Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2023 – 04:39 PM EDT

PDB ID	:	8GJA
Title	:	RAD51C-XRCC3 structure
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Deposited on	:	2023-03-15
Resolution	:	2.60 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:

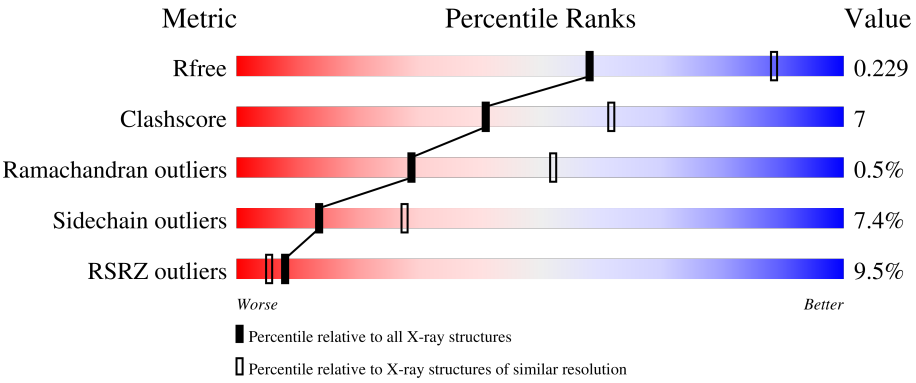
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	287	6% 79% 13% • 6%
1	C	287	7% 82% 12% • 5%
1	E	287	2% 82% 8% 10%
2	B	347	16% 71% 20% 5% •
2	D	347	10% 73% 19% • •

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Mol	Chain	Length	Quality of chain
2	F	347	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14549 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.

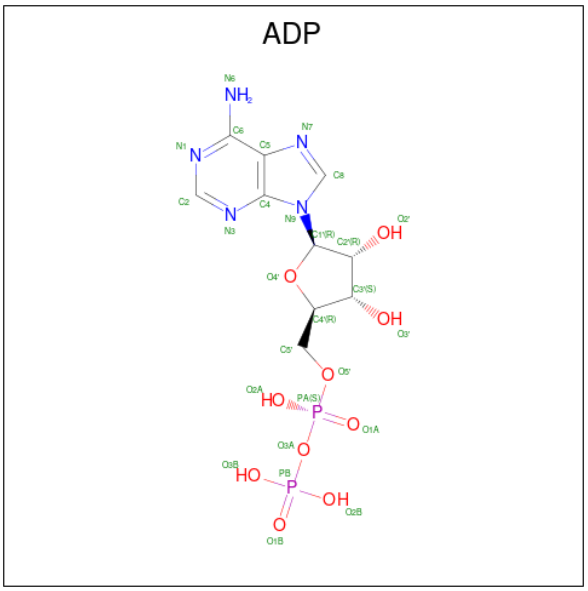
- Molecule 1 is a protein called RAD51C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	1	0
			2101	1340	357	393	11			
1	C	274	Total	C	N	O	S	0	0	0
			2131	1356	361	403	11			
1	E	259	Total	C	N	O	S	0	0	0
			2023	1292	343	378	10			

- Molecule 2 is a protein called XRCC3.

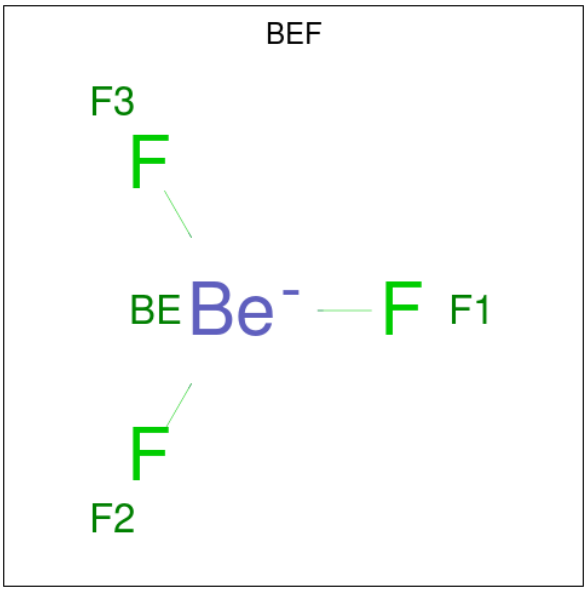
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	335	Total	C	N	O	S	0	1	0
			2619	1647	483	472	17			
2	D	336	Total	C	N	O	S	0	0	0
			2632	1656	479	479	18			
2	F	342	Total	C	N	O	S	0	0	0
			2686	1690	492	487	17			

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Be F 4 1 3	0	0
4	B	1	Total Be F 4 1 3	0	0
4	C	1	Total Be F 4 1 3	0	0
4	D	1	Total Be F 4 1 3	0	0
4	E	1	Total Be F 4 1 3	0	0

- Molecule 5 is water.

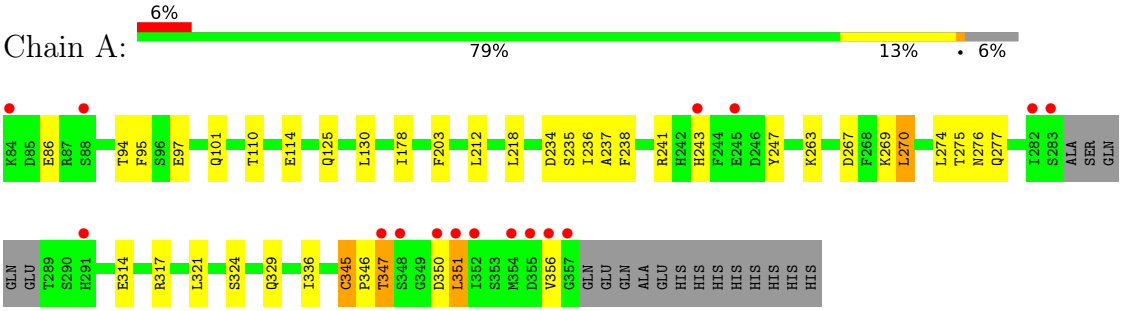
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	28	Total O 28 28	0	0
5	B	37	Total O 37 37	0	0
5	C	28	Total O 28 28	0	0
5	D	28	Total O 28 28	0	0
5	E	26	Total O 26 26	0	0
5	F	28	Total O 28 28	0	0

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.

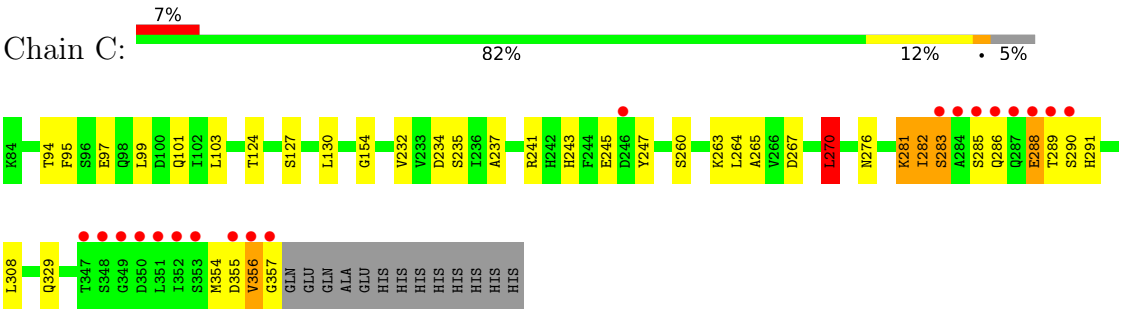
• Molecule 1: RAD51C

Chain A:



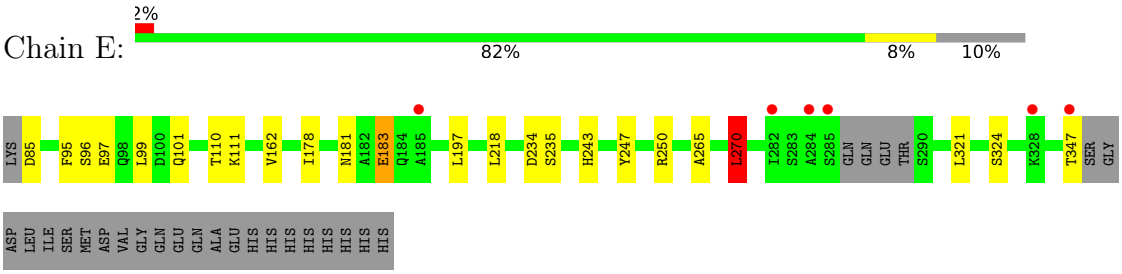
• Molecule 1: RAD51C

Chain C:



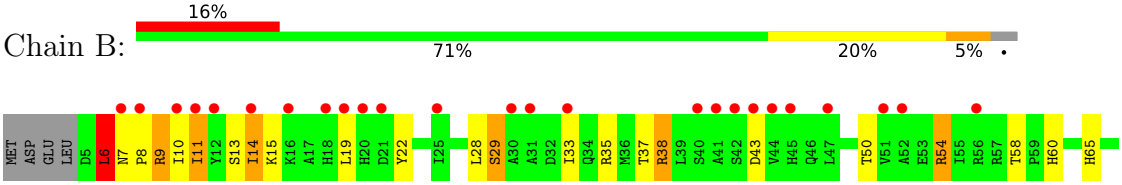
• Molecule 1: RAD51C

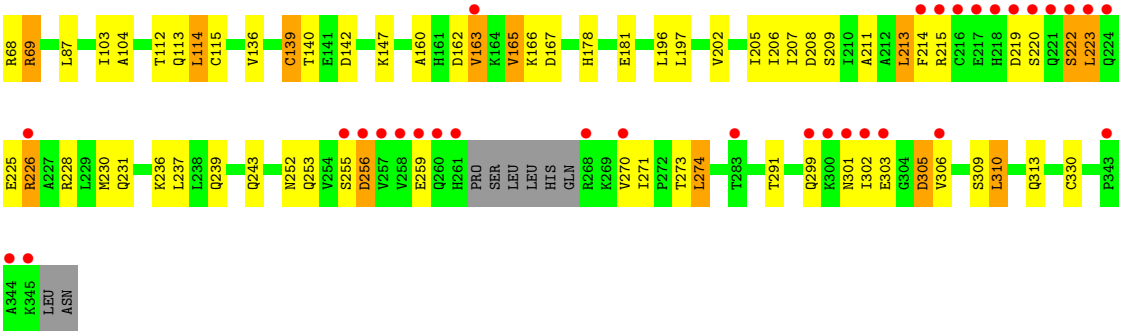
Chain E:



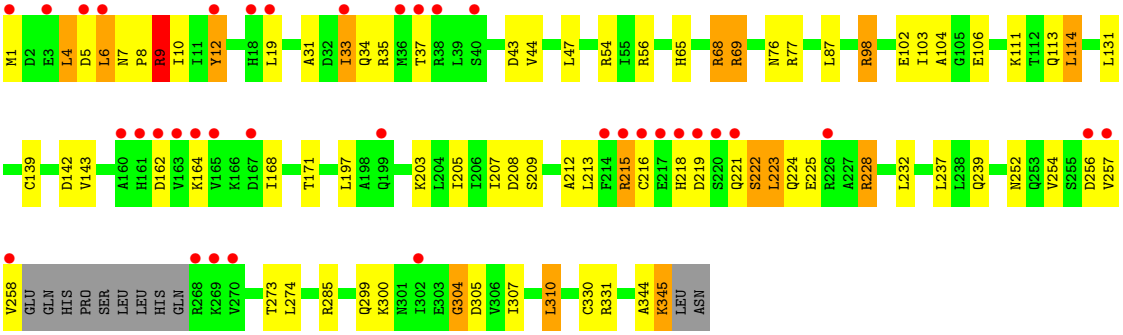
• Molecule 2: XRCC3

Chain B:

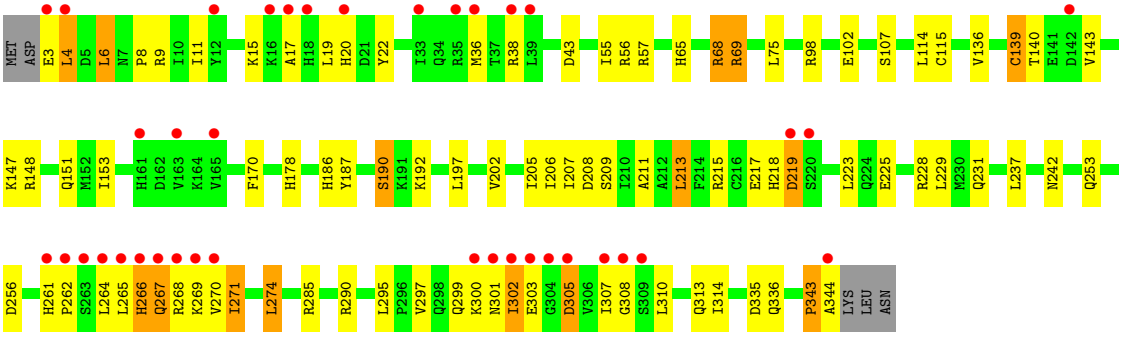




• Molecule 2: XRCC3



• Molecule 2: XRCC3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.94Å 112.30Å 259.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.33 – 2.60 38.33 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.0 (38.33-2.60) 93.0 (38.33-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.186 , 0.232 0.184 , 0.229	Depositor DCC
R_{free} test set	1865 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.8	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	0.96	EDS
Total number of atoms	14549	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% 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: BEF, ADP

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	0.26	0/2145	0.54	2/2909 (0.1%)
1	C	0.27	0/2173	0.57	2/2949 (0.1%)
1	E	0.25	0/2064	0.51	1/2802 (0.0%)
2	B	0.26	0/2664	0.56	1/3605 (0.0%)
2	D	0.27	0/2672	0.61	5/3613 (0.1%)
2	F	0.27	0/2730	0.59	3/3695 (0.1%)
All	All	0.26	0/14448	0.57	14/19573 (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	C	0	1
2	D	0	3
All	All	0	4

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	281	LYS	C-N-CA	9.38	145.15	121.70
2	D	9	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	C	270	LEU	CA-CB-CG	6.99	131.37	115.30
2	D	68	ARG	C-N-CA	6.87	138.87	121.70
1	A	351	LEU	CA-CB-CG	6.70	130.71	115.30
2	D	222	SER	C-N-CA	6.69	138.43	121.70
1	E	270	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	270	LEU	CA-CB-CG	6.09	129.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	68	ARG	C-N-CA	6.09	136.91	121.70
2	F	19	LEU	CA-CB-CG	5.59	128.15	115.30
2	F	68	ARG	C-N-CA	5.44	135.30	121.70
2	D	9	ARG	CD-NE-CZ	5.25	130.95	123.60
2	F	267	GLN	C-N-CA	5.22	134.74	121.70
2	D	219	ASP	C-N-CA	5.11	134.48	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	288	GLU	Peptide
2	D	304	GLY	Peptide
2	D	305	ASP	Peptide
2	D	5	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2101	0	2115	20	0
1	C	2131	0	2135	22	0
1	E	2023	0	2033	10	0
2	B	2619	0	2679	58	0
2	D	2632	0	2714	54	0
2	F	2686	0	2763	54	0
3	A	27	0	12	1	0
3	B	27	0	12	2	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
4	A	4	0	0	1	0
4	B	4	0	0	0	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	0	1	0
5	B	37	0	0	0	0
5	C	28	0	0	0	0
5	D	28	0	0	0	0
5	E	26	0	0	0	0
5	F	28	0	0	0	0
All	All	14549	0	14511	204	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 7.

