Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 06:04 PM EDT

PDB ID	:	8ENK
Title	:	Crystal structure of UAP56 in complex with Tho1, the yeast homolog of human SARNP
Authors	:	Xie, Y.; Ren, Y.
Deposited on	:	2022-09-30
Resolution	:	2.50 Å(reported)

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

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

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

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

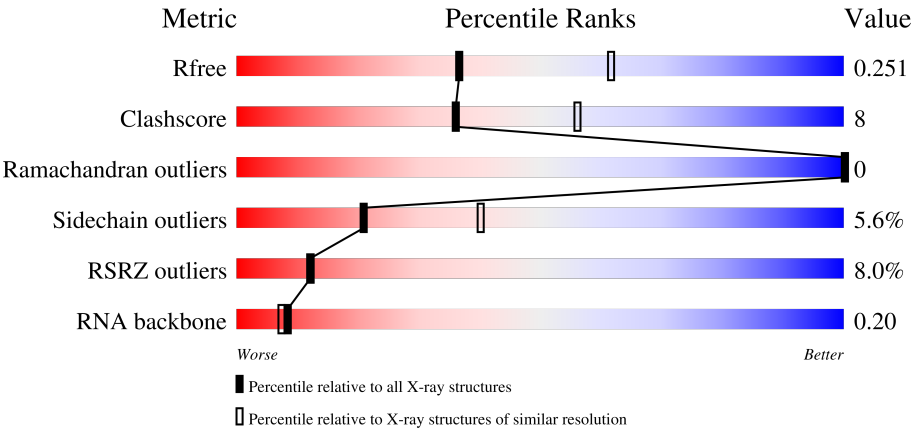
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	390	6% 76% 19%
1	B	390	9% 69% 27%
2	E	61	10% 67% 18% 13%
3	M	15	7% 7% 20% 13% 60%

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Mol	Chain	Length	Quality of chain
3	N	15	13% 13% 7% 67%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6879 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 Spliceosome RNA helicase DDX39B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			3069	1956	533	558	22			
1	B	381	Total	C	N	O	S	0	0	0
			3081	1962	535	562	22			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	expression tag	UNP Q13838
A	40	ALA	-	expression tag	UNP Q13838
A	41	MET	-	expression tag	UNP Q13838
A	42	GLY	-	expression tag	UNP Q13838
A	43	SER	-	expression tag	UNP Q13838
B	39	GLY	-	expression tag	UNP Q13838
B	40	ALA	-	expression tag	UNP Q13838
B	41	MET	-	expression tag	UNP Q13838
B	42	GLY	-	expression tag	UNP Q13838
B	43	SER	-	expression tag	UNP Q13838

- Molecule 2 is a protein called Protein THO1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	53	Total	C	N	O	0	0	0
			428	266	79	83			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	118	GLY	-	expression tag	UNP P40040
E	119	ALA	-	expression tag	UNP P40040
E	120	MET	-	expression tag	UNP P40040
E	121	GLY	-	expression tag	UNP P40040

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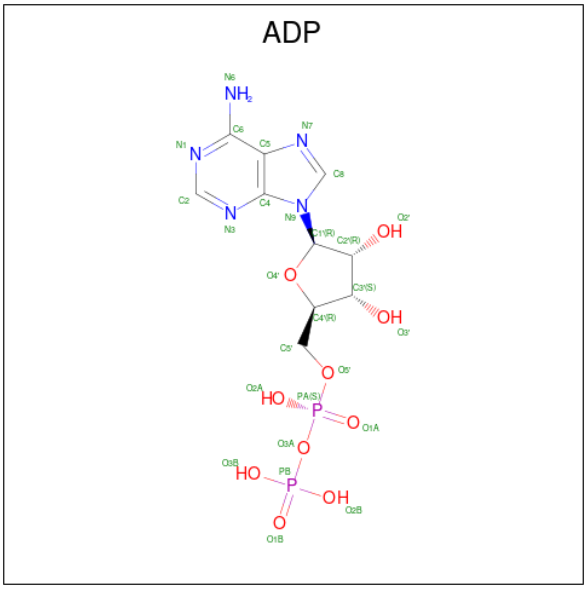
Chain	Residue	Modelled	Actual	Comment	Reference
E	122	SER	-	expression tag	UNP P40040

- Molecule 3 is a RNA chain called RNA.

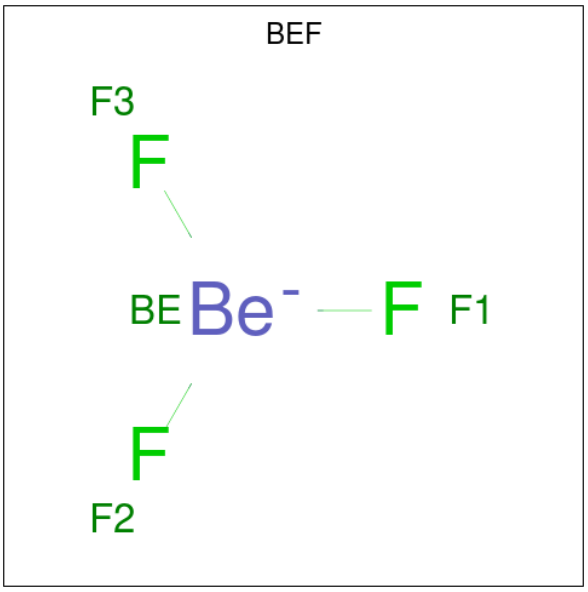
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			
3	N	5	Total	C	N	O	P	0	0	0
			100	45	10	40	5			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Be F 4 1 3	0	0
5	B	1	Total Be F 4 1 3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0

- Molecule 7 is water.

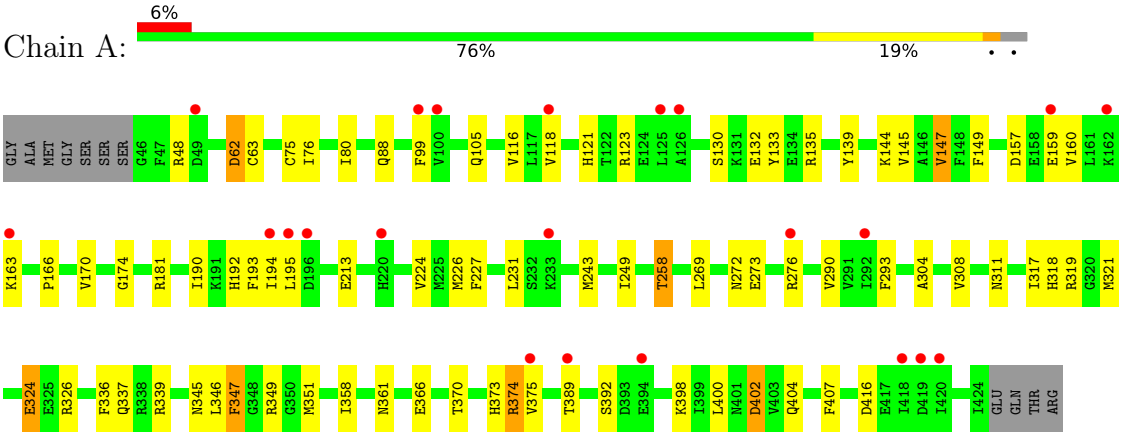
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	8	Total O 8 8	0	0
7	B	9	Total O 9 9	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

