



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:27 PM BST

PDB ID : 5OF3  
Title : Crystal structure of the heterotrimeric PriSLX primase from *S. solfataricus*.  
Authors : Pellegrini, L.; Holzer, S.  
Deposited on : 2017-07-10  
Resolution : 2.91 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

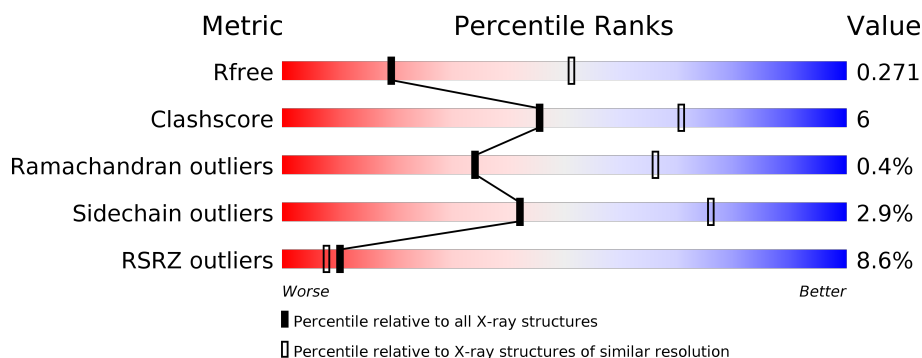
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	330	<div> <div>76%</div> <div>20%</div> <div>••</div> </div>
1	D	330	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>••</div> </div>
2	B	307	<div> <div>13%</div> <div>72%</div> <div>18%</div> <div>• 9%</div> </div>
2	E	307	<div> <div>18%</div> <div>69%</div> <div>19%</div> <div>• 11%</div> </div>
3	C	154	<div> <div>%</div> <div>58%</div> <div>11%</div> <div>31%</div> </div>
3	F	154	<div> <div>11%</div> <div>49%</div> <div>14%</div> <div>• 36%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11540 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 DNA primase small subunit PriS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	1	0
			2566	1634	438	481	13			
1	D	319	Total	C	N	O	S	0	0	0
			2558	1629	437	480	12			

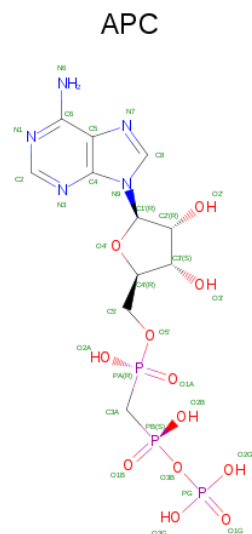
- Molecule 2 is a protein called DNA primase large subunit PriL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2302	1496	380	420	6			
2	E	273	Total	C	N	O	S	0	1	0
			2262	1473	371	412	6			

- Molecule 3 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	107	Total	C	N	O	S	0	0	0
			895	579	152	162	2			
3	F	98	Total	C	N	O	S	0	0	0
			827	537	140	148	2			

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
4	D	1	Total 31	C 11	N 5	O 12	P 3	0	0
4	C	1	Total 31	C 11	N 5	O 12	P 3	0	0
4	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mn 1 1	0	0
5	D	1	Total Mn 1 1	0	0
5	C	1	Total Mn 1 1	0	0
5	F	1	Total Mn 1 1	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0

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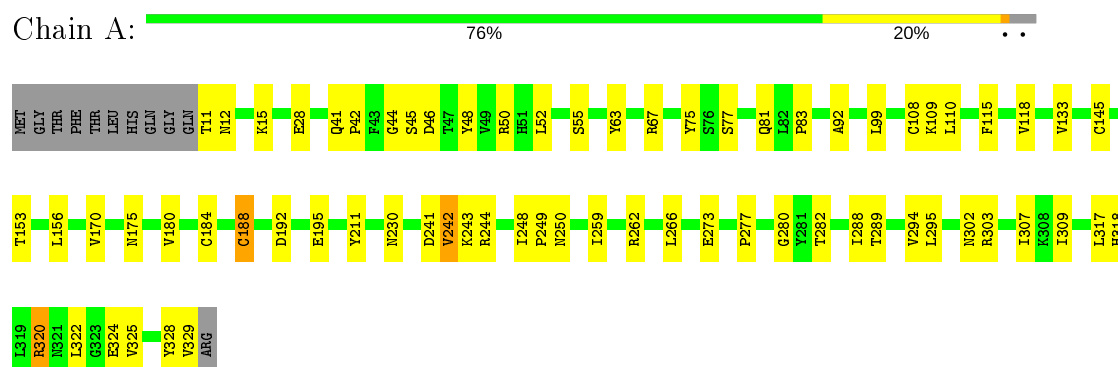
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Zn	0	0
			1	1		

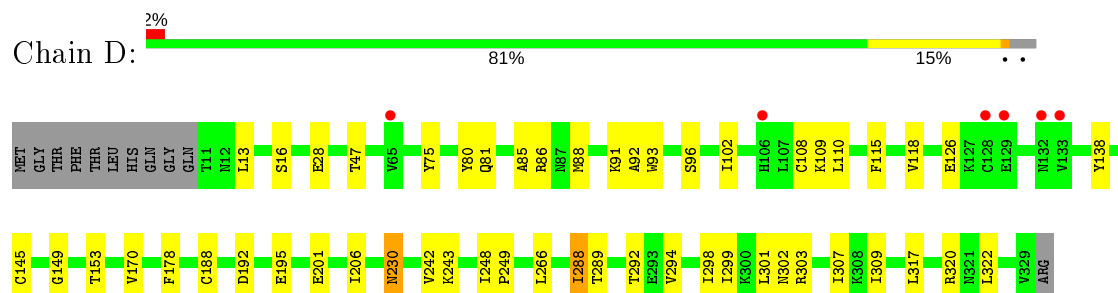
### 3 Residue-property plots [i](#)

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.

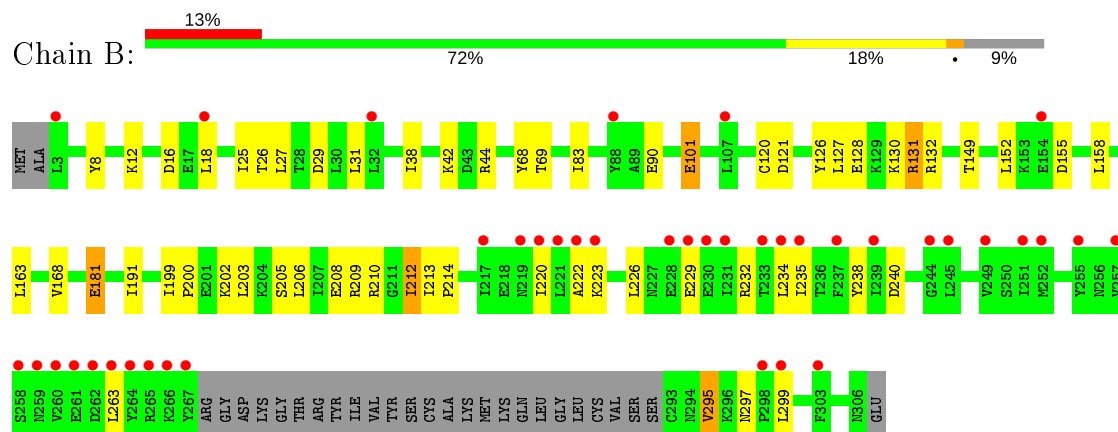
- Molecule 1: DNA primase small subunit PriS



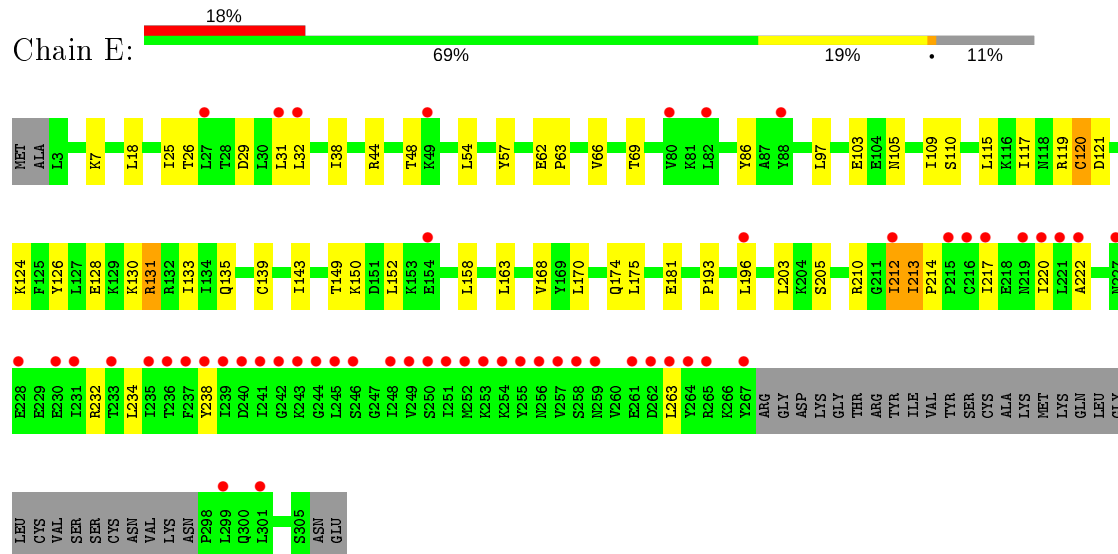
- Molecule 1: DNA primase small subunit PriS