All (204) 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)
2:F:136:VAL:HG23	2:F:202:VAL:HG11	1.54	0.88
2:B:11:ILE:HD12	2:B:14:ILE:HD11	1.60	0.83
2:B:309:SER:OG	2:F:270:VAL:O	1.99	0.80
2:B:256:ASP:HB2	2:B:270:VAL:HG12	1.63	0.80
1:C:281:LYS:HA	1:C:282:ILE:HB	1.64	0.78
2:F:299:GLN:HG3	2:F:307:ILE:HB	1.64	0.78
2:F:267:GLN:HB3	2:F:269:LYS:H	1.50	0.76
2:D:331:ARG:HH22	2:D:345:LYS:H	1.35	0.75
2:F:262:PRO:HA	2:F:265:LEU:HG	1.69	0.75
2:D:31:ALA:HA	2:D:34:GLN:HE21	1.50	0.74
2:F:266:HIS:HB2	2:F:268:ARG:HG3	1.72	0.72
2:B:220:SER:HA	2:B:223:LEU:HB2	1.70	0.72
1:C:265:ALA:HA	1:C:270:LEU:HD22	1.70	0.71
2:B:219:ASP:O	2:B:223:LEU:N	2.24	0.70
2:B:219:ASP:HB3	2:B:222:SER:HB3	1.74	0.69
2:D:331:ARG:NH2	2:D:345:LYS:H	1.89	0.69
2:F:9:ARG:NH2	2:F:43:ASP:OD2	2.26	0.69
2:D:215:ARG:NH2	2:D:273:THR:O	2.27	0.68
2:B:222:SER:O	2:B:226:ARG:N	2.27	0.67
2:D:76:ASN:O	2:D:98:ARG:NH1	2.28	0.66
2:D:300:LYS:HB3	2:D:304:GLY:O	1.95	0.66
2:F:3:GLU:HG3	2:F:20:HIS:HB2	1.77	0.66
2:F:290:ARG:NH2	2:F:313:GLN:OE1	2.29	0.66
2:D:33:ILE:HG21	2:D:44:VAL:HB	1.78	0.65
2:B:291:THR:O	2:B:313:GLN:NE2	2.30	0.64
2:F:186:HIS:O	2:F:190:SER:OG	2.16	0.64
2:D:197:LEU:HD11	2:D:205:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:ARG:HE	2:D:273:THR:HG23	1.62	0.64
2:F:4:LEU:H	2:F:4:LEU:HD12	1.62	0.63
2:B:163:VAL:HG21	2:D:68:ARG:HG3	1.80	0.63
2:F:17:ALA:HB1	2:F:36:MET:HG3	1.81	0.62
2:D:54:ARG:NH2	2:F:268:ARG:HB2	2.14	0.62
2:D:113:GLN:HG2	3:D:1000:ADP:O2A	2.00	0.60
2:B:197:LEU:HD11	2:B:205:ILE:HD11	1.83	0.60
2:D:56:ARG:HD2	2:F:265:LEU:HB2	1.84	0.60
2:F:207:ILE:HD12	2:F:237:LEU:HD11	1.83	0.60
2:D:223:LEU:HD22	2:D:223:LEU:H	1.67	0.58
2:B:239:GLN:NE2	2:B:243:GLN:OE1	2.36	0.57
2:B:301:ASN:OD1	2:B:302:ILE:N	2.37	0.57
2:D:207:ILE:HD12	2:D:237:LEU:HD11	1.86	0.57
2:B:10:ILE:HD11	2:B:43:ASP:HB3	1.85	0.57
1:C:263:LYS:NZ	1:C:267:ASP:OD2	2.37	0.57
2:B:211:ALA:HA	2:B:274:LEU:HD11	1.86	0.57
1:A:97:GLU:O	1:A:101:GLN:HG2	2.04	0.56
2:B:160:ALA:O	2:B:166:LYS:NZ	2.36	0.56
2:F:217:GLU:O	2:F:218:HIS:ND1	2.36	0.56
1:A:263:LYS:NZ	1:A:267:ASP:OD2	2.39	0.56
1:C:97:GLU:O	1:C:101:GLN:HG2	2.06	0.56
2:B:305:ASP:OD2	2:D:56:ARG:NH2	2.40	0.55
2:F:148:ARG:NH2	2:F:335:ASP:O	2.37	0.55
2:F:215:ARG:NH1	2:F:256:ASP:OD1	2.38	0.55
2:F:98:ARG:NH1	2:F:242:ASN:O	2.39	0.55
2:B:11:ILE:HG23	2:B:15:LYS:HG2	1.88	0.55
2:F:115:CYS:HB3	2:F:206:ILE:HD13	1.88	0.55
2:B:207:ILE:HD12	2:B:237:LEU:HD11	1.89	0.55
2:D:33:ILE:O	2:D:37:THR:HG22	2.07	0.54
1:A:345:CYS:O	1:A:347:THR:HA	2.08	0.54
2:B:11:ILE:HG13	2:B:15:LYS:HE3	1.90	0.54
2:B:115:CYS:HB3	2:B:206:ILE:HD13	1.90	0.54
2:F:148:ARG:HH12	2:F:336:GLN:HA	1.72	0.54
1:E:181:ASN:HB3	1:E:183:GLU:OE1	2.09	0.53
2:F:151:GLN:NE2	2:F:336:GLN:HG3	2.24	0.53
2:D:106:GLU:O	2:D:111:LYS:NZ	2.41	0.52
2:D:54:ARG:HH22	2:F:268:ARG:HB2	1.73	0.52
2:D:331:ARG:HH21	2:D:344:ALA:HA	1.75	0.52
2:D:6:LEU:HD11	2:D:10:ILE:HG21	1.91	0.51
2:F:299:GLN:CD	2:F:301:ASN:H	2.13	0.51
1:A:317:ARG:NH1	5:A:1102:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:GLU:OE2	2:B:228:ARG:NH2	2.36	0.51
2:B:8:PRO:HA	2:B:11:ILE:HB	1.93	0.51
2:B:230:MET:HE3	2:B:274:LEU:HG	1.91	0.51
1:E:265:ALA:HA	1:E:270:LEU:HD22	1.91	0.51
2:F:302:ILE:N	2:F:303:GLU:HA	2.26	0.50
1:A:238:PHE:O	1:A:241[B]:ARG:NH1	2.39	0.50
2:F:65:HIS:O	2:F:69:ARG:HA	2.12	0.50
2:B:303:GLU:OE1	2:D:98:ARG:NH2	2.44	0.50
2:B:214:PHE:CZ	2:B:226:ARG:HB3	2.47	0.49
2:B:259:GLU:HB3	2:B:271:ILE:HD12	1.93	0.49
2:D:10:ILE:CD1	2:D:47:LEU:HB2	2.42	0.49
1:A:125:GLN:HG3	1:A:336:ILE:HD13	1.93	0.49
1:C:154:GLY:O	2:D:77:ARG:NH2	2.45	0.49
2:B:54:ARG:HD2	2:B:54:ARG:O	2.12	0.49
2:B:103:ILE:HD13	2:B:114:LEU:HD13	1.95	0.49
2:D:307:ILE:O	2:D:307:ILE:HG13	2.13	0.49
2:D:54:ARG:HH21	2:F:268:ARG:N	2.11	0.48
2:B:163:VAL:HG11	2:D:68:ARG:HD2	1.94	0.48
2:D:212:ALA:O	2:D:216:CYS:HB2	2.13	0.48
2:D:56:ARG:HG3	2:F:265:LEU:O	2.13	0.48
2:F:305:ASP:N	2:F:305:ASP:OD1	2.47	0.48
2:F:197:LEU:HD11	2:F:205:ILE:HD11	1.95	0.48
2:F:211:ALA:HB2	2:F:274:LEU:HD22	1.96	0.48
2:D:9:ARG:NH1	2:D:10:ILE:HB	2.28	0.48
1:A:241[A]:ARG:NH1	1:A:277:GLN:OE1	2.47	0.47
2:F:211:ALA:HB1	2:F:256:ASP:HB3	1.96	0.47
2:F:11:ILE:O	2:F:15:LYS:HG3	2.14	0.47
1:A:110:THR:HG22	1:A:269:LYS:HA	1.96	0.47
2:D:54:ARG:HH21	2:F:268:ARG:H	1.62	0.47
1:A:94:THR:HG22	1:A:130:LEU:HD21	1.97	0.47
1:C:243:HIS:CE1	2:D:228:ARG:HB3	2.50	0.47
2:F:225:GLU:OE1	2:F:228:ARG:NH1	2.48	0.46
1:C:127:SER:HB3	1:C:232:VAL:HG11	1.97	0.46
1:E:97:GLU:O	1:E:101:GLN:HG2	2.16	0.46
2:F:102:GLU:OE1	2:F:285:ARG:HD3	2.16	0.46
1:A:203:PHE:CE1	2:B:60:HIS:HB2	2.51	0.45
2:B:196:LEU:HB3	2:B:202:VAL:HG21	1.99	0.45
2:D:10:ILE:HD11	2:D:47:LEU:HB2	1.99	0.45
2:F:299:GLN:N	2:F:308:GLY:O	2.47	0.45
2:B:11:ILE:HG23	2:B:15:LYS:CG	2.46	0.45
2:B:302:ILE:HG13	2:B:303:GLU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:THR:HB	2:F:213:LEU:HD13	1.99	0.45
2:F:295:LEU:HD13	2:F:314:ILE:HD11	1.99	0.45
2:B:208:ASP:HA	2:B:209:SER:HA	1.76	0.45
2:B:140:THR:HB	2:B:213:LEU:HD13	1.99	0.45
2:D:345:LYS:HE2	2:D:345:LYS:HB3	1.77	0.45
2:F:3:GLU:HG2	2:F:15:LYS:NZ	2.32	0.45
2:F:215:ARG:HA	2:F:271:ILE:HG21	1.99	0.45
2:F:22:TYR:HB3	2:F:55:ILE:HD11	1.97	0.45
1:C:289:THR:CB	1:C:291:HIS:HB2	2.47	0.44
1:C:281:LYS:HA	1:C:282:ILE:CB	2.39	0.44
1:A:237:ALA:HB2	1:A:276:ASN:OD1	2.18	0.44
2:B:6:LEU:HB3	2:B:7:ASN:H	1.68	0.44
2:F:299:GLN:CG	2:F:300:LYS:H	2.31	0.44
2:F:299:GLN:NE2	2:F:305:ASP:HB2	2.32	0.44
2:D:131:LEU:HB3	2:D:203:LYS:HE3	2.00	0.44
2:D:164:LYS:O	2:D:168:ILE:HG13	2.16	0.44
2:B:253:GLN:O	2:B:273:THR:OG1	2.26	0.44
2:D:54:ARG:HA	2:D:54:ARG:HD2	1.70	0.44
2:D:257:VAL:HG22	2:D:258:VAL:H	1.82	0.44
2:F:343:PRO:HB2	2:F:344:ALA:H	1.66	0.44
2:B:230:MET:CE	2:B:274:LEU:HG	2.47	0.44
1:C:282:ILE:O	1:C:283:SER:HB3	2.18	0.44
2:D:215:ARG:NE	2:D:273:THR:HG23	2.29	0.44
2:B:223:LEU:HD12	2:B:223:LEU:HA	1.87	0.44
2:D:208:ASP:HA	2:D:209:SER:HA	1.72	0.44
1:E:243:HIS:HB3	1:E:250:ARG:HB2	2.00	0.44
2:B:213:LEU:HD12	2:B:213:LEU:HA	1.74	0.44
2:B:299:GLN:HG3	2:B:310:LEU:HD22	2.00	0.44
2:D:228:ARG:HA	2:D:228:ARG:HD2	1.74	0.44
2:B:113:GLN:HG2	3:B:1000:ADP:O1A	2.18	0.43
1:C:124:THR:OG1	4:C:1001:BEF:F2	2.26	0.43
2:D:4:LEU:H	2:D:4:LEU:HD23	1.83	0.43
1:C:94:THR:HG22	1:C:130:LEU:HD21	2.00	0.43
2:D:225:GLU:OE1	2:D:225:GLU:N	2.46	0.43
2:F:107:SER:HA	2:F:253:GLN:HE22	1.83	0.43
2:B:104:ALA:HA	2:B:252:ASN:O	2.18	0.43
1:C:237:ALA:HB2	1:C:276:ASN:OD1	2.18	0.43
2:F:68:ARG:H	2:F:69:ARG:HA	1.83	0.43
2:B:162:ASP:O	2:B:165:VAL:HG13	2.18	0.43
2:D:65:HIS:O	2:D:69:ARG:HA	2.19	0.43
2:B:29:SER:O	2:B:33:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:ASN:HA	2:D:8:PRO:HD3	1.91	0.43
2:F:68:ARG:N	2:F:69:ARG:HA	2.34	0.43
2:F:187:TYR:CE2	2:F:192:LYS:HE3	2.54	0.43
1:C:329:GLN:HG2	1:C:355:ASP:HB2	2.00	0.43
2:F:68:ARG:HD3	2:F:68:ARG:HA	1.76	0.43
1:E:321:LEU:HD11	1:E:324:SER:HB3	2.00	0.43
2:B:7:ASN:OD1	2:B:9:ARG:HG3	2.19	0.43
2:B:28:LEU:HD23	2:B:28:LEU:HA	1.87	0.43
2:B:181:GLU:HG2	2:B:215:ARG:HH21	1.84	0.43
1:C:356:VAL:HA	1:C:357:GLY:HA3	1.59	0.42
2:F:208:ASP:HA	2:F:209:SER:HA	1.85	0.42
1:C:260:SER:O	1:C:264:LEU:HD13	2.19	0.42
2:D:299:GLN:HG3	2:D:310:LEU:HD22	2.00	0.42
1:E:234:ASP:HA	1:E:235:SER:HA	1.70	0.42
2:B:112:THR:HB	3:B:1000:ADP:O1A	2.20	0.42
1:A:114:GLU:HA	1:A:274:LEU:O	2.19	0.42
1:A:321:LEU:HD11	1:A:324:SER:HB3	2.01	0.42
2:F:6:LEU:HA	2:F:6:LEU:HD12	1.77	0.42
1:A:241[A]:ARG:HH12	1:A:277:GLN:HB2	1.85	0.42
1:A:243:HIS:CE1	2:B:228:ARG:HG3	2.55	0.42
2:F:153:ILE:HD13	2:F:170:PHE:HB2	2.01	0.42
1:C:247:TYR:HD1	1:C:247:TYR:HA	1.76	0.42
2:F:139:CYS:O	2:F:178:HIS:HA	2.20	0.41
1:A:247:TYR:HD1	1:A:247:TYR:HA	1.71	0.41
2:B:7:ASN:O	2:B:11:ILE:HD13	2.20	0.41
2:D:142:ASP:OD1	2:D:143:VAL:N	2.50	0.41
2:B:236:LYS:HD2	2:B:236:LYS:HA	1.88	0.41
2:D:6:LEU:HD11	2:D:10:ILE:HD13	2.02	0.41
2:D:102:GLU:OE1	2:D:285:ARG:HD3	2.20	0.41
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.89	0.41
2:D:103:ILE:HD13	2:D:114:LEU:HD13	2.01	0.41
1:E:218:LEU:HD23	1:E:218:LEU:HA	1.92	0.41
1:E:110:THR:O	1:E:111:LYS:HD3	2.21	0.41
1:A:236:ILE:HG22	1:A:275:THR:O	2.20	0.41
1:A:234:ASP:HA	1:A:235:SER:HA	1.74	0.41
2:B:38:ARG:H	2:B:38:ARG:HG2	1.54	0.41
1:C:286:GLN:NE2	1:C:286:GLN:HA	2.36	0.41
2:D:9:ARG:O	2:D:12:TYR:HD1	2.03	0.41
2:D:224:GLN:O	2:D:228:ARG:HG2	2.20	0.41
1:C:281:LYS:NZ	1:C:291:HIS:HB3	2.35	0.41
1:E:162:VAL:HG22	1:E:197:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:LEU:HD12	2:B:310:LEU:HA	1.91	0.40
1:C:234:ASP:HA	1:C:235:SER:HA	1.85	0.40
2:D:104:ALA:HA	2:D:252:ASN:O	2.22	0.40
2:B:65:HIS:O	2:B:69:ARG:HA	2.21	0.40
2:B:136:VAL:HG12	2:B:202:VAL:HG11	2.02	0.40
1:C:103:LEU:HD21	1:C:308:LEU:HD11	2.03	0.40
1:E:96:SER:OG	1:E:99:LEU:HB2	2.22	0.40
2:B:139:CYS:O	2:B:178[A]:HIS:HA	2.22	0.40
1:A:178:ILE:HD13	1:A:178:ILE:HA	1.94	0.40
3:A:1000:ADP:O2B	4:A:1001:BEF:F1	2.30	0.40
2:B:139:CYS:O	2:B:178[B]:HIS:HA	2.22	0.40
1:C:355:ASP:OD1	1:C:356:VAL:N	2.54	0.40
2:D:9:ARG:HH12	2:D:43:ASP:HB3	1.86	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	266/287 (93%)	260 (98%)	5 (2%)	1 (0%)	34	57
1	C	272/287 (95%)	261 (96%)	9 (3%)	2 (1%)	22	43
1	E	255/287 (89%)	253 (99%)	2 (1%)	0	100	100
2	B	332/347 (96%)	320 (96%)	11 (3%)	1 (0%)	41	64
2	D	332/347 (96%)	324 (98%)	8 (2%)	0	100	100
2	F	340/347 (98%)	323 (95%)	12 (4%)	5 (2%)	10	21
All	All	1797/1902 (94%)	1741 (97%)	47 (3%)	9 (0%)	29	52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	282	ILE
2	F	8	PRO
2	F	343	PRO
2	F	274	LEU
1	A	346	PRO
1	C	283	SER
2	F	219	ASP
2	B	6	LEU
2	F	302	ILE