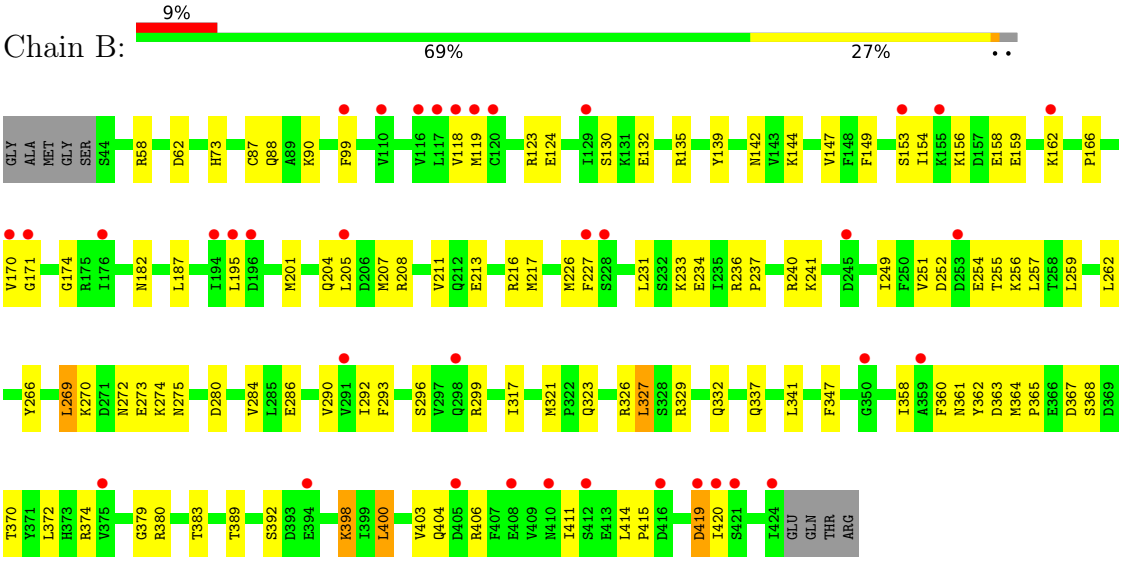
• Molecule 1: Spliceosome RNA helicase DDX39B

Chain A:



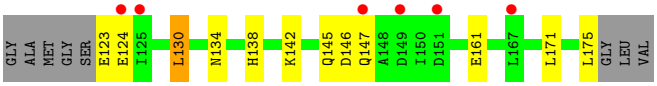
• Molecule 1: Spliceosome RNA helicase DDX39B

Chain B:



• Molecule 2: Protein THO1

Chain E:



• Molecule 3: RNA

• Molecule 3: RNA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.53Å 96.79Å 126.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.50 29.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.72-2.50) 99.8 (29.72-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.224 , 0.253 0.223 , 0.251	Depositor DCC
R_{free} test set	1993 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6879	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, BEF, 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	0.27	0/3124	0.52	0/4205
1	B	0.27	0/3136	0.52	0/4221
2	E	0.24	0/430	0.45	0/572
3	M	0.28	0/131	0.98	0/200
3	N	0.24	0/109	0.74	0/166
All	All	0.27	0/6930	0.53	0/9364

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	3069	0	3113	46	0
1	B	3081	0	3123	63	0
2	E	428	0	440	2	0
3	M	120	0	61	4	0
3	N	100	0	51	2	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	8	0	0	0	0
7	B	9	0	0	0	0
All	All	6879	0	6812	110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (110) 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:63:CYS:HB2	1:A:135:ARG:HH21	1.49	0.77
1:A:345:ASN:ND2	1:A:366:GLU:OE2	2.24	0.70
1:B:174:GLY:HA3	3:N:5:U:H5"	1.75	0.69
1:A:132:GLU:OE2	1:A:135:ARG:NH1	2.29	0.66
1:A:174:GLY:HA3	3:M:5:U:H5"	1.79	0.65
1:B:88:GLN:HB2	1:B:231:LEU:HD12	1.78	0.64
2:E:130:LEU:O	2:E:134:ASN:ND2	2.31	0.63
1:B:153:SER:HB3	1:B:156:LYS:HD2	1.80	0.62
1:B:290:VAL:HG22	1:B:358:ILE:HB	1.81	0.61
1:B:118:VAL:HB	1:B:170:VAL:HG12	1.84	0.60
1:A:269:LEU:HG	1:A:273:GLU:HB2	1.85	0.59
1:B:159:GLU:HA	1:B:162:LYS:HE2	1.85	0.59
1:B:205:LEU:HD13	1:B:208:ARG:HD2	1.84	0.59
1:B:270:LYS:HB2	1:B:273:GLU:HG3	1.85	0.59
1:B:299:ARG:NH2	1:B:363:ASP:OD1	2.33	0.57
1:A:195:LEU:HB2	1:A:226:MET:HG2	1.87	0.56
1:B:317:ILE:HG22	1:B:341:LEU:HD11	1.87	0.56
1:A:317:ILE:HD11	1:A:347:PHE:HB2	1.87	0.56
1:B:286:GLU:HB3	1:B:420:ILE:HD11	1.87	0.56
1:A:123:ARG:HG2	1:A:149:PHE:HB2	1.88	0.55
1:B:254:GLU:HG2	1:B:257:LEU:HD12	1.88	0.55
1:B:370:THR:O	1:B:374:ARG:HG3	2.06	0.55
1:B:62:ASP:OD2	1:B:139:TYR:OH	2.23	0.55
1:B:142:ASN:N	1:B:142:ASN:OD1	2.41	0.54
1:A:349:ARG:HB3	1:A:373:HIS:HB3	1.88	0.54
1:A:339:ARG:NH2	2:E:142:LYS:O	2.40	0.54
1:B:201:MET:HG3	1:B:207:MET:SD	2.47	0.54
1:A:290:VAL:HG12	1:A:358:ILE:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:GLY:HA2	1:B:383:THR:HG23	1.88	0.54
1:B:132:GLU:OE2	1:B:135:ARG:NH1	2.34	0.53
1:B:144:LYS:HB2	1:B:166:PRO:HA	1.91	0.53
1:B:233:LYS:HA	1:B:236:ARG:HD2	1.90	0.53
1:B:233:LYS:H	1:B:233:LYS:HD2	1.75	0.52
1:A:398:LYS:NZ	1:A:402:ASP:OD2	2.42	0.52
1:A:118:VAL:HG22	1:A:194:ILE:HB	1.92	0.52
1:B:323:GLN:HE21	1:B:327:LEU:HD13	1.75	0.51
1:B:414:LEU:HD12	1:B:415:PRO:HD2	1.91	0.51
1:B:147:VAL:HG23	1:B:170:VAL:HG23	1.91	0.51
1:B:280:ASP:O	1:B:284:VAL:HG12	2.10	0.51
1:A:258:THR:HG22	1:A:407:PHE:HB3	1.93	0.51
1:A:370:THR:O	1:A:374:ARG:HB2	2.10	0.51
1:A:130:SER:HB3	1:A:147:VAL:HG13	1.92	0.51
1:A:400:LEU:O	1:A:404:GLN:HG2	2.11	0.50
1:B:275:ASN:OD1	1:B:362:TYR:OH	2.27	0.50
1:B:368:SER:OG	1:B:406:ARG:NH1	2.45	0.50
1:B:204:GLN:HB3	1:B:207:MET:HB3	1.92	0.50
1:B:419:ASP:N	1:B:419:ASP:OD1	2.44	0.50
1:A:159:GLU:HG3	1:A:163:LYS:HE2	1.93	0.50
1:A:62:ASP:OD2	1:A:139:TYR:OH	2.23	0.49
1:A:133:TYR:HB3	1:A:145:VAL:HG11	1.94	0.49
1:A:361:ASN:HB2	1:A:389:THR:HA	1.94	0.49
1:A:76:ILE:O	1:A:80:ILE:HG12	2.11	0.49
1:B:237:PRO:O	1:B:241:LYS:HG2	2.12	0.49
1:A:347:PHE:CG	1:A:351:MET:HG3	2.48	0.49
1:B:213:GLU:OE1	1:B:216:ARG:NH2	2.36	0.49
1:B:124:GLU:OE1	1:B:326:ARG:NH2	2.45	0.48
1:A:319:ARG:NH1	3:M:4:U:OP2	2.44	0.48
1:B:321:MET:HE1	1:B:329:ARG:HD2	1.95	0.48
1:A:193:PHE:HB3	1:A:224:VAL:HG12	1.95	0.48
1:B:123:ARG:HG2	1:B:149:PHE:HB2	1.96	0.48
1:A:269:LEU:O	1:A:392:SER:HA	2.13	0.48
1:B:236:ARG:NH1	1:B:252:ASP:OD1	2.44	0.48
1:B:204:GLN:O	1:B:208:ARG:N	2.37	0.48
1:B:293:PHE:CG	1:B:374:ARG:HD2	2.48	0.47
1:B:130:SER:HB3	1:B:170:VAL:HG21	1.95	0.47
1:B:364:MET:SD	1:B:365:PRO:HD2	2.54	0.47
1:A:80:ILE:HD12	1:A:105:GLN:HG2	1.95	0.47
1:A:48:ARG:H	1:A:48:ARG:HG3	1.50	0.47
1:A:88:GLN:HB2	1:A:231:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LYS:HE3	1:B:392:SER:HB2	1.98	0.47
1:B:195:LEU:HB2	1:B:226:MET:HG2	1.95	0.46
1:B:259:LEU:HB2	1:B:262:LEU:HD12	1.97	0.46
1:B:266:TYR:HD1	1:B:411:ILE:HG22	1.81	0.46
1:A:144:LYS:HB2	1:A:166:PRO:HA	1.96	0.46
1:A:347:PHE:CD1	1:A:351:MET:HG3	2.51	0.46
1:A:75:CYS:SG	1:A:249:ILE:HG13	2.56	0.46
1:A:324:GLU:H	1:A:324:GLU:HG2	1.46	0.45
1:B:296:SER:HA	3:N:2:U:H5'	1.98	0.45
1:B:58:ARG:HG2	1:B:139:TYR:CE2	2.52	0.45
1:B:292:ILE:HA	1:B:360:PHE:HB2	1.98	0.45
1:B:380:ARG:O	1:B:383:THR:HG22	2.16	0.45
1:A:318:HIS:CE1	1:A:321:MET:HG3	2.51	0.45
1:B:361:ASN:HB2	1:B:389:THR:HA	1.98	0.45
1:A:147:VAL:HA	1:A:170:VAL:O	2.17	0.44
1:A:157:ASP:O	1:A:160:VAL:HG12	2.18	0.44
1:A:346:LEU:HD13	3:M:3:U:H5"	1.99	0.44
1:B:237:PRO:HA	1:B:240:ARG:HB2	1.99	0.43
1:B:257:LEU:HD23	1:B:257:LEU:HA	1.86	0.43
1:B:251:VAL:HG21	1:B:257:LEU:HD21	2.00	0.43
1:B:87:CYS:HA	1:B:249:ILE:HB	2.01	0.43
1:A:321:MET:HB2	1:A:326:ARG:HG3	2.00	0.43
1:B:400:LEU:HA	1:B:403:VAL:HG12	2.01	0.42
1:A:99:PHE:HB3	1:A:227:PHE:CE1	2.54	0.42
1:A:190:ILE:O	1:A:190:ILE:HG13	2.19	0.42
1:A:293:PHE:CE2	1:A:374:ARG:HG2	2.55	0.42
1:B:269:LEU:HD11	1:B:274:LYS:HA	2.02	0.42
1:A:116:VAL:HG22	1:A:192:HIS:HB2	2.01	0.42
1:B:187:LEU:HD12	1:B:217:MET:HE3	2.01	0.42
1:B:205:LEU:HA	1:B:208:ARG:HB3	2.01	0.42
1:B:99:PHE:HB3	1:B:227:PHE:CE1	2.55	0.41
1:B:398:LYS:HB2	1:B:398:LYS:HE2	1.76	0.41
1:A:345:ASN:HB2	3:M:2:U:O2'	2.21	0.41
1:B:158:GLU:OE2	1:B:182:ASN:ND2	2.52	0.41
1:A:304:ALA:O	1:A:308:VAL:HG23	2.21	0.41
1:B:147:VAL:HA	1:B:170:VAL:O	2.20	0.41
1:B:332:GLN:HB2	1:B:337:GLN:HB2	2.01	0.41
1:B:208:ARG:O	1:B:211:VAL:HG12	2.20	0.41
1:A:181:ARG:HH21	1:A:213:GLU:CD	2.24	0.41
1:B:119:MET:HA	1:B:171:GLY:O	2.21	0.41
1:A:224:VAL:HG23	1:A:243:MET:HG2	2.03	0.41

