2	1:C:421:HIS:CD2	2.29	0.68
1:B:241:TYR:OH	1:E:359:ASP:OD2	2.07	0.68
1:B:264:GLU:HG2	1:B:265:ARG:HG3	1.76	0.68
1:B:60:HIS:HA	1:B:63:ALA:HB3	1.76	0.67
1:A:306:VAL:HG23	1:A:450:LEU:HD21	1.75	0.67
1:C:264:GLU:HG2	1:C:265:ARG:HG3	1.75	0.67
1:B:109:ARG:NH1	1:B:356:GLU:OE2	2.28	0.67
1:F:264:GLU:HG2	1:F:265:ARG:HG3	1.76	0.66
1:D:418:THR:H	1:D:421:HIS:CE1	2.14	0.66
1:E:367:THR:HG21	1:E:428:SER:HB3	1.78	0.66
1:D:98:MET:HE2	1:D:278:ILE:HD11	1.77	0.65
1:D:367:THR:HG21	1:D:428:SER:HB3	1.79	0.65
1:A:86:PRO:HD2	1:A:89:GLN:NE2	2.12	0.65
1:F:367:THR:HG21	1:F:428:SER:HB3	1.80	0.64
1:F:232:ASN:ND2	1:F:385:SER:HB2	2.09	0.64
1:C:233:HIS:HB3	1:C:293:ALA:HB2	1.80	0.64
1:C:233:HIS:O	1:C:237:VAL:HG23	1.98	0.64
1:F:80:ARG:HE	1:F:156:GLU:CD	2.05	0.64
1:B:81:HIS:CE1	1:B:84:ARG:HD3	2.33	0.63
1:B:232:ASN:HB2	1:B:291:ASP:HB3	1.80	0.63
1:D:417:LEU:H	1:D:421:HIS:HE1	1.46	0.63
1:A:420:ASP:OD1	1:A:421:HIS:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:HIS:CE1	1:F:239:LEU:HD13	2.33	0.63
1:A:376:ARG:HD2	1:A:421:HIS:CE1	2.34	0.63
1:C:57:ASN:HB2	1:C:59:GLN:HG3	1.79	0.63
1:D:412:ARG:NH1	1:D:426:TRP:O	2.32	0.63
1:C:233:HIS:HE1	1:F:239:LEU:HD13	1.63	0.62
1:E:409:THR:O	1:E:412:ARG:NH1	2.32	0.62
1:B:120:ARG:HH21	1:B:164:ASP:HB3	1.63	0.62
1:F:408:GLY:N	1:F:411:ASN:OD1	2.24	0.62
1:F:80:ARG:NE	1:F:156:GLU:OE1	2.30	0.61
1:F:224:ASN:ND2	1:F:226:GLN:HG2	2.15	0.61
1:B:408:GLY:N	1:B:411:ASN:OD1	2.27	0.61
1:E:69:TYR:O	1:E:73:LEU:HG	1.99	0.61
1:C:414:ARG:HB3	1:C:423:PRO:HB2	1.81	0.61
1:F:212:GLY:HA2	1:F:341:ARG:HH21	1.66	0.61
1:E:86:PRO:HD2	1:E:89:GLN:NE2	2.16	0.61
1:B:237:VAL:HG21	1:E:239:LEU:HG	1.82	0.60
1:D:60:HIS:CD2	1:D:64:GLU:HB2	2.37	0.60
1:A:81:HIS:CD2	1:A:82:PRO:HD2	2.36	0.60
1:C:234:HIS:NE2	1:C:407:GLY:O	2.35	0.60
1:B:289:ARG:HH22	1:B:357:TYR:HD2	1.48	0.59
1:A:233:HIS:ND1	1:A:291:ASP:OD1	2.35	0.59
1:B:367:THR:HG21	1:B:428:SER:HB3	1.84	0.59
1:C:237:VAL:HG21	1:F:239:LEU:CD2	2.32	0.59
1:E:98:MET:HE1	1:E:324:LEU:HD22	1.82	0.59
1:C:120:ARG:HH21	1:C:164:ASP:HB3	1.67	0.59
1:C:246:MET:HG3	1:C:295:ILE:HG12	1.85	0.59
1:B:224:ASN:ND2	1:B:226:GLN:HG2	2.16	0.59
1:F:246:MET:HG3	1:F:295:ILE:HG12	1.85	0.59
1:D:403:GLY:HA2	1:D:432:LEU:HB2	1.85	0.58
1:E:122:ARG:NH1	2:E:1001:ATP:O1B	2.36	0.58
1:B:85:LEU:HD12	1:B:162:TRP:CD1	2.39	0.58
1:D:289:ARG:HD3	1:D:406:TRP:CZ2	2.39	0.58
1:B:98:MET:HE2	1:B:278:ILE:HD11	1.86	0.58
1:E:238:ASP:OD2	1:E:243:ASN:CB	2.48	0.57
1:D:224:ASN:ND2	1:D:226:GLN:HG2	2.18	0.57
1:F:403:GLY:HA2	1:F:432:LEU:HB2	1.86	0.57
1:F:204:GLN:NE2	1:F:249:PRO:O	2.30	0.56
1:C:234:HIS:CD2	1:C:407:GLY:O	2.58	0.56
1:C:363:ILE:HD12	1:F:241:TYR:CE2	2.39	0.56
1:F:120:ARG:HH21	1:F:164:ASP:HB3	1.69	0.56
1:C:238:ASP:HB3	1:C:239:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:HIS:CG	1:D:241:TYR:HE2	2.23	0.56
1:B:212:GLY:HA2	1:B:341:ARG:HH21	1.71	0.56
1:A:403:GLY:HA2	1:A:432:LEU:HB2	1.87	0.56
1:E:238:ASP:C	1:E:239:LEU:HD22	2.31	0.56
1:E:403:GLY:HA2	1:E:432:LEU:HB2	1.87	0.56
1:B:241:TYR:CE2	1:E:361:LYS:HD2	2.41	0.56
1:B:403:GLY:HA2	1:B:432:LEU:HB2	1.87	0.56
1:E:289:ARG:NH1	1:E:367:THR:OG1	2.36	0.55
1:A:53:TRP:O	1:A:55:THR:HG23	2.06	0.55
1:A:303:ILE:O	1:A:306:VAL:HG22	2.07	0.55
1:D:208:HIS:CG	1:D:241:TYR:CE2	2.94	0.55
1:B:81:HIS:NE2	1:B:85:LEU:HD22	2.22	0.54
1:C:119:PHE:HB2	1:C:126:LEU:HD22	1.88	0.54
1:E:409:THR:HG22	1:E:412:ARG:HH12	1.72	0.54
1:E:207:SER:CB	1:E:243:ASN:HB3	2.36	0.54
1:F:212:GLY:HA2	1:F:341:ARG:NH2	2.23	0.54
1:A:363:ILE:HG13	1:D:241:TYR:OH	2.07	0.54
1:C:98:MET:HE2	1:C:278:ILE:HD11	1.89	0.54
1:E:78:LEU:C	1:E:80:ARG:H	2.15	0.54
1:C:52:LEU:HB2	1:F:52:LEU:HB2	1.90	0.54
1:E:289:ARG:HH22	1:E:357:TYR:HD2	1.56	0.54
1:C:109:ARG:HH12	1:C:358:ASN:HD22	1.55	0.54
1:A:241:TYR:OH	1:D:359:ASP:OD2	2.20	0.53
1:D:208:HIS:CD2	1:D:241:TYR:HE2	2.26	0.53
1:C:109:ARG:NH1	1:C:358:ASN:HD22	2.06	0.53
1:E:338:LYS:HE3	1:E:346:THR:OG1	2.08	0.53
1:F:93:SER:HB2	1:F:325:GLN:HA	1.90	0.53
1:C:361:LYS:HB2	1:F:241:TYR:OH	2.09	0.53
1:E:450:LEU:O	1:E:454:VAL:HG13	2.09	0.53
1:B:236:ALA:HB1	1:B:263:VAL:HG21	1.91	0.52
1:B:241:TYR:CZ	1:E:361:LYS:HD2	2.45	0.52
1:E:119:PHE:HB2	1:E:126:LEU:HD22	1.91	0.52
1:F:85:LEU:HD12	1:F:89:GLN:NE2	2.24	0.52
1:E:414:ARG:HB3	1:E:423:PRO:HB2	1.91	0.52
1:A:191:LYS:HB3	1:A:196:ASP:HB2	1.92	0.52
1:E:191:LYS:HB3	1:E:196:ASP:HB2	1.91	0.52
1:B:81:HIS:HE1	1:B:84:ARG:CG	2.23	0.52
1:D:93:SER:HB2	1:D:325:GLN:HA	1.91	0.52
1:E:120:ARG:HH21	1:E:164:ASP:HB3	1.74	0.52
1:C:113:LEU:HD11	1:C:137:ALA:HB2	1.92	0.52
1:F:408:GLY:O	1:F:411:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD12	1:A:89:GLN:NE2	2.25	0.51
1:C:57:ASN:HB2	1:C:59:GLN:CG	2.39	0.51
1:D:385:SER:HB3	1:D:407:GLY:HA2	1.92	0.51
1:E:153:ALA:O	1:E:154:ILE:HG12	2.10	0.51
1:A:367:THR:HG21	1:A:428:SER:HB2	1.91	0.51
1:F:172:TYR:HA	1:F:413:GLY:HA3	1.92	0.51
1:F:289:ARG:HD3	1:F:406:TRP:CZ2	2.45	0.51
1:C:97:LEU:HD21	1:C:328:LEU:HD11	1.92	0.51
1:D:187:GLU:HG2	1:F:419:SER:OG	2.10	0.51
1:D:289:ARG:NH1	1:D:367:THR:OG1	2.41	0.51
1:D:289:ARG:HH11	1:D:367:THR:HG1	1.59	0.51
1:B:212:GLY:C	1:B:341:ARG:HE	2.19	0.51
1:C:236:ALA:HB1	1:C:263:VAL:HG21	1.91	0.51
1:C:233:HIS:CE1	1:F:239:LEU:CD1	2.95	0.50
1:D:451:GLN:O	1:D:455:GLN:HG2	2.11	0.50
1:C:334:ARG:HG2	1:C:391:LEU:HD22	1.93	0.50
1:D:236:ALA:HB2	1:D:263:VAL:HG21	1.93	0.50
1:A:239:LEU:HD11	1:D:234:HIS:CD2	2.47	0.50
1:F:231:THR:O	1:F:293:ALA:N	2.45	0.50
1:B:85:LEU:HD12	1:B:162:TRP:CG	2.47	0.49
1:C:238:ASP:O	1:C:239:LEU:HB2	2.11	0.49
1:D:68:ASN:OD1	1:D:72:ASN:ND2	2.45	0.49
1:B:51:PHE:HE2	1:E:53:TRP:CD2	2.30	0.49
1:B:231:THR:O	1:B:293:ALA:N	2.45	0.49
1:F:238:ASP:HB2	1:F:241:TYR:O	2.12	0.49
1:B:220:ARG:HH22	1:B:226:GLN:HG3	1.77	0.49
1:F:338:LYS:HD3	1:F:405:ILE:HD11	1.95	0.49
1:B:154:ILE:HD12	1:B:164:ASP:HA	1.93	0.49
1:B:56:SER:HB3	1:E:49:ALA:HA	1.95	0.49
1:D:417:LEU:HB2	1:D:421:HIS:CE1	2.48	0.49
1:F:233:HIS:O	1:F:237:VAL:HG23	2.12	0.49
1:B:233:HIS:CD2	1:E:239:LEU:HD12	2.48	0.49
1:B:405:ILE:HD13	1:B:427:THR:HG21	1.95	0.49
1:C:93:SER:HB2	1:C:325:GLN:HA	1.95	0.49
1:F:233:HIS:CE1	1:F:291:ASP:HA	2.48	0.49
1:F:275:TRP:CD1	1:F:288:VAL:HG11	2.48	0.49
1:C:241:TYR:CE2	1:F:363:ILE:HD12	2.48	0.49
1:B:275:TRP:CD1	1:B:288:VAL:HG11	2.48	0.48
1:C:74:GLN:HA	1:C:77:LEU:CD1	2.43	0.48
1:C:338:LYS:HG2	1:C:339:VAL:N	2.28	0.48
1:E:188:LEU:O	1:E:192:LEU:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:LEU:HD22	1:E:239:LEU:N	2.28	0.48
1:F:237:VAL:HG12	1:F:238:ASP:H	1.78	0.48
1:B:397:GLU:OE1	1:B:397:GLU:N	2.40	0.48
1:C:58:LEU:HD23	1:C:61:CYS:SG	2.54	0.48
1:F:212:GLY:C	1:F:341:ARG:HE	2.22	0.48
1:B:58:LEU:HG	1:B:61:CYS:HB3	1.96	0.48
1:B:263:VAL:HA	1:B:295:ILE:HG13	1.96	0.48
1:D:74:GLN:O	1:D:77:LEU:HG	2.14	0.48
1:D:106:LYS:HA	1:D:109:ARG:HG2	1.96	0.48
1:E:74:GLN:C	1:E:76:GLY:H	2.22	0.48
1:F:338:LYS:HG2	1:F:339:VAL:N	2.29	0.48
1:B:188:LEU:O	1:B:192:LEU:HD13	2.14	0.47