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	236/252 (94%)	225 (95%)	11 (5%)	26 50
1	C	239/252 (95%)	229 (96%)	10 (4%)	30 55
1	E	227/252 (90%)	220 (97%)	7 (3%)	40 66
2	B	290/307 (94%)	255 (88%)	35 (12%)	5 9
2	D	295/307 (96%)	265 (90%)	30 (10%)	7 14
2	F	301/307 (98%)	277 (92%)	24 (8%)	12 24
All	All	1588/1677 (95%)	1471 (93%)	117 (7%)	13 28

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	GLU
1	A	95	PHE
1	A	212	LEU
1	A	270	LEU
1	A	314	GLU
1	A	329	GLN
1	A	345	CYS
1	A	347	THR
1	A	350	ASP
1	A	351	LEU

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Mol	Chain	Res	Type
1	A	356	VAL
2	B	6	LEU
2	B	9	ARG
2	B	11	ILE
2	B	13	SER
2	B	14	ILE
2	B	19	LEU
2	B	22	TYR
2	B	29	SER
2	B	35	ARG
2	B	37	THR
2	B	38	ARG
2	B	50	THR
2	B	54	ARG
2	B	58	THR
2	B	69	ARG
2	B	87	LEU
2	B	114	LEU
2	B	139	CYS
2	B	142	ASP
2	B	147	LYS
2	B	163	VAL
2	B	165	VAL
2	B	167	ASP
2	B	213	LEU
2	B	222	SER
2	B	223	LEU
2	B	226	ARG
2	B	231	GLN
2	B	255	SER
2	B	256	ASP
2	B	274	LEU
2	B	305	ASP
2	B	306	VAL
2	B	310	LEU
2	B	330	CYS
1	C	95	PHE
1	C	99	LEU
1	C	241	ARG
1	C	245	GLU
1	C	270	LEU
1	C	285	SER

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Mol	Chain	Res	Type
1	C	288	GLU
1	C	290	SER
1	C	354	MET
1	C	356	VAL
2	D	1	MET
2	D	4	LEU
2	D	6	LEU
2	D	9	ARG
2	D	12	TYR
2	D	19	LEU
2	D	33	ILE
2	D	35	ARG
2	D	69	ARG
2	D	87	LEU
2	D	98	ARG
2	D	114	LEU
2	D	139	CYS
2	D	162	ASP
2	D	171	THR
2	D	213	LEU
2	D	215	ARG
2	D	218	HIS
2	D	221	GLN
2	D	222	SER
2	D	223	LEU
2	D	228	ARG
2	D	232	LEU
2	D	239	GLN
2	D	254	VAL
2	D	256	ASP
2	D	274	LEU
2	D	310	LEU
2	D	330	CYS
2	D	345	LYS
1	E	85	ASP
1	E	95	PHE
1	E	178	ILE
1	E	183	GLU
1	E	247	TYR
1	E	270	LEU
1	E	347	THR
2	F	4	LEU

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Mol	Chain	Res	Type
2	F	6	LEU
2	F	38	ARG
2	F	56	ARG
2	F	57	ARG
2	F	69	ARG
2	F	75	LEU
2	F	114	LEU
2	F	139	CYS
2	F	143	VAL
2	F	147	LYS
2	F	190	SER
2	F	213	LEU
2	F	219	ASP
2	F	223	LEU
2	F	229	LEU
2	F	231	GLN
2	F	261	HIS
2	F	264	LEU
2	F	266	HIS
2	F	271	ILE
2	F	297	VAL
2	F	305	ASP
2	F	310	LEU

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

Mol	Chain	Res	Type
2	D	34	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BEF	E	1001	3	0,3,3	-	-	-		
3	ADP	D	1000	4	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)
4	BEF	C	1001	3	0,3,3	-	-	-		
4	BEF	B	1001	3	0,3,3	-	-	-		
3	ADP	B	1000	4	24,29,29	0.96	1 (4%)	29,45,45	1.44	4 (13%)
3	ADP	A	1000	4	24,29,29	0.95	1 (4%)	29,45,45	1.28	4 (13%)
4	BEF	D	1001	3	0,3,3	-	-	-		
3	ADP	F	1000	-	24,29,29	0.95	1 (4%)	29,45,45	1.42	4 (13%)
4	BEF	A	1001	3	0,3,3	-	-	-		
3	ADP	E	1000	4	24,29,29	0.94	1 (4%)	29,45,45	1.27	4 (13%)
3	ADP	C	1000	4	24,29,29	1.00	1 (4%)	29,45,45	1.25	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	1000	4	-	3/12/32/32	0/3/3/3
3	ADP	B	1000	4	-	3/12/32/32	0/3/3/3
3	ADP	A	1000	4	-	5/12/32/32	0/3/3/3
3	ADP	F	1000	-	-	2/12/32/32	0/3/3/3
3	ADP	E	1000	4	-	6/12/32/32	0/3/3/3
3	ADP	C	1000	4	-	2/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	ADP	C5-C4	2.53	1.47	1.40
3	D	1000	ADP	C5-C4	2.52	1.47	1.40
3	F	1000	ADP	C5-C4	2.51	1.47	1.40
3	E	1000	ADP	C5-C4	2.47	1.47	1.40
3	C	1000	ADP	C5-C4	2.42	1.47	1.40
3	A	1000	ADP	C5-C4	2.42	1.47	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1000	ADP	C3'-C2'-C1'	3.56	106.33	100.98
3	D	1000	ADP	PA-O3A-PB	-3.19	121.88	132.83
3	F	1000	ADP	N3-C2-N1	-3.17	123.73	128.68
3	E	1000	ADP	N3-C2-N1	-3.15	123.76	128.68
3	D	1000	ADP	N3-C2-N1	-3.14	123.76	128.68
3	B	1000	ADP	N3-C2-N1	-3.14	123.77	128.68
3	C	1000	ADP	N3-C2-N1	-3.07	123.87	128.68
3	A	1000	ADP	N3-C2-N1	-3.07	123.89	128.68
3	C	1000	ADP	PA-O3A-PB	-2.97	122.63	132.83
3	B	1000	ADP	PA-O3A-PB	-2.91	122.85	132.83
3	B	1000	ADP	C4-C5-N7	-2.85	106.42	109.40
3	A	1000	ADP	PA-O3A-PB	-2.81	123.18	132.83
3	B	1000	ADP	C3'-C2'-C1'	2.77	105.15	100.98
3	D	1000	ADP	C4-C5-N7	-2.73	106.55	109.40
3	D	1000	ADP	C3'-C2'-C1'	2.64	104.95	100.98
3	E	1000	ADP	C4-C5-N7	-2.63	106.66	109.40
3	F	1000	ADP	C4-C5-N7	-2.60	106.69	109.40
3	E	1000	ADP	C3'-C2'-C1'	2.55	104.82	100.98
3	F	1000	ADP	PA-O3A-PB	-2.53	124.13	132.83
3	A	1000	ADP	C4-C5-N7	-2.53	106.76	109.40
3	E	1000	ADP	PA-O3A-PB	-2.41	124.55	132.83
3	A	1000	ADP	C3'-C2'-C1'	2.40	104.59	100.98
3	C	1000	ADP	C4-C5-N7	-2.34	106.96	109.40

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	ADP	C5'-O5'-PA-O1A
3	B	1000	ADP	C5'-O5'-PA-O2A
3	C	1000	ADP	PA-O3A-PB-O2B
3	C	1000	ADP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	D	1000	ADP	C5'-O5'-PA-O1A
3	E	1000	ADP	PA-O3A-PB-O2B
3	E	1000	ADP	PA-O3A-PB-O3B
3	E	1000	ADP	C5'-O5'-PA-O2A
3	F	1000	ADP	PA-O3A-PB-O3B
3	A	1000	ADP	C5'-O5'-PA-O3A
3	B	1000	ADP	C5'-O5'-PA-O3A
3	E	1000	ADP	C5'-O5'-PA-O3A
3	A	1000	ADP	C5'-O5'-PA-O2A
3	B	1000	ADP	C5'-O5'-PA-O1A
3	D	1000	ADP	C5'-O5'-PA-O2A
3	E	1000	ADP	C5'-O5'-PA-O1A
3	E	1000	ADP	PA-O3A-PB-O1B
3	A	1000	ADP	PA-O3A-PB-O2B
3	F	1000	ADP	PA-O3A-PB-O2B
3	D	1000	ADP	C5'-O5'-PA-O3A
3	A	1000	ADP	C3'-C4'-C5'-O5'

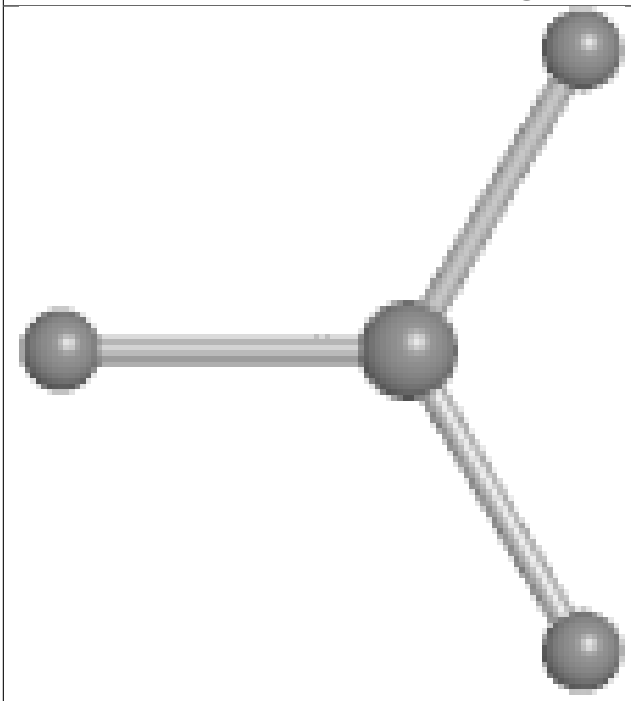
There are no ring outliers.

5 monomers are involved in 5 short contacts:

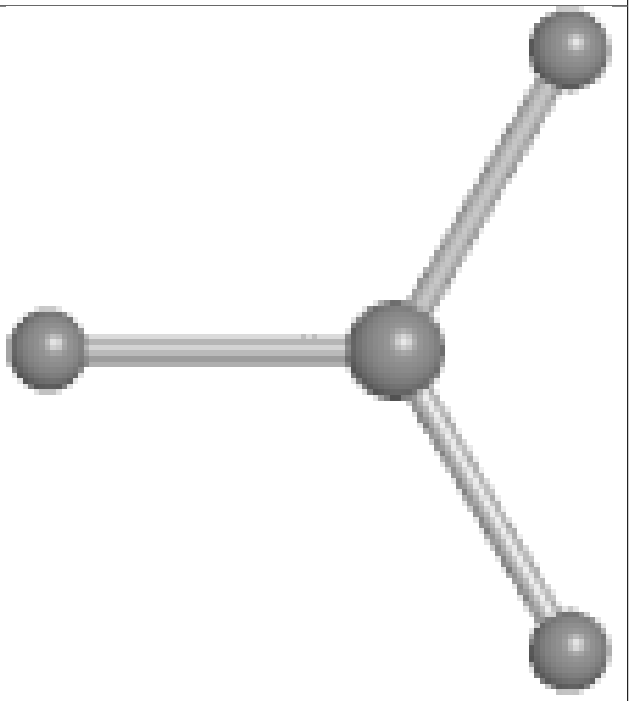
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1000	ADP	1	0
4	C	1001	BEF	1	0
3	B	1000	ADP	2	0
3	A	1000	ADP	1	0
4	A	1001	BEF	1	0

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 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.