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	377/390 (97%)	372 (99%)	5 (1%)	0	100	100
1	B	379/390 (97%)	371 (98%)	8 (2%)	0	100	100
2	E	51/61 (84%)	49 (96%)	2 (4%)	0	100	100
All	All	807/841 (96%)	792 (98%)	15 (2%)	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	342/350 (98%)	327 (96%)	15 (4%)	28	52
1	B	344/350 (98%)	328 (95%)	16 (5%)	26	49
2	E	46/50 (92%)	36 (78%)	10 (22%)	1	1
All	All	732/750 (98%)	691 (94%)	41 (6%)	21	40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	121	HIS

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Mol	Chain	Res	Type
1	A	147	VAL
1	A	258	THR
1	A	272	ASN
1	A	276	ARG
1	A	311	ASN
1	A	324	GLU
1	A	336	PHE
1	A	337	GLN
1	A	347	PHE
1	A	374	ARG
1	A	375	VAL
1	A	402	ASP
1	A	416	ASP
1	B	73	HIS
1	B	90	LYS
1	B	154	ILE
1	B	234	GLU
1	B	255	THR
1	B	256	LYS
1	B	269	LEU
1	B	272	ASN
1	B	327	LEU
1	B	347	PHE
1	B	367	ASP
1	B	372	LEU
1	B	398	LYS
1	B	400	LEU
1	B	404	GLN
1	B	419	ASP
2	E	123	GLU
2	E	124	GLU
2	E	130	LEU
2	E	138	HIS
2	E	145	GLN
2	E	146	ASP
2	E	147	GLN
2	E	161	GLU
2	E	171	LEU
2	E	175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	88	GLN
1	B	121	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	M	5/15 (33%)	3 (60%)	0
3	N	4/15 (26%)	2 (50%)	0
All	All	9/30 (30%)	5 (55%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	M	4	U
3	M	5	U
3	M	6	U
3	N	5	U
3	N	6	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 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	ADP	A	1000	6,5	24,29,29	0.95	1 (4%)	29,45,45	1.34	3 (10%)
5	BEF	B	1001	4	0,3,3	-	-	-		
5	BEF	A	1001	4	0,3,3	-	-	-		
4	ADP	B	1000	6,5	24,29,29	0.94	1 (4%)	29,45,45	1.36	4 (13%)

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	ADP	A	1000	6,5	-	2/12/32/32	0/3/3/3
4	ADP	B	1000	6,5	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1000	ADP	C5-C4	2.40	1.47	1.40
4	A	1000	ADP	C5-C4	2.33	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1000	ADP	N3-C2-N1	-3.51	123.20	128.68
4	A	1000	ADP	N3-C2-N1	-3.28	123.55	128.68
4	B	1000	ADP	C4-C5-N7	-2.94	106.34	109.40
4	A	1000	ADP	C4-C5-N7	-2.81	106.47	109.40
4	A	1000	ADP	PA-O3A-PB	-2.79	123.27	132.83
4	B	1000	ADP	PA-O3A-PB	-2.54	124.10	132.83
4	B	1000	ADP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