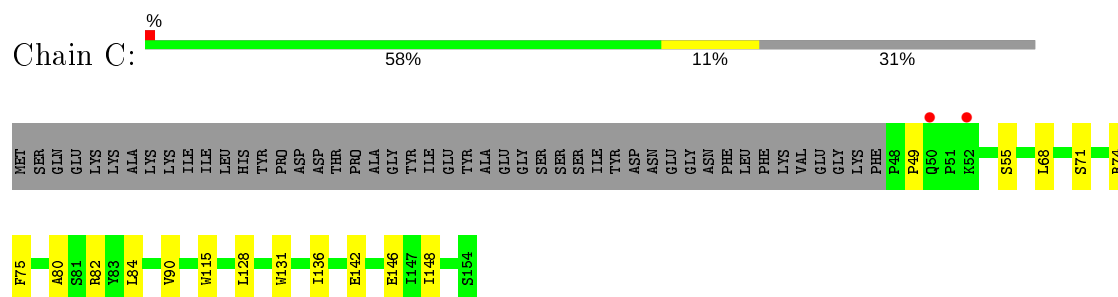
- Molecule 2: DNA primase large subunit PriL



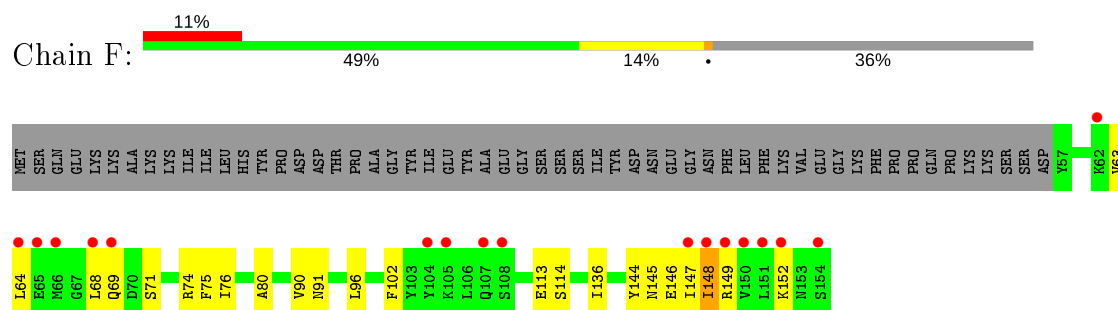
- Molecule 2: DNA primase large subunit PriL



- Molecule 3: Uncharacterized protein



- Molecule 3: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.89Å 104.89Å 229.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.91 – 2.91 47.71 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.91-2.91) 100.0 (47.71-2.91)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.228 , 0.271 0.227 , 0.271	Depositor DCC
$R_{free}$ test set	2677 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APC, ZN, MN

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	0.25	0/2619	0.44	0/3539
1	D	0.24	0/2611	0.44	0/3529
2	B	0.24	0/2340	0.41	0/3148
2	E	0.24	0/2300	0.40	0/3093
3	C	0.23	0/913	0.38	0/1224
3	F	0.24	0/842	0.38	0/1128
All	All	0.24	0/11625	0.42	0/15661