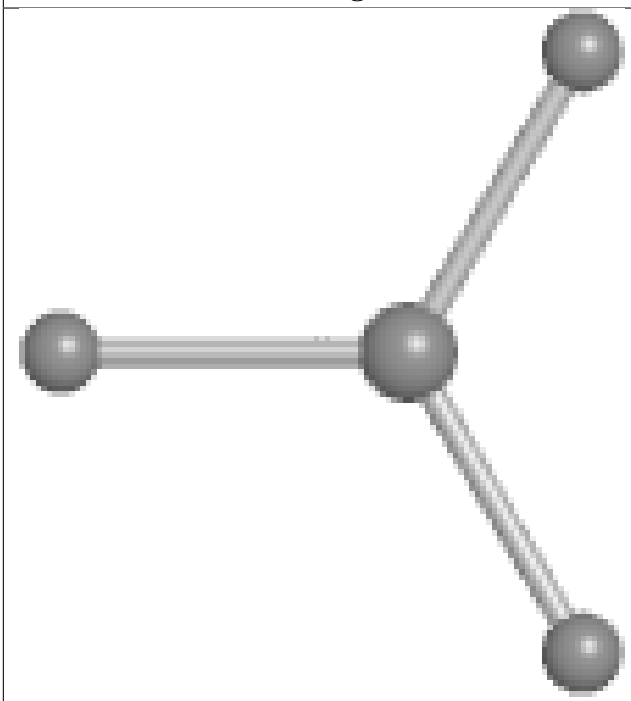
Ligand BEF E 1001



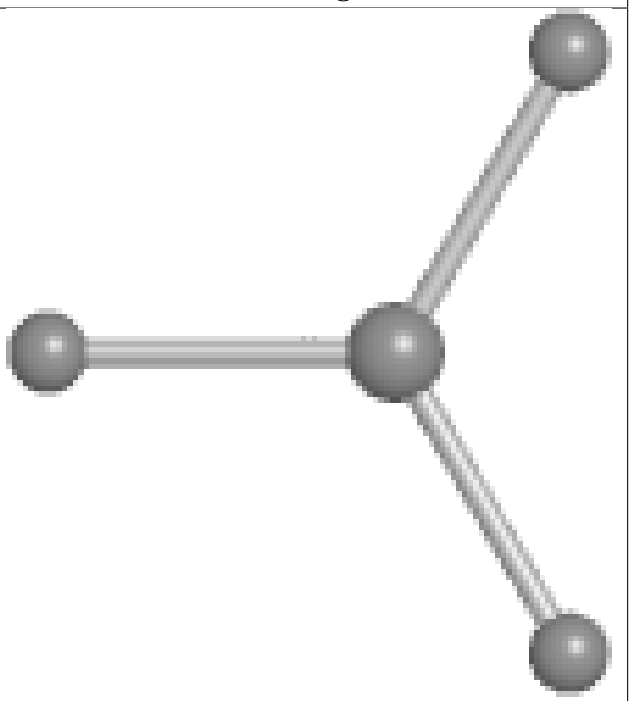
Bond lengths



Bond angles

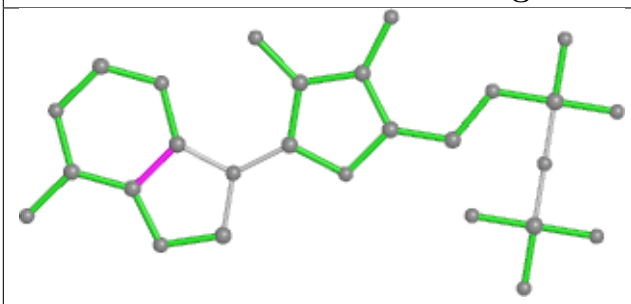


Torsions

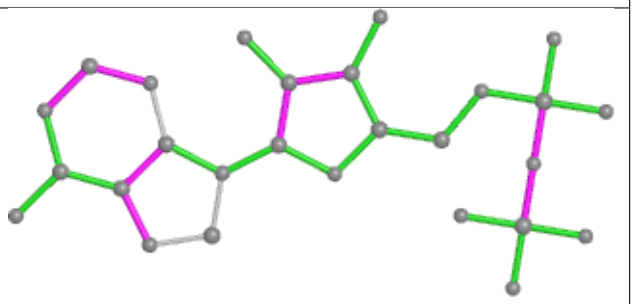


Rings

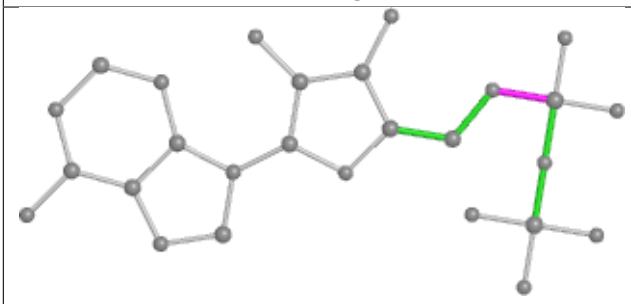
Ligand ADP D 1000



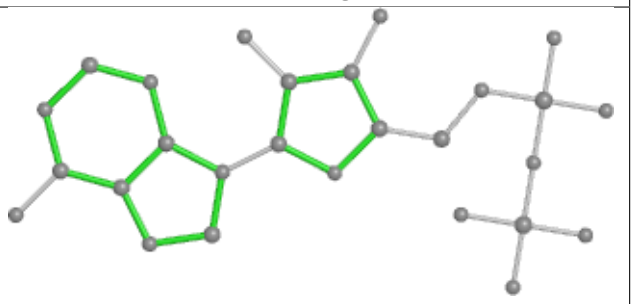
Bond lengths



Bond angles

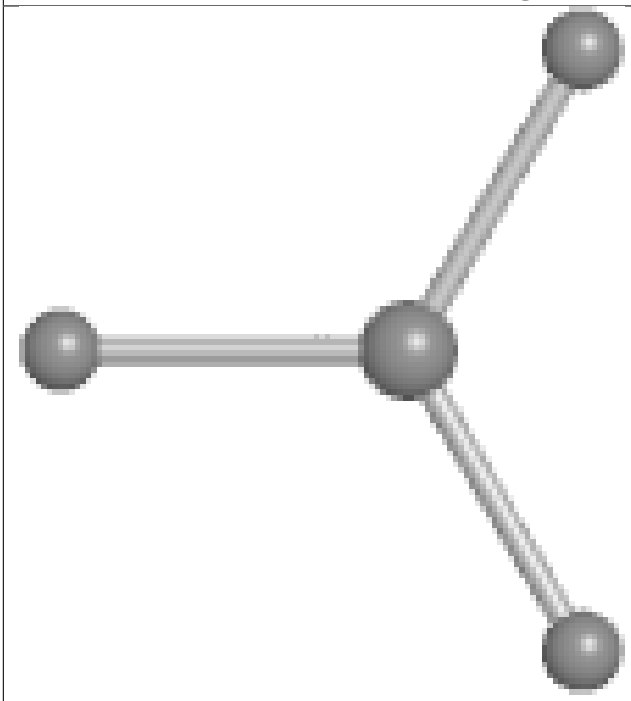


Torsions



Rings

Ligand BEF C 1001



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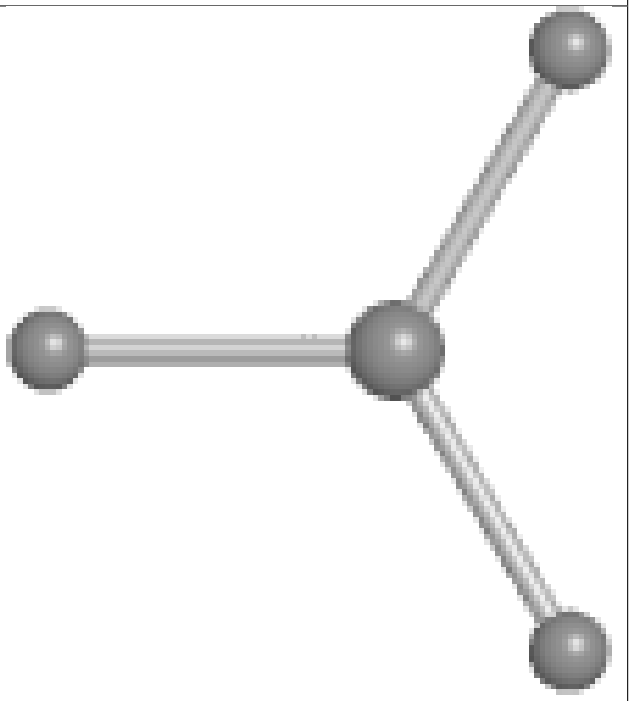
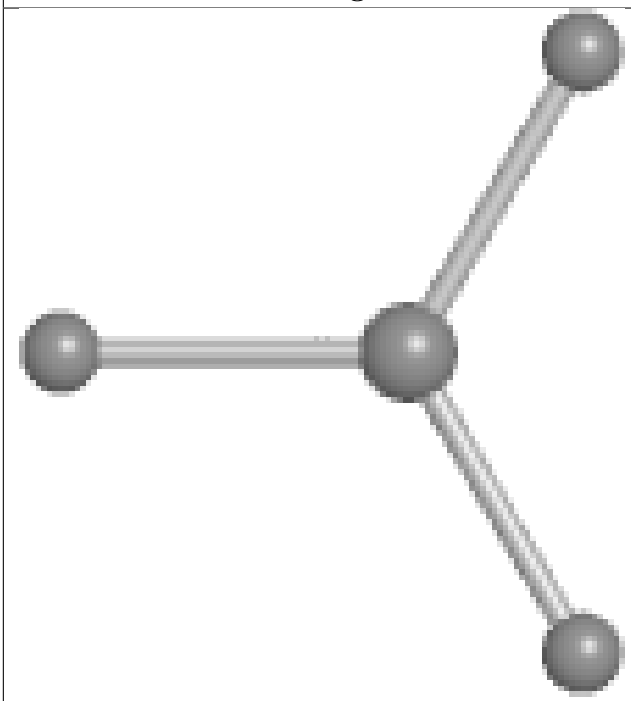


Bond angles



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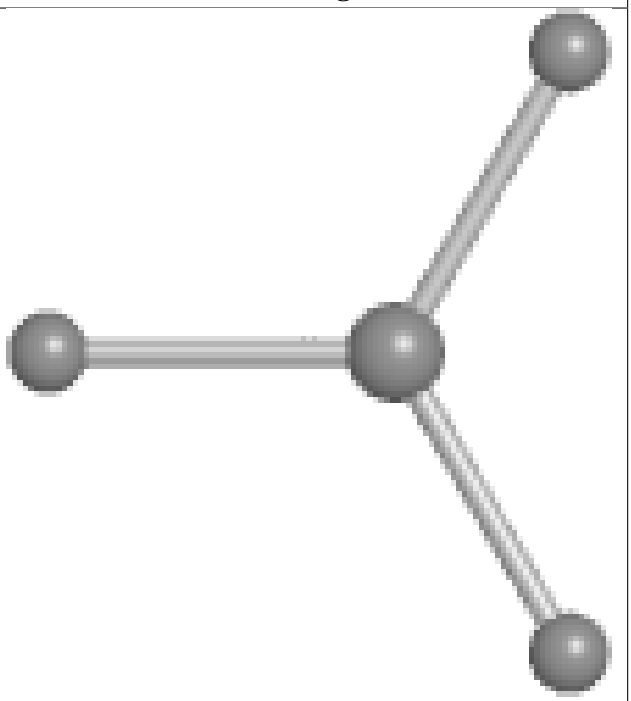

Rings

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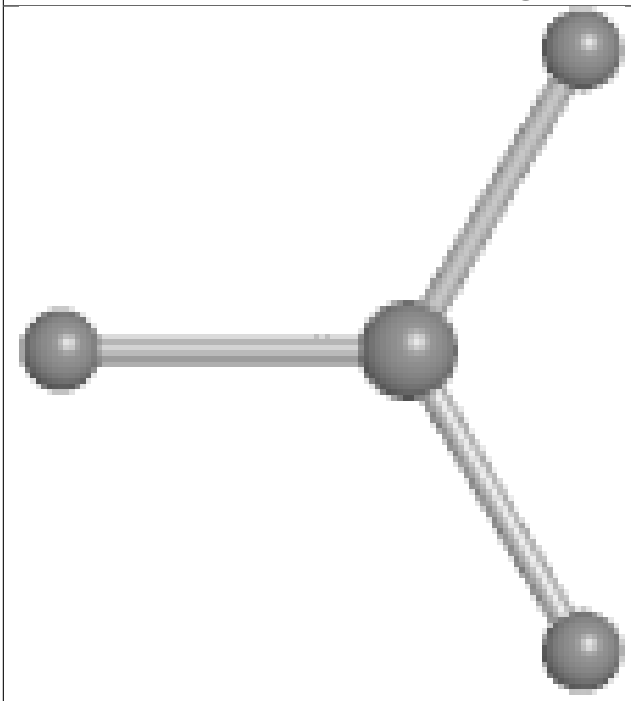

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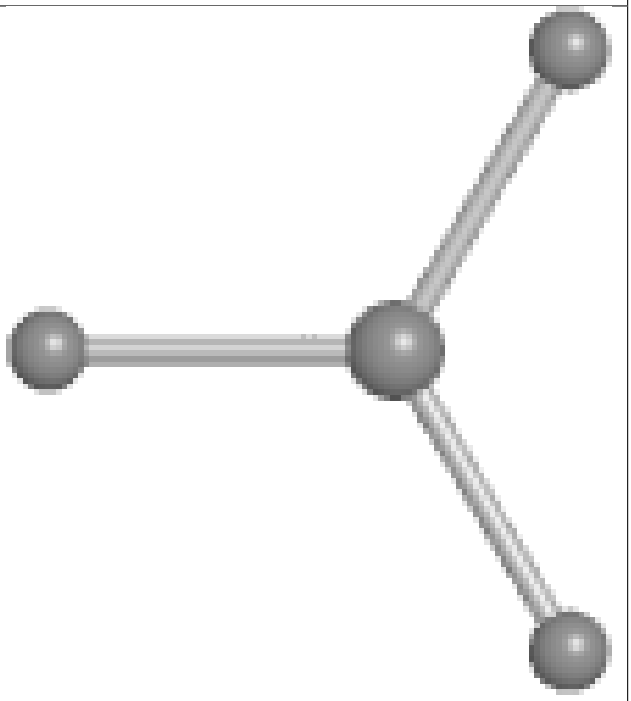

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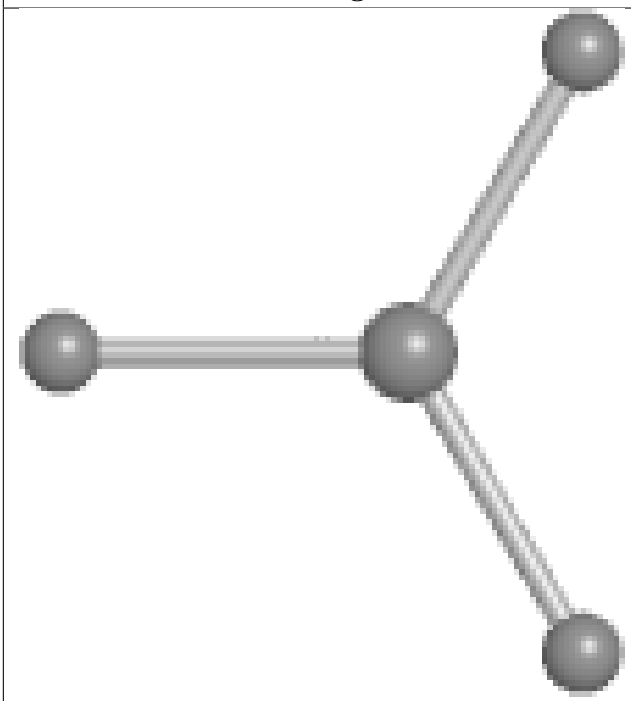

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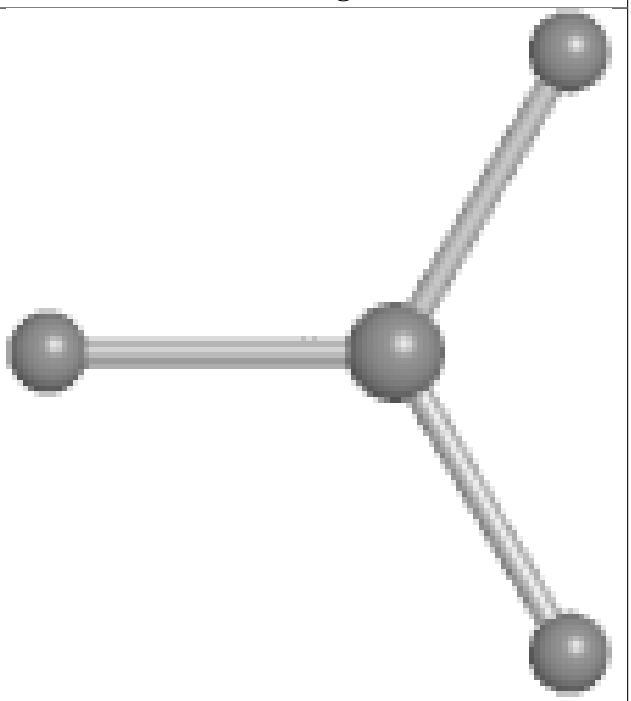
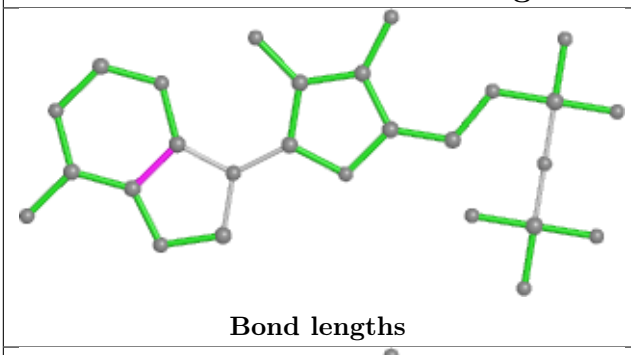