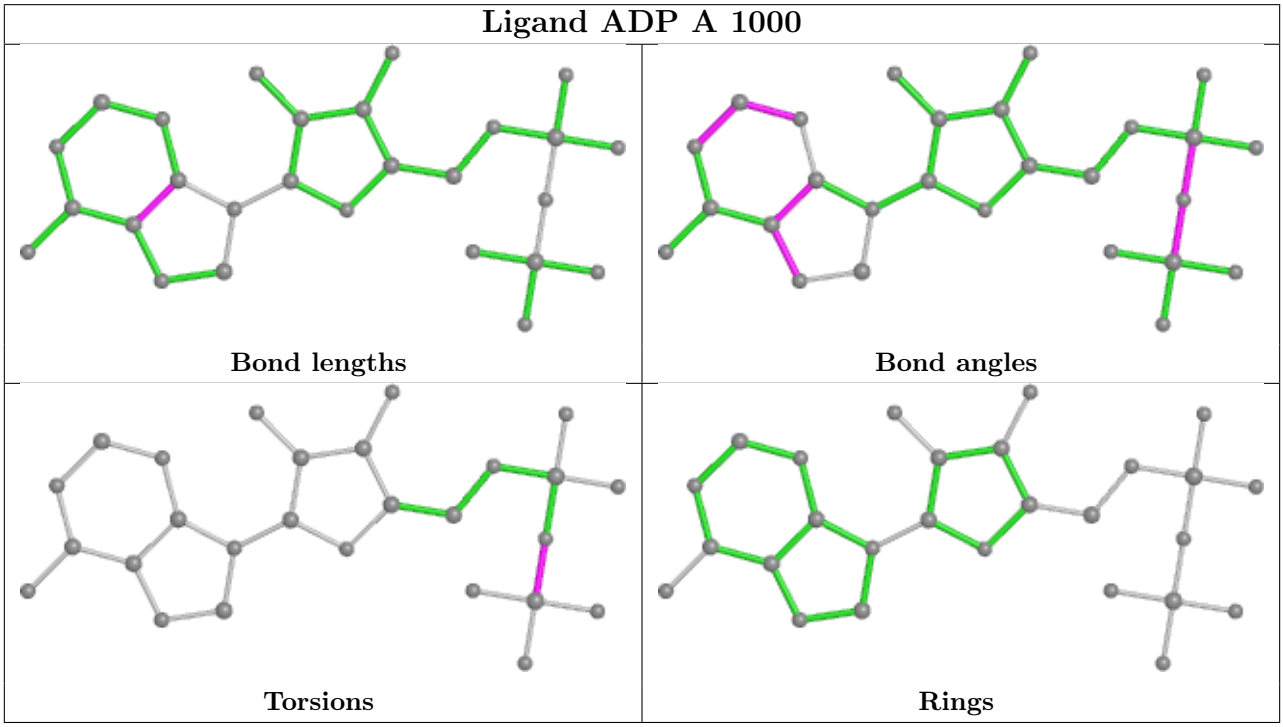
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1000	ADP	PA-O3A-PB-O2B
4	B	1000	ADP	PA-O3A-PB-O1B
4	A	1000	ADP	PA-O3A-PB-O3B
4	B	1000	ADP	PA-O3A-PB-O3B

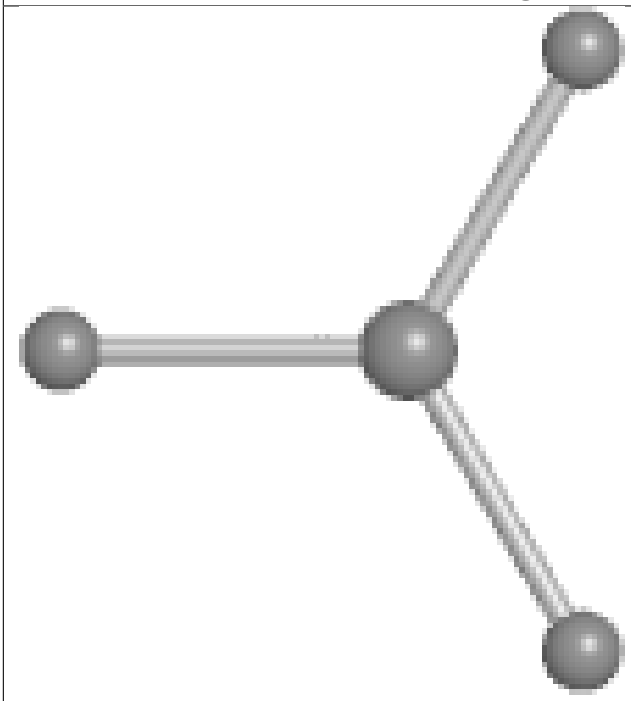
There are no ring outliers.

No monomer is involved in short contacts.

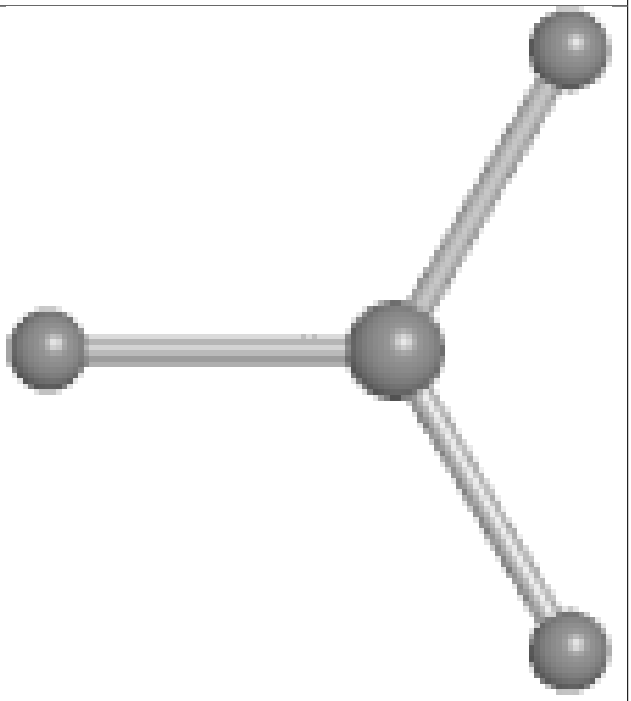
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