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2566	0	2549	40	0
1	D	2558	0	2537	30	0
2	B	2302	0	2420	32	0
2	E	2262	0	2380	33	0
3	C	895	0	929	9	0
3	F	827	0	859	13	0
4	A	31	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	31	0	14	0	0
4	D	31	0	14	0	0
4	F	31	0	14	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
All	All	11540	0	11730	149	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 6.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:HB3	1:A:15:LYS:HB2	1.65	0.77
3:F:74:ARG:HD3	4:F:1001:APC:H1'	1.73	0.71
2:E:205:SER:HB2	2:E:210:ARG:HB2	1.72	0.70
3:F:68:LEU:HD22	3:F:146:GLU:HG3	1.72	0.70
1:D:28:GLU:HB2	1:D:249:PRO:HG2	1.73	0.69
1:A:48:TYR:OH	4:A:1001:APC:N6	2.26	0.68
1:A:28:GLU:HB2	1:A:249:PRO:HG2	1.76	0.67
3:F:96:LEU:HD11	3:F:113:GLU:HG2	1.78	0.66
1:A:81:GLN:HB2	1:A:92:ALA:HB3	1.79	0.64
1:D:93:TRP:HE1	1:D:96:SER:HB3	1.62	0.61
1:A:170:VAL:HG11	1:A:266:LEU:HD21	1.82	0.61
3:C:68:LEU:HD22	3:C:146:GLU:HG3	1.83	0.60
2:B:202:LYS:O	2:B:206:LEU:N	2.33	0.59
2:E:117:ILE:HG21	2:E:175:LEU:HD13	1.85	0.58
1:A:42:PRO:HG2	1:A:45:SER:HB3	1.85	0.58
1:A:289:THR:HG22	1:A:302:ASN:HA	1.86	0.58
1:A:115:PHE:CD1	1:A:288:ILE:HD11	2.39	0.57
2:B:27:LEU:HD21	2:B:69:THR:HG22	1.88	0.56
1:A:118:VAL:HG21	1:A:133:VAL:HG21	1.87	0.55
2:E:25:ILE:HG23	2:E:29:ASP:HB2	1.89	0.55
1:A:318:HIS:CD2	1:A:324:GLU:HA	2.42	0.55
1:D:192:ASP:OD2	2:E:150:LYS:NZ	2.32	0.55
2:B:31:LEU:HD22	2:B:38:ILE:HG13	1.88	0.54
2:E:220:ILE:HG21	2:E:234:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:GLU:O	2:B:131:ARG:HD3	2.08	0.54
1:D:317:LEU:HD22	1:D:322:LEU:HD12	1.91	0.53
2:E:31:LEU:HD22	2:E:38:ILE:HG13	1.90	0.53
1:A:318:HIS:HD2	1:A:325:VAL:H	1.55	0.53
1:D:301:LEU:HD11	1:D:317:LEU:HD13	1.89	0.53
2:E:120[B]:CYS:SG	2:E:121:ASP:N	2.82	0.53
1:A:242:VAL:HG12	1:A:243:LYS:HG3	1.91	0.53
2:B:8:TYR:OH	2:B:101:GLU:OE1	2.27	0.52
2:E:126:TYR:HB3	2:E:130:LYS:HA	1.92	0.52
2:E:18:LEU:HD13	2:E:26:THR:HA	1.92	0.52
1:A:110:LEU:HD21	1:A:145:CYS:SG	2.49	0.52
2:B:126:TYR:HB3	2:B:130:LYS:HA	1.92	0.52
2:B:223:LYS:HB2	2:B:226:LEU:HD23	1.92	0.51
1:A:184:CYS:HB2	1:A:188:CYS:HB2	1.93	0.51
1:A:77:SER:HB3	1:A:99:LEU:HD11	1.92	0.51
3:F:76:ILE:HA	3:F:80:ALA:HB3	1.92	0.51
2:E:163:LEU:HG	2:E:168:VAL:HG22	1.93	0.51
2:B:205:SER:HB2	2:B:210:ARG:HB2	1.92	0.51
1:D:115:PHE:CD1	1:D:288:ILE:HD11	2.46	0.51
1:A:250:ASN:HA	1:A:259:ILE:HG23	1.92	0.51
1:D:80:TYR:CD2	1:D:91:LYS:HB3	2.46	0.51
2:B:83:ILE:HD13	2:B:191:ILE:HG21	1.93	0.51
2:B:220:ILE:HD13	2:B:234:LEU:HB2	1.94	0.50
1:A:273:GLU:HA	1:A:295:LEU:HD13	1.93	0.50
2:B:212:ILE:HG22	2:B:213:ILE:H	1.77	0.50
2:B:18:LEU:HD13	2:B:26:THR:HA	1.94	0.49
2:E:48:THR:HG21	2:E:86:TYR:HD1	1.76	0.49
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.93	0.49
2:E:44:ARG:NH2	2:E:54:LEU:HB3	2.28	0.49
1:D:289:THR:HG22	1:D:302:ASN:HA	1.94	0.49
2:E:103:GLU:OE1	2:E:119:ARG:HD2	2.12	0.49
1:A:259:ILE:HD11	1:A:277:PRO:HB3	1.95	0.49
2:E:212:ILE:HG22	2:E:213:ILE:H	1.78	0.49
1:A:55:SER:HB3	1:D:88:MET:HG2	1.94	0.48
3:F:64:LEU:HD21	3:F:80:ALA:HB1	1.95	0.48
1:D:75:TYR:HD2	1:D:248:ILE:HG12	1.78	0.48
4:F:1001:APC:H8	4:F:1001:APC:O5'	2.12	0.48
1:A:241:ASP:HB2	1:A:244:ARG:HG2	1.95	0.48
1:A:317:LEU:HD22	1:A:322:LEU:HD12	1.94	0.48
1:A:192:ASP:HB2	1:A:195:GLU:HG3	1.96	0.48
2:B:44:ARG:NH2	2:B:90:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:220:ILE:HD13	2:E:234:LEU:HD13	1.95	0.48
3:C:71:SER:HB3	3:C:74:ARG:NH2	2.29	0.48
1:A:52:LEU:HD23	1:D:47:THR:HG22	1.95	0.48
1:A:63:TYR:HA	1:A:67:ARG:HG2	1.96	0.47
1:D:170:VAL:HG11	1:D:266:LEU:HD21	1.96	0.47
2:B:229:GLU:OE2	2:B:232:ARG:NH2	2.47	0.47
1:D:153:THR:HG21	1:D:178:PHE:HB2	1.95	0.47
3:F:90:VAL:HG23	3:F:91:ASN:O	2.14	0.47
1:A:294:VAL:HG21	1:A:317:LEU:HD21	1.96	0.47
2:E:31:LEU:HD21	2:E:69:THR:HG21	1.97	0.47
1:A:41:GLN:HB2	1:A:48:TYR:CE2	2.50	0.47
3:F:145:ASN:HB3	3:F:149:ARG:CZ	2.45	0.47
1:A:118:VAL:O	1:A:303:ARG:NH2	2.48	0.46
2:B:235:ILE:HG21	2:B:263:LEU:HB3	1.97	0.46
3:C:82:ARG:HD3	3:C:128:LEU:HB3	1.95	0.46
3:F:148:ILE:HG23	3:F:152:LYS:HE2	1.97	0.46
1:A:280:GLY:HA3	1:A:328:TYR:HE1	1.80	0.46
2:B:220:ILE:HD13	2:B:234:LEU:HD13	1.98	0.46
1:D:149:GLY:O	1:D:153:THR:HG23	2.15	0.46
1:D:85:ALA:O	1:D:91:LYS:HE3	2.15	0.46
2:B:163:LEU:HG	2:B:168:VAL:HG22	1.97	0.46
1:D:242:VAL:HG12	1:D:243:LYS:HG3	1.98	0.46
2:B:127:LEU:HD23	2:B:132:ARG:HH11	1.80	0.46
2:E:124:LYS:HG2	2:E:135:GLN:HG2	1.97	0.45
1:A:318:HIS:HD2	1:A:324:GLU:HA	1.81	0.45
2:B:158:LEU:HD11	2:B:163:LEU:HD21	1.98	0.45
1:A:75:TYR:HD2	1:A:248:ILE:HG12	1.81	0.45
2:B:213:ILE:HG22	2:B:214:PRO:HD2	1.99	0.45
2:B:200:PRO:O	2:B:203:LEU:N	2.50	0.45
1:A:92:ALA:HB1	3:C:115:TRP:CD1	2.53	0.44
2:B:12:LYS:O	2:B:68:TYR:OH	2.30	0.44
2:E:126:TYR:CE1	2:E:133:ILE:HG12	2.52	0.44
1:A:175:ASN:OD1	1:A:320:ARG:NH2	2.51	0.44
1:D:294:VAL:HG21	1:D:317:LEU:HD21	1.99	0.44
1:D:188:CYS:HB2	2:E:143:ILE:HD11	1.99	0.44
2:E:149:THR:HA	2:E:152:LEU:HD12	1.98	0.44
1:D:192:ASP:HB2	1:D:195:GLU:HG3	1.99	0.44
1:D:110:LEU:HD21	1:D:145:CYS:SG	2.58	0.44
1:D:118:VAL:O	1:D:303:ARG:NH2	2.50	0.43
1:A:83:PRO:HD2	1:D:86:ARG:NH2	2.33	0.43
2:E:7:LYS:HB3	2:E:97:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:105:ASN:O	2:E:109:ILE:HG13	2.18	0.43
2:B:240:ASP:O	3:C:49:PRO:HG3	2.18	0.43
1:A:44:GLY:HA3	1:D:126:GLU:OE1	2.18	0.43
1:A:322:LEU:HA	1:A:322:LEU:HD23	1.78	0.43
2:E:110:SER:HB2	2:E:115:LEU:HB2	2.00	0.43
3:F:63:VAL:HG21	3:F:147:ILE:HG23	2.01	0.43
2:E:232:ARG:HA	2:E:263:LEU:HD21	2.01	0.43
2:E:32:LEU:HD21	2:E:203:LEU:HB2	2.00	0.43
2:B:200:PRO:O	2:B:202:LYS:N	2.52	0.42
2:E:170:LEU:HD22	2:E:174:GLN:HB3	2.00	0.42
2:B:205:SER:HA	2:B:208:GLU:HB2	2.00	0.42
3:C:142:GLU:HG3	3:C:142:GLU:H	1.64	0.42
3:F:75:PHE:CE2	3:F:80:ALA:HB2	2.53	0.42
3:F:136:ILE:HG22	3:F:144:TYR:HB2	2.00	0.42
2:B:42:LYS:HE3	2:B:209:ARG:HG3	2.02	0.42
1:A:282:THR:HB	1:A:325:VAL:HG13	2.02	0.42
2:B:152:LEU:HD21	2:B:181:GLU:HG3	2.01	0.42
1:D:138:TYR:HE2	1:D:292:THR:HG21	1.83	0.42
2:E:139:CYS:HA	2:E:168:VAL:O	2.20	0.42
3:C:75:PHE:CE2	3:C:80:ALA:HB2	2.55	0.42
2:E:158:LEU:HD11	2:E:163:LEU:HD21	2.02	0.42
2:E:57:TYR:O	2:E:63:PRO:HB3	2.20	0.42
1:D:13:LEU:O	1:D:16:SER:OG	2.35	0.41
1:D:81:GLN:HB2	1:D:92:ALA:HB3	2.02	0.41
1:D:307:ILE:HG22	1:D:309:ILE:HG23	2.02	0.41
2:E:214:PRO:HG2	2:E:217:ILE:HD13	2.02	0.41
1:D:298:ILE:O	1:D:299:ILE:HD12	2.20	0.41
2:E:193:PRO:HA	2:E:196:LEU:HD13	2.02	0.41
2:E:128:GLU:O	2:E:131:ARG:HD3	2.20	0.41
2:B:199:ILE:HG23	2:B:203:LEU:HD23	2.03	0.41
1:D:201:GLU:HG2	1:D:206:ILE:HG13	2.03	0.41
3:F:71:SER:HB3	3:F:74:ARG:NH2	2.36	0.41
2:B:149:THR:HA	2:B:152:LEU:HD12	2.03	0.41
2:B:83:ILE:HG23	2:B:191:ILE:HD12	2.03	0.41
3:C:84:LEU:O	3:C:90:VAL:HG22	2.21	0.41
3:F:64:LEU:HA	3:F:102:PHE:CD1	2.56	0.41
2:E:62:GLU:O	2:E:66:VAL:HG23	2.21	0.40
1:A:307:ILE:HG22	1:A:309:ILE:HG23	2.02	0.40
3:C:131:TRP:HE3	3:C:136:ILE:HG12	1.87	0.40
1:A:156:LEU:HD23	1:A:180:VAL:HG21	2.03	0.40
1:A:211:TYR:HB3	2:B:127:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:ASN:OD1	1:D:230:ASN:N	2.51	0.40
1:A:230:ASN:OD1	1:A:230:ASN:N	2.53	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	318/330 (96%)	302 (95%)	15 (5%)	1 (0%)	41	71
1	D	317/330 (96%)	302 (95%)	14 (4%)	1 (0%)	41	71
2	B	275/307 (90%)	253 (92%)	20 (7%)	2 (1%)	22	54
2	E	270/307 (88%)	253 (94%)	16 (6%)	1 (0%)	34	66
3	C	105/154 (68%)	92 (88%)	12 (11%)	1 (1%)	15	45
3	F	96/154 (62%)	89 (93%)	7 (7%)	0	100	100
All	All	1381/1582 (87%)	1291 (94%)	84 (6%)	6 (0%)	34	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	LYS
2	B	295	VAL
2	B	222	ALA
3	C	55	SER
1	D	109	LYS
2	E	222	ALA

### 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	285/293 (97%)	275 (96%)	10 (4%)	36	70
1	D	284/293 (97%)	279 (98%)	5 (2%)	59	85
2	B	261/284 (92%)	249 (95%)	12 (5%)	27	60
2	E	256/284 (90%)	249 (97%)	7 (3%)	44	77
3	C	100/140 (71%)	99 (99%)	1 (1%)	76	92
3	F	91/140 (65%)	88 (97%)	3 (3%)	38	72
All	All	1277/1434 (89%)	1239 (97%)	38 (3%)	42	75

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	46	ASP
1	A	50	ARG
1	A	108	CYS
1	A	153	THR
1	A	188	CYS
1	A	242	VAL
1	A	262	ARG
1	A	320	ARG
1	A	329	VAL
2	B	16	ASP
2	B	101	GLU
2	B	120	CYS
2	B	121	ASP
2	B	131	ARG
2	B	155	ASP
2	B	181	GLU
2	B	212	ILE
2	B	238	TYR
2	B	295	VAL
2	B	297	ASN
2	B	299	LEU

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Mol	Chain	Res	Type
1	D	102	ILE
1	D	108	CYS
1	D	230	ASN
1	D	288	ILE
1	D	320	ARG
2	E	120[A]	CYS
2	E	120[B]	CYS
2	E	131	ARG
2	E	181	GLU
2	E	212	ILE
2	E	213	ILE
2	E	238	TYR
3	C	148	ILE
3	F	69	GLN
3	F	114	SER
3	F	148	ILE

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

Mol	Chain	Res	Type
1	A	318	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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.