Rings

Ligand ADP B 1000



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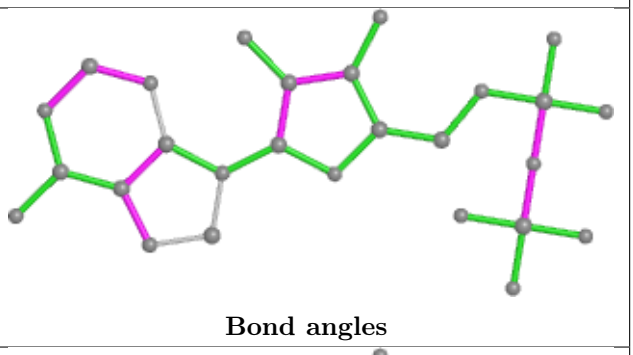
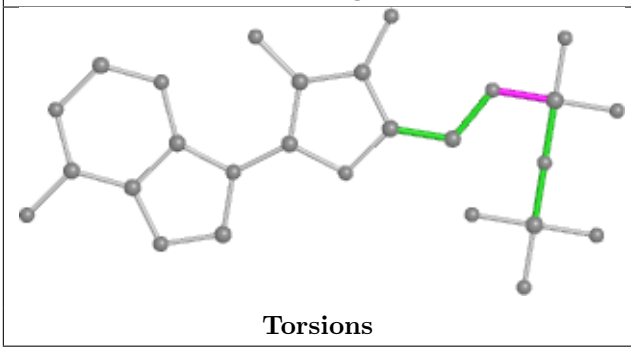


Bond angles



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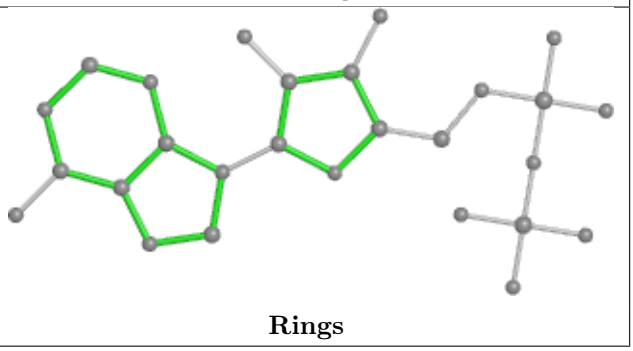
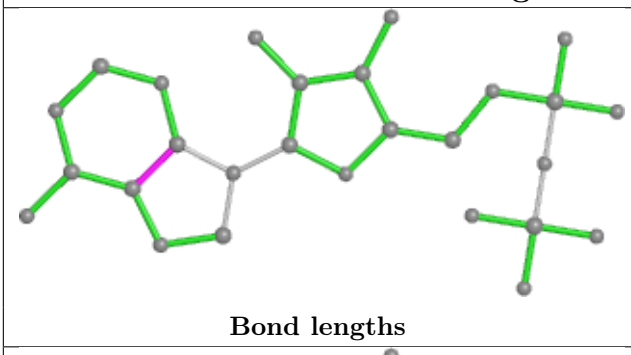


Rings

Ligand ADP A 1000



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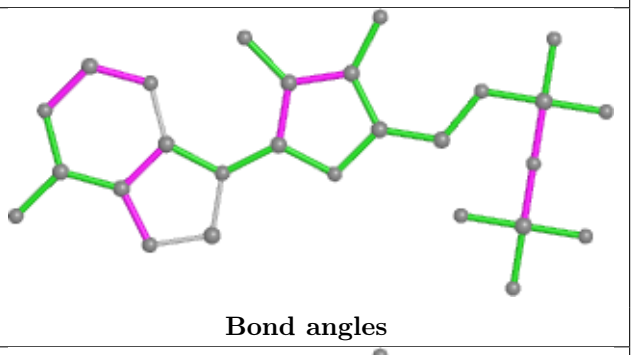
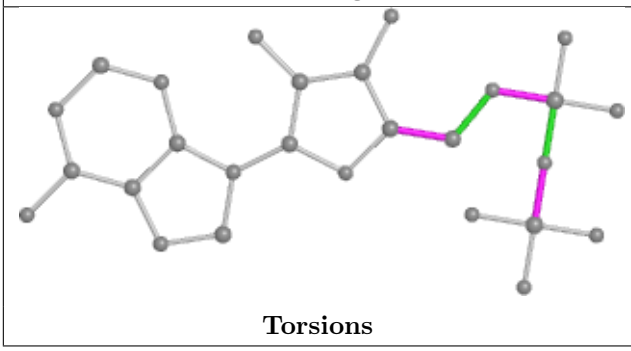


Bond angles



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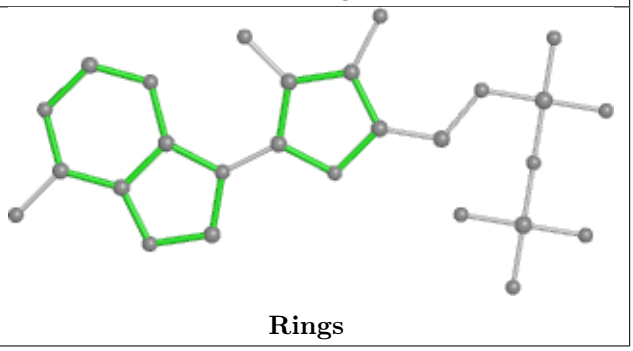
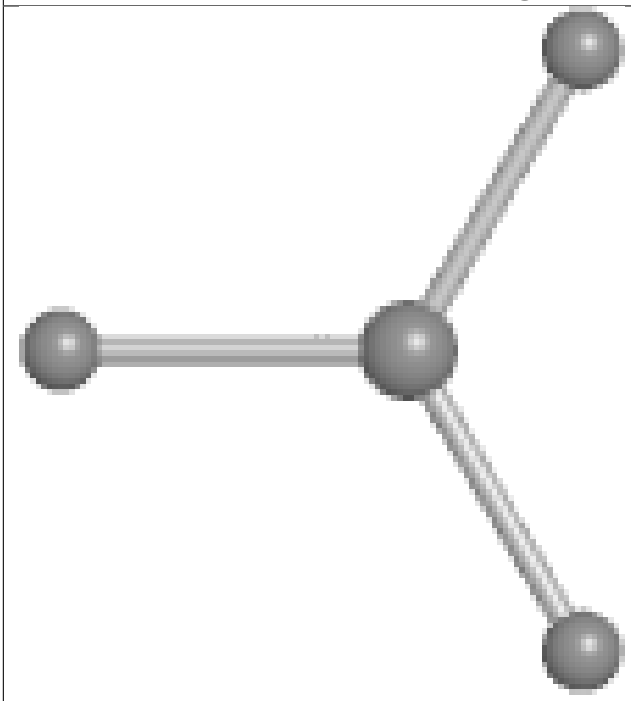


Rings

Ligand BEF D 1001



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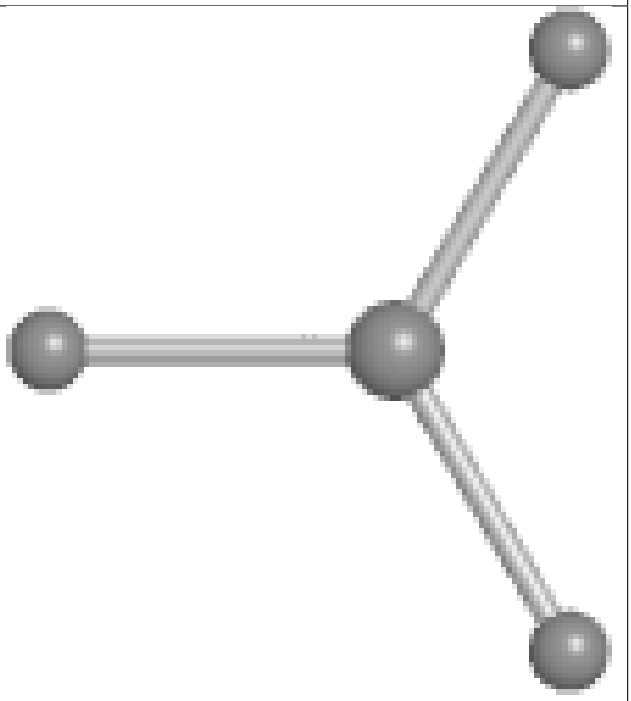
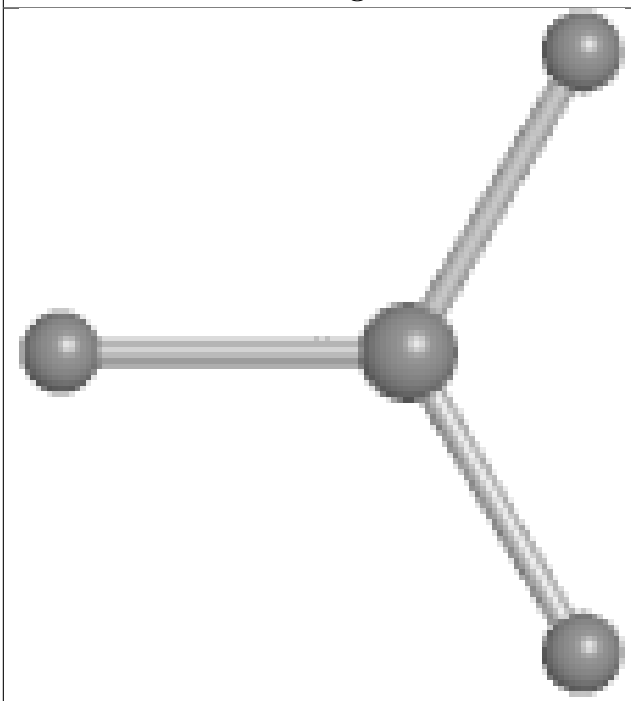
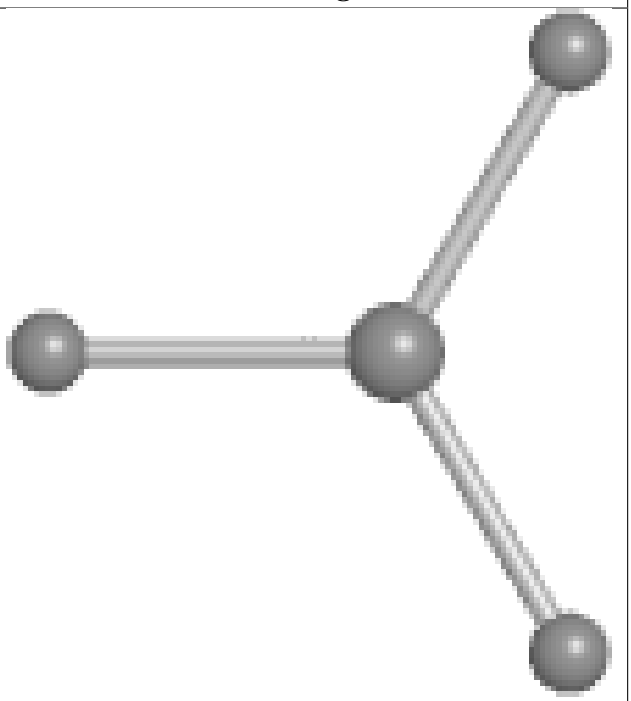