1:C:48:ALA:HB3	1:F:55:THR:OG1	2.14	0.47
1:C:104:HIS:O	1:C:108:LEU:HB2	2.13	0.47
1:E:338:LYS:HG2	1:E:339:VAL:N	2.29	0.47
1:B:246:MET:HG3	1:B:295:ILE:HG12	1.95	0.47
1:A:306:VAL:CG2	1:A:450:LEU:HD21	2.44	0.47
1:B:338:LYS:HD3	1:B:405:ILE:CD1	2.44	0.47
1:A:265:ARG:NH2	1:A:440:GLU:OE1	2.48	0.47
1:B:244:GLN:O	1:B:263:VAL:HG23	2.14	0.47
1:C:450:LEU:O	1:C:454:VAL:HG13	2.15	0.47
1:F:397:GLU:OE1	1:F:397:GLU:N	2.41	0.47
1:E:79:PRO:HB3	1:E:156:GLU:OE2	2.15	0.47
1:C:289:ARG:HH22	1:C:357:TYR:HD2	1.63	0.47
1:F:233:HIS:CE1	1:F:268:SER:HA	2.50	0.46
1:F:289:ARG:HH22	1:F:357:TYR:HD2	1.61	0.46
1:B:85:LEU:HA	1:B:85:LEU:HD13	1.72	0.46
1:D:338:LYS:HD3	1:D:405:ILE:HD11	1.97	0.46
1:B:302:ASP:OD1	1:B:304:SER:OG	2.21	0.46
1:C:323:ASP:HB3	1:C:326:CYS:SG	2.55	0.46
1:E:453:ALA:HA	1:E:456:GLN:HE21	1.81	0.46
1:B:234:HIS:ND1	1:B:407:GLY:O	2.48	0.46
1:F:239:LEU:O	1:F:239:LEU:HG	2.16	0.46
1:A:246:MET:HG3	1:A:295:ILE:HG12	1.96	0.46
1:B:289:ARG:HD3	1:B:406:TRP:CZ2	2.51	0.46
1:C:376:ARG:HD2	1:C:421:HIS:CG	2.50	0.46
1:E:376:ARG:CZ	1:E:421:HIS:ND1	2.79	0.46
1:F:233:HIS:CE1	1:F:291:ASP:CG	2.94	0.46
1:C:85:LEU:HB3	1:C:162:TRP:CD1	2.51	0.46
1:E:146:ASN:OD1	1:E:149:GLN:N	2.45	0.46
1:B:338:LYS:HD3	1:B:405:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:VAL:HG21	1:C:441:LEU:HD13	1.98	0.46
1:C:232:ASN:HD21	1:C:385:SER:HB3	1.81	0.46
1:E:263:VAL:HA	1:E:295:ILE:HG13	1.97	0.46
1:E:451:GLN:O	1:E:454:VAL:HG22	2.16	0.46
1:F:184:MET:HE2	1:F:184:MET:HB2	1.77	0.46
1:F:456:GLN:O	1:F:456:GLN:HG3	2.15	0.46
1:F:220:ARG:HH22	1:F:226:GLN:HG3	1.79	0.46
1:C:397:GLU:OE1	1:C:397:GLU:N	2.40	0.45
1:E:86:PRO:HD2	1:E:89:GLN:HE21	1.81	0.45
1:A:71:GLY:O	1:A:74:GLN:HB3	2.15	0.45
1:E:275:TRP:CD1	1:E:288:VAL:HG11	2.51	0.45
1:F:233:HIS:CD2	1:F:234:HIS:HD2	2.35	0.45
1:F:405:ILE:HD13	1:F:427:THR:HG21	1.99	0.45
1:A:85:LEU:HD12	1:A:89:GLN:HE21	1.82	0.45
1:A:451:GLN:HA	1:A:454:VAL:HG12	1.99	0.45
1:E:89:GLN:O	1:E:161:VAL:HA	2.15	0.45
1:F:135:PHE:HB3	1:F:170:PHE:CB	2.47	0.45
1:A:219:LYS:HB3	1:A:444:ILE:HD11	1.99	0.45
1:D:152:PRO:O	1:D:165:VAL:HB	2.17	0.45
1:B:109:ARG:HA	1:B:112:SER:OG	2.16	0.45
1:D:74:GLN:OE1	1:D:77:LEU:HD11	2.17	0.45
1:F:142:LYS:HA	1:F:145:LEU:HD12	1.98	0.44
1:B:338:LYS:HE3	1:B:346:THR:OG1	2.17	0.44
1:B:414:ARG:HB3	1:B:423:PRO:HB2	1.99	0.44
1:C:87:LYS:HE2	1:C:90:GLN:OE1	2.17	0.44
1:B:142:LYS:HA	1:B:145:LEU:HD12	1.99	0.44
1:D:78:LEU:N	1:D:79:PRO:HD3	2.33	0.44
1:D:395:ASP:OD1	1:D:395:ASP:C	2.60	0.44
1:E:220:ARG:NH2	1:E:224:ASN:HB3	2.33	0.44
1:F:93:SER:HB2	1:F:324:LEU:O	2.17	0.44
1:A:244:GLN:HG2	1:A:262:ALA:HB1	1.98	0.44
1:B:135:PHE:HB3	1:B:170:PHE:CB	2.47	0.44
1:B:318:ASP:O	1:B:400:ARG:HD2	2.18	0.44
1:C:58:LEU:HB3	1:C:61:CYS:SG	2.58	0.44
1:F:445:ILE:HG13	1:F:446:THR:HG23	2.00	0.44
1:E:338:LYS:HD3	1:E:405:ILE:HD11	1.99	0.44
1:E:220:ARG:HH21	1:E:224:ASN:HB3	1.83	0.43
1:F:236:ALA:HB1	1:F:263:VAL:HG21	2.00	0.43
1:C:85:LEU:HD13	1:C:85:LEU:HA	1.84	0.43
1:C:246:MET:HE3	1:C:246:MET:HB3	1.93	0.43
1:E:405:ILE:HD13	1:E:427:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ALA:HA	1:F:56:SER:HB3	2.01	0.43
1:A:294:PHE:HB2	1:A:441:LEU:HD11	2.01	0.43
1:D:60:HIS:CE1	1:D:63:ALA:HB3	2.54	0.43
1:F:390:ILE:HA	1:F:401:PRO:HA	2.00	0.43
1:C:116:ALA:HB2	1:C:355:LEU:HD12	2.01	0.43
1:D:60:HIS:O	1:D:60:HIS:CG	2.71	0.43
1:F:219:LYS:HB3	1:F:444:ILE:HD11	1.99	0.43
1:B:81:HIS:CE1	1:B:84:ARG:CD	3.02	0.43
1:D:107:ILE:HD12	1:D:107:ILE:HA	1.92	0.43
1:E:122:ARG:CZ	2:E:1001:ATP:O1B	2.67	0.43
1:B:105:SER:HB2	1:B:109:ARG:CZ	2.48	0.42
1:D:409:THR:HG22	1:D:410:ALA:N	2.34	0.42
1:E:236:ALA:HB1	1:E:263:VAL:HG21	2.00	0.42
1:A:93:SER:HB2	1:A:325:GLN:HA	2.01	0.42
1:A:338:LYS:HD3	1:A:405:ILE:HD11	2.01	0.42
1:D:59:GLN:HA	1:D:60:HIS:HA	1.77	0.42
1:D:80:ARG:C	1:D:82:PRO:HD2	2.44	0.42
1:B:234:HIS:CE1	1:B:407:GLY:O	2.72	0.42
1:E:236:ALA:CB	1:E:263:VAL:HG21	2.49	0.42
1:A:63:ALA:O	1:A:66:ARG:HB3	2.19	0.42
1:B:338:LYS:HG2	1:B:339:VAL:N	2.32	0.42
1:C:453:ALA:HA	1:C:456:GLN:HE21	1.83	0.42
1:C:74:GLN:HA	1:C:77:LEU:HD11	2.01	0.42
1:E:351:MET:HB2	1:E:370:LEU:HD22	2.01	0.42
1:C:228:GLY:HA2	1:C:297:PHE:CD2	2.54	0.42
1:C:367:THR:HG21	1:C:428:SER:HB3	2.01	0.42
1:A:265:ARG:HA	1:D:51:PHE:O	2.19	0.42
1:D:154:ILE:HD13	1:D:164:ASP:HA	2.02	0.42
1:C:239:LEU:HA	1:C:239:LEU:HD13	1.76	0.42
1:C:338:LYS:HE3	1:C:346:THR:OG1	2.19	0.42
1:D:338:LYS:HE3	1:D:338:LYS:HB3	1.85	0.42
1:E:156:GLU:O	1:E:156:GLU:HG3	2.20	0.42
1:E:244:GLN:O	1:E:263:VAL:HG23	2.20	0.42
1:F:406:TRP:CZ2	1:F:408:GLY:HA3	2.54	0.42
1:B:191:LYS:HB3	1:B:196:ASP:HB2	2.02	0.42
1:C:238:ASP:OD1	1:C:239:LEU:N	2.52	0.42
1:A:228:GLY:HA2	1:A:297:PHE:CD2	2.54	0.41
1:A:351:MET:HB2	1:A:370:LEU:HD22	2.02	0.41
1:B:93:SER:HB2	1:B:325:GLN:HA	2.02	0.41
1:A:113:LEU:HD11	1:A:137:ALA:HB2	2.01	0.41
1:A:451:GLN:O	1:A:454:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.86	0.41
1:C:109:ARG:HH12	1:C:358:ASN:ND2	2.17	0.41
1:D:104:HIS:HB3	1:D:107:ILE:HG22	2.02	0.41
1:C:55:THR:HG1	1:F:47:SER:N	2.18	0.41
1:C:403:GLY:HA2	1:C:432:LEU:HB2	2.02	0.41
1:E:81:HIS:CD2	1:E:82:PRO:HD3	2.56	0.41
1:E:233:HIS:HA	1:E:293:ALA:HB2	2.02	0.41
1:C:361:LYS:HD2	1:F:241:TYR:CZ	2.55	0.41
1:E:367:THR:CG2	1:E:428:SER:HB3	2.47	0.41
1:F:338:LYS:HD3	1:F:405:ILE:CD1	2.50	0.41
1:F:388:LEU:HD23	1:F:404:ILE:HG22	2.01	0.41
1:B:232:ASN:ND2	1:B:385:SER:HB2	2.27	0.41
1:B:213:THR:OG1	1:B:341:ARG:HG2	2.20	0.41
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.93	0.41
1:C:376:ARG:HD2	1:C:421:HIS:NE2	2.36	0.41
1:F:89:GLN:O	1:F:161:VAL:HA	2.21	0.41
1:A:239:LEU:HA	1:A:239:LEU:HD12	1.75	0.41
1:C:418:THR:OG1	1:C:420:ASP:OD1	2.32	0.41
1:D:338:LYS:HG2	1:D:339:VAL:N	2.35	0.41
1:E:246:MET:HG3	1:E:295:ILE:HG12	2.02	0.41
1:B:233:HIS:NE2	1:B:234:HIS:CD2	2.89	0.41
1:C:109:ARG:HH22	1:C:358:ASN:ND2	2.19	0.41
1:A:416:LYS:HE3	1:A:416:LYS:HB3	1.95	0.41
1:B:120:ARG:NH2	1:B:164:ASP:HB3	2.33	0.41
1:C:102:ALA:HA	1:C:105:SER:OG	2.21	0.41
1:C:231:THR:O	1:C:293:ALA:N	2.54	0.40
1:E:80:ARG:HA	1:E:81:HIS:HA	1.53	0.40
1:E:323:ASP:HB3	1:E:326:CYS:SG	2.61	0.40
1:B:79:PRO:C	1:B:80:ARG:HG3	2.45	0.40
1:B:219:LYS:HB3	1:B:444:ILE:HD11	2.03	0.40
1:C:156:GLU:O	1:C:156:GLU:HG3	2.21	0.40
1:C:233:HIS:O	1:C:237:VAL:N	2.54	0.40
1:E:87:LYS:HD3	1:E:87:LYS:O	2.21	0.40
1:F:376:ARG:HD2	1:F:421:HIS:CG	2.56	0.40
1:B:134:VAL:HG21	1:B:151:LEU:HD22	2.02	0.40
1:D:266:ALA:HA	1:D:292:GLY:O	2.22	0.40
1:A:62:ALA:O	1:A:279:TYR:HE1	2.04	0.40
1:A:338:LYS:HE3	1:A:346:THR:OG1	2.21	0.40
1:B:105:SER:CB	1:B:109:ARG:HH22	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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%)	327 (98%)	6 (2%)	51	72
1	B	334/342 (98%)	326 (98%)	8 (2%)	43	67
1	C	334/342 (98%)	328 (98%)	6 (2%)	51	72
1	D	334/342 (98%)	329 (98%)	5 (2%)	57	76
1	E	334/342 (98%)	330 (99%)	4 (1%)	63	79
1	F	334/342 (98%)	329 (98%)	5 (2%)	57	76
All	All	2003/2052 (98%)	1969 (98%)	34 (2%)	53	73