In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	APC	F	1001	5	27,33,33	0.79	0	31,52,52	1.14	3 (9%)
4	APC	C	1001	5	27,33,33	0.84	0	31,52,52	1.17	3 (9%)
4	APC	D	1001	5	27,33,33	0.77	0	31,52,52	1.12	3 (9%)
4	APC	A	1001	5	27,33,33	0.82	1 (3%)	31,52,52	1.20	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	APC	F	1001	5	-	10/15/38/38	0/3/3/3
4	APC	C	1001	5	-	9/15/38/38	0/3/3/3
4	APC	D	1001	5	-	9/15/38/38	0/3/3/3
4	APC	A	1001	5	-	5/15/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	APC	PB-O2B	-2.00	1.51	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1001	APC	O1B-PB-C3A	4.34	120.54	109.07
4	D	1001	APC	O1B-PB-C3A	4.22	120.23	109.07
4	A	1001	APC	O2B-PB-C3A	3.54	121.07	106.58
4	A	1001	APC	O1A-PA-C3A	3.47	118.24	109.07
4	C	1001	APC	O2B-PB-C3A	3.44	120.64	106.58
4	C	1001	APC	O1A-PA-C3A	3.40	118.06	109.07
4	D	1001	APC	O2A-PA-C3A	2.99	118.82	106.58
4	F	1001	APC	O2A-PA-C3A	2.96	118.67	106.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1001	APC	C5-C6-N6	2.32	123.87	120.35
4	C	1001	APC	C5-C6-N6	2.30	123.85	120.35
4	A	1001	APC	C5-C6-N6	2.26	123.79	120.35
4	D	1001	APC	C5-C6-N6	2.24	123.76	120.35

There are no chirality outliers.

All (33) torsion outliers are listed below:

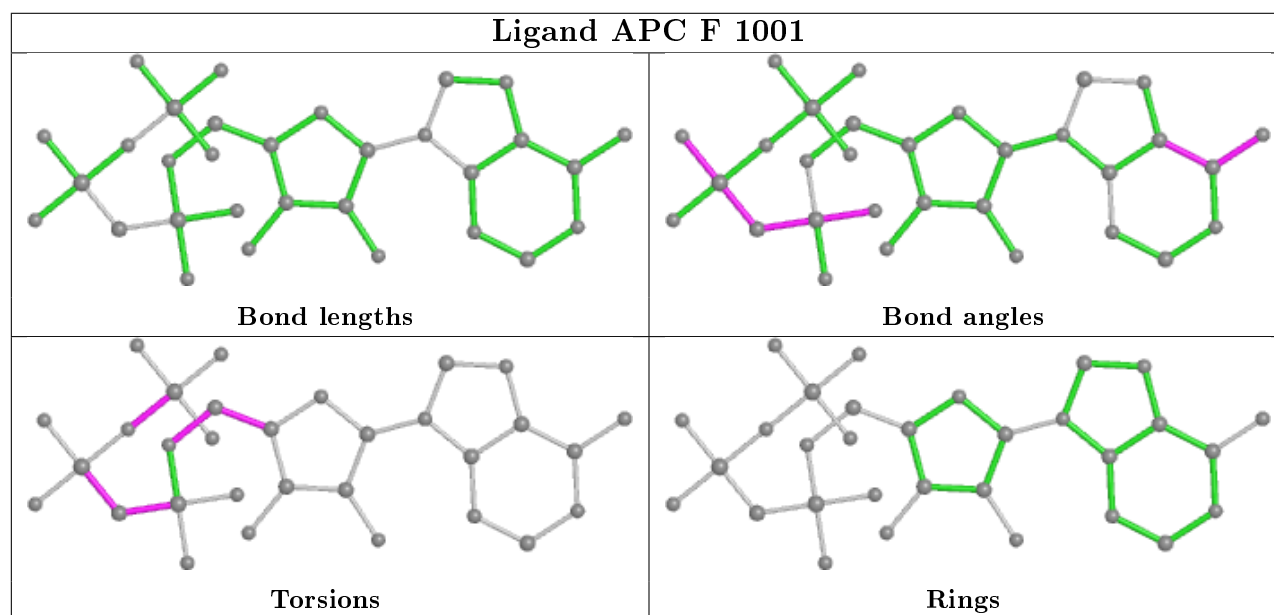
Mol	Chain	Res	Type	Atoms
4	F	1001	APC	PA-C3A-PB-O1B
4	F	1001	APC	PA-C3A-PB-O2B
4	F	1001	APC	PA-C3A-PB-O3B
4	F	1001	APC	PB-C3A-PA-O1A
4	F	1001	APC	PB-C3A-PA-O2A
4	F	1001	APC	PB-C3A-PA-O5'
4	F	1001	APC	O4'-C4'-C5'-O5'
4	F	1001	APC	C3'-C4'-C5'-O5'
4	C	1001	APC	PB-O3B-PG-O2G
4	C	1001	APC	PA-C3A-PB-O1B
4	C	1001	APC	PA-C3A-PB-O2B
4	C	1001	APC	PA-C3A-PB-O3B
4	C	1001	APC	C5'-O5'-PA-O1A
4	D	1001	APC	PB-O3B-PG-O2G
4	D	1001	APC	PB-O3B-PG-O3G
4	D	1001	APC	PA-C3A-PB-O1B
4	D	1001	APC	PA-C3A-PB-O3B
4	D	1001	APC	C5'-O5'-PA-O1A
4	A	1001	APC	PB-O3B-PG-O3G
4	A	1001	APC	PA-C3A-PB-O1B
4	A	1001	APC	PA-C3A-PB-O2B
4	A	1001	APC	PA-C3A-PB-O3B
4	A	1001	APC	C5'-O5'-PA-O2A
4	F	1001	APC	C4'-C5'-O5'-PA
4	F	1001	APC	PB-O3B-PG-O3G
4	D	1001	APC	PA-C3A-PB-O2B
4	C	1001	APC	C5'-O5'-PA-O2A
4	D	1001	APC	C5'-O5'-PA-O2A
4	D	1001	APC	O4'-C4'-C5'-O5'
4	C	1001	APC	PB-O3B-PG-O3G
4	C	1001	APC	O4'-C4'-C5'-O5'
4	C	1001	APC	C3'-C4'-C5'-O5'
4	D	1001	APC	C3'-C4'-C5'-O5'

There are no ring outliers.

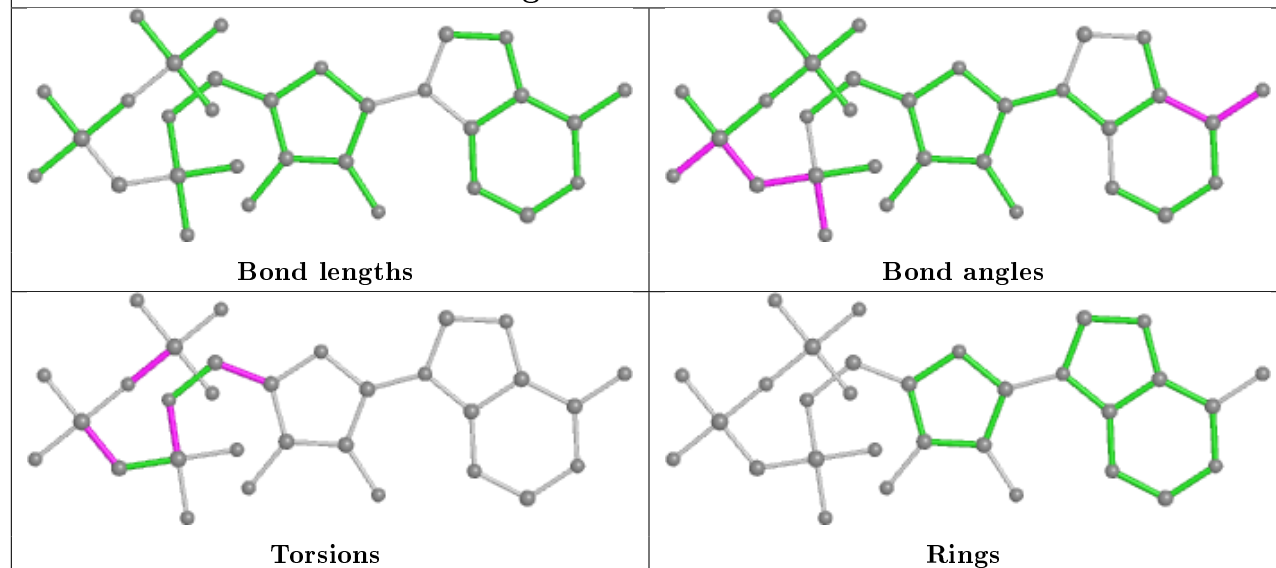
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1001	APC	2	0
4	A	1001	APC	1	0