Bond angles

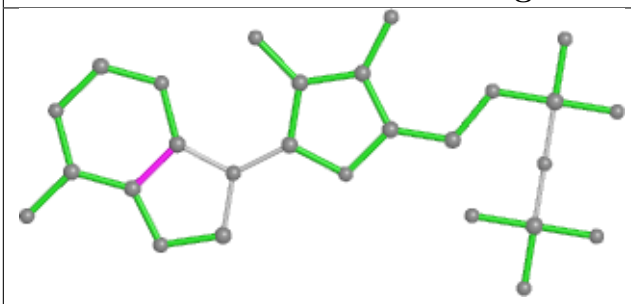


Torsions

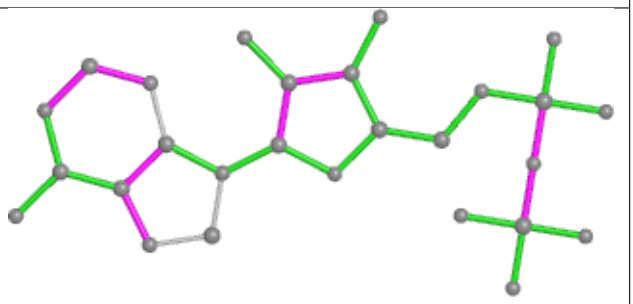


Rings

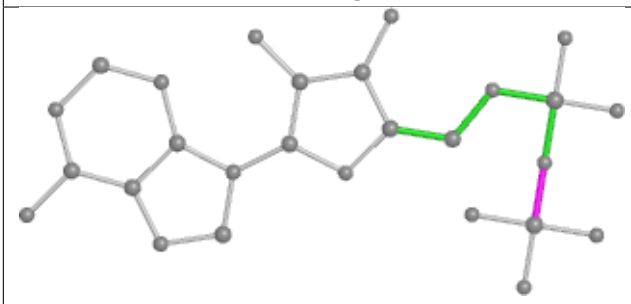
Ligand ADP F 1000



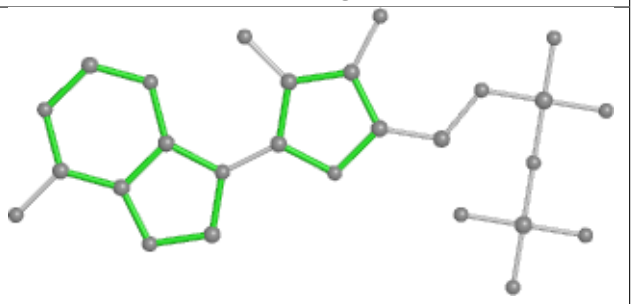
Bond lengths



Bond angles

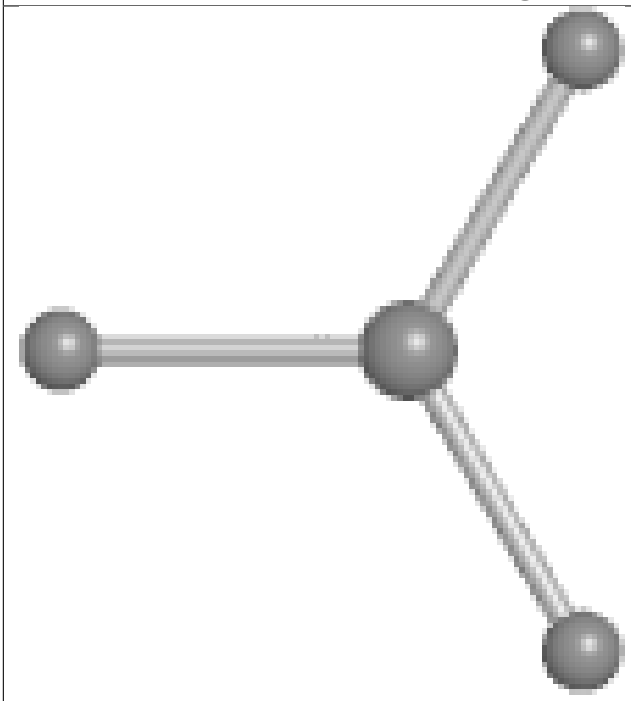


Torsions

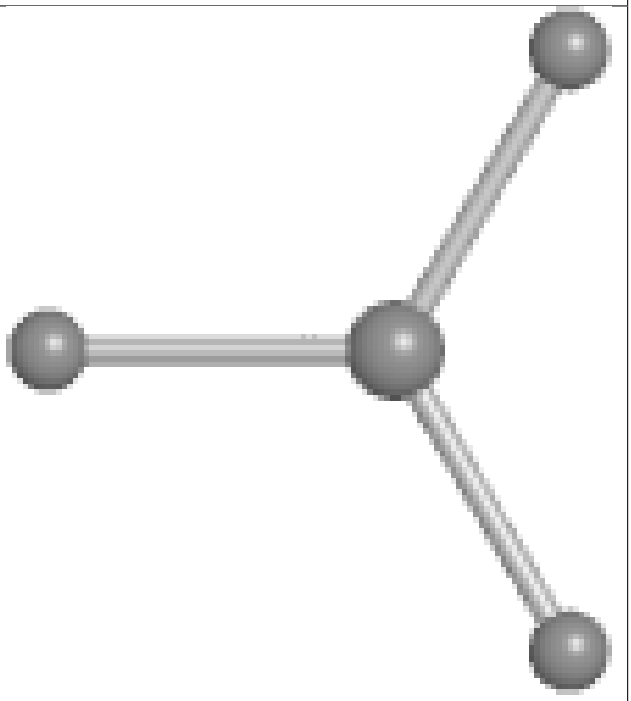


Rings

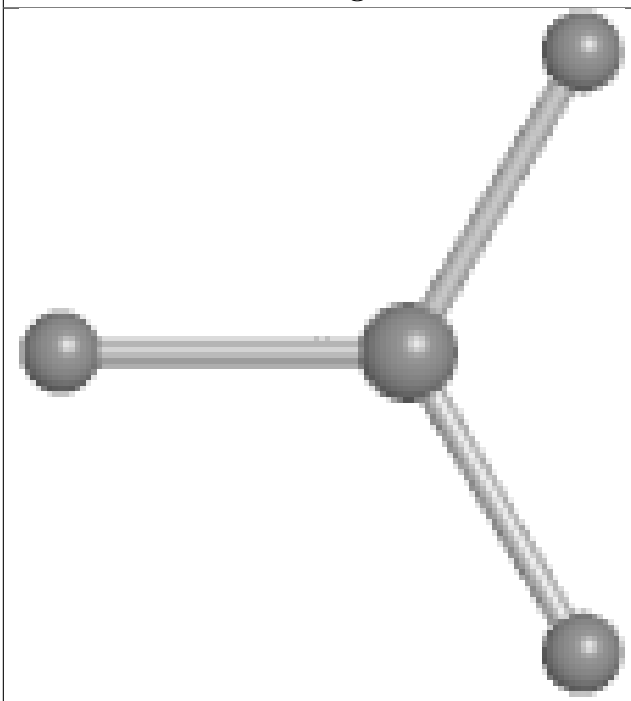
Ligand BEF A 1001



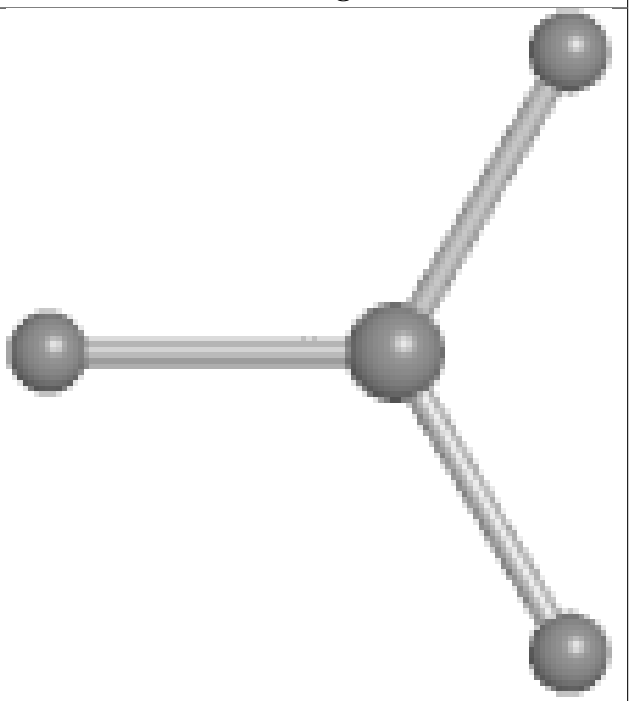
Bond lengths



Bond angles

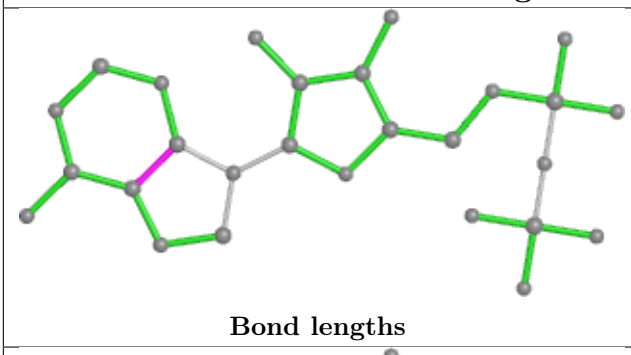


Torsions



Rings

Ligand ADP E 1000



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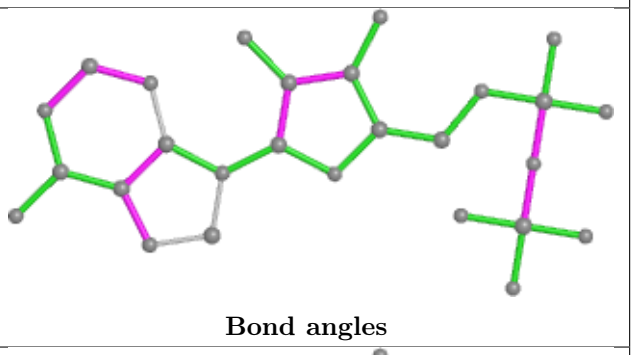

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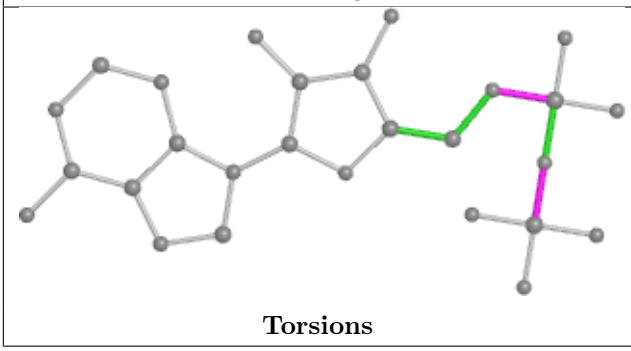

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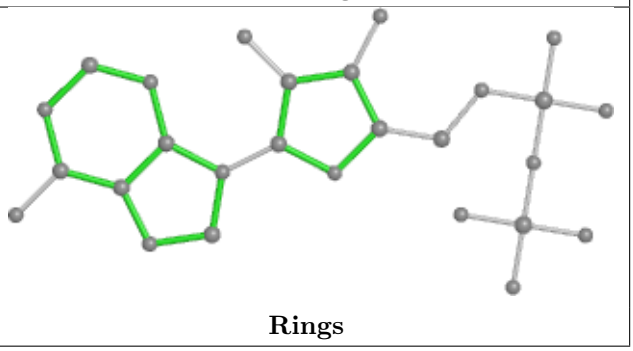
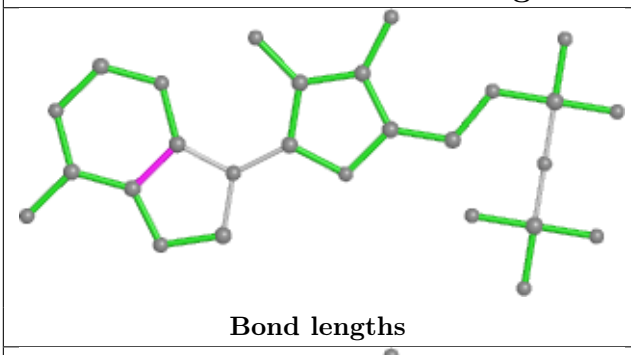
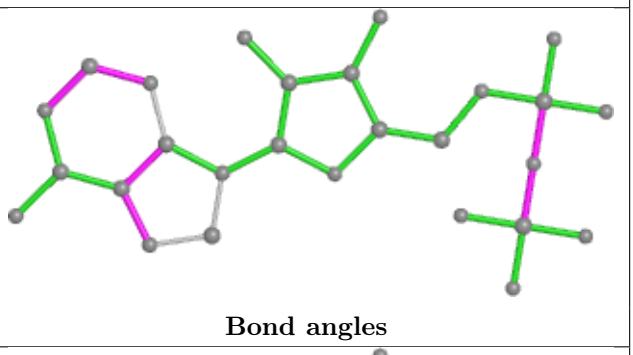


Rings

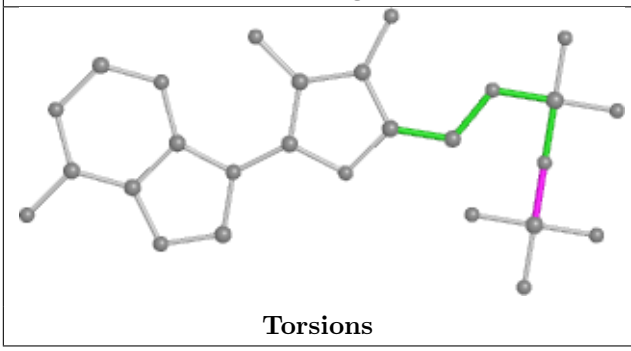
Ligand ADP C 1000



Bond lengths



Bond angles



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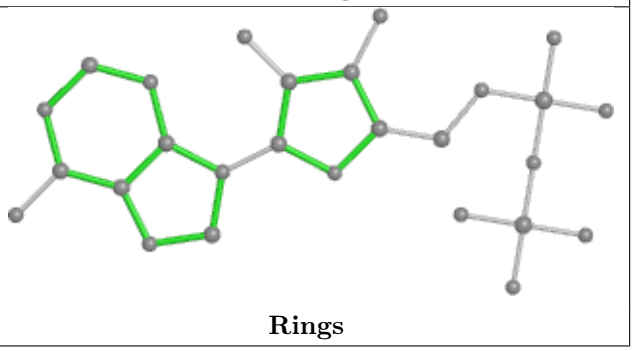

Rings

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	269/287 (93%)	0.08	16 (5%)	22	17	35, 65, 138, 186	0
1	C	274/287 (95%)	0.13	19 (6%)	16	12	33, 58, 161, 251	0
1	E	259/287 (90%)	-0.04	6 (2%)	60	54	41, 63, 118, 208	0
2	B	335/347 (96%)	0.66	57 (17%)	1	1	27, 63, 188, 237	0
2	D	336/347 (96%)	0.27	36 (10%)	6	3	32, 71, 159, 242	0
2	F	342/347 (98%)	0.41	38 (11%)	5	3	38, 67, 155, 221	0
All	All	1815/1902 (95%)	0.27	172 (9%)	8	5	27, 65, 164, 251	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	217	GLU	11.6
1	C	352	ILE	10.2
1	C	349	GLY	9.5
1	C	348	SER	9.3
2	B	345	LYS	9.0
2	B	344	ALA	8.8
2	F	302	ILE	8.5
2	F	307	ILE	8.3
1	C	350	ASP	8.1
1	E	284	ALA	7.8
2	B	258	VAL	7.8
2	B	41	ALA	7.7
2	B	218	HIS	7.5
2	F	301	ASN	7.4
2	B	259	GLU	6.9
1	C	357	GLY	6.8
2	F	266	HIS	6.8
2	B	20	HIS	6.6
2	B	42	SER	6.5

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Mol	Chain	Res	Type	RSRZ
1	C	285	SER	6.3
2	B	220	SER	6.2
2	F	12	TYR	6.2
2	B	257	VAL	6.2
2	B	219	ASP	6.1
1	C	288	GLU	6.1
2	B	31	ALA	6.1
2	B	221	GLN	5.7
2	B	44	VAL	5.6
2	B	256	ASP	5.6
2	F	33	ILE	5.5
1	A	356	VAL	5.4
2	D	40	SER	5.4
2	D	218	HIS	5.3
2	B	14	ILE	5.3
2	F	344	ALA	5.3
2	D	220	SER	5.1
2	B	19	LEU	4.9
2	B	216	CYS	4.9
2	D	216	CYS	4.9
2	D	163	VAL	4.8
1	C	287	GLN	4.7
2	F	38	ARG	4.6
2	F	304	GLY	4.5
1	A	355	ASP	4.5
2	F	268	ARG	4.4
2	D	258	VAL	4.4
2	D	5	ASP	4.4
2	B	8	PRO	4.3
2	F	265	LEU	4.3
1	C	284	ALA	4.3
1	A	352	ILE	4.2
2	B	47	LEU	4.2
2	B	303	GLU	4.2
2	B	33	ILE	4.2
2	F	18	HIS	4.2
2	B	301	ASN	4.2
1	E	282	ILE	4.1
2	B	7	ASN	4.1
2	D	257	VAL	4.1
2	B	43	ASP	4.1
2	F	308	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	160	ALA	4.0
1	C	351	LEU	4.0
2	D	161	HIS	4.0
2	B	302	ILE	4.0
2	B	300	LYS	4.0
2	D	3	GLU	3.9
2	D	12	TYR	3.8
2	B	224	GLN	3.8
2	F	300	LYS	3.8
2	F	36	MET	3.7
2	F	262	PRO	3.7
2	F	305	ASP	3.6
1	A	84	LYS	3.6
2	B	255	SER	3.6
2	B	18	HIS	3.6
1	A	347	THR	3.5
2	F	35	ARG	3.5
2	D	165	VAL	3.5
2	B	215	ARG	3.5
1	E	285	SER	3.4
2	F	264	LEU	3.4
1	C	290	SER	3.4
2	B	226	ARG	3.4
2	D	217	GLU	3.4
1	C	353	SER	3.4
2	B	16	LYS	3.3
1	A	351	LEU	3.3
1	A	243	HIS	3.3
2	F	267	GLN	3.3
1	A	348	SER	3.3
2	B	52	ALA	3.3
2	F	309	SER	3.2
2	D	221	GLN	3.2
2	B	10	ILE	3.2
2	D	162	ASP	3.1
2	F	3	GLU	3.1
2	D	38	ARG	3.1
1	A	245	GLU	3.1
1	A	354	MET	3.1
2	B	261	HIS	3.1
2	D	215	ARG	3.1
1	E	185	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	199	GLN	3.0
2	B	222	SER	3.0
2	F	220	SER	3.0
1	C	289	THR	3.0
2	B	25	ILE	3.0
1	C	283	SER	2.9
1	A	357	GLY	2.9
1	E	347	THR	2.9
2	F	269	LYS	2.9
2	F	161	HIS	2.9
2	F	20	HIS	2.9
2	B	223	LEU	2.9
2	B	51	VAL	2.9
2	D	219	ASP	2.8
1	A	282	ILE	2.8
2	B	260	GLN	2.8
2	F	142	ASP	2.8
2	D	37	THR	2.8
2	B	343	PRO	2.8
2	D	1	MET	2.8
2	F	263	SER	2.8
1	C	347	THR	2.7
2	B	56	ARG	2.7
2	B	268	ARG	2.7
2	B	45	HIS	2.7
2	D	167	ASP	2.7
2	F	303	GLU	2.6
2	B	21	ASP	2.6
2	D	256	ASP	2.6
2	D	33	ILE	2.5
1	A	283	SER	2.5
2	F	17	ALA	2.4
2	F	261	HIS	2.4
1	A	350	ASP	2.4
2	D	19	LEU	2.4
2	F	4	LEU	2.4
2	B	11	ILE	2.4
2	D	302	ILE	2.4
2	F	163	VAL	2.4
2	B	270	VAL	2.4
1	E	328	LYS	2.3
2	D	214	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	270	VAL	2.3
2	D	226	ARG	2.3
2	B	214	PHE	2.3
2	F	219	ASP	2.3
2	D	164	LYS	2.3
2	D	269	LYS	2.2
1	C	356	VAL	2.2
2	F	165	VAL	2.2
2	D	36	MET	2.2
1	C	355	ASP	2.2
2	D	18	HIS	2.2
2	B	283	THR	2.2
2	B	306	VAL	2.1
2	F	16	LYS	2.1
2	D	268	ARG	2.1
2	F	39	LEU	2.1
2	B	30	ALA	2.1
2	F	270	VAL	2.1
1	C	286	GLN	2.1
2	B	12	TYR	2.1
1	C	246	ASP	2.1
2	B	163	VAL	2.1
2	B	299	GLN	2.1
2	B	40	SER	2.1
2	D	6	LEU	2.0
1	A	291	HIS	2.0
1	A	88	SER	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,