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

Mol	Chain	Res	Type
1	A	99	THR
1	A	227	VAL
1	A	237	VAL
1	A	363	ILE
1	A	377	GLN
1	A	409	THR
1	B	68	ASN
1	B	85	LEU
1	B	154	ILE
1	B	192	LEU
1	B	237	VAL
1	B	304	SER
1	B	306	VAL
1	B	405	ILE
1	C	78	LEU
1	C	108	LEU
1	C	183	GLN
1	C	227	VAL
1	C	258	VAL
1	C	404	ILE
1	D	138	ARG
1	D	239	LEU
1	D	321	VAL
1	D	358	ASN
1	D	418	THR
1	E	192	LEU
1	E	235	VAL
1	E	258	VAL
1	E	306	VAL
1	F	64	GLU
1	F	154	ILE
1	F	187	GLU
1	F	291	ASP
1	F	405	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	89	GLN
1	A	204	GLN

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Mol	Chain	Res	Type
1	A	208	HIS
1	B	59	GLN
1	B	234	HIS
1	B	421	HIS
1	C	233	HIS
1	C	335	GLN
1	C	358	ASN
1	C	456	GLN
1	D	60	HIS
1	D	72	ASN
1	D	451	GLN
1	E	59	GLN
1	E	224	ASN
1	E	234	HIS
1	E	456	GLN
1	F	234	HIS
1	F	335	GLN

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 oligosaccharides 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	D	1001	3	32,33,33	1.45	5 (15%)	48,52,52	1.71	7 (14%)
2	ATP	F	1001	3	32,33,33	1.46	5 (15%)	48,52,52	1.75	8 (16%)
2	ATP	A	1001	3	32,33,33	1.48	7 (21%)	48,52,52	1.75	7 (14%)
2	ATP	B	1001	3	32,33,33	1.40	4 (12%)	48,52,52	1.76	8 (16%)
2	ATP	C	1001	3	32,33,33	1.38	5 (15%)	48,52,52	1.77	10 (20%)
2	ATP	E	1001	3	32,33,33	1.37	5 (15%)	48,52,52	2.14	14 (29%)

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	D	1001	3	-	2/22/38/38	0/3/3/3
2	ATP	F	1001	3	-	2/22/38/38	0/3/3/3
2	ATP	A	1001	3	-	2/22/38/38	0/3/3/3
2	ATP	B	1001	3	-	2/22/38/38	0/3/3/3
2	ATP	C	1001	3	-	2/22/38/38	0/3/3/3
2	ATP	E	1001	3	-	2/22/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	ATP	C5-C4	4.84	1.47	1.39
2	F	1001	ATP	C5-C4	4.80	1.47	1.39
2	A	1001	ATP	C5-C4	4.78	1.47	1.39
2	E	1001	ATP	C5-C4	4.65	1.47	1.39
2	B	1001	ATP	C5-C4	4.65	1.47	1.39
2	C	1001	ATP	C5-C4	4.62	1.47	1.39
2	F	1001	ATP	C5-C6	2.81	1.48	1.41
2	C	1001	ATP	C5-C6	2.78	1.48	1.41
2	E	1001	ATP	C5-C6	2.76	1.48	1.41
2	B	1001	ATP	C5-C6	2.75	1.48	1.41
2	D	1001	ATP	C5-C6	2.57	1.48	1.41
2	A	1001	ATP	PA-O3A	2.56	1.62	1.59
2	A	1001	ATP	C5-C6	2.47	1.47	1.41
2	D	1001	ATP	C8-N7	2.46	1.36	1.31
2	D	1001	ATP	C5-N7	-2.44	1.34	1.39
2	A	1001	ATP	C8-N7	2.44	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1001	ATP	C8-N7	2.43	1.36	1.31
2	C	1001	ATP	C8-N7	2.41	1.36	1.31
2	B	1001	ATP	C8-N7	2.40	1.36	1.31
2	A	1001	ATP	PB-O3A	2.38	1.62	1.59
2	A	1001	ATP	C5-N7	-2.36	1.34	1.39
2	C	1001	ATP	PB-O3B	2.35	1.62	1.59
2	B	1001	ATP	C5-N7	-2.33	1.34	1.39
2	E	1001	ATP	C8-N7	2.32	1.36	1.31
2	E	1001	ATP	C5-N7	-2.30	1.34	1.39
2	F	1001	ATP	C5-N7	-2.28	1.34	1.39
2	F	1001	ATP	PA-O3A	2.16	1.61	1.59
2	D	1001	ATP	PA-O3A	2.15	1.61	1.59
2	C	1001	ATP	C5-N7	-2.14	1.35	1.39
2	E	1001	ATP	PB-O3A	-2.10	1.57	1.59
2	A	1001	ATP	PB-O3B	2.02	1.61	1.59

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1001	ATP	O3A-PB-O1B	-7.48	88.21	110.70
2	F	1001	ATP	C5-C4-N3	-6.07	118.36	126.72
2	A	1001	ATP	C5-C4-N3	-6.06	118.37	126.72
2	B	1001	ATP	C5-C4-N3	-6.03	118.41	126.72
2	D	1001	ATP	C5-C4-N3	-5.92	118.57	126.72
2	E	1001	ATP	C5-C4-N3	-5.78	118.75	126.72
2	C	1001	ATP	C5-C4-N3	-5.76	118.79	126.72
2	A	1001	ATP	N3-C4-N9	4.81	135.34	127.17
2	C	1001	ATP	N3-C4-N9	4.56	134.93	127.17
2	D	1001	ATP	N3-C4-N9	4.54	134.89	127.17
2	E	1001	ATP	N3-C4-N9	4.51	134.83	127.17
2	F	1001	ATP	N3-C4-N9	4.42	134.69	127.17
2	B	1001	ATP	N3-C4-N9	4.39	134.64	127.17
2	B	1001	ATP	C4-C5-N7	-3.98	106.04	110.58
2	F	1001	ATP	C4-C5-N7	-3.90	106.13	110.58
2	A	1001	ATP	C2-N3-C4	3.71	120.90	111.83
2	C	1001	ATP	C2-N3-C4	3.71	120.90	111.83
2	B	1001	ATP	C2-N3-C4	3.70	120.86	111.83
2	F	1001	ATP	C2-N3-C4	3.66	120.77	111.83
2	D	1001	ATP	C2-N3-C4	3.62	120.68	111.83
2	E	1001	ATP	C2-N3-C4	3.61	120.65	111.83
2	C	1001	ATP	C4-C5-N7	-3.60	106.47	110.58
2	E	1001	ATP	C4-C5-N7	-3.56	106.51	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ATP	C4-C5-N7	-3.30	106.81	110.58
2	D	1001	ATP	C4-C5-N7	-3.24	106.88	110.58
2	A	1001	ATP	N3-C2-N1	-3.22	123.72	128.58
2	C	1001	ATP	N3-C2-N1	-3.20	123.73	128.58
2	D	1001	ATP	N3-C2-N1	-3.08	123.92	128.58
2	E	1001	ATP	N3-C2-N1	-3.05	123.96	128.58
2	B	1001	ATP	N3-C2-N1	-3.04	123.98	128.58
2	C	1001	ATP	C4-N9-C8	2.98	108.87	105.74
2	E	1001	ATP	O2B-PB-O1B	2.93	126.06	112.44
2	F	1001	ATP	N3-C2-N1	-2.90	124.20	128.58
2	B	1001	ATP	C5-N7-C8	2.77	107.81	103.45
2	C	1001	ATP	C5-N7-C8	2.71	107.72	103.45
2	E	1001	ATP	C4-N9-C8	2.67	108.54	105.74
2	F	1001	ATP	C5-N7-C8	2.66	107.63	103.45
2	E	1001	ATP	C5-N7-C8	2.55	107.46	103.45
2	A	1001	ATP	C5-N7-C8	2.44	107.28	103.45
2	A	1001	ATP	C4-N9-C8	2.38	108.24	105.74
2	C	1001	ATP	N9-C8-N7	-2.31	110.67	113.94
2	E	1001	ATP	O3G-PG-O2G	2.30	116.42	107.80
2	C	1001	ATP	C6-C5-N7	2.27	136.47	132.09
2	B	1001	ATP	C4-N9-C8	2.26	108.11	105.74
2	D	1001	ATP	C5-N7-C8	2.22	106.94	103.45
2	B	1001	ATP	C6-C5-N7	2.21	136.36	132.09
2	E	1001	ATP	O2B-PB-O3B	2.19	113.19	107.27
2	F	1001	ATP	C6-C5-N7	2.13	136.19	132.09
2	F	1001	ATP	C4-N9-C8	2.12	107.97	105.74
2	E	1001	ATP	O3B-PG-O1G	-2.12	99.91	111.04
2	E	1001	ATP	C6-C5-N7	2.10	136.15	132.09
2	D	1001	ATP	C3'-C2'-C1'	2.07	105.38	101.46
2	C	1001	ATP	C3'-C2'-C1'	2.03	105.30	101.46
2	E	1001	ATP	N9-C8-N7	-2.02	111.07	113.94