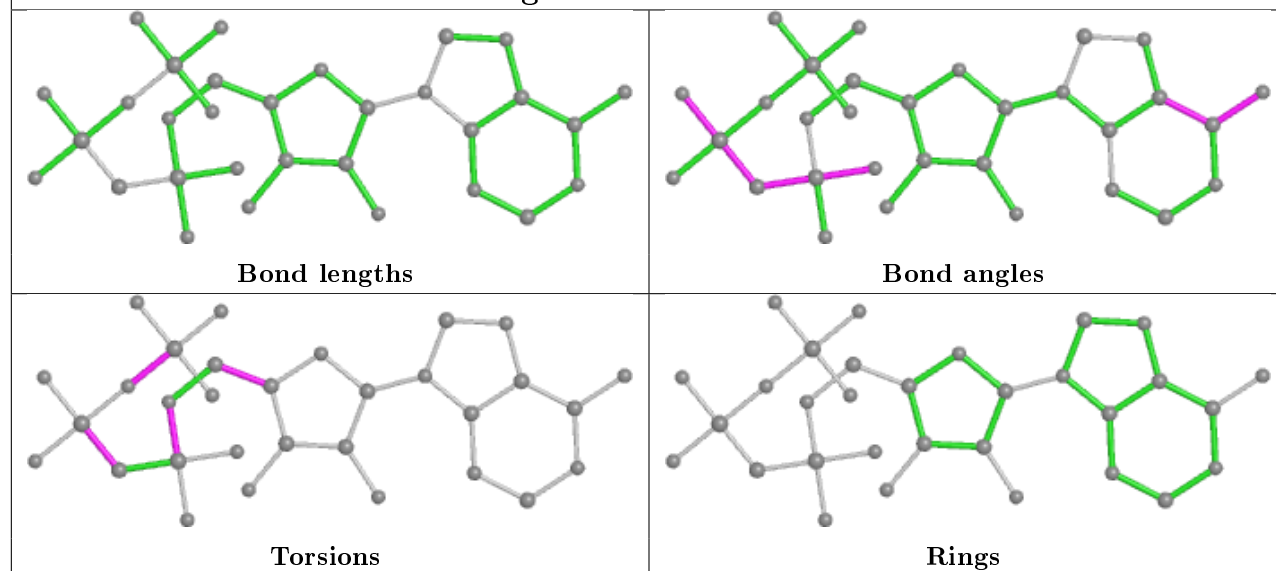
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

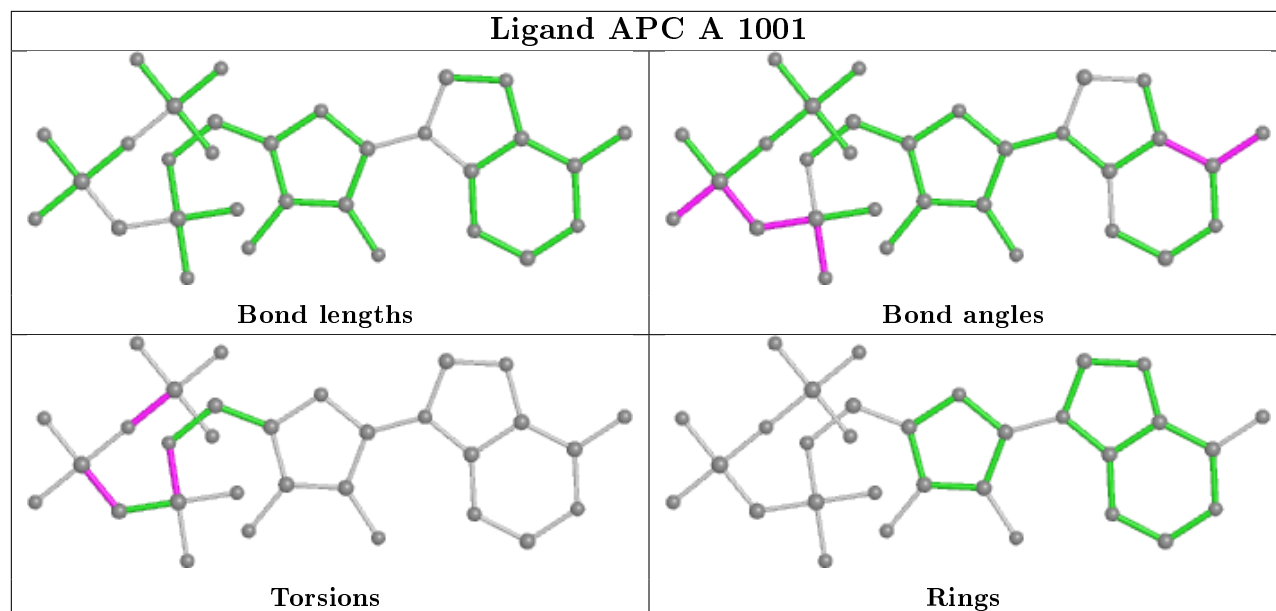


## Ligand APC C 1001



## Ligand APC D 1001





## 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	319/330 (96%)	-0.05	0 100 100	46, 70, 107, 146	0
1	D	319/330 (96%)	0.15	6 (1%) 66 65	48, 79, 128, 167	0
2	B	279/307 (90%)	0.76	41 (14%) 2 1	55, 107, 200, 221	0
2	E	273/307 (88%)	0.94	54 (19%) 1 0	55, 112, 218, 238	0
3	C	107/154 (69%)	0.07	2 (1%) 66 65	65, 102, 147, 168	0
3	F	98/154 (63%)	0.53	17 (17%) 1 1	80, 129, 166, 173	0
All	All	1395/1582 (88%)	0.40	120 (8%) 10 8	46, 92, 189, 238	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	264	TYR	12.6
2	E	244	GLY	12.1
2	E	252	MET	10.6
2	B	299	LEU	7.6
2	E	267	TYR	7.4
2	B	265	ARG	7.3
2	E	251	ILE	7.2
2	E	222	ALA	7.1
2	E	249	VAL	7.0
2	E	264	TYR	6.9
2	E	241	ILE	6.9
2	E	255	TYR	6.3
2	E	245	LEU	6.3
3	F	66	MET	6.1
2	B	259	ASN	6.0
2	E	299	LEU	6.0
2	B	262	ASP	6.0
2	B	230	GLU	6.0
2	E	263	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
2	B	263	LEU	5.8
2	E	237	PHE	5.8
2	E	235	ILE	5.7
2	E	233	THR	5.4
2	E	248	ILE	5.3
3	F	65	GLU	5.3
2	E	256	ASN	5.2
2	E	254	LYS	5.2
3	F	68	LEU	5.1
2	B	261	GLU	5.0
2	E	239	ILE	5.0
2	E	259	ASN	4.9
2	B	233	THR	4.9
2	B	260	VAL	4.8
2	B	235	ILE	4.7
2	E	240	ASP	4.7
2	B	298	PRO	4.7
2	B	222	ALA	4.5
2	B	267	TYR	4.5
3	F	69	GLN	4.4
2	E	243	LYS	4.4
2	E	217	ILE	4.2
2	B	251	ILE	4.0
2	E	246	SER	3.9
2	B	249	VAL	3.9
2	E	258	SER	3.8
2	E	215	PRO	3.8
2	E	242	GLY	3.7
2	E	265	ARG	3.7
2	E	230	GLU	3.7
3	F	107	GLN	3.6
1	D	132	ASN	3.6
2	B	244	GLY	3.5
2	E	262	ASP	3.4
2	E	250	SER	3.4
2	B	234	LEU	3.4
2	E	231	ILE	3.4
2	B	257	VAL	3.4
2	E	301	LEU	3.3
2	B	231	ILE	3.3
2	E	220	ILE	3.3
3	F	151	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	106	HIS	3.2
2	B	228	GLU	3.1
2	B	258	SER	3.1
2	E	238	TYR	3.1
2	E	253	LYS	3.1
2	B	220	ILE	3.0
2	B	221	LEU	2.9
2	B	239	ILE	2.9
3	F	154	SER	2.9
2	B	303	PHE	2.9
2	B	229	GLU	2.9
2	E	236	THR	2.9
2	E	49	LYS	2.8
2	E	216	CYS	2.8
2	B	88	TYR	2.8
2	B	237	PHE	2.8
2	E	219	ASN	2.7
3	F	147	ILE	2.7
3	C	50	GLN	2.7
2	E	257	VAL	2.7
2	E	227	ASN	2.6
3	F	105	LYS	2.6
2	E	196	LEU	2.6
2	B	154	GLU	2.6
2	E	80	VAL	2.6
2	B	245	LEU	2.5
2	B	219	ASN	2.5
3	F	150	VAL	2.5
3	F	108	SER	2.5
2	B	255	TYR	2.5
2	B	223	LYS	2.4
2	B	217	ILE	2.4
2	E	31	LEU	2.4
2	E	221	LEU	2.3
3	F	62	LYS	2.3
2	E	82	LEU	2.3
2	E	261	GLU	2.3
3	F	64	LEU	2.3
2	E	228	GLU	2.3
1	D	133	VAL	2.2
3	F	152	LYS	2.2
2	E	88	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	52	LYS	2.2
1	D	129	GLU	2.2
2	B	266	LYS	2.2
2	B	32	LEU	2.1
2	B	107	LEU	2.1
2	E	212	ILE	2.1
2	E	27	LEU	2.1
3	F	148	ILE	2.1
2	B	252	MET	2.1
1	D	128	CYS	2.1
2	B	3	LEU	2.1
2	B	18	LEU	2.0
3	F	149	ARG	2.0
3	F	104	TYR	2.0
1	D	65	VAL	2.0
2	E	154	GLU	2.0
2	E	32	LEU	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.