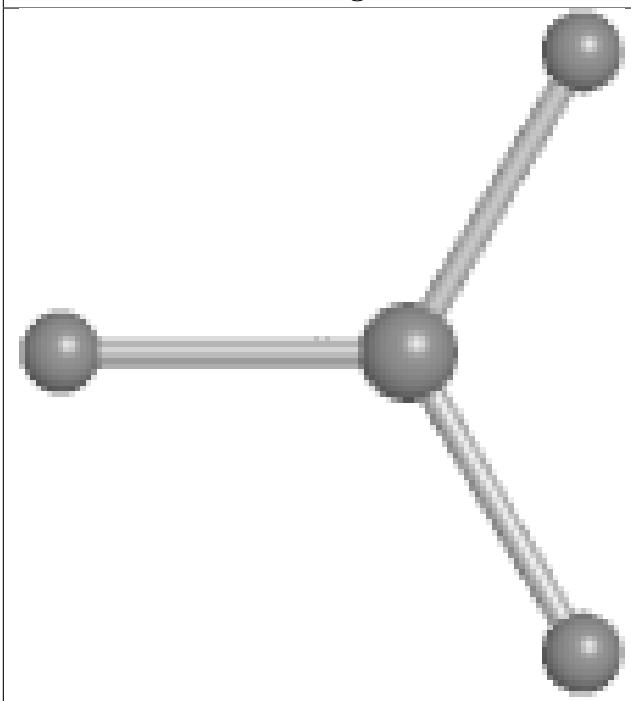
Ligand BEF B 1001



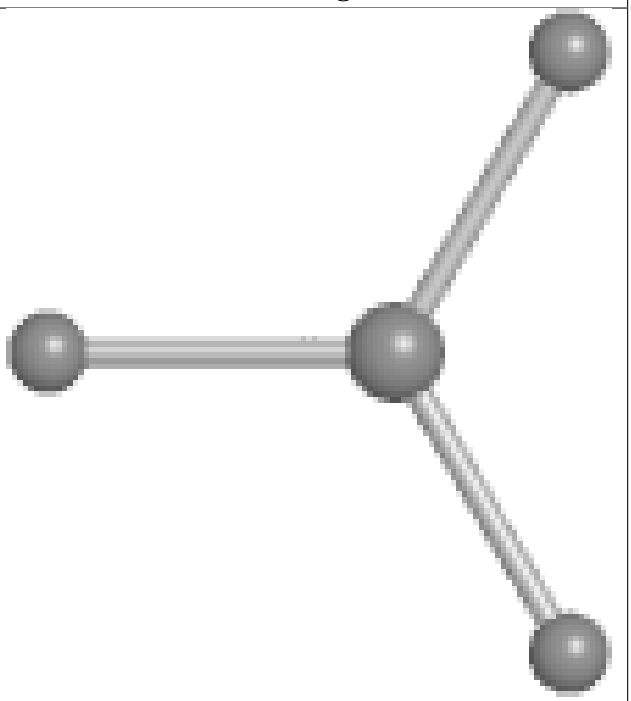
Bond lengths



Bond angles

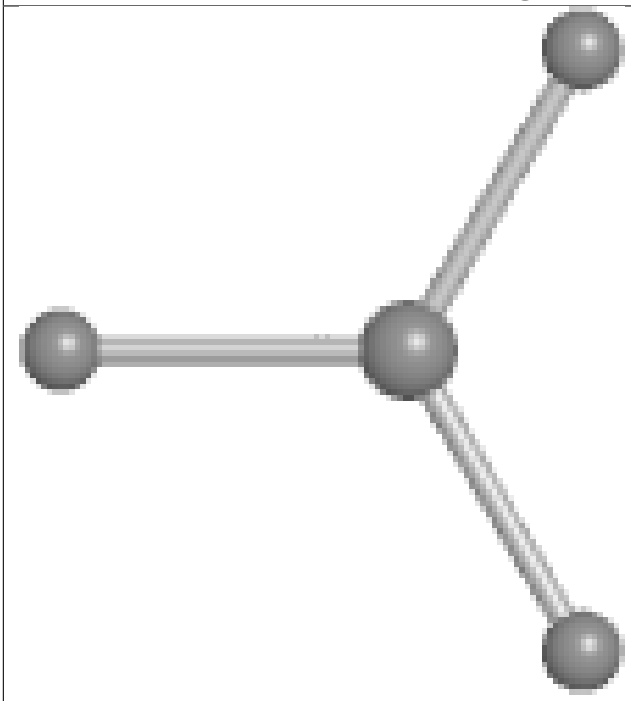


Torsions

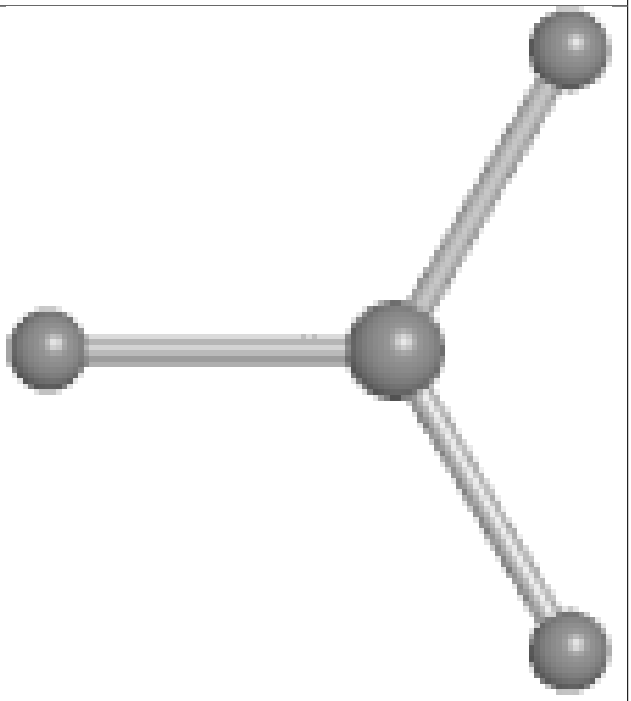


Rings

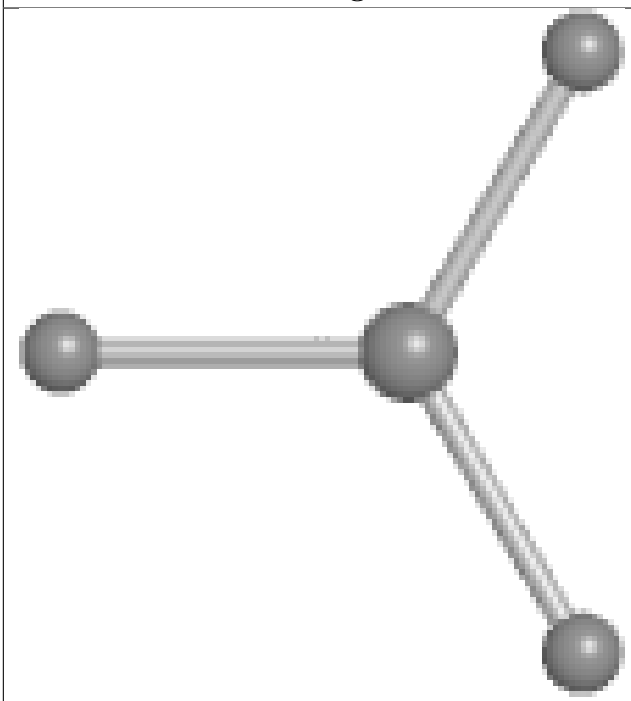
Ligand BEF A 1001



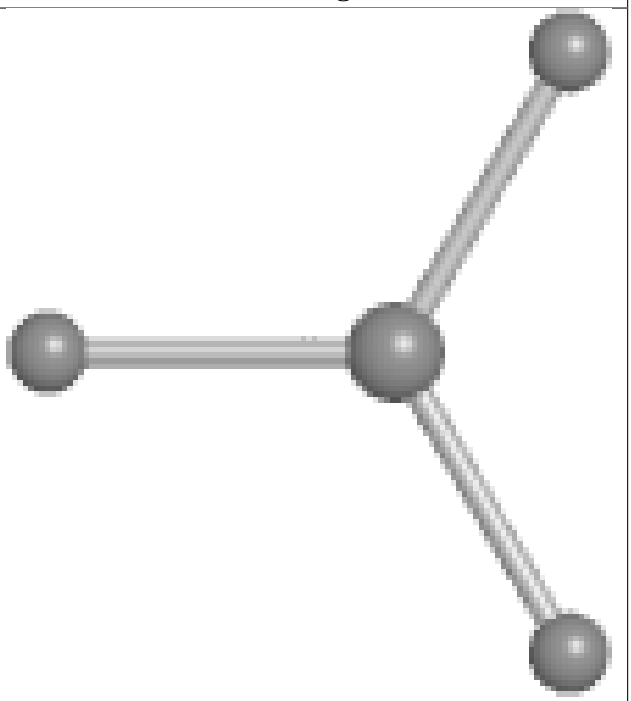
Bond lengths



Bond angles

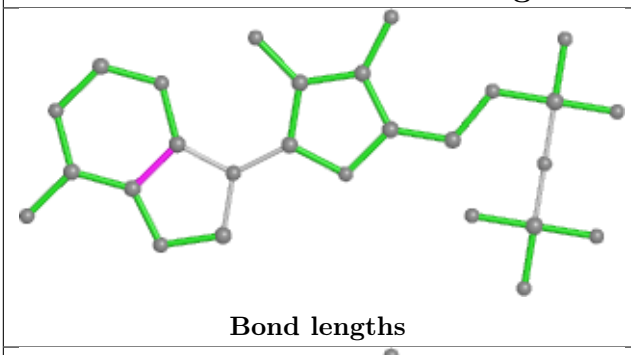


Torsions

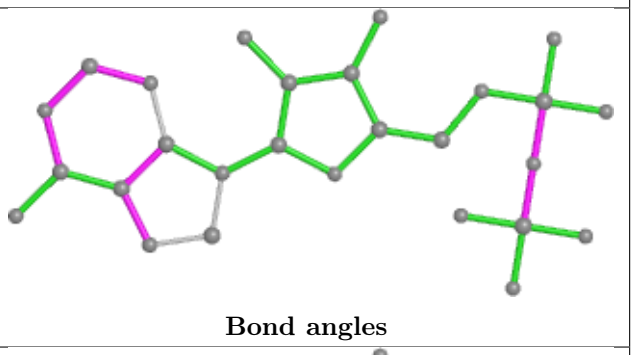


Rings

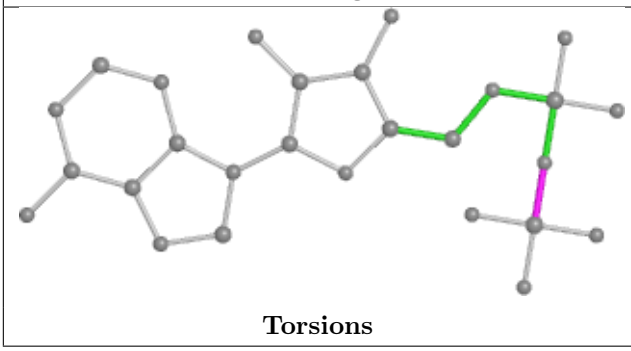
Ligand ADP B 1000



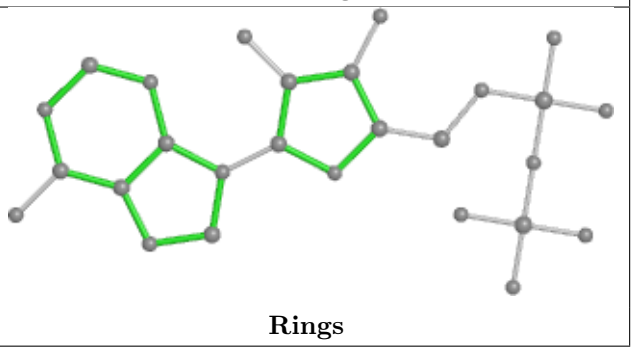
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	379/390 (97%)	0.29	22 (5%) 23 24	43, 64, 95, 128	0
1	B	381/390 (97%)	0.45	37 (9%) 7 7	46, 71, 105, 130	0
2	E	53/61 (86%)	0.64	6 (11%) 5 4	68, 81, 103, 110	0
3	M	6/15 (40%)	0.06	1 (16%) 1 1	56, 63, 77, 109	0
3	N	5/15 (33%)	-0.11	0 100 100	77, 78, 86, 99	0
All	All	824/871 (94%)	0.38	66 (8%) 12 12	43, 69, 100, 130	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	VAL	4.6
1	B	410	ASN	4.2
1	B	205	LEU	4.0
1	B	194	ILE	3.7
1	A	420	ILE	3.7
1	B	117	LEU	3.4
1	B	419	ASP	3.4
2	E	167	LEU	3.3
1	B	412	SER	3.3
1	A	99	PHE	3.3
1	B	110	VAL	3.3
1	B	195	LEU	3.2
1	B	421	SER	3.2
2	E	125	ILE	3.2
1	B	405	ASP	3.2
1	A	118	VAL	3.1
1	A	418	ILE	3.0
2	E	124	GLU	3.0
1	B	424	ILE	2.9