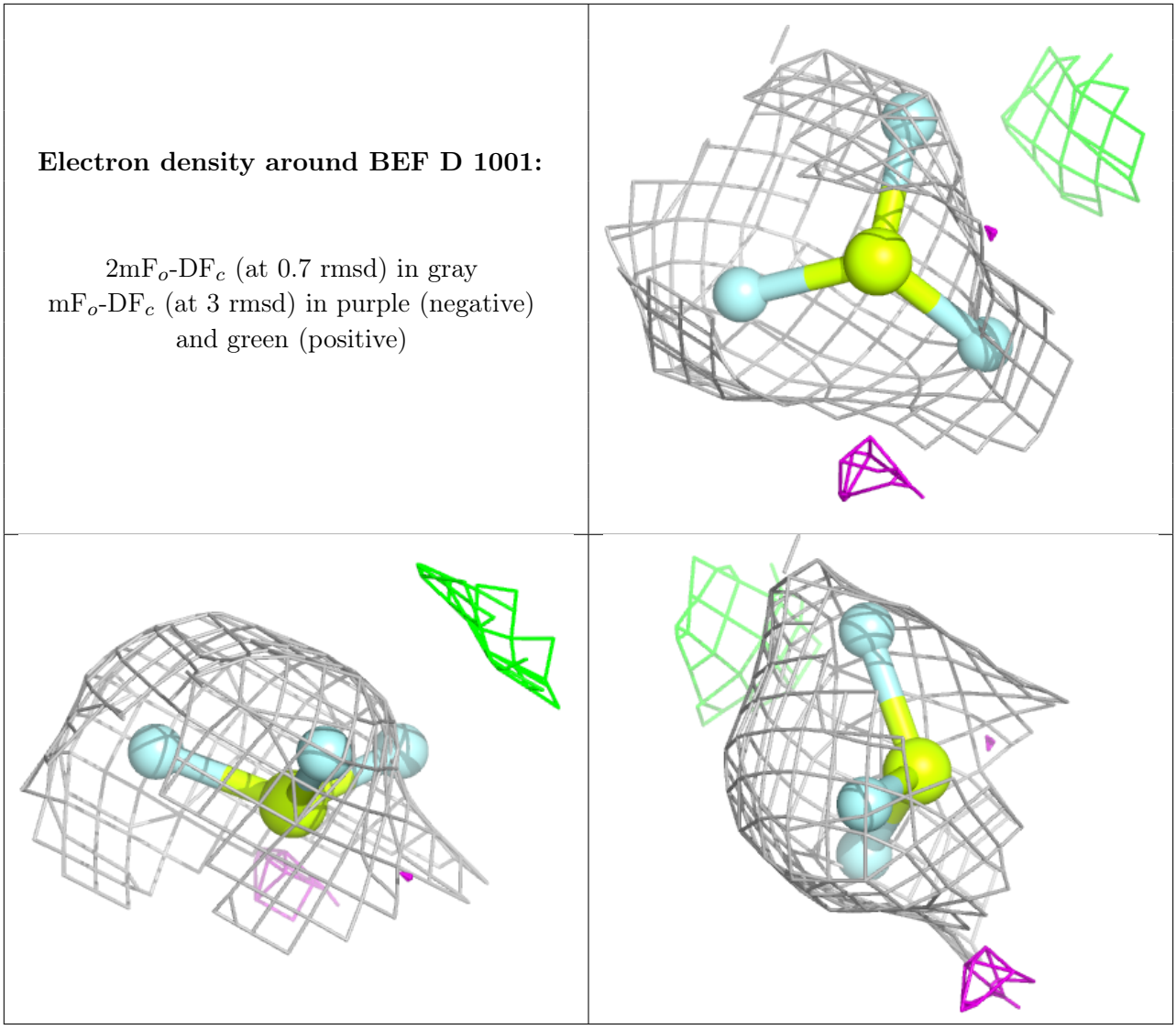
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BEF	D	1001	4/4	0.89	0.15	64,72,79,87	0
4	BEF	C	1001	4/4	0.90	0.31	38,40,44,54	0
4	BEF	B	1001	4/4	0.94	0.11	59,68,70,79	0
3	ADP	F	1000	27/27	0.94	0.18	68,89,102,113	0
4	BEF	A	1001	4/4	0.94	0.28	40,42,45,54	0
4	BEF	E	1001	4/4	0.94	0.38	43,47,49,65	0
3	ADP	B	1000	27/27	0.96	0.11	46,59,69,82	0
3	ADP	D	1000	27/27	0.96	0.11	48,60,77,85	0
3	ADP	A	1000	27/27	0.97	0.20	30,38,43,45	0
3	ADP	C	1000	27/27	0.98	0.18	27,35,44,49	0
3	ADP	E	1000	27/27	0.98	0.17	35,43,50,55	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.

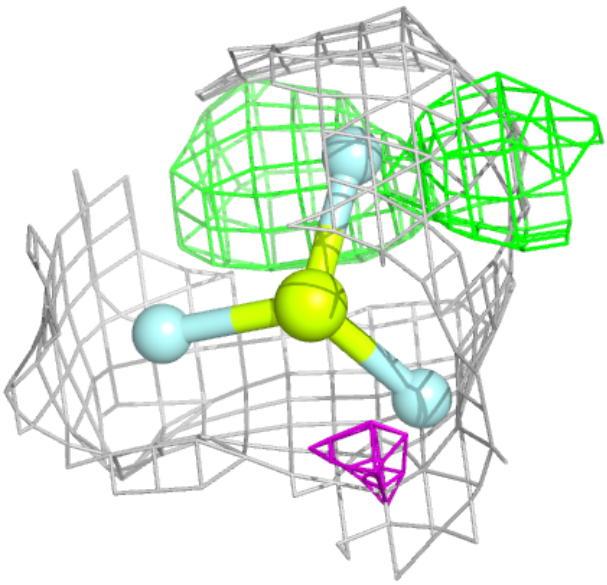
Electron density around BEF D 1001:

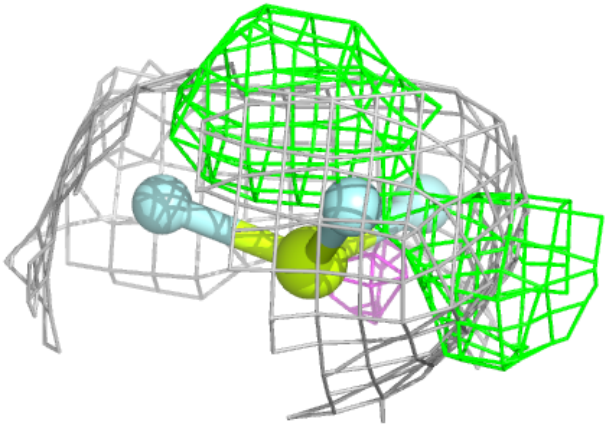
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

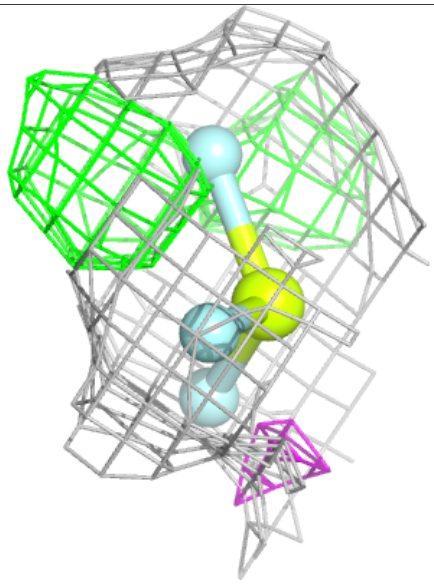


Electron density around BEF C 1001:

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

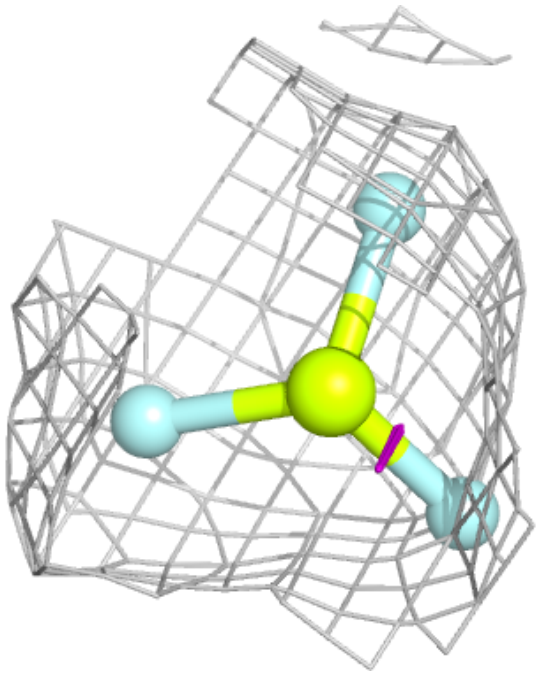


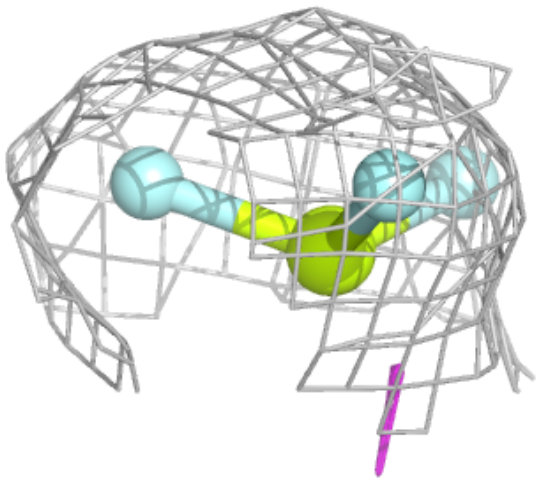


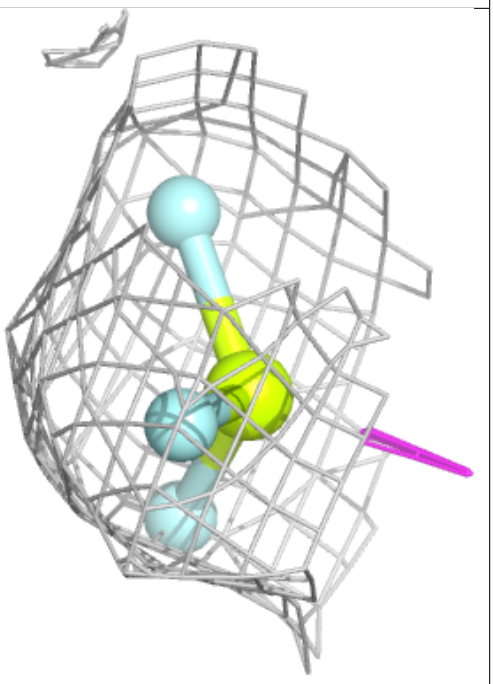


Electron density around BEF B 1001:

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

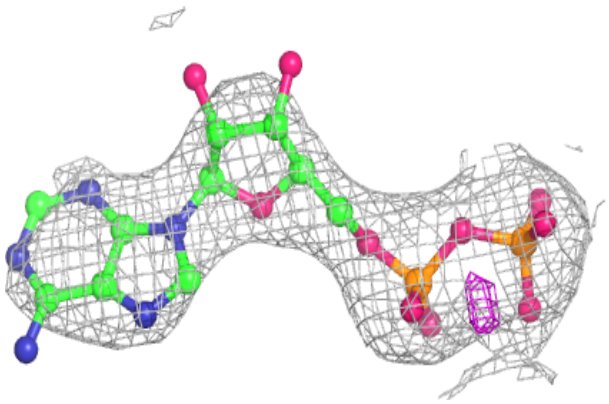


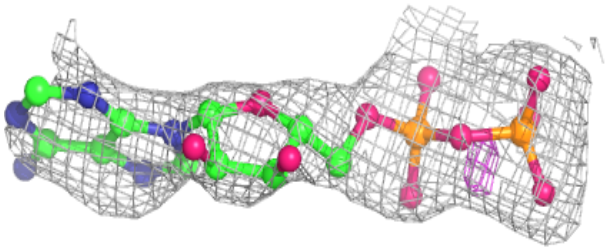


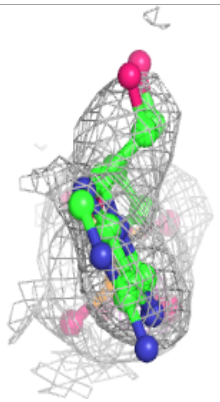


Electron density around ADP F 1000:

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

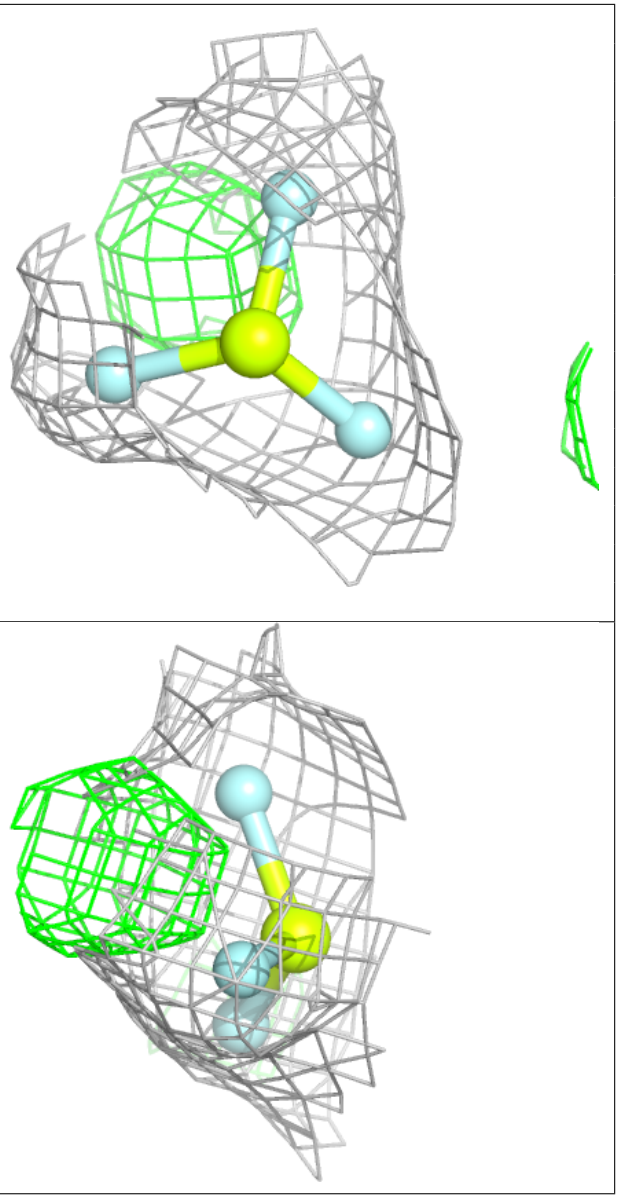






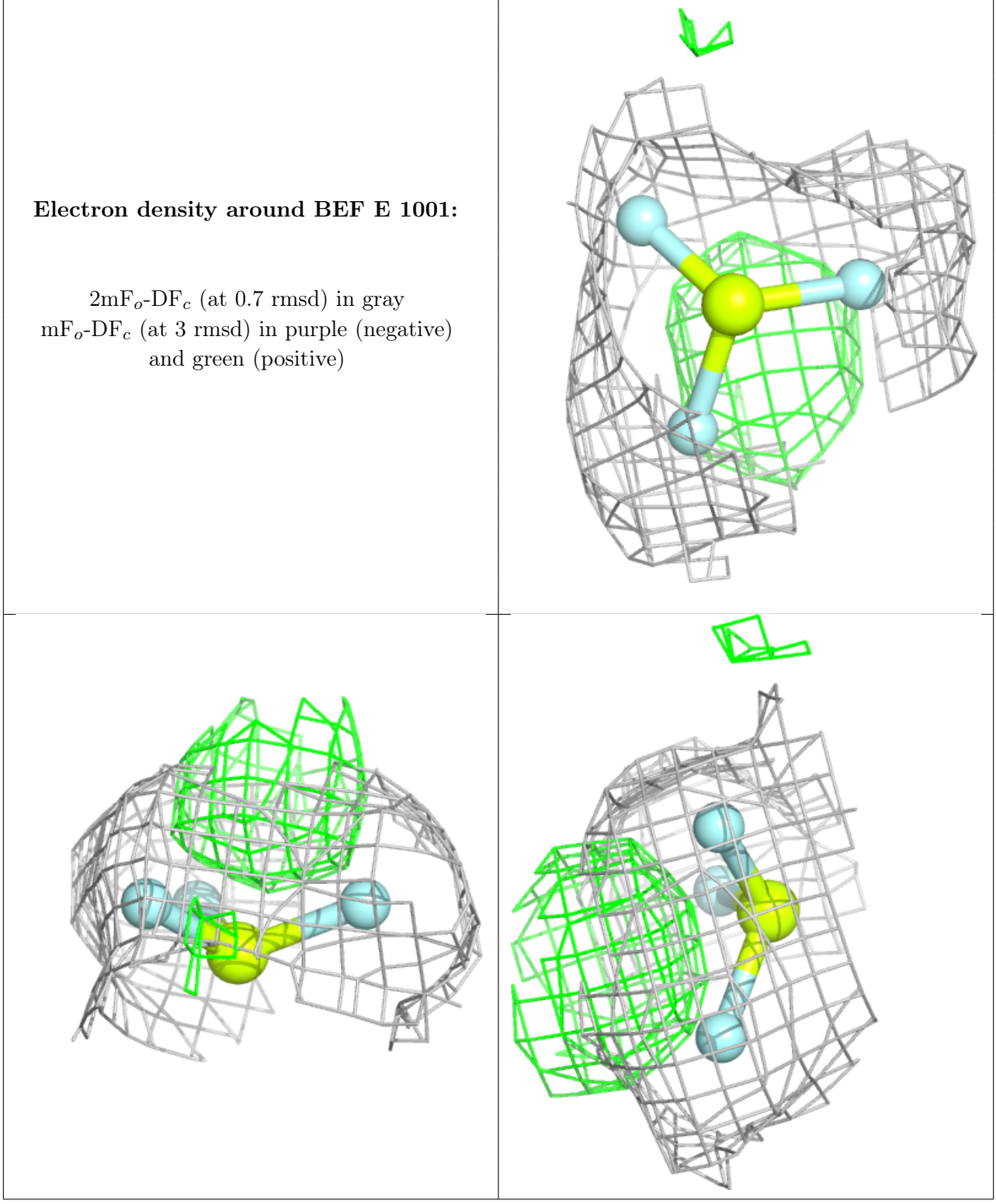
Electron density around BEF A 1001:

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



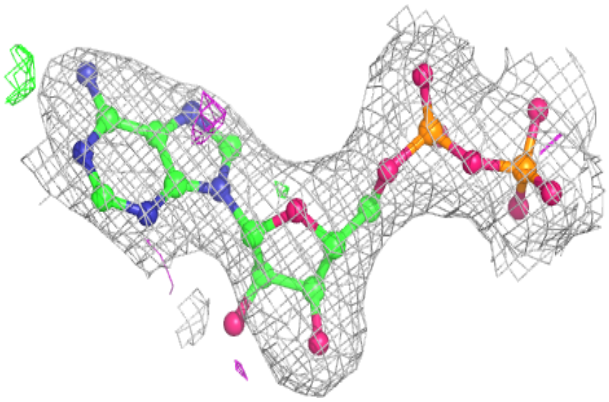
Electron density around BEF E 1001:

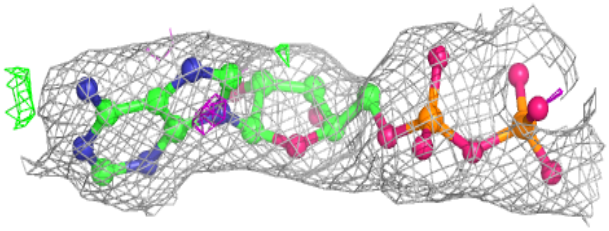
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

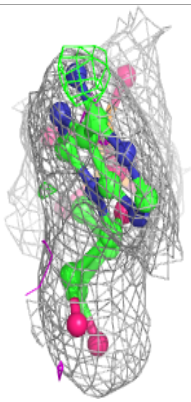


Electron density around ADP B 1000:

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

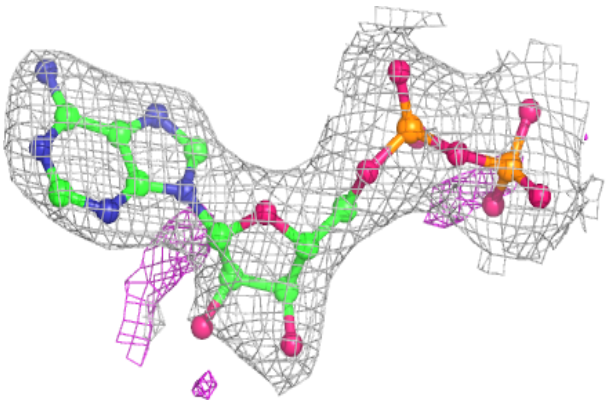


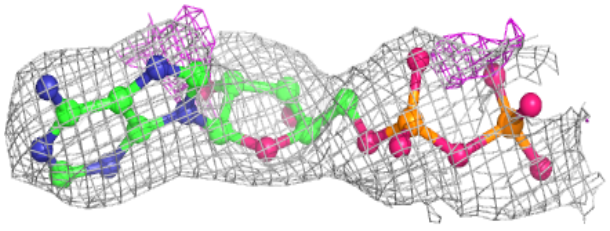


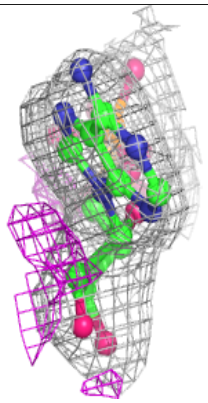


Electron density around ADP D 1000:

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

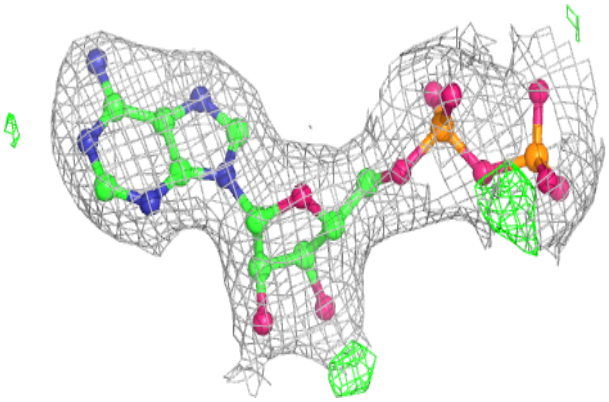


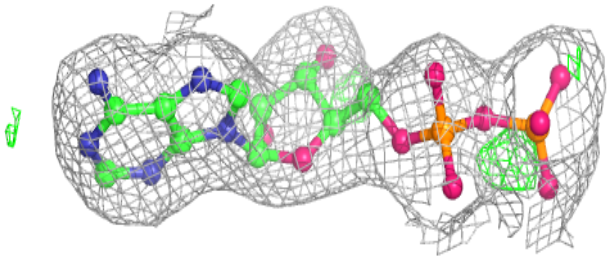


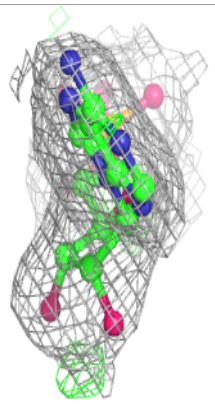


Electron density around ADP A 1000:

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

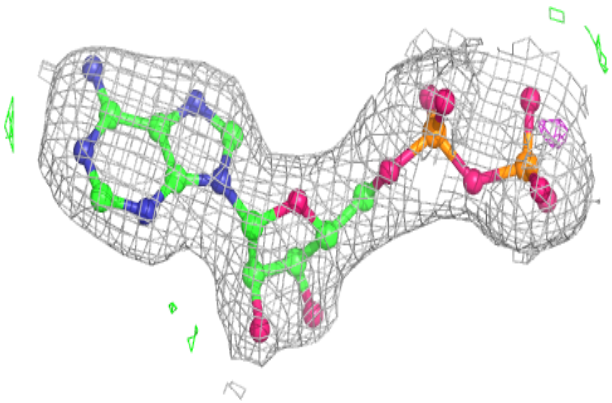


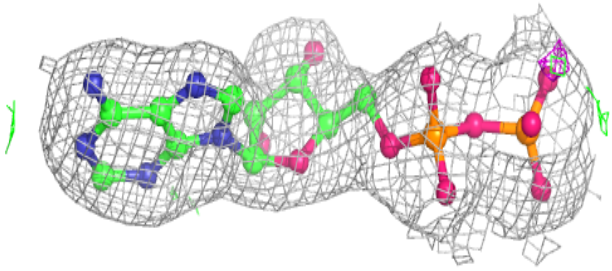


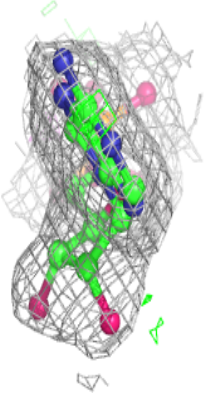


Electron density around ADP C 1000:

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

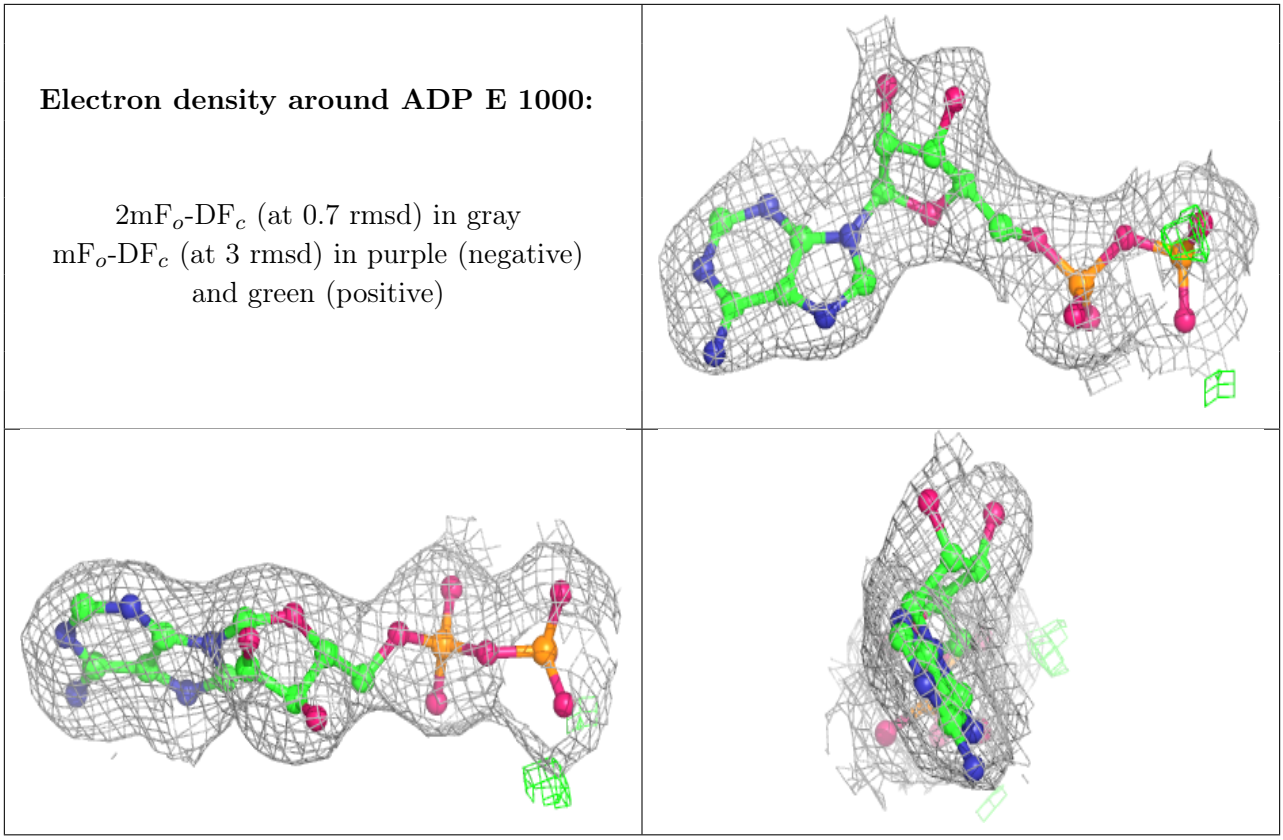






Electron density around ADP E 1000:

$2mF_o$-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.