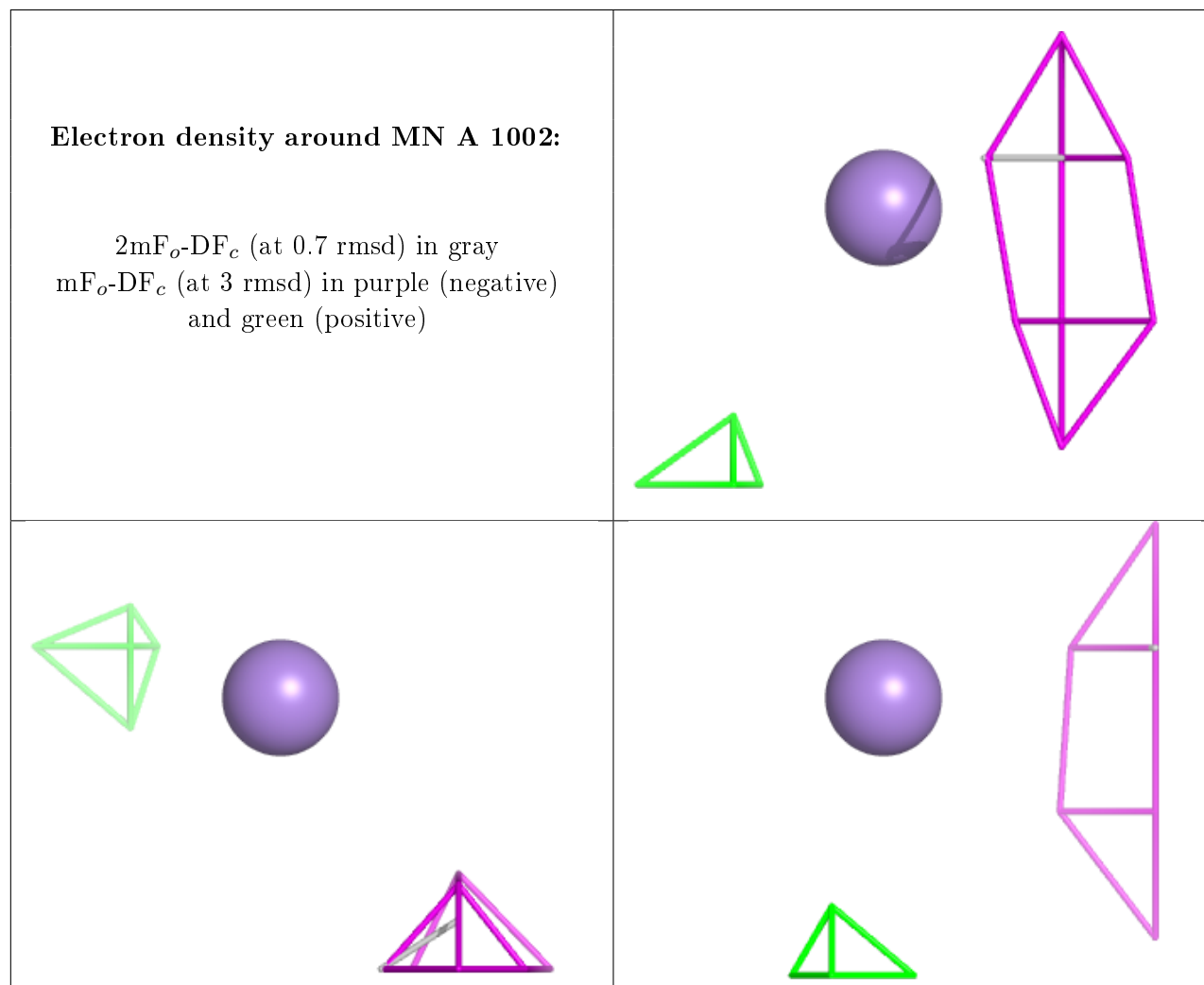
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MN	A	1002	1/1	0.73	0.09	97,97,97,97	1
4	APC	F	1001	31/31	0.83	0.28	90,127,142,145	31
5	MN	C	1002	1/1	0.84	0.10	112,112,112,112	0
6	ZN	D	1003	1/1	0.86	0.04	142,142,142,142	0
4	APC	A	1001	31/31	0.89	0.25	53,85,98,108	31
4	APC	C	1001	31/31	0.93	0.21	79,107,127,132	31

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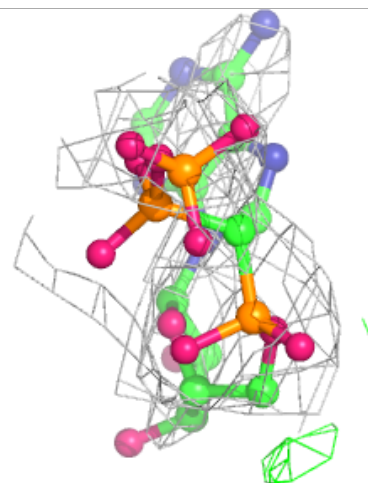
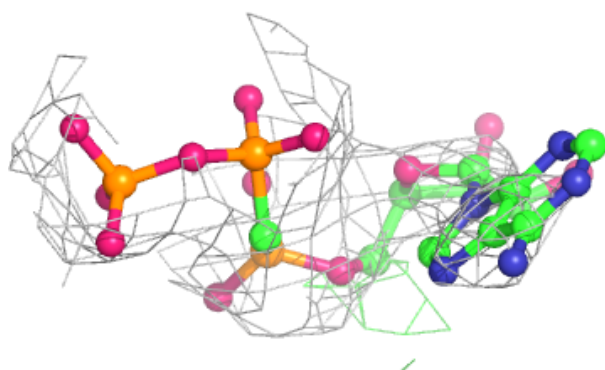
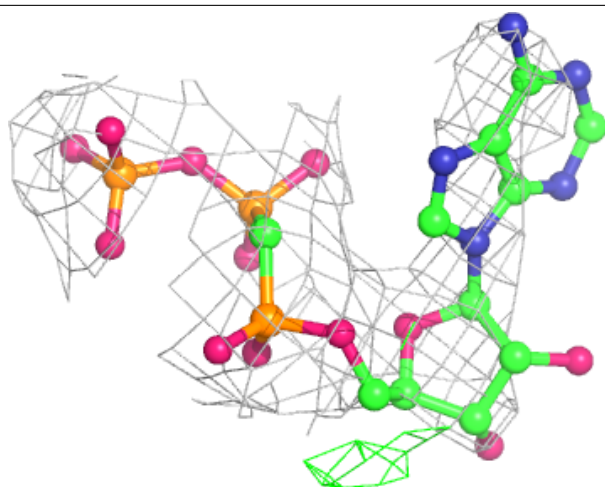
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MN	F	1002	1/1	0.93	0.09	118,118,118,118	1
5	MN	D	1002	1/1	0.96	0.21	70,70,70,70	0
4	APC	D	1001	31/31	0.98	0.20	42,68,78,86	0
6	ZN	A	1003	1/1	0.99	0.13	91,91,91,91	0