1	B	394	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	100	VAL	2.9
1	B	170	VAL	2.9
1	A	394	GLU	2.9
1	B	228	SER	2.8
1	A	375	VAL	2.8
2	E	151	ASP	2.8
1	A	195	LEU	2.7
1	B	162	LYS	2.7
1	A	220	HIS	2.7
1	B	420	ILE	2.6
1	B	359	ALA	2.5
1	B	227	PHE	2.5
1	B	298	GLN	2.5
1	A	292	ILE	2.5
1	A	419	ASP	2.4
1	A	126	ALA	2.4
1	B	120	CYS	2.4
1	B	291	VAL	2.4
1	B	375	VAL	2.4
1	A	233	LYS	2.4
1	A	276	ARG	2.4
1	A	49	ASP	2.3
1	B	119	MET	2.3
1	A	159	GLU	2.3
1	A	163	LYS	2.3
1	B	253	ASP	2.3
1	B	196	ASP	2.3
1	B	171	GLY	2.3
1	B	153	SER	2.2
1	B	116	VAL	2.2
1	A	194	ILE	2.2
1	B	155	LYS	2.2
1	A	162	LYS	2.1
2	E	147	GLN	2.1
1	A	125	LEU	2.1
1	B	350	GLY	2.1
1	B	99	PHE	2.1
1	B	129	ILE	2.1
1	B	416	ASP	2.1
1	B	245	ASP	2.0
1	B	176	ILE	2.0
1	A	389	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	408	GLU	2.0
2	E	149	ASP	2.0
3	M	1	U	2.0
1	A	196	ASP	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)

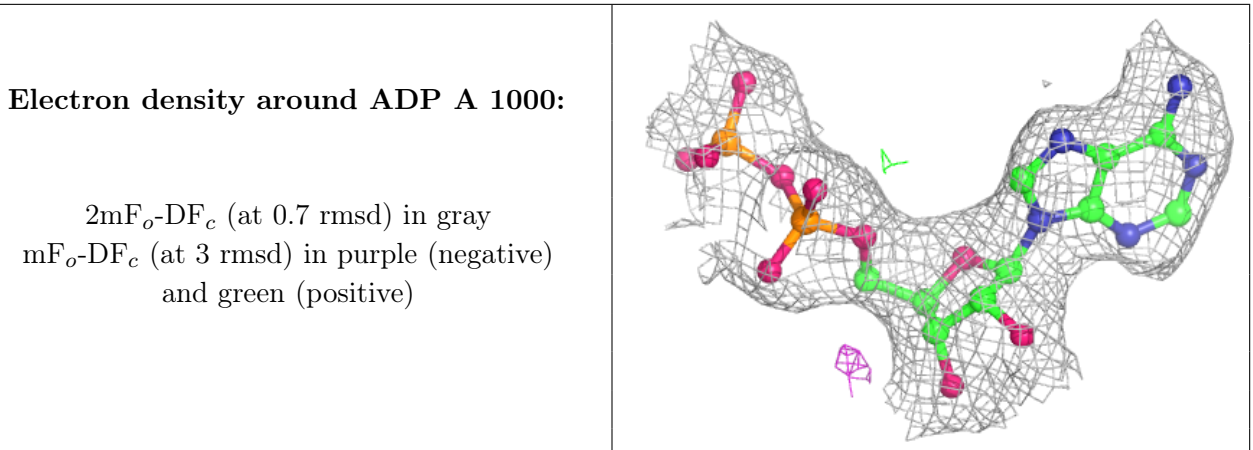
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ADP	A	1000	27/27	0.93	0.15	47,55,66,68	0
4	ADP	B	1000	27/27	0.94	0.14	47,52,57,57	0
6	MG	B	1002	1/1	0.96	0.22	54,54,54,54	0
5	BEF	B	1001	4/4	0.97	0.28	51,53,53,54	0
6	MG	A	1002	1/1	0.97	0.20	50,50,50,50	0
5	BEF	A	1001	4/4	0.97	0.22	49,49,50,51	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.