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

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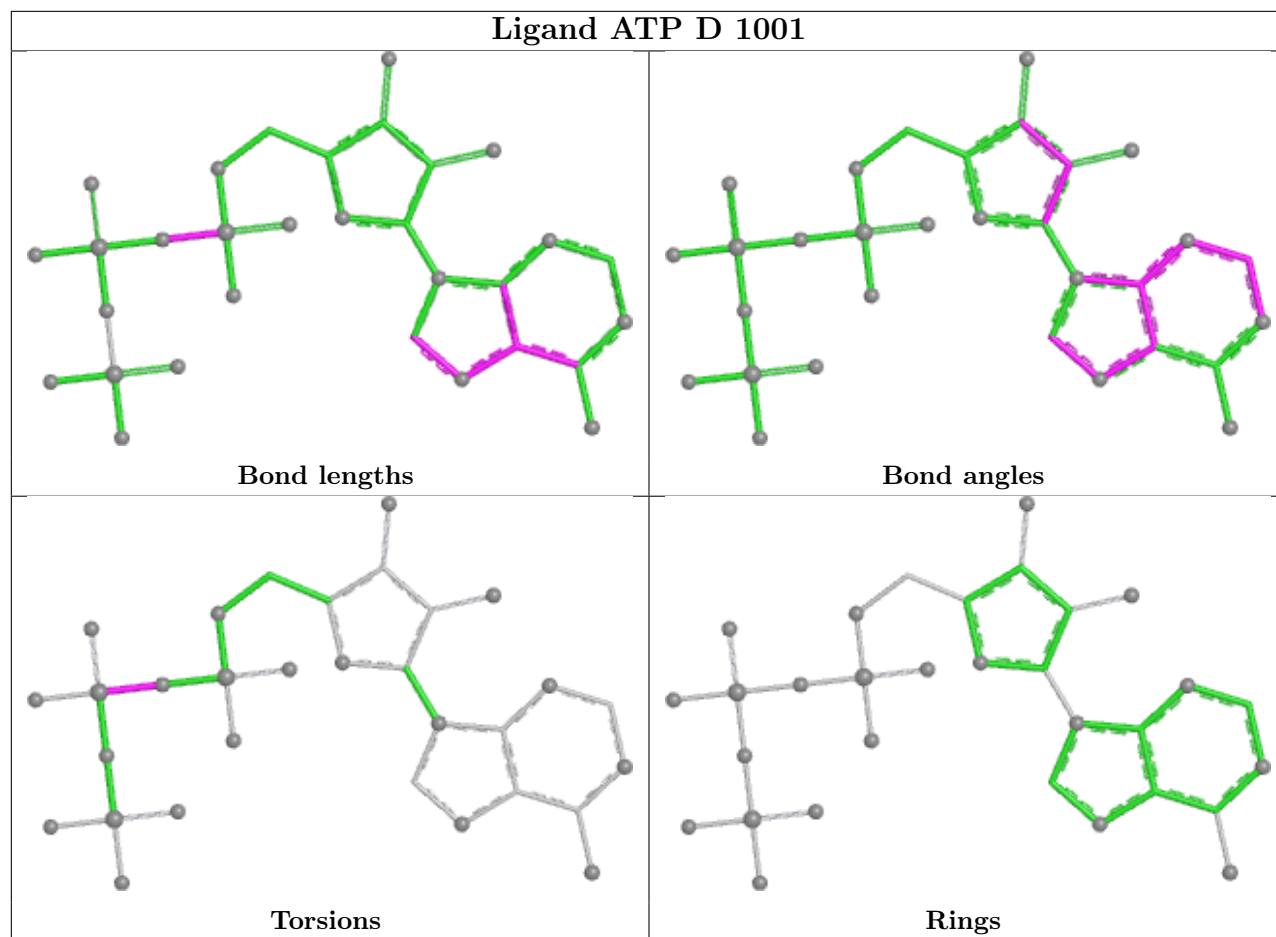
Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	PA-O3A-PB-O1B
2	B	1001	ATP	PA-O3A-PB-O1B
2	C	1001	ATP	PA-O3A-PB-O1B
2	D	1001	ATP	PA-O3A-PB-O1B
2	E	1001	ATP	PA-O3A-PB-O1B
2	F	1001	ATP	PA-O3A-PB-O1B

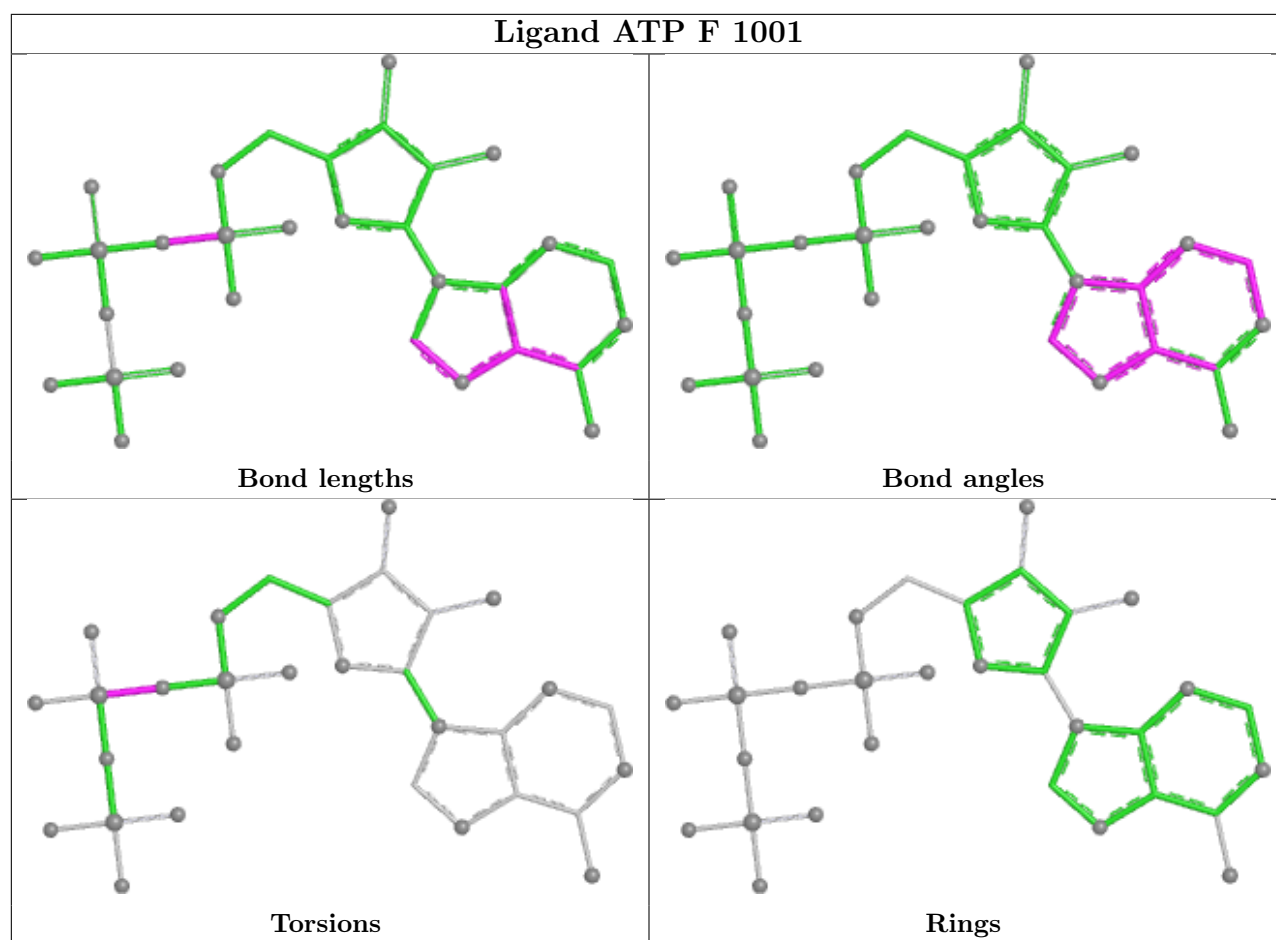
There are no ring outliers.

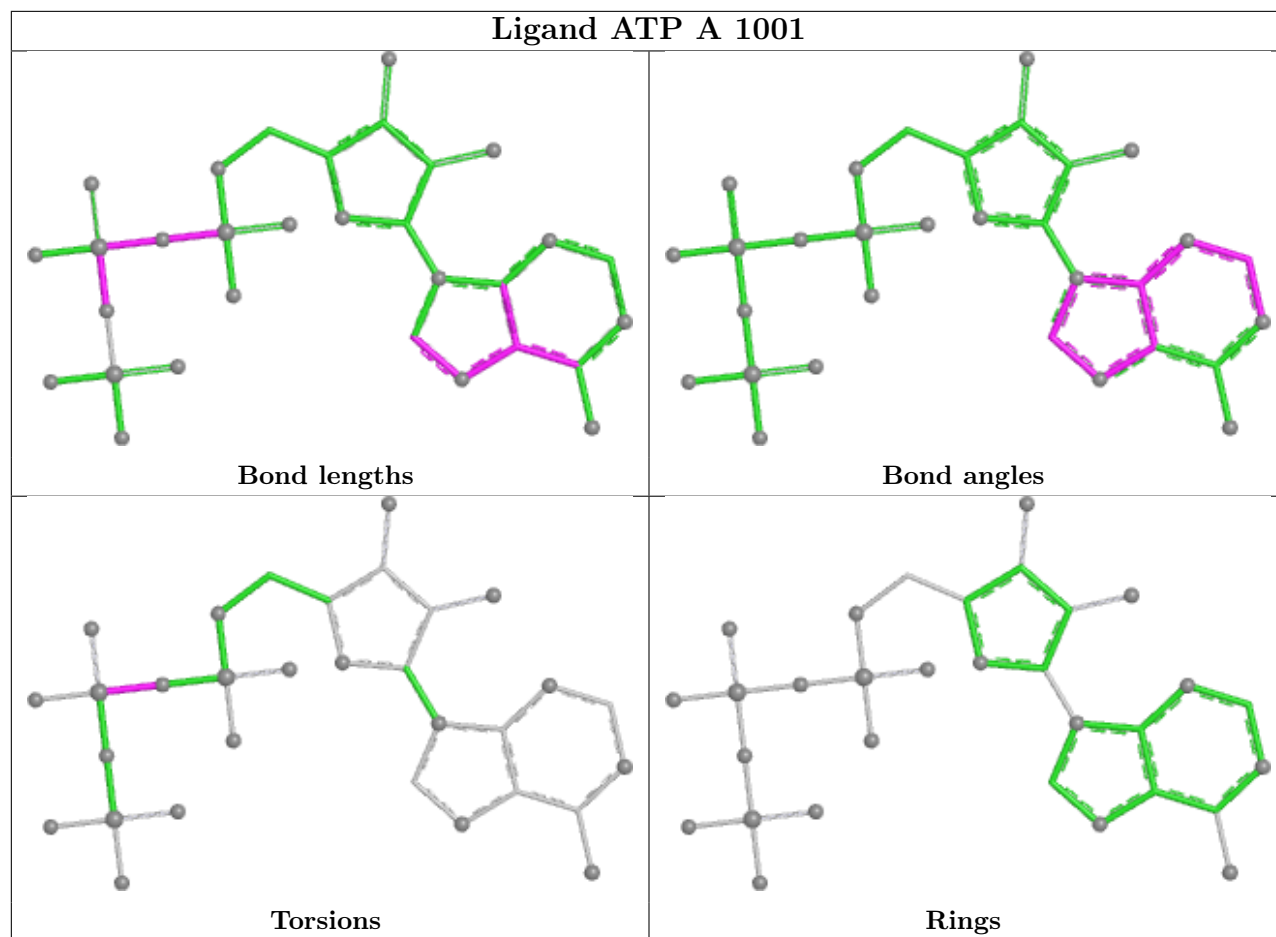
1 monomer is involved in 2 short contacts:

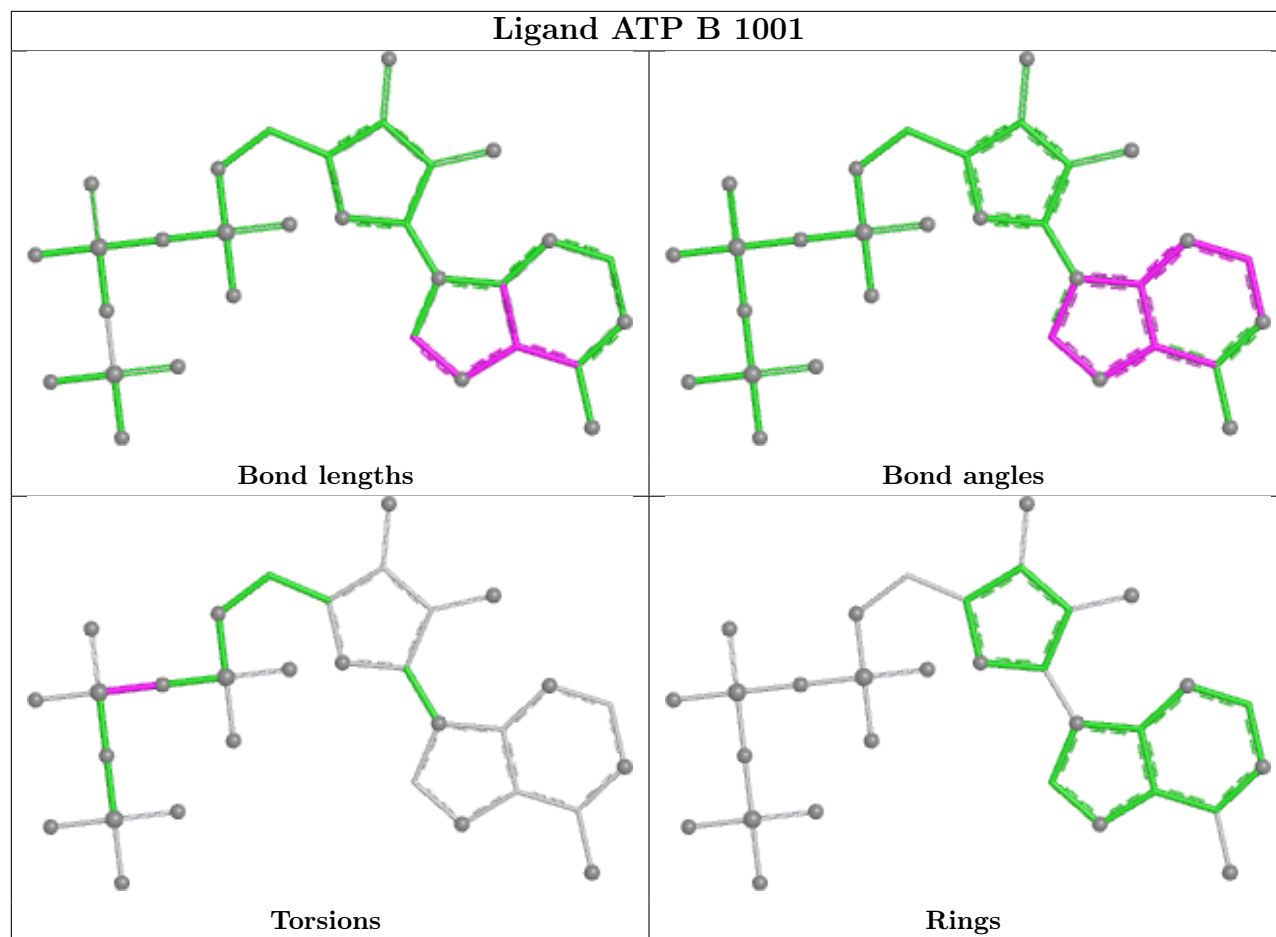
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1001	ATP	2	0

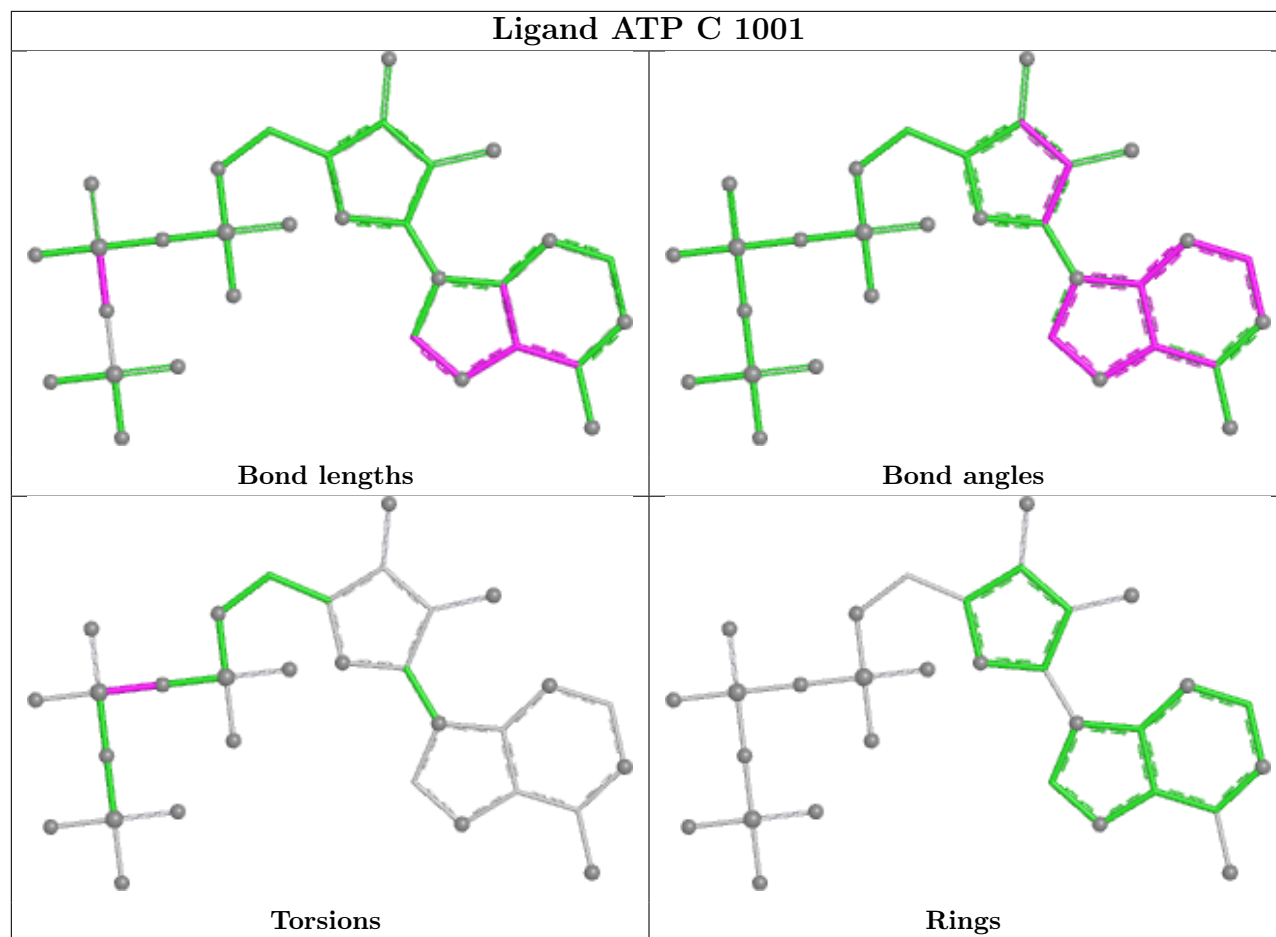
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

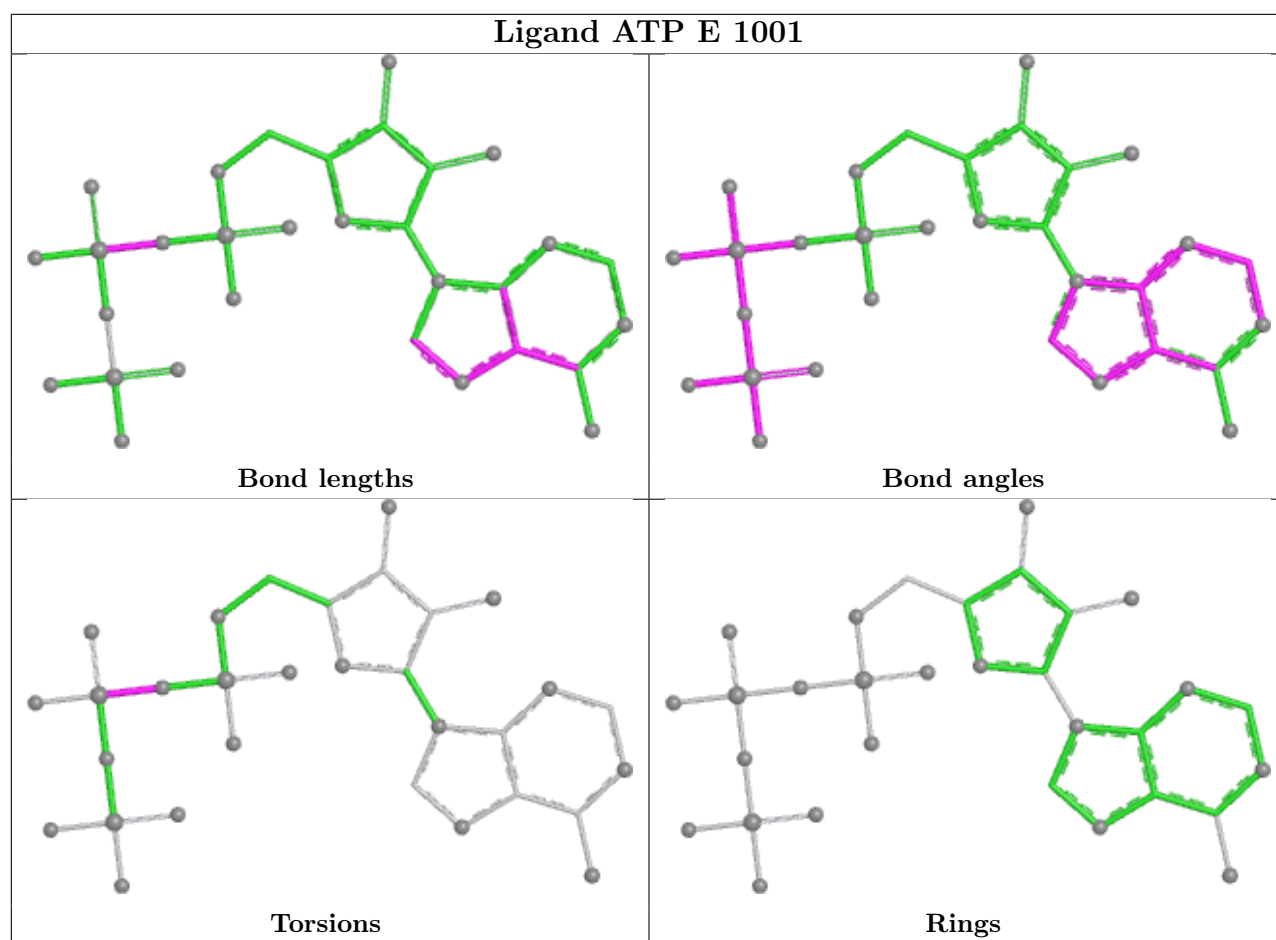












5.7 Other polymers [i](#)

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, 95th 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	401/413 (97%)	-0.14	4 (0%) 79 74	38, 64, 116, 191	0
1	B	402/413 (97%)	-0.25	4 (0%) 79 74	37, 60, 106, 160	0
1	C	402/413 (97%)	-0.11	7 (1%) 69 62	38, 68, 116, 157	0
1	D	402/413 (97%)	-0.16	9 (2%) 62 54	39, 63, 114, 188	0
1	E	402/413 (97%)	-0.11	10 (2%) 58 50	43, 68, 120, 189	0
1	F	402/413 (97%)	-0.27	4 (0%) 79 74	36, 59, 104, 150	0
All	All	2411/2478 (97%)	-0.17	38 (1%) 70 63	36, 63, 115, 191	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	236	ALA	4.3
1	B	78	LEU	4.1
1	C	236	ALA	3.9
1	D	241	TYR	3.8
1	C	237	VAL	3.5
1	E	237	VAL	3.5
1	C	78	LEU	3.2
1	B	79	PRO	3.2
1	B	237	VAL	3.1
1	E	79	PRO	3.0
1	A	78	LEU	2.9
1	C	411	ASN	2.9
1	F	56	SER	2.9
1	B	58	LEU	2.9
1	A	79	PRO	2.8
1	F	237	VAL	2.7
1	A	412	ARG	2.7
1	E	234	HIS	2.7
1	E	82	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	82	PRO	2.5
1	E	233	HIS	2.4
1	D	239	LEU	2.4
1	D	183	GLN	2.4
1	E	58	LEU	2.4
1	D	56	SER	2.4
1	F	240	ASP	2.3
1	E	77	LEU	2.3
1	D	238	ASP	2.3
1	A	233	HIS	2.3
1	E	78	LEU	2.2
1	E	62	ALA	2.2
1	D	85	LEU	2.2
1	F	58	LEU	2.2
1	C	82	PRO	2.1
1	C	412	ARG	2.1
1	C	85	LEU	2.1
1	D	443	ILE	2.1
1	D	87	LYS	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 oligosaccharides 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, 95th 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.