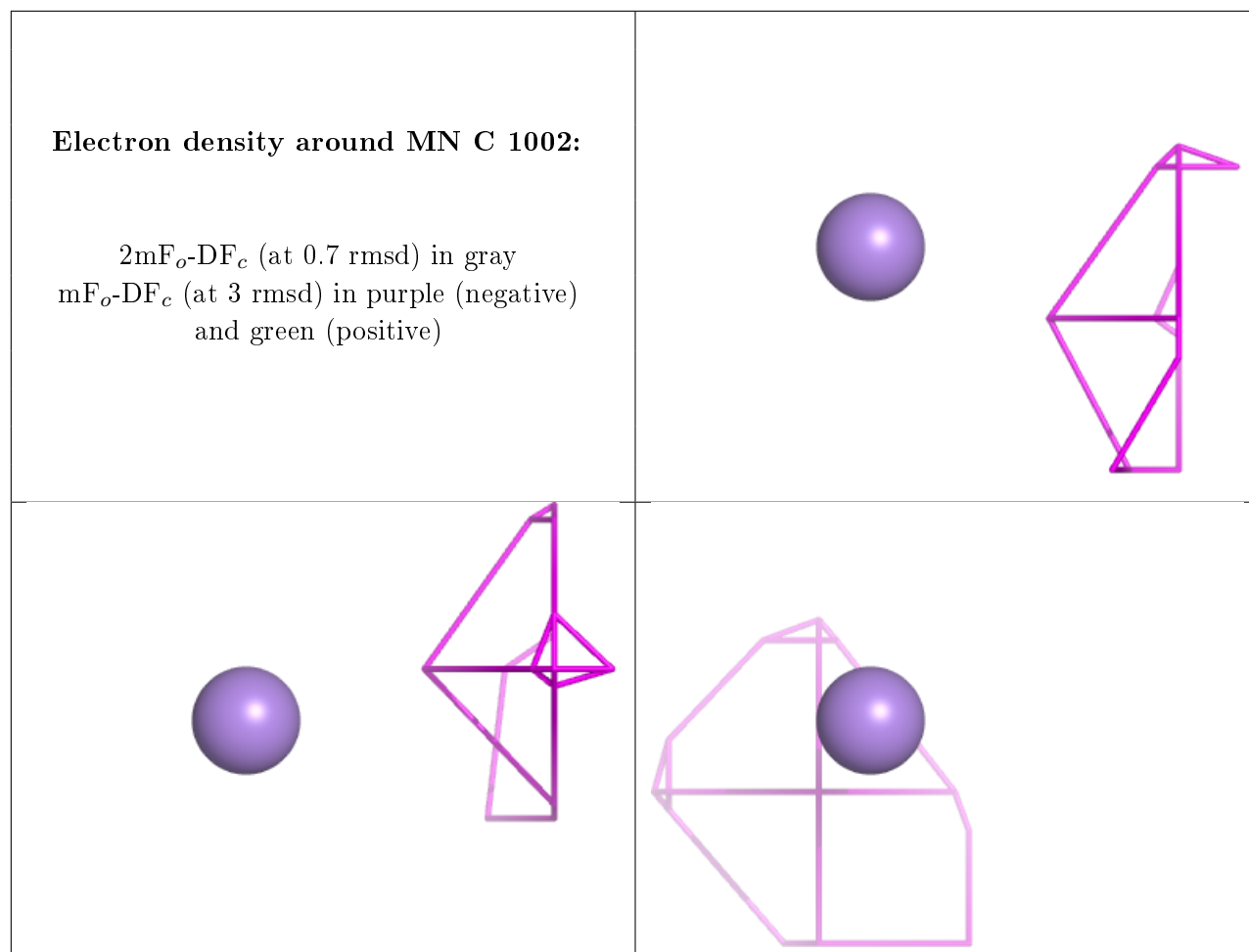
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around APC F 1001:**

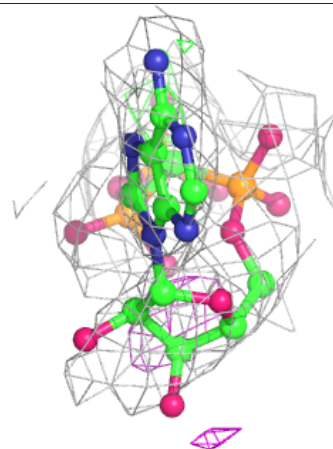
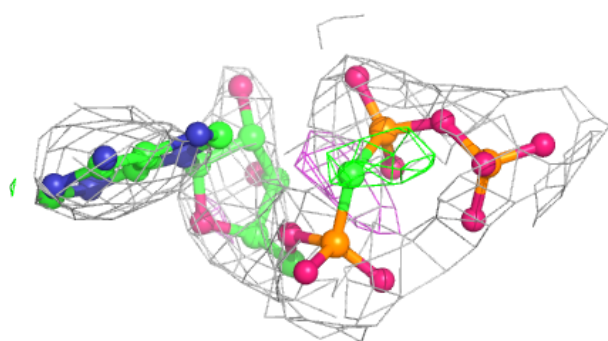
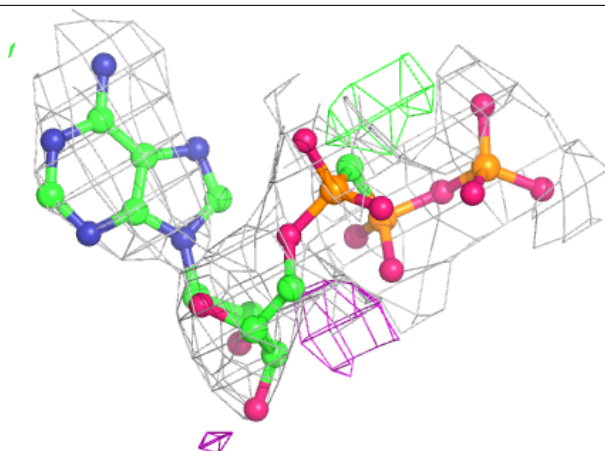
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





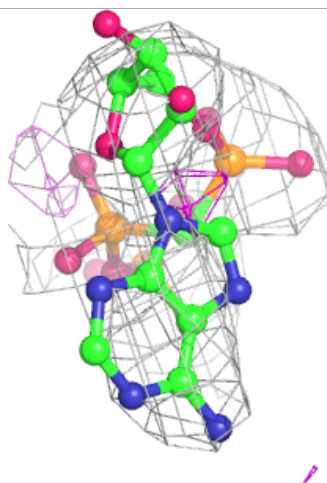
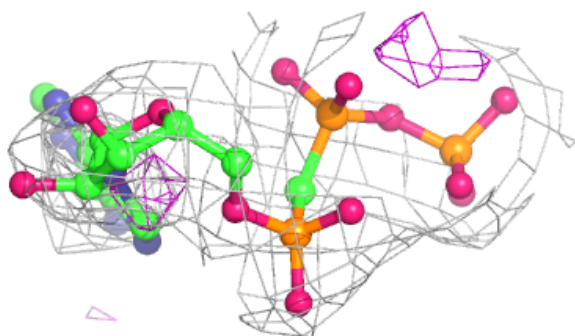
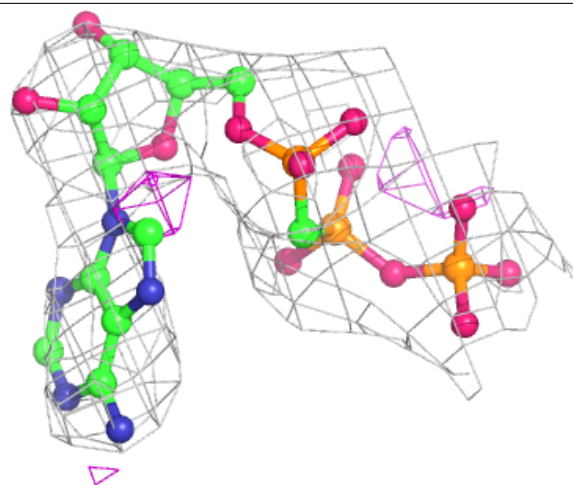
**Electron density around APC A 1001:**

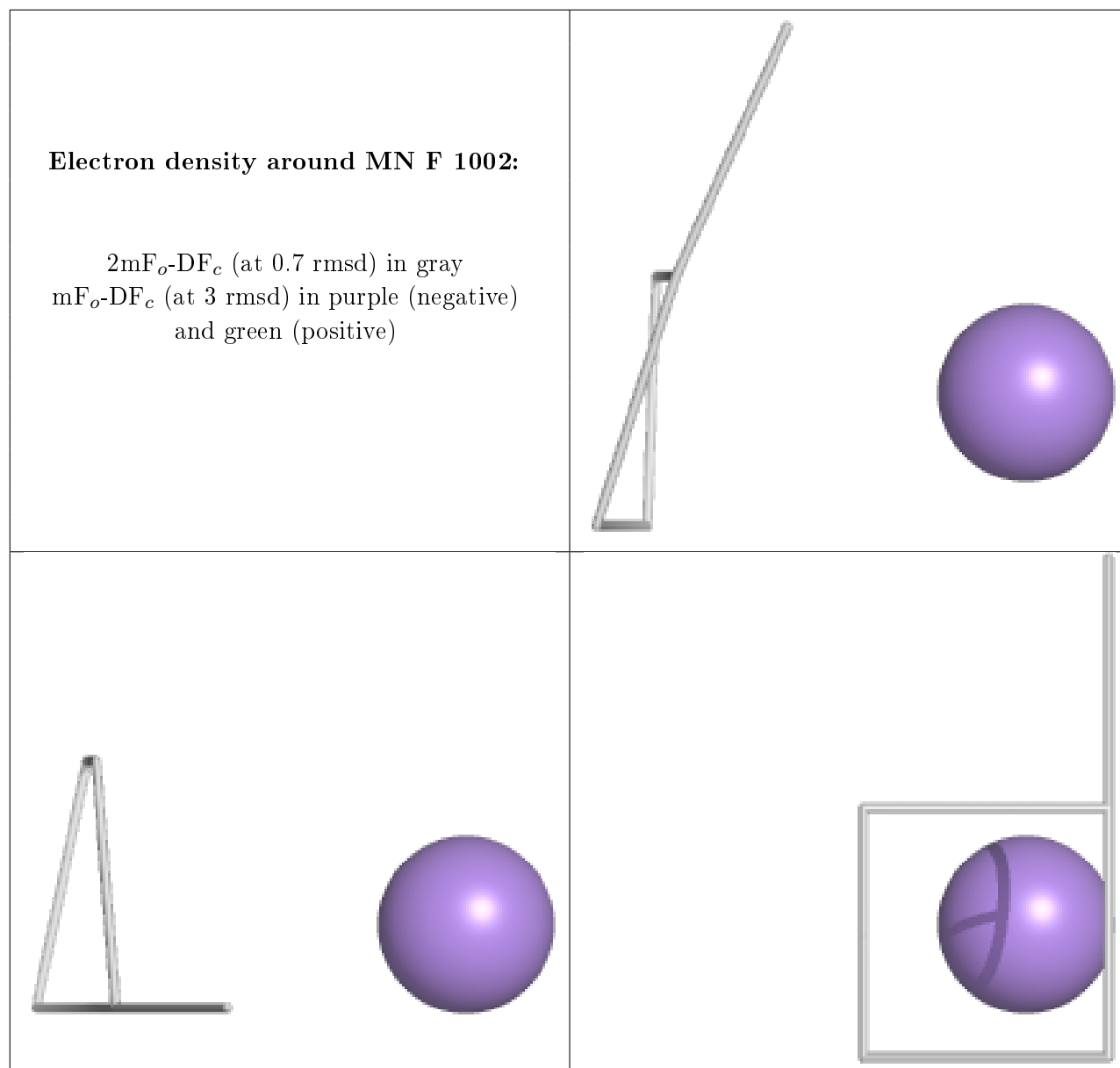
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