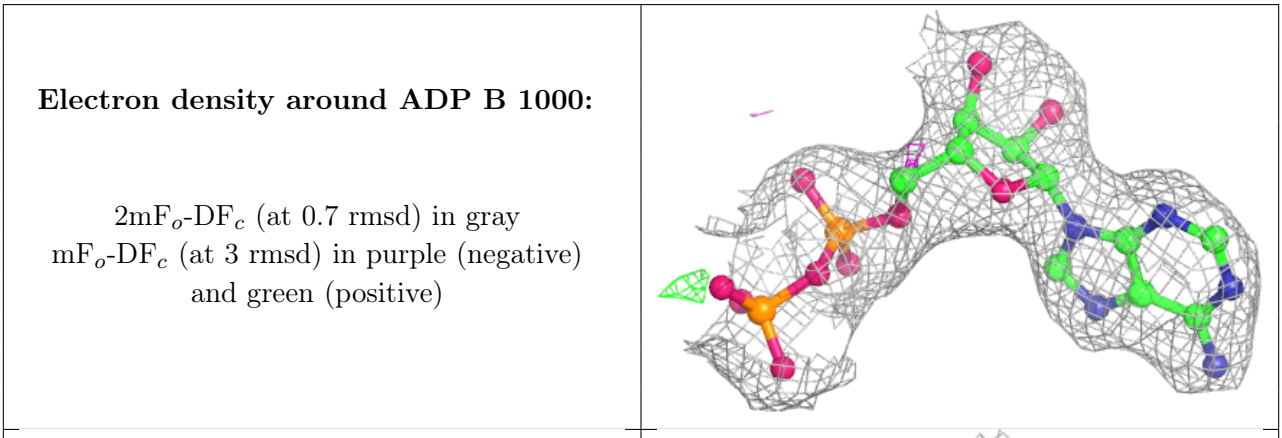
Electron density around ADP A 1000:

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



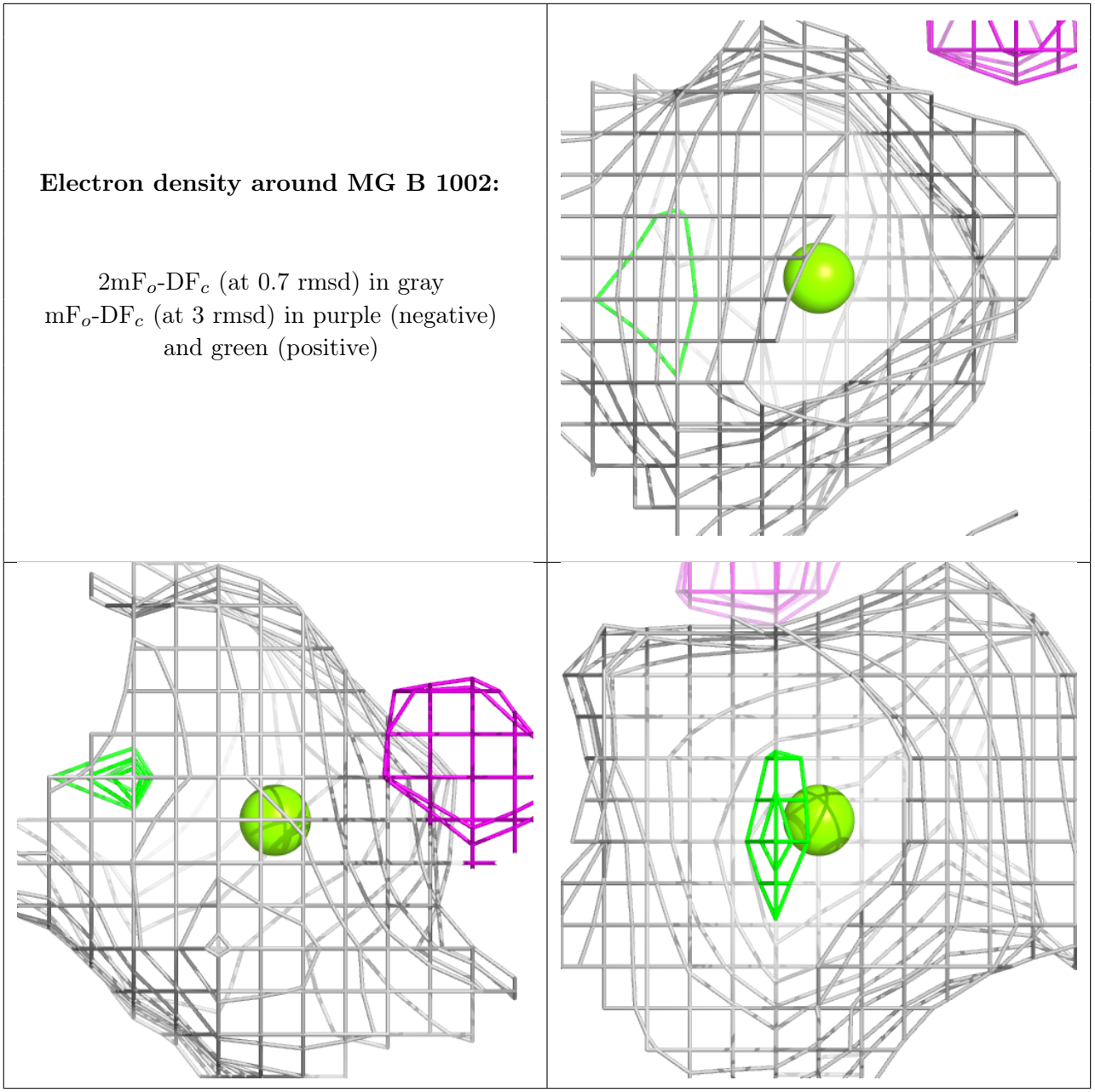
Electron density around ADP B 1000:

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



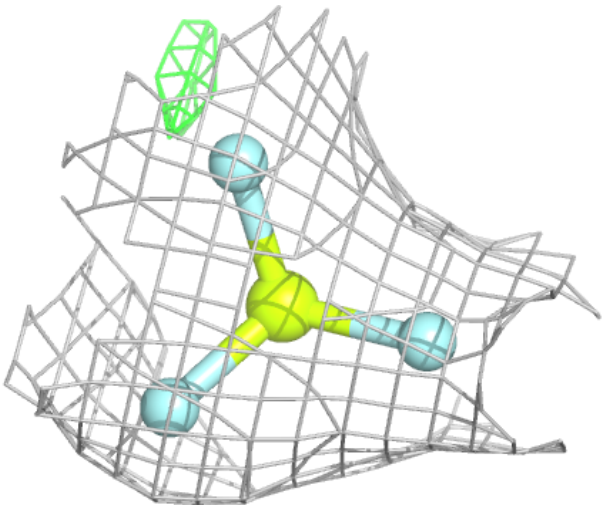
Electron density around MG B 1002:

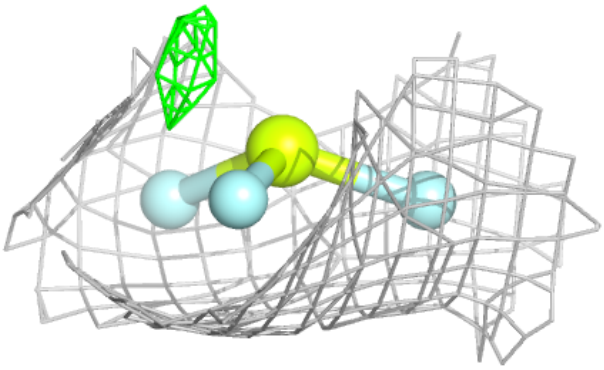
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

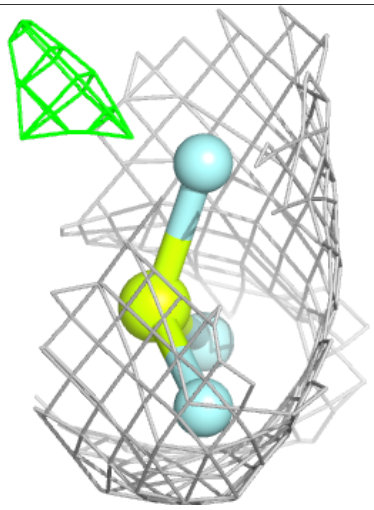


Electron density around BEF B 1001:

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

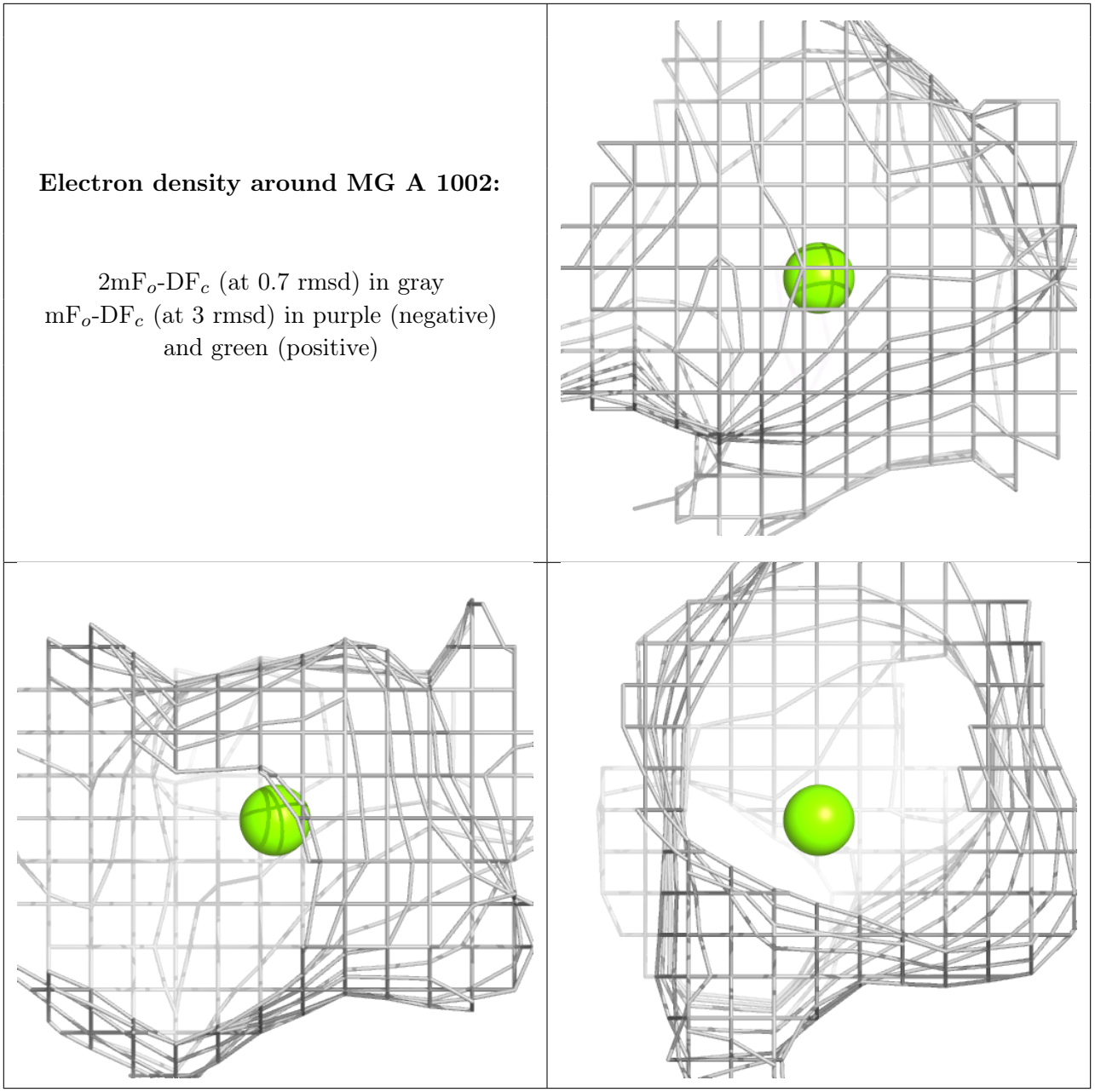






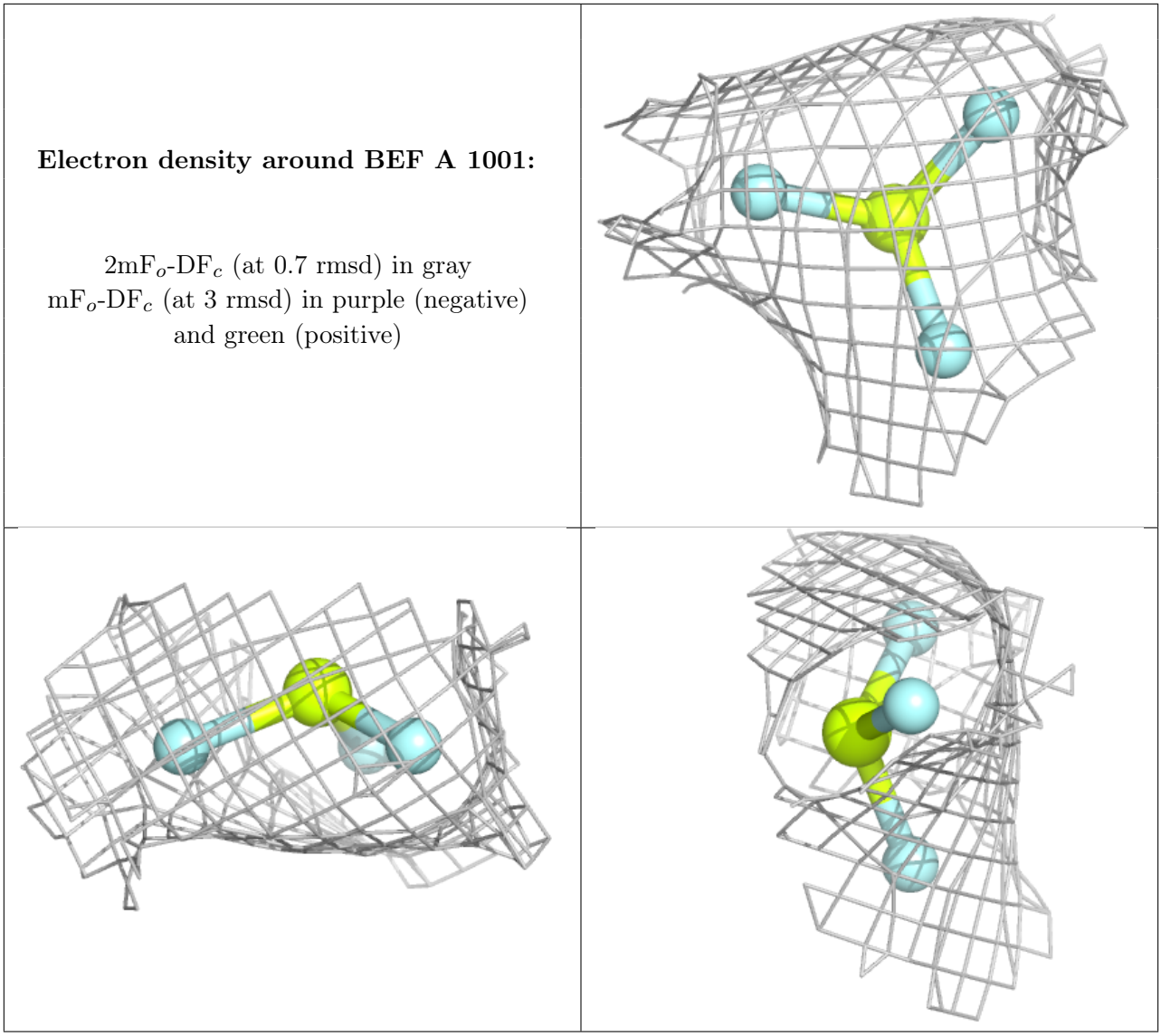
Electron density around MG A 1002:

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



Electron density around BEF 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)



6.5 Other polymers

There are no such residues in this entry.