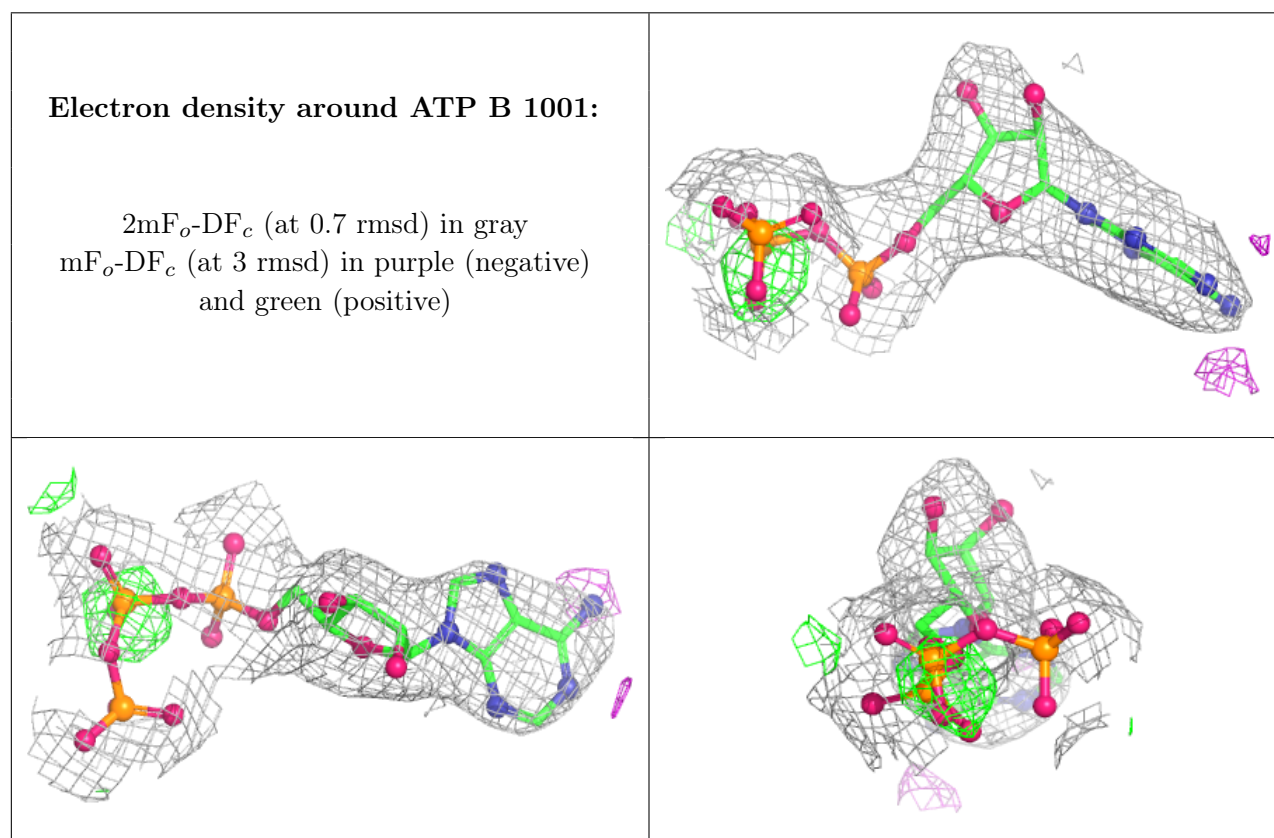
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	B	1001	31/31	0.95	0.07	41,51,64,84	0
2	ATP	C	1001	31/31	0.95	0.07	51,65,77,87	0
2	ATP	F	1001	31/31	0.95	0.07	44,53,65,72	0
2	ATP	E	1001	31/31	0.96	0.07	48,63,73,89	0

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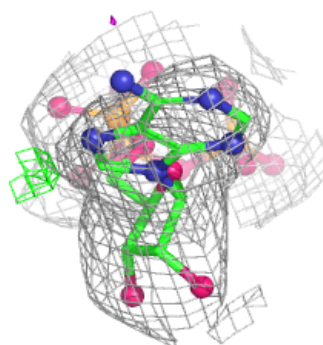
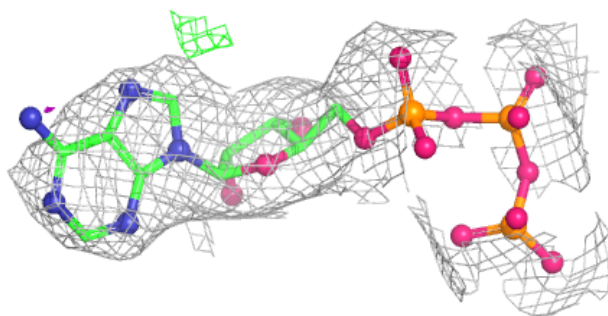
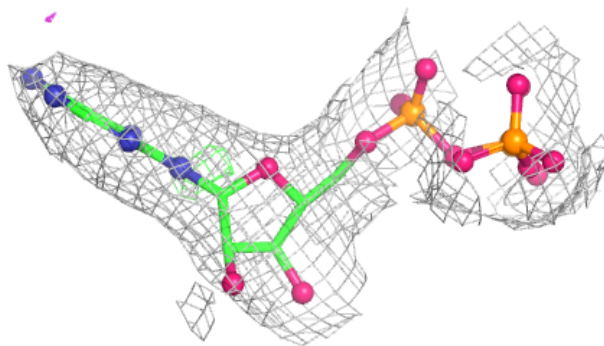
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	A	1001	31/31	0.96	0.07	39,50,67,75	0
2	ATP	D	1001	31/31	0.97	0.06	40,51,64,69	0
3	MG	A	1002	1/1	0.98	0.10	55,55,55,55	0
3	MG	C	1002	1/1	0.98	0.06	49,49,49,49	0
3	MG	B	1002	1/1	0.99	0.08	48,48,48,48	0
3	MG	D	1002	1/1	0.99	0.09	48,48,48,48	0
3	MG	E	1002	1/1	0.99	0.05	54,54,54,54	0
3	MG	F	1002	1/1	0.99	0.07	49,49,49,49	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.

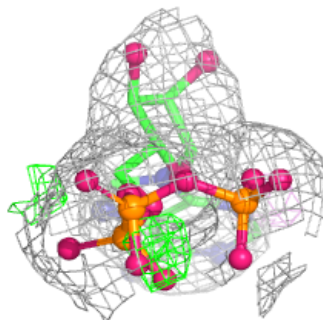
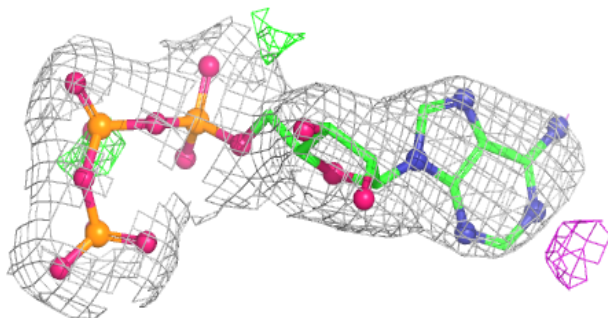
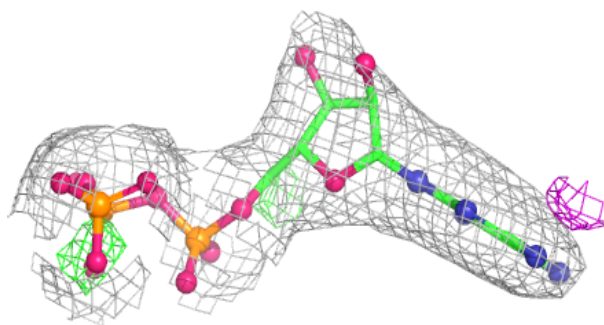


Electron density around ATP C 1001:

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

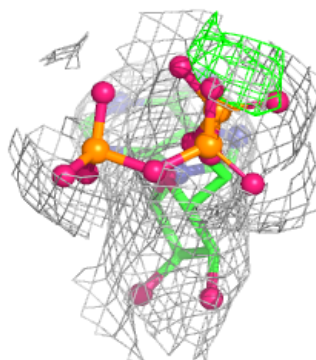
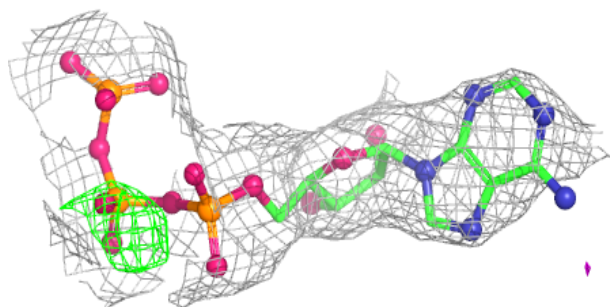
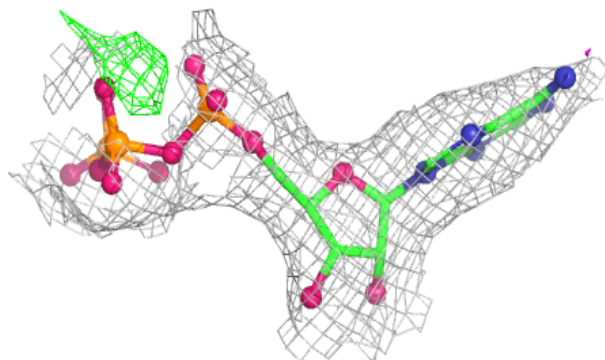
**Electron density around ATP F 1001:**

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

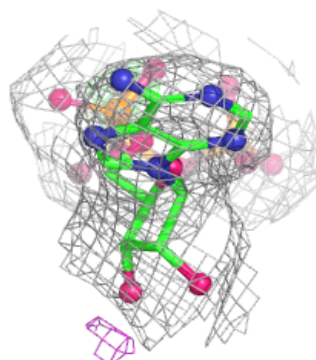
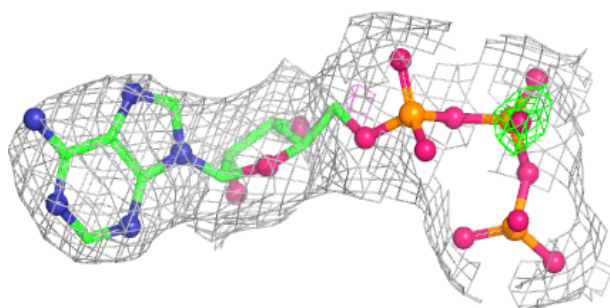
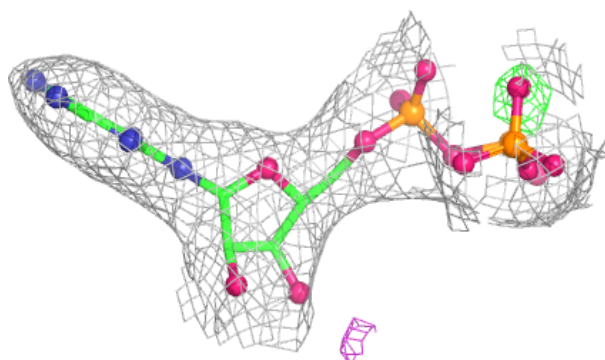