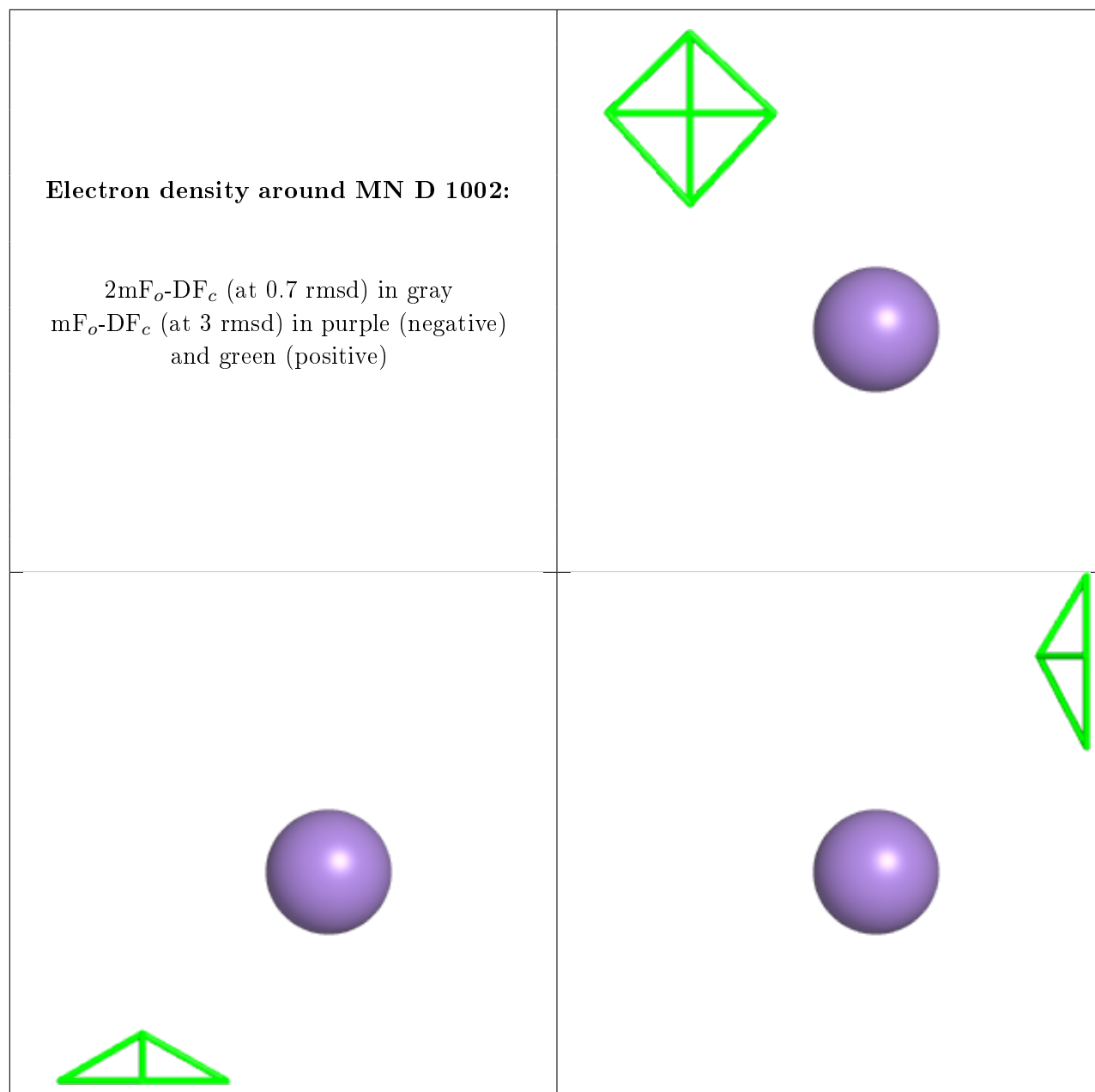


**Electron density around APC C 1001:**

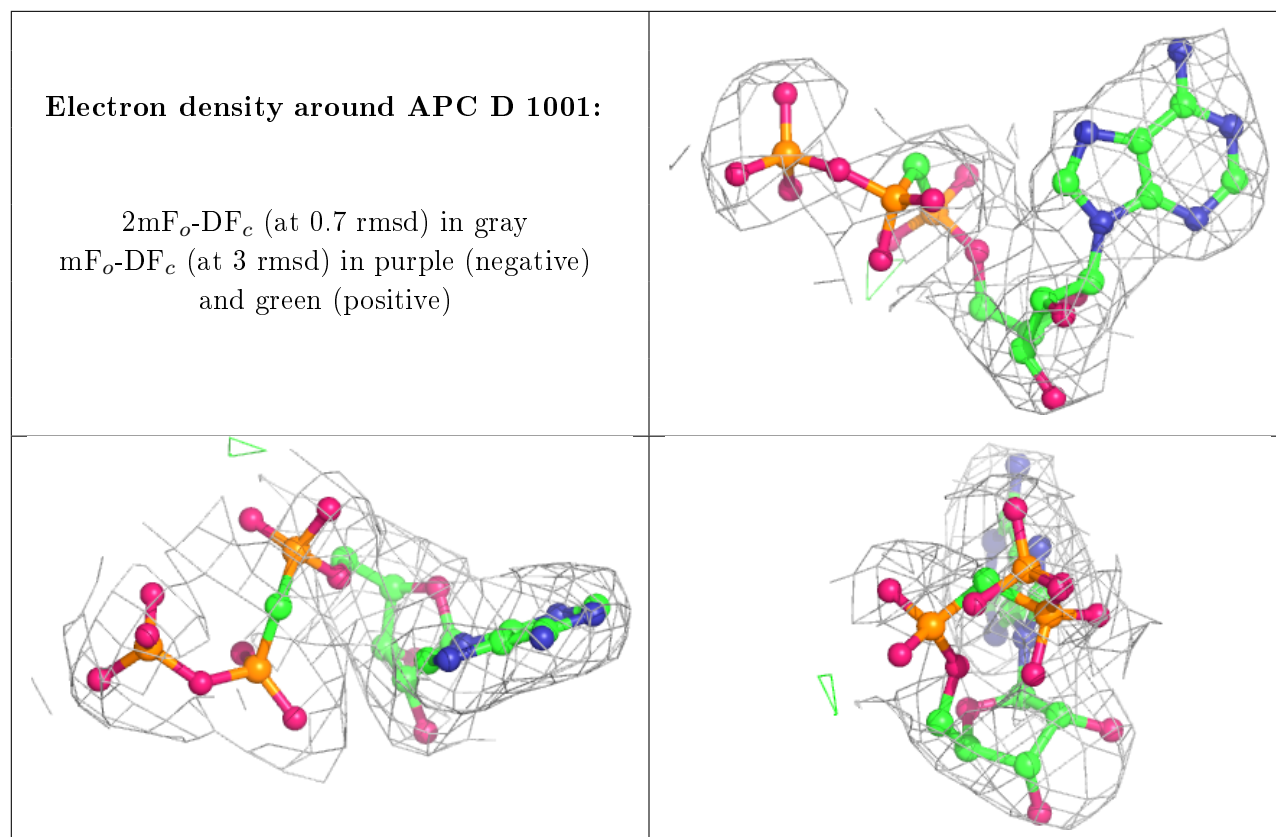
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)











## 6.5 Other polymers [i](#)

There are no such residues in this entry.