Electron density around ATP E 1001:

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

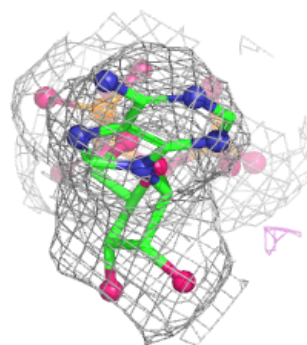
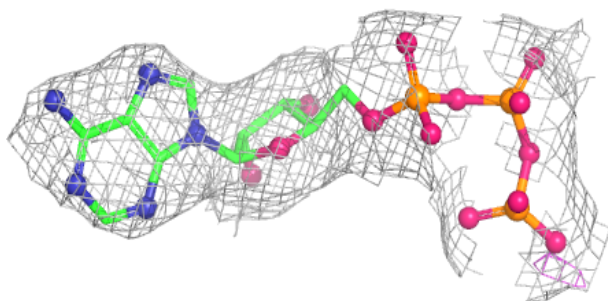
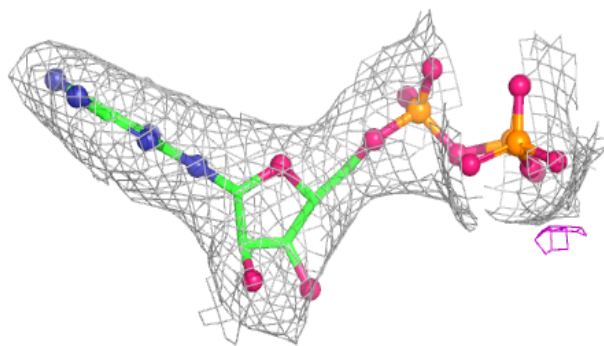
**Electron density around ATP A 1001:**

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



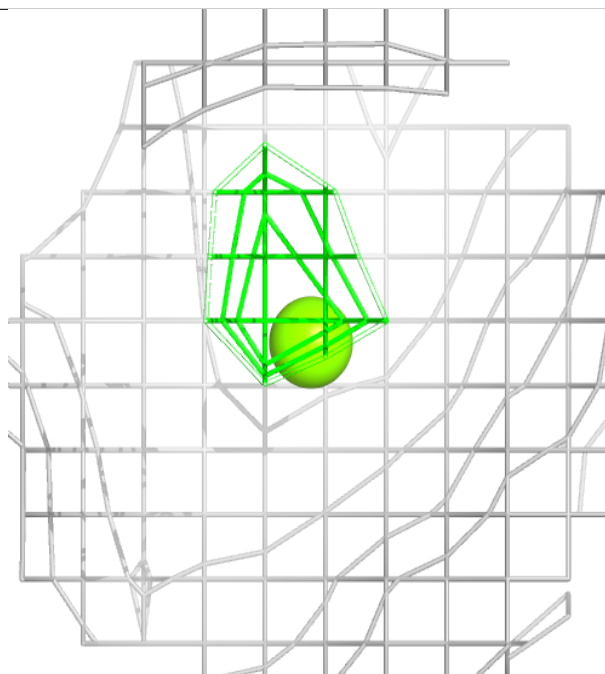
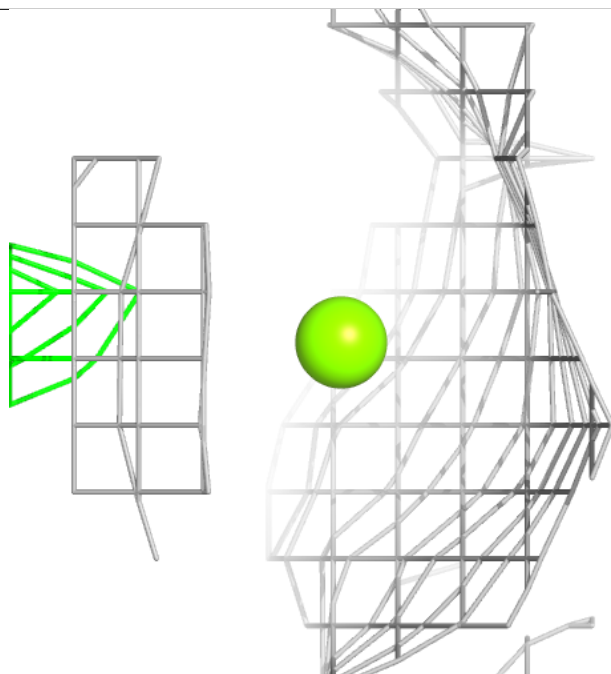
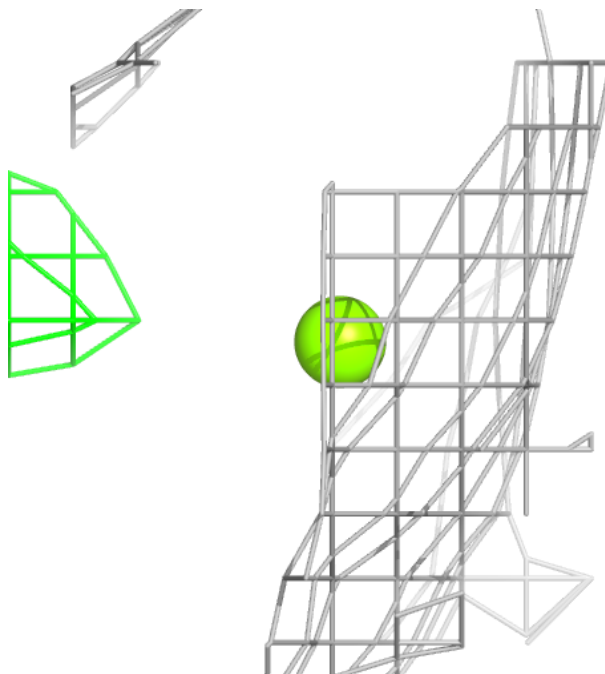
Electron density around ATP D 1001:

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



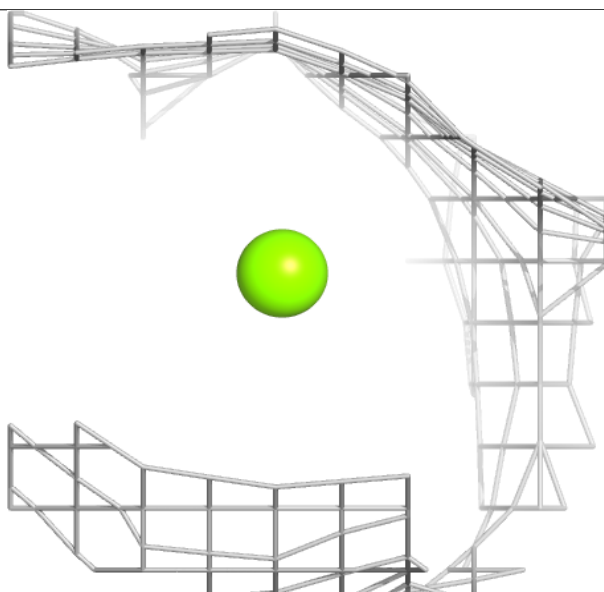
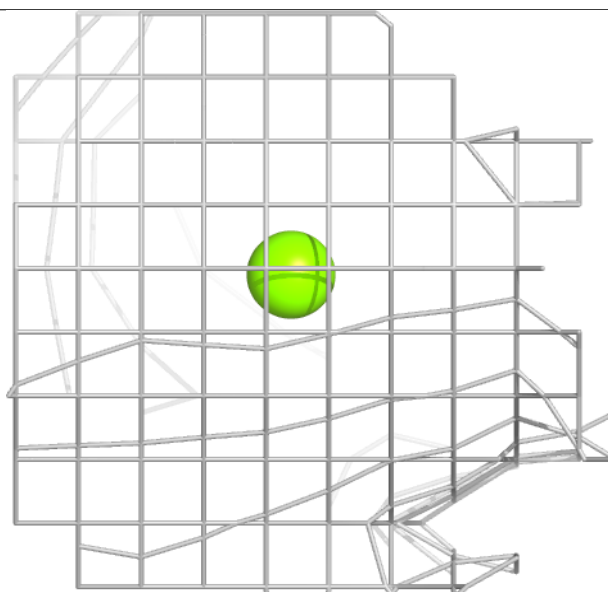
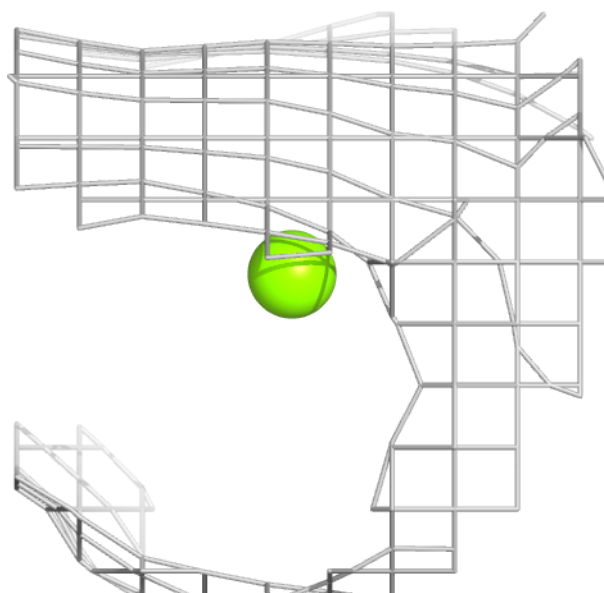
Electron density around MG A 1002:

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



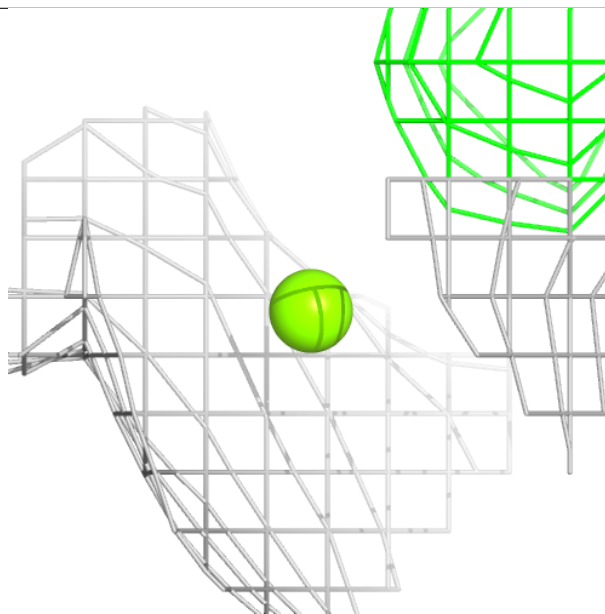
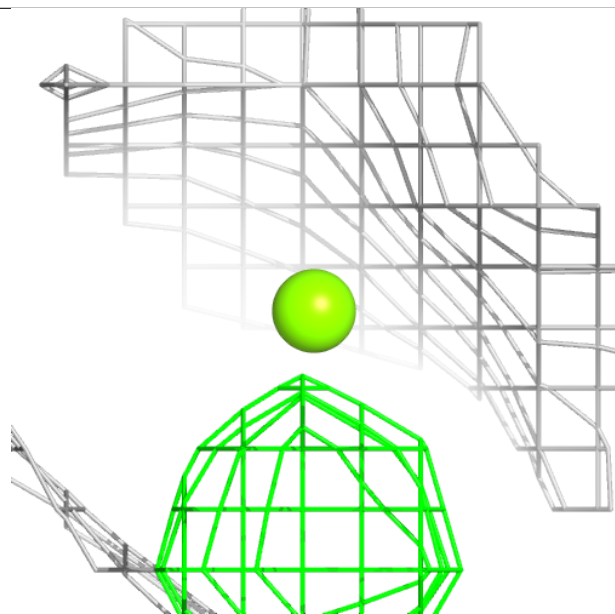
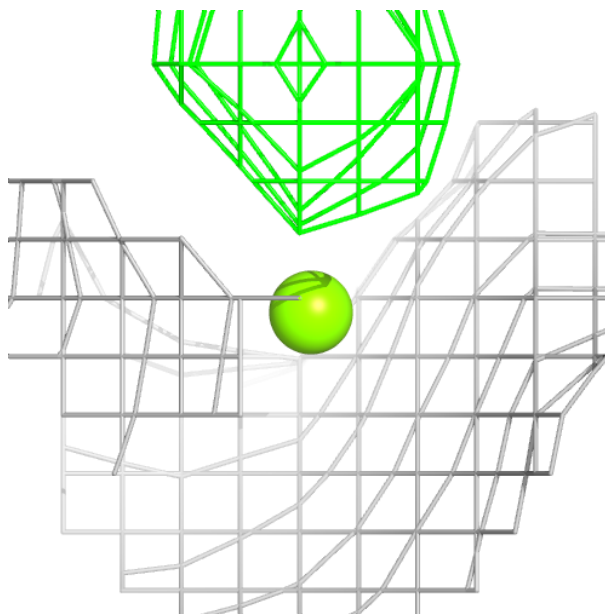
Electron density around MG C 1002:

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



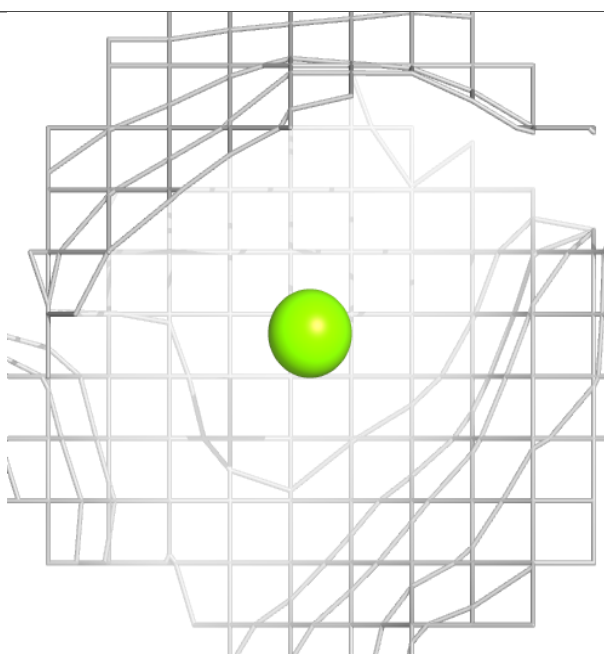
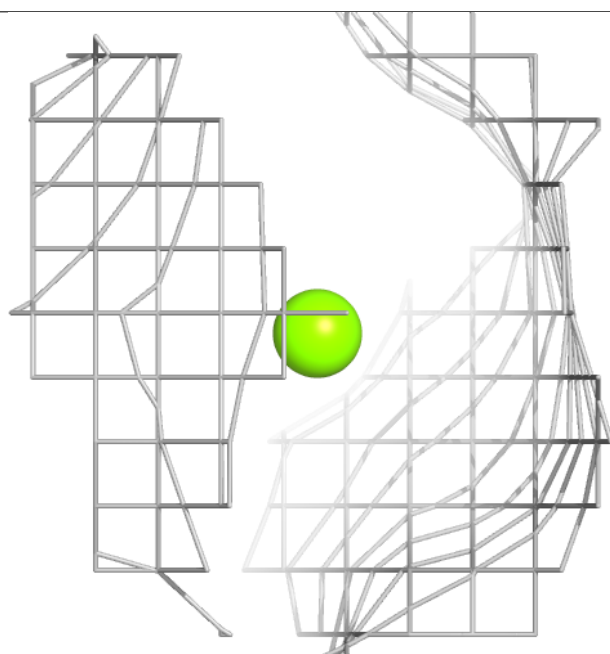
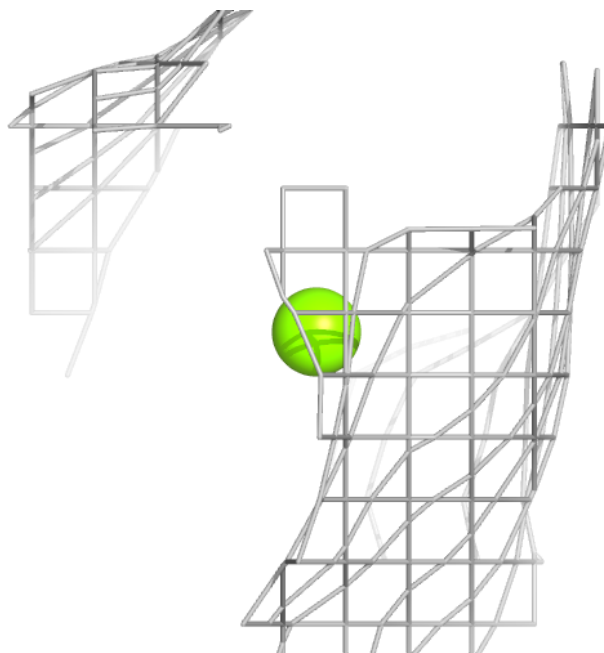
Electron density around MG B 1002:

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



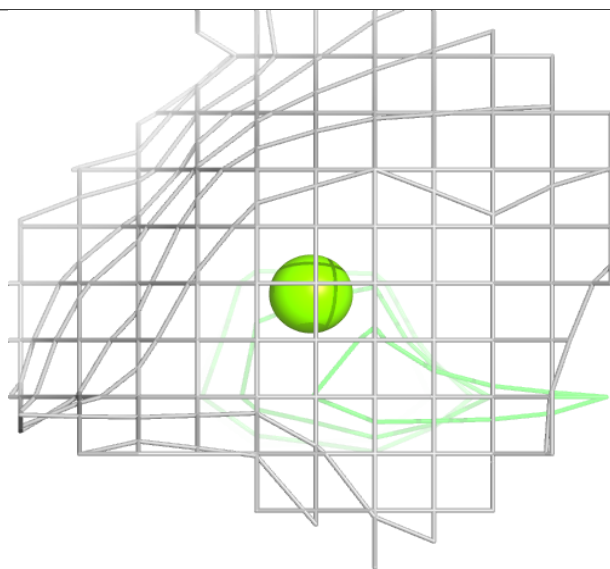
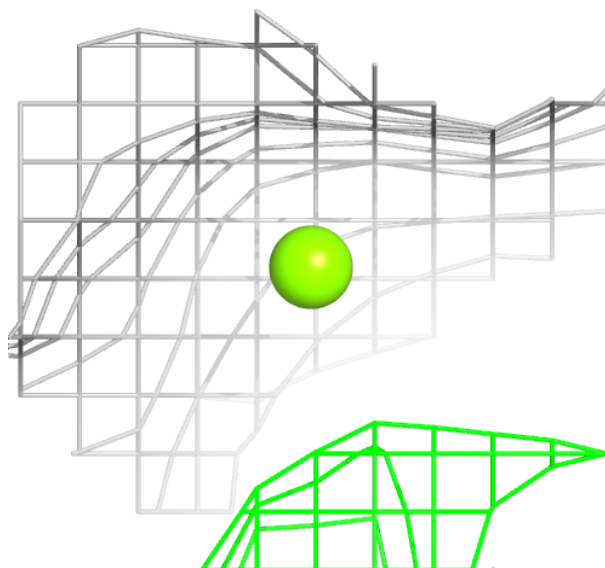
Electron density around MG D 1002:

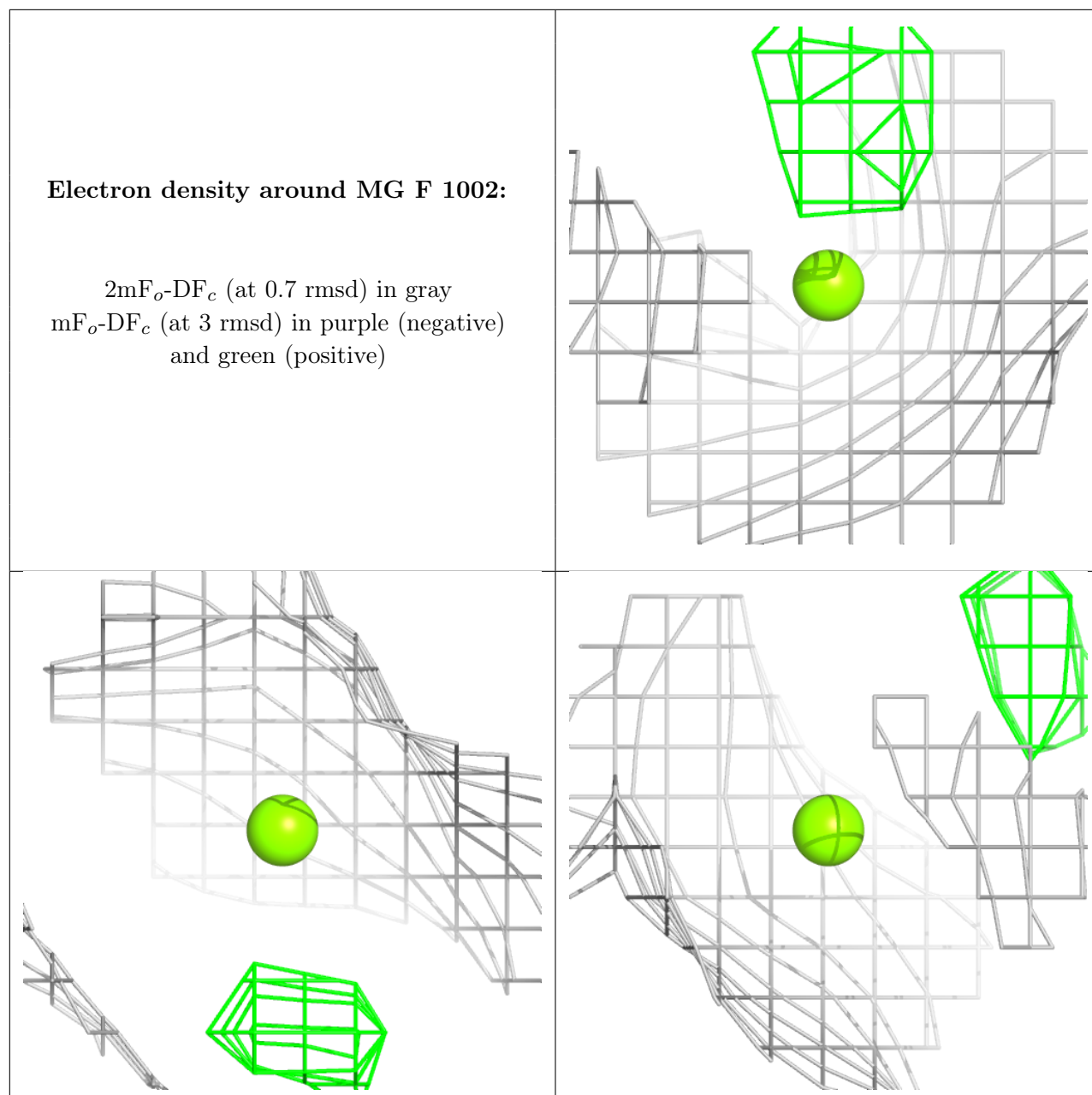
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG E 1002:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.